

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0131 A Wavelength=0.71073

Cell: a=9.370(4) b=12.462(6) c=16.242(7)
 alpha=102.593(9) beta=95.875(8) gamma=105.085(8)

Temperature: 293 K

	Calculated	Reported
Volume	1761.5(14)	1761.5(13)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C37 H26 Co N5 O4, 2(H2 O)	?
Sum formula	C37 H30 Co N5 O6	C37 H30 Co N5 O6
Mr	699.59	699.59
Dx,g cm-3	1.319	1.319
Z	2	2
Mu (mm-1)	0.539	0.539
F000	724.0	724.0
F000'	724.99	
h,k,lmax	11,14,19	11,14,19
Nref	6206	6040
Tmin,Tmax	0.908,0.953	0.891,0.953
Tmin'	0.888	

Correction method= MULTI-SCAN

Data completeness= 0.973 Theta(max)= 25.000

R(reflections)= 0.0874(3687) wR2(reflections)= 0.1577(6040)

S = 1.004 Npar= 454

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 A

PLAT213_ALERT_2_A Atom C11	has ADP max/min Ratio	5.2 prola
PLAT213_ALERT_2_A Atom C15	has ADP max/min Ratio	6.7 prola
PLAT241_ALERT_2_A Check High	Ueq as Compared to Neighbors for	C15
PLAT245_ALERT_2_A U(iso) H3W	Smaller than U(eq) O2W by ...	0.126 AngSq

PLAT245_ALERT_2_A	U(iso) H4W	Smaller than U(eq) O2W	by ...	0.126	AngSq
PLAT415_ALERT_2_A	Short Inter D-H..H-X	H1W	.. H16	..	1.73 Ang.
PLAT417_ALERT_2_A	Short Inter D-H..H-D	H2W	.. H4W	..	1.45 Ang.
PLAT601_ALERT_2_A	Structure Contains Solvent Accessible VOIDS of			279	A**3

Alert level B

PLAT213_ALERT_2_B	Atom C7	has ADP max/min Ratio	4.3	prola
PLAT213_ALERT_2_B	Atom C9	has ADP max/min Ratio	4.2	prola
PLAT213_ALERT_2_B	Atom C10	has ADP max/min Ratio	4.3	prola
PLAT220_ALERT_2_B	Large Non-Solvent	C	Ueq(max)/Ueq(min)	...	8.6 Ratio
PLAT222_ALERT_3_B	Large Non-Solvent	H	Uiso(max)/Uiso(min)	..	7.7 Ratio
PLAT420_ALERT_2_B	D-H Without Acceptor	O2W	- H3W	...	?

Alert level C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	Low	0.979	
PLAT048_ALERT_1_C	MoietyFormula	Not Given	?	
PLAT125_ALERT_4_C	No '_symmetry_space_group_name_Hall'	Given	?	
PLAT213_ALERT_2_C	Atom N3	has ADP max/min Ratio	3.4	prola
PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio	4.0	prola
PLAT213_ALERT_2_C	Atom C6	has ADP max/min Ratio	3.5	prola
PLAT213_ALERT_2_C	Atom C8	has ADP max/min Ratio	3.2	prola
PLAT213_ALERT_2_C	Atom C12	has ADP max/min Ratio	3.7	prola
PLAT213_ALERT_2_C	Atom C13	has ADP max/min Ratio	3.3	prola
PLAT213_ALERT_2_C	Atom C14	has ADP max/min Ratio	3.6	prola
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C6	
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C11	
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C12	
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C14	
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C28	
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C34	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		C10	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		C13	
PLAT245_ALERT_2_C	U(iso) H1W	Smaller than U(eq) O1W	by ...	0.049	AngSq
PLAT245_ALERT_2_C	U(iso) H2W	Smaller than U(eq) O1W	by ...	0.049	AngSq
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		4.0	
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0131	Ang
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond	C12 - C13	...	1.34	Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond	C13 - C14	...	1.34	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H8	.. H15	..	1.99 Ang.

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6
PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension	3
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.20
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffn_ambient_temperature	293 K
PLAT343_ALERT_2_G	Check sp? Angle Range in Main Residue for	C13
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	6

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

37 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
missing. This is required for a full paper submission (but is
optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
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RESPONSE: ...
;
_vrf_PLAT213_I
;
PROBLEM: Atom C11          has ADP max/min Ratio .....      5.2 prola
RESPONSE: ...
;
_vrf_PLAT241_I
;
PROBLEM: Check High      Ueq as Compared to Neighbors for      C15
RESPONSE: ...
;
_vrf_PLAT245_I
;
PROBLEM: U(iso) H3W      Smaller than U(eq) O2W      by ...      0.126 AngSq
RESPONSE: ...
;
_vrf_PLAT415_I
;
PROBLEM: Short Inter D-H..H-X      H1W      ..      H16      ..      1.73 Ang.
RESPONSE: ...
;
_vrf_PLAT417_I
;
PROBLEM: Short Inter D-H..H-D      H2W      ..      H4W      ..      1.45 Ang.
RESPONSE: ...
;
_vrf_PLAT601_I
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of .      279 A**3
RESPONSE: ...
;
# end Validation Reply Form

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If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

