

```

#\#CIF_1.1

# CIF produced by WinGX routine CIF_UPDATE
# Created on 2013-07-31 at 15:57:18
# Using CIFtbx version 2.6.2 16 Jun 1998

# Dictionary name : cif_core.dic
# Dictionary vers : 2.4
# Request file    : c:\wingx\files\archive.reqdat
# CIF files read  : gl567_2 gl567_2_od

#----- SECTION 1. GLOBAL INFORMATION -----#
data_global

#----- AUDIT DETAILS -----#
_audit_creation_date      2013-07-31
_audit_creation_method    'WinGX routine CIF_UPDATE'
_audit_conform_dict_name  cif_core.dic
_audit_conform_dict_version 2.4
_audit_conform_dict_location ftp://ftp.iucr.org/pub/cif_core.dic
_audit_update_record      ?

#----- AUTHOR DETAILS -----#

#----- SECTION 2. COMPOUND(S) DETAILS -----#
data_gl567_2

_audit_creation_date      2013-07-31T15:57:18-00:00
_audit_creation_method    'WinGX routine CIF_UPDATE'
_audit_author_name        'V. Kahlenberg'
_audit_contact_author     'V. Kahlenberg'
_audit_contact_author_address
;
  Institut f\"ur Mineralogie und Petrographie
  Leopold-Franzens-Universit\"at Innsbruck
  Innrain 52
  A-6020 Innsbruck
  Austria
;
_audit_contact_author_email Volker.Kahlenberg@uibk.ac.at
_audit_contact_author_fax '+43 512 507 2926'
_audit_contact_author_phone '+43 512 507 5503'

_audit_conform_dict_name  cif_core.dic
_audit_conform_dict_version 2.4
_audit_conform_dict_location ftp://ftp.iucr.org/pub/cif_core.dic
_publ_requested_category  FO

#-----#
#          CHEMICAL INFORMATION          #
#-----#

_chemical_name_systematic
;
?
;
_chemical_formula_sum      'C11 H13 N O4'
_chemical_formula_moiety  'C11 H11 N O3, H2 O'
_chemical_formula_weight  223.22
_chemical_absolute_configuration unk

```

```
#-----#
#                               #
#                               #
#-----#
```

UNIT CELL INFORMATION

```
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M  'C 1 c 1'
_symmetry_space_group_name_Hall 'C -2yc'
loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'
  'x, -y, z+1/2'
  'x+1/2, y+1/2, z'
  'x+1/2, -y+1/2, z+1/2'

_cell_length_a                  4.7469(3)
_cell_length_b                  16.5037(11)
_cell_length_c                  13.1660(9)
_cell_angle_alpha               90
_cell_angle_beta                95.426(7)
_cell_angle_gamma               90
_cell_volume                     1026.82(12)
_cell_formula_units_Z           4
_cell_measurement_temperature   173(2)
_cell_measurement_reflns_used   1783
_cell_measurement_theta_min     3.3702
_cell_measurement_theta_max     67.2878
```

```
#-----#
#                               #
#                               #
#-----#
```

CRYSTAL INFORMATION

```
_exptl_crystal_description      'platy fragment'
_exptl_crystal_colour           colourless
_exptl_crystal_size_max         0.18
_exptl_crystal_size_mid         0.16
_exptl_crystal_size_min         0.04
_exptl_crystal_density_diffn    1.444
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000            472
_exptl_special_details
;
?
```

```
#-----#
#                               #
#                               #
#-----#
```

ABSORPTION CORRECTION

```
_exptl_absorpt_coefficient_mu   0.93
_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_process_details
;
```

```
  CrysAlisPro, Agilent Technologies,
  Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
  (compiled Jul 11 2012,15:38:31)
  Empirical absorption correction using spherical harmonics,
  implemented in SCALE3 ABSPACK scaling algorithm.
```

```
_exptl_absorpt_correction_T_min 0.94873
_exptl_absorpt_correction_T_max 1
```

```
#-----#
#                               #
#                               #
#-----#
```

DATA COLLECTION

```

#-----#
_diffrn_ambient_temperature          173(2)
_diffrn_radiation_wavelength         1.5418
_diffrn_radiation_type               CuK\alpha
_diffrn_radiation_monochromator       mirror
_diffrn_detector_area_resol_mean     10.3575
_diffrn_orient_matrix_ub_11          0.2317761
_diffrn_orient_matrix_ub_12          0.0560854
_diffrn_orient_matrix_ub_13          0.0506406
_diffrn_orient_matrix_ub_21          0.1180111
_diffrn_orient_matrix_ub_22          -0.0707372
_diffrn_orient_matrix_ub_23          0.067624
_diffrn_orient_matrix_ub_31          0.1970399
_diffrn_orient_matrix_ub_32          -0.0236084
_diffrn_orient_matrix_ub_33          -0.0816786
_diffrn_measurement_device_type       'Xcalibur, Ruby, Gemini ultra'
_diffrn_measurement_method            '\w scans'
_diffrn_reflns_av_R_equivalents      0.0301
_diffrn_reflns_av_unetI/netI         0.0244
_diffrn_reflns_number                 4219
_diffrn_reflns_limit_h_min            -5
_diffrn_reflns_limit_h_max            5
_diffrn_reflns_limit_k_min            -19
_diffrn_reflns_limit_k_max            19
_diffrn_reflns_limit_l_min            -15
_diffrn_reflns_limit_l_max            9
_diffrn_reflns_theta_min              5.36
_diffrn_reflns_theta_max              67.36
_diffrn_reflns_theta_full             67.36
_diffrn_measured_fraction_theta_full 0.995
_diffrn_measured_fraction_theta_max  0.995
_reflns_number_total                  1221
_reflns_number_gt                     1161
_reflns_threshold_expression           >2\s(I)

#-----#
#                                     COMPUTER PROGRAMS USED                                     #
#-----#

_computing_data_collection
;
    CrysAlisPro, Agilent Technologies,
    Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
    (compiled Jul 11 2012,15:38:31)
;
_computing_cell_refinement
;
    CrysAlisPro, Agilent Technologies,
    Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
    (compiled Jul 11 2012,15:38:31)
;
_computing_data_reduction
;
    CrysAlisPro, Agilent Technologies,
    Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
    (compiled Jul 11 2012,15:38:31)
;
_computing_structure_solution          'SIR2002 (Burla et al., 2003)'
_computing_structure_refinement       'SHELXL-97 (Sheldrick, 2008)'

#-----#

```

```

#                               STRUCTURE SOLUTION                               #
#-----#

_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom

#-----#
#                               REFINEMENT INFORMATION                               #
#-----#

_refine_special_details
;
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\|s(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^)+(0.1673P)^2^+0.2782P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment        mixed
_refine_ls_extinction_method          none
_refine_ls_number_reflns             1221
_refine_ls_number_parameters          150
_refine_ls_number_restraints          6
_refine_ls_R_factor_all               0.0541
_refine_ls_R_factor_gt               0.0524
_refine_ls_wR_factor_ref              0.1582
_refine_ls_wR_factor_gt               0.154
_refine_ls_goodness_of_fit_ref        1.07
_refine_ls_restrained_S_all           1.069
_refine_ls_shift/su_max                0
_refine_ls_shift/su_mean               0
_refine_ls_abs_structure_details
      'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack         0.7(4)
_refine_diff_density_max               0.454
_refine_diff_density_min               -0.526
_refine_diff_density_rms               0.093

#-----#
#                               ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS     #
#-----#

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
C C 0.0181 0.0091 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0311 0.018 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0492 0.0322 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group

O1 O 0.5135(6) 0.17149(15) 0.5050(2) 0.0351(8) Uani 1 1 d . . .
O2 O 0.4725(7) 0.32503(15) 0.4818(3) 0.0377(8) Uani 1 1 d . . .
O3 O -0.2784(7) 0.04966(17) 0.2538(3) 0.0417(8) Uani 1 1 d . . .
N1 N -0.2942(7) 0.29530(19) 0.2244(3) 0.0308(8) Uani 1 1 d D . .
H1 H -0.274(12) 0.3454(15) 0.211(4) 0.037 Uiso 1 1 d D . .
C10 C 0.4427(13) 0.4112(3) 0.4771(4) 0.0492(13) Uani 1 1 d . . .
H10A H 0.4658 0.4299 0.4077 0.074 Uiso 1 1 calc R . .
H10B H 0.5875 0.4364 0.525 0.074 Uiso 1 1 calc R . .
H10C H 0.2545 0.4265 0.4955 0.074 Uiso 1 1 calc R . .
C9 C 0.2905(9) 0.2813(3) 0.4236(3) 0.0300(9) Uani 1 1 d . . .
C7 C -0.0964(8) 0.2614(2) 0.2937(3) 0.0296(9) Uani 1 1 d . . .
C6 C -0.4773(9) 0.2502(3) 0.1662(3) 0.0314(9) Uani 1 1 d . . .
H6 H -0.6098 0.2763 0.1183 0.038 Uiso 1 1 calc R . .
C5 C -0.4807(9) 0.1673(3) 0.1732(4) 0.0351(10) Uani 1 1 d . . .
H5 H -0.615 0.137 0.1307 0.042 Uiso 1 1 calc R . .
C3 C -0.0847(8) 0.1775(2) 0.3053(3) 0.0298(10) Uani 1 1 d . . .
C1 C 0.3127(8) 0.1954(3) 0.4365(3) 0.0315(10) Uani 1 1 d . . .
C4 C -0.2830(8) 0.1264(2) 0.2441(4) 0.0334(10) Uani 1 1 d . . .
C2 C 0.1263(9) 0.1461(2) 0.3785(3) 0.0336(10) Uani 1 1 d . . .
H2 H 0.1394 0.0891 0.3877 0.04 Uiso 1 1 calc R . .
C11 C 0.5586(11) 0.0860(2) 0.5137(4) 0.0437(11) Uani 1 1 d . . .
H11A H 0.3924 0.0604 0.5389 0.065 Uiso 1 1 calc R . .
H11B H 0.7255 0.0754 0.5615 0.065 Uiso 1 1 calc R . .
H11C H 0.5887 0.0636 0.4466 0.065 Uiso 1 1 calc R . .
C8 C 0.0896(10) 0.3135(2) 0.3536(4) 0.0354(10) Uani 1 1 d . . .
H8 H 0.0749 0.3706 0.3452 0.042 Uiso 1 1 calc R . .
O4 O 0.7055(7) 0.46611(17) 0.2208(3) 0.0449(9) Uani 1 1 d D . .
H41 H 0.5693 0.4907 0.2464 0.067 Uiso 1 1 d RD . .
H42 H 0.8531 0.4959 0.2272 0.067 Uiso 1 1 d RD . .

loop_

_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12

O1 0.0423(17) 0.0214(14) 0.0406(16) -0.0005(11) -0.0012(14) 0.0034(11)
O2 0.0461(18) 0.0222(14) 0.0437(17) -0.0049(11) -0.0008(15) -0.0038(11)
O3 0.0338(14) 0.0289(13) 0.061(2) -0.0069(14) -0.0008(13) -0.0015(12)
N1 0.0272(15) 0.0317(15) 0.0333(17) 0.0047(14) 0.0027(13) 0.0028(14)
C10 0.072(3) 0.0182(19) 0.055(3) -0.0012(18) -0.006(3) -0.0014(18)
C9 0.0288(18) 0.0291(18) 0.032(2) -0.0022(17) 0.0003(16) 0.0009(16)
C7 0.0228(17) 0.036(2) 0.0301(19) 0.0040(18) 0.0031(15) 0.0018(16)
C6 0.0265(19) 0.040(2) 0.0275(19) 0.0014(17) -0.0001(15) 0.0021(16)
C5 0.030(2) 0.036(2) 0.039(2) -0.0105(19) 0.0013(17) -0.0059(17)
C3 0.0194(17) 0.038(2) 0.032(2) 0.0030(17) 0.0017(16) 0.0024(16)
C1 0.024(2) 0.035(2) 0.035(2) -0.0072(18) 0.0008(17) 0.0002(16)
C4 0.0228(17) 0.0320(19) 0.046(3) -0.0051(17) 0.0051(18) 0.0015(16)
C2 0.0327(19) 0.0284(18) 0.039(2) -0.0024(17) 0.0020(18) 0.0035(17)
C11 0.054(3) 0.0211(18) 0.054(3) 0.0069(18) -0.005(2) 0.0041(17)
C8 0.034(2) 0.0278(18) 0.045(3) -0.0004(17) 0.0046(19) 0.0018(16)

04 0.0363(16) 0.0292(12) 0.069(2) -0.0049(13) 0.0055(15) 0.0004(12)

```
#-----#  
#                               #  
#           MOLECULAR GEOMETRY           #  
#-----#
```

_geom_special_details

;

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

;

loop_

_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag

O1 C1 1.309(6) . ?
O1 C11 1.430(5) . ?
O2 C9 1.315(5) . ?
O2 C10 1.431(5) . ?
O3 C4 1.273(5) . ?
N1 C6 1.331(6) . ?
N1 C7 1.366(5) . ?
N1 H1 0.85(2) . ?
C10 H10A 0.98 . ?
C10 H10B 0.98 . ?
C10 H10C 0.98 . ?
C9 C8 1.370(7) . ?
C9 C1 1.431(6) . ?
C7 C3 1.392(5) . ?
C7 C8 1.418(6) . ?
C6 C5 1.371(6) . ?
C6 H6 0.95 . ?
C5 C4 1.430(6) . ?
C5 H5 0.95 . ?
C3 C2 1.421(6) . ?
C3 C4 1.451(6) . ?
C1 C2 1.378(6) . ?
C2 H2 0.95 . ?
C11 H11A 0.98 . ?
C11 H11B 0.98 . ?
C11 H11C 0.98 . ?
C8 H8 0.95 . ?
O4 H41 0.8588 . ?
O4 H42 0.8538 . ?

loop_

_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_3
_geom_angle_publ_flag

C1 O1 C11 116.5(3) . . ?
C9 O2 C10 117.6(4) . . ?
C6 N1 C7 121.7(3) . . ?
C6 N1 H1 120(4) . . ?

C7 N1 H1 117(4) . . ?
O2 C10 H10A 109.5 . . ?
O2 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
O2 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
O2 C9 C8 123.8(4) . . ?
O2 C9 C1 115.9(4) . . ?
C8 C9 C1 120.2(4) . . ?
N1 C7 C3 119.9(4) . . ?
N1 C7 C8 118.3(4) . . ?
C3 C7 C8 121.8(4) . . ?
N1 C6 C5 122.0(4) . . ?
N1 C6 H6 119 . . ?
C5 C6 H6 119 . . ?
C6 C5 C4 120.3(4) . . ?
C6 C5 H5 119.9 . . ?
C4 C5 H5 119.9 . . ?
C7 C3 C2 117.1(4) . . ?
C7 C3 C4 120.0(4) . . ?
C2 C3 C4 122.9(3) . . ?
O1 C1 C2 126.3(4) . . ?
O1 C1 C9 114.9(3) . . ?
C2 C1 C9 118.9(4) . . ?
O3 C4 C5 122.7(4) . . ?
O3 C4 C3 121.3(4) . . ?
C5 C4 C3 116.1(3) . . ?
C1 C2 C3 122.4(3) . . ?
C1 C2 H2 118.8 . . ?
C3 C2 H2 118.8 . . ?
O1 C11 H11A 109.5 . . ?
O1 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
O1 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
C9 C8 C7 119.7(4) . . ?
C9 C8 H8 120.1 . . ?
C7 C8 H8 120.1 . . ?
H41 O4 H42 109.3 . . ?

loop_

_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C10 O2 C9 C8 5.3(7) ?
C10 O2 C9 C1 -175.1(4) ?
C6 N1 C7 C3 -0.5(6) ?
C6 N1 C7 C8 -179.4(4) ?
C7 N1 C6 C5 0.8(7) ?
N1 C6 C5 C4 -0.3(7) ?
N1 C7 C3 C2 179.8(4) ?
C8 C7 C3 C2 -1.3(5) ?
N1 C7 C3 C4 -0.3(5) ?
C8 C7 C3 C4 178.6(4) ?
C11 O1 C1 C2 5.9(6) ?

C11 O1 C1 C9 -174.7(3) ?
O2 C9 C1 O1 -0.1(5) ?
C8 C9 C1 O1 179.5(4) ?
O2 C9 C1 C2 179.4(3) ?
C8 C9 C1 C2 -1.0(6) ?
C6 C5 C4 O3 179.7(4) ?
C6 C5 C4 C3 -0.4(6) ?
C7 C3 C4 O3 -179.4(4) ?
C2 C3 C4 O3 0.5(6) ?
C7 C3 C4 C5 0.7(6) ?
C2 C3 C4 C5 -179.4(4) ?
O1 C1 C2 C3 -179.7(4) ?
C9 C1 C2 C3 0.9(6) ?
C7 C3 C2 C1 0.2(6) ?
C4 C3 C2 C1 -179.7(4) ?
O2 C9 C8 C7 179.6(4) ?
C1 C9 C8 C7 -0.1(6) ?
N1 C7 C8 C9 -179.9(4) ?
C3 C7 C8 C9 1.2(6) ?

loop_

_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A

O4 H41 O3 0.86 1.93 2.749(4) 160 3
O4 H42 O3 0.85 1.96 2.809(4) 170.8 3_655
N1 H1 O4 0.85(2) 2.00(3) 2.819(4) 161(5) 1_455

END of CIF


```

#\#CIF_1.1

# CIF produced by WinGX routine CIF_UPDATE
# Created on 2013-07-29 at 13:18:49
# Using CIFtbx version 2.6.2 16 Jun 1998

# Dictionary name : cif_core.dic
# Dictionary vers : 2.4
# Request file    : c:\wingx\files\archive.reqdat
# CIF files read  : gl576_1 gl576_1_od

#----- SECTION 1. GLOBAL INFORMATION -----#
data_global

#----- AUDIT DETAILS -----#

_audit_creation_date      2013-07-29
_audit_creation_method    'WinGX routine CIF_UPDATE'
_audit_conform_dict_name  cif_core.dic
_audit_conform_dict_version 2.4
_audit_conform_dict_location ftp://ftp.iucr.org/pub/cif_core.dic
_audit_update_record      ?

#----- AUTHOR DETAILS -----#

#----- SECTION 2. COMPOUND(S) DETAILS -----#
data_gl576_1

_audit_creation_date      2013-07-29T13:18:49-00:00
_audit_creation_method    'WinGX routine CIF_UPDATE'
_audit_author_name        'V. Kahlenberg'
_audit_contact_author     'V. Kahlenberg'
_audit_contact_author_address
;
  Institut f\"ur Mineralogie und Petrographie
  Leopold-Franzens-Universit\"at Innsbruck
  Innrain 52
  A-6020 Innsbruck
  Austria
;
_audit_contact_author_email Volker.Kahlenberg@uibk.ac.at
_audit_contact_author_fax '+43 512 507 2926'
_audit_contact_author_phone '+43 512 507 5503'

_audit_conform_dict_name  cif_core.dic
_audit_conform_dict_version 2.4
_audit_conform_dict_location ftp://ftp.iucr.org/pub/cif_core.dic
_publ_requested_category  FO

#-----#
#          CHEMICAL INFORMATION          #
#-----#

_chemical_name_systematic
;
?
;
_chemical_formula_sum      'C12 H12 F N O3'
_chemical_formula_moiety  'C12 H12 F N O3'
_chemical_formula_weight   237.23

```

```
#-----#
#                               #
#                               #
#-----#
```

UNIT CELL INFORMATION

```
_symmetry_cell_setting      orthorhombic
_symmetry_space_group_name_H-M  'P n m a'
_symmetry_space_group_name_Hall '-P 2ac 2n'
```

loop_

 _symmetry_equiv_pos_as_xyz

```
'x, y, z'
'-x+1/2, -y, z+1/2'
'x+1/2, -y+1/2, -z+1/2'
'-x, y+1/2, -z'
'-x, -y, -z'
'x-1/2, y, -z-1/2'
'-x-1/2, y-1/2, z-1/2'
'x, -y-1/2, z'
```

```
_cell_length_a      13.0264(6)
_cell_length_b      6.9982(5)
_cell_length_c      12.1392(6)
_cell_angle_alpha   90
_cell_angle_beta    90
_cell_angle_gamma   90
_cell_volume        1106.63(11)
_cell_formula_units_Z 4
_cell_measurement_temperature 173(2)
_cell_measurement_reflns_used 1224
_cell_measurement_theta_min 3.3899
_cell_measurement_theta_max 67.3217
```

```
#-----#
#                               #
#                               #
#-----#
```

CRYSTAL INFORMATION

```
_exptl_crystal_description 'platy fragment'
_exptl_crystal_colour      colourless
_exptl_crystal_size_max    0.4
_exptl_crystal_size_mid    0.32
_exptl_crystal_size_min    0.16
_exptl_crystal_density_diffrn 1.424
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000      496
_exptl_special_details
```

;

?

;

```
#-----#
#                               #
#                               #
#-----#
```

ABSORPTION CORRECTION

```
_exptl_absorpt_coefficient_mu 0.965
_exptl_absorpt_correction_type multi-scan
_exptl_absorpt_process_details
```

;

CrysAlisPro, Agilent Technologies,
Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)

Empirical absorption correction using spherical harmonics,
implemented in SCALE3 ABSPACK scaling algorithm.

;

_exptl_absorpt_correction_T_min 0.72469
_exptl_absorpt_correction_T_max 1

#-----#
DATA COLLECTION #
#-----#

_diffrn_ambient_temperature 173(2)
_diffrn_radiation_wavelength 1.5418
_diffrn_radiation_type CuK\a
_diffrn_radiation_monochromator mirror
_diffrn_detector_area_resol_mean 10.3575
_diffrn_orient_matrix_ub_11 0.0282368
_diffrn_orient_matrix_ub_12 -0.0032562
_diffrn_orient_matrix_ub_13 -0.1230591
_diffrn_orient_matrix_ub_21 0.0035884
_diffrn_orient_matrix_ub_22 -0.2199795
_diffrn_orient_matrix_ub_23 0.002761
_diffrn_orient_matrix_ub_31 -0.1148223
_diffrn_orient_matrix_ub_32 -0.0079857
_diffrn_orient_matrix_ub_33 -0.0307244
_diffrn_measurement_device_type 'Xcalibur, Ruby, Gemini ultra'
_diffrn_measurement_method '\w scans'
_diffrn_reflsv_av_R_equivalents 0.0256
_diffrn_reflsv_av_unetI/netI 0.0197
_diffrn_reflsv_number 3313
_diffrn_reflsv_limit_h_min -15
_diffrn_reflsv_limit_h_max 10
_diffrn_reflsv_limit_k_min -8
_diffrn_reflsv_limit_k_max 5
_diffrn_reflsv_limit_l_min -14
_diffrn_reflsv_limit_l_max 13
_diffrn_reflsv_theta_min 4.98
_diffrn_reflsv_theta_max 67.43
_diffrn_reflsv_theta_full 67.43
_diffrn_measured_fraction_theta_full 0.99
_diffrn_measured_fraction_theta_max 0.99
_reflsv_number_total 1077
_reflsv_number_gt 903
_reflsv_threshold_expression >2\s(I)

#-----#
COMPUTER PROGRAMS USED #
#-----#

_computing_data_collection
;
CrysAlisPro, Agilent Technologies,
Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)
;
_computing_cell_refinement
;
CrysAlisPro, Agilent Technologies,
Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)
;
_computing_data_reduction
;
CrysAlisPro, Agilent Technologies,
Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)

```

;
_computing_structure_solution      'SIR2002 (Burla et al., 2003)'
_computing_structure_refinement    'SHELXL-97 (Sheldrick, 2008)'

#-----#
#                               STRUCTURE SOLUTION                               #
#-----#

_atom_sites_solution_primary       direct
_atom_sites_solution_secondary     difmap
_atom_sites_solution_hydrogens     geom

#-----#
#                               REFINEMENT INFORMATION                           #
#-----#

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2σ(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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/[σ2(Fo2)+(0.0654P)2+0.1085P] where P=(Fo2+2Fc2)/3'
_refine_ls_hydrogen_treatment      mixed
_refine_ls_extinction_method       none
_refine_ls_number_reflns           1077
_refine_ls_number_parameters        107
_refine_ls_number_restraints        4
_refine_ls_R_factor_all             0.0426
_refine_ls_R_factor_gt              0.0356
_refine_ls_wR_factor_ref            0.108
_refine_ls_wR_factor_gt             0.1019
_refine_ls_goodness_of_fit_ref      1.061
_refine_ls_restrained_S_all         1.059
_refine_ls_shift/su_max             0
_refine_ls_shift/su_mean            0
_refine_diff_density_max            0.185
_refine_diff_density_min            -0.177
_refine_diff_density_rms            0.036

#-----#
#                               ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS   #
#-----#

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
C C 0.0181 0.0091 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0311 0.018 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0492 0.0322 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F F 0.0727 0.0534 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

```

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_adp_type
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
F1 F 0.44603(10) 0.25 -0.11234(9) 0.0579(4) Uani 1 2 d S . .
O2 O 0.60000(9) 0.25 0.50245(11) 0.0447(4) Uani 1 2 d S . .
O3 O 0.29204(10) 0.25 0.39722(11) 0.0545(5) Uani 1 2 d S . .
O1 O 0.54330(10) 0.25 0.67486(11) 0.0479(4) Uani 1 2 d S . .
N1 N 0.45845(11) 0.25 0.34212(13) 0.0358(4) Uani 1 2 d SD . .
H1 H 0.5196(13) 0.25 0.3678(17) 0.043 Uiso 1 2 d SD . .
C11 C 0.35694(14) 0.25 0.16956(16) 0.0391(5) Uani 1 2 d S . .
H11 H 0.2941 0.25 0.2093 0.047 Uiso 1 2 calc SR . .
C15 C 0.54138(14) 0.25 0.16649(16) 0.0377(5) Uani 1 2 d S . .
H15 H 0.605 0.25 0.2048 0.045 Uiso 1 2 calc SR . .
C2 C 0.34546(10) 0.3553(2) 0.61550(11) 0.0410(4) Uani 1 1 d . . .
H2A H 0.376 0.4209 0.6799 0.049 Uiso 1 1 calc R . .
H2B H 0.2854 0.4209 0.5828 0.049 Uiso 1 1 calc R . .
C12 C 0.35622(15) 0.25 0.05493(16) 0.0416(5) Uani 1 2 d S . .
H12 H 0.2931 0.25 0.0156 0.05 Uiso 1 2 calc SR . .
C1 C 0.41843(14) 0.25 0.53719(14) 0.0338(4) Uani 1 2 d S . .
C10 C 0.45007(13) 0.25 0.22575(15) 0.0340(4) Uani 1 2 d S . .
C14 C 0.54102(15) 0.25 0.05260(16) 0.0424(5) Uani 1 2 d S . .
H14 H 0.6034 0.25 0.0121 0.051 Uiso 1 2 calc SR . .
C3 C 0.52947(14) 0.25 0.56715(15) 0.0328(4) Uani 1 2 d S . .
C13 C 0.44788(15) 0.25 -0.00040(16) 0.0411(5) Uani 1 2 d S . .
C6 C 0.38376(14) 0.25 0.41861(15) 0.0362(4) Uani 1 2 d S . .
C5 C 0.64857(16) 0.25 0.71298(17) 0.0504(6) Uani 1 2 d SD . .
H5B H 0.6833(13) 0.3664(14) 0.6881(8) 0.076 Uiso 1 1 d D . .
H5A H 0.6444(17) 0.25 0.7936(2) 0.076 Uiso 1 2 d SD . .

```

```

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_23
  _atom_site_aniso_U_13
  _atom_site_aniso_U_12
F1 0.0626(9) 0.0836(10) 0.0274(6) 0 0.0003(5) 0
O2 0.0318(7) 0.0692(10) 0.0329(7) 0 0.0010(6) 0
O3 0.0283(7) 0.0985(13) 0.0368(8) 0 -0.0002(6) 0
O1 0.0377(7) 0.0773(11) 0.0287(7) 0 -0.0031(5) 0
N1 0.0267(7) 0.0527(10) 0.0281(8) 0 0.0001(6) 0
C11 0.0318(9) 0.0514(12) 0.0342(10) 0 -0.0002(7) 0
C15 0.0323(9) 0.0465(11) 0.0344(10) 0 -0.0002(7) 0
C2 0.0378(7) 0.0488(9) 0.0364(7) -0.0033(6) 0.0074(5) 0.0056(6)
C12 0.0371(10) 0.0525(12) 0.0352(10) 0 -0.0069(8) 0
C1 0.0314(9) 0.0408(10) 0.0290(9) 0 0.0041(7) 0
C10 0.0339(9) 0.0376(10) 0.0305(10) 0 -0.0006(7) 0
C14 0.0382(10) 0.0538(12) 0.0352(10) 0 0.0059(8) 0
C3 0.0343(9) 0.0347(9) 0.0293(9) 0 -0.0010(7) 0
C13 0.0502(11) 0.0455(11) 0.0275(9) 0 -0.0004(8) 0
C6 0.0314(9) 0.0445(10) 0.0327(9) 0 0.0016(8) 0
C5 0.0416(11) 0.0745(15) 0.0352(10) 0 -0.0104(9) 0

```

```
#-----#  
#           MOLECULAR GEOMETRY           #  
#-----#
```

```
_geom_special_details
```

```
;
```

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

```
;
```

```
loop_
```

```
  _geom_bond_atom_site_label_1  
  _geom_bond_atom_site_label_2  
  _geom_bond_distance  
  _geom_bond_site_symmetry_2  
  _geom_bond_publ_flag
```

```
F1 C13 1.359(2) . ?  
O2 C3 1.209(2) . ?  
O3 C6 1.223(2) . ?  
O1 C3 1.320(2) . ?  
O1 C5 1.447(2) . ?  
N1 C6 1.345(2) . ?  
N1 C10 1.417(2) . ?  
N1 H1 0.855(16) . ?  
C11 C12 1.392(3) . ?  
C11 C10 1.392(3) . ?  
C11 H11 0.95 . ?  
C15 C14 1.383(3) . ?  
C15 C10 1.390(3) . ?  
C15 H15 0.95 . ?  
C2 C2 1.473(3) 8_565 ?  
C2 C1 1.5329(19) . ?  
C2 H2A 0.99 . ?  
C2 H2B 0.99 . ?  
C12 C13 1.370(3) . ?  
C12 H12 0.95 . ?  
C1 C3 1.491(2) . ?  
C1 C6 1.509(3) . ?  
C1 C2 1.5329(19) 8_565 ?  
C14 C13 1.373(3) . ?  
C14 H14 0.95 . ?  
C5 H5B 0.9799(11) . ?  
C5 H5A 0.9799(10) . ?
```

```
loop_
```

```
  _geom_angle_atom_site_label_1  
  _geom_angle_atom_site_label_2  
  _geom_angle_atom_site_label_3  
  _geom_angle  
  _geom_angle_site_symmetry_1  
  _geom_angle_site_symmetry_3  
  _geom_angle_publ_flag
```

```
C3 O1 C5 116.49(15) . . ?  
C6 N1 C10 129.24(16) . . ?  
C6 N1 H1 115.0(15) . . ?  
C10 N1 H1 115.8(15) . . ?  
C12 C11 C10 119.74(17) . . ?  
C12 C11 H11 120.1 . . ?  
C10 C11 H11 120.1 . . ?
```

C14 C15 C10 120.97(17) . . ?
C14 C15 H15 119.5 . . ?
C10 C15 H15 119.5 . . ?
C2 C2 C1 61.28(6) 8_565 . ?
C2 C2 H2A 117.6 8_565 . ?
C1 C2 H2A 117.6 . . ?
C2 C2 H2B 117.6 8_565 . ?
C1 C2 H2B 117.6 . . ?
H2A C2 H2B 114.7 . . ?
C13 C12 C11 118.97(18) . . ?
C13 C12 H12 120.5 . . ?
C11 C12 H12 120.5 . . ?
C3 C1 C6 121.53(15) . . ?
C3 C1 C2 116.75(13) . 8_565 ?
C6 C1 C2 113.96(13) . 8_565 ?
C3 C1 C2 116.75(13) . . ?
C6 C1 C2 113.96(13) . . ?
C2 C1 C2 57.44(13) 8_565 . ?
C15 C10 C11 119.49(16) . . ?
C15 C10 N1 116.74(16) . . ?
C11 C10 N1 123.77(16) . . ?
C13 C14 C15 118.13(18) . . ?
C13 C14 H14 120.9 . . ?
C15 C14 H14 120.9 . . ?
O2 C3 O1 122.68(16) . . ?
O2 C3 C1 125.37(16) . . ?
O1 C3 C1 111.96(15) . . ?
F1 C13 C12 118.34(17) . . ?
F1 C13 C14 118.95(17) . . ?
C12 C13 C14 122.70(18) . . ?
O3 C6 N1 124.07(17) . . ?
O3 C6 C1 119.68(16) . . ?
N1 C6 C1 116.25(16) . . ?
O1 C5 H5B 109.8(10) . . ?
O1 C5 H5A 105.5(13) . . ?
H5B C5 H5A 109.47(16) . . ?

loop_

_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C10 C11 C12 C13 0 ?
C2 C2 C1 C3 -106.03(10) 8_565 ?
C2 C2 C1 C6 104.09(10) 8_565 ?
C14 C15 C10 C11 0 ?
C14 C15 C10 N1 180 ?
C12 C11 C10 C15 0 ?
C12 C11 C10 N1 180 ?
C6 N1 C10 C15 180 ?
C6 N1 C10 C11 0 ?
C10 C15 C14 C13 0 ?
C5 O1 C3 O2 0 ?
C5 O1 C3 C1 180 ?
C6 C1 C3 O2 0 ?
C2 C1 C3 O2 147.45(8) 8_565 ?
C2 C1 C3 O2 -147.45(8) ?
C6 C1 C3 O1 180 ?

C2 C1 C3 O1 -32.55(8) 8_565 . . . ?
C2 C1 C3 O1 32.55(8) . . . ?
C11 C12 C13 F1 180 . . . ?
C11 C12 C13 C14 0 . . . ?
C15 C14 C13 F1 180 . . . ?
C15 C14 C13 C12 0 . . . ?
C10 N1 C6 O3 0 . . . ?
C10 N1 C6 C1 180 . . . ?
C3 C1 C6 O3 180 . . . ?
C2 C1 C6 O3 31.72(8) 8_565 . . . ?
C2 C1 C6 O3 -31.72(8) . . . ?
C3 C1 C6 N1 0 . . . ?
C2 C1 C6 N1 -148.28(8) 8_565 . . . ?
C2 C1 C6 N1 148.28(8) . . . ?

loop_

_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A

N1 H1 O2 0.855(16) 1.942(18) 2.6811(19) 144(2) .

END of CIF


```

#\#CIF_1.1

# CIF produced by WinGX routine CIF_UPDATE
# Created on 2014-01-19 at 22:05:51
# Using CIFTbx version 2.6.2 16 Jun 1998

# Dictionary name : cif_core.dic
# Dictionary vers : 2.4
# Request file    : c:\wingx\files\archive.reqdat
# CIF files read  : gl579_1 gl579_1_od

#----- SECTION 1. GLOBAL INFORMATION -----#
data_global

#----- AUDIT DETAILS -----#
_audit_creation_date          2014-01-19
_audit_creation_method        'WinGX routine CIF_UPDATE'
_audit_contact_author         'V. Kahlenberg'
_audit_contact_author_address
;
Institut f\"ur Mineralogie und Petrographie
Leopold-Franzens-Universit\"at Innsbruck
Innrain 52
A-6020 Innsbruck
Austria
;
_audit_contact_author_email   Volker.Kahlenberg@uibk.ac.at
_audit_contact_author_phone   '+43 512 507 5503'

_audit_conform_dict_name      cif_core.dic
_audit_conform_dict_version    2.4
_audit_conform_dict_location   ftp://ftp.iucr.org/pub/cif_core.dic
_audit_update_record          ?

#----- AUTHOR DETAILS -----#

#----- SECTION 2. COMPOUND(S) DETAILS -----#
data_gl579_1

_audit_creation_date          2014-01-19T22:05:51-00:00
_audit_creation_method        'WinGX routine CIF_UPDATE'
_audit_conform_dict_name      cif_core.dic
_audit_conform_dict_version    2.4
_audit_conform_dict_location   ftp://ftp.iucr.org/pub/cif_core.dic
_publ_requested_category      FO

#-----#
#          CHEMICAL INFORMATION          #
#-----#

_chemical_name_systematic
;
?
;
_chemical_formula_sum         'C17 H14 F2 N2 O2'
_chemical_formula_moiety      'C17 H14 F2 N2 O2'
_chemical_formula_weight      316.3

#-----#
#          UNIT CELL INFORMATION          #
#-----#

```

```

#-----#
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_space_group_name_Hall '-P 1'
loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'
  '-x, -y, -z'

_cell_length_a                 8.6443(4)
_cell_length_b                 11.2465(5)
_cell_length_c                 15.7852(8)
_cell_angle_alpha              100.013(4)
_cell_angle_beta               94.434(4)
_cell_angle_gamma              93.114(4)
_cell_volume                   1503.12(12)
_cell_formula_units_Z          4
_cell_measurement_temperature  173(2)
_cell_measurement_reflns_used  4586
_cell_measurement_theta_min    2.8038
_cell_measurement_theta_max    28.8114

#-----#
#                               CRYSTAL INFORMATION                               #
#-----#

_exptl_crystal_description     'prismatic fragment'
_exptl_crystal_colour          colourless
_exptl_crystal_size_max        0.52
_exptl_crystal_size_mid        0.2
_exptl_crystal_size_min        0.2
_exptl_crystal_density_diffn   1.398
_exptl_crystal_density_method  'not measured'
_exptl_crystal_F_000           656
_exptl_special_details
;
?
;

#-----#
#                               ABSORPTION CORRECTION                               #
#-----#

_exptl_absorpt_coefficient_mu   0.109
_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_process_details
;
  CrysAlisPro, Agilent Technologies,
  Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
  (compiled Jul 11 2012,15:38:31)
  Empirical absorption correction using spherical harmonics,
  implemented in SCALE3 ABSPACK scaling algorithm.
;
_exptl_absorpt_correction_T_min 0.91558
_exptl_absorpt_correction_T_max 1

#-----#
#                               DATA COLLECTION                               #
#-----#

_diffn_ambient_temperature     173(2)
_diffn_radiation_wavelength    0.71073
_diffn_radiation_type           MoK\alpha

```

```

_diffrn_radiation_monochromator      graphite
_diffrn_detector_area_resol_mean    10.3575
_diffrn_orient_matrix_ub_11         0.0579333
_diffrn_orient_matrix_ub_12         0.0404344
_diffrn_orient_matrix_ub_13         0.0258365
_diffrn_orient_matrix_ub_21         -0.0560603
_diffrn_orient_matrix_ub_22         0.0431
_diffrn_orient_matrix_ub_23         0.0092966
_diffrn_orient_matrix_ub_31         -0.0175152
_diffrn_orient_matrix_ub_32         -0.0250742
_diffrn_orient_matrix_ub_33         0.0366664
_diffrn_measurement_device_type      'Xcalibur, Ruby, Gemini ultra'
_diffrn_measurement_method           '\w scans'
_diffrn_reflns_av_R_equivalents      0.0196
_diffrn_reflns_av_unetI/netI        0.0322
_diffrn_reflns_number                9200
_diffrn_reflns_limit_h_min           -10
_diffrn_reflns_limit_h_max           10
_diffrn_reflns_limit_k_min           -12
_diffrn_reflns_limit_k_max           13
_diffrn_reflns_limit_l_min           -18
_diffrn_reflns_limit_l_max           19
_diffrn_reflns_theta_min             2.81
_diffrn_reflns_theta_max             25.35
_diffrn_reflns_theta_full            25.35
_diffrn_measured_fraction_theta_full 0.988
_diffrn_measured_fraction_theta_max 0.988
_reflns_number_total                 5455
_reflns_number_gt                    4585
_reflns_threshold_expression         >2sigma(I)

#-----#
#                COMPUTER PROGRAMS USED                #
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;
    CrysAlisPro, Agilent Technologies,
    Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
    (compiled Jul 11 2012,15:38:31)
;
_computing_cell_refinement
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    CrysAlisPro, Agilent Technologies,
    Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
    (compiled Jul 11 2012,15:38:31)
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_computing_data_reduction
;
    CrysAlisPro, Agilent Technologies,
    Version 1.171.36.20 (release 27-06-2012 CrysAlis171 .NET)
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;
_computing_structure_solution        'SIR2002 (Burla et al., 2003)'
_computing_structure_refinement     'SHELXL-97 (Sheldrick, 1997)'

#-----#
#                STRUCTURE SOLUTION                #
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_atom_sites_solution_primary         direct
_atom_sites_solution_secondary       difmap

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_atom_sites_solution_hydrogens          geom

#-----#
#                               REFINEMENT INFORMATION                               #
#-----#

_refine_special_details
;
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^ > 2sigma(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        Fsqr
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0391P)^2^+0.3963P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment          mixed
_refine_ls_extinction_method           none
_refine_ls_number_reflns               5455
_refine_ls_number_parameters           431
_refine_ls_number_restraints           4
_refine_ls_R_factor_all                 0.0461
_refine_ls_R_factor_gt                 0.0364
_refine_ls_wR_factor_ref               0.091
_refine_ls_wR_factor_gt               0.0845
_refine_ls_goodness_of_fit_ref         1.029
_refine_ls_restrained_S_all            1.029
_refine_ls_shift/su_max                0
_refine_ls_shift/su_mean               0
_refine_diff_density_max               0.223
_refine_diff_density_min               -0.221
_refine_diff_density_rms               0.04

#-----#
#                               ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS       #
#-----#

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  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.006 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F F 0.0171 0.0103 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity

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_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group

O1B	O	0.99620(11)	0.49382(10)	0.60707(7)	0.0290(2)	Uani	1	1	d
F1B	F	1.05955(12)	1.08212(8)	0.64373(6)	0.0448(3)	Uani	1	1	d
O1A	O	1.01091(11)	1.06762(9)	0.10434(6)	0.0270(2)	Uani	1	1	d
F1A	F	1.05353(12)	0.51634(9)	0.14778(8)	0.0537(3)	Uani	1	1	d
N2A	N	0.69018(14)	1.05106(11)	-0.08893(8)	0.0232(3)	Uani	1	1	d	D	.	.	.
N1B	N	0.81171(13)	0.61012(11)	0.56090(8)	0.0237(3)	Uani	1	1	d	D	.	.	.
F2A	F	0.38825(13)	1.00250(11)	-0.41567(6)	0.0548(3)	Uani	1	1	d
N1A	N	0.80353(13)	0.92956(11)	0.07086(8)	0.0229(3)	Uani	1	1	d	D	.	.	.
F2B	F	0.38837(12)	0.52230(11)	0.09616(6)	0.0545(3)	Uani	1	1	d
O2B	O	0.50203(10)	0.34733(9)	0.46644(6)	0.0274(2)	Uani	1	1	d
O2A	O	0.51370(11)	1.14986(9)	-0.00909(7)	0.0280(2)	Uani	1	1	d
N2B	N	0.68763(13)	0.43676(11)	0.39943(8)	0.0243(3)	Uani	1	1	d	D	.	.	.
C6B	C	0.63489(15)	0.39205(12)	0.46612(9)	0.0215(3)	Uani	1	1	d
C6A	C	0.64340(15)	1.11078(12)	-0.01490(9)	0.0207(3)	Uani	1	1	d
C9B	C	0.88352(15)	0.72880(13)	0.58403(9)	0.0225(3)	Uani	1	1	d
C10A	C	0.82355(17)	0.71423(14)	0.04103(10)	0.0281(3)	Uani	1	1	d
H10A	H	0.7478	0.7097	-0.0048	0.034	Uiso	1	1	calc	R	.	.	.
C1A	C	0.76512(16)	1.13611(13)	0.06031(9)	0.0222(3)	Uani	1	1	d
C1B	C	0.75396(15)	0.39599(13)	0.54188(9)	0.0221(3)	Uani	1	1	d
C16A	C	0.60643(16)	1.03838(13)	-0.17152(9)	0.0233(3)	Uani	1	1	d
C21B	C	0.67588(17)	0.53224(15)	0.27548(10)	0.0304(3)	Uani	1	1	d
H21B	H	0.7737	0.5694	0.2956	0.036	Uiso	1	1	calc	R	.	.	.
C9A	C	0.87503(15)	0.82548(13)	0.08990(9)	0.0222(3)	Uani	1	1	d
C12B	C	1.00043(18)	0.96492(14)	0.62403(10)	0.0312(4)	Uani	1	1	d
C17A	C	0.51699(19)	1.12898(15)	-0.19376(10)	0.0343(4)	Uani	1	1	d
H17A	H	0.507	1.1983	-0.1533	0.041	Uiso	1	1	calc	R	.	.	.
C14B	C	1.00411(18)	0.76226(14)	0.64834(10)	0.0300(3)	Uani	1	1	d
H14B	H	1.0446	0.7051	0.6783	0.036	Uiso	1	1	calc	R	.	.	.
C11A	C	0.88405(18)	0.60945(14)	0.05989(11)	0.0330(4)	Uani	1	1	d
H11A	H	0.8499	0.5343	0.0273	0.04	Uiso	1	1	calc	R	.	.	.
C10B	C	0.82237(17)	0.81548(14)	0.54089(10)	0.0279(3)	Uani	1	1	d
H10B	H	0.7416	0.7928	0.4977	0.034	Uiso	1	1	calc	R	.	.	.
C11B	C	0.87964(18)	0.93455(15)	0.56120(10)	0.0318(4)	Uani	1	1	d
H11B	H	0.8373	0.9929	0.533	0.038	Uiso	1	1	calc	R	.	.	.
C12A	C	0.99560(18)	0.61922(15)	0.12783(11)	0.0343(4)	Uani	1	1	d
C4A	C	0.87315(15)	1.04158(13)	0.07945(8)	0.0205(3)	Uani	1	1	d
C2B	C	0.70298(18)	0.33391(14)	0.61410(10)	0.0309(4)	Uani	1	1	d
H2B1	H	0.746	0.3673	0.6725	0.037	Uiso	1	1	calc	R	.	.	.
H2B2	H	0.5962	0.3005	0.6093	0.037	Uiso	1	1	calc	R	.	.	.
C19A	C	0.46061(19)	1.01452(16)	-0.33441(10)	0.0354(4)	Uani	1	1	d
C16B	C	0.60447(15)	0.45424(13)	0.32193(9)	0.0229(3)	Uani	1	1	d
C4B	C	0.86658(15)	0.50395(13)	0.57194(8)	0.0215(3)	Uani	1	1	d
C14A	C	0.98856(18)	0.83276(14)	0.15809(10)	0.0300(3)	Uani	1	1	d
H14A	H	1.0235	0.9075	0.1911	0.036	Uiso	1	1	calc	R	.	.	.
C13B	C	1.06417(19)	0.88206(15)	0.66772(10)	0.0349(4)	Uani	1	1	d
H13B	H	1.1466	0.9055	0.7098	0.042	Uiso	1	1	calc	R	.	.	.
C21A	C	0.62209(19)	0.93680(15)	-0.23245(10)	0.0347(4)	Uani	1	1	d
H21A	H	0.6827	0.8762	-0.218	0.042	Uiso	1	1	calc	R	.	.	.
C19B	C	0.45951(19)	0.49907(16)	0.17086(10)	0.0348(4)	Uani	1	1	d
C17B	C	0.45913(16)	0.39745(14)	0.29077(9)	0.0268(3)	Uani	1	1	d
H17B	H	0.4109	0.3441	0.321	0.032	Uiso	1	1	calc	R	.	.	.
C3B	C	0.80858(18)	0.27362(14)	0.55377(10)	0.0319(4)	Uani	1	1	d
H3B1	H	0.7663	0.2033	0.5122	0.038	Uiso	1	1	calc	R	.	.	.
H3B2	H	0.9161	0.2702	0.5753	0.038	Uiso	1	1	calc	R	.	.	.
C20A	C	0.5483(2)	0.92420(16)	-0.31500(10)	0.0392(4)	Uani	1	1	d
H20A	H	0.5585	0.8557	-0.3561	0.047	Uiso	1	1	calc	R	.	.	.
C18B	C	0.38624(18)	0.42061(15)	0.21430(10)	0.0328(4)	Uani	1	1	d
H18B	H	0.289	0.3832	0.193	0.039	Uiso	1	1	calc	R	.	.	.
C18A	C	0.4427(2)	1.11625(16)	-0.27600(11)	0.0403(4)	Uani	1	1	d
H18A	H	0.3816	1.1761	-0.2912	0.048	Uiso	1	1	calc	R	.	.	.

C20B C 0.60327(18) 0.55530(16) 0.19971(10) 0.0362(4) Uani 1 1 d . . .
H20B H 0.6509 0.608 0.1688 0.043 Uiso 1 1 calc R . . .
C13A C 1.04953(19) 0.72786(16) 0.17671(11) 0.0376(4) Uani 1 1 d . . .
H13A H 1.1262 0.7315 0.222 0.045 Uiso 1 1 calc R . . .
C2A C 0.7238(2) 1.22269(16) 0.13825(10) 0.0392(4) Uani 1 1 d . . .
H2A1 H 0.6195 1.2505 0.1372 0.047 Uiso 1 1 calc R . . .
H2A2 H 0.7678 1.2118 0.1946 0.047 Uiso 1 1 calc R . . .
C3A C 0.8304(2) 1.26612(14) 0.07976(12) 0.0399(4) Uani 1 1 d . . .
H3A1 H 0.9395 1.2818 0.1004 0.048 Uiso 1 1 calc R . . .
H3A2 H 0.7912 1.3204 0.043 0.048 Uiso 1 1 calc R . . .
H8A H 0.7044(16) 0.9172(15) 0.0500(10) 0.036(5) Uiso 1 1 d D . . .
H15A H 0.7814(17) 1.0219(15) -0.0862(11) 0.033(4) Uiso 1 1 d D . . .
H15B H 0.7870(16) 0.4628(15) 0.4047(10) 0.033(4) Uiso 1 1 d D . . .
H8B H 0.7161(17) 0.6085(15) 0.5390(10) 0.035(5) Uiso 1 1 d D . . .

loop_

_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
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F1B 0.0608(6) 0.0295(5) 0.0408(6) 0.0057(4) -0.0050(5) -0.0109(5)
O1A 0.0176(5) 0.0283(6) 0.0336(6) 0.0039(5) -0.0043(4) 0.0025(4)
F1A 0.0504(6) 0.0357(6) 0.0821(8) 0.0296(6) -0.0013(6) 0.0168(5)
N2A 0.0187(6) 0.0261(7) 0.0248(6) 0.0047(5) -0.0016(5) 0.0067(5)
N1B 0.0143(6) 0.0269(7) 0.0288(7) 0.0045(5) -0.0030(5) 0.0011(5)
F2A 0.0587(7) 0.0726(8) 0.0283(5) 0.0036(5) -0.0161(5) 0.0095(6)
N1A 0.0167(6) 0.0229(6) 0.0296(7) 0.0080(5) -0.0028(5) 0.0031(5)
F2B 0.0494(6) 0.0824(8) 0.0348(5) 0.0253(6) -0.0117(5) 0.0075(6)
O2B 0.0154(5) 0.0319(6) 0.0355(6) 0.0100(5) -0.0011(4) -0.0014(4)
O2A 0.0181(5) 0.0315(6) 0.0340(6) 0.0046(5) -0.0003(4) 0.0071(4)
N2B 0.0145(6) 0.0325(7) 0.0259(6) 0.0072(5) -0.0020(5) -0.0002(5)
C6B 0.0173(7) 0.0196(7) 0.0269(7) 0.0022(6) 0.0011(6) 0.0043(6)
C6A 0.0179(7) 0.0172(7) 0.0279(8) 0.0072(6) -0.0001(6) 0.0013(5)
C9B 0.0182(7) 0.0281(8) 0.0215(7) 0.0043(6) 0.0036(6) 0.0005(6)
C10A 0.0261(8) 0.0277(8) 0.0310(8) 0.0083(7) -0.0010(6) 0.0024(6)
C1A 0.0207(7) 0.0202(7) 0.0256(7) 0.0050(6) -0.0008(6) 0.0027(6)
C1B 0.0167(7) 0.0251(8) 0.0254(7) 0.0065(6) 0.0009(6) 0.0037(6)
C16A 0.0200(7) 0.0260(8) 0.0243(7) 0.0067(6) -0.0011(6) 0.0012(6)
C21B 0.0219(7) 0.0366(9) 0.0337(8) 0.0105(7) -0.0009(6) 0.0015(6)
C9A 0.0191(7) 0.0255(8) 0.0242(7) 0.0086(6) 0.0044(6) 0.0056(6)
C12B 0.0383(9) 0.0264(8) 0.0277(8) 0.0037(7) 0.0035(7) -0.0049(7)
C17A 0.0418(9) 0.0294(9) 0.0298(8) 0.0022(7) -0.0065(7) 0.0088(7)
C14B 0.0317(8) 0.0310(9) 0.0265(8) 0.0067(7) -0.0041(6) 0.0007(7)
C11A 0.0351(9) 0.0231(8) 0.0417(9) 0.0067(7) 0.0057(7) 0.0040(7)
C10B 0.0221(7) 0.0350(9) 0.0272(8) 0.0095(7) -0.0015(6) -0.0009(6)
C11B 0.0329(8) 0.0326(9) 0.0324(8) 0.0137(7) 0.0008(7) 0.0013(7)
C12A 0.0310(8) 0.0286(9) 0.0498(10) 0.0206(8) 0.0061(8) 0.0124(7)
C4A 0.0198(7) 0.0247(8) 0.0170(7) 0.0031(6) 0.0003(5) 0.0045(6)
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C19A 0.0321(8) 0.0491(11) 0.0234(8) 0.0068(7) -0.0077(7) 0.0005(8)
C16B 0.0191(7) 0.0262(8) 0.0233(7) 0.0028(6) 0.0007(6) 0.0073(6)
C4B 0.0160(7) 0.0306(8) 0.0187(7) 0.0060(6) 0.0027(6) 0.0026(6)
C14A 0.0335(8) 0.0268(8) 0.0293(8) 0.0065(7) -0.0038(7) 0.0043(7)
C13B 0.0377(9) 0.0364(9) 0.0274(8) 0.0038(7) -0.0086(7) -0.0044(7)
C21A 0.0368(9) 0.0335(9) 0.0334(9) 0.0037(7) -0.0017(7) 0.0129(7)
C19B 0.0329(9) 0.0469(10) 0.0257(8) 0.0092(7) -0.0041(7) 0.0128(8)
C17B 0.0219(7) 0.0296(8) 0.0280(8) 0.0034(6) -0.0005(6) 0.0022(6)
C3B 0.0301(8) 0.0266(8) 0.0394(9) 0.0095(7) -0.0059(7) 0.0065(7)
C20A 0.0447(10) 0.0397(10) 0.0289(9) -0.0046(7) -0.0021(7) 0.0067(8)
C18B 0.0254(8) 0.0411(10) 0.0288(8) 0.0011(7) -0.0061(7) 0.0026(7)

C18A 0.0461(10) 0.0395(10) 0.0352(9) 0.0091(8) -0.0099(8) 0.0138(8)
C20B 0.0326(9) 0.0448(10) 0.0354(9) 0.0172(8) 0.0046(7) 0.0067(8)
C13A 0.0344(9) 0.0406(10) 0.0399(9) 0.0170(8) -0.0090(7) 0.0071(8)
C2A 0.0437(10) 0.0403(10) 0.0300(9) -0.0051(7) -0.0076(7) 0.0212(8)
C3A 0.0386(9) 0.0210(8) 0.0565(11) 0.0067(8) -0.0170(8) -0.0005(7)

#-----#
MOLECULAR GEOMETRY #
#-----#

_geom_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.

;

loop_

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_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2
_geom_bond_publ_flag

O1B C4B 1.2311(15) . ?
F1B C12B 1.3619(18) . ?
O1A C4A 1.2280(16) . ?
F1A C12A 1.3616(17) . ?
N2A C6A 1.3453(18) . ?
N2A C16A 1.4221(18) . ?
N2A H15A 0.871(13) . ?
N1B C4B 1.3425(18) . ?
N1B C9B 1.4162(19) . ?
N1B H8B 0.869(13) . ?
F2A C19A 1.3642(17) . ?
N1A C4A 1.3466(19) . ?
N1A C9A 1.4194(17) . ?
N1A H8A 0.888(13) . ?
F2B C19B 1.3599(17) . ?
O2B C6B 1.2292(17) . ?
O2A C6A 1.2304(16) . ?
N2B C6B 1.3425(19) . ?
N2B C16B 1.4195(17) . ?
N2B H15B 0.886(14) . ?
C6B C1B 1.5093(18) . ?
C6A C1A 1.5014(19) . ?
C9B C14B 1.386(2) . ?
C9B C10B 1.387(2) . ?
C10A C9A 1.382(2) . ?
C10A C11A 1.384(2) . ?
C10A H10A 0.93 . ?
C1A C4A 1.5065(18) . ?
C1A C3A 1.509(2) . ?
C1A C2A 1.509(2) . ?
C1B C4B 1.499(2) . ?
C1B C3B 1.5162(19) . ?
C1B C2B 1.517(2) . ?
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C16A C17A 1.388(2) . ?
C21B C20B 1.379(2) . ?
C21B C16B 1.387(2) . ?
C21B H21B 0.93 . ?

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C12B C13B 1.367(2) . ?
C12B C11B 1.369(2) . ?
C17A C18A 1.384(2) . ?
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C14B C13B 1.391(2) . ?
C14B H14B 0.93 . ?
C11A C12A 1.371(2) . ?
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C10B C11B 1.377(2) . ?
C10B H10B 0.93 . ?
C11B H11B 0.93 . ?
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C2B H2B2 0.97 . ?
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C9A N1A H8A 115.4(11) . . ?
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C6B N2B H15B 116.7(11) . . ?
C16B N2B H15B 114.1(11) . . ?
O2B C6B N2B 124.06(13) . . ?
O2B C6B C1B 121.05(13) . . ?
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C4B C1B C6B 121.12(11) . . ?
C4B C1B C3B 117.18(11) . . ?
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C3B C2B H2B2 117.7 . . ?
C1B C2B H2B2 117.7 . . ?
H2B1 C2B H2B2 114.8 . . ?
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C21B C16B C17B 119.43(13) . . ?

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C16B C17B H17B 120.1 . . ?
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C1B C3B H3B2 117.7 . . ?
H3B1 C3B H3B2 114.8 . . ?
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C14A C13A H13A 120.4 . . ?
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C3A C2A H2A2 117.7 . . ?
C1A C2A H2A2 117.7 . . ?
H2A1 C2A H2A2 114.8 . . ?
C2A C3A C1A 60.73(11) . . ?
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C2A C1A C4A O1A -70.68(18) ?
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C3B C1B C4B O1B -2.07(19) ?
C2B C1B C4B O1B 63.09(17) ?
C6B C1B C4B N1B 31.94(17) ?
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C2B C1B C4B N1B -114.04(13) ?
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N1A C9A C14A C13A 176.88(14) ?
F1B C12B C13B C14B 179.70(14) ?
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C9B C14B C13B C12B 1.4(2) ?

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 N2B C16B C17B C18B 179.74(13) ?
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 F2B C19B C20B C21B 179.90(14) ?
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 C16B C21B C20B C19B -0.4(2) ?
 F1A C12A C13A C14A -178.51(14) ?
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 C9A C14A C13A C12A -0.5(2) ?
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 C4A C1A C2A C3A 107.43(14) ?
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 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A

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 N2A H15A O1A 0.871(13) 2.120(14) 2.9793(15) 168.7(15) 2_775
 N2B H15B O1B 0.886(14) 1.941(14) 2.8159(15) 169.0(16) 2_766
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END of CIF

data_s412

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_shelx_SHELXL_version_number '2014/7'  
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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'H' 'H' 0.0000 0.0000  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'N' 'N' 0.0061 0.0033  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'O' 'O' 0.0106 0.0060  
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_space_group_name_Hall      'C -2yc'
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_shelx_space_group_comment

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;  
The symmetry employed for this shelxl refinement is uniquely defined  
by the following loop, which should always be used as a source of  
symmetry information in preference to the above space-group names.  
They are only intended as comments.  
;
```

loop_

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'x, -y, z+1/2'  
'x+1/2, y+1/2, z'  
'x+1/2, -y+1/2, z+1/2'  
  
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_cell_length_b              9.5212(4)  
_cell_length_c              7.6800(6)  
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_cell_angle_beta            92.652(3)  
_cell_angle_gamma           90  
_cell_volume                1448.54(13)  
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_diffn_reflns_limit_h_min         -23
_diffn_reflns_limit_h_max         23
_diffn_reflns_limit_k_min         -11
_diffn_reflns_limit_k_max         11
_diffn_reflns_limit_l_min         -9
_diffn_reflns_limit_l_max         9
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_reflns_number_gt                 2254
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_reflns_special_details
;
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.
;

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_computing_cell_refinement        ?
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_computing_structure_solution     ?
_computing_structure_refinement   'SHELXL-2014/7 (Sheldrick, 2014)'
_computing_molecular_graphics     ?

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hydrogens at N2 were found and refined isotropically with bond restraints
(d=87pm).
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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0489P)^2^+0.2380P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    ?
_atom_sites_solution_hydrogens    mixed
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      'SHELXL-2014/7 (Sheldrick 2014'
_refine_ls_extinction_coef        0.013(3)
_refine_ls_extinction_expression  'Fc^^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_abs_structure_details
;
Flack x determined using 987 quotients [(I+)-(I-)]/[(I+)+(I-)]
(Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
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_refine_ls_shift/su_mean          0.000

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_atom_site_fract_z
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O1 O 0.87450(11) 0.4839(2) 0.6688(3) 0.0419(6) Uani 1 1 d . . . . .
O2 O 0.75894(11) 0.4735(2) 0.4985(3) 0.0485(6) Uani 1 1 d . . . . .
O3 O 0.95643(10) -0.01690(18) 0.7278(3) 0.0373(5) Uani 1 1 d . . . . .
N1 N 0.76110(13) -0.0325(2) 0.5002(3) 0.0368(6) Uani 1 1 d . . . . .
N2 N 1.13970(13) -0.4629(3) 0.7443(4) 0.0375(6) Uani 1 1 d D . . . . .
H2N H 1.1559(14) -0.476(3) 0.639(3) 0.033(8) Uiso 1 1 d D . . . . .
H1N H 1.1699(15) -0.459(4) 0.837(4) 0.046(10) Uiso 1 1 d D . . . . .
C1 C 0.85197(14) 0.3525(3) 0.6264(4) 0.0337(7) Uani 1 1 d . . . . .
C2 C 0.78710(14) 0.3460(3) 0.5365(4) 0.0352(7) Uani 1 1 d . . . . .
C3 C 0.75890(15) 0.2192(3) 0.4977(4) 0.0367(7) Uani 1 1 d . . . . .
H3 H 0.7157 0.2157 0.4423 0.044 Uiso 1 1 calc R U . . .

```

```

C4 C 0.79307(14) 0.0920(3) 0.5388(3) 0.0309(7) Uani 1 1 d . . . . .
C6 C 0.79493(14) -0.1491(3) 0.5385(4) 0.0384(8) Uani 1 1 d . . . . .
H6 H 0.7733 -0.2351 0.5137 0.046 Uiso 1 1 calc R U . . .
C7 C 0.86064(15) -0.1537(3) 0.6134(4) 0.0357(7) Uani 1 1 d . . . . .
H7 H 0.8824 -0.2399 0.6363 0.043 Uiso 1 1 calc R U . . .
C8 C 0.89213(14) -0.0293(3) 0.6522(4) 0.0307(7) Uani 1 1 d . . . . .
C9 C 0.85848(14) 0.0986(3) 0.6184(3) 0.0296(7) Uani 1 1 d . . . . .
C10 C 0.88683(14) 0.2317(3) 0.6612(4) 0.0315(7) Uani 1 1 d . . . . .
H10 H 0.9304 0.2366 0.7144 0.038 Uiso 1 1 calc R U . . .
C11 C 1.00041(13) -0.1327(3) 0.7290(4) 0.0322(7) Uani 1 1 d . . . . .
C12 C 1.01940(14) -0.1931(3) 0.5752(4) 0.0356(7) Uani 1 1 d . . . . .
H12 H 1.0008 -0.1607 0.4678 0.043 Uiso 1 1 calc R U . . .
C13 C 1.06590(15) -0.3015(3) 0.5800(4) 0.0353(7) Uani 1 1 d . . . . .
H13 H 1.0778 -0.3440 0.4753 0.042 Uiso 1 1 calc R U . . .
C14 C 1.09533(14) -0.3488(3) 0.7379(4) 0.0318(7) Uani 1 1 d . . . . .
C15 C 1.07620(15) -0.2842(3) 0.8901(4) 0.0352(7) Uani 1 1 d . . . . .
H15 H 1.0955 -0.3141 0.9979 0.042 Uiso 1 1 calc R U . . .
C16 C 1.02910(14) -0.1764(3) 0.8862(4) 0.0332(7) Uani 1 1 d . . . . .
H16 H 1.0169 -0.1334 0.9904 0.040 Uiso 1 1 calc R U . . .
C17 C 0.93687(18) 0.4899(3) 0.7696(5) 0.0467(9) Uani 1 1 d . . . . .
H17A H 0.9728 0.4524 0.7019 0.070 Uiso 1 1 calc R U . . .
H17B H 0.9332 0.4348 0.8750 0.070 Uiso 1 1 calc R U . . .
H17C H 0.9469 0.5867 0.8004 0.070 Uiso 1 1 calc R U . . .
C18 C 0.69605(19) 0.4737(4) 0.4008(6) 0.0616(11) Uani 1 1 d . . . . .
H18A H 0.6618 0.4303 0.4690 0.092 Uiso 1 1 calc R U . . .
H18B H 0.7005 0.4214 0.2936 0.092 Uiso 1 1 calc R U . . .
H18C H 0.6830 0.5697 0.3734 0.092 Uiso 1 1 calc R U . . .

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loop_
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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
O1 0.0383(12) 0.0254(11) 0.0614(14) 0.0019(10) -0.0044(10) -0.0015(9)
O2 0.0376(13) 0.0321(12) 0.0749(16) 0.0086(11) -0.0057(10) 0.0096(9)
O3 0.0315(11) 0.0260(10) 0.0534(13) -0.0035(9) -0.0095(9) 0.0059(9)
N1 0.0303(13) 0.0335(14) 0.0463(14) -0.0051(12) -0.0013(11) -0.0007(11)
N2 0.0302(13) 0.0350(14) 0.0472(17) -0.0015(12) -0.0001(12) 0.0076(11)
C1 0.0306(17) 0.0294(16) 0.0415(17) 0.0011(12) 0.0044(13) -0.0030(12)
C2 0.0299(16) 0.0278(15) 0.0479(19) 0.0053(12) 0.0033(13) 0.0059(12)
C3 0.0265(15) 0.0368(17) 0.0464(18) 0.0015(14) -0.0012(12) 0.0028(12)
C4 0.0286(16) 0.0310(16) 0.0333(16) -0.0002(11) 0.0011(12) 0.0000(12)
C6 0.0340(18) 0.0289(15) 0.052(2) -0.0048(13) 0.0022(15) -0.0015(13)
C7 0.0340(16) 0.0258(15) 0.0472(18) -0.0003(13) 0.0019(13) 0.0015(13)
C8 0.0268(16) 0.0314(16) 0.0338(16) -0.0003(12) -0.0003(12) 0.0010(11)
C9 0.0259(14) 0.0298(16) 0.0332(16) -0.0008(11) 0.0027(12) 0.0022(11)
C10 0.0264(15) 0.0292(16) 0.0387(16) 0.0003(12) 0.0003(12) 0.0022(11)
C11 0.0253(14) 0.0239(14) 0.0469(17) 0.0001(12) -0.0043(12) 0.0004(11)
C12 0.0331(16) 0.0358(15) 0.0370(16) 0.0038(13) -0.0060(12) -0.0001(12)
C13 0.0330(16) 0.0350(15) 0.0378(16) -0.0037(13) 0.0019(12) 0.0009(13)
C14 0.0249(14) 0.0295(14) 0.0410(17) 0.0016(13) -0.0006(12) -0.0033(12)
C15 0.0329(15) 0.0323(15) 0.0396(17) 0.0037(13) -0.0071(13) 0.0011(12)
C16 0.0315(15) 0.0315(14) 0.0365(16) -0.0022(12) -0.0003(12) 0.0023(12)
C17 0.046(2) 0.0321(16) 0.061(2) -0.0006(15) -0.0094(16) -0.0052(14)
C18 0.047(2) 0.049(2) 0.087(3) 0.011(2) -0.0144(19) 0.0143(17)

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_geom_special_details
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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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O1 C17 1.430(4) . ?
O2 C2 1.362(3) . ?
O2 C18 1.425(4) . ?
O3 C8 1.381(3) . ?
O3 C11 1.406(3) . ?
N1 C6 1.324(4) . ?
N1 C4 1.370(4) . ?
N2 C14 1.398(4) . ?
N2 H2N 0.89(2) . ?
N2 H1N 0.91(2) . ?
C1 C10 1.362(4) . ?
C1 C2 1.433(4) . ?
C2 C3 1.358(4) . ?
C3 C4 1.416(4) . ?
C3 H3 0.9400 . ?
C4 C9 1.410(3) . ?
C6 C7 1.400(4) . ?
C6 H6 0.9400 . ?
C7 C8 1.366(4) . ?
C7 H7 0.9400 . ?
C8 C9 1.406(4) . ?
C9 C10 1.419(4) . ?
C10 H10 0.9400 . ?
C11 C16 1.375(4) . ?
C11 C12 1.382(4) . ?
C12 C13 1.384(4) . ?
C12 H12 0.9400 . ?
C13 C14 1.396(4) . ?
C13 H13 0.9400 . ?
C14 C15 1.389(4) . ?
C15 C16 1.387(4) . ?
C15 H15 0.9400 . ?
C16 H16 0.9400 . ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C17 H17C 0.9700 . ?
C18 H18A 0.9700 . ?
C18 H18B 0.9700 . ?
C18 H18C 0.9700 . ?
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  _geom_angle_site_symmetry_3
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C1 O1 C17 115.6(2) . . ?
C2 O2 C18 117.0(3) . . ?
C8 O3 C11 119.8(2) . . ?
C6 N1 C4 116.9(2) . . ?
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C14 N2 H2N 109.1(19) . . ?
C14 N2 H1N 113(2) . . ?
H2N N2 H1N 117(3) . . ?
O1 C1 C10 124.8(3) . . ?
O1 C1 C2 115.6(2) . . ?
C10 C1 C2 119.6(3) . . ?
C3 C2 O2 125.8(3) . . ?
C3 C2 C1 119.7(3) . . ?
O2 C2 C1 114.5(3) . . ?
C2 C3 C4 121.6(3) . . ?
C2 C3 H3 119.2 . . ?
C4 C3 H3 119.2 . . ?
N1 C4 C9 122.7(3) . . ?
N1 C4 C3 118.7(2) . . ?
C9 C4 C3 118.7(3) . . ?
N1 C6 C7 124.8(3) . . ?
N1 C6 H6 117.6 . . ?
C7 C6 H6 117.6 . . ?
C8 C7 C6 118.0(3) . . ?
C8 C7 H7 121.0 . . ?
C6 C7 H7 121.0 . . ?
C7 C8 O3 124.7(3) . . ?
C7 C8 C9 120.2(2) . . ?
O3 C8 C9 115.1(2) . . ?
C8 C9 C4 117.4(3) . . ?
C8 C9 C10 123.4(2) . . ?
C4 C9 C10 119.1(2) . . ?
C1 C10 C9 121.1(2) . . ?
C1 C10 H10 119.4 . . ?
C9 C10 H10 119.4 . . ?
C16 C11 C12 120.5(2) . . ?
C16 C11 O3 118.3(3) . . ?
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C11 C12 C13 119.7(3) . . ?
C11 C12 H12 120.1 . . ?
C13 C12 H12 120.1 . . ?
C12 C13 C14 121.0(3) . . ?
C12 C13 H13 119.5 . . ?
C14 C13 H13 119.5 . . ?
C15 C14 C13 118.0(3) . . ?
C15 C14 N2 120.7(3) . . ?
C13 C14 N2 121.2(3) . . ?
C16 C15 C14 121.3(3) . . ?
C16 C15 H15 119.4 . . ?
C14 C15 H15 119.4 . . ?
C11 C16 C15 119.6(3) . . ?
C11 C16 H16 120.2 . . ?
C15 C16 H16 120.2 . . ?
O1 C17 H17A 109.5 . . ?
O1 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
O1 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
O2 C18 H18A 109.5 . . ?
O2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
O2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?

_refine_diff_density_max 0.167
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_refine_diff_density_rms 0.035

_shelx_res_file

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s412.res created by SHELXL-2014/7

TITL p in Cc
CELL 0.71073 19.8309 9.5212 7.6800 90.000 92.652 90.000
ZERR 4.00 0.0004 0.0004 0.0006 0.000 0.003 0.000
LATT -7
SYMM X, -Y, 0.5+Z
SFAC C H N O
UNIT 68 64 8 12
L.S. 10
ACTA
TEMP -40
OMIT 0 50
OMIT 2 0 0
OMIT -2 8 -1
OMIT -9 1 7
OMIT 11 1 -8
OMIT -7 1 8
OMIT 11 9 -2
BOND
BOND \$H
FMAP 2
PLAN 10
DFIX 0.87 0.02 N2 H1N N2 H2N
WGHT 0.048900 0.238000
EXTI 0.013438
FVAR 0.67463
O1 4 0.874500 0.483884 0.668787 11.00000 0.03828 0.02544 =
0.06138 0.00186 -0.00443 -0.00150
O2 4 0.758941 0.473481 0.498525 11.00000 0.03755 0.03212 =
0.07492 0.00862 -0.00569 0.00958
O3 4 0.956426 -0.016901 0.727770 11.00000 0.03152 0.02601 =
0.05344 -0.00348 -0.00951 0.00588
N1 3 0.761099 -0.032492 0.500184 11.00000 0.03034 0.03352 =
0.04626 -0.00510 -0.00125 -0.00070
N2 3 1.139703 -0.462946 0.744317 11.00000 0.03020 0.03496 =
0.04721 -0.00147 -0.00006 0.00756
H2N 2 1.155859 -0.475856 0.639293 11.00000 0.03310
H1N 2 1.169883 -0.458935 0.836548 11.00000 0.04627
C1 1 0.851973 0.352531 0.626383 11.00000 0.03057 0.02940 =
0.04145 0.00105 0.00436 -0.00295
C2 1 0.787099 0.345969 0.536496 11.00000 0.02991 0.02779 =
0.04792 0.00526 0.00334 0.00592
C3 1 0.758897 0.219173 0.497706 11.00000 0.02654 0.03682 =
0.04642 0.00150 -0.00123 0.00278
AFIX 43
H3 2 0.715663 0.215730 0.442273 11.00000 -1.20000
AFIX 0
C4 1 0.793074 0.091992 0.538784 11.00000 0.02859 0.03096 =
0.03325 -0.00021 0.00114 0.00001
C6 1 0.794931 -0.149122 0.538517 11.00000 0.03403 0.02886 =
0.05238 -0.00477 0.00225 -0.00154
AFIX 43
H6 2 0.773284 -0.235123 0.513672 11.00000 -1.20000
AFIX 0
C7 1 0.860637 -0.153718 0.613403 11.00000 0.03402 0.02580 =
0.04723 -0.00027 0.00186 0.00146
AFIX 43
H7 2 0.882422 -0.239886 0.636287 11.00000 -1.20000

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AFIX 0
C8 1 0.892126 -0.029252 0.652202 11.00000 0.02682 0.03138 =
0.03375 -0.00028 -0.00025 0.00102
C9 1 0.858483 0.098556 0.618444 11.00000 0.02595 0.02985 =
0.03325 -0.00077 0.00271 0.00216
C10 1 0.886829 0.231672 0.661165 11.00000 0.02640 0.02920 =
0.03873 0.00025 0.00034 0.00219
AFIX 43
H10 2 0.930413 0.236567 0.714390 11.00000 -1.20000
AFIX 0
C11 1 1.000413 -0.132719 0.729033 11.00000 0.02534 0.02391 =
0.04688 0.00011 -0.00429 0.00036
C12 1 1.019402 -0.193110 0.575194 11.00000 0.03315 0.03576 =
0.03704 0.00385 -0.00597 -0.00007
AFIX 43
H12 2 1.000813 -0.160667 0.467787 11.00000 -1.20000
AFIX 0
C13 1 1.065897 -0.301541 0.579960 11.00000 0.03304 0.03499 =
0.03784 -0.00367 0.00187 0.00090
AFIX 43
H13 2 1.077843 -0.344041 0.475296 11.00000 -1.20000
AFIX 0
C14 1 1.095333 -0.348764 0.737898 11.00000 0.02488 0.02950 =
0.04097 0.00155 -0.00065 -0.00326
C15 1 1.076197 -0.284190 0.890140 11.00000 0.03289 0.03227 =
0.03961 0.00368 -0.00708 0.00110
AFIX 43
H15 2 1.095538 -0.314135 0.997872 11.00000 -1.20000
AFIX 0
C16 1 1.029096 -0.176364 0.886243 11.00000 0.03147 0.03153 =
0.03651 -0.00222 -0.00033 0.00226
AFIX 43
H16 2 1.016873 -0.133429 0.990393 11.00000 -1.20000
AFIX 0
C17 1 0.936866 0.489933 0.769623 11.00000 0.04614 0.03214 =
0.06075 -0.00058 -0.00940 -0.00522
AFIX 137
H17A 2 0.972807 0.452363 0.701886 11.00000 -1.50000
H17B 2 0.933182 0.434804 0.874968 11.00000 -1.50000
H17C 2 0.946923 0.586738 0.800427 11.00000 -1.50000
AFIX 0
C18 1 0.696050 0.473737 0.400841 11.00000 0.04707 0.04913 =
0.08711 0.01100 -0.01443 0.01425
AFIX 137
H18A 2 0.661758 0.430271 0.469027 11.00000 -1.50000
H18B 2 0.700545 0.421404 0.293636 11.00000 -1.50000
H18C 2 0.683048 0.569709 0.373385 11.00000 -1.50000

AFIX 0
HKLF 4

REM p in Cc
REM R1 = 0.0378 for 2254 Fo > 4sig(Fo) and 0.0432 for all 2492 data
REM 210 parameters refined using 4 restraints

END

WGHT 0.0489 0.2404

REM Highest difference peak 0.167, deepest hole -0.150, 1-sigma level 0.035
Q1 1 0.7658 -0.2830 0.5091 11.00000 0.05 0.17
Q2 1 0.9566 0.0193 0.9283 11.00000 0.05 0.15
Q3 1 0.9559 -0.0045 0.5259 11.00000 0.05 0.15
Q4 1 0.7899 0.6026 0.5519 11.00000 0.05 0.15

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Q5	1	0.8544	0.5992	0.6041	11.00000	0.05	0.14
Q6	1	0.8786	0.5165	0.9499	11.00000	0.05	0.13
Q7	1	0.8877	-0.2824	0.6652	11.00000	0.05	0.12
Q8	1	0.9354	0.4906	0.5632	11.00000	0.05	0.12
Q9	1	1.0736	-0.2858	1.0795	11.00000	0.05	0.12
Q10	1	1.0190	-0.1731	1.1480	11.00000	0.05	0.12

;

_shelx_res_checksum 61924

_shelx_hkl_file

;

-23	-1	-1	14.59	3.67
-23	-1	0	18.40	4.20
-23	1	-1	13.47	2.79
-23	1	0	27.25	3.55
-23	1	1	6.81	3.03
-23	3	0	5.71	4.49
-23	3	1	5.52	4.23
-22	-4	-1	25.70	5.07
-22	-4	0	38.81	5.98
-22	-2	-2	-1.80	5.68
-22	-2	0	51.12	8.15
-22	-2	2	38.69	6.34
-22	-2	3	7.90	3.32
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-22	0	-2	255.04	21.72
-22	0	-1	2.59	2.09
-22	0	0	53.58	5.12
-22	0	1	-0.50	2.51
-22	0	2	164.35	13.59
-22	2	-2	3.61	2.20
-22	2	0	53.14	3.94
-22	2	1	8.88	4.59
-22	2	2	43.03	4.72
-22	2	3	3.31	2.62
-22	4	-1	30.80	3.44
-22	4	0	48.86	7.27
-22	4	1	9.00	5.40
-21	-5	-1	17.14	9.52
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-21	-5	2	-1.30	3.69
-21	-3	-3	24.70	5.27
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-21	-3	0	12.82	3.79
-21	-3	1	31.58	4.16
-21	-3	2	81.90	7.96
-21	-3	3	56.55	12.33
-21	-3	4	59.60	7.10
-21	-1	-3	123.21	16.87
-21	-1	-2	8.18	2.97
-21	-1	-1	83.91	8.43
-21	-1	0	30.25	6.16
-21	-1	2	36.60	4.72
-21	-1	3	45.56	8.37
-21	1	-3	155.50	9.98
-21	1	-2	10.50	3.30
-21	1	-1	79.92	8.76
-21	1	0	26.32	3.28
-21	1	1	15.60	3.32
-21	1	2	39.44	4.14
-21	1	3	42.25	4.16
-21	3	-3	19.98	4.29
-21	3	-2	-9.00	3.48
-21	3	-1	23.14	4.23

-21	3	0	14.82	2.46
-21	3	1	31.47	3.14
-21	3	2	68.56	8.11
-21	5	-1	5.11	4.79
-21	5	0	14.52	4.50
-21	5	1	5.11	4.70
-21	5	2	6.00	4.80
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-20	-4	3	143.04	11.48
-20	-2	-4	0.20	3.73
-20	-2	-2	10.82	2.90
-20	-2	-1	-3.31	3.89
-20	-2	0	66.26	6.67
-20	-2	1	20.34	3.52
-20	-2	2	20.61	5.72
-20	-2	3	29.92	4.38
-20	-2	4	32.95	5.17
-20	-2	5	1.80	3.48
-20	0	-4	56.55	4.36
-20	0	-3	-0.20	1.81
-20	0	-2	279.56	20.06
-20	0	-1	-0.40	2.29
-20	0	0	122.54	7.08
-20	0	1	0.00	1.00
-20	0	2	5.52	2.73
-20	0	3	-0.10	2.43
-20	0	4	112.15	12.28
-20	0	5	0.71	3.41
-20	2	-4	9.99	2.72
-20	2	-3	2.50	3.10
-20	2	-2	8.82	3.03
-20	2	-1	0.30	1.80
-20	2	0	62.57	4.27
-20	2	1	16.32	2.02
-20	2	2	27.56	8.51
-20	2	3	31.02	3.34
-20	2	4	32.49	4.22
-20	4	-3	47.75	6.77
-20	4	-2	39.69	4.03
-20	4	-1	5.29	2.12
-20	4	0	63.20	5.25
-20	4	1	27.88	4.01
-20	4	2	205.92	13.49
-20	4	3	141.85	22.39
-20	6	-1	9.12	5.62
-20	6	0	6.60	4.52
-20	6	1	20.70	18.56
-19	-5	-3	3.39	2.98
-19	-5	-1	19.01	3.92
-19	-5	0	1.69	2.60
-19	-5	1	42.64	5.35
-19	-5	2	78.85	15.45
-19	-5	3	82.45	11.44
-19	-5	4	133.63	17.11
-19	-3	-4	22.00	14.26
-19	-3	-3	19.10	3.58
-19	-3	-2	10.18	3.13
-19	-3	-1	1.49	1.59
-19	-3	0	125.66	8.74
-19	-3	1	196.28	14.01
-19	-3	2	193.77	15.59
-19	-3	3	84.09	8.99
-19	-3	5	22.56	5.32

-19	-1	-5	-3.20	3.19
-19	-1	-4	16.89	2.63
-19	-1	-3	151.78	8.87
-19	-1	-2	147.62	6.56
-19	-1	-1	0.30	1.31
-19	-1	0	192.38	14.98
-19	-1	1	37.95	5.67
-19	-1	3	99.80	8.19
-19	-1	4	118.59	11.11
-19	-1	5	7.40	2.77
-19	1	-5	-0.79	3.28
-19	1	-4	11.42	3.38
-19	1	-3	136.89	7.02
-19	1	-2	141.13	8.08
-19	1	-1	2.50	1.71
-19	1	0	183.33	9.48
-19	1	1	26.94	3.84
-19	1	2	131.10	8.70
-19	1	3	95.84	7.64
-19	1	4	116.86	11.46
-19	1	5	14.06	3.30
-19	3	-4	5.52	3.29
-19	3	-3	29.70	3.49
-19	3	-2	1.10	2.79
-19	3	-1	8.18	2.80
-19	3	0	121.22	8.37
-19	3	1	199.94	9.62
-19	3	2	176.62	10.37
-19	3	3	91.58	7.46
-19	5	-3	2.69	4.30
-19	5	-2	22.75	4.58
-19	5	-1	17.81	4.30
-19	5	0	1.80	3.89
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-19	5	2	89.11	8.12
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-19	5	4	127.92	14.48
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-18	-6	-2	14.21	3.47
-18	-6	1	55.06	5.94
-18	-6	2	2.99	3.60
-18	-4	-3	6.50	2.91
-18	-4	-2	7.78	2.51
-18	-4	-1	19.54	3.54
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-18	-4	2	491.51	34.59
-18	-4	3	161.29	12.19
-18	-4	4	144.96	10.60
-18	-2	-5	7.51	9.43
-18	-2	-4	14.82	2.93
-18	-2	-3	64.48	5.94
-18	-2	-2	73.27	5.65
-18	-2	-1	65.61	4.54
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-18	-2	4	50.41	9.23
-18	-2	5	30.25	4.29
-18	-2	6	1.90	3.39
-18	0	-5	-0.40	1.69
-18	0	-4	115.56	6.66
-18	0	-3	1.30	1.30
-18	0	-2	347.08	15.28
-18	0	-1	0.90	1.10

-18	0	0	181.71	7.28
-18	0	1	2.10	1.91
-18	0	2	3.69	2.11
-18	0	3	2.59	2.00
-18	0	4	219.63	15.12
-18	0	5	-0.71	2.91
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-18	2	-5	6.00	2.11
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-18	2	-3	90.06	5.12
-18	2	-2	86.12	5.20
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-18	2	2	29.27	2.38
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-18	2	5	30.58	3.98
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-18	4	-3	15.92	3.59
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-18	6	-3	3.10	3.20
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-18	6	1	58.06	12.34
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-18	6	3	11.49	4.61
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-17	-7	0	21.90	4.40
-17	-7	2	65.93	7.47
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-17	-5	-1	104.24	5.31
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-17	-5	2	164.61	12.57
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-17	-5	5	2.99	4.08
-17	-3	-5	48.16	5.14
-17	-3	-4	10.69	3.60
-17	-3	-3	35.64	3.94
-17	-3	-2	4.71	2.91
-17	-3	-1	56.85	3.32
-17	-3	0	256.64	16.34
-17	-3	1	119.46	9.18
-17	-3	2	136.89	10.30
-17	-3	4	130.87	11.44
-17	-3	6	3.61	3.19
-17	-1	-5	34.34	4.81
-17	-1	-4	128.60	6.80
-17	-1	-3	61.00	2.97
-17	-1	-2	97.02	4.14
-17	-1	-1	3.10	0.99
-17	-1	0	126.56	6.75
-17	-1	1	24.40	3.26
-17	-1	2	51.12	4.15
-17	-1	4	26.63	3.92
-17	-1	5	24.21	4.03
-17	-1	6	10.11	3.37
-17	1	-6	3.69	3.49

-17	1	-5	27.04	2.60
-17	1	-4	117.07	6.49
-17	1	-3	55.06	3.56
-17	1	-2	95.84	4.11
-17	1	-1	4.80	1.10
-17	1	0	134.79	7.89
-17	1	1	29.70	2.18
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-17	1	4	26.21	3.07
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-17	3	-5	50.27	4.54
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-17	3	-3	34.93	2.95
-17	3	-2	8.01	1.58
-17	3	-1	62.09	4.26
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-17	3	3	170.82	8.10
-17	3	4	126.11	10.56
-17	5	-4	7.67	2.38
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-17	5	4	3.50	3.59
-17	7	-2	-0.50	4.32
-17	7	-1	31.02	5.35
-17	7	0	27.14	4.48
-17	7	1	72.59	16.87
-17	7	2	65.61	6.80
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-16	-8	-1	7.51	2.90
-16	-8	0	8.88	2.21
-16	-8	1	16.32	4.69
-16	-6	-4	15.52	4.41
-16	-6	-3	2.79	3.21
-16	-6	-1	10.37	2.19
-16	-6	0	12.82	3.08
-16	-6	1	157.50	10.54
-16	-6	2	1.10	2.50
-16	-6	3	6.50	2.81
-16	-6	4	8.82	3.33
-16	-6	5	16.56	9.69
-16	-4	-5	28.52	3.95
-16	-4	-4	12.82	2.72
-16	-4	-3	109.20	8.15
-16	-4	-2	109.83	5.24
-16	-4	-1	294.47	16.82
-16	-4	0	1428.08	58.95
-16	-4	1	298.60	16.59
-16	-4	2	246.80	18.22
-16	-4	3	206.50	18.68
-16	-4	4	0.30	3.52
-16	-4	5	9.92	3.40
-16	-4	6	8.53	3.68
-16	-2	-6	0.20	3.12
-16	-2	-5	4.88	2.92
-16	-2	-4	88.17	4.51
-16	-2	-3	145.93	9.18

-16	-2	-2	69.06	4.32
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-16	-2	2	4.08	1.98
-16	-2	3	168.48	12.72
-16	-2	4	110.04	10.70
-16	-2	5	11.83	5.09
-16	0	-6	7.78	3.91
-16	0	-5	-0.71	1.92
-16	0	-4	179.83	6.70
-16	0	-3	1.00	1.10
-16	0	-2	41.47	2.19
-16	0	-1	-1.21	1.21
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-16	0	1	2.99	1.21
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-16	0	4	166.67	14.72
-16	0	5	-1.30	2.01
-16	0	6	38.19	6.06
-16	0	7	-2.19	3.49
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-16	2	-4	74.13	3.96
-16	2	-3	143.76	6.71
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-16	4	-4	6.81	2.09
-16	4	-3	98.21	6.14
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-16	4	3	203.06	20.23
-16	4	4	-5.02	2.69
-16	6	-4	7.08	2.39
-16	6	-3	0.40	1.59
-16	6	-2	3.10	1.41
-16	6	-1	21.62	3.72
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-16	6	1	160.02	12.65
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-16	8	-2	5.52	3.81
-16	8	-1	24.50	12.38
-16	8	0	12.11	7.10
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-15	-7	-1	11.02	3.12
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-15	-5	-5	3.61	2.62
-15	-5	-3	23.23	3.18
-15	-5	-2	25.40	1.81
-15	-5	-1	78.32	3.72
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-15	-5	2	198.53	15.22
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-15	-3	-6	1.90	2.90
-15	-3	-4	90.44	8.18
-15	-3	-3	130.64	5.94
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-15	-3	2	203.06	10.83
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-15	-1	-5	13.18	1.67
-15	-1	-4	8.82	1.31
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-15	-1	-2	67.73	3.13
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-15	-1	3	61.62	5.49
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-15	1	-2	67.57	2.63
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-15	5	-3	20.61	2.18
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-13	-7	-5	13.40	3.07
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-13	-3	-7	4.71	3.39
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-13	-3	-2	285.27	13.17
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-13	-1	-5	17.14	1.74
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-9	-5	-7	25.00	4.50
-9	-5	-6	55.50	4.17
-9	-5	-5	19.98	2.86
-9	-5	-4	207.94	13.27
-9	-5	-3	186.60	7.38
-9	-5	-2	18.58	1.81
-9	-5	-1	153.26	10.15
-9	-5	0	43.96	2.25
-9	-5	1	350.81	20.60
-9	-5	2	93.90	8.91
-9	-5	3	98.21	5.15
-9	-5	4	431.39	31.16
-9	-5	5	2.19	2.60
-9	-5	6	3.50	2.81
-9	-5	7	22.18	40.60
-9	-3	-8	5.62	3.79
-9	-3	-7	74.30	8.62
-9	-3	-6	223.80	11.67
-9	-3	-5	94.48	6.42
-9	-3	-4	5.29	1.89
-9	-3	-3	103.84	4.28
-9	-3	-2	149.33	6.11
-9	-3	-1	89.30	6.80
-9	-3	0	1163.49	75.04
-9	-3	1	406.83	19.77
-9	-3	2	498.18	20.98
-9	-3	3	144.24	5.28
-9	-3	4	49.70	2.96
-9	-3	5	9.61	2.11
-9	-3	6	287.64	23.40
-9	-1	-6	20.79	2.10
-9	-1	-5	9.30	1.10
-9	-1	-4	22.00	1.03
-9	-1	-3	174.77	4.76
-9	-1	-2	277.56	7.66
-9	-1	-1	134.33	4.17
-9	-1	0	152.52	5.93
-9	-1	1	68.72	4.48
-9	-1	2	293.09	11.64
-9	-1	3	137.59	5.86
-9	-1	4	124.10	4.23
-9	-1	5	53.73	2.49
-9	-1	6	90.25	5.32
-9	1	-7	7.29	2.32
-9	1	-6	19.01	6.98

-9	1	-5	9.99	1.39
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-9	1	-3	176.09	5.84
-9	1	-2	286.62	7.11
-9	1	-1	134.79	3.48
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-9	1	4	130.42	6.85
-9	1	5	57.61	4.40
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-9	3	-2	135.72	6.06
-9	3	-1	84.27	5.51
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-9	9	-4	2.40	3.69
-9	9	-3	8.12	3.82
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-9	9	1	30.25	7.59
-9	9	2	1.10	2.60
-9	9	3	10.18	7.72
-9	9	4	4.20	3.69
-8	-10	-3	11.63	3.48
-8	-10	-2	11.02	3.12

-8	-10	-1	9.00	3.30
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-8	-10	2	15.37	2.59
-8	-10	3	0.79	2.08
-8	-8	-4	12.32	3.09
-8	-8	-3	166.93	7.75
-8	-8	-2	60.06	6.04
-8	-8	-1	192.10	8.59
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-8	-8	2	11.02	1.59
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-8	-8	5	417.38	24.52
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-8	-6	-4	85.93	3.15
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-8	-4	5	5.11	1.99
-8	-4	6	15.29	3.36
-8	-2	-8	3.88	3.31
-8	-2	-7	22.28	5.00
-8	-2	-6	112.15	4.87
-8	-2	-5	29.38	1.84
-8	-2	-4	1.39	0.59
-8	-2	-3	304.15	8.37
-8	-2	-2	390.06	12.24
-8	-2	-1	243.36	12.17
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-8	-2	4	29.70	2.18
-8	-2	5	60.22	4.19
-8	-2	6	2.31	1.31
-8	0	-7	-0.10	1.82
-8	0	-6	43.03	3.41
-8	0	-5	-0.10	1.22
-8	0	-4	95.84	3.52
-8	0	-3	-0.30	0.51

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-8	0	4	1130.30	72.62
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-8	2	-5	24.11	1.96
-8	2	-4	1.69	0.91
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-8	10	-1	11.29	3.83
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-7	-9	-2	14.82	1.39
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-7	-9	0	13.62	1.48
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-6	4	7	103.43	14.85
-6	6	-7	45.16	6.05
-6	6	-6	5.29	3.31
-6	6	-5	24.60	3.67
-6	6	-4	301.02	16.31

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-6	6	1	191.27	8.85
-6	6	2	24.50	1.68
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-6	6	4	252.81	12.40
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-6	8	-6	40.96	5.63
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-6	8	3	354.19	13.55
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-6	8	5	469.59	29.90
-6	10	-3	26.11	7.05
-6	10	-2	12.39	3.87
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-5	-11	-1	23.23	2.89
-5	-11	0	14.59	2.29
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-5	-9	-4	-0.30	1.61
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-5	-9	-2	-0.10	1.92
-5	-9	-1	107.12	5.18
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-5	-9	1	22.47	2.46
-5	-9	2	13.40	2.49
-5	-9	3	15.60	2.37
-5	-9	4	14.90	2.32
-5	-9	5	7.78	2.40
-5	-7	-6	-0.50	2.41
-5	-7	-5	19.10	2.80
-5	-7	-4	34.46	2.35
-5	-7	-3	72.08	3.91
-5	-7	-2	229.52	7.88
-5	-7	-1	10.11	1.21
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-5	-7	2	550.84	18.78
-5	-7	3	413.72	13.83
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-5	-7	6	-0.20	2.11
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-5	-5	-7	23.91	4.50
-5	-5	-6	42.38	3.91
-5	-5	-5	4.80	2.19
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-5	-5	-3	98.41	3.97
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-5	-5	7	17.31	4.08
-5	-5	8	14.36	2.80
-5	-3	-8	14.06	3.53
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-5	-3	-4	106.09	7.62
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-5	-3	0	334.89	11.35
-5	-3	1	1069.94	44.49
-5	-3	2	203.06	6.56
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-5	-3	6	8.82	4.10
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-5	-1	-7	8.12	1.48
-5	-1	-6	25.30	2.21
-5	-1	-5	35.16	2.25
-5	-1	-4	11.42	1.01
-5	-1	-3	971.57	26.81
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-5	-1	-1	124.10	3.79
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-5	-1	3	523.49	22.88
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-5	1	-6	24.30	2.17
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-5	1	-4	14.82	1.69
-5	1	-3	980.32	37.57
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-4	-2	-1	818.53	33.19
-4	-2	0	5728.98	317.90
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-4	0	-8	14.36	2.58
-4	0	-7	-2.50	1.39
-4	0	-6	359.86	23.14
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-4	0	-2	2258.15	65.58
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-3	9	-1	30.25	3.30
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-3	9	1	17.64	1.76
-3	9	2	6.20	2.49
-3	9	3	151.78	8.38
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-3	11	-2	56.55	6.47
-3	11	-1	13.76	3.86
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-2	-10	-3	71.57	10.15
-2	-10	-2	115.13	7.51
-2	-10	-1	57.46	4.24
-2	-10	0	73.27	4.45
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-2	-8	-4	56.25	3.30
-2	-8	-3	192.93	8.61
-2	-8	-2	31.25	1.68
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-2	-6	-7	10.50	2.72
-2	-6	-5	5.02	0.72
-2	-6	-4	0.10	0.61
-2	-6	-3	35.88	1.56
-2	-6	-2	42.64	1.44
-2	-6	-1	193.49	7.51
-2	-6	0	160.53	5.32
-2	-6	1	363.28	12.20
-2	-6	2	393.23	10.71
-2	-6	3	2.89	1.09
-2	-6	4	7.67	1.50
-2	-6	5	30.36	2.64
-2	-6	6	40.96	3.97
-2	-6	7	-1.99	2.68
-2	-4	-8	36.00	7.68
-2	-4	-7	10.30	3.40

-2	-4	-6	50.55	4.12
-2	-4	-5	79.03	6.05
-2	-4	-4	641.10	19.75
-2	-4	-3	897.60	28.16
-2	-4	-2	1858.47	56.04
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-2	-4	3	40.32	1.52
-2	-4	4	476.99	15.72
-2	-4	5	239.01	10.20
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-2	-4	7	52.56	4.35
-2	-4	8	58.06	8.84
-2	-2	-7	76.04	5.41
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-2	6	6	37.82	3.44
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-2	8	-5	16.08	4.33
-2	8	-4	50.98	4.71
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-1	-7	0	279.56	11.04
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-1	-7	2	213.74	7.31
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-1	-5	-7	2.19	2.19
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1	-5	-7	7.51	1.81
1	-5	-6	15.68	1.19
1	-5	-5	6.60	0.51

1	-5	-4	3.39	0.40
1	-5	-3	2.69	0.49
1	-5	-2	67.40	2.79
1	-5	-1	317.55	12.12
1	-5	0	86.68	2.61
1	-5	1	30.80	2.33
1	-5	2	22.47	1.23
1	-5	3	21.16	1.29
1	-5	4	53.58	2.64
1	-5	5	3.88	1.38
1	-5	6	2.31	3.10
1	-5	7	2.50	2.50
1	-5	8	17.89	4.31
1	-3	-7	16.56	1.71
1	-3	-6	2.31	0.70
1	-3	-5	171.61	5.50
1	-3	-4	3.39	0.40
1	-3	-3	766.74	19.38
1	-3	-2	201.92	6.25
1	-3	-1	14.36	0.91
1	-3	0	1296.72	42.49
1	-3	1	225.00	7.50
1	-3	2	114.06	3.63
1	-3	3	977.19	40.01
1	-3	4	39.94	1.90
1	-3	5	18.49	1.29
1	-3	6	0.79	1.30
1	-3	7	2.99	1.90
1	-3	8	0.79	2.79
1	-1	-8	5.62	1.99
1	-1	-6	5.62	1.18
1	-1	-5	29.59	1.41
1	-1	-4	199.09	9.31
1	-1	-3	330.51	13.82
1	-1	-2	137.83	3.99
1	-1	-1	885.66	107.73
1	-1	0	556.49	15.57
1	-1	1	4366.57	210.13
1	-1	2	1365.30	45.82
1	-1	3	268.96	8.20
1	-1	4	176.36	6.91
1	-1	5	305.55	12.59
1	-1	6	44.22	2.53
1	-1	7	129.28	6.59
1	-1	8	29.38	3.04
1	1	-9	2.69	2.59
1	1	-8	7.02	2.23
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1	1	3	259.53	7.41
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1	1	6	45.43	1.89
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1	3	5	21.62	1.40
1	3	6	1.69	0.81
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1	5	-6	19.89	2.94
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1	5	1	28.84	1.83
1	5	2	26.83	1.24
1	5	3	18.58	1.12
1	5	4	58.06	4.42
1	5	5	4.20	0.98
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1	7	-6	9.99	2.97
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1	7	3	89.30	4.72
1	7	4	6.00	0.98
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1	9	-5	30.69	9.97
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1	9	2	17.81	2.03
1	9	3	240.87	28.56
1	11	-2	4.20	3.40
1	11	-1	10.30	4.62
1	11	0	24.50	4.26
1	11	1	21.81	3.18
1	11	2	46.24	7.75
2	-10	-3	82.81	10.56
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2	-10	-1	138.53	11.53
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2	-10	4	13.69	3.40

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2	-8	4	57.61	5.01
2	-8	5	17.64	3.28
2	-8	6	5.62	4.12
2	-6	-7	-0.20	1.61
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2	-6	-5	31.25	1.34
2	-6	-4	7.29	0.81
2	-6	-3	3.10	0.81
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2	-6	-1	370.95	9.63
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2	-6	1	192.38	6.93
2	-6	2	38.19	1.85
2	-6	3	36.84	2.31
2	-6	4	0.71	1.41
2	-6	5	12.18	4.12
2	-6	6	56.55	3.91
2	-6	7	8.41	2.61
2	-4	-7	45.56	4.72
2	-4	-6	176.89	6.92
2	-4	-5	237.78	9.87
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2	-4	-2	410.47	15.40
2	-4	-1	219.34	8.00
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2	-4	4	633.53	24.16
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2	-2	-8	5.20	2.01
2	-2	-7	14.06	1.12
2	-2	-6	17.31	1.41
2	-2	-5	7.78	0.78
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2	-2	-3	205.92	5.74
2	-2	-2	1928.97	77.30
2	-2	-1	4020.83	121.75
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2	-2	5	28.41	1.71
2	-2	6	20.07	2.06
2	-2	7	75.52	5.74
2	-2	8	-0.71	3.11
2	0	-9	6.10	4.59
2	0	-8	124.99	12.75
2	0	-7	3.10	1.58
2	0	-6	593.41	24.85

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2	0	-1	7.29	0.49
2	0	0	1536.64	99.57
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2	0	2	22.47	0.85
2	0	3	0.30	0.51
2	0	4	629.01	21.07
2	0	5	-0.20	0.91
2	0	6	1483.79	60.86
2	0	7	-0.40	1.40
2	0	8	78.15	5.13
2	2	-9	8.53	3.21
2	2	-8	5.20	2.60
2	2	-7	17.31	2.66
2	2	-6	15.92	1.52
2	2	-5	7.51	1.10
2	2	-4	214.33	6.73
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2	2	4	40.20	1.14
2	2	5	32.15	0.91
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2	4	-6	196.28	9.81
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2	4	1	791.30	30.38
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2	6	-5	41.09	3.59
2	6	-4	9.49	2.77
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2	6	2	43.96	1.72
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2	8	-4	147.87	11.92
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2	8	3	216.38	13.83
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3	-11	1	13.18	4.07
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3	-9	-1	15.76	1.27
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3	1	4	191.82	6.37
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3	9	3	26.63	2.99
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4	0	2	2266.71	85.70
4	0	3	0.71	0.50
4	0	4	616.03	19.36
4	0	5	6.20	5.08
4	0	6	353.82	13.54
4	0	7	-1.80	1.50
4	0	8	13.76	1.93
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4	2	3	16.40	0.81
4	2	4	101.61	4.84
4	2	5	287.30	17.97
4	2	6	251.86	15.55
4	2	7	77.62	4.41
4	4	-8	33.52	6.83
4	4	-7	23.72	3.51
4	4	-6	160.28	10.38
4	4	-5	6.40	1.32
4	4	-4	250.27	8.86
4	4	-3	140.19	5.21
4	4	-2	388.48	12.22
4	4	-1	147.14	6.31
4	4	0	2277.20	82.08
4	4	1	832.32	31.16

4	4	2	1536.64	61.15
4	6	-7	10.63	3.00
4	6	-6	8.29	2.88
4	6	-5	2.69	2.49
4	6	-4	62.73	3.64
4	6	-3	31.92	2.15
4	6	-2	419.43	18.43
4	6	-1	24.01	2.16
4	6	0	50.84	2.28
4	6	1	148.84	5.12
4	6	2	23.81	1.46
4	6	3	197.12	10.95
4	8	-6	12.18	4.12
4	8	-5	307.30	24.54
4	8	-4	71.06	6.41
4	8	-3	2053.90	82.48
4	8	-2	72.42	5.11
4	8	-1	168.74	9.87
4	8	0	109.20	5.85
4	8	1	23.04	2.78
4	8	2	5.62	1.42
4	8	3	16.00	2.00
4	10	-4	15.21	3.98
4	10	-3	39.69	4.91
4	10	-2	10.82	4.08
4	10	-1	6.71	3.11
4	10	0	18.92	2.78
4	10	1	49.84	3.95
4	10	2	47.06	5.90
5	-11	-1	2.59	2.70
5	-11	0	18.92	3.83
5	-11	1	33.76	6.39
5	-9	-4	10.18	2.49
5	-9	-3	13.69	2.29
5	-9	-2	12.53	1.91
5	-9	-1	30.80	3.55
5	-9	0	56.55	6.17
5	-9	1	121.00	6.82
5	-9	2	6.00	2.50
5	-9	3	3.50	2.51
5	-9	4	9.61	31.00
5	-9	5	21.72	6.34
5	-7	-6	-0.40	1.89
5	-7	-5	78.32	4.60
5	-7	-4	266.02	11.42
5	-7	-3	398.00	19.95
5	-7	-2	572.64	29.67
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5	-7	1	8.12	1.48
5	-7	2	229.83	9.40
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5	-7	4	32.95	3.21
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5	-7	6	1.30	4.90
5	-5	-6	32.38	1.59
5	-5	-5	44.36	1.60
5	-5	-4	5.71	0.48
5	-5	-3	108.58	3.13
5	-5	-2	116.21	4.31
5	-5	-1	76.04	3.66
5	-5	0	332.70	11.67
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5	-5	8	12.60	3.69
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5	-3	-4	165.12	3.60
5	-3	-3	10.11	0.51
5	-3	-2	201.92	5.97
5	-3	-1	1129.63	34.28
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5	-3	3	53.00	2.33
5	-3	4	112.36	5.09
5	-3	5	8.58	1.29
5	-3	6	136.66	7.72
5	-3	7	82.26	6.89
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5	-1	-7	52.85	2.47
5	-1	-6	430.15	14.93
5	-1	-5	121.66	4.41
5	-1	-4	576.00	18.24
5	-1	-3	528.08	12.87
5	-1	-2	178.22	4.81
5	-1	-1	129.50	5.69
5	-1	0	3389.57	109.45
5	-1	1	116.42	3.67
5	-1	2	135.26	4.19
5	-1	3	992.88	33.40
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5	-1	6	30.69	1.99
5	-1	7	14.59	2.37
5	-1	8	10.82	2.11
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5	1	-8	14.82	3.31
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5	1	-4	593.90	17.06
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5	1	-1	136.19	5.37
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5	1	2	129.28	3.87
5	1	3	1001.72	29.12
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5	1	5	35.76	1.55
5	1	6	30.25	1.21
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5	3	-6	15.21	2.57
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5	3	-3	13.69	1.11
5	3	-2	206.21	6.89
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5	5	-6	38.07	4.32
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5	5	1	394.02	11.12
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5	7	2	225.60	10.81
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5	9	-2	5.38	2.60
5	9	-1	26.32	4.10
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5	9	1	102.82	7.10
5	9	2	-2.10	1.80
5	9	3	3.80	1.91
5	11	-1	4.20	7.01
5	11	0	25.70	5.48
5	11	1	37.33	4.77
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6	-10	1	2.89	2.58
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6	-8	-5	465.70	49.20
6	-8	-4	42.64	3.92
6	-8	-3	366.34	14.93
6	-8	-2	31.36	2.58
6	-8	-1	17.81	2.36
6	-8	0	20.98	2.11
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6	-6	-6	-0.50	1.11
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6	-6	-3	238.70	13.60
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6	-6	7	35.76	5.14
6	-4	-7	111.72	8.88
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6	-4	-2	533.61	18.94
6	-4	-1	2295.37	92.95
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6	-4	3	171.61	6.81
6	-4	4	32.72	1.94
6	-4	5	84.46	3.68
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6	-4	7	182.79	12.71
6	-4	8	248.38	27.42
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6	-2	-5	44.89	1.74
6	-2	-4	222.31	5.67
6	-2	-3	179.56	4.82
6	-2	-2	353.06	12.03
6	-2	-1	1106.23	29.93
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6	0	-7	-1.69	2.00
6	0	-6	765.08	26.00
6	0	-5	-1.00	0.80
6	0	-3	0.20	0.50
6	0	-2	235.93	6.14
6	0	-1	0.00	1.00
6	0	0	921.73	26.72
6	0	1	0.20	0.40
6	0	2	2149.25	72.32
6	0	3	1.30	0.59
6	0	5	-0.20	0.60
6	0	6	12.32	1.90
6	0	7	1.21	1.10
6	2	-8	4.41	3.02
6	2	-7	131.79	8.50
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6	2	-5	44.76	2.14
6	2	-4	219.34	6.81
6	2	-3	190.16	8.00
6	2	-2	384.94	17.27
6	2	-1	1120.91	36.16
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6	2	1	299.29	20.41

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6	2	3	107.54	4.36
6	2	4	316.13	14.22
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6	2	6	216.09	12.05
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6	4	-6	28.73	3.75
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7	-7	-5	62.57	6.17
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8	0	-6	1096.27	35.10
8	0	-5	0.10	0.71
8	0	-4	1158.72	32.00
8	0	-3	0.59	0.49
8	0	-2	27.98	1.38
8	0	-1	-0.59	0.69
8	0	0	2091.23	74.08
8	0	1	-0.50	0.50
8	0	2	5757.77	295.93
8	0	3	-0.10	0.61
8	0	4	92.93	4.05
8	0	5	0.20	0.70
8	0	6	43.56	2.11
8	0	7	-0.79	1.00
8	2	-8	12.60	3.27
8	2	-7	10.63	3.13
8	2	-6	1.59	1.49
8	2	-5	68.06	3.13
8	2	-4	30.91	1.67
8	2	-3	46.24	2.04
8	2	-2	136.66	8.18
8	2	-1	393.63	13.09

8	2	0	108.16	3.12
8	2	1	249.64	9.16
8	2	2	408.85	16.98
8	2	3	314.35	19.15
8	2	4	1.39	0.90
8	2	5	30.91	2.11
8	2	6	119.90	6.13
8	4	-8	26.63	5.78
8	4	-7	57.30	6.06
8	4	-6	11.22	2.68
8	4	-5	5.02	1.79
8	4	-4	17.47	2.01
8	4	-3	122.54	5.76
8	4	-2	1287.37	67.45
8	4	-1	201.92	11.08
8	4	0	165.89	6.96
8	4	1	451.56	21.25
8	4	2	64.16	2.56
8	4	3	182.79	5.41
8	6	-7	2.19	4.29
8	6	-6	26.01	4.08
8	6	-5	33.99	3.61
8	6	-4	7.40	4.41
8	6	-3	542.89	26.10
8	6	-2	55.95	3.44
8	6	-1	37.09	2.31
8	6	0	17.98	1.78
8	6	1	112.57	6.79
8	6	2	246.49	9.11
8	6	3	450.29	14.01
8	8	-5	431.39	25.75
8	8	-4	65.45	9.87
8	8	-3	37.45	3.92
8	8	-2	19.62	4.43
8	8	-1	80.28	6.45
8	8	0	58.06	5.03
8	8	1	195.72	13.43
8	8	2	57.61	4.86
8	8	3	160.78	11.41
8	10	-3	3.80	3.59
8	10	-2	18.06	5.18
8	10	-1	8.70	3.42
8	10	0	34.46	4.93
8	10	1	13.10	3.19
9	-9	-4	4.28	2.19
9	-9	-3	2.89	2.11
9	-9	-2	2.31	2.61
9	-9	-1	11.49	2.58
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9	-9	1	11.49	2.37
9	-9	2	4.20	2.58
9	-9	3	7.08	5.00
9	-9	4	0.90	3.91
9	-7	-6	82.63	10.36
9	-7	-5	69.39	4.83
9	-7	-4	24.01	2.25
9	-7	-3	7.02	1.48
9	-7	-2	14.21	1.58
9	-7	-1	35.64	2.63
9	-7	1	20.43	2.53
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9	-5	-7	3.80	3.00
9	-5	-6	4.28	1.20
9	-5	-5	2.31	0.61
9	-5	-4	429.32	17.40
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9	-5	-2	89.11	3.96
9	-5	-1	347.45	12.68
9	-5	0	41.47	2.32
9	-5	1	164.10	7.43
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9	-5	3	187.42	6.57
9	-5	4	210.54	11.03
9	-5	5	24.80	2.79
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9	-3	5	98.41	5.36
9	-3	6	206.78	10.93
9	-3	7	63.04	6.03
9	-1	-8	58.68	8.58
9	-1	-7	36.60	2.90
9	-1	-6	103.02	3.86
9	-1	-5	52.13	2.17
9	-1	-4	121.22	4.40
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9	-1	-2	299.98	7.62
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9	1	-7	46.51	4.36
9	1	-6	104.04	5.10
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9	1	-3	142.09	3.81
9	1	-2	293.78	6.86
9	1	-1	72.42	2.55
9	1	0	153.02	4.21
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9	1	2	285.95	10.15
9	1	3	179.83	6.17
9	1	4	26.32	1.74
9	1	5	9.61	0.81
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9	3	-7	15.21	2.89
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9	3	1	90.63	5.14
9	3	2	143.52	4.31
9	3	3	105.47	3.70
9	3	4	5.62	0.52
9	5	-7	1.99	2.99
9	5	-6	5.90	2.82
9	5	-5	-1.10	2.31
9	5	-4	438.06	25.12
9	5	-3	102.01	5.05
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9	7	2	74.82	3.11
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9	9	-1	16.16	2.97
9	9	0	32.15	3.52
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10	-4	2	3.10	1.41
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10	-4	6	454.12	26.85
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10	-2	-8	5.02	3.23
10	-2	-7	60.22	3.41
10	-2	-6	5.81	1.21
10	-2	-5	18.84	1.82
10	-2	-4	169.26	4.94
10	-2	-3	81.36	2.16
10	-2	-2	16.40	1.22
10	-2	-1	121.22	3.08
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10	0	-6	563.11	22.31
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10	0	-4	26.32	1.44
10	0	-3	0.90	0.89
10	0	-2	928.42	25.59
10	0	-1	0.30	0.51
10	0	0	3153.95	95.47
10	0	1	0.40	0.59
10	0	2	1158.72	44.25
10	0	3	2.50	0.79
10	0	4	141.13	4.99
10	0	5	0.30	0.70
10	0	6	0.59	0.89
10	2	-8	2.69	2.79
10	2	-7	59.60	5.56
10	2	-6	9.18	2.30
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12	0	5	1.30	1.39
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12	2	-5	2.19	1.51
12	2	-4	30.25	1.76
12	2	-3	136.19	4.43
12	2	-2	181.44	6.20
12	2	-1	157.00	5.01
12	2	0	302.76	9.05
12	2	1	55.65	2.54
12	2	2	530.84	23.50
12	2	3	139.00	8.96
12	2	4	76.04	4.01
12	2	5	7.62	1.32
12	4	-7	6.92	3.63
12	4	-6	42.12	4.41
12	4	-5	157.75	8.29
12	4	-4	16.97	2.80
12	4	-3	21.44	2.78
12	4	-2	410.87	16.22
12	4	-1	47.20	3.71
12	4	0	96.04	3.14
12	4	1	315.06	10.30
12	4	2	1842.13	66.10
12	4	3	1685.92	64.87
12	4	4	869.66	30.08
12	6	-6	12.53	3.47
12	6	-5	25.30	4.43
12	6	-4	4.58	2.61
12	6	-3	38.32	3.96

12	6	-2	4.08	1.78
12	6	-1	286.29	17.26
12	6	0	245.86	11.60
12	6	1	10.18	2.49
12	6	2	2.40	1.12
12	6	3	107.74	4.36
12	8	-4	2.99	3.60
12	8	-3	66.75	6.37
12	8	-2	0.50	2.61
12	8	-1	203.92	17.42
12	8	0	25.20	3.31
12	8	1	55.65	4.03
12	8	2	43.82	5.16
13	-9	-2	5.90	4.18
13	-9	-1	14.59	3.59
13	-9	0	7.62	2.93
13	-9	1	13.32	3.29
13	-9	2	3.20	3.29
13	-7	-5	2.50	2.81
13	-7	-4	28.84	3.11
13	-7	-3	47.75	4.28
13	-7	-2	53.44	4.24
13	-7	-1	10.50	2.20
13	-7	0	59.14	4.92
13	-7	1	2.10	2.20
13	-7	2	5.02	2.60
13	-7	3	54.91	5.63
13	-7	4	8.29	2.48
13	-7	5	19.27	3.69
13	-5	-6	73.10	7.52
13	-5	-5	12.32	1.83
13	-5	-4	57.46	4.40
13	-5	-3	30.36	2.42
13	-5	-2	6.92	1.89
13	-5	-1	133.63	8.79
13	-5	0	322.92	16.89
13	-5	1	95.26	6.25
13	-5	2	72.93	5.12
13	-5	3	174.24	9.77
13	-5	4	3.10	2.29
13	-5	5	29.38	3.79
13	-5	6	95.65	9.39
13	-3	-7	7.51	2.79
13	-3	-6	12.89	3.02
13	-3	-5	49.00	2.94
13	-3	-4	300.68	10.75
13	-3	-3	39.56	1.76
13	-3	-2	53.14	2.62
13	-3	-1	76.56	5.07
13	-3	0	105.88	4.53
13	-3	1	186.60	6.83
13	-3	2	272.25	10.89
13	-3	3	157.00	6.52
13	-3	4	382.98	18.40
13	-3	5	33.18	3.00
13	-3	6	3.20	1.90
13	-3	7	8.41	2.73
13	-1	-7	28.84	4.62
13	-1	-6	30.25	2.53
13	-1	-5	6.60	1.28
13	-1	-4	45.83	2.03
13	-1	-3	43.43	1.58
13	-1	-2	53.14	2.19
13	-1	-1	70.06	2.51

13	-1	0	371.33	10.79
13	-1	1	58.68	3.06
13	-1	2	118.59	5.01
13	-1	3	9.18	1.21
13	-1	4	41.73	3.75
13	-1	5	19.62	1.86
13	-1	6	77.26	4.39
13	1	-7	30.14	3.73
13	1	-6	41.34	3.99
13	1	-5	8.70	1.48
13	1	-4	43.16	2.50
13	1	-3	46.65	3.01
13	1	-2	55.65	2.24
13	1	-1	74.13	2.93
13	1	0	382.98	10.96
13	1	1	60.06	2.17
13	1	2	118.81	4.80
13	1	3	6.00	1.08
13	1	4	32.72	1.83
13	1	5	15.76	1.27
13	3	-7	16.97	5.19
13	3	-6	18.92	3.13
13	3	-5	57.15	4.08
13	3	-4	315.77	14.57
13	3	-3	38.94	2.37
13	3	-2	58.68	2.45
13	3	-1	72.93	3.93
13	3	0	109.20	4.60
13	3	1	195.16	5.87
13	3	2	275.89	9.30
13	3	3	163.07	6.64
13	3	4	390.46	13.83
13	3	5	33.99	1.98
13	5	-6	90.25	8.93
13	5	-5	8.01	3.00
13	5	-4	54.76	6.36
13	5	-3	30.36	3.75
13	5	-2	6.20	3.39
13	5	-1	129.50	6.60
13	5	0	297.22	15.52
13	5	1	99.20	5.58
13	5	2	71.40	4.06
13	5	3	179.29	7.23
13	5	4	4.08	0.81
13	7	-5	6.20	3.98
13	7	-4	30.25	5.06
13	7	-3	57.46	4.85
13	7	-2	37.58	4.05
13	7	-1	7.90	2.59
13	7	0	54.46	4.58
13	7	1	6.81	2.40
13	7	2	7.29	2.11
13	9	-2	2.31	3.71
13	9	-1	15.68	4.28
13	9	0	5.71	2.92
13	9	1	10.30	2.89
14	-8	-4	2.89	2.89
14	-8	-3	148.35	15.59
14	-8	-2	11.63	2.39
14	-8	-1	87.42	7.29
14	-8	0	7.78	3.79
14	-8	1	14.52	3.12
14	-8	2	56.85	9.80
14	-8	3	33.99	4.08

14	-6	-5	6.10	2.22
14	-6	-4	1.30	2.01
14	-6	-3	14.90	2.78
14	-6	-2	135.72	6.99
14	-6	-1	164.35	12.05
14	-6	0	44.76	3.75
14	-6	1	388.09	17.73
14	-6	2	6.20	2.99
14	-6	3	13.76	2.89
14	-6	4	15.92	3.11
14	-6	5	89.49	7.95
14	-4	-7	23.43	6.00
14	-4	-6	73.96	7.05
14	-4	-5	15.76	1.83
14	-4	-4	91.20	4.97
14	-4	-3	237.47	9.55
14	-4	-2	30.47	2.76
14	-4	-1	209.09	13.88
14	-4	0	606.64	21.67
14	-4	2	1259.54	63.17
14	-4	3	147.87	8.27
14	-4	4	43.96	3.85
14	-4	5	10.82	43.95
14	-4	6	22.00	3.94
14	-2	-7	6.30	4.52
14	-2	-6	22.28	4.15
14	-2	-5	13.03	3.03
14	-2	-4	2.79	1.00
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14	-2	6	2.99	2.11
14	0	-7	2.50	2.81
14	0	-6	64.96	5.64
14	0	-5	0.30	1.10
14	0	-4	342.25	15.17
14	0	-3	-1.30	1.30
14	0	-2	831.75	25.38
14	0	-1	1.80	0.91
14	0	0	510.31	14.46
14	0	1	-1.10	1.20
14	0	2	181.44	6.74
14	0	3	1.80	1.50
14	0	4	91.97	4.03
14	0	5	0.20	1.01
14	0	6	323.64	14.03
14	2	-7	7.40	3.81
14	2	-6	7.40	3.37
14	2	-5	14.06	3.08
14	2	-4	0.71	1.31
14	2	-3	30.91	2.11
14	2	-2	49.00	2.24
14	2	-1	37.33	1.83
14	2	0	102.01	3.64
14	2	1	8.53	0.99
14	2	2	463.11	16.36
14	2	3	97.42	5.33
14	2	4	19.71	2.84

14	2	5	3.31	1.71
14	4	-7	42.77	6.15
14	4	-6	79.92	8.22
14	4	-5	16.32	3.07
14	4	-4	99.20	7.17
14	4	-3	219.63	9.78
14	4	-2	40.58	3.18
14	4	-1	267.98	14.41
14	4	0	623.00	20.97
14	4	1	936.36	31.21
14	4	2	1251.74	41.75
14	4	3	149.57	6.11
14	4	4	51.98	2.88
14	6	-5	32.26	54.07
14	6	-4	5.90	4.52
14	6	-3	9.99	3.29
14	6	-2	127.46	11.06
14	6	-1	154.01	11.91
14	6	0	40.58	3.06
14	6	1	381.81	16.02
14	6	2	9.99	2.40
14	6	3	11.90	1.93
14	8	-4	2.31	3.50
14	8	-3	166.93	14.99
14	8	-2	12.67	2.99
14	8	-1	74.30	7.76
14	8	0	12.11	2.99
14	8	1	9.61	2.91
15	-7	-4	7.51	2.90
15	-7	-3	4.88	3.01
15	-7	-2	1.30	2.30
15	-7	-1	89.87	7.20
15	-7	0	33.76	4.42
15	-7	1	25.30	3.32
15	-7	2	40.96	4.48
15	-7	3	8.41	2.78
15	-7	4	-3.80	2.61
15	-5	-6	9.99	3.29
15	-5	-5	8.18	2.12
15	-5	-4	5.90	2.62
15	-5	-3	12.32	2.32
15	-5	-2	200.51	8.50
15	-5	-1	46.51	3.96
15	-5	0	564.06	31.35
15	-5	1	92.74	6.93
15	-5	2	27.04	3.43
15	-5	3	18.84	2.78
15	-5	4	10.18	2.68
15	-5	5	1.30	2.39
15	-3	-7	11.02	3.78
15	-3	-6	4.08	3.39
15	-3	-5	4.49	2.29
15	-3	-4	153.76	7.69
15	-3	-3	18.40	1.46
15	-3	-2	194.60	8.93
15	-3	-1	152.77	7.91
15	-3	0	243.05	10.60
15	-3	1	210.25	9.86
15	-3	2	765.63	33.20
15	-3	3	140.90	6.88
15	-3	4	95.84	5.29
15	-3	5	9.42	2.33
15	-3	6	-1.69	2.60
15	-1	-7	18.66	3.63

15	-1	-6	-0.30	2.41
15	-1	-5	14.90	4.09
15	-1	-4	21.72	1.86
15	-1	-3	55.20	2.67
15	-1	-2	105.06	3.08
15	-1	-1	177.69	6.40
15	-1	0	40.07	2.15
15	-1	1	1.59	1.79
15	-1	2	68.56	4.31
15	-1	3	35.05	2.49
15	-1	4	11.49	3.32
15	-1	5	12.60	1.77
15	-1	6	12.53	2.48
15	1	-7	15.52	4.18
15	1	-6	-0.79	2.69
15	1	-5	8.70	2.71
15	1	-4	22.94	2.11
15	1	-3	54.76	3.26
15	1	-2	105.27	3.90
15	1	-1	186.60	6.56
15	1	0	43.56	1.98
15	1	1	0.40	1.59
15	1	2	70.56	4.03
15	1	3	33.76	2.56
15	1	4	12.60	1.63
15	1	5	13.62	3.32
15	3	-7	8.70	4.19
15	3	-6	13.03	3.68
15	3	-5	6.40	2.58
15	3	-4	149.57	7.58
15	3	-3	21.90	2.71
15	3	-2	207.65	8.36
15	3	-1	171.09	6.02
15	3	0	240.25	8.68
15	3	1	217.86	7.68
15	3	2	824.84	32.17
15	3	3	144.24	6.73
15	3	4	92.54	5.39
15	3	5	11.90	2.07
15	5	-6	13.99	3.81
15	5	-5	15.37	3.06
15	5	-4	8.29	3.28
15	5	-3	12.67	2.71
15	5	-2	197.12	11.23
15	5	-1	40.32	3.30
15	5	0	556.49	30.20
15	5	1	78.32	4.60
15	5	2	26.63	3.10
15	5	3	23.72	2.14
15	7	-4	13.32	4.38
15	7	-3	-0.10	2.73
15	7	-2	0.59	2.79
15	7	-1	83.91	5.86
15	7	0	29.92	2.95
15	7	1	20.98	2.47
15	7	2	38.94	5.24
16	-8	-2	23.43	4.55
16	-8	-1	17.72	3.87
16	-8	0	17.89	4.06
16	-8	1	23.81	13.86
16	-6	-5	7.18	3.11
16	-6	-4	11.83	4.82
16	-6	-3	6.60	2.72
16	-6	-2	3.88	2.88

16	-6	-1	164.87	8.22
16	-6	0	17.64	2.69
16	-6	1	20.07	3.23
16	-6	2	2.79	3.31
16	-6	3	1.49	3.10
16	-6	4	12.18	3.07
16	-4	-6	6.92	3.21
16	-4	-5	10.89	1.98
16	-4	-4	0.40	1.59
16	-4	-3	218.74	10.94
16	-4	-2	283.25	16.49
16	-4	-1	334.16	16.45
16	-4	0	1457.71	61.85
16	-4	1	309.06	18.99
16	-4	2	119.68	6.78
16	-4	3	108.78	7.93
16	-4	4	8.88	2.80
16	-4	5	44.49	5.20
16	-2	-6	0.00	1.00
16	-2	-5	9.49	2.71
16	-2	-4	98.60	5.56
16	-2	-3	164.61	5.39
16	-2	-2	3.31	1.09
16	-2	-1	11.02	1.33
16	-2	0	152.52	7.16
16	-2	1	6.92	2.10
16	-2	2	60.06	3.25
16	-2	3	140.19	9.24
16	-2	4	85.19	7.94
16	-2	5	8.12	2.51
16	-2	6	5.90	3.30
16	0	-7	4.08	3.11
16	0	-6	53.29	4.96
16	0	-5	2.19	1.39
16	0	-4	172.92	11.31
16	0	-3	-0.10	1.32
16	0	-2	108.78	4.59
16	0	-1	0.71	0.91
16	0	0	468.29	12.98
16	0	1	-0.59	1.09
16	0	2	36.00	2.76
16	0	3	4.00	1.80
16	0	4	187.42	9.86
16	0	5	1.39	1.49
16	2	-6	-1.59	3.18
16	2	-5	12.60	2.98
16	2	-4	119.46	6.78
16	2	-3	154.50	6.96
16	2	-2	5.02	1.52
16	2	-1	11.97	1.52
16	2	0	153.02	7.17
16	2	1	7.62	1.38
16	2	2	74.13	3.79
16	2	3	148.60	18.53
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16	4	-5	9.00	3.30
16	4	-4	-1.80	2.39
16	4	-3	217.27	11.79
16	4	-2	241.18	11.18
16	4	-1	329.06	14.15
16	4	0	1410.00	67.59
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16	4	2	116.64	6.70

16	4	3	110.25	8.40
16	4	4	7.90	2.08
16	6	-5	2.79	4.88
16	6	-4	2.99	3.29
16	6	-3	3.50	2.92
16	6	-2	1.30	3.31
16	6	-1	164.10	13.83
16	6	0	15.13	2.18
16	6	1	23.43	2.81
16	6	2	1.10	2.71
16	8	-2	23.81	4.98
16	8	-1	20.07	4.12
16	8	0	22.28	10.48
16	8	1	15.76	3.33
17	-7	-3	16.48	4.71
17	-7	-2	48.86	6.15
17	-7	-1	88.74	8.29
17	-7	0	27.56	3.78
17	-7	1	29.48	7.38
17	-7	2	0.71	2.30
17	-5	-5	7.90	2.81
17	-5	-4	1.80	3.19
17	-5	-3	27.35	3.45
17	-5	-2	182.52	11.89
17	-5	-1	126.34	7.19
17	-5	0	40.96	3.97
17	-5	1	116.86	8.43
17	-5	2	11.97	2.63
17	-5	3	50.27	4.54
17	-5	4	12.89	3.02
17	-3	-6	4.80	3.20
17	-3	-5	6.92	3.89
17	-3	-4	138.77	7.77
17	-3	-3	156.00	10.99
17	-3	-2	136.89	10.30
17	-3	-1	105.27	6.36
17	-3	0	288.32	17.66
17	-3	1	70.56	6.89
17	-3	2	10.89	4.22
17	-3	3	35.28	4.04
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17	-1	-6	9.67	3.48
17	-1	-5	16.56	3.01
17	-1	-4	22.66	2.19
17	-1	-3	17.72	4.38
17	-1	-2	53.73	2.64
17	-1	-1	27.46	2.10
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17	-1	1	1.99	1.30
17	-1	2	99.00	5.77
17	-1	3	60.84	4.37
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17	-1	5	30.25	3.30
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17	1	-4	29.38	3.79
17	1	-3	8.70	1.71
17	1	-2	55.95	2.99
17	1	-1	25.20	2.31
17	1	0	124.99	5.37
17	1	1	4.80	2.01
17	1	2	84.82	10.32
17	1	3	59.29	6.01

17	1	4	118.16	11.09
17	3	-6	0.71	3.21
17	3	-5	-1.10	2.79
17	3	-4	145.20	11.81
17	3	-3	176.62	11.16
17	3	-2	143.28	11.49
17	3	-1	100.20	5.21
17	3	0	288.32	12.90
17	3	1	60.37	4.66
17	3	2	5.52	1.41
17	3	3	34.46	3.05
17	3	4	9.30	2.07
17	5	-5	6.50	3.62
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17	5	-3	32.72	48.16
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17	5	-1	110.04	8.81
17	5	0	43.16	3.94
17	5	1	110.25	7.77
17	5	2	15.60	2.21
17	5	3	48.16	4.58
17	7	-3	17.72	4.04
17	7	-2	54.02	5.59
17	7	-1	73.62	7.72
17	7	0	32.95	4.25
17	7	1	33.29	5.65
18	-6	-3	10.30	3.79
18	-6	-2	8.12	3.08
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18	-6	0	8.88	3.10
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18	-6	3	8.29	2.71
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18	-2	-2	21.16	1.84
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18	0	-6	111.09	13.07
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18	0	-3	0.79	1.50
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18	0	-1	-2.10	1.39
18	0	0	163.58	8.70
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18	2	-6	1.59	4.59
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18	2	-4	52.71	6.10
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19	1	-1	38.32	3.96
19	1	0	186.60	9.02

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20	-6	0	16.08	8.66
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20	-4	-4	114.06	8.12
20	-4	-3	131.10	11.22
20	-4	-2	206.50	13.80
20	-4	-1	30.69	8.31
20	-4	0	63.68	5.91
20	-4	1	5.11	2.71
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20	-2	-3	24.21	2.56
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20	-2	-1	18.66	3.02
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20	-2	2	10.63	2.93
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20	6	1	5.02	3.00
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21	-1	3	126.79	10.13
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22	2	0	50.13	5.95
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