

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CCCDC_2260010, _CCDC_2260009

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: _CCDC_2260009

Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073
Cell:	a=21.266(2) alpha=90	b=19.1361(16) beta=90.517(3) c=25.447(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	10355.2(15)	10355.0(16)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	3(C30 H24 Mn N6 O6), 6(Cl O4), 3(H2 O), O	3(C30 H24 Mn N6 O6), 6(Cl O4), 4(H2 O)
Sum formula	C90 H78 Cl6 Mn3 N18 O46	C90 H80 Cl6 Mn3 N18 O46
Mr	2525.22	2527.24
Dx, g cm ⁻³	1.620	1.621
Z	4	4
Mu (mm ⁻¹)	0.620	0.620
F000	5156.0	5164.0
F000'	5166.32	
h, k, lmax	28, 25, 34	28, 25, 33
Nref	26029	25850
Tmin, Tmax	0.911, 0.943	0.630, 0.714
Tmin'	0.876	

Correction method= # Reported T Limits: Tmin=0.630 Tmax=0.714
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 28.407

R(reflections)= 0.0531(22753)

wR2(reflections)=
0.1421(25850)

S = 1.069

Npar= 1483

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT214_ALERT_2_B	Atom O162	(Anion/Solvent) ADP max/min Ratio	5.2 prolat
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O4W Check

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
	Calc: C90 H78 Cl6 Mn3 N18 O46		
	Rep.: C90 H80 Cl6 Mn3 N18 O46		
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ	Please Check
	Calc: 3(C30 H24 Mn N6 O6), 6(Cl O4), 3(H2 O), O		
	Rep.: 3(C30 H24 Mn N6 O6), 6(Cl O4), 4(H2 O)		
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		Cl2 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		Cl4 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		Cl5 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl6	0.119 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.021 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		7 Note
	1 1 0, -1 0 1, -1 1 1, 0 1 1, 1 0 1, 1 1 1,		
	0 0 2,		
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	22 Report
	0 2 0, 0 8 0, 2 1 0, 10 9 0, -1 9 1, 2 18 1,		
	-11 0 3, -8 9 3, 0 8 3, 10 1 4, 10 9 4, 0 9 5,		
	-10 1 6, -10 8 6, 0 17 7, -10 1 8, 11 8 8, 0 8 9,		
	11 0 9, -1 8 12, -9 0 21, 0 8 27,		
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1 Check
	-10 1 12,		
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.75Ang From O164		1.54 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.03Ang From O4W	.	0.54 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.99Ang From O111	.	-0.69 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.02Ang From O131	.	-0.67 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.67Ang From O112	.	-0.59 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C90 H80 Cl6 Mn3 N18 O46
Atom count from the _atom_site data: C90 H78 Cl6 Mn3 N18 O46

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C90 H80 Cl6 Mn3 N18 O46
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	360.00	360.00	0.00
H	320.00	312.00	8.00
Cl	24.00	24.00	0.00

Mn	12.00	12.00	0.00	
N	72.00	72.00	0.00	
O	184.00	184.00	0.00	
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms				6 Report
H11W	H12W	H21W	H22W	H31W H32W
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large				24.34 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as				mixed Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn2	--O41	. 5.3 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn3	--O72	. 6.4 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C11 Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C13 Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C16 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O162	..C910	. 2.98 Ang.
		x,y,z =		1_555 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #				9 Note
	C1	O4		
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1	(II)	.	2.26 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn2	(II)	.	2.28 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn3	(II)	.	2.32 Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		143 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			17 Note
	0 2 0,	2 1 0,	-10 1 6,	11 0 9, -11 0 3,
	-1 8 12,	-10 8 6,	11 8 8,	-10 1 8, 10 1 4,
	-9 0 21,	0 8 27,	10 9 0,	0 9 5, 0 8 3,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value				6.22 Note
Predicted wR2: Based on SigI**2 2.28 or SHELX Weight 13.69				
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.				1 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 20 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 5 ALERT type 5 Informative message, check

Datablock: CCCDC_2260010

Bond precision: C-C = 0.0105 A Wavelength=0.71073

Cell: a=21.302(3) b=19.101(3) c=25.487(4)
 alpha=90 beta=90.354(5) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	10370(3)	10370(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	3(C30 H24 Mn N6 O6), 6(Cl O4), 4(O)	3(C30 H24 Mn N6 O6), 6(Cl O4), 4(H2 O)
Sum formula	C90 H72 Cl6 Mn3 N18 O46	C90 H80 Cl6 Mn3 N18 O46
Mr	2519.18	2527.24
Dx, g cm ⁻³	1.614	1.619
Z	4	4
Mu (mm ⁻¹)	0.619	0.619
F000	5132.0	5164.0
F000'	5142.32	
h,k,lmax	28,25,34	28,25,34
Nref	26149	25615
Tmin,Tmax	0.893,0.933	0.601,0.746
Tmin'	0.885	

Correction method= # Reported T Limits: Tmin=0.601 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.980 Theta(max)= 28.433

R(reflections)= 0.1002(20710)

wR2(reflections)=
0.2710(25615)

S = 1.096 Npar= 1468

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O1W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O2W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O3W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O4W Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O3W	..O11	2.83 Ang.
		x,y,z =	1_555 Check
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		4 Check
	12 1 8, -11 13 8, 2 3 12, 12 5 14,		

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
	Calc.: C90 H72 Cl6 Mn3 N18 O46		
	Rep.: C90 H80 Cl6 Mn3 N18 O46		
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ	Please Check

Calc: 3(C30 H24 Mn N6 O6), 6(Cl O4), 4(O)
Rep.: 3(C30 H24 Mn N6 O6), 6(Cl O4), 4(H2 O)

PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	8.06	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.33	Report
PLAT220_ALERT_2_C	NonSolvent Resd 3 C Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C15 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C11	0.131	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01047	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact O2W ..051 .	2.87	Ang.
	x,y,z =	1_555	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact O3W ..031 .	2.90	Ang.
	x,y,z =	1_555	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	17.822	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.853	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	8	Note
	1 1 0, 2 0 0, -1 0 1, -1 1 1, 0 1 1, 1 0 1,		
	1 1 1, 0 0 2,		
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	275	Report
	0 2 0, 1 2 0, 2 1 0, 3 5 0, 3 13 0, 8 1 0,		
	9 8 0, 9 12 0, 10 3 0, 11 3 0, 13 4 0, 13 8 0,		
	14 10 0, 17 4 0, 18 8 0, 19 8 0, -18 10 1, -13 8 1,		
	-12 8 1, -11 19 1, -8 1 1, -8 2 1, -7 11 1, -6 1 1,		
	-6 5 1, 11 13 1, 12 5 1, 14 3 1, 15 7 1, 20 1 1,		
	-17 10 2, -15 11 2, -14 4 2, -13 16 2, -11 7 2, -8 6 2,		
	-6 3 2, -1 18 2, 1 16 2, 2 0 2, 4 2 2, 6 3 2,		
	6 4 2, 8 2 2, 10 3 2, 12 6 2, 15 11 2, 17 6 2,		
	17 12 2, 22 2 2, -21 6 3, -19 3 3, -19 9 3, -17 6 3,		
	-14 1 3, -12 3 3, -8 3 3, -8 9 3, -5 12 3, 5 14 3,		
	7 7 3, 7 11 3, 8 7 3, -19 5 4, -19 7 4, -13 6 4,		
	-7 12 4, -5 10 4, -4 4 4, -2 5 4, 0 2 4, 3 11 4,		
	4 0 4, 4 2 4, 5 8 4, 7 5 4, 9 8 4, 11 13 4,		
	16 0 4, 21 5 4, -18 8 5, -9 4 5, -2 1 5, 0 4 5,		
	0 6 5, 13 10 5, 20 9 5, -20 5 6, -16 0 6, -13 8 6,		
	-12 6 6, -11 5 6, -11 11 6, -9 8 6, -5 10 6, -1 12 6,		
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.75Ang From O92	1.68	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.02Ang From O123	0.99	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.80Ang From O122	-0.74	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.47Ang From O4W	-0.66	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.53Ang From O72	-0.64	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H18	-0.36	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H28	-0.41	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H82	-0.35	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H93	-0.36	eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C90 H80 Cl6 Mn3 N18 O46
Atom count from the _atom_site data: C90 H72 Cl6 Mn3 N18 O46

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C90 H80 Cl6 Mn3 N18 O46
TEST: Compare cell contents of formula and atom_site data

	atom	Z*formula	cif sites	diff						
	C	360.00	360.00	0.00						
	H	320.00	288.00	32.00						
	Cl	24.00	24.00	0.00						
	Mn	12.00	12.00	0.00						
	N	72.00	72.00	0.00						
	O	184.00	184.00	0.00						
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	121.50	Why ?						
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn3 --O72 .	5.3 s.u.							
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		Cl1 Check							
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		Cl2 Check							
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		Cl3 Check							
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		Cl4 Check							
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		Cl6 Check							
PLAT432_ALERT_2_G	Short Inter X...Y Contact O112 ..C910 .	2.99 Ang.			x,y,z =	1_555	Check			
PLAT432_ALERT_2_G	Short Inter X...Y Contact C22 ..C58 .	3.20 Ang.			1-x,1-y,1-z =	3_666	Check			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	4 Note								
	Cl O4									
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	5 Note								
	Cl O4									
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1 (II) .	2.29 Info								
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn2 (II) .	2.30 Info								
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn3 (II) .	2.37 Info								
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	248 Note								
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	20 Note								
	0 2 0,	2 1 0,	-7 13 8,	-6 1 1,	0 2 8,	0 2 4,				
	8 2 2,	7 15 10,	10 3 0,	-11 11 6,	-16 5 10,	-4 4 4,				
	-6 1 15,	6 3 2,	9 8 0,	14 4 14,	7 11 8,	8 7 3,				
	-8 1 1,	-13 8 6,								
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check								
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.88 Note								
	Predicted wR2: Based on SigI**2	5.55 or SHELX Weight	25.45							
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density.	0 Info								

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

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# start Validation Reply Form
_vrf_PLAT214__CCDC_2260009
;
PROBLEM: Atom O162          (Anion/Solvent) ADP max/min Ratio          5.2 prolat
RESPONSE: ...
;
_vrf_PLAT306__CCDC_2260009
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) .....          04W Check
RESPONSE: ...
;
_vrf_PLAT041__CCDC_2260009
;
PROBLEM: Calc. and Reported SumFormula      Strings      Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT042__CCDC_2260009
;
PROBLEM: Calc. and Reported MoietyFormula Strings      Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT068__CCDC_2260009
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...      Please Check
RESPONSE: ...
;
_vrf_PLAT244__CCDC_2260009
;
PROBLEM: Low      'Solvent' Ueq as Compared to Neighbors of      C12 Check
RESPONSE: ...
;
_vrf_PLAT260__CCDC_2260009
;
PROBLEM: Large Average Ueq of Residue Including      C16      0.119 Check
RESPONSE: ...
;
_vrf_PLAT906__CCDC_2260009
;
PROBLEM: Large K Value in the Analysis of Variance .....      3.021 Check
RESPONSE: ...
;
_vrf_PLAT910__CCDC_2260009
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min).      7 Note
RESPONSE: ...
;
_vrf_PLAT911__CCDC_2260009
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      22 Report
RESPONSE: ...
;
_vrf_PLAT934__CCDC_2260009
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..      1 Check
RESPONSE: ...
;
_vrf_PLAT971__CCDC_2260009

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;
PROBLEM: Check Calcd Resid. Dens.  2.75Ang From O164          1.54 eA-3
RESPONSE: ...
;
_vrf_PLAT975__CCDC_2260009
;
PROBLEM: Check Calcd Resid. Dens.  1.03Ang From O4W          .      0.54 eA-3
RESPONSE: ...
;
_vrf_PLAT976__CCDC_2260009
;
PROBLEM: Check Calcd Resid. Dens.  0.99Ang From O111          .      -0.69 eA-3
RESPONSE: ...
;
_vrf_PLAT306__CCDC_2260010
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) .....      O1W Check
RESPONSE: ...
;
_vrf_PLAT430__CCDC_2260010
;
PROBLEM: Short Inter D...A Contact  O3W          ..O11          .      2.83 Ang.
RESPONSE: ...
;
_vrf_PLAT934__CCDC_2260010
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..      4 Check
RESPONSE: ...
;
_vrf_PLAT041__CCDC_2260010
;
PROBLEM: Calc. and Reported SumFormula      Strings      Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT042__CCDC_2260010
;
PROBLEM: Calc. and Reported MoietyFormula Strings      Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT043__CCDC_2260010
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..      8.06 Check
RESPONSE: ...
;
_vrf_PLAT068__CCDC_2260010
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...      Please Check
RESPONSE: ...
;
_vrf_PLAT084__CCDC_2260010
;
PROBLEM: High wR2 Value (i.e. > 0.25) .....      0.27 Report
RESPONSE: ...
;
_vrf_PLAT094__CCDC_2260010
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....      2.33 Report

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RESPONSE: ...
;
_vrf_PLAT220_CCCDC_2260010
;
PROBLEM: NonSolvent   Resd 3   C   Ueq(max)/Ueq(min) Range           3.6 Ratio
RESPONSE: ...
;
_vrf_PLAT244_CCCDC_2260010
;
PROBLEM: Low        'Solvent' Ueq as Compared to Neighbors of       C15 Check
RESPONSE: ...
;
_vrf_PLAT260_CCCDC_2260010
;
PROBLEM: Large Average Ueq of Residue Including           C11       0.131 Check
RESPONSE: ...
;
_vrf_PLAT341_CCCDC_2260010
;
PROBLEM: Low Bond Precision on   C-C Bonds .....           0.01047 Ang.
RESPONSE: ...
;
_vrf_PLAT906_CCCDC_2260010
;
PROBLEM: Large K Value in the Analysis of Variance .....   17.822 Check
RESPONSE: ...
;
_vrf_PLAT910_CCCDC_2260010
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min).       8 Note
RESPONSE: ...
;
_vrf_PLAT911_CCCDC_2260010
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=           0.600       275 Report
RESPONSE: ...
;
_vrf_PLAT971_CCCDC_2260010
;
PROBLEM: Check Calcd Resid. Dens.   0.75Ang From O92           1.68 eA-3
RESPONSE: ...
;
_vrf_PLAT975_CCCDC_2260010
;
PROBLEM: Check Calcd Resid. Dens.   1.02Ang From O123           .           0.99 eA-3
RESPONSE: ...
;
_vrf_PLAT976_CCCDC_2260010
;
PROBLEM: Check Calcd Resid. Dens.   0.80Ang From O122           .           -0.74 eA-3
RESPONSE: ...
;
_vrf_PLAT977_CCCDC_2260010
;

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PROBLEM: Check Negative Difference Density on H18 . -0.36 eA-3
RESPONSE: ...
;
end Validation Reply Form

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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