SUPPORTING INFORMATION

Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 3_{10}-helix secondary structures †

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General Experimental Methods

Chemicals were obtained from commercial sources and used without further purification. Preparative RP-HPLC analyses were performed using a DENALI C-18 column (10 mm, 250_22 mm). Two mobile phases were used: A=94.9% water, 5% MeCN, 0.1% TFA; B=95% MeCN, 4.9% water, 0.1% TFA. ESI mass spectra were recorded on an LCQ Advantage spectrometer. NMR spectroscopic analysis: NMR spectroscopic experiments were carried out on either 200 MHz spectrometer (200 and 50 MHz for \(^1\)H and \(^{13}\)C, respectively), 500 MHz spectrometer (500 and 125 MHz for \(^1\)H and \(^{13}\)C, respectively) or 300 MHz spectrometer (300 and 75 MHz for \(^1\)H and \(^{13}\)C, respectively) To take advantage of the magnetic field value, measurements that required temperatures higher than room temperature for observing coalescence were performed in an apparatus with a \(^1\)H resonance frequency of 300 MHz spectrometer. 2D-NOESY experiments on peptides 2a and 2b were performed at different mixing times (300, 500 ms). Chemical shifts are given in ppm relative to CDCl\(_3\) or CD\(_3\)CN, CD\(_3\)OD as internal standards, and coupling constants J are reported in hertz (Hz). The MW mediated reaction were performed using MW reactor with IR temperature detector.
Two dimensional NMR experiments

Compound 2b
Protons signal assignment:
AR 453 F2
HMBCgp (Jn=8 Hz) in CD3CN a T=300K.
AR 453 F2
NOESYph in CD3CN at T=300K
Amide protons region of the NOESY spectrum ($\tau_m$ 500ms, BBI probe, 300K, 500MHz) of peptide 2b in CD$_3$CN (20mM). Sequential short range NH$_i$-NH$_{i+1}$ signals.
Compound 2a
Protons signals assignments:
AR 441 F1
HMBC in CD3CN a T=300K, Jn=8Hz
AR 441 F1
HSQC in CD3CN at T=300K
AR 441 F1
NOESY in CD3CN, T=300K, tmix=500ms
1) Amide protons region of the NOESY spectrum ($\tau_m$ 500 ms, BBI probe, 300 K, 500 MHz) of peptide 2a in CD$_3$CN (20 mM). Sequential short range NH$_i$-NH$_{i+1}$ signals.

2) Amide protons region of the NOESY spectrum ($\tau_m$ 300 ms, BBI probe, 300 K, 300 MHz) of peptide 2a in CD$_3$CN (8 mM). Sequential short range NH$_i$-NH$_{i+1}$ signals.
Non magnetic equivalence (NME) evaluation

Compound 2a

Aib chemical shift (26ppm.60-22.72 ppm.), NME = 3.88 ppm;
Compound 2b

Aib (26.26 ppm-23.19 ppm), NME = 3.07 ppm;
VT-NMR, DMSO\textsubscript{d6} titration

Compound 2b

Variation temperature NMR for compound 2b
DMSO$_{d6}$ titration NMR of compound 2b
Compound 2a

Variation temperature NMR of compound 2a
DMSO$_{d6}$ titration NMR of compound 2a
NMR

Compound 6a
\[ ^1H \text{NMR (200 MHz, CDCl}_3, 25^\circ\text{C}): \delta = 8.60 (s, 1H, Ph), 7.32-7.35 (m, 2H, Ph), 7.24-7.27 (m, 2H, Ph), 7.02-7.04 (m, 1H, Ph), 3.90-3.76 (s br, 2H, CH\text{}_2\text{Br}), 3.60-3.7 (m, 1H, Ph), 1.21-1.17 (m, 2H, 5-H, 7-H), 2.32 (4-H), 1.92-1.87 (m, 6-H, 1H, 7a-H), 1.45 (11-H, 7b-H), 0.98-0.96 (m, 8CH\text{}_2, 9-CH\text{}_2, \text{CH}_3). \]

\[ \text{MS (EI+): } m/z = 377\text{A (M+H)}. \]

\[ \text{C}_{17}\text{H}_{11}\text{O}_5\text{S} (377.3); \text{calcd C, 63.60; H, 7.50; N, 7.38; S, 12.75; found C, 63.30; H, 7.43; N, 7.39; S, 12.52.} \]

\[ \text{IR (KBr): } v = 3198, 2963, 1723, 1605, 1490, 1221. \]
Compound 7a
Compound 10
Compound 11

- TFA\(^+\)H\(_3\)N

\(\text{Me} \quad \text{Me} \quad \text{Me} \quad \text{NH}_2\)

\(\text{Me} \quad \text{Me} \quad \text{O} \quad \text{Me} \quad \text{O} \quad \text{N} \quad \text{H}\)

\(\text{Me} \quad \text{Me} \quad \text{O} \quad \text{Me} \quad \text{O} \quad \text{N} \quad \text{H}_2\)

S28
Compound 4

ARP436_3H
AR 436

1H NMR

δ (ppm)
0  1  2  3  4  5  6  7  8  9  10  11  12

6.1  3.2  3.0

4.1  4.2  4.3  4.4  4.5  4.6  4.7  4.8  4.9  5.0  5.1  5.2

-1  -2

-1500  -1000  -500  0  500  1000  1500  2000  2500  3000  3500  4000  4500  5000
Compound 14

Boc_amminalC_1Hefd copy
Boc amminal C
Compound 15
Compound 16b
Compound 17a

17a
Compound 17b

[Chemical structure image]

[1H NMR spectrum image]
Compound 2a (0.08 mM)

Acquisition in 0.08mM concentration use in VT-NMR and DMSO$_6$ titration present different chemical shifts for amide protons and is reported below
Compound 2b

AR 453 F2
1H in CD3CN at T=300K
Computational Analysis

Methods

Theoretical calculations A preliminary Low Mode conformational search was performed for Ac-(R,R,R,S)-NRB-NMe using MOE software with the MMFF94x force field and the Born solvation model. To obtain a charge set compatible with the ff99SB force field, the two lowest energy conformations were optimized at the HF/6-31G(d) level and two different spatial orientation were used to derive orientation- and conformation-independent Resp charges, using the Gaussian 09 package. Accordingly to standard amino acids, charge restraints of −0.4157, 0.2719, 0.5973 and −0.5679 were imposed to backbone nitrogen, hydrogen, carbonyl carbon and oxygen, respectively. The REMD simulation protocol has been previously optimized. The simulations (12 replicas distributed over the following temperatures: 260.00, 283.25, 308.53, 335.98, 365.78, 398.13, 433.19, 471.31, 512.66, 557.47, 606.14 and 658.94 K) were originated from the extended configuration of peptides 2a and 2b. A short equilibration run (200 ps) was performed on each replica prior to the actual production run, then REMD simulations were conducted on each peptide for 50 ns at constant temperature by using Langevin dynamics (ntt = 3) with different seeds (ig) for every simulation. A time step of 0.002 ps and an infinite cut-off for electrostatic were requested, and the SHAKE algorithm was used in order to constrain all bonds involving hydrogens. Exchanges were attempted every 2 ps and were on average accepted with a 55% probability. For H-bond analyses the following parameters were used: donor-acceptor distance: 4.0 Å, angle cutoff: 30°. Cluster analyses were performed with ptraj (AmberTools13) by using the average-linkage algorithm, as suggested by Shao and coworkers, by sampling one every two frames and using the pairwise mass weighted rmsd between frames as a metric. A total of 5 cluster were requested on the basis of the pseudo-F statistical analysis, and SSR/SST ratio (R-squared value). Pushing the REMD runs up to 250 ns did not provide significant variations to the results of trajectory analyses, proofing that the simulation was fully converged for the parameters of interest.
Most representative geometries obtained from the cluster analysis of the final 25 ns of the 308.5 K $ff99SB$ REMD trajectory for 2a peptide having (R,R,R)-NRB at position 2
Most representative geometries obtained from the cluster analysis of the final 25 ns of the 308.5 K \textit{ff99SB} REMD trajectory for \textit{2b} peptide having (\textit{S,S,R})-NRB at position 2.
X-ray diffraction

Single crystals of 6a were grown by slow evaporation from a mixture 1:1 of ethyl acetoacetate and chloroform, while those of compound 2b by slow evaporation from a solution of acetonitrile. X-ray diffraction data were collected at room temperature and 150(2) K, for 6a and 2b, respectively, on a three-circle Bruker SMART APEX II diffractometer equipped with a CCD area detector and an Oxford Cryostream N\textsubscript{2} device. Diffraction data were recorded for both compounds using \( \omega \)-scans (0.5 deg/frame) with graphite monochromated Mo Ka radiation (\( \lambda = 0.71073 \) Å) up to a 2\( \theta \) Bragg angle of 55.0\(^\circ\). The SAINT-Plus\textsuperscript{9} program package was used to perform the data reduction, whereas the collected structure factor amplitudes were corrected for beam anisotropy effects and for absorption using the program SADABS.\textsuperscript{10} The structures were solved by direct methods with the SHELXS97\textsuperscript{11} program and refined by full-matrix least-squares procedures on \( F^2 \), using all data, by application of the SHELXL-97\textsuperscript{4} and SHELXL2013\textsuperscript{4} programs, for compound 6a and 2b respectively, with all non-H atoms anisotropic. For compound 6a the coordinates of the H atoms bonded to nitrogen atoms and to atom C19 were refined, while all the other were included in the model at geometrically calculated positions and in riding modes, as it was done for all H atoms of compound 2b. Crystal structure data have been deposited at the Cambridge Crystallographic Data Centre, and allocated the deposition numbers CCDC 989313 and CCDC 989314 for 6a and 2b, respectively.

Crystal data for compound 6a: C\textsubscript{20}H\textsubscript{28}N\textsubscript{2}O\textsubscript{3}S, M = 376.50, orthorhombic, space group \( P2_12_12_1 \), \( a =11.545(2) \) Å, \( b = 13.276(3) \) Å, \( c =13.627(3) \) Å, \( V = 2088.6(7) \) Å\textsuperscript{3}, \( Z = 4 \), \( Z' = 1 \); \( \rho_{calc} = 1.197 \) Mg m\textsuperscript{-3}, \( \mu = 0.18 \) mm\textsuperscript{-1}, 27663 reflections measured, 4800 independent reflections (\( R_{int} = 0.044 \)), \( \theta_{max} = 27.51^\circ \), \( T = 293(2) \) K. Flack parameter: -0.03(9). The final \( R_1 \) values were 0.0468 [ \( I > 2\sigma(I) \)] and 0.0738 (all data). The final \( wR(F^2) \) values were 0.1082 [ \( I > 2\sigma(I) \)] and 0.1231 (all data). Data/restraints/parameters 4800/0/242. Goodness-of-fit on \( F^2 = 1.019 \). The largest difference peak and hole were 0.286 and -0.243 e Å\textsuperscript{-3}, respectively.
Stereoview of the molecular structure of compound 6a at 298 K, showing 30% probability displacement ellipsoids.
Packing of 6a.

a) projection along cell axis $a$.

b) projection along cell axis $b$;

c) projection along cell axis $c$;
Crystal data for compound 2b: C_{30}H_{42}N_{6}O_{6}S, M = 614.75, monoclinic, space group P2_1, a = 11.829(2) Å, b = 9.0852(18) Å, c = 31.098(6) Å, V = 3340.7(12) Å³, Z = 4, Z' = 2; \rho_{calcd} = 1.222 \text{ Mg m}^{-3}, \mu = 0.15 \text{ mm}^{-1}, 72594 reflections measured, 15364 independent reflections (R_{int} = 0.045), \theta_{max} = 27.51^\circ, T = 150(2) K. Flack parameter: 0.01(2). The final R_1 values were 0.0502 [I > 2\sigma(I)] and 0.0795 (all data). The final wR(F^2) values were 0.1113 [I > 2\sigma(I)] and 0.1235 (all data). Data/restraints/parameters 15364/1/788. Goodness-of-fit on F2 = 1.039. The largest difference peak and hole were 0.566 and -0.392 e Å^{-3}, respectively.

Figure S 1 Stereoview of the molecular structure of compound 2b at 150 K, showing 50% probability displacement ellipsoids, 4i and 4ii two different conformers of peptide 2b in the crystal cell
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(1S,2R,3R,4R)-ethyl 2-((S)-2-aminopropanamido)-3-(benzylthio)bicyclo[2.2.1]heptane-2-carboxylate

_CHEMICAL_NAME_SYSTEMATIC_ (1S,2R,3R,4R)-ethyl 2-((S)-2-aminopropanamido)-3-(benzylthio)bicyclo[2.2.1]heptane-2-carboxylate

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_CHEMICAL_MELTING_POINT_ ?

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_computing_data_reduction 'SAINT+ (Bruker AXS, Madison (USA) 1994-1996)'
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_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics 'Diamond v3.2i (Brandenburg, 2012)'

S64
Refinement of $F^2$ against ALL reflections. The weighted R-factor $wR$ and
goodness of fit $S$ are based on $F^2$, conventional R-factors $R$ are based
on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of
$F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on $F^2$ are statistically about twice as large as those based on $F$, and R-
factors based on ALL data will be even larger.

Refine LS structure factor coef Fsqd
Refine LS matrix type full
Refine LS weighting scheme calc
Refine LS weighting details
'calc $w=1/[(s^2(Fo^2)+(0.0553P)^2+0.3574P)]$ where $P=(Fo^2+2Fc^2)/3$'
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Atom sites solution secondary difmap
Atom sites solution hydrogens geom
Refine LS hydrogen treatment mixed
Refine LS extinction method none
Refine LS extinction coef ?
Refine LS abs structure details
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H1 H -0.2026 -0.1773 0.6813 0.124 Uiso 1 1 calc R . .
C2 C -0.0517(4) -0.2357(3) 0.7237(3) 0.1089(13) Uani 1 1 d . . .
H2 H -0.0816 -0.2956 0.7486 0.131 Uiso 1 1 calc R . .
C3 C 0.0688(3) -0.2168(2) 0.7256(3) 0.0843(9) Uani 1 1 d . . .
H3 H 0.1195 -0.2647 0.7509 0.101 Uiso 1 1 calc R . .
C4 C 0.1097(2) -0.1281(2) 0.6903(2) 0.0625(7) Uani 1 1 d . . .
C5 C 0.0327(3) -0.0582(3) 0.6532(2) 0.0769(8) Uani 1 1 d . . .
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C6 C -0.0831(3) -0.0777(3) 0.6515(3) 0.0919(10) Uani 1 1 d . . .
H6 H -0.1341 -0.0298 0.6269 0.110 Uiso 1 1 calc R . .
C7 C 0.2371(2) -0.1042(2) 0.6924(2) 0.0768(8) Uani 1 1 d . . .
H7A H 0.2613 -0.0773 0.6295 0.092 Uiso 1 1 calc R . .
H7B H 0.2813 -0.1649 0.7054 0.092 Uiso 1 1 calc R . .
C8 C 0.4180(18) 0.00043(19) 0.78580(18) 0.0565(6) Uani 1 1 d . . .
H8 H 0.4513 -0.0670 0.7775 0.068 Uiso 1 1 calc R . .
C9 C 0.47324(18) 0.07184(18) 0.70475(19) 0.0527(5) Uani 1 1 d . . .
C10 C 0.5508(2) 0.1413(2) 0.7681(2) 0.0670(7) Uani 1 1 d . . .
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C11 C 0.4748(3) 0.2152(2) 0.8240(2) 0.0774(8) Uani 1 1 d . . .
H11A H 0.4195 0.2476 0.7807 0.093 Uiso 1 1 calc R . .
H11B H 0.5212 0.2665 0.8562 0.093 Uiso 1 1 calc R . .
C12 C 0.4130(3) 0.1474(2) 0.8999(2) 0.0790(8) Uani 1 1 d . . .
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H12B H 0.3299 0.1467 0.8891 0.095 Uiso 1 1 calc R . .
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C20  C 0.3163(4)  0.3311(3)  0.5058(5)  0.159(3)  Uani 1 1 d . . .
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H20C H 0.3098  0.3587  0.5707  0.238  Uiso 1 1 calc R . . .
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N2   N 0.2064(3)  0.1807(3)  0.5412(3)  0.1516(19) Uani 1 1 d . . .
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H2B  H 0.1527   0.1975  0.4964   0.227  Uiso 1 1 d . . .
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O2   O 0.48084(18) -0.03372(16) 0.56474(15) 0.0770(5) Uani 1 1 d . . .
O3   O 0.51496(17)  0.20144(18) 0.55176(18) 0.0911(7) Uani 1 1 d . . .
S1   S 0.26240(5) -0.01211(5) 0.78841(5)  0.06035(18) Uani 1 1 d . . .
HN1  H 0.315(2)  0.110(2)  0.6581(19) 0.064(8)  Uiso 1 1 d . . .
H19  H 0.326(3)  0.194(2)  0.450(2)  0.077  Uiso 1 1 d . . .

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C4  0.0500(13)  0.0746(17)  0.0629(16) -0.0078(13)  0.0041(12) -0.0044(12)
C5  0.0645(18)  0.098(2)  0.0683(17)  0.0025(16)  0.0029(14)  0.0049(16)
C6  0.063(2)    0.127(3)  0.086(2) -0.007(2) -0.0078(17)  0.006(2)
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#------------------ SUBMISSION DETAILS --------------------------------------#

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_diffrn_reflns_theta_min  1.825
Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.
Refine LS structure factor coef: Fsqd
Refine LS matrix type: full
Refine LS weighting scheme: calc
Refine LS weighting details:
\[ w = \frac{1}{s^2(Fo^2) + (0.0650P)^2 + 0.1731P} \]
where \( P = (Fo^2 + 2Fc^2)/3 \)
Atom sites solution primary: ?
Atom sites solution secondary: ?
Atom sites solution hydrogens: geom
Refine LS hydrogen treatment: constr
Refine LS extinction method: SHELXL
Refine LS extinction coef: 0.0021(6)
Refine LS extinction expression:
\[ Fc^* = kFc\left[1 + 0.001xFc^2|l^3|/\sin(2\theta)\right]^{-1/4} \]
Refine LS abs structure details
Flack x determined using 4302 quotients \([(I+)-(I-)]/[|I+|+|I-|)]\)

Refine LS abs structure Flack: 0.01(2)
Chemical absolute configuration: 'rmad'
Refine LS number reflns: 15364
Refine LS number parameters: 788
Refine LS number restraints: 1
Refine LS R_factor_all: 0.0795
Refine LS R_factor_gt: 0.0502
Refine LS wR_factor_ref: 0.1235
Refine LS wR_factor_gt: 0.1113
Refine LS goodness of fit ref: 1.039
Refine LS restrained S_all: 1.039
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_refine_ls_shift/su_mean  0.000

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_site_symmetry_order
_atom_site_calc_flag
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_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
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_atom_site_disorder_group
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O1A O 0.77319(19) 0.3001(3) 0.91003(8) 0.0236(6) Uani 1 1 d . . . . .
O2A O 0.9310(2) 0.0395(3) 0.98508(8) 0.0326(6) Uani 1 1 d . . . . .
O3A O 0.59932(18) -0.0058(3) 0.87904(8) 0.0239(6) Uani 1 1 d . . . . .
O4A O 1.0932(2) -0.0637(3) 0.89809(9) 0.0347(7) Uani 1 1 d . . . . .
O5A O 0.4534(2) 0.0156(3) 0.97587(8) 0.0355(7) Uani 1 1 d . . . . .
O6A O 1.2037(2) 0.3181(4) 0.91189(11) 0.0529(9) Uani 1 1 d . . . . .
N1A N 0.6563(2) 0.1838(3) 0.95431(9) 0.0214(7) Uani 1 1 d . . . . .
HN1A H 0.5887 0.1555 0.9596 0.026 Uiso 1 1 calc R U . .
N2A N 0.8110(2) -0.0351(3) 0.93143(9) 0.0228(7) Uani 1 1 d . . . . .
HN2A H 0.7424 -0.0357 0.9215 0.027 Uiso 1 1 calc R U . .
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H14A H 0.6515 0.1610 1.0383 0.058 Uiso 1 1 calc R U . . .
H14B H 0.7620 0.0687 1.0465 0.058 Uiso 1 1 calc R U . . .
H14C H 0.6598 0.0003 1.0202 0.058 Uiso 1 1 calc R U . . .
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C16A C 0.4049(3) -0.0585(4) 0.89130(12) 0.0266(8) Uani 1 1 d . . .
H16A H 0.4333 -0.1541 0.9014 0.032 Uiso 1 1 calc R U . . .
C17A C 0.3549(3) 0.0229(4) 0.96314(13) 0.0294(9) Uani 1 1 d . . .
C18A C 1.0496(3) 0.2210(5) 0.86943(12) 0.0317(9) Uani 1 1 d . . .
H18A H 1.1107 0.1675 0.8556 0.038 Uiso 1 1 calc R U . . .
C19A C 0.8971(3) -0.1217(4) 0.90930(12) 0.0249(8) Uani 1 1 d . . .
C20A C 0.5839(3) 0.5093(4) 0.83930(12) 0.0288(9) Uani 1 1 d . . .
H20A H 0.6216 0.5642 0.8167 0.035 Uiso 1 1 calc R U . . .
C21A C 0.4564(3) 0.5187(4) 0.83844(13) 0.0315(9) Uani 1 1 d . . .
H21A H 0.4105 0.5439 0.8148 0.038 Uiso 1 1 calc R U . . .
C22A C 0.6104(3) 0.5605(4) 0.88554(12) 0.0281(9) Uani 1 1 d . . .
H22A H 0.6881 0.5414 0.8947 0.034 Uiso 1 1 calc R U . . .
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C23A C 1.1013(3) 0.3050(5) 0.90783(14) 0.0343(10) Uani 1 1 d . . .
C24A C 0.5264(3) 0.4544(4) 0.90544(12) 0.0236(8) Uani 1 1 d . . .
H24A H 0.5171 0.4638 0.9365 0.028 Uiso 1 1 calc R U . . .
C25A C 0.4217(3) 0.4847(4) 0.87745(13) 0.0271(8) Uani 1 1 d . . .
H25A H 0.3471 0.4802 0.8860 0.032 Uiso 1 1 calc R U . . .
C26A C 0.8442(3) -0.1781(5) 0.86755(13) 0.0310(9) Uani 1 1 d . . .
H26A H 0.7807 -0.2397 0.8737 0.047 Uiso 1 1 calc R U . . .
H26B H 0.8990 -0.2341 0.8523 0.047 Uiso 1 1 calc R U . . .
H26C H 0.8193 -0.0964 0.8502 0.047 Uiso 1 1 calc R U . . .
C27A C 0.9414(3) -0.2507(5) 0.93625(15) 0.0397(10) Uani 1 1 d . . .
H27A H 0.9739 -0.2145 0.9628 0.060 Uiso 1 1 calc R U . . .
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C2A 0.0240(18) 0.033(2) 0.0216(19) -0.0016(17) 0.0021(15) 0.0079(17)
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_all_special_details

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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N3B C9B C24B C25B -57.7(4) . . . . ?
C11B C9B C24B C25B -176.7(3) . . . . ?
C8B C9B C24B C25B 66.2(3) . . . . ?
N3B C9B C24B C22B -161.6(3) . . . . ?
C11B C9B C24B C22B 79.4(3) . . . . ?
C8B C9B C24B C22B -37.7(3) . . . . ?
C20B C21B C25B C24B 1.6(4) . . . . ?
C22B C24B C25B C21B 32.5(4) . . . . ?
C9B C24B C25B C21B -72.0(4) . . . . ?

_refine_diff_density_max  0.566
_refine_diff_density_min -0.392
_refine_diff_density_rms  0.054

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1 MOE, Chemical Computing Group Inc., Montreal, Canada, MOE v2012.10 edn., 2012


