

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	C-C = 0.0010 A	Wavelength=0.71073
Cell:	a=7.0287(10)	b=12.9457(19) c=18.578(3)
	alpha=90	beta=90.850(6) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1690.3(4)	1690.3(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C11 H18 Cl2 Fe N4, Cl O4	C11 H18 Cl2 Fe N4, Cl O4
Sum formula	C11 H18 Cl3 Fe N4 O4	C11 H18 Cl3 Fe N4 O4
Mr	432.49	435.52
Dx,g cm-3	1.699	1.711
Z	4	4
Mu (mm-1)	1.389	1.390
F000	884.0	896.0
F000'	887.43	
h,k,lmax	14,26,37	14,26,37
Nref	15150	15087
Tmin,Tmax	0.612,0.801	0.690,0.810
Tmin'	0.590	

Correction method= # Reported T Limits: Tmin=0.690 Tmax=0.810
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 46.620

R(reflections)= 0.0289(12351) wR2(reflections)= 0.0727(15087)

S = 1.050 Npar= 220

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

CHEMW01_ALERT_1_C The difference between the given and expected weight for compound is greater 1 mass unit. Check that all hydrogen atoms have been taken into account.

PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	3.03	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.50	Report
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H12 .. CL3 ..	2.91	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4 .. CL2 ..	2.86	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9B .. CL2 ..	2.91	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9A .. CL1 ..	2.96	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8A .. CL2 ..	2.85	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4 .. CL2 ..	2.86	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9B .. CL2 ..	2.91	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9A .. CL1 ..	2.96	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8A .. CL2 ..	2.85	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8A .. CL2 ..	2.85	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9A .. CL1 ..	2.96	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9B .. CL2 ..	2.91	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4 .. CL2 ..	2.86	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8A .. CL2 ..	2.85	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9A .. CL1 ..	2.96	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9B .. CL2 ..	2.91	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4 .. CL2 ..	2.86	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8A .. CL2 ..	2.85	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9A .. CL1 ..	2.96	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H9B .. CL2 ..	2.91	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4 .. CL2 ..	2.86	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H12 .. CL3 ..	2.91	Ang.

Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	Please Do !
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- N1 ..	8.6 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- N2 ..	7.4 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- N3 ..	11.4 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- N4 ..	6.9 su
PLAT793_ALERT_4_G	The Model has Chirality at N1	(Centro SPGR)	R Verify
PLAT793_ALERT_4_G	The Model has Chirality at N2	(Centro SPGR)	R Verify
PLAT793_ALERT_4_G	The Model has Chirality at N3	(Centro SPGR)	S Verify

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
26 **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
5 **ALERT type 2** Indicator that the structure model may be wrong or deficient
0 **ALERT type 3** Indicator that the structure quality may be low
25 **ALERT type 4** Improvement, methodology, query or suggestion
1 **ALERT type 5** Informative message, check

checkCIF publication errors

Alert level A

PUBL003_ALERT_1_A The contact author's name is missing,
_publ_contact_author_name.
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'
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).

5 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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 a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

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

```
# start Validation Reply Form
_vrf_PUBL003_GLOBAL
;
PROBLEM: The contact author's name is 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: ...
```

```

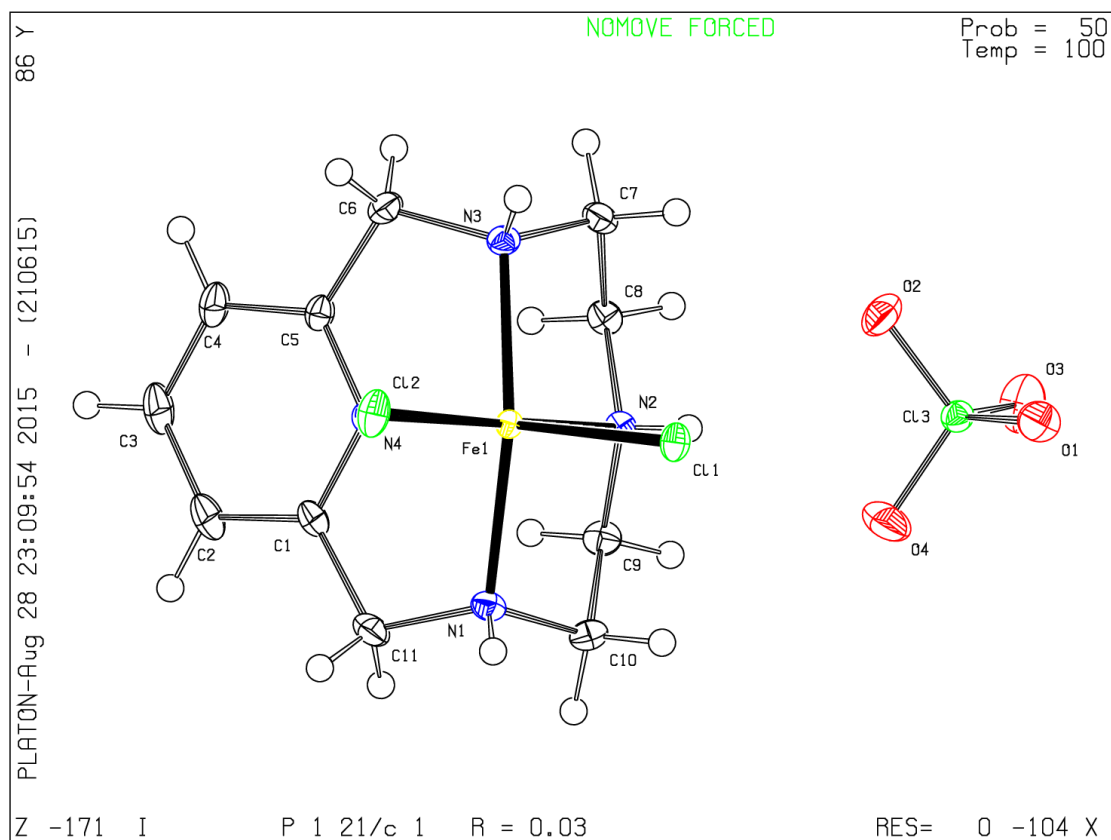
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
# end Validation Reply Form

```

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 21/06/2015; check.def file version of 21/06/2015

Datablock I - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0017 Å Wavelength=0.71073

Cell: a=9.2816(7) b=12.7956(9) c=14.4652(11)
 alpha=90 beta=95.565(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1709.8(2)	1709.8(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C11 H18 Cl2 Fe N4 O, Cl O4	C11 H18 Cl2 Fe N4 O, Cl O4
Sum formula	C11 H18 Cl3 Fe N4 O5	C11 H18 Cl3 Fe N4 O5
Mr	448.49	448.49
Dx,g cm-3	1.742	1.742
Z	4	4
Mu (mm-1)	1.381	1.381
F000	916.0	916.0
F000'	919.47	
h,k,lmax	14,20,23	14,20,22
Nref	7524	7088
Tmin,Tmax	0.745,0.802	0.750,0.810
Tmin'	0.731	

Correction method= # Reported T Limits: Tmin=0.750 Tmax=0.810
AbsCorr = MULTI-SCAN

Data completeness= 0.942 Theta(max)= 34.990

R(reflections)= 0.0307(5977) wR2(reflections)= 0.0828(7088)

S = 1.024 Npar= 230

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

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full	Low	0.942	Note
PLAT480_ALERT_4_B	Long H...A H-Bond Reported H1	..	CL2 ..	3.32	Ang.
PLAT482_ALERT_4_B	Small D-H..A Angle Rep for N1	..	CL2 ..	85.40	Degree

Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.14	Report
-------------------	---	------	------	--------

Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- N3 ..	7.5 su
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #		4 Do !
	CL2 -FE1 -N2 -C9	-113.10 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #		9 Do !
	CL2 -FE1 -N2 -C8	15.80 0.50 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #		25 Do !
	CL1 -FE1 -N4 -C1	73.40 0.20 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #		30 Do !
	CL1 -FE1 -N4 -C5	-105.60 0.20 1.555 1.555 1.555	1.555
PLAT793_ALERT_4_G	The Model has Chirality at N1	(Centro SPGR)	S Verify
PLAT793_ALERT_4_G	The Model has Chirality at N2	(Centro SPGR)	R Verify
PLAT793_ALERT_4_G	The Model has Chirality at N3	(Centro SPGR)	R Verify

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

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

checkCIF publication errors

Alert level A

PUBL003_ALERT_1_A The contact author's name is missing,
_publ_contact_author_name.
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'
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).

- 5 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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 a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

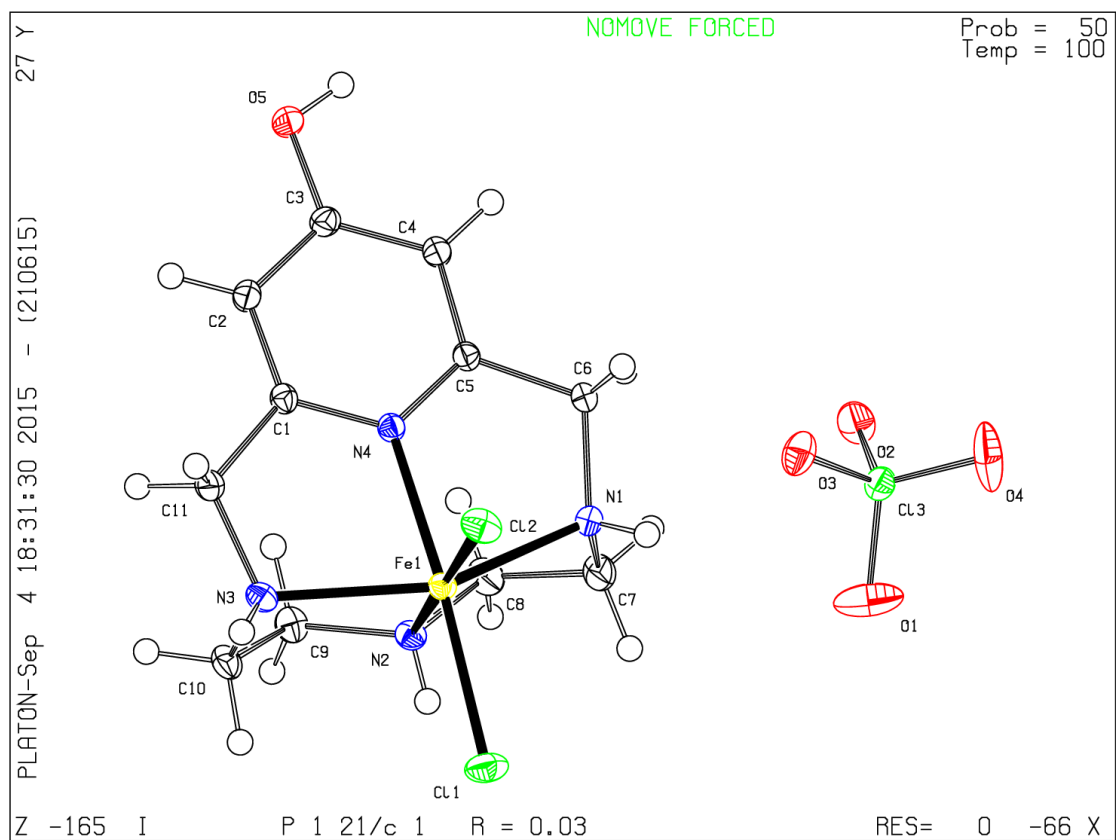
Validation response form

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

```
# start Validation Reply Form
_vrf_PUBL003_GLOBAL
;
PROBLEM: The contact author's name is 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_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: ...
;
# end Validation Reply Form
```

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.

Datablock I - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073
Cell:	a=7.0773(3)	b=9.4652(4) c=12.9941(6)
	alpha=85.329(2)	beta=81.642(2) gamma=89.546(2)
Temperature:	100 K	
	Calculated	Reported
Volume	858.34(7)	858.34(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C11 H18 Cl2 Fe N4 O, Cl O4	C11 H18 Cl2 Fe N4 O, Cl O4
Sum formula	C11 H18 Cl3 Fe N4 O5	C11 H18 Cl3 Fe N4 O5
Mr	448.49	448.49
Dx,g cm-3	1.735	1.735
Z	2	2
Mu (mm-1)	1.375	1.375
F000	458.0	458.0
F000'	459.73	
h,k,lmax	9,12,16	9,12,16
Nref	3805	3797
Tmin,Tmax	0.820,0.934	0.810,0.940
Tmin'	0.803	

Correction method= # Reported T Limits: Tmin=0.810 Tmax=0.940
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.160

R(reflections)= 0.0358(3041) wR2(reflections)= 0.0779(3797)

S = 0.954 Npar= 239

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

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C13 Check



Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 5 Report
 PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed Check
 PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00200 Degree
 PLAT301_ALERT_3_G Main Residue Disorder Percentage = 16 Note
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 5 Do !
 CL2 -FE1 -N1 -C11 -51.70 0.70 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 10 Do !
 CL2 -FE1 -N1 -C1 77.80 0.70 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 !
 CL1 -FE1 -N3 -C8 110.70 0.60 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 !
 CL1 -FE1 -N3 -C4 -75.60 0.60 1.555 1.555 1.555 1.555
 PLAT793_ALERT_4_G The Model has Chirality at N1 (Centro SPGR) R Verify
 PLAT793_ALERT_4_G The Model has Chirality at N2 (Centro SPGR) S Verify
 PLAT793_ALERT_4_G The Model has Chirality at N4 (Centro SPGR) R Verify

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

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

checkCIF publication errors



Alert level A

PUBL003_ALERT_1_A The contact author's name is missing,
 _publ_contact_author_name.
 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'
 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).

5 **ALERT level A** = Data missing that is essential or data in wrong format
 0 **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 a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

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

```
# start Validation Reply Form
_vrf_PUBL003_GLOBAL
;
PROBLEM: The contact author's name is 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_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: ...
;
# end Validation Reply Form
```

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 21/06/2015; check.def file version of 21/06/2015

Datablock I - ellipsoid plot

