

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) 2, 4, 5, 6, taphen

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: taphen

Bond precision:	C-C = 0.0040 A	Wavelength=0.71069
Cell:	a=3.8606(2) b=14.8724(7) c=17.6816(8)	
	alpha=105.797(2) beta=95.852(2) gamma=93.668(1)	
Temperature:	150 K	
	Calculated	Reported
Volume	967.31(8)	967.31(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C10 H6 N4), C H2 Cl2	2(C10 H6 N4), C H2 Cl2
Sum formula	C21 H14 Cl2 N8	C21 H14 Cl2 Co0 N8
Mr	449.30	449.30
Dx,g cm-3	1.543	1.543
Z	2	2
Mu (mm-1)	0.365	0.365
F000	460.0	460.0
F000'	460.71	
h,k,lmax	5,19,22	5,19,22
Nref	4414	4092
Tmin,Tmax	0.957,0.964	0.939,1.085
Tmin'	0.903	
Correction method=	# Reported T Limits: Tmin=0.939	
Tmax=1.085 AbsCorr =	MULTI-SCAN	
Data completeness=	0.927	Theta(max)= 27.519
R(reflections)=	0.0538(3706)	wR2(reflections)= 0.1750(4092)
S =	1.020	Npar= 322

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 value Low . 0.940 Why?
Author Response: the quality of the crystal did not allow an full measurment at high angles

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.786	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	210	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2	Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	12.35	Check

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CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
      symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z      2
From the CIF: _chemical_formula_sum   C21 H14 Cl2 Co0 N8
TEST: Compare cell contents of formula and atom site data

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atom	Z*formula	cif sites	diff	
C	42.00	42.00	0.00	
H	28.00	28.00	0.00	
Cl	4.00	4.00	0.00	
Co	2.00	0.00	2.00	
N	16.00	16.00	0.00	
PLAT072 ALERT 2 G	SHELXL First Parameter in WGHT Unusually Large			0.10 Report
PLAT883 ALERT 1 G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600			112 Note
PLAT913 ALERT 3 G	Missing # of Very Strong Reflections in FCF			3 Note
PLAT933 ALERT 2 G	Number of OMIT Records in Embedded .res File ...			5 Note
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density.			9 Info

- ```
0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
5 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
```

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

Bond precision: C-C = 0.0128 A Wavelength=0.71069
Cell: a=6.8917(2) b=14.0417(4) c=14.0951(4)
alpha=90 beta=101.345(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	1337.35(7)	1337.35(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H12 N4 Pt [+ solvent]	C12 H12 N4 Pt
Sum formula	C12 H12 N4 Pt [+ solvent]	C12 H12 N4 Pt
Mr	407.34	407.35
Dx,g cm-3	2.023	2.023
Z	4	4
Mu (mm-1)	10.476	10.476
F000	760.0	760.0
F000'	753.89	
h,k,lmax	9,19,19	9,19,19
Nref	3951	3931
Tmin,Tmax	0.296,0.811	0.845,1.185
Tmin'	0.042	
Correction method= # Reported T Limits: Tmin=0.845		
Tmax=1.185 AbsCorr = MULTI-SCAN		
Data completeness=	0.995	Theta(max)= 30.157
R(reflections)=	0.0406(3264)	wR2(reflections)= 0.0983(3931)
S =	1.074	Npar= 156

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

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01278	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.994	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.77A From N3	0.63	eA-3

 Alert level G

PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF	Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.89	Why ?
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	121	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Pt1 (II) .	1.86	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	19	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

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

Datablock: 4

Bond precision:	C-C = 0.0279 A	Wavelength=0.71069
Cell:	a=13.4500(3) b=15.9392(3) c=19.6119(4)	
	alpha=88.664(1) beta=72.997(1) gamma=69.298(1)	
Temperature:	150 K	
	Calculated	Reported
Volume	3745.97(14)	3745.97(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H42 N4 Pt Yb [+ solvent]	C32 H42 N4 Pt Yb
Sum formula	C32 H42 N4 Pt Yb [+ solvent]	C32 H42 N4 Pt Yb
Mr	850.82	850.82
Dx,g cm-3	1.509	1.509
Z	4	4
Mu (mm-1)	6.233	6.233
F000	1640.0	1640.0
F000'	1632.61	
h,k,lmax	16,18,23	16,18,23
Nref	13208	13184
Tmin,Tmax	0.645,0.940	0.864,1.290
Tmin'	0.531	
Correction method=	# Reported T Limits: Tmin=0.864	
Tmax=1.290 AbsCorr =	MULTI-SCAN	
Data completeness=	0.998	Theta(max)= 25.025
R(reflections)=	0.0792(10158)	wR2(reflections)= 0.2086(13184)
S =	1.086	Npar= 703

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

PLAT213_ALERT_2_B	Atom C27	has ADP max/min Ratio	4.2	prolat
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Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_B Atom C60 has ADP max/min Ratio 4.7 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.02793 Ang.

Author Response: additional refinement or tentative disordered model did not improved the C-C bond precision

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT213_ALERT_2_C Atom N1 has ADP max/min Ratio 3.6 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio 3.2 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_C Atom C14 has ADP max/min Ratio 3.4 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_C Atom C32 has ADP max/min Ratio 3.8 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_C Atom C48 has ADP max/min Ratio 3.4 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_C Atom C52 has ADP max/min Ratio 3.1 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT213_ALERT_2_C Atom C57 has ADP max/min Ratio 3.3 prolat

Author Response: additional refinement or tentative disordered model did not improved the anisotropy of the thermal elispoids

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio

PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 3.5 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd 2 H Uiso(max)/Uiso(min) Range 4.3 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference N3 --C6 . 0.17 Ang.

And 6 other PLAT234 Alerts

PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C2 . 0.23 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C14 --C15 . 0.22 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C23 --C24 . 0.20 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference N8 --C39 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C55 --C56 . 0.21 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C56 --C57 . 0.18 Ang.

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.1 Note

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H63 ..H72 . 2.07 Ang.

2-x,-y,1-z = 2_756 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.014 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.013 Check

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	20	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		1	Check
PLAT923_ALERT_1_C	S Values in the CIF and FCF Differ by		0.014	Check
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Pt2		1.39	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H25		-0.33	eA-3
And 2 other PLAT977 Alerts				
PLAT977_ALERT_2_C	Check Negative Difference Density on H34		-0.34	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H75		-0.41	eA-3

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		6	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		95.20	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.001	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		!	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pt1 (II) .		1.81	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pt2 (II) .		1.87	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		36	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please	Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		60%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		4	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		5	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

- 0

ALERT level A

= Most likely a serious problem - resolve or explain
- 3

ALERT level B

= A potentially serious problem, consider carefully
- 29

ALERT level C

= Check. Ensure it is not caused by an omission or oversight
- 16

ALERT level G

= General information/check it is not something unexpected
- 4

ALERT type 1

CIF construction/syntax error, inconsistent or missing data
- 21

ALERT type 2

Indicator that the structure model may be wrong or deficient
- 10

ALERT type 3

Indicator that the structure quality may be low
- 11

ALERT type 4

Improvement, methodology, query or suggestion
- 2

ALERT type 5

Informative message, check

Datablock: 5

Bond precision:	C-C = 0.0159 A	Wavelength=0.71069
Cell:	a=8.6458(2) b=16.9907(3) c=17.5855(3)	
	alpha=92.099(1) beta=90.278(1) gamma=103.004(1)	
Temperature:	150 K	
	Calculated	Reported
Volume	2515.11(9)	2515.11(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H72 N4 Pd Yb2 [+ solvent]	C52 H72 N4 Pd Yb2
Sum formula	C52 H72 N4 Pd Yb2 [+ solvent]	C52 H72 N4 Pd Yb2
Mr	1205.62	1205.61
Dx, g cm-3	1.592	1.592
Z	2	2
Mu (mm-1)	4.078	4.078
F000	1196.0	1196.0
F000'	1192.83	
h,k,lmax	12,23,24	12,23,24
Nref	14718	14668
Tmin,Tmax	0.783,0.816	0.899,1.117
Tmin'	0.665	
Correction method= # Reported T Limits: Tmin=0.899		
Tmax=1.117 AbsCorr = MULTI-SCAN		
Data completeness= 0.997 Theta(max)= 30.030		
R(reflections)= 0.0652(10831) wR2(reflections)= 0.1830(14668)		
S = 0.952 Npar= 561		

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
[PLAT351_ALERT_3_B](#) Long C-H (X0.96,N1.08A) C51 - H51B . 1.24 Ang.

Author Response: This issue comes from a disorder. CH50 and H51B do not belong to the same PART

[PLAT973_ALERT_2_B](#) Check Calcd Positive Resid. Density on Yb02 1.56 eA-3

Alert level C
[PLAT220_ALERT_2_C](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
[PLAT222_ALERT_3_C](#) Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.1 Ratio
[PLAT342_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.01586 Ang.
[PLAT350_ALERT_3_C](#) Short C-H (X0.96,N1.08A) C51 - H51C . 0.81 Ang.
[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 6.069 Check
[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report
[PLAT975_ALERT_2_C](#) Check Calcd Resid. Dens. 0.95A From C51 1.14 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H17C -0.43 eA-3
And 2 other PLAT977 Alerts

[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H18A -0.43 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H52C -0.51 eA-3
[PLAT978_ALERT_2_C](#) Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G
[PLAT083_ALERT_2_G](#) SHELXL Second Parameter in WGHT Unusually Large 44.48 Why ?
[PLAT154_ALERT_1_G](#) The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
[PLAT164_ALERT_4_G](#) Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 3 Note
[PLAT343_ALERT_2_G](#) Unusual Angle Range in Main Residue for C51 Check
[PLAT343_ALERT_2_G](#) Unusual sp? Angle Range in Main Residue for C52 Check
[PLAT380_ALERT_4_G](#) Incorrectly? Oriented X(sp2)-Methyl Moiety C18 Check
[PLAT380_ALERT_4_G](#) Incorrectly? Oriented X(sp2)-Methyl Moiety C39 Check
[PLAT605_ALERT_4_G](#) Largest Solvent Accessible VOID in the Structure 157 A**3
[PLAT720_ALERT_4_G](#) Number of Unusual/Non-Standard Labels 3 Note
[PLAT869_ALERT_4_G](#) ALERTS Related to the Use of SQUEEZE Suppressed ! Info
[PLAT883_ALERT_1_G](#) No Info/Value for _atom_sites_solution_primary . Please Do !
[PLAT910_ALERT_3_G](#) Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
[PLAT912_ALERT_4_G](#) Missing # of FCF Reflections Above STh/L= 0.600 31 Note
[PLAT913_ALERT_3_G](#) Missing # of Very Strong Reflections in FCF 2 Note
[PLAT933_ALERT_2_G](#) Number of OMIT Records in Embedded .res File ... 14 Note

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- 2 **ALERT level B** = A potentially serious problem, consider carefully
- 11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 15 **ALERT level G** = General information/check it is not something unexpected

- 2 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
- 8 ALERT type 3 Indicator that the structure quality may be low
- 7 ALERT type 4 Improvement, methodology, query or suggestion
- 0 ALERT type 5 Informative message, check

Datablock: 6

Bond precision:	C-C = 0.0205 A	Wavelength=0.71073
Cell:	a=8.6444(4) b=16.9738(6) c=17.6073(8)	
	alpha=91.943(3) beta=90.393(2) gamma=102.997(3)	
Temperature:	150 K	
	Calculated	Reported
Volume	2515.58(19)	2515.58(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H72 N4 Pt Yb2 [+ solvent]	C52 H72 N4 Pt Yb2
Sum formula	C52 H72 N4 Pt Yb2 [+ solvent]	C52 H72 N4 Pt Yb2
Mr	1294.30	1294.30
Dx,g cm-3	1.709	1.709
Z	2	2

Mu (mm-1)	6.497	6.497
F000	1260.0	1260.0
F000'	1255.69	
h,k,lmax	10,20,21	10,20,21
Nref	9225	9118
Tmin,Tmax	0.585,0.878	0.922,1.145
Tmin'	0.141	
Correction method= # Reported T Limits: Tmin=0.922		
Tmax=1.145 AbsCorr = MULTI-SCAN		
Data completeness= 0.988	Theta(max)= 25.349	
R(reflections)= 0.0613(6938)	wR2(reflections)= 0.1273(9118)	
S = 1.102	Npar= 554	

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 C19 has ADP max/min Ratio 6.3 prolat

Author Response: Additional refinement did not improved the problem on the methyl atoms of the cp rings.

 **Alert level B**
[PLAT342_ALERT_3_B](#) Low Bond Precision on C-C Bonds 0.02047 Ang.

Author Response: additional refinement or tentative disordered model did not improved the C-C bond precision

 **Alert level C**
[PLAT213_ALERT_2_C](#) Atom C47 has ADP max/min Ratio 3.6 prolat

Author Response: Additional refinement did not improved the problem on the methyl atoms of the cp rings.

[PLAT213_ALERT_2_C](#) Atom C48 has ADP max/min Ratio 3.8 prolat

Author Response: Additional refinement did not improved the problem on the methyl atoms of the cp rings.

[PLAT213_ALERT_2_C](#) Atom C49 has ADP max/min Ratio 3.3 prolat

Author Response: Additional refinement did not improved the problem on the methyl atoms of the cp rings.

[PLAT220_ALERT_2_C](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.7 Ratio
[PLAT222_ALERT_3_C](#) Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.9 Ratio
[PLAT234_ALERT_4_C](#) Large Hirshfeld Difference C2 --C3 . 0.16 Ang.
[PLAT234_ALERT_4_C](#) Large Hirshfeld Difference C12 --C13 . 0.16 Ang.
[PLAT412_ALERT_2_C](#) Short Intra XH3 .. XHn H18 ..H52B . 1.88 Ang.
x,y,z = 1_555 Check
[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 4.817 Check
[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= 0.600 100 Report
[PLAT973_ALERT_2_C](#) Check Calcd Positive Resid. Density on Yb2 1.18 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H3 -0.33 eA-3

And 5 other PLAT977 Alerts

[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H18 -0.59 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H22 -0.38 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H51B -0.47 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H51C -0.45 eA-3
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H52A -0.37 eA-3

[PLAT978_ALERT_2_C](#) Number C-C Bonds with Positive Residual Density. 0 Info

 **Alert level G**
[PLAT083_ALERT_2_G](#) SHELXL Second Parameter in WGHT Unusually Large 51.24 Why ?

PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C51 Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C52 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		160 A**3
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		3 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		2 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		2 Note

1	ALERT level A	= Most likely a serious problem - resolve or explain
1	ALERT level B	= A potentially serious problem, consider carefully
19	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
9	ALERT level G	= General information/check it is not something unexpected
1	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
18	ALERT type 2	Indicator that the structure model may be wrong or deficient
6	ALERT type 3	Indicator that the structure quality may be low
5	ALERT type 4	Improvement, methodology, query or suggestion
0	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

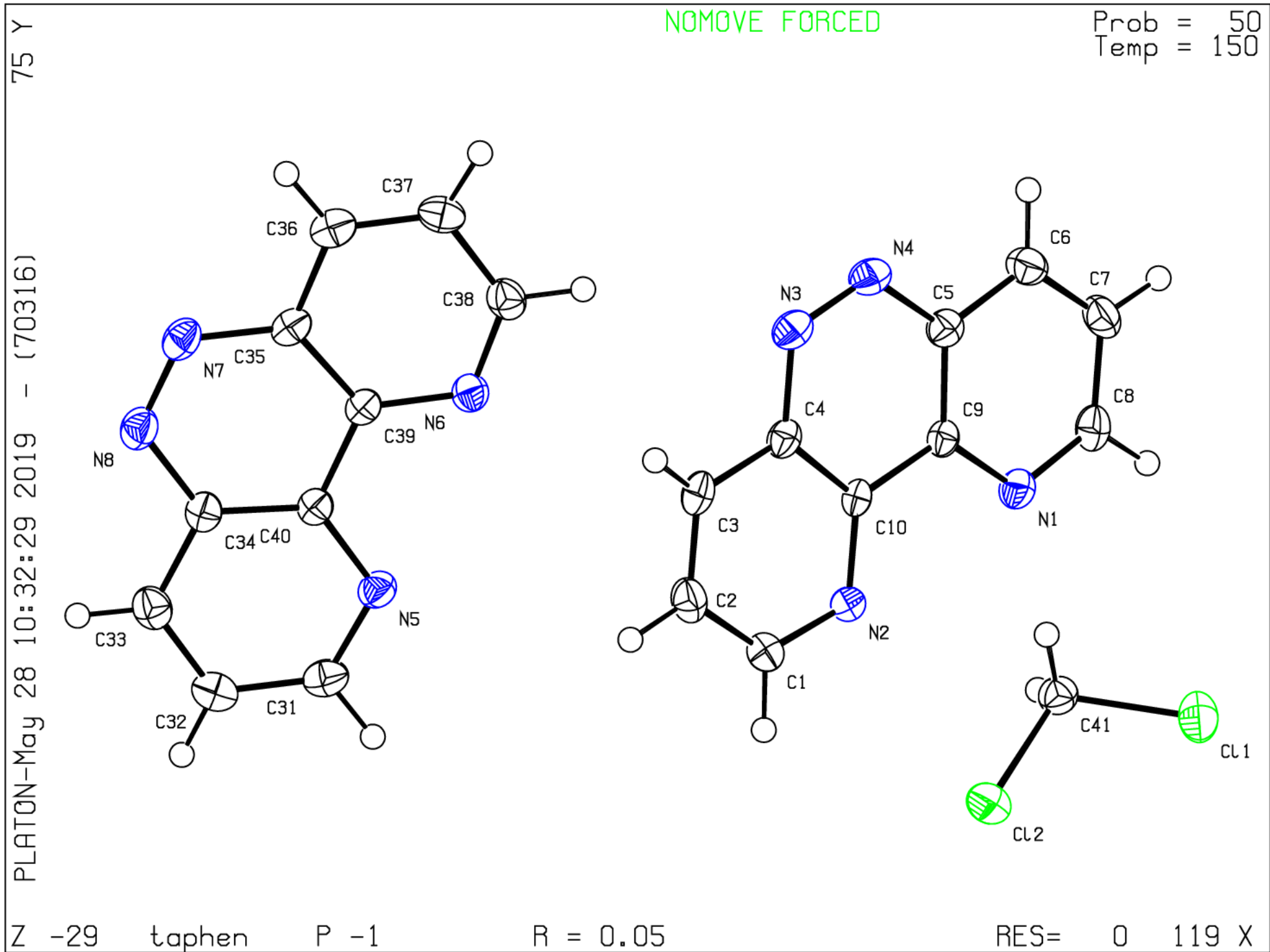
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

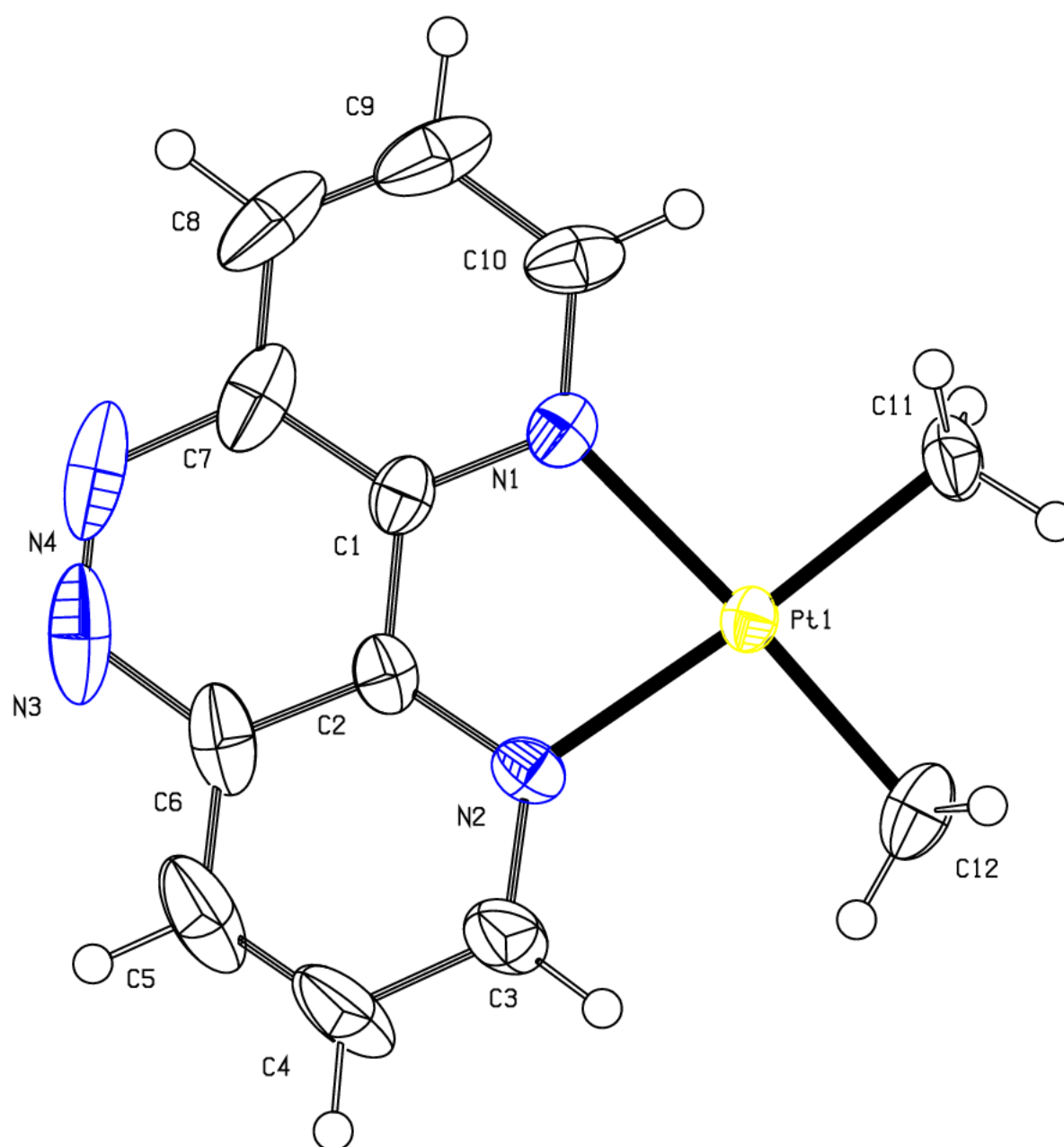
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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

Datablock taphen - ellipsoid plot

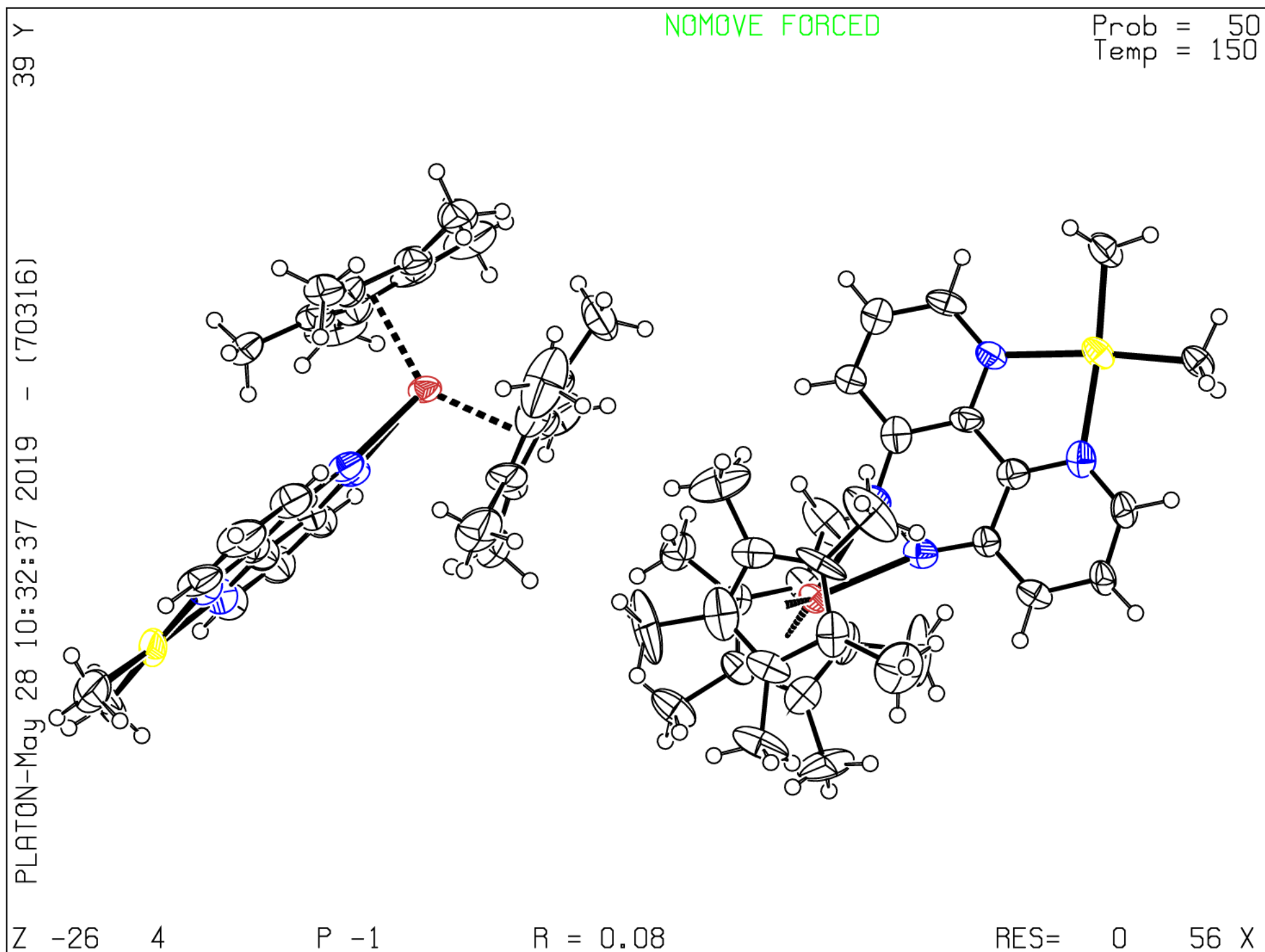


Datablock 2 - ellipsoid plot

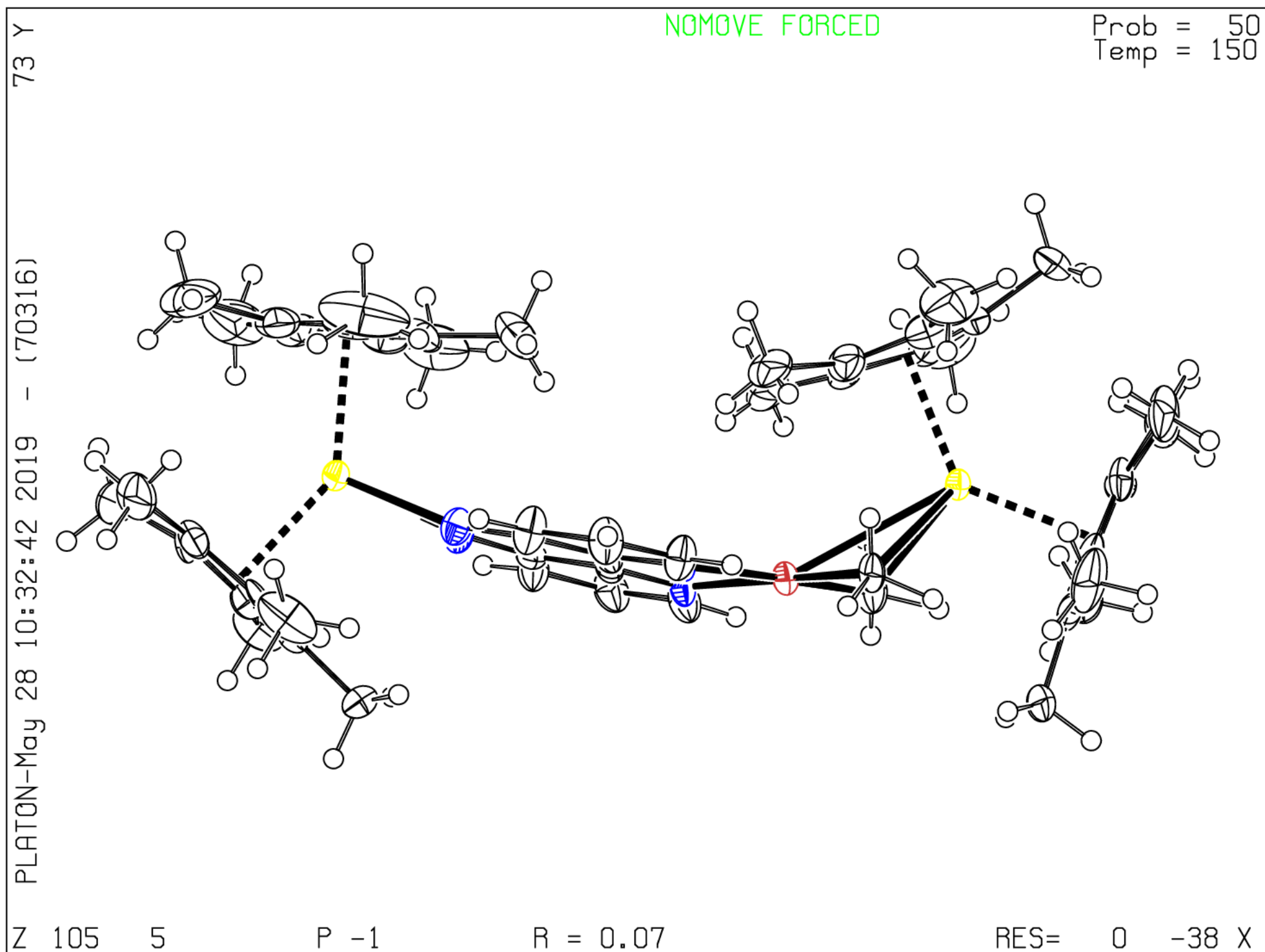


Z -104 2 P 21/c R = 0.04 RES= 0 -135 X

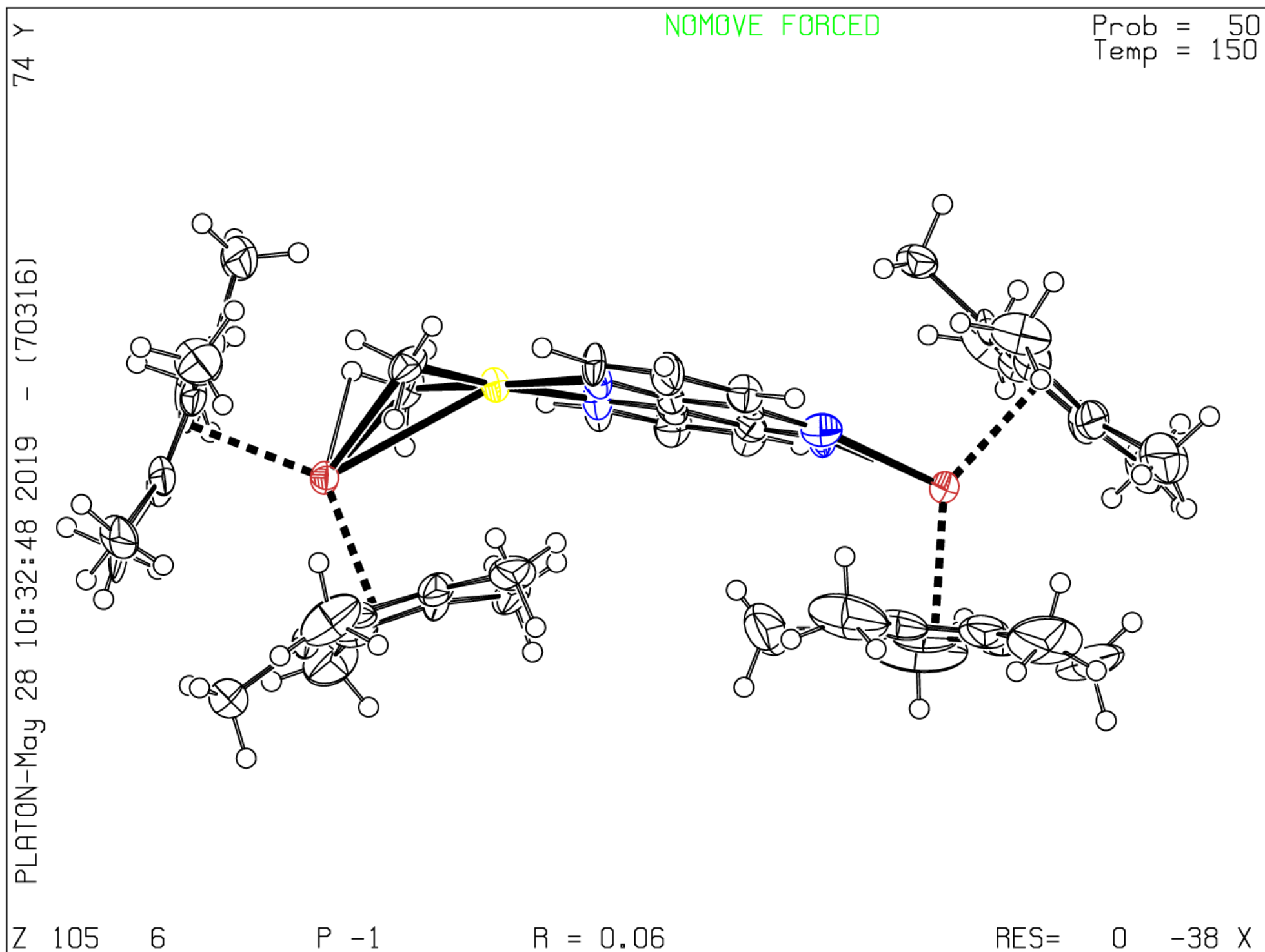
Datablock 4 - ellipsoid plot



Datablock 5 - ellipsoid plot



Datablock 6 - ellipsoid plot



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