

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) mo_dm15738_0m

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No syntax errors found.
Please wait while processing

CIF dictionary
Interpreting this report

Structure factor report

Datablock: mo_dm15738_0m

Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073	
Cell:	a=15.801(2)	b=13.9759(18)	c=19.829(3)
	alpha=90	beta=97.419(3)	gamma=90
Temperature: 133 K			
	Calculated	Reported	
Volume	4342.2(10)	4342.3(10)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C47 H57 Mg N3 O2 Si2	?	
Sum formula	C47 H57 Mg N3 O2 Si2	C47 H57 Mg N3 O2 Si2	
Mr	776.45	776.44	
Dx, g cm ⁻³	1.188	1.188	
Z	4	4	
Mu (mm ⁻¹)	0.137	0.137	
F000	1664.0	1664.0	
F000'	1665.32		
h, k, lmax	19, 17, 24	19, 17, 24	
Nref	8547	8546	
Tmin, Tmax	0.972, 0.982	0.637, 0.746	
Tmin'	0.972		
Correction method= # Reported T Limits: Tmin=0.637 Tmax=0.746 AbsCorr = MULTI-SCAN			
Data completeness= 1.000	Theta(max)= 26.000		
R(reflections)= 0.0520(5012)	wR2(reflections)= 0.1285(8546)		
S = 1.003	Npar= 557		

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

[PLAT410_ALERT_2_B](#) Short Intra H...H Contact H8A .. H22C .. 1.80 Ang.

● Alert level C

[PLAT410_ALERT_2_C](#) Short Intra H...H Contact H7B .. H17' .. 1.91 Ang.

[PLAT410_ALERT_2_C](#) Short Intra H...H Contact H8A .. H22A .. 1.98 Ang.

[PLAT905_ALERT_3_C](#) Negative K value in the Analysis of Variance ... -3.655 Report

● Alert level G

[PLAT003_ALERT_2_G](#) Number of Uiso or Uij Restrained non-H Atoms ... 12 Report

[PLAT300_ALERT_4_G](#) Atom Site Occupancy of >C17 is Constrained at 0.700 Check

And 33 other PLAT300 Alerts

[More ...](#)

PLAT301_ALERT_3_G Main Residue Disorder	Percentage =	11	Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints		72	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...		1	Report

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
34 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock mo_dm15738_0m - ellipsoid plot



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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) mo_dm15804_0m

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[CIF dictionary](#)
[Interpreting this report](#)

Structure factor report

Datablock: mo_dm15804_0m

Bond precision:	C-C = 0.0093 Å	Wavelength=0.71073
Cell:	a=11.371 (4) b=19.871 (7) c=20.675 (7)	
	alpha=90 beta=90 gamma=90	
Temperature: 296 K		
	Calculated	Reported
Volume	4672 (3)	4671 (3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C51 H57 Mg N3 O2 Si2	?
Sum formula	C51 H57 Mg N3 O2 Si2	C51 H57 Mg N3 O2 Si2
Mr	824.49	824.48
Dx, g cm ⁻³	1.172	1.172
Z	4	4
Mu (mm ⁻¹)	0.131	0.131
F000	1760.0	1760.0
F000'	1761.36	
h, k, lmax	13, 24, 25	13, 24, 25
Nref	8688 [4829]	8688
Tmin, Tmax	0.974, 0.983	0.630, 0.746
Tmin'	0.972	
Correction method= # Reported T Limits: Tmin=0.630 Tmax=0.746 AbsCorr = MULTI-SCAN		
Data completeness= 1.80/1.00	Theta(max)= 25.499	
R(reflections)= 0.0538 (4547)	wR2(reflections)= 0.1251 (8688)	
S = 0.985	Npar= 550	

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

[PLAT213_ALERT_2_C](#) Atom C51 has ADP max/min Ratio 3.2 prolat
[PLAT220_ALERT_2_C](#) Large Non-Solvent C Ueq(max)/Ueq(min) Range 5.9 Ratio
[PLAT222_ALERT_3_C](#) Large Non-Solvent H Uiso(max)/Uiso(min) ... 6.5 Ratio
[PLAT241_ALERT_2_C](#) High Ueq as Compared to Neighbors for C18 Check
[PLAT241_ALERT_2_C](#) High Ueq as Compared to Neighbors for C23 Check
[PLAT242_ALERT_2_C](#) Low Ueq as Compared to Neighbors for Si1 Check

And 2 other PLAT242 Alerts

More ...

[PLAT331_ALERT_2_C](#) Small Average Phenyl C-C Dist. C21 -C26 1.36 Ang.
[PLAT334_ALERT_2_C](#) Small Average Benzene C-C Dist. C14 -C19 1.37 Ang.
[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.0093 Ang.
[PLAT905_ALERT_3_C](#) Negative K value in the Analysis of Variance ... -0.149 Report

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of >C50 is Constrained at	0.600	Check
And 7 other PLAT300 Alerts			
More ...			
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =	2	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	35	Check
	N3 -SI1 -MG1 1.555 1.555 1.555 31.23 Deg.		
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	48	Check
	N3 -SI2 -MG1 1.555 1.555 1.555 35.12 Deg.		
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	70	Check
	O1 -C1 -MG1 1.555 1.555 1.555 34.30 Deg.		
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	109	Check
	N2 -C10 -MG1 1.555 1.555 1.555 42.70 Deg.		
PLAT791_ALERT_4_G	The Model has Chirality at C11 (Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	The Model has Chirality at C12 (Chiral SPGR)	R	Verify
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 and su ..	0.11	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 10 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

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Datablock mo_dm15804_0m - ellipsoid plot



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- Test a new CIF entry

checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: mo_dm15237_0m

Bond precision:	C-C = 0.0115 A	Wavelength=0.71073
Cell:	a=22.132(5) b=11.214(3) c=19.876(5)	
	alpha=90 beta=98.636(4) gamma=90	
Temperature: 130 K		
	Calculated	Reported
Volume	4877(2)	4877(2)
Space group	C 2	C 1 2 1
Hall group	C 2y	C 2y
Moiety formula	2(C50 H57 Mg N3 O2 Si2), C7 H8	C50 H57 Mg N3 O2 Si2, C3.5 H4
Sum formula	C107 H122 Mg2 N6 O4 Si4	C53.50 H61 Mg N3 O2 Si2
Mr	1717.09	858.54
Dx, g cm ⁻³	1.169	1.169
Z	2	4
Mu (mm ⁻¹)	0.128	0.128
F000	1836.0	1836.0
F000'	1837.39	
h, k, lmax	31, 15, 28	31, 15, 28
Nref	14754[7723]	12718
Tmin, Tmax	0.977, 0.994	0.597, 0.746
Tmin'	0.969	
Correction method= # Reported T Limits:	Tmin=0.597 Tmax=0.746 AbsCorr = MULTI-SCAN	
Data completeness= 1.65/0.86	Theta(max)= 30.412	
R(reflections)= 0.0751(4605)	wR2(reflections)= 0.1824(12718)	
S = 0.907	Npar= 564	

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

[PLAT026_ALERT_3_B](#) Ratio Observed / Unique Reflections too Low 36 %
[PLAT340_ALERT_3_B](#) Low Bond Precision on C-C Bonds 0.0115 Ang.

Alert level C

[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
[PLAT244_ALERT_4_C](#) Low 'Solvent' Ueq as Compared to Neighbors of C54 Check
[PLAT601_ALERT_2_C](#) Structure Contains Solvent Accessible VOIDS of . 41 Ang3

Alert level G

[PLAT042_ALERT_1_G](#) Calc. and Reported MoietyFormula Strings Differ Please Check
[PLAT045_ALERT_1_G](#) Calculated and Reported Z Differ by 0.50 Ratio
[PLAT779_ALERT_4_G](#) Suspect or Irrelevant (Bond) Angle in CIF # 1 Check
 N3 -Si1 -Mg1 1.555 1.555 35.40 Deg.

And 3 other PLAT779 Alerts

More ...

[PLAT789_ALERT_4_G](#) Atoms with Negative _atom_site_disorder_group # 3 Check
[PLAT791_ALERT_4_G](#) The Model has Chirality at C11 (Chiral SPGR) R Verify

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

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

7 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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Datablock mo_dm15237_0m - ellipsoid plot



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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) dm16274

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[CIF dictionary](#)
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Structure factor report

Datablock: dm16274

Bond precision:	C-C = 0.0056 Å	Wavelength=0.71073	
Cell:	a=22.162(3)	b=11.2330(13)	c=19.873(3)
	alpha=90	beta=98.551(5)	gamma=90
Temperature: 130 K			
	Calculated	Reported	
Volume	4892.3(11)	4892.2(12)	
Space group	C 2	C 1 2 1	
Hall group	C 2y	C 2y	
Moiety formula	2(C50 H57 Mg N3 O2 Si2), C7 H8	C50 H57 Mg N3 O2 Si2, C3.5 H4	
Sum formula	C107 H122 Mg2 N6 O4 Si4	C53.50 H61 Mg N3 O2 Si2	
Mr	1717.09	858.54	
Dx, g cm ⁻³	1.166	1.166	
Z	2	4	
Mu (mm ⁻¹)	0.128	0.128	
F000	1836.0	1836.0	
F000'	1837.39		
h, k, lmax	31, 15, 28	31, 15, 28	
Nref	14767 [7729]	11794	
Tmin, Tmax	0.985, 0.994	0.661, 0.746	
Tmin'	0.981		
Correction method= # Reported T Limits: Tmin=0.661 Tmax=0.746 AbsCorr = MULTI-SCAN			
Data completeness= 1.53/0.80	Theta(max)= 30.386		
R(reflections)= 0.0497(6590)	wR2(reflections)= 0.1039(11794)		
S = 0.941	Npar= 564		

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● Alert level C

[PLAT244_ALERT_4_C](#) Low 'Solvent' Ueq as Compared to Neighbors of C52 Check
[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00557 Ang.
[PLAT601_ALERT_2_C](#) Structure Contains Solvent Accessible VOIDS of . 39 Ang3
[PLAT905_ALERT_3_C](#) Negative K value in the Analysis of Variance ... -1.014 Report
[PLAT915_ALERT_3_C](#) No Flack x Check Done: Low Friedel Pair Coverage 59 %
[PLAT978_ALERT_2_C](#) Number C-C Bonds with Positive Residual Density 0 Note

● Alert level G

[PLAT042_ALERT_1_G](#) Calc. and Reported MoietyFormula Strings Differ Please Check
[PLAT045_ALERT_1_G](#) Calculated and Reported Z Differ by a Factor ... 0.50 Check
[PLAT300_ALERT_4_G](#) Atom Site Occupancy of *H51A is Constrained at 0.5 Check

And 2 other PLAT300 Alerts

[More ...](#)

PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp ²)-Methyl Moiety	C25 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	1 Check
	N3 -SI1 -MG1 1.555 1.555 1.555 35.52 Deg.	
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	11 Check
	N3 -SI2 -MG1 1.555 1.555 1.555 33.47 Deg.	
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	63 Check
	O1 -C1 -MG1 1.555 1.555 1.555 36.09 Deg.	
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	122 Check
	N1 -C16 -MG1 1.555 1.555 1.555 43.22 Deg.	
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	3 Check
PLAT791_ALERT_4_G	The Model has Chirality at C18 (Chiral SPGR)	S Verify
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	64 Note

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Datablock dm16274 - ellipsoid plot



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