

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) 3a, 4b, 4e, 5a2-TMEDA, 5b, 6b

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: 3a

Bond precision:	C-C = 0.0051 Å	Wavelength=1.54184
Cell:	a=11.9440(4) b=12.0368(6) c=22.8595(9)	
	alpha=91.871(4) beta=104.635(3) gamma=112.172(4)	
Temperature:	173 K	
	Calculated	Reported
Volume	2914.5(2)	2914.5(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C55 H90 Mg N2 P2 Pd, 0.5(C6 H14)	C55 H90 Mg N2 P2 Pd, 0.5(C6 H14)
Sum formula	C58 H97 Mg N2 P2 Pd	C58 H97 Mg N2 P2 Pd
Mr	1015.03	1015.02
Dx, g cm ⁻³	1.157	1.157
Z	2	2
Mu (mm ⁻¹)	3.444	3.444
F000	1094.0	1094.0
F000'	1097.90	
h,k,lmax	14,14,28	14,14,28
Nref	11727	11034
Tmin,Tmax	0.343,0.930	0.405,0.928
Tmin'	0.178	
Correction method=	# Reported T Limits: Tmin=0.405 Tmax=0.928	
AbsCorr =	ANALYTICAL	
Data completeness=	0.941	Theta(max)= 73.483
R(reflections)=	0.0353(9204)	wR2(reflections)= 0.0893(11034)
S =	1.017	Npar= 613

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

PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.6 Ratio
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600 213 Report

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	12 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% Note
PLAT303_ALERT_2_G	Full Occupancy Atom H1 with # Connections	2.00 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	5.22 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	4.78 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	40 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	43 Note
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).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	480 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.5 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 4b

Bond precision:	C-C = 0.0039 A	Wavelength=0.71073
Cell:	a=14.8444(3) b=16.0913(2) c=16.9949(3)	
	alpha=96.1668(14) beta=97.1851(15) gamma=97.9294(14)	
Temperature:	173 K	
	Calculated	Reported
Volume	3956.87(12)	3956.85(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C76 H117 Mg2 N4 P Pt, C6 H14	C76 H117 Mg2 N4 P Pt, C6 H14
Sum formula	C82 H131 Mg2 N4 P Pt	C82 H131 Mg2 N4 P Pt
Mr	1447.59	1447.58
Dx,g cm-3	1.215	1.215
Z	2	2
Mu (mm-1)	1.852	1.852
F000	1536.0	1536.0
F000'	1533.35	
h,k,lmax	19,21,22	19,21,22
Nref	19784	16946
Tmin,Tmax	0.484,0.530	0.581,0.641
Tmin'	0.475	
Correction method=	# Reported T Limits: Tmin=0.581 Tmax=0.641	
AbsCorr =	ANALYTICAL	
Data completeness=	0.857	Theta(max)= 28.353
R(reflections)=	0.0272(15062)	wR2(reflections)= 0.0591(16946)
S =	1.044	Npar= 841

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). 12 Note

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.5 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35 Check

And 2 other PLAT242 Alerts

[Less ...](#)

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C44 Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C65 Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C84 Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	C81 0.102 Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.600 27 Report

Alert level G

PLAT303_ALERT_2_G	Full Occupancy Atom H1	with # Connections	2.00 Check
PLAT303_ALERT_2_G	Full Occupancy Atom H2	with # Connections	2.00 Check
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	2797 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.1 Low
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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 4e

Bond precision:	C-C = 0.0047 A	Wavelength=0.71073
Cell:	a=14.6246(5) b=16.6683(5) c=26.2662(8)	
	alpha=90 beta=103.526(3) gamma=90	
Temperature:	173 K	
	Calculated	Reported
Volume	6225.3(3)	6225.2(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C122 H184 N10 Pd2 Zn4, C6 H14	C122 H184 N10 Pd2 Zn4, C6 H14
Sum formula	C128 H198 N10 Pd2 Zn4	C128 H198 N10 Pd2 Zn4
Mr	2351.34	2351.23
Dx, g cm ⁻³	1.254	1.254
Z	2	2
Mu (mm ⁻¹)	1.091	1.091
F000	2496.0	2496.0
F000'	2494.85	
h, k, lmax	19, 22, 34	18, 21, 34
Nref	15313	12392
Tmin, Tmax	0.901, 0.926	0.959, 1.000
Tmin'	0.858	
Correction method=	# Reported T Limits: Tmin=0.959 Tmax=1.000	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.809	Theta(max)= 28.191
R(reflections)=	0.0378(8972)	wR2(reflections)= 0.0790(12392)
S =	0.974	Npar= 680

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	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	3.7 Ratio
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C000 Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C013 Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	C01Y	0.164 Check
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C01Y - C020	1.42 Ang.
PLAT910_ALERT_3_C	Missing	# of FCF Reflection(s) Below Theta(Min).		9 Note
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.600	135 Report

●Alert level G

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	Please Check
PLAT303_ALERT_2_G	Full Occupancy Atom H9BA	with # Connections	2.00 Check
PLAT303_ALERT_2_G	Full Occupancy Atom H0CA	with # Connections	2.00 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		170 Note
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	2707 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.7 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1 Info

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7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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- 2 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 5a2-TMEDA

Bond precision:	C-C = 0.0078 Å	Wavelength=1.54184
Cell:	a=13.7691(2)	b=25.5240(4) c=21.1334(4)
	alpha=90	beta=95.1714(17) gamma=90
Temperature: 173 K		
	Calculated	Reported
Volume	7396.9(2)	7396.9(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C122 H188 Mg4 N10 Pt2, 2(C7 H8) [solvent]	[+ C122 H188 Mg4 N10 Pt2, 2(C7 H8), 2.25(C6 H14)]
Sum formula	C136 H204 Mg4 N10 Pt2 [+ solvent]	C149.50 H235.50 Mg4 N10 Pt2
Mr	2466.50	2660.39
Dx, g cm-3	1.107	1.194
Z	2	2
Mu (mm-1)	3.984	4.017
F000	2588.0	2813.0
F000'	2576.11	
h,k,lmax	17,31,26	17,30,25
Nref	14874	14179
Tmin,Tmax	0.782,0.852	0.543,0.871
Tmin'	0.327	
Correction method=	# Reported T Limits: Tmin=0.543 Tmax=0.871	
AbsCorr =	ANALYTICAL	
Data completeness=	0.953	Theta(max)= 73.385
R(reflections)=	0.0442(10088)	wR2(reflections)= 0.1150(14179)
S =	0.964	Npar= 728

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	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.7 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	4.2 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C70	--C71 .	0.24 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C71	--C72 .	0.24 Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C15	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C24	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.9 Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C70	0.119 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	184 Report

●Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C149.5 H235.5 Mg4 N10 Pt2

Atom count from the _atom_site data: C136 H204 Mg4 N10 Pt2

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

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 C149.50 H235.50 Mg4 N10 Pt2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	299.00	272.00	27.00
H	471.00	408.00	63.00
Mg	8.00	8.00	0.00
N	20.00	20.00	0.00
Pt	4.00	4.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check

PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 0.83 %

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report

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

PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C71 --C76 . 6.4 s.u.

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note

PLAT303_ALERT_2_G Full Occupancy Atom H1A with # Connections 2.00 Check

And 3 other PLAT303 Alerts

Less ...

PLAT303_ALERT_2_G Full Occupancy Atom H1B with # Connections 2.00 Check

PLAT303_ALERT_2_G Full Occupancy Atom H1C with # Connections 2.00 Check

PLAT303_ALERT_2_G Full Occupancy Atom H1D with # Connections 2.00 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 8.76 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 6.24 Check

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C70 Check

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 42.70 Deg.

N31 -C31 -MG2 1_555 1_555 1_555 # 72 Check

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 42.20 Deg.

N33 -C33 -MG2 1_555 1_555 1_555 # 82 Check

PLAT860_ALERT_3_G Number of Least-Squares Restraints 43 Note

PLAT869_ALERT_3_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 463 Note

PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 5 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.7 Low

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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29 **ALERT level G** = General information/check it is not something unexpected

4 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

15 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

Datablock: 5b

Bond precision: C-C = 0.0048 A Wavelength=1.54184

Cell: a=13.8262(3) b=19.0434(3) c=14.1627(3)

alpha=90 beta=108.739(3) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	3531.34(14)	3531.34(14)

Space group	I 2/m	I 2/m
Hall group	-I 2y	-I 2y
Moiety formula	C58 H86 N4 Pt Zn2, 2(C6 H14)	C58 H86 N4 Pt Zn2, 2(C6 H14)
Sum formula	C70 H114 N4 Pt Zn2	C70 H114 N4 Pt Zn2
Mr	1337.51	1337.48
Dx,g cm-3	1.258	1.258
Z	2	2
Mu (mm-1)	4.703	4.703
F000	1400.0	1400.0
F000'	1387.20	
h,k,lmax	17,23,17	16,23,17
Nref	3683	3476
Tmin,Tmax	0.490,0.640	0.562,0.703
Tmin'	0.445	
Correction method= # Reported T Limits: Tmin=0.562 Tmax=0.703		
AbsCorr = ANALYTICAL		
Data completeness= 0.944	Theta(max)= 73.577	
R(reflections)= 0.0285(3288)	wR2(reflections)= 0.0750(3476)	
S = 1.051	Npar= 217	

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

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C21	0.114	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H1A ..H1B	.	1.91	Ang.
	-x,y,1-z = 2_556	Check		
PLAT410_ALERT_2_C	Short Intra H...H Contact H1A ..H1B	.	1.91	Ang.
	-x,y,1-z = 2_556	Check		
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	58	Report

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C21 Constrained at	0.5	Check

And 19 other PLAT300 Alerts

Less ...

PLAT300_ALERT_4_G	Atom Site Occupancy of C22	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26C	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note	
PLAT303_ALERT_2_G	Full Occupancy Atom H1A with # Connections	2.00	Check	
PLAT303_ALERT_2_G	Full Occupancy Atom H1B with # Connections	2.00	Check	
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	20	Check	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	16	Note	
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	141	Note	
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note	

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

Datablock: 6b

Bond precision: C-C = 0.0062 Å Wavelength=1.54184
Cell: a=16.2798(5) b=13.0600(5) c=45.8501(10)
alpha=90 beta=93.226(2) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	9732.9(5)	9732.9(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C87 H126 Mg3 N6 Pt [+ solvent]	C87 H126 Mg3 N6 Pt, C7 H8, C6 H14
Sum formula	C87 H126 Mg3 N6 Pt [+ solvent]	C100 H148 Mg3 N6 Pt
Mr	1523.96	1702.26
Dx, g cm ⁻³	1.040	1.162
Z	4	4
Mu (mm ⁻¹)	3.172	3.220
F000	3216.0	3616.0
F000'	3206.13	
h,k,lmax	20,16,57	20,15,55
Nref	19601	18623
Tmin,Tmax	0.812,0.876	0.592,0.890
Tmin'	0.324	

Correction method= # Reported T Limits: Tmin=0.592 Tmax=0.890
AbsCorr = ANALYTICAL
Data completeness= 0.950 Theta(max)= 73.505
R(reflections)= 0.0376(14088) wR2(reflections)= 0.0897(18623)
S = 0.982 Npar= 951

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 NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.5 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C57 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 230 Report

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C100 H148 Mg3 N6 Pt1
Atom count from the _atom_site data: C87 H126 Mg3 N6 Pt1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C100 H148 Mg3 N6 Pt
TEST: Compare cell contents of formula and atom_site data

atom Z*formula cif sites diff

C	400.00	348.00	52.00
H	592.00	504.00	88.00
Mg	12.00	12.00	0.00
N	24.00	24.00	0.00
Pt	4.00	4.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	21	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	16	Report
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please	Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	1.50	%
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	9	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	9%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H1 with # Connections	3.00	Check

And 2 other PLAT303 Alerts

Less ...

PLAT303_ALERT_2_G	Full Occupancy Atom H2 with # Connections	3.00	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H3 with # Connections	3.00	Check

PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H4B ..H14A .	1.97	Ang.
	x,y,z = 1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H5C ..H29A .	2.01	Ang.
	x,y,z = 1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H8A ..H14F .	2.14	Ang.
	x,y,z = 1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H22A ..H28B .	1.95	Ang.
	x,y,z = 1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H38A ..H44F .	1.89	Ang.
	x,y,z = 1_555	Check	

PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	72	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).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	671	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	12	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.6	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ	2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	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
29 **ALERT level G** = General information/check it is not something unexpected

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 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
1 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

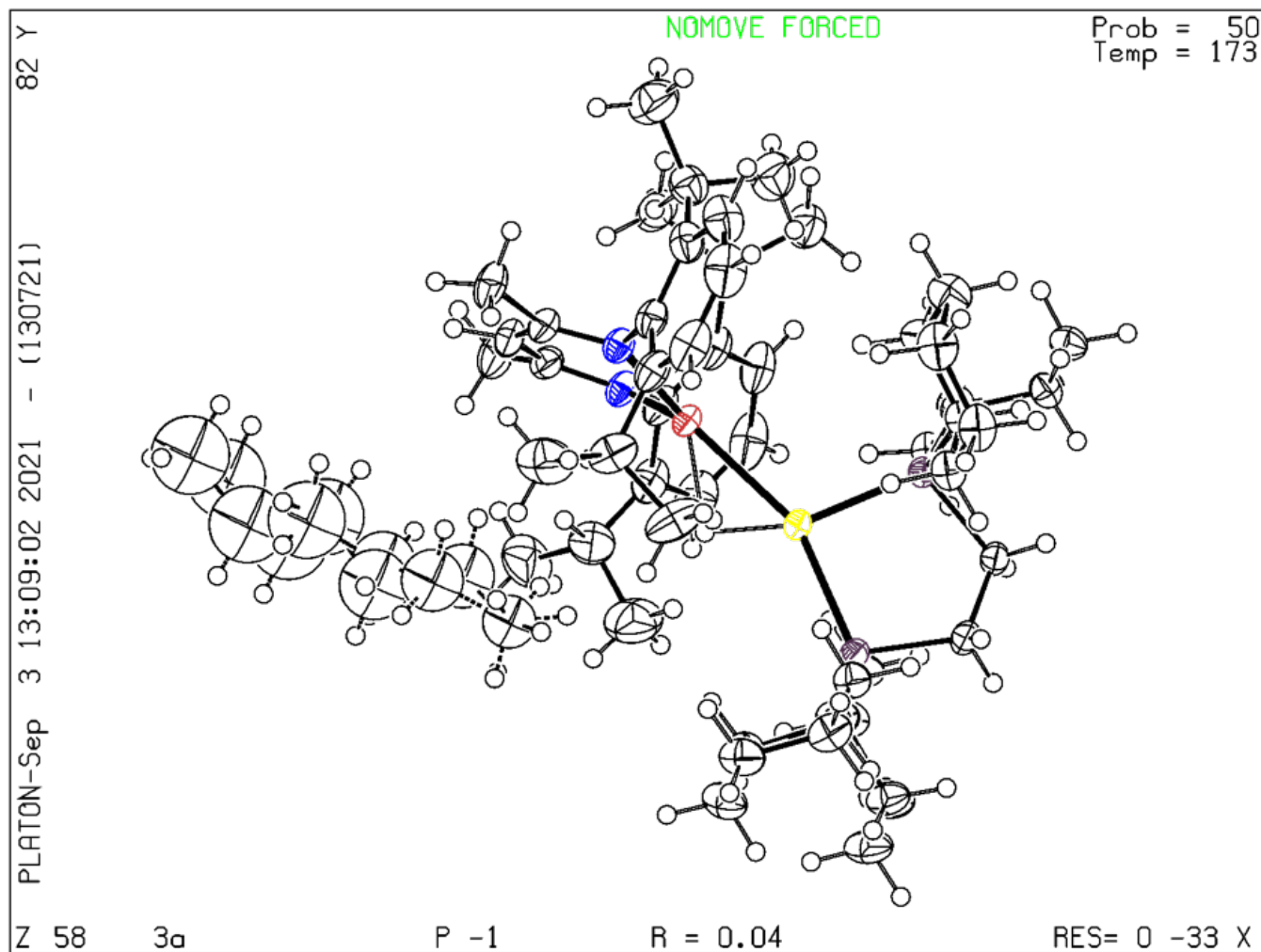
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

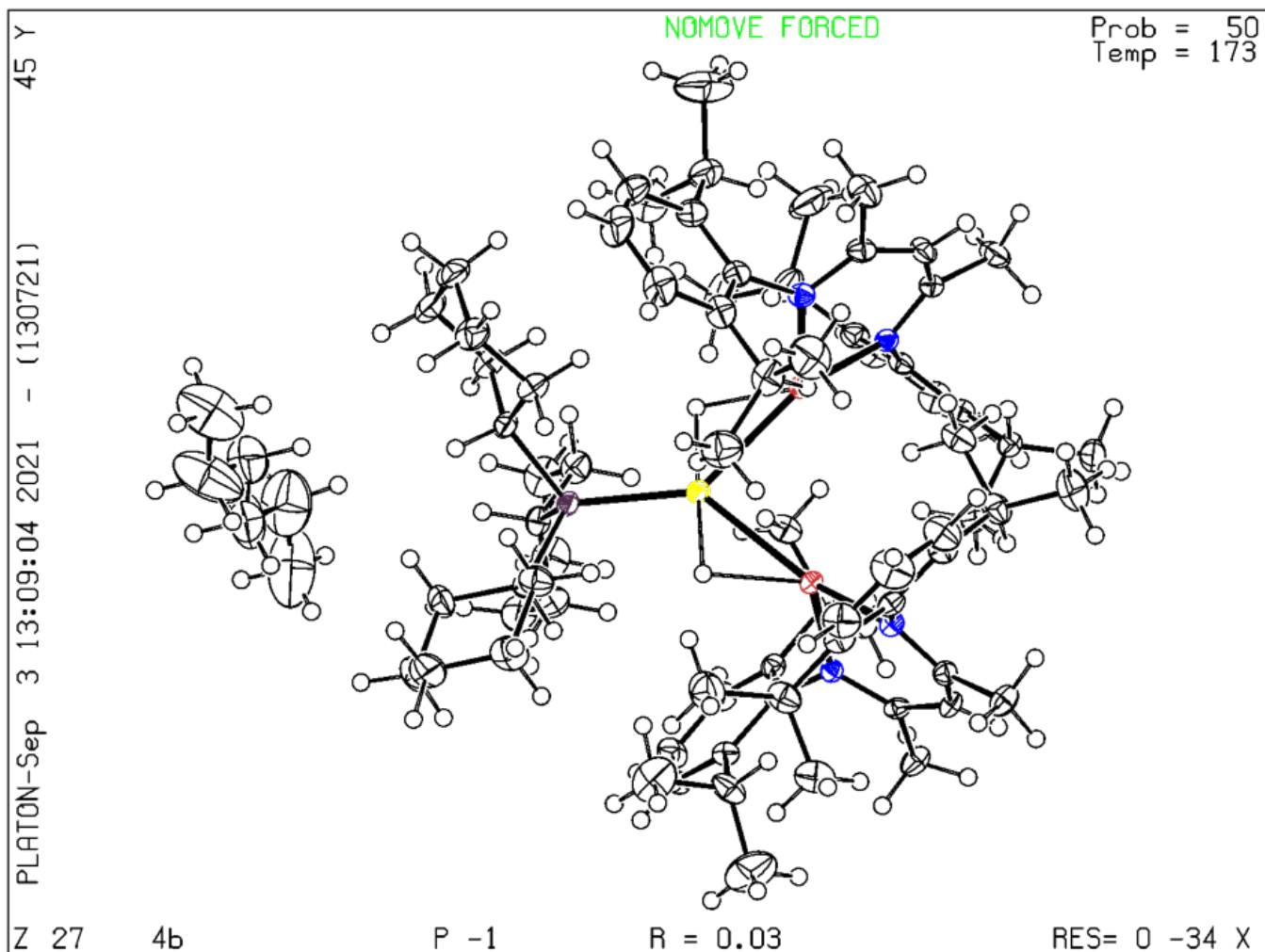
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

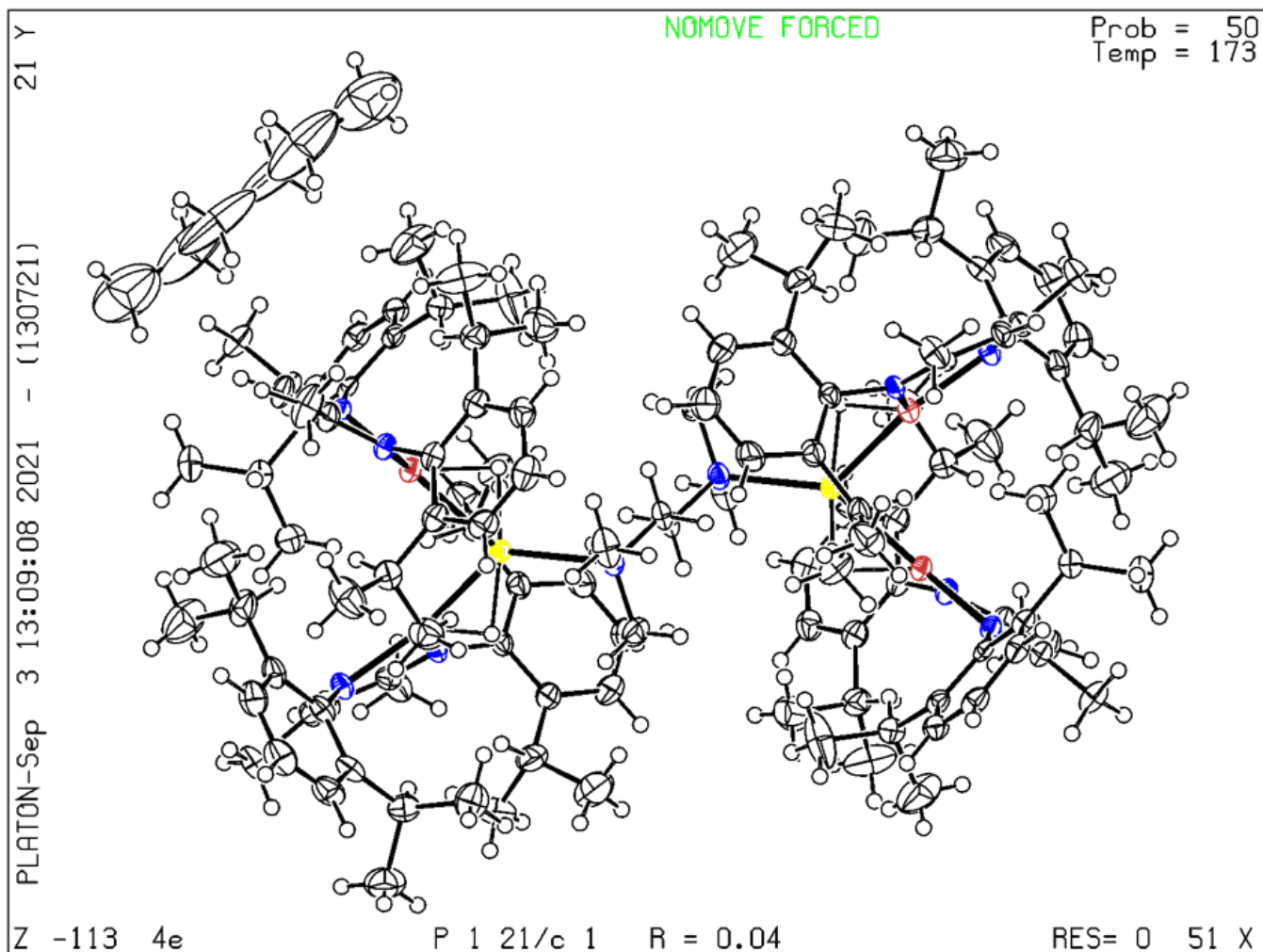
Datablock 3a - ellipsoid plot



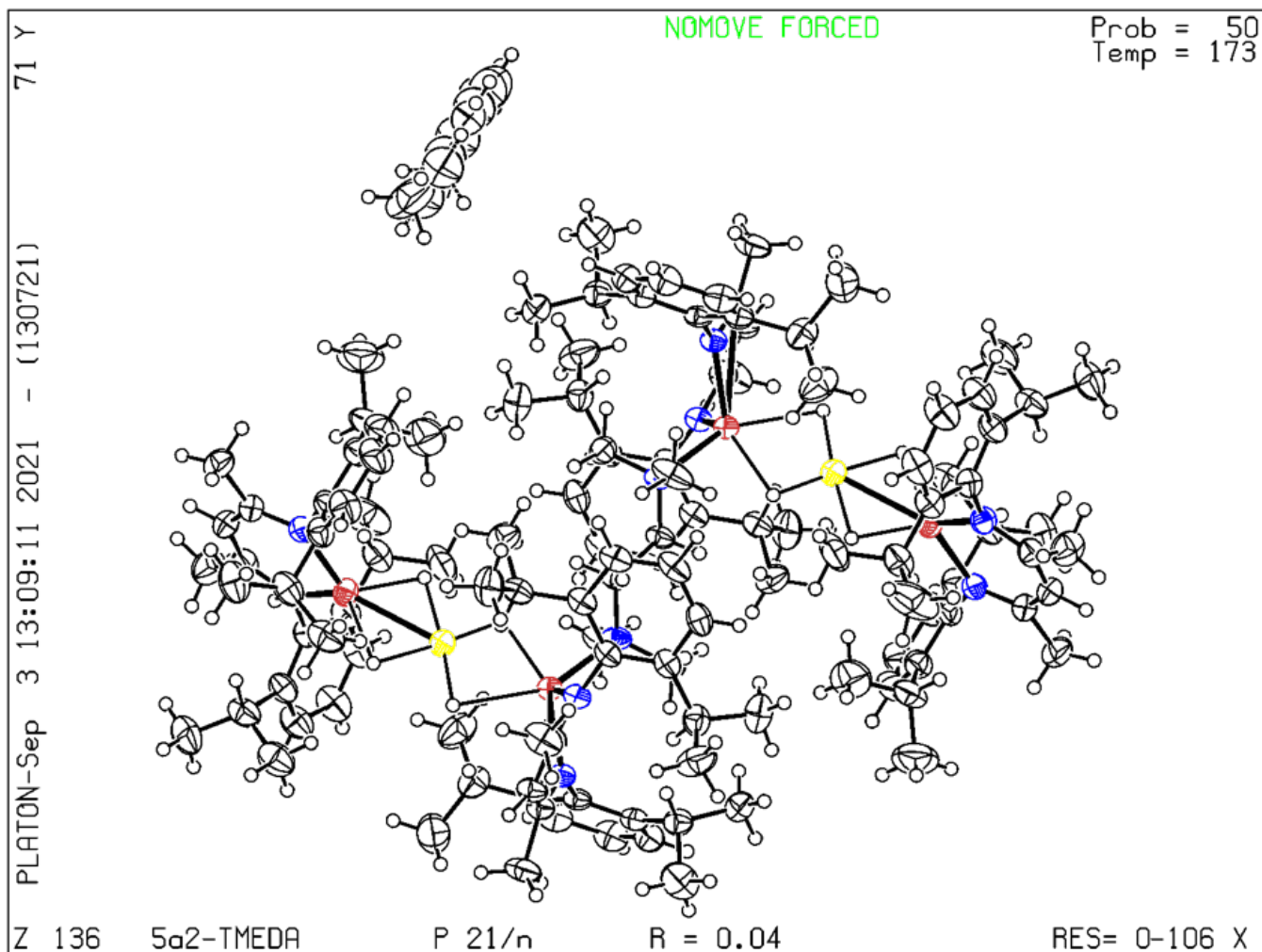
Datablock 4b - ellipsoid plot



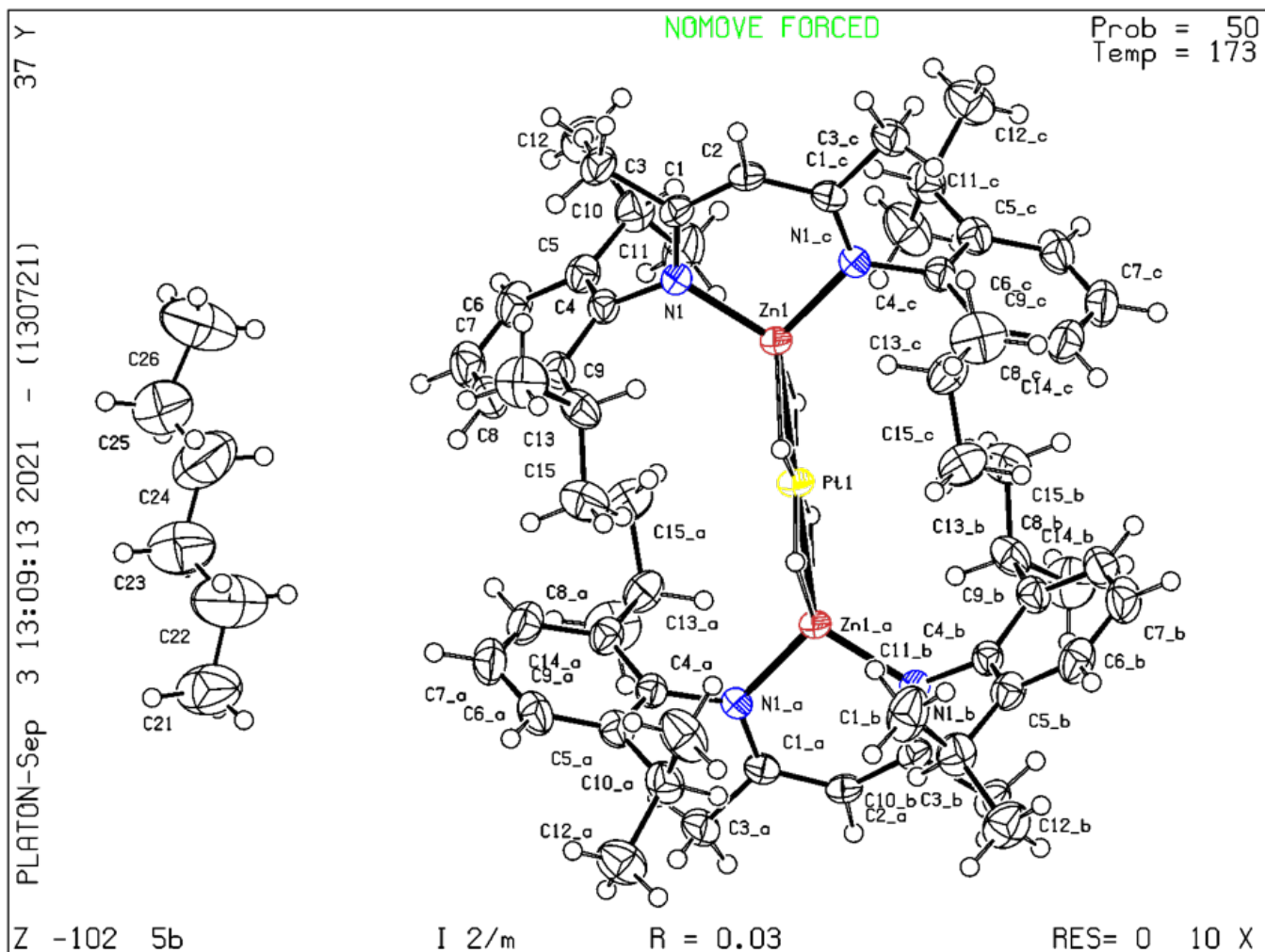
Datablock 4e - ellipsoid plot



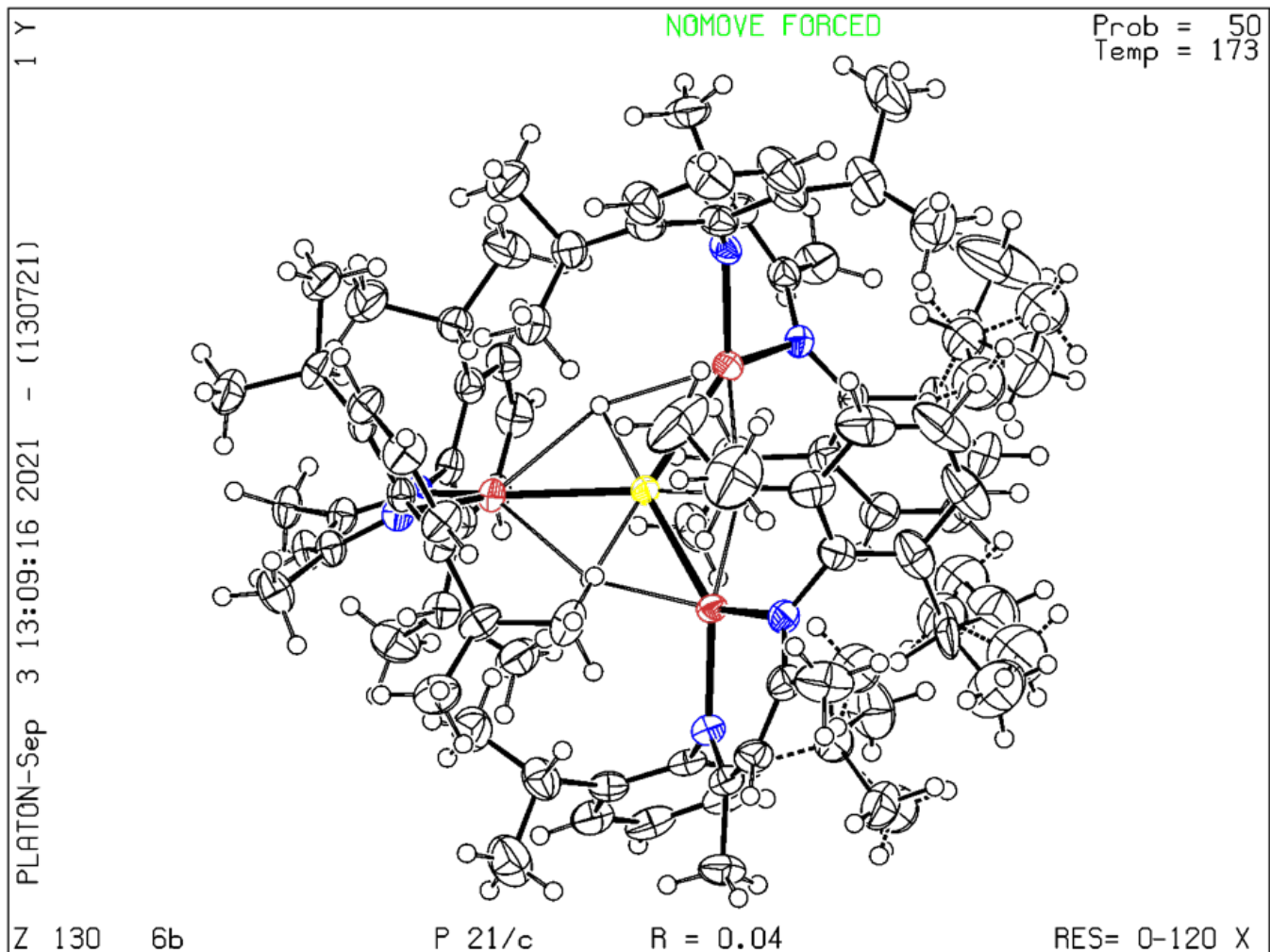
Datablock 5a2-TMEDA - ellipsoid plot



Datablock 5b - ellipsoid plot



Datablock 6b - ellipsoid plot



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