# Noncovalent Interactions within a Synthetic Receptor Can Reinforce Guest Binding

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*Publication date:*
2006

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_audit_creation_date        04-05-28
_audit_creation_method CRYSTALS_ver_12.20
#******************************************************************************
#==============================================================================

_chemical_name_systematic         # IUPAC name, in full
;
?
;

_chemical_melting_point           ?

# choose from 'full, fullcycle, atomblock, userblock, diagonal, sparse'
_refine_ls_matrix_type            full

# choose from 'heavy, direct, difmap, geom'
_atom_sites_solution_primary      direct

# _atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens    geom

# choose from 'none, undef, noref, refall, refxyz, refU, constr, mixed'
_refine_ls_hydrogen_treatment     mixed

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_cell_angle_alpha                 90
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_cell_angle_beta                  93.196(10)
_cell_length_c                    26.4260(10)
_cell_angle_gamma                 90
_cell_volume                      5490.3(6)

_symmetry_cell_setting            'Monoclinic'
_symmetry_space_group_name_H-M    'P 1 21 1 '
loop_
 _symmetry_equiv_pos_as_xyz
 'x,y,z'
 '-x,y+1/2,-z'

# choose from: rm (reference molecule of
# known chirality), ad (anomolous
# dispersion - ie. Flack param), rmad
# (both rm and ad), syn (known from
# synthetic pathway), unk (unknown)
# or . (not applicable).

_chemical_absolute_configuration  'syn'

loop_
_atom_type_symbol
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_Cromer_Mann_a1
_atom_type_scat_Cromer_Mann_b1
_atom_type_scat_Cromer_Mann_a2
_atom_type_scat_Cromer_Mann_b2
_atom_type_scat_Cromer_Mann_a3
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_atom_type_scat_Cromer_Mann_b3
_atom_type_scat_Cromer_Mann_a4
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_atom_type_scat_Cromer_Mann_c
_atom_type_scat_source
 'C   '    0.0020    0.0020    2.3100   20.8439
    1.0200   10.2075    1.5886    0.5687    0.8650   51.6512    0.2156
'International_Tables_Vol_IV_Table_2.2B'
 'H   '    0.0000    0.0000    0.4930   10.5109
    0.3229   26.1257    0.1402    3.1424    0.0408   57.7997    0.0030
'International_Tables_Vol_IV_Table_2.2B'
 'N   '    0.0040    0.0030   12.2126    0.0057
    3.1322    9.8933    2.0125   28.9975    1.1663    0.5826  -11.5290
'International_Tables_Vol_IV_Table_2.2B'
 'O   '    0.0080    0.0060    3.0485   13.2771
    2.2868    5.7011    1.5463    0.3239    0.8670   32.9089    0.2508
'International_Tables_Vol_IV_Table_2.2B'
 'S   '    0.1100    0.1240    6.9053    1.4679
    5.2034   22.2151    1.4379    0.2536    1.5863   56.1720    0.8669
'International_Tables_Vol_IV_Table_2.2B'


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_chemical_formula_moiety
;
C69 H70 N18 O13 S4, C16 H36 N, C16 H36 N, O4 S, H2 O
;
_chemical_compound_source
;
synthesis as described
;
_chemical_formula_weight           2086.66
_cell_measurement_reflns_used            13502
_cell_measurement_theta_min              2.18
_cell_measurement_theta_max              22.28
_cell_measurement_temperature          150(2)
_exptl_crystal_description         ' block '
_exptl_crystal_colour              ' colourless '
_exptl_crystal_size_min           0.04
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_exptl_crystal_density_diffrn     1.261
_exptl_crystal_density_meas       ?
# Non-dispersive F(000):
_exptl_crystal_F_000              2223.000
_exptl_absorpt_coefficient_mu     0.178
 _computing_data_collection        'Bruker SMART (Bruker AXS, 1994)'
_computing_cell_refinement        'Bruker SAINT (Bruker AXS, 1994)'
_computing_data_reduction         'Bruker SAINT (Bruker AXS, 1994)'
_computing_structure_solution     'SHELXTL v6.12 (Bruker AXS, 2001)'
_computing_structure_refinement
;
 CRYSTALS (Watkin et al 2001)
;
_computing_publication_material
;
 CRYSTALS (Watkin et al 2001)
;
_computing_molecular_graphics
;
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 CAMERON (Watkin et al 1996)
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_diffrn_radiation_wavelength      0.6923
_diffrn_radiation_type            ' synchrotron '
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_diffrn_measurement_device_type   'Bruker SMART CCD'
_diffrn_measurement_method        'Thin slice \w-scans'
_exptl_absorpt_process_details
;

  Correction applied by SADABS - note that the transmission factors are
  not real since they include corrections for beam decay and possibly
  crystal decay (the two cannot be distinguished).
  The numbers listed in the CIF are those calculated by CRYSTALS.
;
_exptl_absorpt_correction_T_min   1.00
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_exptl_absorpt_correction_type    multi-scan
_diffrn_standards_interval_time   0
_diffrn_standards_interval_count  0
_diffrn_standards_number          0
_diffrn_standards_decay_%         0.00
_diffrn_ambient_temperature        150(2)
_diffrn_reflns_number             35394
_reflns_number_total              8281
_diffrn_reflns_av_R_equivalents   0.04
# Number of reflections with Friedels Law is 8281
# Number of reflections without Friedels Law is 0
# Theoretical number of reflections is about 7972
_diffrn_reflns_theta_min          1.712
_diffrn_reflns_theta_max          23.346
_diffrn_measured_fraction_theta_max 0.997
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_diffrn_reflns_limit_h_min        -14
_diffrn_reflns_limit_h_max        14
_diffrn_reflns_limit_k_min        -17
_diffrn_reflns_limit_k_max        17
_diffrn_reflns_limit_l_min        -29
_diffrn_reflns_limit_l_max        29
_reflns_limit_h_min               -14
_reflns_limit_h_max               14
_reflns_limit_k_min               0
_reflns_limit_k_max               17
_reflns_limit_l_min               0
_reflns_limit_l_max               29
_refine_diff_density_min          -0.95
_refine_diff_density_max          1.35
_refine_ls_number_reflns          5124
_refine_ls_number_restraints      344
_refine_ls_number_parameters      979

#_refine_ls_R_factor_ref          0.1128
_refine_ls_wR_factor_ref          0.1248
_refine_ls_goodness_of_fit_ref    1.1570

#_reflns_number_all               8231
_refine_ls_R_factor_all           0.1431
_refine_ls_wR_factor_all          0.1534
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# The I/u(I) cutoff below was used for refinement as
# well as the _gt R-factors:
_reflns_threshold_expression      I>2.00u(I)
_reflns_number_gt                 5124
_refine_ls_R_factor_gt            0.1128
_refine_ls_wR_factor_gt           0.1248

_refine_ls_shift/su_max           0.013418
_refine_ls_structure_factor_coef  F
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
;
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
 [weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~]*T~n-1~(x)]
 where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
 Method = Robust Weighting (Prince, 1982)
 W = [weight] * [1-(deltaF/6*sigmaF)^2^]^2^
 A~i~ are:
 1.13 1.35 0.484
;

_exptl_special_details
;

Guest SO4(2-) disordered over two positions was modelled
with refined occupancies:
site (S100, O100, O200, O300, O400) occ 0.538 and
site (S101, O101, O201, O301, O401) occ 0.462

S-alkyl bridge also disordered over two postions was modelled with
refined occupancies:
site (S200, S300, C340, C350, C360, O500, S400, S500) 0.662
and site (S201, S301, C341, C351, C361, O501, S401, S501) 0.338

Butyl chains are disordered - restrained and isotropic refinement
A part of one of the butyl chains modeleled over two positions
with refined occupancies: (C871, C881, C891) occ 0.505
and c(870, C880, C890) occ 0.495
;

## ------------------REFERENCES ----------------------##
## Insert your own references - in alphabetic order
_publ_section_references
;


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SMART: Area-Detector Software Package; Madison, WI.


Siemens Industrial Automation, Inc (1995).
SAINT: Area-Detector Integration Software.; Madison, WI.


Betteridge, P.W., Carruthers, J.R., Cooper, R.I.,
Prout, K., Watkin, D.J. (2003). J. Appl. Cryst. 36, 1487.

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Springer-Verlag, New York, 1982.
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crystal structures. Univ. of Gottingen, Federal Republic of Germany.

Watkin D.J. (1994),
Acta Cryst, A50, 411-437

Watkin, D.J., Prout, C.K. & Pearce, L.J. (1996) CAMERON, Chemical
Crystallography Laboratory, OXFORD, UK.
;

# Uequiv = arithmetic mean of Ui
# i.e. Ueqiv = (U1+U2+U3)/3

# Replace trailing . with the number of unfound
# hydrogen atoms attaced to relavent atom

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_adp_type
_atom_site_refinement_flags_posn
_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
_atom_site_attached_hydrogens
N1 N -0.1742(8) 0.4740(6) 0.8088(4) 0.0440 1.0000 Uani . . . . . .
N3 N -0.2285(8) 0.7701(7) 0.8567(4) 0.0449 1.0000 Uani . . . . . .
N4 N -0.1704(8) 0.9886(7) 0.8832(4) 0.0429 1.0000 Uani . . . . . .
N6 N -0.2535(8) 0.8995(7) 0.7044(3) 0.0428 1.0000 Uani . . . . . .
N7 N -0.2229(9) 0.8297(7) 0.5735(3) 0.0437 1.0000 Uani . . . . . .
N9 N -0.2541(8) 0.6154(7) 0.7070(4) 0.0453 1.0000 Uani . . . . . .
N10 N 0.0887(8) 0.7126(6) 0.5735(4) 0.0407 1.0000 Uani . . . . . .
N12 N 0.1574(7) 0.9159(7) 0.7142(4) 0.0453 1.0000 Uani . . . . . .
N13 N 0.1194(8) 1.0557(6) 0.8190(4) 0.0450 1.0000 Uani . . . . . .
N15 N 0.1828(8) 0.7557(7) 0.8520(4) 0.0413 1.0000 Uani . . . . . .
N16 N 0.1282(8) 0.5332(7) 0.8754(4) 0.0447 1.0000 Uani . . . . . .
N18 N 0.1701(8) 0.6354(7) 0.6997(4) 0.0424 1.0000 Uani . . . . . .
O5 O -0.3596(7) 0.9116(6) 0.6318(3) 0.0497 1.0000 Uani . . . . . .
O6 O -0.3266(9) 0.4979(8) 0.7350(5) 0.0859 1.0000 Uani . . . . . .
O7 O -0.2610(8) 0.4166(6) 0.8722(4) 0.0630 1.0000 Uani . . . . . .
O8 O -0.3192(7) 0.8675(6) 0.8969(3) 0.0526 1.0000 Uani . . . . . .
O10 O -0.3274(9) 0.7692(7) 0.5131(3) 0.0671 1.0000 Uani . . . . . .
O11 O -0.2656(8) 1.1069(6) 0.8780(4) 0.0587 1.0000 Uani . . . . . .
O12 O 0.1812(8) 0.7763(8) 0.5164(4) 0.0681 1.0000 Uani . . . . . .
O13 O 0.2588(7) 1.0197(6) 0.7468(4) 0.0504 1.0000 Uani . . . . . .
O14 O 0.2310(10) 1.1058(6) 0.8803(4) 0.0759 1.0000 Uani . . . . . .
O15 O 0.2805(7) 0.6532(6) 0.8908(4) 0.0538 1.0000 Uani . . . . . .
O16 O 0.2220(9) 0.4172(6) 0.8707(4) 0.0628 1.0000 Uani . . . . . .
O17 O 0.2400(7) 0.6171(6) 0.6238(4) 0.0556 1.0000 Uani . . . . . .
C1 C -0.2439(11) 0.4777(8) 0.8440(5) 0.0478 1.0000 Uani . . . . . .
N2 N -0.2451(6) 0.6303(5) 0.8508(3) 0.0433 1.0000 Uani . . . . . .

```
C2 C -0.2990(7) 0.5594(6) 0.8503(4) 0.0456 1.0000 Uani . . . . . .
C3 C -0.3999(8) 0.5573(6) 0.8613(4) 0.0606 1.0000 Uani . . . . . .
C4 C -0.4500(7) 0.6357(8) 0.8678(4) 0.0782 1.0000 Uani . . . . . .
C5 C -0.3971(7) 0.7074(7) 0.8664(4) 0.0595 1.0000 Uani . . . . . .
C6 C -0.2917(7) 0.7003(6) 0.8578(3) 0.0413 1.0000 Uani . . . . . .
C7 C -0.2413(10) 0.8449(8) 0.8755(5) 0.0392 1.0000 Uani . . . . . .
C8 C -0.1515(9) 0.9021(8) 0.8718(5) 0.0410 1.0000 Uani . . . . . .
C9 C -0.0619(10) 0.8800(9) 0.9110(5) 0.0561 1.0000 Uani D U . 3 1 .
C11 C -0.1023(11) 1.0237(9) 0.9268(6) 0.0584 1.0000 Uani D U . 3 1 .
C12 C -0.2460(10) 1.0368(8) 0.8608(5) 0.0417 1.0000 Uani . . . . . .
N5 N -0.2572(6) 0.9647(5) 0.7809(3) 0.0382 1.0000 Uani . . . . . .
C13 C -0.3090(7) 1.0070(6) 0.8171(4) 0.0415 1.0000 Uani . . . . . .
C14 C -0.4100(8) 1.0321(6) 0.8094(4) 0.0542 1.0000 Uani . . . . . .
C15 C -0.4646(7) 1.0035(8) 0.7670(4) 0.0509 1.0000 Uani . . . . . .
C16 C -0.4168(7) 0.9598(7) 0.7308(4) 0.0541 1.0000 Uani . . . . . .
C17 C -0.3146(7) 0.9402(6) 0.7388(3) 0.0461 1.0000 Uani . . . . . .
C18 C -0.2818(10) 0.8900(7) 0.6519(4) 0.0353 1.0000 Uani . . . . . .
C19 C -0.1886(9) 0.8536(7) 0.6257(4) 0.0338 1.0000 Uani . . . . . .
C20 C -0.1070(9) 0.9229(9) 0.6183(4) 0.0466 1.0000 Uani D U . 4 1 .
C22 C -0.1767(12) 0.8841(10) 0.5366(6) 0.0677 1.0000 Uani D U . 4 1 .
C23 C -0.2974(10) 0.7736(10) 0.5589(5) 0.0504 1.0000 Uani . . . . . .
N8 N -0.2839(5) 0.6941(5) 0.6354(2) 0.0383 1.0000 Uani . . . . . .
C24 C -0.3423(7) 0.7209(6) 0.5957(3) 0.0424 1.0000 Uani . . . . . .
C25 C -0.4446(8) 0.6899(7) 0.5851(4) 0.0443 1.0000 Uani . . . . . .
C26 C -0.4858(8) 0.6347(9) 0.6172(5) 0.0895 1.0000 Uani . . . . . .
C27 C -0.4247(8) 0.6091(8) 0.6599(4) 0.0703 1.0000 Uani . . . . . .
C28 C -0.3225(7) 0.6393(6) 0.6672(3) 0.0484 1.0000 Uani . . . . . .
C29 C -0.2553(12) 0.5464(9) 0.7364(5) 0.0535 1.0000 Uani . . . . . .
C30 C -0.1594(10) 0.5349(9) 0.7700(5) 0.0490 1.0000 Uani . . . . . .
C31 C -0.0734(12) 0.4987(10) 0.7392(6) 0.0592 1.0000 Uani . . . . . .
C32 C -0.0282(13) 0.4287(9) 0.7703(7) 0.0819 1.0000 Uani D U . 5 1 .
C33 C -0.1166(12) 0.3973(9) 0.8008(6) 0.0594 1.0000 Uani . . . . . .
C36 C -0.0603(14) 0.6322(11) 0.5687(6) 0.0844 1.0000 Uani D U . 5 1 .
C37 C 0.0237(11) 0.6684(9) 0.5368(5) 0.0515 1.0000 Uani . . . . . .
C38 C 0.1622(10) 0.7667(9) 0.5608(5) 0.0445 1.0000 Uani . . . . . .
N11 N 0.1678(5) 0.8437(5) 0.6399(2) 0.0391 1.0000 Uani . . . . . .
C39 C 0.2218(7) 0.8115(6) 0.6039(3) 0.0450 1.0000 Uani . . . . . .
C40 C 0.3281(8) 0.8231(7) 0.5990(4) 0.0816 1.0000 Uani . . . . . .
C41 C 0.3863(8) 0.8611(9) 0.6370(5) 0.0734 1.0000 Uani . . . . . .
C42 C 0.3272(8) 0.8943(8) 0.6784(4) 0.0746 1.0000 Uani . . . . . .
C43 C 0.2185(7) 0.8849(6) 0.6760(3) 0.0417 1.0000 Uani . . . . . .
C44 C 0.1760(11) 0.9785(9) 0.7450(5) 0.0504 1.0000 Uani . . . . . .
C45 C 0.0885(9) 1.0002(8) 0.7771(5) 0.0389 1.0000 Uani . . . . . .
C46 C 0.0054(12) 1.0506(11) 0.7475(6) 0.0616 1.0000 Uani . . . . . .
C47 C -0.0299(13) 1.1142(11) 0.7865(7) 0.0694 1.0000 Uani . . . . . .
C48 C 0.0610(12) 1.1345(10) 0.8167(6) 0.0634 1.0000 Uani . . . . . .
C49 C 0.1999(11) 1.0464(9) 0.8540(5) 0.0496 1.0000 Uani . . . . . .
N14 N 0.2016(5) 0.8950(5) 0.8520(3) 0.0388 1.0000 Uani . . . . . .
C50 C 0.2580(7) 0.9671(6) 0.8555(3) 0.0441 1.0000 Uani . . . . . .
C51 C 0.3650(8) 0.9682(7) 0.8684(4) 0.0587 1.0000 Uani . . . . . .
C52 C 0.4103(8) 0.8885(7) 0.8743(4) 0.0526 1.0000 Uani . . . . . .
C53 C 0.3550(7) 0.8153(8) 0.8678(4) 0.0581 1.0000 Uani . . . . . .
C54 C 0.2495(7) 0.8210(6) 0.8569(3) 0.0477 1.0000 Uani . . . . . .
C55 C 0.2024(11) 0.6787(9) 0.8696(5) 0.0447 1.0000 Uani . . . . . .
C56 C 0.1065(10) 0.6207(8) 0.8660(4) 0.0423 1.0000 Uani . . . . . .
C57 C 0.0316(9) 0.6430(9) 0.9064(5) 0.0492 1.0000 Uani D U . 2 1 .
C59 C 0.0810(12) 0.5022(9) 0.9205(5) 0.0624 1.0000 Uani D U . 2 1 .
C60 C 0.1986(11) 0.4843(8) 0.8532(5) 0.0442 1.0000 Uani . . . . . .
N17 N 0.1902(5) 0.5643(5) 0.7738(3) 0.0431 1.0000 Uani . . . . . .
C61 C 0.2516(7) 0.5171(6) 0.8091(3) 0.0403 1.0000 Uani . . . . . .
C62 C 0.3451(8) 0.4887(7) 0.7988(4) 0.0577 1.0000 Uani . . . . . .
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C63 C 0.3890(8) 0.5220(7) 0.7544(4) 0.0811 1.0000 Uani . . . . . .
C64 C 0.3382(7) 0.5703(8) 0.7239(4) 0.0734 1.0000 Uani . . . . . .
C65 C 0.2310(7) 0.5883(6) 0.7310(3) 0.0498 1.0000 Uani . . . . . .
C66 C 0.1716(11) 0.6433(8) 0.6490(5) 0.0438 1.0000 Uani . . . . . .
C67 C 0.0758(9) 0.6825(8) 0.6262(4) 0.0365 1.0000 Uani . . . . . .
C68 C -0.0120(12) 0.6169(10) 0.6177(5) 0.0594 1.0000 Uani . . . . . .
S100 S -0.0552(1) 0.7638(1) 0.7569(1) 0.0345 0.5382 Uani D U . 6 1 .
O100 O -0.0199(1) 0.7781(1) 0.8093(1) 0.0408 0.5382 Uani D U . 6 1 .
O200 O -0.0292(1) 0.8314(1) 0.7246(1) 0.0397 0.5382 Uani D U . 6 1 .
O300 O -0.1644(1) 0.7520(1) 0.7545(1) 0.0470 0.5382 Uani D U . 6 1 .
O400 O -0.0118(1) 0.6882(1) 0.7403(1) 0.0505 0.5382 Uani D U . 6 1 .
S101 S -0.0266(1) 0.7686(1) 0.7545(1) 0.0367 0.4618 Uani D U . 6 2 .
O101 O -0.0529(1) 0.7468(1) 0.8052(1) 0.0464 0.4618 Uani D U . 6 2 .
O201 O -0.0578(1) 0.8530(1) 0.7426(1) 0.0401 0.4618 Uani D U . 6 2 .
O301 O 0.0825(1) 0.7590(1) 0.7505(1) 0.0521 0.4618 Uani D U . 6 2 .
O401 O -0.0763(1) 0.7118(1) 0.7197(1) 0.0456 0.4618 Uani D U . 6 2 .
S200 S 0.0573(7) 0.3528(6) 0.7463(4) 0.0853 0.651(18) Uani D U P 5 1 .
S300 S -0.0332(10) 0.2993(6) 0.6916(4) 0.0986 0.651(18) Uani D U P 5 1 .
C340 C 0.003(3) 0.366(2) 0.6405(12) 0.1236 0.651(18) Uani D U P 5 1 .
C350 C -0.088(3) 0.404(3) 0.6074(10) 0.1290 0.651(18) Uani D U P 5 1 .
C360 C -0.183(3) 0.355(2) 0.6027(16) 0.1436 0.651(18) Uani D U P 5 1 .
O500 O -0.170(3) 0.275(2) 0.5835(11) 0.1596 0.651(18) Uani D U P 5 1 0.651
S400 S -0.0418(12) 0.4405(8) 0.5471(5) 0.1156 0.651(18) Uani D U P 5 1 .
S500 S -0.1333(11) 0.5457(8) 0.5400(5) 0.1032 0.651(18) Uani D U P 5 1 .
S201 S 0.006(2) 0.3471(14) 0.7249(10) 0.1259 0.349(18) Uani D U P 5 2 .
S301 S -0.106(3) 0.3202(14) 0.6713(10) 0.1378 0.349(18) Uani D U P 5 2 .
C341 C -0.065(6) 0.376(4) 0.616(2) 0.1273 0.349(18) Uani D U P 5 2 .
C351 C -0.148(5) 0.428(4) 0.5852(17) 0.1176 0.349(18) Uani D U P 5 2 .
C361 C -0.249(5) 0.394(4) 0.596(3) 0.1218 0.349(18) Uani D U P 5 2 .
O501 O -0.290(3) 0.330(3) 0.5666(18) 0.1182 0.349(18) Uani D U P 5 2 0.349
S401 S -0.0942(16) 0.4699(11) 0.5287(8) 0.0922 0.349(18) Uani D U P 5 2 .
S501 S -0.1681(14) 0.5799(11) 0.5384(10) 0.0801 0.349(18) Uani D U P 5 2 .
N19 N 0.4518(6) 0.1563(6) 0.6036(4) 0.1092(19) 1.0000 Uiso D U . . . .
C70 C 0.4713(10) 0.1207(7) 0.5500(4) 0.112(2) 1.0000 Uiso D U . . . .
C71 C 0.4704(8) 0.0238(7) 0.5492(4) 0.115(2) 1.0000 Uiso D U . . . .
C72 C 0.4555(9) -0.0032(9) 0.4909(4) 0.118(3) 1.0000 Uiso D U . . . .
C73 C 0.4496(11) -0.1032(10) 0.4906(6) 0.120(3) 1.0000 Uiso D U . . . .
C74 C 0.3581(8) 0.1183(8) 0.6283(4) 0.106(2) 1.0000 Uiso D U . . . .
C75 C 0.2536(9) 0.1357(7) 0.5964(4) 0.106(2) 1.0000 Uiso D U . . . .
C76 C 0.1643(8) 0.0969(8) 0.6281(5) 0.106(2) 1.0000 Uiso D U . . . .
C77 C 0.0614(10) 0.1243(10) 0.6011(6) 0.106(3) 1.0000 Uiso D U . . . .
C78 C 0.4431(8) 0.2482(7) 0.5932(4) 0.113(2) 1.0000 Uiso D U . . . .
C79 C 0.4494(8) 0.3003(7) 0.6427(5) 0.118(2) 1.0000 Uiso D U . . . .
C80 C 0.3357(9) 0.3296(7) 0.6516(5) 0.122(3) 1.0000 Uiso D U . . . .
C81 C 0.3131(11) 0.4047(10) 0.6149(8) 0.124(3) 1.0000 Uiso D U . . . .
C82 C 0.5445(11) 0.1291(14) 0.6399(6) 0.109(2) 1.0000 Uiso D U . . . .
C83 C 0.6508(11) 0.1553(13) 0.6196(6) 0.109(3) 1.0000 Uiso D U . . . .
C84 C 0.7370(12) 0.1276(12) 0.6619(7) 0.110(3) 1.0000 Uiso D U . . . .
C85 C 0.7138(17) 0.1767(16) 0.7108(7) 0.111(3) 1.0000 Uiso D U . . . .
O103 O 0.3086(17) 0.6216(16) 0.5153(8) 0.160(7) 1.0000 Uiso . . . . . 2
N20 N 0.4707(6) 0.2779(6) 0.9535(4) 0.1919(19) 1.0000 Uiso D U . . . .
C90 C 0.5673(10) 0.2532(7) 0.9865(4) 0.193(2) 1.0000 Uiso D U . . . .
C91 C 0.6654(8) 0.2982(7) 0.9699(4) 0.193(2) 1.0000 Uiso D U . . . .
C92 C 0.7562(9) 0.2706(9) 1.0081(4) 0.195(3) 1.0000 Uiso D U . . . .
C93 C 0.8621(11) 0.2870(10) 0.9794(6) 0.195(3) 1.0000 Uiso D U . . . .
C94 C 0.4684(8) 0.3766(8) 0.9487(4) 0.193(2) 1.0000 Uiso D U . . . .
C95 C 0.4357(9) 0.4204(7) 0.9996(4) 0.194(2) 1.0000 Uiso D U . . . .
C96 C 0.3854(8) 0.5079(8) 0.9830(5) 0.194(2) 1.0000 Uiso D U . . . .
C97 C 0.4253(10) 0.5730(10) 1.0243(6) 0.195(3) 1.0000 Uiso D U . . . .
C98 C 0.3658(8) 0.2465(7) 0.9729(4) 0.194(2) 1.0000 Uiso D U . . . .
C99 C 0.3717(8) 0.1520(7) 0.9909(5) 0.196(2) 1.0000 Uiso D U . . . .
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C100 C 0.2564(9) 0.1251(7) 1.0012(5) 0.197(3) 1.0000 Uiso D U . . . .
C101 C 0.2563(11) 0.0256(10) 1.0041(8) 0.198(3) 1.0000 Uiso D U . . . .
C86 C 0.4889(15) 0.2463(13) 0.9004(8) 0.190(3) 1.0000 Uiso D U . 1 1 .
C870 C 0.392(4) 0.261(5) 0.8625(13) 0.189(3) 0.48(3) Uiso D U P 1 2 .
C880 C 0.408(5) 0.203(4) 0.8149(18) 0.188(4) 0.48(3) Uiso D U P 1 2 .
C890 C 0.325(6) 0.232(5) 0.7725(16) 0.187(4) 0.48(3) Uiso D U P 1 2 .
C871 C 0.536(5) 0.315(2) 0.8668(13) 0.189(3) 0.52(3) Uiso D U P 1 1 .
C881 C 0.569(4) 0.270(4) 0.8179(12) 0.187(4) 0.52(3) Uiso D U P 1 1 .
C891 C 0.689(4) 0.256(5) 0.825(3) 0.186(4) 0.52(3) Uiso D U P 1 1 .
C580 C 0.052(3) 0.5824(14) 0.9489(8) 0.0547 0.39(3) Uani D U P 2 2 .
C581 C -0.0098(14) 0.5590(11) 0.9216(9) 0.0566 0.61(3) Uani D U P 2 1 .
C110 C -0.0154(14) 0.9618(11) 0.9293(9) 0.0574 0.66(3) Uani D U P 3 1 .
C111 C -0.073(3) 0.9418(14) 0.9536(9) 0.0570 0.34(3) Uani D U P 3 2 .
C21 C -0.141(2) 0.9592(13) 0.5670(7) 0.0612 0.53(3) Uani D U P 4 1 .
C210 C -0.0751(16) 0.908(2) 0.5651(7) 0.0568 0.47(3) Uani D U P 4 2 .
H1 H -0.1712 0.7625 0.8400 0.0558 1.0000 Uiso . . . . . .
H2 H -0.1895 0.8842 0.7167 0.0505 1.0000 Uiso . . . . . .
H3 H -0.1971 0.6463 0.7111 0.0541 1.0000 Uiso . . . . . .
H4 H 0.0973 0.8887 0.7174 0.0556 1.0000 Uiso . . . . . .
H5 H 0.1179 0.7627 0.8383 0.0499 1.0000 Uiso . . . . . .
H6 H 0.1115 0.6525 0.7128 0.0499 1.0000 Uiso . . . . . .
H31 H -0.4375 0.5034 0.8647 0.0722 1.0000 Uiso . . . . . .
H41 H -0.5255 0.6370 0.8734 0.0936 1.0000 Uiso . . . . . .
H51 H -0.4308 0.7627 0.8712 0.0708 1.0000 Uiso . . . . . .
H81 H -0.1356 0.8947 0.8355 0.0495 1.0000 Uiso . . . . . .
H141 H -0.4427 1.0700 0.8339 0.0656 1.0000 Uiso . . . . . .
H151 H -0.5403 1.0148 0.7626 0.0609 1.0000 Uiso . . . . . .
H161 H -0.4559 0.9424 0.6988 0.0644 1.0000 Uiso . . . . . .
H191 H -0.1602 0.8063 0.6468 0.0402 1.0000 Uiso . . . . . .
H251 H -0.4858 0.7089 0.5541 0.0535 1.0000 Uiso . . . . . .
H261 H -0.5575 0.6129 0.6107 0.1077 1.0000 Uiso . . . . . .
H271 H -0.4532 0.5697 0.6849 0.0838 1.0000 Uiso . . . . . .
H301 H -0.1420 0.5908 0.7849 0.0589 1.0000 Uiso . . . . . .
H311 H -0.0197 0.5420 0.7336 0.0713 1.0000 Uiso . . . . . .
H312 H -0.1023 0.4776 0.7058 0.0713 1.0000 Uiso . . . . . .
H331 H -0.0905 0.3721 0.8337 0.0717 1.0000 Uiso . . . . . .
H332 H -0.1598 0.3554 0.7812 0.0717 1.0000 Uiso . . . . . .
H371 H -0.0065 0.7071 0.5102 0.0618 1.0000 Uiso . . . . . .
H372 H 0.0628 0.6231 0.5203 0.0618 1.0000 Uiso . . . . . .
H401 H 0.3611 0.8034 0.5679 0.0985 1.0000 Uiso . . . . . .
H411 H 0.4631 0.8660 0.6366 0.0882 1.0000 Uiso . . . . . .
H421 H 0.3633 0.9231 0.7079 0.0893 1.0000 Uiso . . . . . .
H451 H 0.0637 0.9449 0.7890 0.0465 1.0000 Uiso . . . . . .
H461 H 0.0347 1.0794 0.7180 0.0743 1.0000 Uiso . . . . . .
H462 H -0.0531 1.0140 0.7353 0.0743 1.0000 Uiso . . . . . .
H471 H -0.0831 1.0890 0.8079 0.0837 1.0000 Uiso . . . . . .
H472 H -0.0590 1.1650 0.7691 0.0837 1.0000 Uiso . . . . . .
H481 H 0.0435 1.1528 0.8514 0.0766 1.0000 Uiso . . . . . .
H482 H 0.1011 1.1794 0.8004 0.0766 1.0000 Uiso . . . . . .
H511 H 0.4054 1.0210 0.8730 0.0703 1.0000 Uiso . . . . . .
H521 H 0.4859 0.8848 0.8835 0.0625 1.0000 Uiso . . . . . .
H531 H 0.3900 0.7599 0.8709 0.0698 1.0000 Uiso . . . . . .
H561 H 0.0784 0.6292 0.8304 0.0508 1.0000 Uiso . . . . . .
H621 H 0.3824 0.4466 0.8208 0.0694 1.0000 Uiso . . . . . .
H631 H 0.4615 0.5068 0.7471 0.0985 1.0000 Uiso . . . . . .
H641 H 0.3729 0.5958 0.6948 0.0878 1.0000 Uiso . . . . . .
H671 H 0.0602 0.7282 0.6503 0.0437 1.0000 Uiso . . . . . .
H681 H -0.0635 0.6232 0.6443 0.0715 1.0000 Uiso . . . . . .
H682 H 0.0174 0.5593 0.6193 0.0715 1.0000 Uiso . . . . . .
H701 H 0.5401 0.1407 0.5397 0.1344 1.0000 Uiso . . . . . .
H702 H 0.4160 0.1416 0.5253 0.1344 1.0000 Uiso . . . . . .
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H711 H 0.5372 0.0016 0.5644 0.1382 1.0000 Uiso . . . . . .
H712 H 0.4121 0.0021 0.5687 0.1382 1.0000 Uiso . . . . . .
H721 H 0.5153 0.0162 0.4718 0.1418 1.0000 Uiso . . . . . .
H722 H 0.3902 0.0210 0.4753 0.1418 1.0000 Uiso . . . . . .
H731 H 0.4402 -0.1234 0.4548 0.1441 1.0000 Uiso . . . . . .
H732 H 0.5150 -0.1265 0.5066 0.1441 1.0000 Uiso . . . . . .
H733 H 0.3899 -0.1218 0.5101 0.1441 1.0000 Uiso . . . . . .
H741 H 0.3534 0.1429 0.6628 0.1278 1.0000 Uiso . . . . . .
H742 H 0.3683 0.0567 0.6313 0.1278 1.0000 Uiso . . . . . .
H751 H 0.2429 0.1971 0.5919 0.1269 1.0000 Uiso . . . . . .
H752 H 0.2547 0.1084 0.5624 0.1269 1.0000 Uiso . . . . . .
H761 H 0.1693 0.1186 0.6636 0.1271 1.0000 Uiso . . . . . .
H762 H 0.1695 0.0347 0.6286 0.1271 1.0000 Uiso . . . . . .
H771 H 0.0025 0.1014 0.6196 0.1270 1.0000 Uiso . . . . . .
H772 H 0.0575 0.1865 0.6005 0.1270 1.0000 Uiso . . . . . .
H773 H 0.0576 0.1027 0.5655 0.1270 1.0000 Uiso . . . . . .
H781 H 0.5006 0.2653 0.5718 0.1361 1.0000 Uiso . . . . . .
H782 H 0.3754 0.2594 0.5745 0.1361 1.0000 Uiso . . . . . .
H791 H 0.4768 0.2655 0.6718 0.1419 1.0000 Uiso . . . . . .
H792 H 0.4953 0.3498 0.6389 0.1419 1.0000 Uiso . . . . . .
H801 H 0.3301 0.3477 0.6876 0.1470 1.0000 Uiso . . . . . .
H802 H 0.2858 0.2833 0.6438 0.1470 1.0000 Uiso . . . . . .
H811 H 0.2415 0.4257 0.6191 0.1483 1.0000 Uiso . . . . . .
H812 H 0.3638 0.4504 0.6229 0.1483 1.0000 Uiso . . . . . .
H813 H 0.3195 0.3859 0.5791 0.1483 1.0000 Uiso . . . . . .
H821 H 0.5372 0.1557 0.6737 0.1302 1.0000 Uiso . . . . . .
H822 H 0.5431 0.0671 0.6437 0.1302 1.0000 Uiso . . . . . .
H831 H 0.6531 0.2170 0.6144 0.1311 1.0000 Uiso . . . . . .
H832 H 0.6621 0.1263 0.5868 0.1311 1.0000 Uiso . . . . . .
H841 H 0.8074 0.1420 0.6509 0.1317 1.0000 Uiso . . . . . .
H842 H 0.7329 0.0662 0.6681 0.1317 1.0000 Uiso . . . . . .
H851 H 0.7659 0.1616 0.7386 0.1331 1.0000 Uiso . . . . . .
H852 H 0.7176 0.2379 0.7040 0.1331 1.0000 Uiso . . . . . .
H853 H 0.6431 0.1622 0.7212 0.1331 1.0000 Uiso . . . . . .
H901 H 0.5561 0.2680 1.0225 0.2311 1.0000 Uiso . . . . . .
H902 H 0.5778 0.1916 0.9837 0.2311 1.0000 Uiso . . . . . .
H911 H 0.6557 0.3600 0.9714 0.2321 1.0000 Uiso . . . . . .
H912 H 0.6804 0.2816 0.9346 0.2321 1.0000 Uiso . . . . . .
H921 H 0.7559 0.3046 1.0399 0.2336 1.0000 Uiso . . . . . .
H922 H 0.7496 0.2102 1.0167 0.2336 1.0000 Uiso . . . . . .
H931 H 0.9228 0.2704 1.0021 0.2344 1.0000 Uiso . . . . . .
H932 H 0.8675 0.3475 0.9707 0.2344 1.0000 Uiso . . . . . .
H933 H 0.8611 0.2531 0.9476 0.2344 1.0000 Uiso . . . . . .
H941 H 0.5388 0.3966 0.9408 0.2311 1.0000 Uiso . . . . . .
H942 H 0.4177 0.3925 0.9204 0.2311 1.0000 Uiso . . . . . .
H951 H 0.4977 0.4294 1.0232 0.2325 1.0000 Uiso . . . . . .
H952 H 0.3843 0.3852 1.0166 0.2325 1.0000 Uiso . . . . . .
H961 H 0.3083 0.5042 0.9820 0.2329 1.0000 Uiso . . . . . .
H962 H 0.4078 0.5246 0.9489 0.2329 1.0000 Uiso . . . . . .
H971 H 0.3959 0.6292 1.0157 0.2335 1.0000 Uiso . . . . . .
H972 H 0.4029 0.5554 1.0583 0.2335 1.0000 Uiso . . . . . .
H973 H 0.5024 0.5757 1.0251 0.2335 1.0000 Uiso . . . . . .
H981 H 0.3471 0.2821 1.0020 0.2325 1.0000 Uiso . . . . . .
H982 H 0.3113 0.2516 0.9448 0.2325 1.0000 Uiso . . . . . .
H991 H 0.4169 0.1469 1.0227 0.2350 1.0000 Uiso . . . . . .
H992 H 0.3996 0.1162 0.9639 0.2350 1.0000 Uiso . . . . . .
H1001 H 0.2354 0.1494 1.0340 0.2368 1.0000 Uiso . . . . . .
H1002 H 0.2078 0.1447 0.9730 0.2368 1.0000 Uiso . . . . . .
H1011 H 0.1852 0.0055 1.0105 0.2376 1.0000 Uiso . . . . . .
H1012 H 0.3056 0.0069 1.0323 0.2376 1.0000 Uiso . . . . . .
H1013 H 0.2780 0.0022 0.9713 0.2376 1.0000 Uiso . . . . . .
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H861 H 0.5373 0.1978 0.9030 0.2280 1.0000 Uiso . . . . . .
H862 H 0.4214 0.2279 0.8839 0.2280 1.0000 Uiso . . . . . .
H8701 H 0.3271 0.2447 0.8788 0.2262 0.4821 Uiso . . . . . .
H8702 H 0.3877 0.3206 0.8520 0.2262 0.4821 Uiso . . . . . .
H8801 H 0.3977 0.1435 0.8238 0.2251 0.4821 Uiso . . . . . .
H8802 H 0.4795 0.2110 0.8030 0.2251 0.4821 Uiso . . . . . .
H8901 H 0.3324 0.1971 0.7414 0.2247 0.4821 Uiso . . . . . .
H8902 H 0.2545 0.2242 0.7850 0.2247 0.4821 Uiso . . . . . .
H8903 H 0.3363 0.2918 0.7642 0.2247 0.4821 Uiso . . . . . .
H8711 H 0.5976 0.3405 0.8851 0.2264 0.5179 Uiso . . . . . .
H8712 H 0.4836 0.3587 0.8580 0.2264 0.5179 Uiso . . . . . .
H8811 H 0.5325 0.2148 0.8139 0.2248 0.5179 Uiso . . . . . .
H8812 H 0.5517 0.3051 0.7874 0.2248 0.5179 Uiso . . . . . .
H8911 H 0.7139 0.2272 0.7943 0.2234 0.5179 Uiso . . . . . .
H8912 H 0.7048 0.2209 0.8556 0.2234 0.5179 Uiso . . . . . .
H8913 H 0.7241 0.3112 0.8292 0.2234 0.5179 Uiso . . . . . .
H1901 H -0.1089 0.9661 0.6456 0.0554 1.0000 Uiso . . . 4 1 .
H1902 H -0.0359 0.8989 0.6180 0.0554 1.0000 Uiso . . . 4 1 .
H1903 H -0.1980 1.0001 0.5701 0.0733 0.5293 Uiso . . . 4 1 .
H1904 H -0.0814 0.9871 0.5512 0.0733 0.5293 Uiso . . . 4 1 .
H1905 H -0.2290 0.9005 0.5092 0.0810 1.0000 Uiso . . . 4 1 .
H1906 H -0.1172 0.8559 0.5213 0.0810 1.0000 Uiso . . . 4 1 .
H291 H -0.0453 0.9597 0.5506 0.0678 0.4707 Uiso . . . 4 2 .
H292 H -0.0237 0.8617 0.5642 0.0678 0.4707 Uiso . . . 4 2 .
H391 H 0.1098 0.6015 0.9726 0.0663 0.3920 Uiso . . . 2 2 .
H392 H -0.0114 0.5736 0.9683 0.0663 0.3920 Uiso . . . 2 2 .
H491 H 0.0682 0.6715 0.9359 0.0593 1.0000 Uiso . . . . . .
H492 H -0.0251 0.6797 0.8921 0.0593 1.0000 Uiso . . . . . .
H493 H -0.0362 0.5614 0.9564 0.0678 0.6080 Uiso . . . . . .
H494 H -0.0664 0.5402 0.8970 0.0678 0.6080 Uiso . . . . . .
H495 H 0.1281 0.5084 0.9515 0.0754 1.0000 Uiso . . . . . .
H496 H 0.0595 0.4426 0.9166 0.0754 1.0000 Uiso . . . . . .
H591 H -0.0890 0.8485 0.9401 0.0665 1.0000 Uiso . . . . . .
H592 H -0.0088 0.8456 0.8946 0.0665 1.0000 Uiso . . . . . .
H593 H 0.0141 0.9562 0.9649 0.0686 0.6598 Uiso . . . . . .
H594 H 0.0400 0.9798 0.9068 0.0686 0.6598 Uiso . . . . . .
H595 H -0.1392 1.0247 0.9591 0.0696 1.0000 Uiso . . . . . .
H596 H -0.0774 1.0811 0.9192 0.0696 1.0000 Uiso . . . . . .
H691 H -0.0069 0.9478 0.9743 0.0677 0.3402 Uiso . . . 3 2 .
H692 H -0.1290 0.9239 0.9759 0.0677 0.3402 Uiso . . . 3 2 .
H7901 H 0.0455 0.4124 0.6555 0.1496 0.6508 Uiso . . . 5 1 .
H7902 H 0.0458 0.3318 0.6177 0.1496 0.6508 Uiso . . . 5 1 .
H7903 H -0.2114 0.3499 0.6371 0.1727 0.6508 Uiso . . . 5 1 .
H7904 H -0.2342 0.3852 0.5796 0.1727 0.6508 Uiso . . . 5 1 .
H7905 H -0.1113 0.4539 0.6266 0.1556 0.6508 Uiso . . . 5 1 .
H7906 H 0.0313 0.4526 0.7912 0.0997 1.0000 Uiso . . . 5 1 .
H7907 H -0.1178 0.6732 0.5715 0.0999 1.0000 Uiso . . . 5 1 .
H8921 H -0.0086 0.4145 0.6280 0.1531 0.3492 Uiso . . . 5 2 .
H8922 H -0.0375 0.3333 0.5927 0.1531 0.3492 Uiso . . . 5 2 .
H8923 H -0.2432 0.3733 0.6321 0.1480 0.3492 Uiso . . . 5 2 .
H8924 H -0.2991 0.4412 0.5936 0.1480 0.3492 Uiso . . . 5 2 .
H8925 H -0.0923 0.4308 0.5606 0.1417 0.3492 Uiso . . . 5 2 .
loop_
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_atom_site_aniso_U_12
N1 0.049(6) 0.031(6) 0.053(6) 0.010(5) 0.003(5) 0.003(5)
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N3 0.050(6) 0.035(6) 0.052(6) -0.001(5) 0.019(5) 0.001(5)
N4 0.046(6) 0.040(6) 0.044(6) -0.023(5) 0.005(5) -0.004(5)
N6 0.042(6) 0.060(7) 0.025(5) 0.008(5) -0.007(4) -0.002(5)
N7 0.064(7) 0.045(6) 0.022(5) 0.007(5) 0.003(5) -0.005(6)
N9 0.047(6) 0.049(7) 0.039(6) 0.019(5) -0.012(5) -0.012(5)
N10 0.049(6) 0.041(6) 0.032(5) -0.002(5) 0.005(5) -0.004(5)
N12 0.030(6) 0.056(7) 0.051(6) -0.005(6) 0.002(5) -0.021(5)
N13 0.048(6) 0.025(5) 0.063(7) -0.006(5) 0.003(5) -0.004(5)
N15 0.040(6) 0.036(6) 0.046(6) 0.009(5) -0.012(5) -0.001(5)
N16 0.056(7) 0.043(6) 0.038(6) 0.025(5) 0.017(5) 0.005(5)
N18 0.045(6) 0.039(6) 0.042(6) 0.009(5) 0.001(5) 0.012(5)
O5 0.041(5) 0.065(6) 0.041(5) -0.002(5) -0.012(4) 0.012(5)
O6 0.077(8) 0.087(8) 0.092(8) 0.040(7) -0.013(6) -0.031(7)
O7 0.072(7) 0.042(6) 0.077(7) 0.018(5) 0.020(5) 0.000(5)
O8 0.058(6) 0.046(5) 0.054(5) -0.008(5) 0.012(5) 0.006(5)
O10 0.096(7) 0.071(7) 0.033(5) -0.007(5) -0.013(5) -0.038(6)
O11 0.082(7) 0.040(6) 0.054(6) -0.010(5) 0.001(5) 0.017(5)
O12 0.079(7) 0.083(8) 0.043(6) 0.013(5) 0.009(5) -0.014(6)
O13 0.043(5) 0.042(5) 0.066(6) -0.011(4) -0.002(4) -0.007(4)
O14 0.131(10) 0.041(6) 0.053(6) -0.025(5) -0.025(6) 0.004(6)
O15 0.046(6) 0.046(6) 0.068(6) 0.011(5) -0.008(5) 0.006(4)
O16 0.095(8) 0.030(5) 0.064(6) 0.014(5) 0.008(5) 0.010(5)
O17 0.060(6) 0.056(6) 0.053(5) -0.003(5) 0.011(5) 0.005(5)
C1 0.058(9) 0.027(7) 0.059(9) -0.003(6) 0.008(7) 0.005(6)
N2 0.062(4) 0.033(4) 0.036(4) 0.000(3) 0.012(3) 0.001(4)
C2 0.040(5) 0.058(5) 0.040(5) 0.014(4) 0.011(4) -0.008(4)
C3 0.064(7) 0.044(5) 0.073(6) -0.001(5) -0.006(5) 0.017(5)
C4 0.032(5) 0.087(8) 0.115(7) -0.024(6) -0.002(5) 0.016(5)
C5 0.056(6) 0.034(6) 0.087(7) -0.003(5) -0.010(5) -0.007(5)
C6 0.054(6) 0.038(5) 0.032(5) -0.003(4) 0.005(4) 0.008(5)
C7 0.050(8) 0.029(7) 0.038(7) 0.003(6) -0.002(6) 0.009(6)
C8 0.038(7) 0.038(7) 0.048(7) 0.005(6) 0.008(6) 0.007(6)
C9 0.042(7) 0.069(8) 0.055(7) -0.004(6) -0.014(6) -0.001(6)
C11 0.054(8) 0.057(8) 0.063(8) -0.021(7) -0.008(7) -0.003(6)
C12 0.043(8) 0.038(8) 0.044(7) 0.003(6) 0.010(6) 0.001(6)
N5 0.047(4) 0.038(4) 0.029(4) -0.002(3) -0.001(3) 0.011(4)
C13 0.036(5) 0.033(5) 0.055(5) 0.004(4) -0.005(4) 0.002(4)
C14 0.074(7) 0.036(5) 0.055(6) 0.000(5) 0.016(5) 0.005(5)
C15 0.020(5) 0.070(8) 0.062(7) -0.002(6) -0.001(5) 0.003(5)
C16 0.027(6) 0.075(6) 0.059(7) -0.013(5) -0.009(5) 0.007(5)
C17 0.051(6) 0.049(5) 0.037(5) -0.005(4) -0.002(4) -0.002(5)
C18 0.045(8) 0.029(6) 0.032(6) 0.000(5) -0.001(6) 0.004(6)
C19 0.038(7) 0.036(6) 0.027(6) -0.002(5) -0.007(5) -0.014(5)
C20 0.036(7) 0.063(8) 0.040(6) 0.000(6) -0.009(5) -0.010(6)
C22 0.068(8) 0.079(10) 0.056(8) 0.019(7) -0.001(7) -0.018(8)
C23 0.051(8) 0.060(9) 0.040(8) 0.002(7) -0.006(6) -0.010(8)
N8 0.046(4) 0.036(4) 0.033(4) 0.007(3) 0.000(3) -0.003(4)
C24 0.056(5) 0.043(5) 0.029(5) -0.013(4) 0.008(4) -0.001(5)
C25 0.031(6) 0.059(6) 0.044(6) 0.005(6) 0.010(5) 0.014(5)
C26 0.055(6) 0.135(9) 0.079(8) -0.004(8) 0.011(6) -0.038(6)
C27 0.047(6) 0.116(8) 0.046(7) 0.023(6) -0.010(5) -0.040(6)
C28 0.037(5) 0.055(5) 0.054(5) -0.007(5) 0.007(4) -0.002(4)
C29 0.070(10) 0.037(8) 0.054(8) -0.006(7) 0.007(7) -0.023(8)
C30 0.045(8) 0.057(9) 0.046(7) 0.016(7) 0.004(6) -0.005(7)
C31 0.067(9) 0.050(9) 0.062(9) -0.006(7) 0.009(7) 0.009(8)
C32 0.078(9) 0.058(8) 0.113(11) 0.004(8) 0.037(8) 0.002(7)
C33 0.065(10) 0.050(9) 0.064(9) 0.016(7) 0.014(7) 0.013(8)
C36 0.082(9) 0.106(10) 0.062(8) 0.015(8) -0.026(7) -0.031(8)
C37 0.064(9) 0.056(8) 0.035(7) -0.003(6) 0.002(6) -0.006(7)
C38 0.058(8) 0.037(7) 0.039(7) 0.004(6) 0.010(6) 0.004(7)
N11 0.049(4) 0.042(4) 0.026(4) -0.001(3) 0.000(3) 0.003(4)

C39 0.040(5) 0.048(5) 0.046(5) 0.012(4) −0.004(4) 0.001(5)
C40 0.088(6) 0.064(6) 0.094(6) −0.029(6) 0.017(5) −0.009(5)
C41 0.048(6) 0.072(9) 0.100(8) −0.035(8) 0.005(6) 0.013(6)
C42 0.039(6) 0.063(8) 0.121(7) −0.029(6) 0.001(5) −0.011(6)
C43 0.040(5) 0.039(5) 0.046(5) 0.000(5) −0.002(4) −0.004(4)
C44 0.047(8) 0.051(9) 0.054(8) 0.000(7) 0.002(6) −0.013(7)
C45 0.040(7) 0.040(7) 0.036(6) 0.001(6) −0.002(5) 0.009(6)
C46 0.058(9) 0.072(10) 0.056(9) 0.013(8) 0.011(7) 0.019(8)
C47 0.063(10) 0.068(10) 0.079(11) 0.022(9) 0.015(9) 0.025(9)
C48 0.061(10) 0.048(9) 0.083(11) 0.007(8) 0.016(8) 0.013(8)
C49 0.063(9) 0.049(9) 0.035(7) −0.012(7) −0.008(7) 0.008(7)
N14 0.045(4) 0.035(4) 0.035(4) −0.002(3) −0.005(3) 0.005(3)
C50 0.061(5) 0.032(5) 0.036(5) 0.005(4) −0.029(4) 0.001(4)
C51 0.076(6) 0.062(7) 0.037(6) 0.017(5) −0.002(5) 0.022(5)
C52 0.042(6) 0.038(7) 0.076(7) 0.003(6) −0.013(5) 0.001(5)
C53 0.041(6) 0.063(8) 0.071(7) 0.016(6) 0.006(5) 0.009(6)
C54 0.054(6) 0.046(6) 0.041(5) 0.010(4) −0.010(4) 0.024(5)
C55 0.042(8) 0.055(9) 0.038(7) −0.005(7) 0.010(6) 0.008(7)
C56 0.053(8) 0.034(7) 0.040(7) −0.001(6) 0.004(6) −0.006(6)
C57 0.027(6) 0.068(8) 0.053(7) 0.011(6) 0.009(5) 0.002(6)
C59 0.078(9) 0.066(8) 0.045(7) 0.006(6) 0.015(7) −0.007(7)
C60 0.059(9) 0.040(8) 0.033(7) 0.009(6) −0.003(6) 0.007(7)
N17 0.048(4) 0.030(4) 0.053(4) −0.003(3) 0.021(3) −0.010(3)
C61 0.034(5) 0.039(5) 0.049(5) 0.010(4) 0.009(4) 0.010(4)
C62 0.037(6) 0.057(7) 0.079(6) 0.009(5) 0.006(5) 0.003(5)
C63 0.065(6) 0.098(7) 0.083(7) 0.015(6) 0.032(5) 0.020(5)
C64 0.039(6) 0.095(8) 0.085(7) 0.036(6) −0.003(5) 0.029(6)
C65 0.060(6) 0.048(6) 0.044(5) −0.004(4) 0.026(4) −0.001(5)
C66 0.051(8) 0.038(8) 0.044(8) −0.009(6) 0.016(7) −0.002(6)
C67 0.042(7) 0.040(7) 0.028(6) 0.004(5) 0.001(5) −0.007(6)
C68 0.073(10) 0.055(9) 0.051(8) −0.009(7) 0.010(7) −0.018(8)
S100 0.0313 0.0373 0.0350 0.0015 0.0028 0.0029
O100 0.0422 0.0425 0.0375 −0.0041 0.0011 −0.0012
O200 0.0274 0.0489 0.0411 0.0088 −0.0148 −0.0154
O300 0.0313 0.0446 0.0639 −0.0080 −0.0085 0.0012
O400 0.0402 0.0530 0.0592 −0.0044 0.0116 0.0168
S101 0.0343 0.0426 0.0327 0.0041 −0.0021 0.0015
O101 0.0473 0.0519 0.0408 0.0090 0.0089 −0.0012
O201 0.0293 0.0487 0.0410 0.0036 −0.0097 0.0109
O301 0.0401 0.0584 0.0587 −0.0069 0.0106 0.0130
O401 0.0375 0.0410 0.0575 0.0055 −0.0046 −0.0156
S200 0.073(5) 0.062(4) 0.122(7) 0.003(4) 0.026(4) 0.009(4)
S300 0.127(8) 0.073(5) 0.100(6) −0.014(5) 0.046(5) −0.017(5)
C340 0.164(15) 0.100(13) 0.110(12) 0.008(10) 0.034(11) −0.030(13)
C350 0.172(14) 0.111(13) 0.106(11) 0.022(11) 0.026(10) −0.043(12)
C360 0.190(18) 0.132(16) 0.110(15) 0.018(14) 0.019(15) −0.063(15)
O500 0.23(2) 0.131(16) 0.117(16) 0.008(15) −0.005(16) −0.075(18)
S400 0.151(9) 0.097(7) 0.101(7) 0.003(6) 0.031(6) −0.044(6)
S500 0.113(8) 0.116(8) 0.077(5) 0.010(7) −0.026(6) −0.048(6)
S201 0.152(15) 0.083(10) 0.146(13) −0.024(9) 0.045(11) 0.011(11)
S301 0.194(17) 0.080(10) 0.142(13) −0.024(10) 0.035(12) −0.019(12)
C341 0.163(19) 0.085(16) 0.136(16) −0.017(13) 0.015(15) −0.015(15)
C351 0.146(17) 0.087(15) 0.122(14) −0.029(12) 0.021(13) −0.015(14)
C361 0.14(2) 0.100(19) 0.13(2) −0.039(16) 0.047(18) −0.001(17)
O501 0.13(2) 0.11(2) 0.13(2) −0.048(17) 0.070(19) −0.010(18)
S401 0.120(11) 0.060(8) 0.094(10) −0.027(8) −0.019(8) −0.013(7)
S501 0.075(9) 0.070(9) 0.092(9) −0.007(8) −0.027(7) −0.009(6)
C580 0.051(13) 0.065(12) 0.050(12) 0.008(10) 0.019(11) −0.003(11)
C581 0.045(10) 0.081(11) 0.043(10) −0.002(9) 0.000(9) −0.015(9)
C110 0.041(10) 0.065(10) 0.065(11) −0.013(9) −0.003(9) −0.004(8)
C111 0.038(13) 0.067(12) 0.065(13) −0.011(10) −0.012(12) 0.005(12)

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C21 0.063(12) 0.066(12) 0.054(10) 0.019(9) 0.000(10) -0.002(11)
C210 0.052(12) 0.071(13) 0.047(10) 0.019(11) -0.004(9) -0.011(11)
_refine_ls_extinction_method
    'None'
loop_
 _geom_bond_atom_site_label_1
 _geom_bond_site_symmetry_1
 _geom_bond_atom_site_label_2
 _geom_bond_site_symmetry_2
 _geom_bond_distance
 _geom_bond_publ_flag
N1 . C1 . 1.333(18)    yes
N1 . C30 . 1.437(17)    yes
N1 . C33 . 1.462(18)    yes
N3 . C6 . 1.389(14)    yes
N3 . C7 . 1.314(17)    yes
N3 . H1 . 0.894    no
N4 . C8 . 1.442(17)    yes
N4 . C11 . 1.522(17)    yes
N4 . C12 . 1.359(17)    yes
N6 . C17 . 1.401(14)    yes
N6 . C18 . 1.423(15)    yes
N6 . H2 . 0.909    no
N7 . C19 . 1.477(14)    yes
N7 . C22 . 1.462(18)    yes
N7 . C23 . 1.361(17)    yes
N9 . C28 . 1.391(13)    yes
N9 . C29 . 1.353(17)    yes
N9 . H3 . 0.892    no
N10 . C37 . 1.437(17)    yes
N10 . C38 . 1.346(17)    yes
N10 . C67 . 1.492(15)    yes
N12 . C43 . 1.409(14)    yes
N12 . C44 . 1.306(18)    yes
N12 . H4 . 0.901    no
N13 . C45 . 1.459(17)    yes
N13 . C48 . 1.473(18)    yes
N13 . C49 . 1.365(17)    yes
N15 . C54 . 1.361(14)    yes
N15 . C55 . 1.340(18)    yes
N15 . H5 . 0.905    no
N16 . C56 . 1.451(17)    yes
N16 . C59 . 1.457(17)    yes
N16 . C60 . 1.361(17)    yes
N18 . C65 . 1.345(13)    yes
N18 . C66 . 1.347(17)    yes
N18 . H6 . 0.896    no
O5 . C18 . 1.167(14)    yes
O6 . C29 . 1.206(17)    yes
O7 . C1 . 1.259(16)    yes
O8 . C7 . 1.239(15)    yes
O10 . C23 . 1.254(15)    yes
O11 . C12 . 1.243(16)    yes
O12 . C38 . 1.220(15)    yes
O13 . C44 . 1.260(16)    yes
O14 . C49 . 1.234(16)    yes
O15 . C55 . 1.201(15)    yes
O16 . C60 . 1.203(16)    yes
O17 . C66 . 1.213(15)    yes
C1 . C2 . 1.505(16)    yes
N2 . C2 . 1.335(12)    yes
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N2 . C6 . 1.293(11) yes
C2 . C3 . 1.357(14) yes
C3 . C4 . 1.429(15) yes
C3 . H31 . 1.000 no
C4 . C5 . 1.341(15) yes
C4 . H41 . 1.000 no
C5 . C6 . 1.404(13) yes
C5 . H51 . 1.000 no
C7 . C8 . 1.490(19) yes
C8 . C9 . 1.554(18) yes
C8 . H81 . 1.000 no
C9 . C110 . 1.512(16) yes
C9 . H591 . 1.000 no
C9 . H592 . 1.000 no
C11 . C110 . 1.501(16) yes
C11 . H595 . 1.000 no
C11 . H596 . 1.000 no
C12 . C13 . 1.457(17) yes
N5 . C13 . 1.380(12) yes
N5 . C17 . 1.361(11) yes
C13 . C14 . 1.375(14) yes
C14 . C15 . 1.370(15) yes
C14 . H141 . 1.000 no
C15 . C16 . 1.362(15) yes
C15 . H151 . 1.000 no
C16 . C17 . 1.368(13) yes
C16 . H161 . 1.000 no
C18 . C19 . 1.541(17) yes
C19 . C20 . 1.555(17) yes
C19 . H191 . 1.000 no
C20 . C21 . 1.517(17) yes
C20 . H1901 . 1.000 no
C20 . H1902 . 1.000 no
C22 . C21 . 1.508(17) yes
C22 . H1905 . 1.000 no
C22 . H1906 . 1.000 no
C23 . C24 . 1.435(17) yes
N8 . C24 . 1.331(11) yes
N8 . C28 . 1.333(12) yes
C24 . C25 . 1.431(14) yes
C25 . C26 . 1.357(18) yes
C25 . H251 . 1.000 no
C26 . C27 . 1.402(18) yes
C26 . H261 . 1.000 no
C27 . C28 . 1.415(13) yes
C27 . H271 . 1.000 no
C29 . C30 . 1.50(2) yes
C30 . C31 . 1.53(2) yes
C30 . H301 . 1.000 no
C31 . C32 . 1.49(2) yes
C31 . H311 . 1.000 no
C31 . H312 . 1.000 no
C32 . C33 . 1.53(2) yes
C32 . S200 . 1.786(14) yes
C32 . H7906 . 1.000 no
C33 . H331 . 1.000 no
C33 . H332 . 1.000 no
C36 . C37 . 1.53(2) yes
C36 . C68 . 1.43(2) yes
C36 . S500 . 1.822(15) yes
C36 . H7907 . 1.000 no

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C37 . H371 . 1.000    no
C37 . H372 . 1.000    no
C38 . C39 . 1.522(16)    yes
N11 . C39 . 1.317(11)    yes
N11 . C43 . 1.308(11)    yes
C39 . C40 . 1.404(13)    yes
C40 . C41 . 1.364(16)    yes
C40 . H401 . 1.000    no
C41 . C42 . 1.469(17)    yes
C41 . H411 . 1.000    no
C42 . C43 . 1.416(13)    yes
C42 . H421 . 1.000    no
C44 . C45 . 1.496(19)    yes
C45 . C46 . 1.527(19)    yes
C45 . H451 . 1.000    no
C46 . C47 . 1.54(2)    yes
C46 . H461 . 1.000    no
C46 . H462 . 1.000    no
C47 . C48 . 1.43(2)    yes
C47 . H471 . 1.000    no
C47 . H472 . 1.000    no
C48 . H481 . 1.000    no
C48 . H482 . 1.000    no
C49 . C50 . 1.477(17)    yes
N14 . C50 . 1.369(12)    yes
N14 . C54 . 1.342(12)    yes
C50 . C51 . 1.411(13)    yes
C51 . C52 . 1.412(15)    yes
C51 . H511 . 1.000    no
C52 . C53 . 1.381(17)    yes
C52 . H521 . 1.000    no
C53 . C54 . 1.386(14)    yes
C53 . H531 . 1.000    no
C55 . C56 . 1.552(19)    yes
C56 . C57 . 1.523(18)    yes
C56 . H561 . 1.000    no
C57 . C581 . 1.514(16)    yes
C57 . H491 . 1.000    no
C57 . H492 . 1.000    no
C59 . C581 . 1.491(16)    yes
C59 . H495 . 1.000    no
C59 . H496 . 1.000    no
C60 . C61 . 1.482(16)    yes
N17 . C61 . 1.412(11)    yes
N17 . C65 . 1.332(11)    yes
C61 . C62 . 1.338(14)    yes
C62 . C63 . 1.435(15)    yes
C62 . H621 . 1.000    no
C63 . C64 . 1.274(15)    yes
C63 . H631 . 1.000    no
C64 . C65 . 1.444(14)    yes
C64 . H641 . 1.000    no
C66 . C67 . 1.489(19)    yes
C67 . C68 . 1.558(19)    yes
C67 . H671 . 1.000    no
C68 . H681 . 1.000    no
C68 . H682 . 1.000    no
S100 . O100 . 1.45179(10)    yes
S100 . O200 . 1.43345(14)    yes
S100 . O300 . 1.42782(11)    yes
S100 . O400 . 1.41719(13)    yes
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S101 . O101 . 1.44198(9)    yes
S101 . O201 . 1.44275(12)    yes
S101 . O301 . 1.43374(11)    yes
S101 . O401 . 1.42264(15)    yes
S200 . S300 . 2.005(12)    yes
S300 . C340 . 1.802(17)    yes
C340 . C350 . 1.555(19)    yes
C340 . H7901 . 1.000    no
C340 . H7902 . 1.000    no
C340 . H8921 . 0.860    no
C350 . C360 . 1.471(19)    yes
C350 . S400 . 1.826(18)    yes
C350 . H7905 . 1.000    no
C360 . O500 . 1.397(19)    yes
C360 . H7903 . 1.000    no
C360 . H7904 . 1.000    no
S400 . S500 . 2.066(14)    yes
S201 . S301 . 2.021(18)    yes
S301 . C341 . 1.807(19)    yes
C341 . C351 . 1.558(19)    yes
C341 . H8921 . 1.000    no
C341 . H8922 . 1.000    no
C351 . C361 . 1.462(19)    yes
C351 . S401 . 1.814(19)    yes
C351 . H8925 . 1.000    no
C361 . O501 . 1.384(19)    yes
C361 . H8923 . 1.000    no
C361 . H8924 . 1.000    no
S401 . S501 . 2.031(15)    yes
S401 . H8925 . 1.050    no
N19 . C70 . 1.559(12)    yes
N19 . C74 . 1.538(10)    yes
N19 . C78 . 1.501(8)    yes
N19 . C82 . 1.560(14)    yes
C70 . C71 . 1.555(12)    yes
C70 . H701 . 1.000    no
C70 . H702 . 1.000    no
C71 . C72 . 1.602(12)    yes
C71 . H711 . 1.000    no
C71 . H712 . 1.000    no
C72 . C73 . 1.605(16)    yes
C72 . H721 . 1.000    no
C72 . H722 . 1.000    no
C73 . H731 . 1.000    no
C73 . H732 . 1.000    no
C73 . H733 . 1.000    no
C74 . C75 . 1.581(13)    yes
C74 . H741 . 1.000    no
C74 . H742 . 1.000    no
C75 . C76 . 1.594(13)    yes
C75 . H751 . 1.000    no
C75 . H752 . 1.000    no
C76 . C77 . 1.542(10)    yes
C76 . H761 . 1.000    no
C76 . H762 . 1.000    no
C77 . H771 . 1.000    no
C77 . H772 . 1.000    no
C77 . H773 . 1.000    no
C78 . C79 . 1.551(13)    yes
C78 . H781 . 1.000    no
C78 . H782 . 1.000    no
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C79 . C80 . 1.579(10)    yes
C79 . H791 . 1.000    no
C79 . H792 . 1.000    no
C80 . C81 . 1.564(14)    yes
C80 . H801 . 1.000    no
C80 . H802 . 1.000    no
C81 . H811 . 1.000    no
C81 . H812 . 1.000    no
C81 . H813 . 1.000    no
C82 . C83 . 1.565(16)    yes
C82 . H821 . 1.000    no
C82 . H822 . 1.000    no
C83 . C84 . 1.600(16)    yes
C83 . H831 . 1.000    no
C83 . H832 . 1.000    no
C84 . C85 . 1.557(17)    yes
C84 . H841 . 1.000    no
C84 . H842 . 1.000    no
C85 . H851 . 1.000    no
C85 . H852 . 1.000    no
C85 . H853 . 1.000    no
N20 . C90 . 1.538(13)    yes
N20 . C94 . 1.589(13)    yes
N20 . C98 . 1.564(12)    yes
N20 . C86 . 1.523(17)    yes
C90 . C91 . 1.548(13)    yes
C90 . H901 . 1.000    no
C90 . H902 . 1.000    no
C91 . C92 . 1.572(11)    yes
C91 . H911 . 1.000    no
C91 . H912 . 1.000    no
C92 . C93 . 1.628(15)    yes
C92 . H921 . 1.000    no
C92 . H922 . 1.000    no
C93 . H931 . 1.000    no
C93 . H932 . 1.000    no
C93 . H933 . 1.000    no
C94 . C95 . 1.596(13)    yes
C94 . H941 . 1.000    no
C94 . H942 . 1.000    no
C95 . C96 . 1.599(11)    yes
C95 . H951 . 1.000    no
C95 . H952 . 1.000    no
C96 . C97 . 1.576(16)    yes
C96 . H961 . 1.000    no
C96 . H962 . 1.000    no
C97 . H971 . 1.000    no
C97 . H972 . 1.000    no
C97 . H973 . 1.000    no
C98 . C99 . 1.589(11)    yes
C98 . H981 . 1.000    no
C98 . H982 . 1.000    no
C99 . C100 . 1.594(10)    yes
C99 . H991 . 1.000    no
C99 . H992 . 1.000    no
C100 . C101 . 1.598(15)    yes
C100 . H1001 . 1.000    no
C100 . H1002 . 1.000    no
C101 . H1011 . 1.000    no
C101 . H1012 . 1.000    no
C101 . H1013 . 1.000    no
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C86 . C871 . 1.556(19)    yes
C86 . H861 . 1.000    no
C86 . H862 . 1.000    no
C870 . C880 . 1.582(19)    yes
C870 . H8701 . 1.000    no
C870 . H8702 . 1.000    no
C880 . C890 . 1.578(19)    yes
C880 . H8801 . 1.000    no
C880 . H8802 . 1.000    no
C890 . H8901 . 1.000    no
C890 . H8902 . 1.000    no
C890 . H8903 . 1.000    no
C871 . C881 . 1.560(19)    yes
C871 . H8711 . 1.000    no
C871 . H8712 . 1.000    no
C881 . C891 . 1.574(19)    yes
C881 . H8811 . 1.000    no
C881 . H8812 . 1.000    no
C891 . H8911 . 1.000    no
C891 . H8912 . 1.000    no
C891 . H8913 . 1.000    no
C580 . H391 . 1.000    no
C580 . H392 . 1.000    no
C581 . H493 . 1.000    no
C581 . H494 . 1.000    no
C110 . H593 . 1.000    no
C110 . H594 . 1.000    no
C111 . H691 . 1.000    no
C111 . H692 . 1.000    no
C21 . H1903 . 1.000    no
C21 . H1904 . 1.000    no
C210 . H291 . 1.000    no
C210 . H292 . 1.000    no

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C1 . N1 . C33 . 120.7(11)    yes
C30 . N1 . C33 . 112.2(11)    yes
C6 . N3 . C7 . 129.9(10)    yes
C6 . N3 . H1 . 114.221    no
C7 . N3 . H1 . 115.890    no
C8 . N4 . C11 . 114.6(10)    yes
C8 . N4 . C12 . 125.7(10)    yes
C11 . N4 . C12 . 119.6(10)    yes
C17 . N6 . C18 . 123.9(10)    yes
C17 . N6 . H2 . 115.526    no
C18 . N6 . H2 . 120.165    no
C19 . N7 . C22 . 110.8(10)    yes
C19 . N7 . C23 . 127.5(10)    yes
C22 . N7 . C23 . 121.1(10)    yes
C28 . N9 . C29 . 129.2(11)    yes
C28 . N9 . H3 . 115.330    no
C29 . N9 . H3 . 114.968    no
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C37 . N10 . C38 . 123.1(10)    yes
C37 . N10 . C67 . 112.2(10)    yes
C38 . N10 . C67 . 124.1(10)    yes
C43 . N12 . C44 . 128.7(10)    yes
C43 . N12 . H4 . 114.891    no
C44 . N12 . H4 . 116.369    no
C45 . N13 . C48 . 111.9(11)    yes
C45 . N13 . C49 . 128.0(10)    yes
C48 . N13 . C49 . 119.6(12)    yes
C54 . N15 . C55 . 124.8(10)    yes
C54 . N15 . H5 . 121.035    no
C55 . N15 . H5 . 114.019    no
C56 . N16 . C59 . 112.5(10)    yes
C56 . N16 . C60 . 127.8(10)    yes
C59 . N16 . C60 . 118.6(10)    yes
C65 . N18 . C66 . 128.7(10)    yes
C65 . N18 . H6 . 114.573    no
C66 . N18 . H6 . 114.583    no
N1 . C1 . O7 . 121.8(12)    yes
N1 . C1 . C2 . 117.4(11)    yes
O7 . C1 . C2 . 120.7(12)    yes
C2 . N2 . C6 . 119.5(8)    yes
C1 . C2 . N2 . 119.4(9)    yes
C1 . C2 . C3 . 118.2(9)    yes
N2 . C2 . C3 . 122.0(9)    yes
C2 . C3 . C4 . 117.1(9)    yes
C2 . C3 . H31 . 121.473    no
C4 . C3 . H31 . 121.473    no
C3 . C4 . C5 . 121.0(8)    yes
C3 . C4 . H41 . 119.520    no
C5 . C4 . H41 . 119.520    no
C4 . C5 . C6 . 116.0(9)    yes
C4 . C5 . H51 . 121.980    no
C6 . C5 . H51 . 121.981    no
C5 . C6 . N3 . 121.3(9)    yes
C5 . C6 . N2 . 124.2(9)    yes
N3 . C6 . N2 . 114.5(8)    yes
N3 . C7 . O8 . 124.3(12)    yes
N3 . C7 . C8 . 115.0(11)    yes
O8 . C7 . C8 . 120.7(11)    yes
C7 . C8 . N4 . 115.9(10)    yes
C7 . C8 . C9 . 112.0(10)    yes
N4 . C8 . C9 . 102.1(10)    yes
C7 . C8 . H81 . 101.172    no
N4 . C8 . H81 . 111.176    no
C9 . C8 . H81 . 115.143    no
C8 . C9 . C110 . 106.6(12)    yes
C8 . C9 . H591 . 110.191    no
C110 . C9 . H591 . 110.192    no
C8 . C9 . H592 . 110.191    no
C110 . C9 . H592 . 110.192    no
H591 . C9 . H592 . 109.467    no
N4 . C11 . C110 . 101.0(11)    yes
N4 . C11 . H595 . 111.557    no
C110 . C11 . H595 . 111.557    no
N4 . C11 . H596 . 111.558    no
C110 . C11 . H596 . 111.557    no
H595 . C11 . H596 . 109.467    no
N4 . C12 . O11 . 120.9(12)    yes
N4 . C12 . C13 . 121.2(11)    yes
O11 . C12 . C13 . 117.9(11)    yes
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C13 . N5 . C17 . 116.3(7)  yes
C12 . C13 . N5 . 115.9(8)  yes
C12 . C13 . C14 . 120.7(10)  yes
N5 . C13 . C14 . 122.5(9)  yes
C13 . C14 . C15 . 117.9(9)  yes
C13 . C14 . H141 . 121.025  no
C15 . C14 . H141 . 121.025  no
C14 . C15 . C16 . 120.8(8)  yes
C14 . C15 . H151 . 119.604  no
C16 . C15 . H151 . 119.603  no
C15 . C16 . C17 . 119.0(9)  yes
C15 . C16 . H161 . 120.524  no
C17 . C16 . H161 . 120.524  no
N6 . C17 . C16 . 125.8(8)  yes
N6 . C17 . N5 . 111.2(8)  yes
C16 . C17 . N5 . 122.8(8)  yes
N6 . C18 . O5 . 125.6(11)  yes
N6 . C18 . C19 . 108.1(10)  yes
O5 . C18 . C19 . 126.0(10)  yes
C18 . C19 . N7 . 108.3(9)  yes
C18 . C19 . C20 . 110.0(10)  yes
N7 . C19 . C20 . 103.9(8)  yes
C18 . C19 . H191 . 108.183  no
N7 . C19 . H191 . 113.938  no
C20 . C19 . H191 . 112.347  no
C19 . C20 . C21 . 102.9(12)  yes
C19 . C20 . H1901 . 111.091  no
C21 . C20 . H1901 . 111.093  no
C19 . C20 . H1902 . 111.090  no
C21 . C20 . H1902 . 111.092  no
H1901 . C20 . H1902 . 109.467  no
N7 . C22 . C21 . 104.4(13)  yes
N7 . C22 . H1905 . 110.726  no
C21 . C22 . H1905 . 110.725  no
N7 . C22 . H1906 . 110.726  no
C21 . C22 . H1906 . 110.726  no
H1905 . C22 . H1906 . 109.467  no
N7 . C23 . O10 . 119.2(12)  yes
N7 . C23 . C24 . 120.4(10)  yes
O10 . C23 . C24 . 120.4(12)  yes
C24 . N8 . C28 . 119.6(7)  yes
C23 . C24 . N8 . 119.3(9)  yes
C23 . C24 . C25 . 118.6(9)  yes
N8 . C24 . C25 . 121.6(8)  yes
C24 . C25 . C26 . 119.8(10)  yes
C24 . C25 . H251 . 120.107  no
C26 . C25 . H251 . 120.106  no
C25 . C26 . C27 . 118.1(10)  yes
C25 . C26 . H261 . 120.970  no
C27 . C26 . H261 . 120.970  no
C26 . C27 . C28 . 119.5(10)  yes
C26 . C27 . H271 . 120.241  no
C28 . C27 . H271 . 120.241  no
C27 . C28 . N9 . 124.3(9)  yes
C27 . C28 . N8 . 121.4(9)  yes
N9 . C28 . N8 . 114.3(8)  yes
N9 . C29 . O6 . 122.9(14)  yes
N9 . C29 . C30 . 113.9(11)  yes
O6 . C29 . C30 . 123.2(13)  yes
C29 . C30 . N1 . 111.5(11)  yes
C29 . C30 . C31 . 109.7(12)  yes

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N1 . C30 . C31 . 104.6(11)    yes
C29 . C30 . H301 . 106.487    no
N1 . C30 . H301 . 111.436    no
C31 . C30 . H301 . 113.146    no
C30 . C31 . C32 . 105.6(12)    yes
C30 . C31 . H311 . 110.434    no
C32 . C31 . H311 . 110.434    no
C30 . C31 . H312 . 110.433    no
C32 . C31 . H312 . 110.434    no
H311 . C31 . H312 . 109.467    no
C31 . C32 . C33 . 104.8(12)    yes
C31 . C32 . S200 . 123.4(13)    yes
C33 . C32 . S200 . 117.5(11)    yes
C31 . C32 . H7906 . 106.516    no
C33 . C32 . H7906 . 114.514    no
S200 . C32 . H7906 . 88.896    no
C32 . C33 . N1 . 101.8(11)    yes
C32 . C33 . H331 . 111.363    no
N1 . C33 . H331 . 111.363    no
C32 . C33 . H332 . 111.363    no
N1 . C33 . H332 . 111.363    no
H331 . C33 . H332 . 109.467    no
C37 . C36 . C68 . 106.0(12)    yes
C37 . C36 . S500 . 115.4(13)    yes
C68 . C36 . S500 . 116.0(13)    yes
C37 . C36 . H7907 . 110.440    no
C68 . C36 . H7907 . 109.746    no
S500 . C36 . H7907 . 99.073    no
C36 . C37 . N10 . 102.9(10)    yes
C36 . C37 . H371 . 111.082    no
N10 . C37 . H371 . 111.082    no
C36 . C37 . H372 . 111.082    no
N10 . C37 . H372 . 111.082    no
H371 . C37 . H372 . 109.467    no
N10 . C38 . O12 . 120.3(12)    yes
N10 . C38 . C39 . 117.0(10)    yes
O12 . C38 . C39 . 122.6(12)    yes
C39 . N11 . C43 . 117.3(8)    yes
C38 . C39 . N11 . 117.2(8)    yes
C38 . C39 . C40 . 117.0(9)    yes
N11 . C39 . C40 . 125.4(8)    yes
C39 . C40 . C41 . 119.8(9)    yes
C39 . C40 . H401 . 120.102    no
C41 . C40 . H401 . 120.103    no
C40 . C41 . C42 . 114.8(9)    yes
C40 . C41 . H411 . 122.610    no
C42 . C41 . H411 . 122.610    no
C41 . C42 . C43 . 119.2(9)    yes
C41 . C42 . H421 . 120.411    no
C43 . C42 . H421 . 120.411    no
C42 . C43 . N12 . 122.0(9)    yes
C42 . C43 . N11 . 123.0(9)    yes
N12 . C43 . N11 . 114.9(8)    yes
N12 . C44 . O13 . 123.6(13)    yes
N12 . C44 . C45 . 114.4(11)    yes
O13 . C44 . C45 . 121.9(12)    yes
C44 . C45 . N13 . 112.8(10)    yes
C44 . C45 . C46 . 111.6(11)    yes
N13 . C45 . C46 . 102.8(11)    yes
C44 . C45 . H451 . 103.810    no
N13 . C45 . H451 . 112.450    no
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C46 . C45 . H451 . 113.643    no
C45 . C46 . C47 . 103.7(12)    yes
C45 . C46 . H461 . 110.901    no
C47 . C46 . H461 . 110.902    no
C45 . C46 . H462 . 110.901    no
C47 . C46 . H462 . 110.902    no
H461 . C46 . H462 . 109.467    no
C46 . C47 . C48 . 105.0(12)    yes
C46 . C47 . H471 . 110.574    no
C48 . C47 . H471 . 110.574    no
C46 . C47 . H472 . 110.574    no
C48 . C47 . H472 . 110.574    no
H471 . C47 . H472 . 109.467    no
N13 . C48 . C47 . 103.5(13)    yes
N13 . C48 . H481 . 110.944    no
C47 . C48 . H481 . 110.943    no
N13 . C48 . H482 . 110.944    no
C47 . C48 . H482 . 110.943    no
H481 . C48 . H482 . 109.466    no
N13 . C49 . O14 . 120.7(12)    yes
N13 . C49 . C50 . 118.8(11)    yes
O14 . C49 . C50 . 120.0(12)    yes
C50 . N14 . C54 . 119.9(8)    yes
C49 . C50 . N14 . 117.1(9)    yes
C49 . C50 . C51 . 119.3(9)    yes
N14 . C50 . C51 . 122.8(8)    yes
C50 . C51 . C52 . 114.4(9)    yes
C50 . C51 . H511 . 122.816    no
C52 . C51 . H511 . 122.816    no
C51 . C52 . C53 . 123.1(9)    yes
C51 . C52 . H521 . 118.434    no
C53 . C52 . H521 . 118.433    no
C52 . C53 . C54 . 118.0(10)    yes
C52 . C53 . H531 . 121.018    no
C54 . C53 . H531 . 121.018    no
C53 . C54 . N15 . 125.7(10)    yes
C53 . C54 . N14 . 121.7(10)    yes
N15 . C54 . N14 . 112.5(8)    yes
N15 . C55 . O15 . 127.9(13)    yes
N15 . C55 . C56 . 113.3(11)    yes
O15 . C55 . C56 . 118.5(12)    yes
C55 . C56 . N16 . 114.9(11)    yes
C55 . C56 . C57 . 110.9(10)    yes
N16 . C56 . C57 . 103.5(10)    yes
C55 . C56 . H561 . 102.948    no
N16 . C56 . H561 . 110.430    no
C57 . C56 . H561 . 114.492    no
C56 . C57 . C581 . 103.1(12)    yes
C56 . C57 . H491 . 111.035    no
C581 . C57 . H491 . 111.035    no
C56 . C57 . H492 . 111.036    no
C581 . C57 . H492 . 111.035    no
H491 . C57 . H492 . 109.467    no
N16 . C59 . C581 . 100.2(12)    yes
N16 . C59 . H495 . 111.737    no
C581 . C59 . H495 . 111.737    no
N16 . C59 . H496 . 111.737    no
C581 . C59 . H496 . 111.737    no
H495 . C59 . H496 . 109.467    no
N16 . C60 . O16 . 120.7(12)    yes
N16 . C60 . C61 . 119.1(10)    yes
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O16 . C60 . C61 . 120.1(12)    yes
C61 . N17 . C65 . 118.6(7)    yes
C60 . C61 . N17 . 116.1(8)    yes
C60 . C61 . C62 . 120.4(9)    yes
N17 . C61 . C62 . 122.2(8)    yes
C61 . C62 . C63 . 116.5(9)    yes
C61 . C62 . H621 . 121.737    no
C63 . C62 . H621 . 121.737    no
C62 . C63 . C64 . 121.9(10)    yes
C62 . C63 . H631 . 119.069    no
C64 . C63 . H631 . 119.069    no
C63 . C64 . C65 . 120.4(10)    yes
C63 . C64 . H641 . 119.776    no
C65 . C64 . H641 . 119.776    no
C64 . C65 . N18 . 124.7(9)    yes
C64 . C65 . N17 . 119.0(8)    yes
N18 . C65 . N17 . 115.9(8)    yes
N18 . C66 . O17 . 124.3(13)    yes
N18 . C66 . C67 . 112.6(11)    yes
O17 . C66 . C67 . 122.9(12)    yes
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C66 . C67 . H671 . 104.234    no
C68 . C67 . H671 . 114.408    no
C67 . C68 . C36 . 107.1(12)    yes
C67 . C68 . H681 . 110.066    no
C36 . C68 . H681 . 110.066    no
C67 . C68 . H682 . 110.066    no
C36 . C68 . H682 . 110.067    no
H681 . C68 . H682 . 109.466    no
O100 . S100 . O200 . 112.164(11)    yes
O100 . S100 . O300 . 108.860(9)    yes
O200 . S100 . O300 . 109.850(10)    yes
O100 . S100 . O400 . 108.706(11)    yes
O200 . S100 . O400 . 110.646(8)    yes
O300 . S100 . O400 . 106.431(12)    yes
O101 . S101 . O201 . 110.660(10)    yes
O101 . S101 . O301 . 109.212(9)    yes
O201 . S101 . O301 . 110.421(9)    yes
O101 . S101 . O401 . 108.878(11)    yes
O201 . S101 . O401 . 110.346(11)    yes
O301 . S101 . O401 . 107.243(12)    yes
C32 . S200 . S300 . 101.4(8)    yes
S200 . S300 . C340 . 97.0(14)    yes
S300 . C340 . C350 . 116(2)    yes
S300 . C340 . H7901 . 107.855    no
C350 . C340 . H7901 . 107.859    no
S300 . C340 . H7902 . 107.854    no
C350 . C340 . H7902 . 107.858    no
H7901 . C340 . H7902 . 109.465    no
S300 . C340 . H8921 . 140.990    no
C350 . C340 . H8921 . 46.363    no
H7901 . C340 . H8921 . 63.233    no
H7902 . C340 . H8921 . 110.849    no
C340 . C350 . C360 . 116(3)    yes
C340 . C350 . S400 . 110.1(18)    yes
C360 . C350 . S400 . 114(2)    yes
C340 . C350 . H7905 . 106.025    no
C360 . C350 . H7905 . 100.924    no
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S400 . C350 . H7905 . 108.259 no
C360 . C350 . H8921 . 147.654 no
S400 . C350 . H8921 . 92.480 no
H7905 . C350 . H8921 . 86.428 no
C340 . C350 . H8925 . 130.926 no
C360 . C350 . H8925 . 95.791 no
H7905 . C350 . H8925 . 102.891 no
H8921 . C350 . H8925 . 113.382 no
C350 . C360 . O500 . 114(4) yes
C350 . C360 . H7903 . 108.372 no
O500 . C360 . H7903 . 108.373 no
C350 . C360 . H7904 . 108.371 no
O500 . C360 . H7904 . 108.372 no
H7903 . C360 . H7904 . 109.463 no
C350 . C360 . H8923 . 113.487 no
O500 . C360 . H8923 . 125.144 no
C350 . S400 . S500 . 97.2(16) yes
C36 . S500 . S400 . 107.6(9) yes
S201 . S301 . C341 . 103(3) yes
S201 . S301 . H7903 . 149.010 no
S301 . C341 . C351 . 118(3) yes
S301 . C341 . H8921 . 107.388 no
C351 . C341 . H8921 . 107.392 no
S301 . C341 . H8922 . 107.391 no
C351 . C341 . H8922 . 107.393 no
H8921 . C341 . H8922 . 109.467 no
C341 . C351 . C361 . 107(5) yes
C341 . C351 . S401 . 110(3) yes
C361 . C351 . S401 . 134(5) yes
C341 . C351 . H7904 . 109.691 no
C361 . C351 . H7905 . 104.551 no
H7905 . C351 . H8925 . 107.785 no
C351 . C361 . H8923 . 107.095 no
O501 . C361 . H8923 . 107.093 no
C351 . C361 . H8924 . 107.094 no
O501 . C361 . H8924 . 107.089 no
H8923 . C361 . H8924 . 109.465 no
S501 . S401 . H8925 . 114.116 no
C70 . N19 . C74 . 114.4(7) yes
C70 . N19 . C78 . 102.1(5) yes
C74 . N19 . C78 . 114.4(6) yes
C70 . N19 . C82 . 107.3(10) yes
C74 . N19 . C82 . 103.1(6) yes
C78 . N19 . C82 . 115.8(10) yes
N19 . C70 . C71 . 112.1(8) yes
N19 . C70 . H701 . 108.796 no
C71 . C70 . H701 . 108.794 no
N19 . C70 . H702 . 108.799 no
C71 . C70 . H702 . 108.795 no
H701 . C70 . H702 . 109.466 no
C70 . C71 . C72 . 106.5(9) yes
C70 . C71 . H711 . 110.212 no
C72 . C71 . H711 . 110.208 no
C70 . C71 . H712 . 110.212 no
C72 . C71 . H712 . 110.213 no
H711 . C71 . H712 . 109.467 no
C71 . C72 . C73 . 106.1(10) yes
C71 . C72 . H721 . 110.290 no
C73 . C72 . H721 . 110.292 no
C71 . C72 . H722 . 110.284 no
C73 . C72 . H722 . 110.290 no

H721 . C72 . H722 . 109.466 no
C72 . C73 . H731 . 109.465 no
C72 . C73 . H732 . 109.465 no
H731 . C73 . H732 . 109.482 no
C72 . C73 . H733 . 109.463 no
H731 . C73 . H733 . 109.475 no
H732 . C73 . H733 . 109.476 no
N19 . C74 . C75 . 112.2(9) yes
N19 . C74 . H741 . 108.790 no
C75 . C74 . H741 . 108.786 no
N19 . C74 . H742 . 108.792 no
C75 . C74 . H742 . 108.788 no
H741 . C74 . H742 . 109.468 no
C74 . C75 . C76 . 106.1(9) yes
C74 . C75 . H751 . 110.305 no
C76 . C75 . H751 . 110.304 no
C74 . C75 . H752 . 110.306 no
C76 . C75 . H752 . 110.308 no
H751 . C75 . H752 . 109.466 no
C75 . C76 . C77 . 106.4(10) yes
C75 . C76 . H761 . 110.260 no
C77 . C76 . H761 . 110.260 no
C75 . C76 . H762 . 110.255 no
C77 . C76 . H762 . 110.259 no
H761 . C76 . H762 . 109.466 no
C76 . C77 . H771 . 109.465 no
C76 . C77 . H772 . 109.464 no
H771 . C77 . H772 . 109.482 no
C76 . C77 . H773 . 109.463 no
H771 . C77 . H773 . 109.476 no
H772 . C77 . H773 . 109.477 no
N19 . C78 . C79 . 112.0(9) yes
N19 . C78 . H781 . 108.806 no
C79 . C78 . H781 . 108.808 no
N19 . C78 . H782 . 108.805 no
C79 . C78 . H782 . 108.806 no
H781 . C78 . H782 . 109.468 no
C78 . C79 . C80 . 106.3(9) yes
C78 . C79 . H791 . 110.253 no
C80 . C79 . H791 . 110.254 no
C78 . C79 . H792 . 110.253 no
C80 . C79 . H792 . 110.254 no
H791 . C79 . H792 . 109.465 no
C79 . C80 . C81 . 106.3(10) yes
C79 . C80 . H801 . 110.268 no
C81 . C80 . H801 . 110.268 no
C79 . C80 . H802 . 110.267 no
C81 . C80 . H802 . 110.267 no
H801 . C80 . H802 . 109.466 no
C80 . C81 . H811 . 109.469 no
C80 . C81 . H812 . 109.465 no
H811 . C81 . H812 . 109.478 no
C80 . C81 . H813 . 109.465 no
H811 . C81 . H813 . 109.478 no
H812 . C81 . H813 . 109.473 no
N19 . C82 . C83 . 112.2(13) yes
N19 . C82 . H821 . 108.798 no
C83 . C82 . H821 . 108.795 no
N19 . C82 . H822 . 108.798 no
C83 . C82 . H822 . 108.795 no
H821 . C82 . H822 . 109.467 no

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C82 . C83 . C84 . 106.3(13)    yes
C82 . C83 . H831 . 110.262    no
C84 . C83 . H831 . 110.260    no
C82 . C83 . H832 . 110.263    no
C84 . C83 . H832 . 110.263    no
H831 . C83 . H832 . 109.465    no
C83 . C84 . C85 . 106.2(14)    yes
C83 . C84 . H841 . 110.274    no
C85 . C84 . H841 . 110.272    no
C83 . C84 . H842 . 110.270    no
C85 . C84 . H842 . 110.271    no
H841 . C84 . H842 . 109.466    no
C84 . C85 . H851 . 109.468    no
C84 . C85 . H852 . 109.465    no
H851 . C85 . H852 . 109.477    no
C84 . C85 . H853 . 109.466    no
H851 . C85 . H853 . 109.477    no
H852 . C85 . H853 . 109.475    no
C90 . N20 . C94 . 108.3(6)    yes
C90 . N20 . C98 . 115.3(5)    yes
C94 . N20 . C98 . 109.5(4)    yes
C90 . N20 . C86 . 105.9(9)    yes
C94 . N20 . C86 . 105.2(9)    yes
C98 . N20 . C86 . 112.1(9)    yes
N20 . C90 . C91 . 112.1(8)    yes
N20 . C90 . H901 . 108.831    no
C91 . C90 . H901 . 108.827    no
N20 . C90 . H902 . 108.828    no
C91 . C90 . H902 . 108.826    no
H901 . C90 . H902 . 109.466    no
C90 . C91 . C92 . 106.6(9)    yes
C90 . C91 . H911 . 110.183    no
C92 . C91 . H911 . 110.185    no
C90 . C91 . H912 . 110.183    no
C92 . C91 . H912 . 110.180    no
H911 . C91 . H912 . 109.466    no
C91 . C92 . C93 . 106.1(9)    yes
C91 . C92 . H921 . 110.305    no
C93 . C92 . H921 . 110.312    no
C91 . C92 . H922 . 110.310    no
C93 . C92 . H922 . 110.313    no
H921 . C92 . H922 . 109.466    no
C92 . C93 . H931 . 109.464    no
C92 . C93 . H932 . 109.463    no
H931 . C93 . H932 . 109.476    no
C92 . C93 . H933 . 109.465    no
H931 . C93 . H933 . 109.482    no
H932 . C93 . H933 . 109.478    no
N20 . C94 . C95 . 112.1(9)    yes
N20 . C94 . H941 . 108.807    no
C95 . C94 . H941 . 108.806    no
N20 . C94 . H942 . 108.805    no
C95 . C94 . H942 . 108.803    no
H941 . C94 . H942 . 109.466    no
C94 . C95 . C96 . 106.2(9)    yes
C94 . C95 . H951 . 110.277    no
C96 . C95 . H951 . 110.276    no
C94 . C95 . H952 . 110.279    no
C96 . C95 . H952 . 110.276    no
H951 . C95 . H952 . 109.468    no
C95 . C96 . C97 . 106.2(10)    yes
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C95 . C96 . H961 . 110.292 no
C97 . C96 . H961 . 110.294 no
C95 . C96 . H962 . 110.290 no
C97 . C96 . H962 . 110.295 no
H961 . C96 . H962 . 109.467 no
C96 . C97 . H971 . 109.467 no
C96 . C97 . H972 . 109.466 no
H971 . C97 . H972 . 109.482 no
C96 . C97 . H973 . 109.463 no
H971 . C97 . H973 . 109.475 no
H972 . C97 . H973 . 109.474 no
N20 . C98 . C99 . 112.2(8) yes
N20 . C98 . H981 . 108.794 no
C99 . C98 . H981 . 108.790 no
N20 . C98 . H982 . 108.793 no
C99 . C98 . H982 . 108.789 no
H981 . C98 . H982 . 109.467 no
C98 . C99 . C100 . 106.2(8) yes
C98 . C99 . H991 . 110.275 no
C100 . C99 . H991 . 110.275 no
C98 . C99 . H992 . 110.276 no
C100 . C99 . H992 . 110.276 no
H991 . C99 . H992 . 109.464 no
C99 . C100 . C101 . 106.4(9) yes
C99 . C100 . H1001 . 110.244 no
C101 . C100 . H1001 . 110.242 no
C99 . C100 . H1002 . 110.244 no
C101 . C100 . H1002 . 110.243 no
H1001 . C100 . H1002 . 109.467 no
C100 . C101 . H1011 . 109.470 no
C100 . C101 . H1012 . 109.466 no
H1011 . C101 . H1012 . 109.477 no
C100 . C101 . H1013 . 109.465 no
H1011 . C101 . H1013 . 109.476 no
H1012 . C101 . H1013 . 109.472 no
N20 . C86 . C871 . 112.1(2) yes
N20 . C86 . H861 . 108.822 no
C871 . C86 . H861 . 108.819 no
N20 . C86 . H862 . 108.818 no
C871 . C86 . H862 . 108.814 no
H861 . C86 . H862 . 109.468 no
C880 . C870 . H8701 . 110.254 no
C880 . C870 . H8702 . 110.274 no
H862 . C870 . H8702 . 142.854 no
H8701 . C870 . H8702 . 109.466 no
C870 . C880 . C890 . 106.3(2) yes
C870 . C880 . H8801 . 110.271 no
C890 . C880 . H8801 . 110.265 no
C870 . C880 . H8802 . 110.257 no
C890 . C880 . H8802 . 110.266 no
H8801 . C880 . H8802 . 109.462 no
C880 . C890 . H8901 . 109.464 no
C880 . C890 . H8902 . 109.465 no
H8901 . C890 . H8902 . 109.479 no
C880 . C890 . H8903 . 109.463 no
H8901 . C890 . H8903 . 109.475 no
H8902 . C890 . H8903 . 109.481 no
C86 . C871 . C881 . 106.3(2) yes
C86 . C871 . H8711 . 110.265 no
C881 . C871 . H8711 . 110.264 no
C86 . C871 . H8712 . 110.270 no

C881 . C871 . H8712 . 110.266 no
H8711 . C871 . H8712 . 109.465 no
C871 . C881 . C891 . 106.2(2) yes
C871 . C881 . H8811 . 110.272 no
C891 . C881 . H8811 . 110.265 no
C871 . C881 . H8812 . 110.276 no
C891 . C881 . H8812 . 110.285 no
H8811 . C881 . H8812 . 109.467 no
C881 . C891 . H8911 . 109.469 no
C881 . C891 . H8912 . 109.480 no
H8911 . C891 . H8912 . 109.496 no
C881 . C891 . H8913 . 109.451 no
H8911 . C891 . H8913 . 109.459 no
H8912 . C891 . H8913 . 109.472 no
H391 . C580 . H392 . 109.467 no
C57 . C581 . C59 . 104.2(13) yes
C59 . C581 . H392 . 100.951 no
C57 . C581 . H493 . 110.772 no
C59 . C581 . H493 . 110.771 no
C57 . C581 . H494 . 110.772 no
C59 . C581 . H494 . 110.771 no
H493 . C581 . H494 . 109.467 no
C9 . C110 . C11 . 106.0(13) yes
C9 . C110 . H593 . 110.340 no
C11 . C110 . H593 . 110.341 no
C9 . C110 . H594 . 110.340 no
C11 . C110 . H594 . 110.341 no
H593 . C110 . H594 . 109.467 no
C11 . C110 . H691 . 101.086 no
H691 . C111 . H692 . 109.467 no
C20 . C21 . C22 . 103.6(14) yes
C20 . C21 . H1903 . 110.928 no
C22 . C21 . H1903 . 110.927 no
C20 . C21 . H1904 . 110.928 no
C22 . C21 . H1904 . 110.927 no
H1903 . C21 . H1904 . 109.467 no
H291 . C210 . H292 . 109.467 no