

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) maw200916

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: maw200916

Bond precision:	C-C = 0.0106 Å	Wavelength=0.71073
Cell:	a=17.6463(6) b=9.5745(2) c=18.6548(7)	
	alpha=90 beta=115.083(4) gamma=90	
Temperature:	183 K	
	Calculated	Reported
Volume	2854.58(18)	2854.58(16)
Space group	P 21	P21
Hall group	P 2yb	?
Moiety formula	2(C26 H21 N3 O3 Re), 2(F6 P), C4 H8 O	C28 H25 F6 N3 O3.50 P Re
Sum formula	C56 H50 F12 N6 O7 P2 Re2	C56 H50 F12 N6 O7 P2 Re2
Mr	1581.38	1581.36
Dx,g cm-3	1.840	1.840
Z	2	2
Mu (mm-1)	4.390	4.390
F000	1544.0	1544.0
F000'	1541.24	
h,k,lmax	25,13,26	25,13,26
Nref	17400[9177]	17390
Tmin,Tmax	0.412,0.674	0.182,0.693
Tmin'	0.074	

Correction method= # Reported T Limits: Tmin=0.182 Tmax=0.693
AbsCorr = ANALYTICAL

Data completeness= 1.89/1.00 Theta(max)= 30.510

R(reflections)= 0.0327(15898) wR2(reflections)= 0.0815(17390)

S = 1.033 Npar= 752

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 C

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	6	Check
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C19 -- C20 ..	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C39 -- C40 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference P2 -- F4 ..	0.16	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C17	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	O61	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C63	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C62	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C64	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.1	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01057	Ang.
PLAT397_ALERT_2_C	Deviating C-O-C Angle from 120 Deg for O61	108.3	Degree
PLAT430_ALERT_2_C	Short Inter D...A Contact O2 .. O32 ..	2.90	Ang.
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.72A From Rel	1.61	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Residual Density on Rel	1.17	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Note

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and _chemical_formula_moiety. This is
 usually due to the moiety formula being in the wrong format.
 Atom count from _chemical_formula_sum: C56 H50 F12 N6 O7 P2 Re2
 Atom count from _chemical_formula_moiety: C28 H25 F6 N3 O3.5 P1 Re1

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9	Note
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2	Units
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Re1 -- C1 ..	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Re2 -- C31 ..	6.5	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F9 is Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F10 is Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F11 is Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F12 is Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F9B is Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F10B is Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F11B is Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F12B is Constrained at	0.4	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)..	57 %	Note
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	1	Do !
	C1 -RE1 -N1 -C14 139.40 1.90 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6	Do !
	C1 -RE1 -N1 -C4 22.00 2.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	11	Do !
	C1 -RE1 -N1 -C24 -97.00 2.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	18	Do !
	C2 -RE1 -N2 -C5 47.40 1.40 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	23	Do !
	C2 -RE1 -N2 -C13 -135.70 1.20 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	27	Do !

C3	-RE1	-N3	-C15	1.50	1.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	32	Do !
C3	-RE1	-N3	-C23	174.80	1.10	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	37	Do !
C31	-RE2	-N31	-C34	19.00	2.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	42	Do !
C31	-RE2	-N31	-C44	-99.00	2.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	47	Do !
C31	-RE2	-N31	-C54	137.00	2.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	51	Do !
C32	-RE2	-N32	-C45	17.40	1.60	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	56	Do !
C32	-RE2	-N32	-C53	-150.90	1.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	63	Do !
C33	-RE2	-N33	-C35	-20.90	1.30	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	68	Do !
C33	-RE2	-N33	-C43	163.00	1.10	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	71	Do !
C3	-RE1	-C1	-O1	19.00	5.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	72	Do !
C2	-RE1	-C1	-O1	-70.00	5.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	73	Do !
N1	-RE1	-C1	-O1	58.00	6.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	74	Do !
N3	-RE1	-C1	-O1	-162.00	5.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	75	Do !
N2	-RE1	-C1	-O1	113.00	5.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	76	Do !
C1	-RE1	-C2	-O2	16.00	0.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	77	Do !
C3	-RE1	-C2	-O2	12.00	0.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	78	Do !
N1	-RE1	-C2	-O2	2.00	0.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	79	Do !
N3	-RE1	-C2	-O2	6.00	0.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	80	Do !
N2	-RE1	-C2	-O2	0.00	0.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	81	Do !
C1	-RE1	-C3	-O3	-141.00	19.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	82	Do !
C2	-RE1	-C3	-O3	-54.00	19.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	83	Do !
N1	-RE1	-C3	-O3	42.00	19.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	84	Do !
N3	-RE1	-C3	-O3	48.00	19.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	85	Do !
N2	-RE1	-C3	-O3	118.00	19.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	148	Do !
C32	-RE2	-C31	-O31	-26.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	149	Do !
C33	-RE2	-C31	-O31	63.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	150	Do !
N32	-RE2	-C31	-O31	159.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	151	Do !
N33	-RE2	-C31	-O31	-116.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	152	Do !
N31	-RE2	-C31	-O31	-97.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	153	Do !
C31	-RE2	-C32	-O32	53.00	18.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	154	Do !
C33	-RE2	-C32	-O32	-34.00	18.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle ...	#	155	Do !

N32 -RE2 -C32 -O32	-160.00	17.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							156 Do !
N33 -RE2 -C32 -O32	154.00	18.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							157 Do !
N31 -RE2 -C32 -O32	-132.00	18.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							158 Do !
C32 -RE2 -C33 -O33	4.00	11.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							159 Do !
C31 -RE2 -C33 -O33	-80.00	11.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							160 Do !
N32 -RE2 -C33 -O33	18.00	0.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							161 Do !
N33 -RE2 -C33 -O33	93.00	11.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							162 Do !
N31 -RE2 -C33 -O33	98.00	11.00	1.555	1.555	1.555	1.555	
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #							36 Check
F9B -P1 -F12	1.555	1.555	1.555				36.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #							47 Check
F12B -P1 -F9	1.555	1.555	1.555				28.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #							52 Check
F11 -P1 -F11B	1.555	1.555	1.555				30.70 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #							3 Note
F6 P							
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #							4 Note
F6 P							
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #							5 Note
C4 H8 O							
PLAT860_ALERT_3_G Number of Least-Squares Restraints							19 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL							2014 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)							4 Note

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

3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
 13 **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
 69 **ALERT type 4** Improvement, methodology, query or suggestion
 1 **ALERT type 5** Informative message, check

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.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

