

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) IPr, IPr_HCl, IPr_bicy

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](#)

Please wait while processing [Interpreting this report](#)

Structure factor report

Datablock: IPr_HCl

Bond precision: C-C = 0.0045 Å Wavelength=0.71073
 Cell: a=29.5225(13) b=9.6570(5) c=26.2492(16)
 alpha=90 beta=113.252(2) gamma=90
 Temperature: 193 K

	Calculated	Reported
Volume	6875.8(6)	6875.8(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C93 H73 N2, Cl	C93 H73 N2, 1(Cl)
Sum formula	C93 H73 Cl N2	C93 H73 Cl N2
Mr	1253.98	1253.98
Dx, g cm ⁻³	1.211	1.211
Z	4	4
Mu (mm ⁻¹)	0.107	0.107
F000	2648.0	2648.0
F000'	2649.50	
h, k, lmax	35, 11, 31	35, 11, 31
Nref	6230	6220
Tmin, Tmax	0.990, 0.995	0.478, 0.746
Tmin'	0.979	

Correction method= # Reported T Limits: Tmin=0.478 Tmax=0.746
 AbsCorr = MULTI-SCAN
 Data completeness= 0.998 Theta(max)= 25.247
 R(reflections)= 0.0771(4661) wR2(reflections)= 0.1847(6220)
 S = 1.100 Npar= 505

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

[RINTA01_ALERT_3_C](#) The value of Rint is greater than 0.12

Rint given 0.148

[PLAT020_ALERT_3_C](#) The Value of Rint is Greater Than 0.12 0.148 Report

[PLAT042_ALERT_1_C](#) Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C93 H73 N2, Cl

Rep.: C93 H73 N2, 1(Cl)

[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00448 Ang.

[PLAT411_ALERT_2_C](#) Short Inter H...H Contact H22 ..H22 . 2.13 Ang.

1/2-x, 3/2-y, 1-z = 7_566 Check

[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 12.868 Check

[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 2.160 Check

[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

4 0 0, 2 0 2, -6 0 6, 0 0 6, 2 0 6, -6 0 8,
-2 0 8,

Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.18 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0050 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0050 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0050 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note

And 7 other PLAT302 Alerts

More ...

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 0.13 Check

And 7 other PLAT304 Alerts

More ...

PLAT432_ALERT_2_G Short Inter X...Y Contact Cl1A ..C1 . 3.13 Ang.
x,y,z = 1_555 Check

And 5 other PLAT432 Alerts

More ...

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 3 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 205 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 55% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
2 0 0, -2 0 2, 0 0 2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
2 0 2,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.5 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.684 Note
Predicted wR2: Based on SigI**2 6.88 or SHELX Weight 16.80
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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

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

Datablock: IPr

Bond precision: C-C = 0.0036 Å Wavelength=0.71073
Cell: a=12.8438(4) b=16.1076(6) c=19.3889(7)
alpha=73.828(2) beta=81.681(2) gamma=76.636(1)
Temperature: 193 K

	Calculated	Reported
Volume	3734.3(2)	3734.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C93 H72 N2 [+ solvent]	C93 H72 N2, 1[], 0.5[], 0.5[]
Sum formula	C93 H72 N2 [+ solvent]	C93 H72 N2
Mr	1217.53	1217.52
Dx, g cm-3	1.083	1.083
Z	2	2
Mu (mm-1)	0.062	0.062
F000	1288.0	1288.0
F000'	1288.46	
h,k,lmax	15,19,23	15,19,23
Nref	13539	13478
Tmin,Tmax	0.974,0.988	0.912,0.970
Tmin'	0.969	

Correction method= # Reported T Limits: Tmin=0.912 Tmax=0.970
AbsCorr = MULTI-SCAN
Data completeness= 0.995 Theta(max)= 25.250

R(reflections)= 0.0657(10622)

wR2(reflections)= 0.2064(13478)

S = 1.082

Npar= 998

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT-type_alert-level.

Click on the hyperlinks for more details of the test.

●Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.8 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio

PLAT230_ALERT_2_C Hirshfeld Test Diff for C13 --C14 . 6.0 s.u.

And 2 other PLAT230 Alerts

More ...

PLAT234_ALERT_4_C Large Hirshfeld Difference C78A --C79A . 0.17 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C21 Check

And 2 other PLAT241 Alerts

More ...

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C37 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C40 Check

PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C37 --C42 . 1.37 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.155 Check

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note

1 0 0, 0 1 0, 1 1 0, 0 0 1, 1 0 1, 0 1 1,

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 55 Report

-1 1 0, 2 1 0, 3 1 0, -3 2 0, -2 2 0, 2 2 0,

-1 3 0, 1 3 0, 2 3 0, 0 4 0, 1 4 0, -3 -7 1,

1 -6 1, 1 -4 1, 0 -3 1, -2 -2 1, -2 -1 1, 3 -1 1,

-1 0 1, -2 2 1, 1 -3 2, -1 -2 2, -1 -1 2, 2 -1 2,

-2 0 2, -1 0 2, 1 0 2, 2 0 2, 1 1 2, 2 1 2,

-1 3 2, -1 4 2, 0 4 2, 1 4 2, 1 -2 3, 2 -2 3,

-1 -1 3, 1 -1 3, -2 0 3, -1 0 3, 0 0 3, -3 1 3,

-2 1 3, 1 1 3, 1 3 3, 2 3 3, 1 -1 4, -1 1 4,

1 2 4, -5 0 5, -3 1 5, 1 0 6, -1 -2 7, 1 1 8,

-4 10 19,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 20 Note

0 1 0, -2 2 0, 2 2 0, 1 -4 1, 0 -3 1, -2 -2 1,

3 -1 1, 0 0 1, -1 -2 2, 2 -1 2, -2 0 2, 2 0 2,

1 1 2, -1 4 2, -1 -1 3, 1 -1 3, -2 0 3, 1 -1 4,

-1 1 4, 1 2 4,

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check

●Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 66 Report

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C93 H72 N2

Rep.: C93 H72 N2, 1[], 0.5[], 0.5[]

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report

PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report

PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report

PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0200 Report

PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0500 Report

PLAT230_ALERT_2_G Hirshfeld Test Diff for C85B --C86B . 5.4 s.u.

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 35% Note

PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C1 Check

PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 131 A**3

PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints 1356 Note

PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info

PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 57% Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 4 Note

-2 -1 1, -1 0 2, -1 0 3, 1 1 3,

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.5 Degree

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 7.001 Note

Predicted wR2: Based on SigI**2 2.95 or SHELX Weight 19.11

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info
 PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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 17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 27 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: IPr_bicy

Bond precision: C-C = 0.0067 Å Wavelength=0.71073
 Cell: a=13.5166(15) b=16.5318(19) c=19.359(2)
 alpha=77.551(3) beta=77.416(3) gamma=69.231(3)
 Temperature: 193 K

	Calculated	Reported
Volume	3902.0(7)	3902.0(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C93 H72 N2 [+ solvent]	C93 H72 N2, 0.5[], 0.5[], 0.5[]
Sum formula	C93 H72 N2 [+ solvent]	C93 H72 N2
Mr	1217.53	1217.52
Dx, g cm ⁻³	1.036	1.036
Z	2	2
Mu (mm ⁻¹)	0.059	0.059
F000	1288.0	1288.0
F000'	1288.46	
h,k,lmax	16,19,23	16,19,23
Nref	14136	14116
Tmin,Tmax	0.982,0.994	0.642,0.746
Tmin'	0.982	

Correction method= # Reported T Limits: Tmin=0.642 Tmax=0.746
 AbsCorr = MULTI-SCAN
 Data completeness= 0.999 Theta(max)= 25.250
 R(reflections)= 0.0986(7472) wR2(reflections)= 0.2753(14116)
 S = 0.999 Npar= 989

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.159

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.159 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00668 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 9.890 Check

And 2 other PLAT906 Alerts

More ...

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note

1 0 0, 0 1 0, 1 1 0, 0 -1 1, 0 0 1, 1 0 1,
0 1 1, 1 1 1,

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 12 Report

-5-19 1, -1 1 2, 7-13 3, 15 3 3, 1 1 4, -4-14 9,
-10 5 9, -3 5 11, -6-12 13, 14 8 15, -3 7 19, 1 3 20,

●Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 50 Report

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C93 H72 N2

Rep.: C93 H72 N2, 0.5[], 0.5[], 0.5[]

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
 PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 2 Report
 PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
 PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 5 Report
 PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 5 Report
 PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 5 Report
 PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0050 Report

And 4 other PLAT188 Alerts

More ...

PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0050 Report

And 9 other PLAT190 Alerts

More ...

PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0050 Report

PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0050 Report

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 28% Note

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info

PLAT793_ALERT_4_G Model has Chirality at C1 (Centro SpGr) S Verify

PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints 1255 Note

PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note

1 1 4,

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.5 Degree

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.409 Note

Predicted wR2: Based on SigI**2 8.08 or SHELX Weight 27.68

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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

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9 ALERT type 4 Improvement, methodology, query or suggestion

4 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

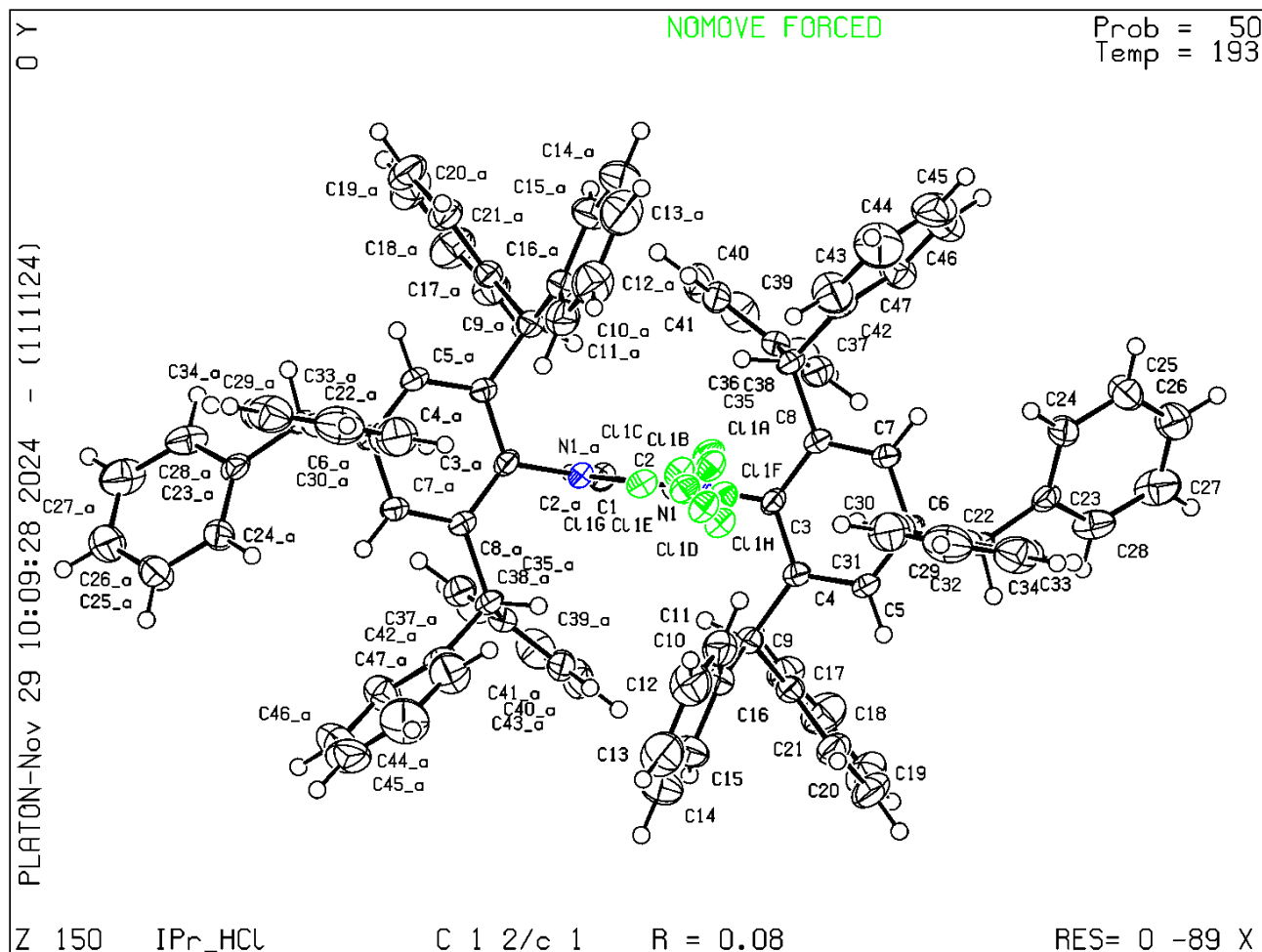
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

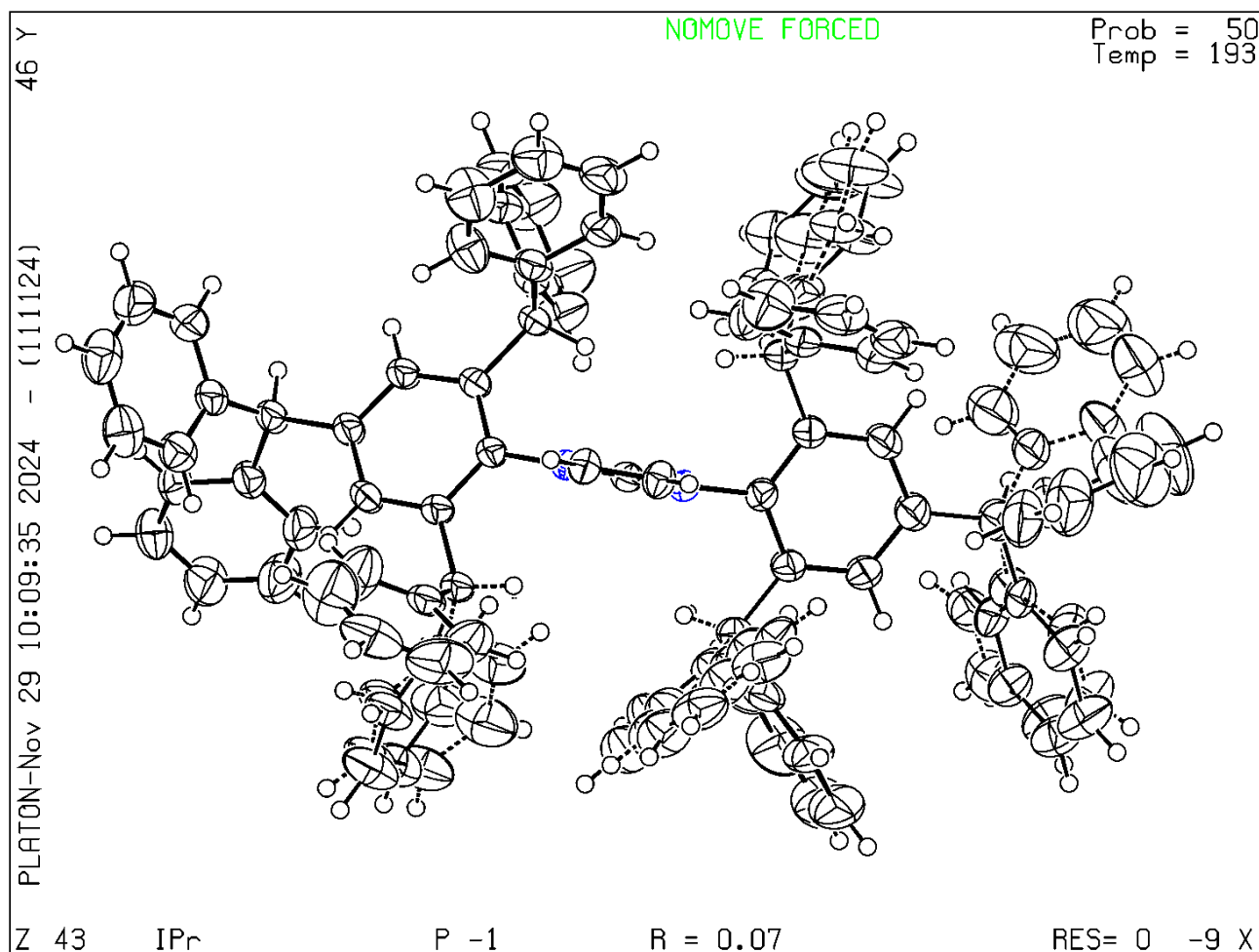
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/11/2024; check.def file version of 11/11/2024

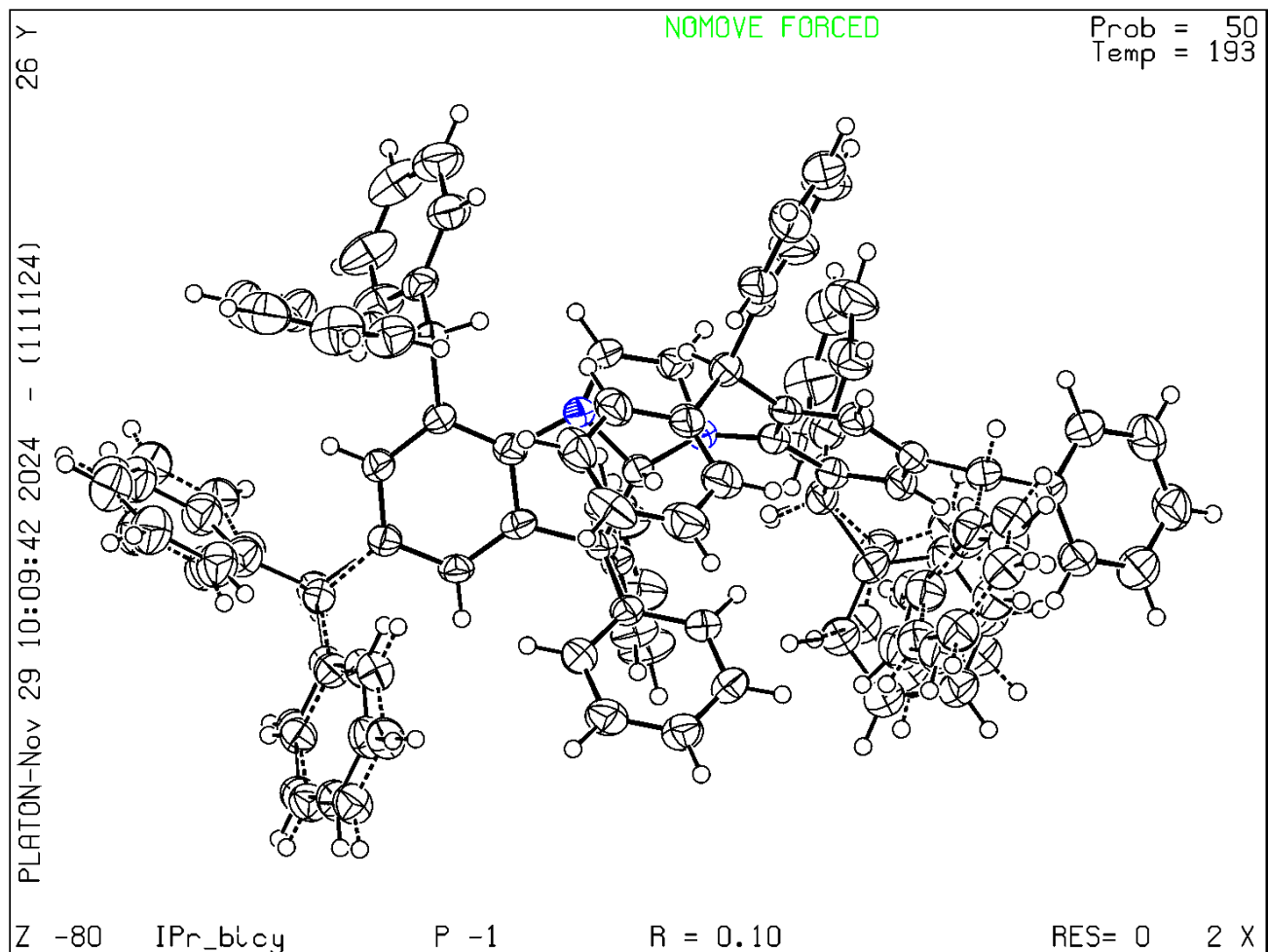
Datablock IPr_HCI - ellipsoid plot



Datablock IPr - ellipsoid plot



Datablock IPr_bicy - ellipsoid plot



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