
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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N Check

 Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.158

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12	0.158 Report
PLAT082_ALERT_2_C High R1 Value	0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.32 Report
PLAT213_ALERT_2_C Atom O00G has ADP max/min Ratio	3.7 prolat
PLAT213_ALERT_2_C Atom O00H has ADP max/min Ratio	4.0 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	4.4 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.4 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.00891 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	40.947 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	4.935 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.160 Check

 Alert level G

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	29 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..	50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0 Info

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 - 1 ALERT type 5 Informative message, check
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-

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-21 Y

PLATON-Sep 24 01:21:22 2022 - (120922)

Z -45

dm_bd_213_autoredP 1 21/c 1 R = 0.12

RES= 0 0 X

NO MOVE FORCED

Prob = 50
Temp = 106

```
R(reflections)= 0.0397( 1955)      wR2(reflections)=
S = 1.058                        0.1076( 2257)
Npar= 175
```

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Alert level C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.594	7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF		5 Note



Alert level G

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	34	Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	74%	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	6	Info

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1 ALERT type 5 Informative message, check
-
-

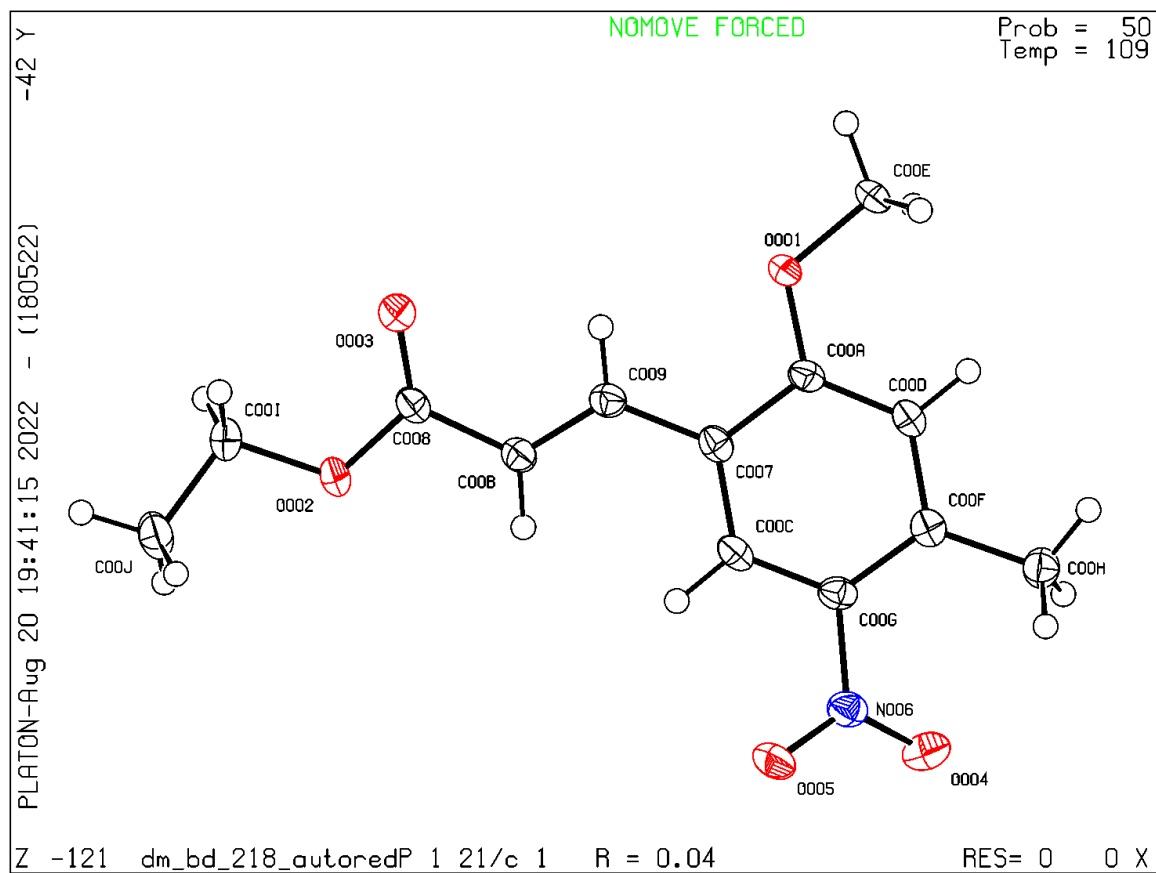
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Alert level C

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.8	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00473	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.665	Check



Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	34	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	47%	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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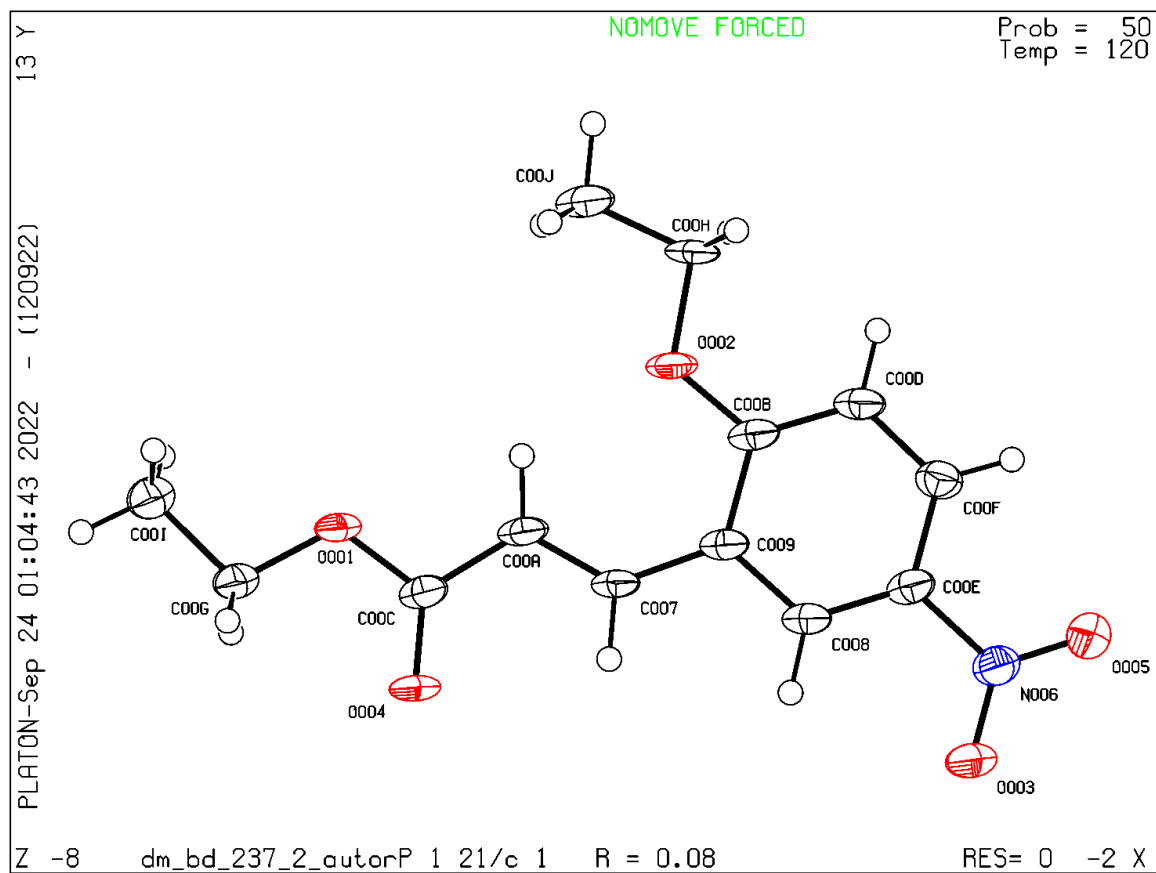
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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm_agj_343_1_autored

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 Interpreting this report

Datablock: dm_agj_343_1_autored

Bond precision: C-C = 0.0067 Å Wavelength=0.71073

Cell: a=18.9612 (9) b=13.2965 (7) c=9.0939 (4)
 alpha=90 beta=102.475 (5) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	2238.60 (19)	2238.60 (19)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H17 F6 N3 O2	C24 H17 F6 N3 O2
Sum formula	C24 H17 F6 N3 O2	C24 H17 F6 N3 O2
Mr	493.41	493.40
Dx, g cm ⁻³	1.464	1.464
Z	4	4
Mu (mm ⁻¹)	0.129	0.129
F000	1008.0	1008.0
F000'	1008.72	
h, k, lmax	22, 15, 10	22, 15, 10
Nref	3942	3942
Tmin, Tmax	0.986, 0.989	
Tmin'	0.986	

Correction method= Not given

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0946 (2660)

wR2(reflections)=
0.2818 (3942)

S = 1.050

Npar= 316

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Alert level B

PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	1.00 eA-3
PLAT213_ALERT_2_B	Atom F00Z has ADP max/min Ratio	4.6 prolat

Alert level C

DIFMN02_ALERT_2_C	The minimum difference density is < -0.1*ZMAX*0.75	
	_refine_diff_density_min given =	-0.700
	Test value =	-0.675
DIFMN03_ALERT_1_C	The minimum difference density is < -0.1*ZMAX*0.75	
	The relevant atom site should be identified.	
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	0.164
PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.164 Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28 Report
PLAT098_ALERT_2_C	Large Reported Min. (Negative) Residual Density	-0.70 eA-3
PLAT213_ALERT_2_C	Atom F00W has ADP max/min Ratio	3.9 prolat
PLAT213_ALERT_2_C	Atom F00X has ADP max/min Ratio	3.7 prolat
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0067 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.968 Check

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.70 Why ?
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C00V Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C00Y Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	52 Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	33% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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