Supplementary material for the article:

Milošev, M. Z.; Jakovljević, K.; Joksović, M. D.; Stanojković, T.; Matić, I. Z.; Perović, M.; Tešić, V.; Kanazir, S.; Mladenović, M.; Rodić, M. V.; et al. Mannich Bases of 1,2,4-Triazole-3-Thione Containing Adamantane Moiety: Synthesis, Preliminary Anticancer Evaluation, and Molecular Modeling Studies. *Chemical Biology and Drug Design* **2017**, *89* (6), 943–952. https://doi.org/10.1111/cbdd.12920

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1m, 1o

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: 1o

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Bond precision:  C-C = 0.0033 A          Wavelength=0.71073

Cell:            a=8.7866(2)     b=18.2502(5)     c=23.2664(6)
                 alpha=90        beta=90          gamma=90
Temperature:     294 K
```

	Calculated	Reported
Volume	3730.94(16)	3730.91(18)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C19 H23 F N4 S	C19 H23 F N4 S
Sum formula	C19 H23 F N4 S	C19 H23 F N4 S
Mr	358.47	358.47
Dx,g cm-3	1.276	1.276
Z	8	8
Mu (mm-1)	0.192	0.192
F000	1520.0	1520.0
F000’	1521.52	
h,k,lmax	11,24,31	11,22,31
Nref	4921	4353
Tmin,Tmax	0.938,0.962	0.951,0.965
Tmin’	0.938	

```
Correction method= # Reported T Limits: Tmin=0.951 Tmax=0.965
AbsCorr = ANALYTICAL

Data completeness= 0.885          Theta(max)= 28.945

R(reflections)= 0.0488( 3044)     wR2(reflections)= 0.1311( 4353)

S = 1.021                 Npar= 316
```

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

PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	4.701 Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	19 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	18 Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	-2 Units
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2 Report
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	36 Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	201 Note
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	500 Note
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	2 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density	4 Note

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

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

Datablock: 1m

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=11.9693(4) b=20.9226(11) c=14.7933(5)
alpha=90 beta=100.784(3) gamma=90
Temperature: 294 K

	Calculated	Reported
Volume	3639.2(3)	3639.2(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C19 H23 F N4 S	C19 H23 F N4 S
Sum formula	C19 H23 F N4 S	C19 H23 F N4 S
Mr	358.47	358.47
Dx,g cm-3	1.309	1.309
Z	8	8
Mu (mm-1)	0.197	0.197
F000	1520.0	1520.0
F000’	1521.52	
h,k,lmax	16,28,20	16,28,20
Nref	9797	8331
Tmin,Tmax	0.966,0.986	0.927,0.987
Tmin’	0.878	

Correction method= # Reported T Limits: Tmin=0.927 Tmax=0.987
AbsCorr = ANALYTICAL

Data completeness= 0.850 Theta(max)= 29.130

R(reflections)= 0.0528(4825) wR2(reflections)= 0.1289(8331)

S = 1.010 Npar= 467

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

PLAT230_ALERT_2_C Hirshfeld Test Diff for S1B -- C1B .. 6.2 s.u.
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C14A -C19A 1.37 Ang.

Author Response: Mogul geometry check didn’t find any significant deviation of the individual phenyl ring bond lengths, as their deviations were less than two sigma away from the average bond length found in the CSD. It should be keept in mind that the ring is substituted, and that anistropic displacement elipsoids show features of increased thermal motion of the atoms.

PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C14B -C19B 1.37 Ang.

Author Response: Mogul geometry check didn't find any significant deviation of the individual phenyl ring bond lengths, as their deviations were less than two sigma away from the average bond length found in the CSD. It should be keept in mind that the ring is substituted, and that anistropic displacement elipsoids show features of increased thermal motion of the atoms.

PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 34 Ang3

Author Response: Maps of difference electron density didn't show posisitve values in the voids. Refinement of the squeezed data didn't improve the model, based on the quality descriptors. Therefore, the initial model was retained with assumption that the voids are empty.

PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 14.266 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.472 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 7 Note

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.66 mm
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1459 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 4 Note

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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

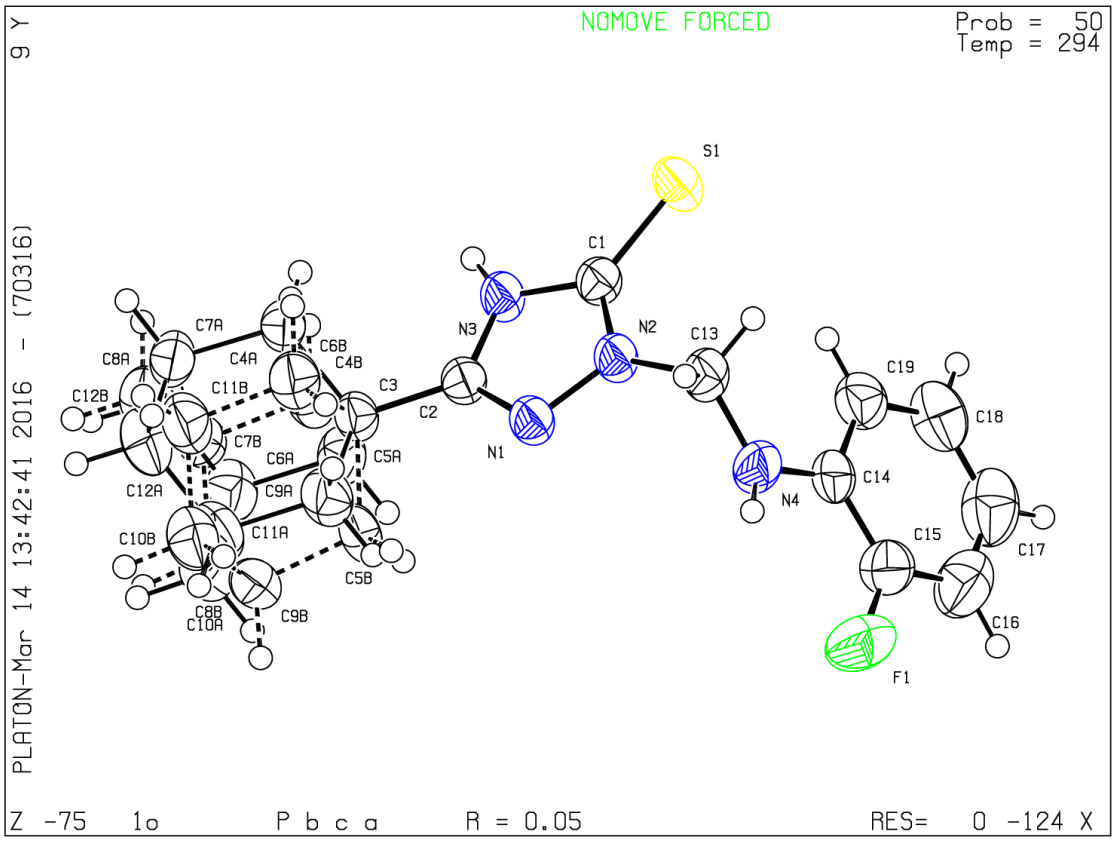
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 07/03/2016; check.def file version of 02/03/2016

Datablock 1o - ellipsoid plot



Datablock 1m - ellipsoid plot