

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) CoNO22L12, CoNO2L12BF4, CoNO32L12, FeCl2L12, FeNO2L12BF4

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.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

[Structure factor report](#)

Datablock: FeNO2L12BF4

Bond precision:	C-C = 0.0080 Å	Wavelength=0.71075
Cell:	a=13.093 (3) b=19.318 (5) c=10.174 (3)	
	alpha=90 beta=90.349 (7) gamma=90	
Temperature:	178 K	

	Calculated	Reported
Volume	2573.3 (12)	2573.3 (12)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C19 H32 Fe N6 O2, B F4	C19 H32 B F4 Fe N6 O2
Sum formula	C19 H32 B F4 Fe N6 O2	C19 H32 B F4 Fe N6 O2
Mr	519.17	519.15
Dx, g cm-3	1.340	1.340
Z	4	4
Mu (mm-1)	0.641	0.640
F000	1084.0	1084.0
F000'	1085.90	
h, k, lmax	16, 25, 13	17, 25, 13
Nref	5916 [2964]	4870
Tmin, Tmax	0.970, 0.981	0.881, 0.981
Tmin'	0.863	

Correction method= # Reported T Limits: Tmin=0.881
Tmax=0.981 AbsCorr = NUMERICAL
Data completeness= 1.64/0.82 Theta(max)= 27.503
R(reflections)= 0.0473 (4507) wR2(reflections)= 0.1365 (4870)
S = 1.042 Npar= 298

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

[PLAT987 ALERT 1 B](#) The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

[PLAT094 ALERT 2 C](#) Ratio of Maximum / Minimum Residual Density 3.15 Report

[PLAT220 ALERT 2 C](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.0 Ratio

[PLAT242 ALERT 2 C](#) Low 'MainMol' Ueq as Compared to Neighbors of C13 Check

And 3 other PLAT242 Alerts

PLAT242 ALERT 2 C	Low	'MainMol' Ueq as Compared to Neighbors of	C17 Check
PLAT242 ALERT 2 C	Low	'MainMol' Ueq as Compared to Neighbors of	C23 Check
PLAT242 ALERT 2 C	Low	'MainMol' Ueq as Compared to Neighbors of	C27 Check
PLAT341 ALERT 3 C	Low	Bond Precision on C-C Bonds	0.008 Ang.
PLAT910 ALERT 3 C	Missing # of FCF Reflection(s) Below Theta(Min).		5 Note
PLAT911 ALERT 3 C	Missing FCF Refl Between Thmin & STh/L=	0.600	2 Report
PLAT915 ALERT 3 C	No Flack x Check Done: Low Friedel Pair Coverage		65 %

Alert level G

PLAT012 ALERT 1 G	N.O.K. _shelx_res_checksum Found in CIF	Please Check
PLAT042 ALERT 1 G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT072 ALERT 2 G	SHELXL First Parameter in WGHT Unusually Large	0.10 Report
PLAT112 ALERT 2 G	ADDSYM Detects New (Pseudo) Symm. Elem	21 93 %Fit
PLAT112 ALERT 2 G	ADDSYM Detects New (Pseudo) Symm. Elem	m 93 %Fit
PLAT113 ALERT 2 G	ADDSYM Suggests Possible Pseudo/New Space Group	Cmc21 Check
PLAT244 ALERT 4 G	Low 'Solvent' Ueq as Compared to Neighbors of	B51 Check
PLAT794 ALERT 5 G	Tentative Bond Valency for Fe (III)	3.89 Info
PLAT882 ALERT 1 G	No Datum for _diffrn_reflns_av unetI/netI	Please Do !
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L=	0.600 12 Note
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density.	1 Info

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- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 1 ALERT type 5 Informative message, check

Datablock: CoNO2L12BF4

Bond precision:	C-C = 0.0127 Å	Wavelength=0.71075
Cell:	a=11.777 (3) b=15.679 (3) c=17.388 (4)	
	alpha=90 beta=108.515 (4) gamma=90	
Temperature: 178 K		
	Calculated	Reported
Volume	3044.5 (12)	3044.5 (12)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C19 H32 Co N6 O2, B F4, C4 H8 O	C23 H40 B Co F4 N6 O3
Sum formula	C23 H40 B Co F4 N6 O3	C23 H40 B Co F4 N6 O3
Mr	594.35	594.34
Dx, g cm-3	1.297	1.297
Z	4	4
Mu (mm-1)	0.621	0.621
F000	1248.0	1248.0
F000'	1249.98	
h, k, lmax	15, 20, 22	15, 20, 22
Nref	6998 [3504]	6765
Tmin, Tmax	0.917, 0.928	0.768, 0.928
Tmin'	0.917	
Correction method=	# Reported T Limits: Tmin=0.768	
Tmax=0.928	AbsCorr = NUMERICAL	
Data completeness=	1.93/0.97	Theta(max)= 27.484
R(reflections)=	0.0536 (5753)	wR2(reflections)= 0.1596 (6765)
S = 0.923	Npar= 343	

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

PLAT360 ALERT 2 B	Short C(sp3)-C(sp3) Bond C63 - C64	1.25 Ang.
PLAT987 ALERT 1 B	The Flack x is >> 0 - Do a BASF/TWIN Refinement	Please Check

Alert level C

PLAT094 ALERT 2 C	Ratio of Maximum / Minimum Residual Density	2.60 Report
PLAT213 ALERT 2 C	Atom Cl8 has ADP max/min Ratio	3.4 prolat
PLAT220 ALERT 2 C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.9 Ratio

PLAT242 ALERT 2 C	Low	'MainMol' Ueq as Compared to Neighbors of	C17	Check
PLAT242 ALERT 2 C	Low	'MainMol' Ueq as Compared to Neighbors of	C27	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	C61	Check
PLAT244 ALERT 4 C	Low	'Solvent' Ueq as Compared to Neighbors of	C62	Check
PLAT250 ALERT 2 C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.1	Note
PLAT260 ALERT 2 C	Large Average Ueq of Residue Including	F51	0.114	Check
PLAT260 ALERT 2 C	Large Average Ueq of Residue Including	O61	0.143	Check
PLAT341 ALERT 3 C	Low Bond Precision on C-C Bonds		0.01268	Ang.
PLAT410 ALERT 2 C	Short Intra H...H Contact H63A ..H64B .		1.91	Ang.
		x,y,z =	1_555	Check
PLAT410 ALERT 2 C	Short Intra H...H Contact H63B ..H64A .		1.92	Ang.
		x,y,z =	1_555	Check
PLAT910 ALERT 3 C	Missing # of FCF Reflection(s) Below Theta(Min).		7	Note
PLAT911 ALERT 3 C	Missing FCF Refl Between Thmin & STh/L= 0.600		5	Report
PLAT934 ALERT 3 C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1	Check
PLAT978 ALERT 2 C	Number C-C Bonds with Positive Residual Density.		0	Info

Alert level G

PLAT042 ALERT 1 G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT072 ALERT 2 G	SHELXL First Parameter in WGHT Unusually Large	0.13	Report
PLAT244 ALERT 4 G	Low 'Solvent' Ueq as Compared to Neighbors of	B51	Check
PLAT398 ALERT 2 G	Deviating C-O-C Angle From 120 for O61	109.9	Degree
PLAT790 ALERT 4 G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	B F4		
PLAT790 ALERT 4 G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	C4 H8 O		
PLAT794 ALERT 5 G	Tentative Bond Valency for Co1 (III) .	3.50	Info
PLAT882 ALERT 1 G	No Datum for _diffrn_reflms_av_unetI/netI	Please	Do !
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	13	Note
PLAT913 ALERT 3 G	Missing # of Very Strong Reflections in FCF	2	Note

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

Datablock: FeCl2L12

Bond precision:	C-C = 0.0022 A	Wavelength=0.71075
Cell:	a=8.9680(14) b=9.8986(15) c=15.939(2)	
	alpha=99.7610(17) beta=92.444(4) gamma=107.572(4)	
Temperature:	178 K	
	Calculated	Reported
Volume	1322.7(3)	1322.7(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C19 H32 Cl2 Fe N4, C3 H6 O	C22 H38 Cl2 Fe N4 O
Sum formula	C22 H38 Cl2 Fe N4 O	C22 H38 Cl2 Fe N4 O
Mr	501.31	501.32
Dx,g cm-3	1.259	1.259
Z	2	2
Mu (mm-1)	0.791	0.790
F000	532.0	532.0
F000'	533.41	
h,k,lmax	11,12,20	11,12,20
Nref	6071	6059
Tmin,Tmax	0.847,0.867	0.814,0.867
Tmin'	0.847	
Correction method=	# Reported T Limits: Tmin=0.814	
Tmax=0.867	AbsCorr = NUMERICAL	
Data completeness=	0.998	Theta(max)= 27.477
R(reflections)=	0.0274(5699)	wR2(reflections)= 0.0755(6059)
S =	1.054	Npar= 271

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

PLAT220 ALERT 2 C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT242 ALERT 2 C	Low 'MainMol' Ueq as Compared to Neighbors of	C23 Check
PLAT244 ALERT 4 C	Low 'Solvent' Ueq as Compared to Neighbors of	C41 Check
PLAT910 ALERT 3 C	Missing # of FCF Reflection(s) Below Theta(Min).	10 Note
PLAT911 ALERT 3 C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report
PLAT977 ALERT 2 C	Check Negative Difference Density on H42A	-0.31 eA-3

And 2 other PLAT977 Alerts

PLAT977 ALERT 2 C	Check Negative Difference Density on H42B	-0.37 eA-3
PLAT977 ALERT 2 C	Check Negative Difference Density on H42C	-0.37 eA-3

Alert level G

PLAT042 ALERT 1 G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Fe1 --Cl32 .	6.3 s.u.
PLAT380 ALERT 4 G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C42 Check
PLAT380 ALERT 4 G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C43 Check
PLAT794 ALERT 5 G	Tentative Bond Valency for Fe1 (II) .	2.03 Info
PLAT882 ALERT 1 G	No Datum for _diffrn_reflms_av_unetI/netI	Please Do !
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density.	11 Info

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 7 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 3 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

Datablock: CoNO32L12

Bond precision:	C-C = 0.0040 A	Wavelength=0.71075
Cell:	a=16.8808(19) b=17.1117(18) c=18.875(2)	
	alpha=90 beta=90 gamma=90	
Temperature:	178 K	
	Calculated	Reported
Volume	5452.2(10)	5452.2(10)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C19 H32 Co N6 O6 [+ solvent]	C19 H32 Co N6 O6
Sum formula	C19 H32 Co N6 O6 [+ solvent]	C19 H32 Co N6 O6
Mr	499.44	499.43
Dx,g cm-3	1.217	1.217
Z	8	8
Mu (mm-1)	0.669	0.669
F000	2104.0	2104.0
F000'	2107.60	
h,k,lmax	21,22,24	21,22,24
Nref	6268	6251
Tmin,Tmax	0.930,0.980	0.919,0.980
Tmin'	0.887	
Correction method=	# Reported T Limits: Tmin=0.919	
Tmax=0.980 AbsCorr =	NUMERICAL	
Data completeness=	0.997 Theta(max)= 27.509	
R(reflections)=	0.0447(4949) wR2(reflections)= 0.1449(6251)	
S = 1.112	Npar= 289	

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

PLAT910 ALERT 3 B	Missing # of FCF Reflection(s) Below Theta(Min).	11 Note
PLAT934 ALERT 3 B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	6 Check

Alert level C

PLAT213 ALERT 2 C	Atom O43 has ADP max/min Ratio	3.6 prolat
PLAT220 ALERT 2 C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1 Ratio

[PLAT220 ALERT 2 C](#) Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 3.8 Ratio
[PLAT413 ALERT 2 C](#) Short Inter XH3 .. XHn H21A ..H28A . 2.09 Ang.
 $1/2-x, -1/2+y, z = 6_655$ Check
[PLAT906 ALERT 3 C](#) Large K Value in the Analysis of Variance 2.916 Check

Alert level G

[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Col --O31 . 5.3 s.u.

And 2 other PLAT232 Alerts

[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Col --O32 . 12.3 s.u.

[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Col --O42 . 7.4 s.u.

[PLAT605 ALERT 4 G](#) Largest Solvent Accessible VOID in the Structure 211 A**3

[PLAT794 ALERT 5 G](#) Tentative Bond Valency for Col (II) . 2.00 Info

[PLAT869 ALERT 4 G](#) ALERTS Related to the Use of SQUEEZE Suppressed ! Info

[PLAT882 ALERT 1 G](#) No Datum for _diffrn_reflns_av_unetI/netI Please Do !

[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600 6 Note

[PLAT913 ALERT 3 G](#) Missing # of Very Strong Reflections in FCF 1 Note

[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 2 Info

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- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 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
 3 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

Datablock: CoNO22L12

Bond precision: C-C = 0.0049 A Wavelength=0.71075

Cell: a=10.0033(15) b=17.788(3) c=16.691(3)

alpha=90 beta=94.743(4) gamma=90

Temperature: 178 K

	Calculated	Reported
Volume	2959.8(9)	2959.8(9)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C19 H32 Co N6 O4, C4 H8 O [+ solvent]	C23 H40 Co N6 O5
Sum formula	C23 H40 Co N6 O5 [+ solvent]	C23 H40 Co N6 O5
Mr	539.54	539.54
Dx, g cm-3	1.211	1.211
Z	4	4
Mu (mm-1)	0.619	0.619
F000	1148.0	1148.0
F000'	1149.80	
h, k, lmax	13, 23, 21	13, 23, 21
Nref	6806	6795
Tmin, Tmax	0.956, 0.976	0.704, 0.976
Tmin'	0.934	

Correction method= # Reported T Limits: Tmin=0.704

Tmax=0.976 AbsCorr = NUMERICAL

Data completeness= 0.998 Theta(max)= 27.521

R(reflections)= 0.0539(5059) wR2(reflections)= 0.1427(6795)

S = 1.069 Npar= 316

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

[PLAT230 ALERT 2 B](#) Hirshfeld Test Diff for O31 --N31 . 9.5 s.u.

[PLAT230 ALERT 2 B](#) Hirshfeld Test Diff for O32 --N31 . 16.0 s.u.

Alert level C

[PLAT230 ALERT 2 C](#) Hirshfeld Test Diff for O42 --N41 . 7.0 s.u.

[PLAT241 ALERT 2 C](#) High 'MainMol' Ueq as Compared to Neighbors of O32 Check

[PLAT241 ALERT 2 C](#) High 'MainMol' Ueq as Compared to Neighbors of O41 Check

[PLAT242 ALERT 2 C](#) Low 'MainMol' Ueq as Compared to Neighbors of Col Check

PLAT242 ALERT 2 C	Low	'MainMol'	Ueq as Compared to Neighbors of	C17	Check
PLAT243 ALERT 4 C	High	'Solvent'	Ueq as Compared to Neighbors of	C51	Check
PLAT243 ALERT 4 C	High	'Solvent'	Ueq as Compared to Neighbors of	C53	Check
PLAT244 ALERT 4 C	Low	'Solvent'	Ueq as Compared to Neighbors of	O51	Check
PLAT244 ALERT 4 C	Low	'Solvent'	Ueq as Compared to Neighbors of	C52	Check
PLAT906 ALERT 3 C	Large K Value in the Analysis of Variance			2.092	Check
PLAT910 ALERT 3 C	Missing # of FCF Reflection(s) Below Theta(Min).			9	Note

Alert level G

PLAT042 ALERT 1 G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Col --032 .	9.6	s.u.
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Col --042 .	8.4	s.u.
PLAT398 ALERT 2 G	Deviating C-O-C Angle From 120 for O51	108.2	Degree
PLAT605 ALERT 4 G	Largest Solvent Accessible VOID in the Structure	138	A**3
PLAT794 ALERT 5 G	Tentative Bond Valency for Col (II) .	1.96	Info
PLAT869 ALERT 4 G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT882 ALERT 1 G	No Datum for _diffrn_reflns_av unetI/netI	Please	Do !
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT913 ALERT 3 G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density.	2	Info

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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

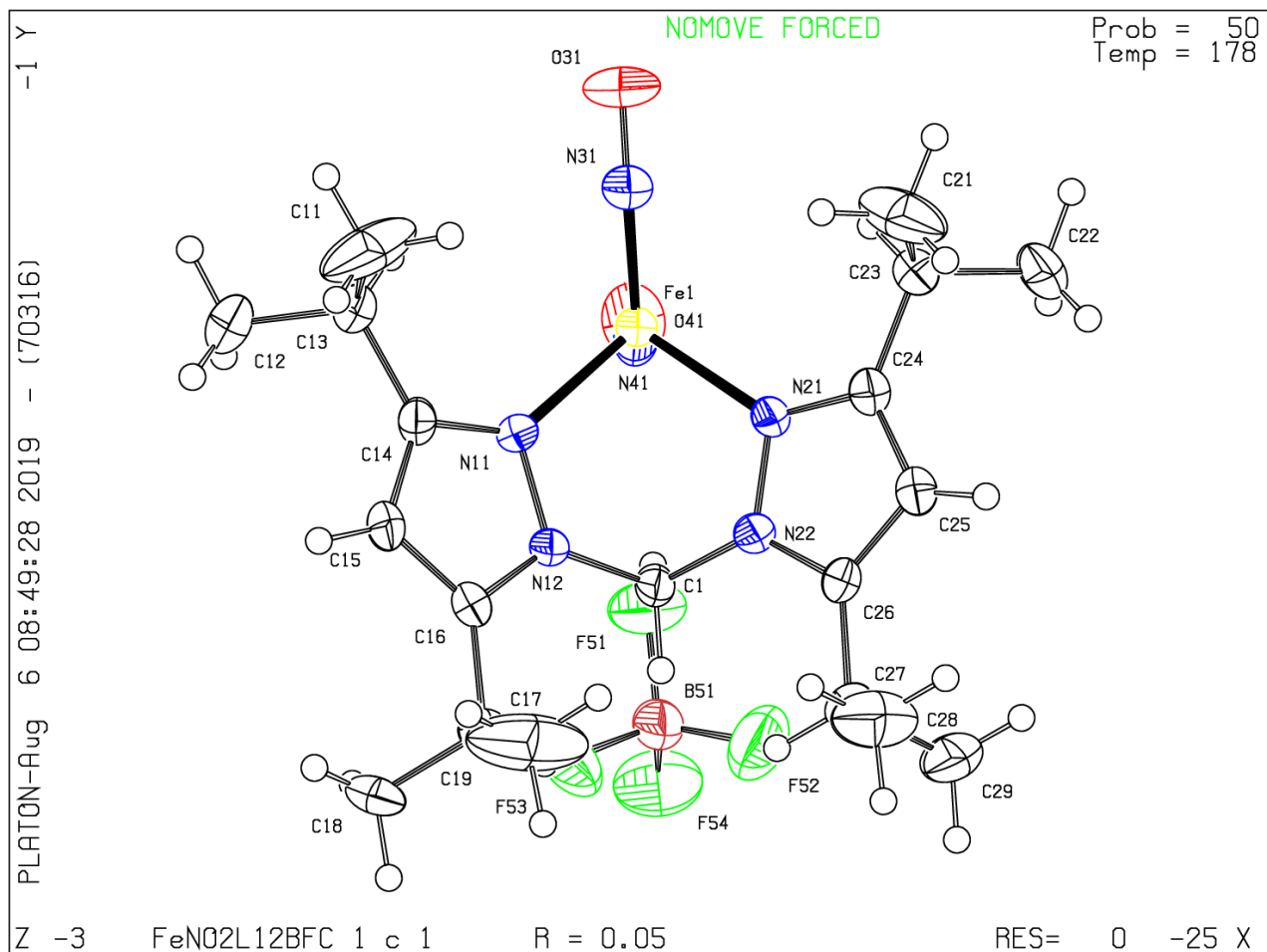
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

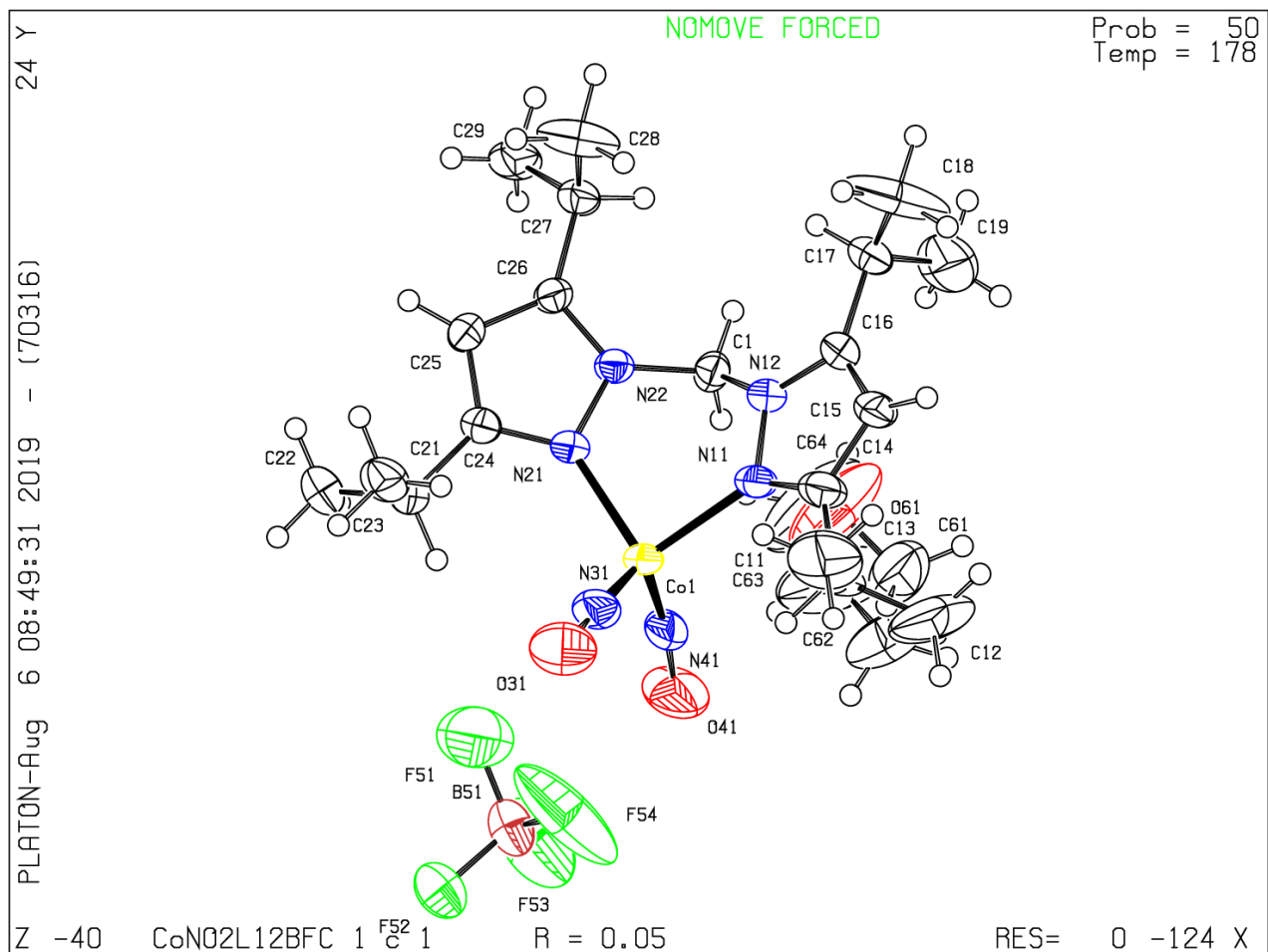
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

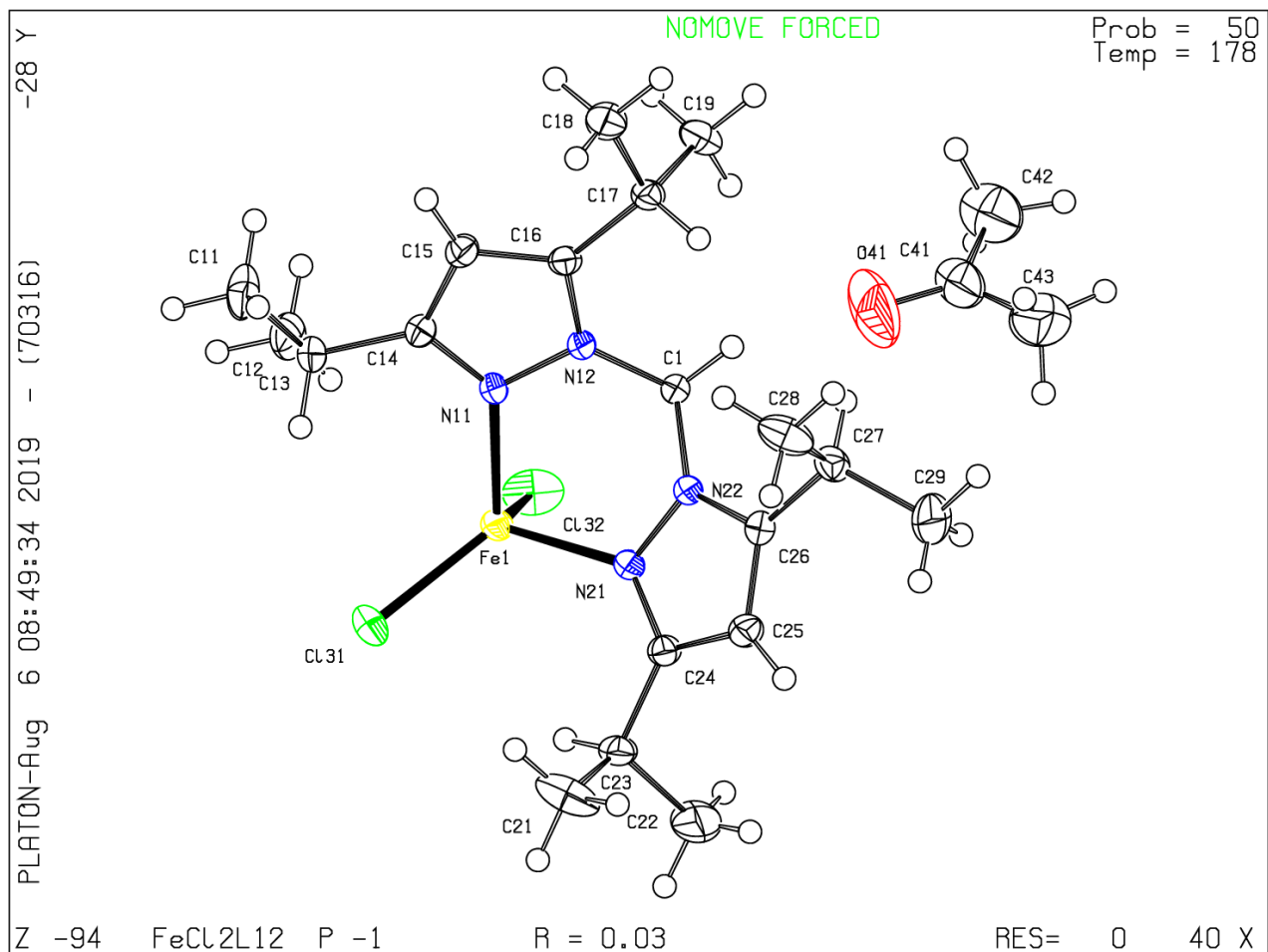
Datablock FeNO2L12BF4 - ellipsoid plot



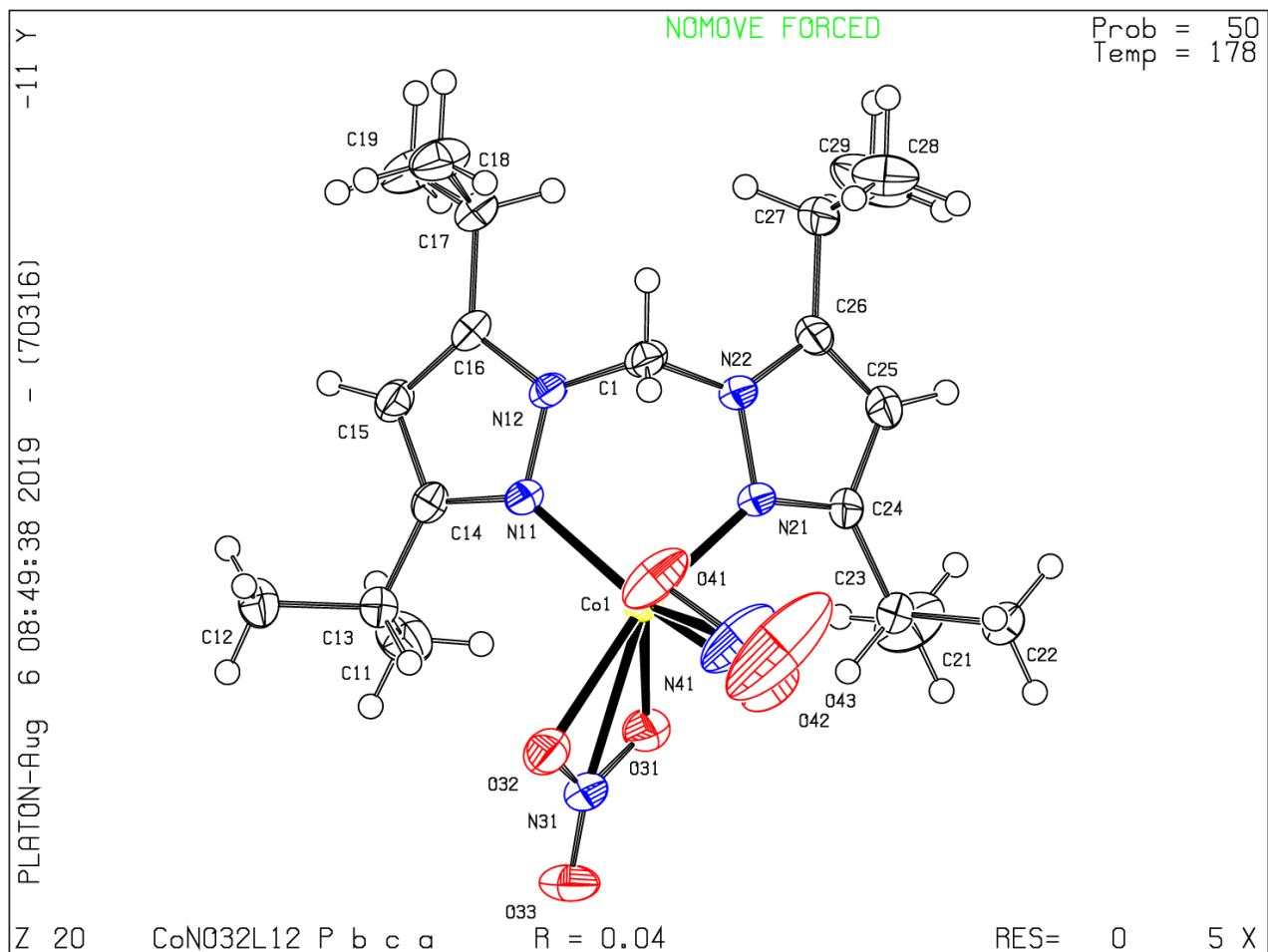
Datablock CoNO2L12BF4 - ellipsoid plot



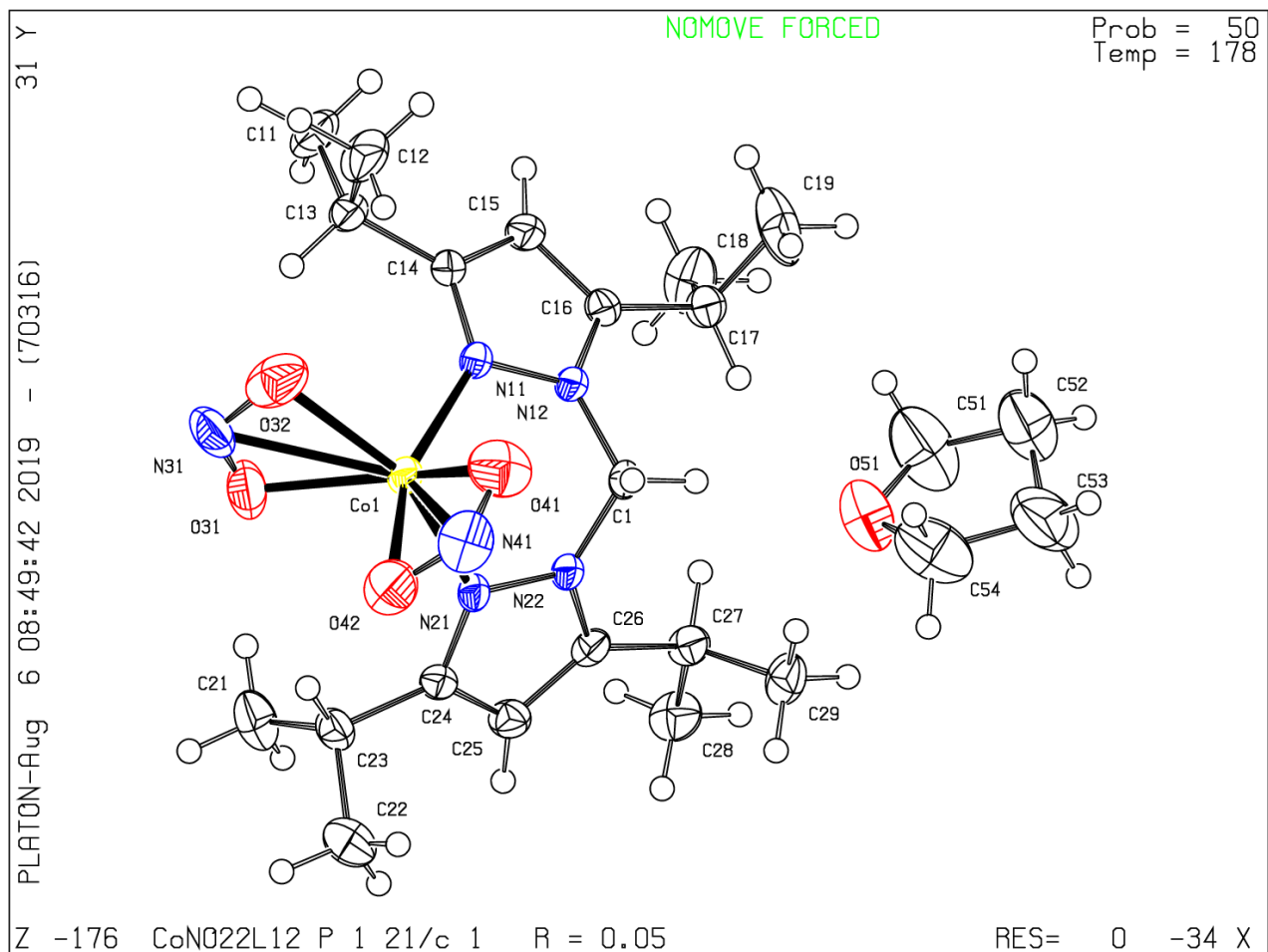
Datablock FeCl2L12 - ellipsoid plot



Datablock CoN032L12 - ellipsoid plot



Datablock CoNO22L12 - ellipsoid plot



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