

## 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) 1f, 2c, 2g

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: 1f

Bond precision:	C-C = 0.0103 Å	Wavelength=0.71073
Cell:	a=9.0622(17)    b=10.8523(14)    c=13.124(2)	
	alpha=85.417(7)    beta=82.59(1)    gamma=89.894(8)	
Temperature: 193 K		

	Calculated	Reported
Volume	1275.8(4)	1275.8(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C11 H14 N4 O6	C11 H14 N4 O6
Sum formula	C11 H14 N4 O6	C11 H14 N4 O6
Mr	298.26	298.26
Dx, g cm <sup>-3</sup>	1.553	1.553
Z	4	4
Mu (mm <sup>-1</sup> )	0.128	0.128
F000	624.0	624.0
F000'	624.36	
h,k,lmax	10,13,15	10,13,15
Nref	4604	4586
Tmin,Tmax	0.988,0.994	0.585,0.746
Tmin'	0.975	

Correction method= # Reported T Limits: Tmin=0.585 Tmax=0.746  
AbsCorr = MULTI-SCAN  
Data completeness= 0.996                      Theta(max)= 25.249  
R(reflections)= 0.1386( 3454)                      wR2(reflections)= 0.3012( 4586)  
S = 1.162                      Npar= 381

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

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density    0.97 eA<sup>-3</sup>  
PLAT213\_ALERT\_2\_B Atom O10                      has ADP max/min Ratio ..... 4.6 oblate  
PLAT213\_ALERT\_2\_B Atom C20                      has ADP max/min Ratio ..... 4.3 prolat  
PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.0103 Å.

### ●Alert level C

CRYSC01\_ALERT\_1\_C The word below has not been recognised as a standard identifier.  
colouless  
CRYSC01\_ALERT\_1\_C No recognised colour has been given for crystal colour.  
DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
The relevant atom site should be identified.

**RINTA01\_ALERT\_3\_C** The value of Rint is greater than 0.12  
 Rint given 0.156

**PLAT020\_ALERT\_3\_C** The Value of Rint is Greater Than 0.12 ..... 0.156 Report

**PLAT082\_ALERT\_2\_C** High R1 Value ..... 0.14 Report

**PLAT084\_ALERT\_3\_C** High wR2 Value (i.e. > 0.25) ..... 0.30 Report

**PLAT213\_ALERT\_2\_C** Atom O2 has ADP max/min Ratio ..... 3.3 prolat

**PLAT213\_ALERT\_2\_C** Atom O11 has ADP max/min Ratio ..... 3.6 prolat

**PLAT220\_ALERT\_2\_C** NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio

**PLAT353\_ALERT\_3\_C** Long N-H (N0.87,N1.01A) N3 - H3N . 1.01 Ang.

**PLAT906\_ALERT\_3\_C** Large K Value in the Analysis of Variance ..... 36.064 Check

**And 2 other PLAT906 Alerts**

More ...

**PLAT911\_ALERT\_3\_C** Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report  
 -1 3 1, -1 4 1, 0-12 2, -2 4 2, -1 4 2, 5-11 3,  
 -1-12 4, 0-12 4, 5-11 4, 5-10 4, 6-10 5, -7 -6 7,  
 -4 -7 9, -7 3 9, -1 -7 12,

**PLAT975\_ALERT\_2\_C** Check Calcd Resid. Dens. 1.06Ang From O9 . 0.60 eA-3

**PLAT977\_ALERT\_2\_C** Check Negative Difference Density on H14 . -0.35 eA-3

## Alert level G

**PLAT003\_ALERT\_2\_G** Number of Uiso or Uij Restrained non-H Atoms ... 15 Report

**PLAT007\_ALERT\_5\_G** Number of Unrefined Donor-H Atoms ..... 6 Report  
 H3N H3O H4N H7N H8N H9O

**PLAT083\_ALERT\_2\_G** SHELXL Second Parameter in WGHT Unusually Large 14.50 Why ?

**PLAT177\_ALERT\_4\_G** The CIF-Embedded .res File Contains DELU Records 2 Report

**PLAT178\_ALERT\_4\_G** The CIF-Embedded .res File Contains SIMU Records 2 Report

**PLAT186\_ALERT\_4\_G** The CIF-Embedded .res File Contains ISOR Records 2 Report

**PLAT188\_ALERT\_3\_G** A Non-default SIMU Restraint Value has been used 0.0020 Report

**PLAT188\_ALERT\_3\_G** A Non-default SIMU Restraint Value has been used 0.0020 Report

**PLAT192\_ALERT\_3\_G** A Non-default DELU Restraint Value for First Par 0.0020 Report

**PLAT192\_ALERT\_3\_G** A Non-default DELU Restraint Value for First Par 0.0020 Report

**PLAT480\_ALERT\_4\_G** Long H...A H-Bond Reported H8B ..O1 . 2.62 Ang.

**PLAT860\_ALERT\_3\_G** Number of Least-Squares Restraints ..... 97 Note

**PLAT883\_ALERT\_1\_G** No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

**PLAT899\_ALERT\_4\_G** SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note

**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). 2 Note  
 0 1 0, 0 0 1,

**PLAT912\_ALERT\_4\_G** Missing # of FCF Reflections Above STh/L= 0.600 1 Note

**PLAT961\_ALERT\_5\_G** Dataset Contains no Negative Intensities ..... Please Check

**PLAT965\_ALERT\_2\_G** The SHELXL WEIGHT Optimisation has not Converged 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 ..... 3.98 Note  
 Predicted wR2: Based on SigI\*\*2 7.57 or SHELX Weight 27.08

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

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

## Datablock: 2c

Bond precision:	C-C = 0.0218 A	Wavelength=0.71073
Cell:	a=16.038(9) b=17.017(7) c=18.571(10)	
	alpha=82.98(2) beta=71.63(3) gamma=88.37(2)	
Temperature: 193 K		
	Calculated	Reported
Volume	4774(4)	4774(4)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C26 H116 Ag N4 Na12 O50, 3(C26 H36 Ag N4 O8) [+ solvent]	C26 H116 Ag N4 Na12 O50, 3(C26 H36 Ag N4 O8)
Sum formula	C104 H224 Ag4 N16 Na12 O74 [+ solvent]	C104 H224 Ag4 N16 Na12 O74
Mr	3590.36	3590.34

Dx,g cm-3	1.249	1.249
Z	1	1
Mu (mm-1)	0.513	0.513
F000	1872.0	1872.0
F000'	1869.76	
h,k,lmax	19,20,22	19,20,22
Nref	34622[ 17311]	33843
Tmin,Tmax	0.884,0.950	0.649,0.746
Tmin'	0.836	
Correction method= # Reported T Limits: Tmin=0.649 Tmax=0.746		
AbsCorr = MULTI-SCAN		
Data completeness=	1.95/0.98	Theta(max)= 25.250
R(reflections)=	0.0708( 28621)	wR2(reflections)= 0.2119( 33843)
S =	1.059	Npar= 1891

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 B

PLAT342\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.02185 Ang.

PLAT416\_ALERT\_2\_B Short Intra D-H..H-D H9E ..H20M . 1.26 Ang.  
x,y,z = 1\_555 Check

#### And 3 other PLAT416 Alerts

More ...

1+x,1+y,z = 1\_665 Check  
PLAT416\_ALERT\_2\_B Short Intra D-H..H-D H17F ..H31A . 1.52 Ang.  
1+x,1+y,z = 1\_665 Check

#### And 4 other PLAT416 Alerts

More ...

PLAT417\_ALERT\_2\_B Short Inter D-H..H-D H8A ..H35A . 1.83 Ang.  
x,1+y,z = 1\_565 Check

PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O1 --H1B . Please Check

#### And 8 other PLAT420 Alerts

More ...

PLAT971\_ALERT\_2\_B Check Calcd Resid. Dens. 2.74Ang From O1 2.61 eA-3  
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 .... 2.84 Report

PLAT214\_ALERT\_2\_C Atom C18D (Anion/Solvent) ADP max/min Ratio 4.6 prolat

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio

#### And 2 other PLAT220 Alerts

More ...

PLAT221\_ALERT\_2\_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 5.3 Ratio

#### And 2 other PLAT221 Alerts

More ...

PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.9 Ratio

PLAT223\_ALERT\_4\_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 6.7 Ratio

#### And 2 other PLAT223 Alerts

More ...

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of Na6 Check

#### And 4 other PLAT241 Alerts

More ...

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Na5 Check

#### And 19 other PLAT242 Alerts

More ...

PLAT309\_ALERT\_2\_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O1C Check

PLAT361\_ALERT\_2\_C Long C(sp3)-C(sp3) Bond C11D - C13D . 1.66 Ang.

PLAT361\_ALERT\_2\_C Long C(sp3)-C(sp3) Bond C19D - C20D . 1.72 Ang.

PLAT363\_ALERT\_2\_C Long C(sp3)-C(sp2) Bond C17D - C18D . 1.63 Ang.

PLAT430\_ALERT\_2\_C Short Inter D...A Contact O4C ..O11 . 2.85 Ang.

x,y,z = 1\_555 Check

PLAT481\_ALERT\_4\_C Long D...A H-Bond Reported O3 ..O7D . 3.55 Ang.

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 213 Report

9 0 0, 12 3 0, 14 4 0, 13 7 0, 8 8 0, -5 12 0,  
-6 -9 1, -12 -6 1, 1 -2 1, -11 -1 1, 1 -1 1, 13 -1 1,  
-12 0 1, 14 0 1, -8 1 1, 11 11 1, 4 -7 2, 7 -6 2,

2 -3 2, 1 -1 2, 2 -1 2, 8 -1 2, 1 1 2, 7 2 2,  
 7 4 2, 14 4 2, 8 5 2, 13 5 2, 13 9 2, 10-12 3,  
 11-11 3, -5-10 3, 7 -4 3, 2 -1 3, 3 -1 3, 0 0 3,  
 5 2 3, 13 5 3, -7 7 3, 14 8 3, 12 10 3, 11 11 3,  
 13 11 3, -6 13 3, -6 14 3, 7-15 4, 6-14 4, 7 -6 4,  
 6 -3 4, 3 -1 4, 4 -1 4, 6 -1 4, 6 1 4, 8 1 4,  
 5 2 4, 6 3 4, 9 4 4, 16 4 4, -11 7 4, -10 9 4,  
 -9 10 4, -14 11 4, 11 11 4, 8-13 5, 8 -8 5, -15 -6 5,  
 5 -3 5, -10 1 5, 8 3 5, 9 4 5, 15 5 5, 6 7 5,  
 7 7 5, 14 8 5, -8 9 5, 7 9 5, 6 12 5, 4 16 5,  
 7-15 6, 10-12 6, 15 -5 6, -15 -4 6, 8 -3 6, 5 -2 6,  
 9 -2 6, 6 -1 6, 9 0 6, 9 2 6, 10 3 6, 17 3 6,  
 3 4 6, 6 6 6, -9 7 6, -4 8 6, -14 9 6, -6 11 6,

PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 3 Check  
 PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.46Ang From O30 1.63 eA-3  
 PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.06Ang From O11 . 1.22 eA-3

#### And 2 other PLAT975 Alerts

More ...

PLAT977\_ALERT\_2\_C Check Negative Difference Density on H12M . -0.34 eA-3

#### And 6 other PLAT977 Alerts

More ...

### Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 74 Report  
 PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
 PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 80 Report  
 H1A H1B H2E H2F H3E H3F H4E H4F H5A H5B H7A  
 H7B H8A H8B H9E H9F H10A H10B H12M H12N H13M H13N  
 PLAT033\_ALERT\_4\_G Flack x Value Deviates > 3.0 \* sigma from Zero . 0.034 Note  
 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  
 PLAT309\_ALERT\_2\_G Single Bonded Oxygen (C-O > 1.3 Ang) ..... O2B Check

#### And 2 other PLAT309 Alerts

More ...

PLAT480\_ALERT\_4\_G Long H...A H-Bond Reported H3F ..O7D . 2.63 Ang.  
 PLAT480\_ALERT\_4\_G Long H...A H-Bond Reported H32B ..O5D . 2.64 Ang.  
 PLAT606\_ALERT\_4\_G Solvent Accessible VOID(S) in Structure ..... ! Info  
 PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 24 Note  
 H7A1 H7A2 H7A3 H8A1 H8A2 H8A3 H7B1 H7B2  
 H7B3 H8B1 H8B2 H8B3 H7C1 H7C2 H7C3 H8C1  
 H8C2 H8C3 H7D1 H7D2 H7D3 H8D1 H8D2 H8D3

PLAT773\_ALERT\_2\_G Check long C-C Bond in CIF: C19D --C20D 1.71 Ang.  
 PLAT774\_ALERT\_1\_G Check X-Y Bond in CIF: Na1 --Na11 .. 4.05 Ang.

#### And 2 other PLAT774 Alerts

More ...

PLAT780\_ALERT\_1\_G Coordinates do not Form a Properly Connected Set Please Do !  
 PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 447 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 !  
 PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
 PLAT909\_ALERT\_3\_G Percentage of I>2sig(I) Data at Theta(Max) Still 68% Note  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note  
 PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities ..... Please Check  
 PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged 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 ..... 4.25 Note  
 Predicted wR2: Based on SigI\*\*2 4.99 or SHELX Weight 20.65  
 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

22 **ALERT level B** = A potentially serious problem, consider carefully

57 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

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

76 ALERT type 2 Indicator that the structure model may be wrong or deficient

9 ALERT type 3 Indicator that the structure quality may be low

15 ALERT type 4 Improvement, methodology, query or suggestion

5 ALERT type 5 Informative message, check

## Datablock: 2g

Bond precision: C-C = 0.0037 Å Wavelength=0.71073  
 Cell: a=8.6893(3) b=11.9503(4) c=15.6733(4)  
 alpha=77.673(1) beta=88.470(1) gamma=75.612(1)  
 Temperature: 193 K

	Calculated	Reported
Volume	1539.52(8)	1539.52(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H32 Ag N4 Na3 O14, 3(H2 O)	C18 H32 Ag N4 Na3 O14, 3(H2 O)
Sum formula	C18 H38 Ag N4 Na3 O17	C18 H38 Ag N4 Na3 O17
Mr	759.36	759.36
Dx, g cm <sup>-3</sup>	1.638	1.638
Z	2	2
Mu (mm <sup>-1</sup> )	0.776	0.776
F000	780.0	780.0
F000'	778.81	
h,k,lmax	10,14,18	10,14,18
Nref	5584	5521
Tmin,Tmax	0.696,0.856	0.627,0.746
Tmin'	0.672	

Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.746  
 AbsCorr = MULTI-SCAN  
 Data completeness= 0.989 Theta(max)= 25.246  
 R(reflections)= 0.0335( 5384) wR2(reflections)= 0.0888( 5521)  
 S = 1.087 Npar= 388

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

[PLAT416\\_ALERT\\_2\\_B](#) Short Intra D-H..H-D H29 ..H113 . 1.43 Ang.  
 1-x,1-y,-z = 2\_665 Check  
[PLAT416\\_ALERT\\_2\\_B](#) Short Intra D-H..H-D H211 ..H214 . 1.19 Ang.  
 1-x,2-y,-z = 2\_675 Check  
[PLAT417\\_ALERT\\_2\\_B](#) Short Inter D-H..H-D H213 ..H216 . 2.02 Ang.  
 x,y,-1+z = 1\_554 Check  
[PLAT417\\_ALERT\\_2\\_B](#) Short Inter D-H..H-D H115 ..H217 . 1.84 Ang.  
 1-x,1-y,1-z = 2\_666 Check  
[PLAT420\\_ALERT\\_2\\_B](#) D-H Bond Without Acceptor O14 --H114 . Please Check  
**And 2 other PLAT420 Alerts**  
[More ...](#)

### ●Alert level C

[PLAT213\\_ALERT\\_2\\_C](#) Atom O1 has ADP max/min Ratio ..... 3.1 prolat  
[PLAT250\\_ALERT\\_2\\_C](#) Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.1 Note  
[PLAT415\\_ALERT\\_2\\_C](#) Short Inter D-H..H-X H3 ..H116 . 2.14 Ang.  
 x,-1+y,z = 1\_545 Check  
[PLAT911\\_ALERT\\_3\\_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 61 Report  
 2 0 0, -1 1 0, 1 1 0, 3 1 0, 5 1 0, 2 2 0,  
 3 3 0, 1 6 0, 2 6 0, -3 -6 1, -2 -3 1, -3 -1 1,  
 -2 -1 1, -1 -1 1, -2 0 1, 2 0 1, 1 1 1, 2 1 1,  
 0 2 1, 2 2 1, -4 4 1, 1 5 1, 3 5 1, 1 8 1,  
 -2 -5 2, 0 -5 2, 0 -3 2, 1 -2 2, 3 -1 2, -3 0 2,  
 -2 0 2, 2 0 2, 1 2 2, 0 3 2, 1 3 2, 1 4 2,  
 2 4 2, 1 5 2, 2 6 2, -2 -3 3, -2 -1 3, -1 0 3,  
 1 0 3, 3 0 3, 0 3 3, 1 3 3, 2 3 3, -4 -6 4,  
 2 -6 4, 1 -5 4, -1 -2 4, 2 -1 4, -1 2 4, 2 5 4,  
 2 6 4, -3 -3 5, 0 -2 6, 0 0 6, 2 0 6, -1 1 7,  
 -2 -1 8,  
[PLAT913\\_ALERT\\_3\\_C](#) Missing # of Very Strong Reflections in FCF .... 9 Note  
 2 0 0, 3 1 0, -2 -3 1, -2 0 1, 2 0 1, -3 0 2,  
 1 5 2, 2 3 3, 0 0 6,  
[PLAT975\\_ALERT\\_2\\_C](#) Check Calcd Resid. Dens. 1.01Ang From O13 . 0.62 eA-3  
**And 7 other PLAT975 Alerts**  
[More ...](#)  
[PLAT976\\_ALERT\\_2\\_C](#) Check Calcd Resid. Dens. 0.83Ang From O13 . -0.73 eA-3  
**And 10 other PLAT976 Alerts**  
[More ...](#)

PLAT977\_ALERT\_2\_C Check Negative Difference Density on H17A . -0.32 eA-3

### And 10 other PLAT977 Alerts

More ...

## Alert level G

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 18 Report

H19 H29 H110 H111 H112 H113 H114 H210 H211 H212 H213

H214 H115 H215 H116 H216 H117 H217

PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Ag1 --C10 . 5.1 s.u.

PLAT480\_ALERT\_4\_G Long H...A H-Bond Reported H19 ..O13 . 2.64 Ang.

PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.10 Ratio

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note

PLAT909\_ALERT\_3\_G Percentage of I>2sig(I) Data at Theta(Max) Still 95% Note

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

0 1 0, 0 0 1,

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 ..... 2.93 Note

Predicted wR2: Based on SigI\*\*2 3.03 or SHELX Weight 8.47

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

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3 ALERT type 4 Improvement, methodology, query or suggestion

5 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

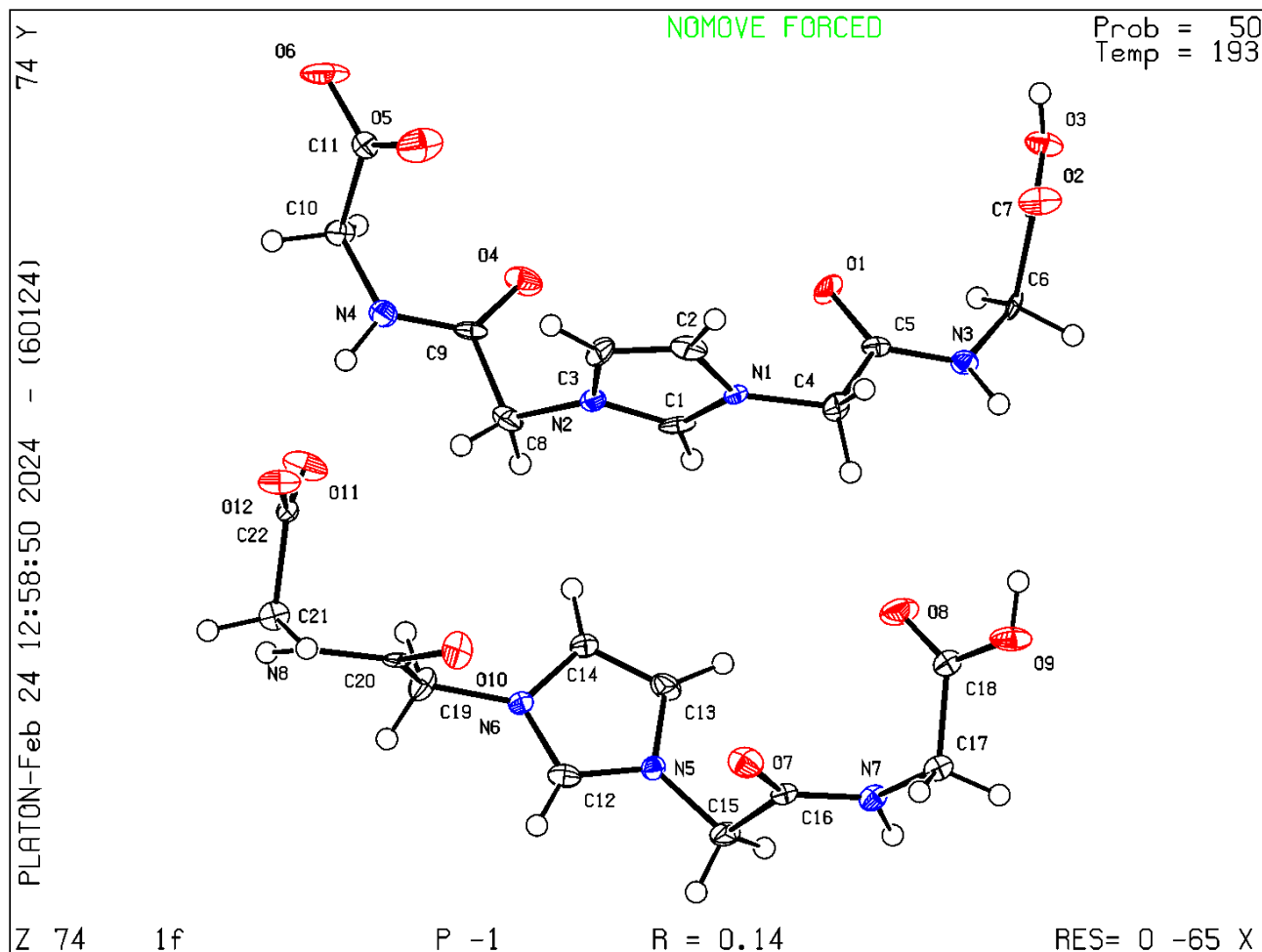
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

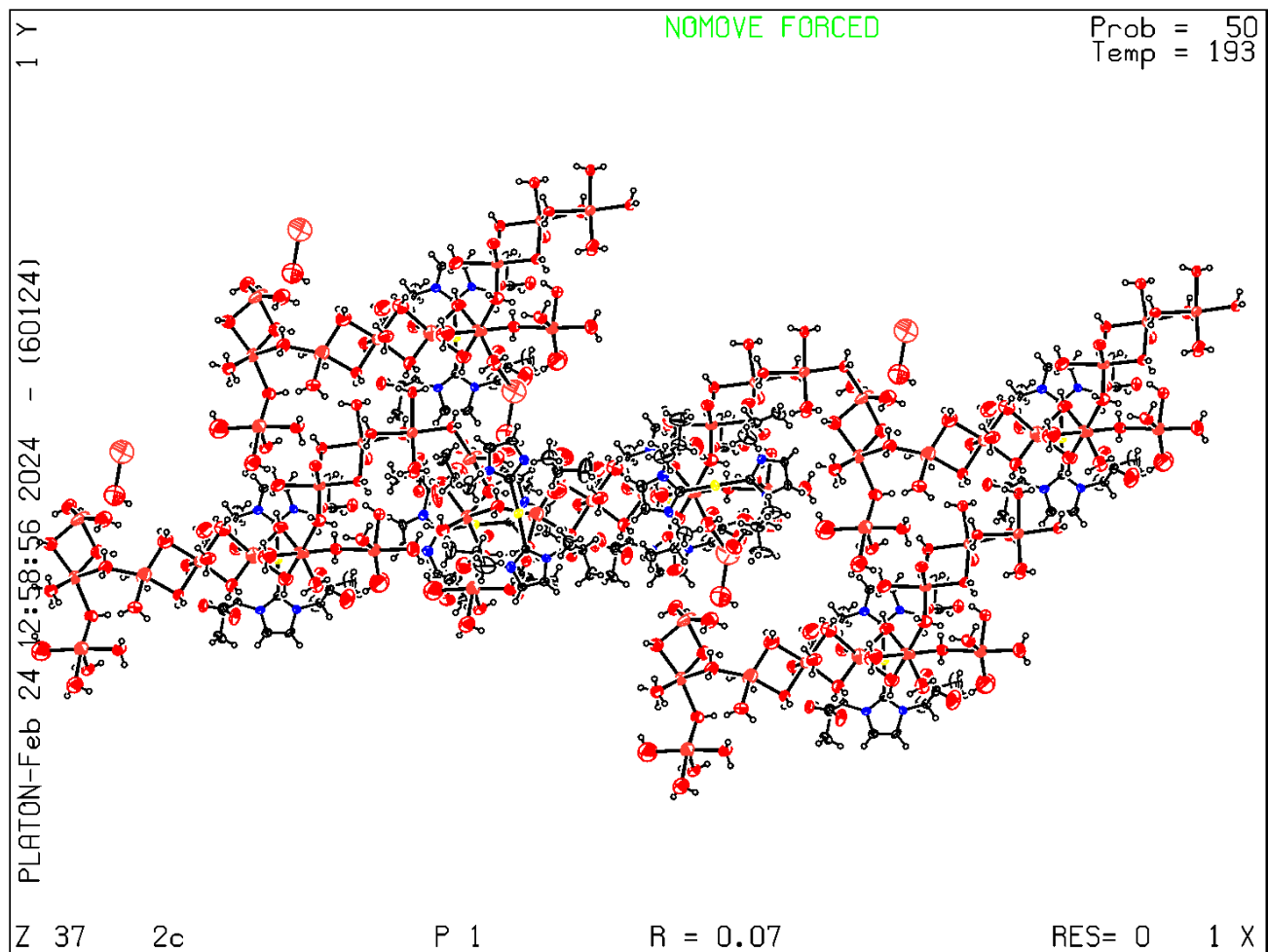
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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## Datablock 1f - ellipsoid plot

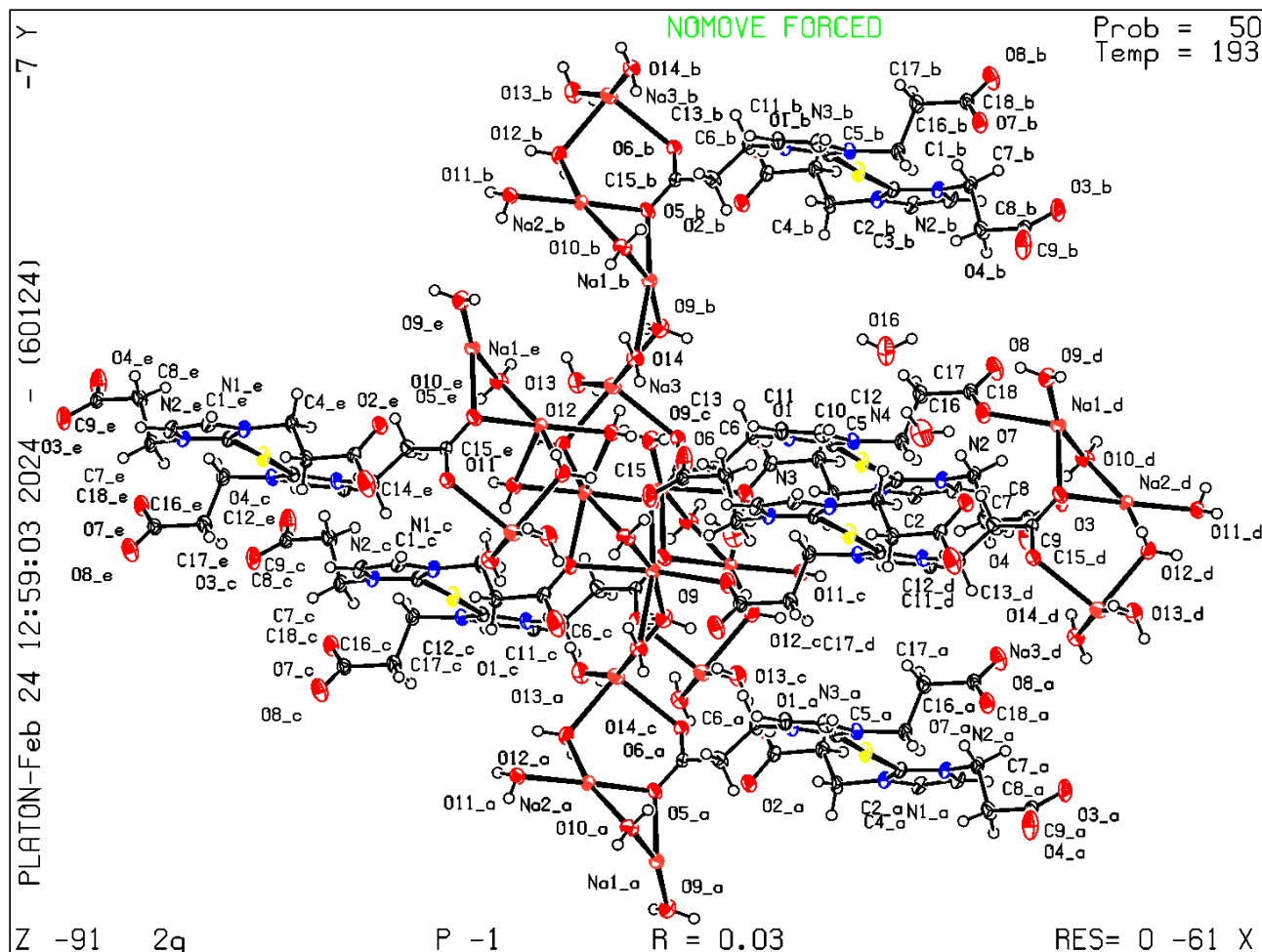


## Datablock 2c - ellipsoid plot



## Datablock 2g - ellipsoid plot





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