Supporting Information

Orally active fumagillin analogues: survival of a reactive warhead under acidic conditions

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General synthetic procedures. Commercially available reagents and solvents were used as purchased without further purification. Fumagillin dicyclohexylamine salt was obtained from CEVA. Compound **3** was prepared according to the published procedure[i]. Analytical LC-MS was performed on a HP-1100 system interfaced with a Finnegan LCQ Advantage electrospray mass spectrometer, using a Phenomenex Luna C8(2) 3 micron columns with CH_3CN / 0.1% aqueous TFA elution. Preparative HPLC was performed on a Gilson system with a Phenomenex Luna C8(2), 5 micron, 100 x 21.2 mm column at a flow rate of 24 mL/min and detection at 214 nm. As appropriate, preparative LC was performed without TFA in the eluting solvents to avoid acid catalyzed degradation. Thin layer chromatography was performed on 250 micron EM Science silica gel 60 plates using UV_{254} or iodine visualization. ^1H and ^{13}C NMR spectra were obtained on a Varian MercuryPlus 400 MHz spectrometer referenced to TMS at 0.0 ppm. In general, final compound purities were 95% or greater as determined by HPLC-MS.

Synthesis of compounds 4 and 5. Compound **3** (1.0 g, 2.4 mmole) was dissolved in 30 mL CH_3CN. To this solution was added 250 mL of 0.1 N HCl. The solution was stirred for 2 days, and then concentrated *in vacuo*. The product was purified by preparative HPLC as follows: injection quantity, ~110 mg; column, Phenomenex Luna, C8, 5 micron, 100 x 21.2mm; mobile phases, "A" = 5 mM NH_4OAc, 0.2% AcOH in H_2O, "B" = 5 mM NH_4OAc, 0.2% AcOH in 3:1 acetonitrile: H_2O; gradient, 32-53% "B" over 20 minutes; flow, 24 mL/min; detection wavelength, 214 nm; temperature, ambient. The yield was 144 mg of **4** (96% pure) and 78 mg of **5** (92% pure). ^1H NMR of compound **4** (400 MHz, CD_3OD) δ 5.41 (m, 1H), 5.26 (t, 1H), 3.96 (dd, 1H), 3.77 (d, 1H), 3.69 (dd, 1H), 3.61 (d, 1H), 3.38 (s, 3H), 3.35 (m, 1H), 2.33 (m, 1H), 2.30 (m, 1H), 2.06 (m, 1H), 2.05 (m, 1H), 2.04 (m, 1H), 1.88 (dd, 1H), 1.69 (s, 3H), 1.67 (m, 2H),1.62 (s, 3H), 1.29 (s, 3H), 0.97 (d, 3H), 0.93 (d, 3H). ^{13}C NMR of compound **4** (100 MHz, CD_3OD) δ

175.5, 157.0, 131.6, 122.2, 85.6, 80.0, 79.3, 77.4, 77.3, 67.7, 60.2, 55.8, 51.4, 30.8, 30.0, 28.0, 25.6, 24.6, 18.3, 16.8, 16.7, 15.4. HRMS for compound **4**: calcd for $C_{22}H_{38}N_2O_7$+H: 443.27518. Found: 443.27479. ^{1}H NMR of compound **5** (400 MHz, CD_3OD) δ 5.30 (m, 1H), 5.24 (t, 1H), 3.98 (d, 1H), 3.64 (d, 1H), 3.52 (m, 1H), 3.50 (d, 1H), 3.32 (s, 3H), 3.28 (m, 1H), 2.34 (m, 1H), 2.20 (m, 1H), 2.08 (m, 1H), 2.02 (m, 1H), 2.01 (m, 1H), 1.97 (m, 1H), 1.79 (m, 1H), 1.71 (s, 3H), 1.62 (s, 3H), 1.53 (m, 1H), 1.25 (s, 3H), 0.99 (d, 3H), 0.96 (d, 3H). ^{13}C NMR of compound **5** (100 MHz, CD_3OD) δ 175.5, 156.9, 132.5, 122.2, 121.5, 88.5, 78.6, 78.1, 77.7, 74.1, 67.0, 60.2, 54.9, 50.0, 31.6, 30.7, 25.7, 24.6, 23.6, 18.6, 18.4, 16.8, 16.7. HRMS for compound **5**: calcd for $C_{22}H_{38}N_2O_7$+H: 443.27518. Found: 443.27447.

Synthesis of compound 6. Compound **3** (1.5g, 3.53mmole) was dissolved in 29.4 mL 1,4-dioxane at room temperature. To the solution was added 4.0 M HCl / 1,4-dioxane (0.973mL, 3.89 mmole). The reaction was stirred at room temperature for 5 minutes, and then concentrated *in vacuo*. The concentrated material was diluted into 30% CH_3CN / H_2O and lyophilized. Crude product was purified by preparative HPLC as follows: injection quantity, ~160mg; column, Phenomenex Luna, C8, 5 micron, 100 x 21.2mm; mobile phases, "A" = 100% H_2O, "B" = 99% CH_3CN, 1% H_2O; gradient, 34-50% "B" over 20 minutes; flow, 24 mL/min; detection wavelength: 214 nm; temperature, ambient, with fractions frozen immediately upon collection. The yield was 0.843 g (1.83mmole) of 99% pure material. Longer reaction time with HCl / 1,4-dioxane caused rapid isomerization to **7** (RRT: 0.75). ^{1}H NMR (400 MHz, CD_3OD) δ 5.31 (m, 1H), 5.25 (t, 1H), 3.94 (d, 1H), 3.77 (m, 1H), 3.62 (br m, 1H), 3.50 (d, 1H), 3.34 (s, 3H), 3.03 (t, 1H), 2.43 (m, 1H), 2.18 (m, 1H), 2.05 (m, 1H), 2.02 (m, 1H), 1.97 (m, 1H), 1.82 (m, 2H), 1.74 (s, 3H), 1.69 (s, 3H), 1.44 (m, 1H), 1.41 (s, 3H), 0.98 (d, 3H), 0.95 (d, 3H). ^{13}C NMR (100

MHz, CD_3OD) δ 175.6, 157.0, 134.4, 118.3, 78.3, 67.2, 61.1, 60.4, 55.6, 50.6, 30.7, 29.3, 27.1, 24.6, 23.4, 18.3, 16.9, 16.6. HRMS: calcd for $C_{22}H_{37}N_2O_6Cl$+H: 461.24129. Found: 461.23927.

Oxidation of 4, 5, and 6. Starting material (0.05 mmole) was dissolved in dry DCM. To this was added TPAP (3.5 mg, 0.01 mmole, 0.2 equiv.), followed by N-methylmorpholine oxide (11 mg, 0.095 mmole, 2 equiv.), and the solution was then stirred under nitrogen for 18 h at room temperature. The solution was filtered through a 1 inch plug of silica gel and eluted with ether (100 mL) and 20% methanol in ether (100 mL). The combined filtrates were concentrated and lyophilized from acetonitrile/water.

Synthesis of compound 7. Compound **3** (0.5 g, 1.17 mmole) was dissolved in 9.8 mL 1,4-dioxane at room temperature. To the solution was added 4.0 M HCl / 1,4-dioxane (0.7 mL, 2.8 mmole, 2.4 equivalents). The reaction was stirred at room temperature for 2 h, and then concentrated *in vacuo*. The concentrated material was brought up in 33% CH_3CN / H_2O and purified by preparative HPLC as follows: column, Phenomenex Luna, C8, 5 micron, 100 x 21.2mm; mobile phases, "A" = 100% H_2O, "B" = 99% CH_3CN, 1% H_2O; gradient, 40-60% "B" over 20 minutes; flow, 24mL/min; detection wavelength, 214nm; temperature, ambient, with fractions frozen immediately upon collection. The yield was 0.292g (54%) of >99% pure material. ^{1}H NMR (400 MHz, CD_3OD) δ 5.37 (s, 1H), 5.3 (br s, 2H), 5.16 (s, 1H), 3.95 (d, 1H), 3.93 (d, 1H), 3.74 (br s, 1H), 3.55 (d, 1H), 3.43 (d, 1H), 3.28 (s, 3H) 3.04 (br s, 1H), 2.43 (br s, H), 2.05 (m, 1H), 1.95 (m, 1H), 1.85 (m, 2H), 1.69 (s, 3H), 1.65 (s, 3H), 1.61 (m, 1H), 0.98 (d, 3H), 0.95 (d, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 175.6, 157.0, 132.3, 120.9, 73.2, 67.3, 60.3, 51.3, 32.8, 30.7, 28.4, 24.6, 23.5, 18.3, 16.9, 16.7.

Synthesis of compound 8. Compound **7** (0.060g, 0.130mmole) was dissolved in 15mL THF. KOtBu (0.024g, 0.209mmole) was added, and the reaction was stirred at room temperature under

dry N_2 gas for 30 minutes. The reaction mixture was then concentrated *in vacuo*,brought up in DCM, washed with H_2O, saturated $NaHCO_3$, H_2O, and brine. The organics were concentrated *in vacuo*, and then brought up in ~50% CH_3CN / H_2O. Crude product was purified by preparative HPLC as follows: injection quantity, ~60mg; column, Phenomenex Luna, C8, 5 micron, 100 x 21.2mm; mobile phases, "A" = 100% H_2O, "B" = 99% CH_3CN, 1% H_2O; gradient, 40-60% "B" over 20 minutes; flow, 24mL/min; detection wavelength, 214nm; temperature, ambient, with fractions frozen immediately upon collection. The overall yield was 0.0365g (0.086mmole) of 99% pure material. ^{1}H NMR (400 MHz, CD_3OD) δ 5.33 (s, 1H), 5.10 (t, 1H), 4.99 (s, 1H), 4.97 (s, 1H), 3.91 (d, 1H), 3.85 (t, 1H), 3.35 (dd, 1H), 3.18 (s, 3H), 2.98 (d, 1H), 2.65 (d, 1H), 2.41 (d, 1H), 2.20 (m, 1H), 2.12 (m, 2H), 1.99 (m, 1H), 1.91 (m, 1H), 1.78 (m, 1H), 1.61 (s, 3H), 1.54 (s, 3H), 1.08 (m, 1H), 0.90 (d, 3H), 0.86 (d, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 175.5, 157.0, 145.3, 131.9, 121.2, 111.5, 111.3, 82.3, 75.9, 68.1, 60.1, 58.4, 56.7, 50.6, 40.9, 33.8, 30.9, 28.2, 25.5, 24.6, 18.4, 16.8, 16.8. HRMS: calcd for $C_{22}H_{36}N_2O_6$+H: 425.26461. Found: 425.26301.

NMR based structure determination. One-dimensional ^{1}H spectra were performed at ambient temperature (~298 K). For each sample, 64-256 scans were recorded. Two-dimensional gradient enhanced DQF-COSY, TOCSY, and ROESY experiments were obtained using an 8 ppm sweep width, with representative additional acquisition and processing parameters as detailed below.

Spectrum	**Scans**	**Increments (States quadrature detection)**	**Other Acquisition Parameters**	**F2 processing**	**F1 processing**	**Final Matrix size**
DQF-COSY	8	2 x 512		Shifted sine bell squared	Shifted sine bell squared	4K x 4K
TOCSY	8	2 x 512	40 ms MLEV spin lock, 2 ms trim pulses	Gaussian	Gaussian	4K x 4K
ROESY	32	2 x 512	200 ms mix time	Gaussian	Gaussian	4K x 4K

^{1}H NMR Assignments of compounds 4 - 8: Proton chemical shifts of the degradants are listed together with those of **3** in Table S1, using the numbering scheme shown in the figure. Proton assignments were made using 2D COSY, TOCSY, and ROESY correlations. When possible, stereospecific assignments were made for H8 and H9 by ROE correlations to H17 and Me7, respectively; and for H14 and H15 by ROE's between H15 and H12. Me2 could be identified by an ROE to H3.

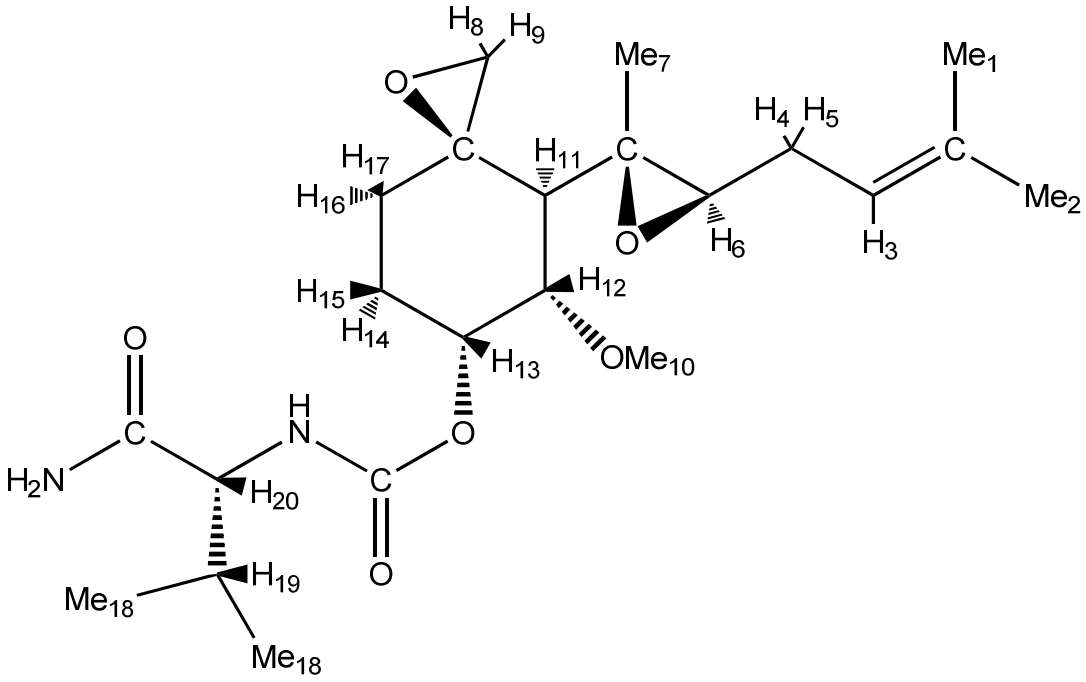

Table S1. ^{1}H Chemical Shift Assignments for 3 and degradants 4 – 8 in CD_3OD, referenced to TMS at 0.0 ppm.

Compound	**3**	**4**	**5**	**6**	**7**	**8**
Resonance						
Me1	1.67	1.62	1.62	1.69	1.65	1.54
Me2	1.75	1.69	1.71	1.74	1.69	1.61
H3	5.24	5.26	5.24	5.25	5.16	5.10
H4,5	2.22, 2.31	2.04, 2.33	2.02, 2.20	2.18, 2.43	2.43	2.12, 2.12
H6	2.64	3.35	3.52	3.03	3.93	3.85
Me7	1.19	1.29	1.25	1.41	5.3	4.97, 4.99
H8	2.56	3.61 or 3.77	3.50 or 3.64	3.50	3.43 or 3.55	2.41
H9	2.96	3.61 or 3.77	3.50 or 3.64	3.77	3.43 or 3.55	2.65
Me10	3.40	3.38	3.32	3.34	3.28	3.18
H11	1.97	2.30	2.34	2.02	3.04	2.98
H12	3.67	3.69	3.28	3.62	3.74	3.35
H13	5.43	5.41	5.30	5.31	5.37	5.33
H14	1.96	1.88	1.97	1.82	1.8 – 2.0	1.91
H15	1.80	2.06	1.53	1.82	1.8 – 2.0	1.78
H16	2.14	1.67	2.01	1.97	1.8 – 2.0	2.20
H17	1.04	1.67	1.79	1.44	1.61	1.08
Me18	0.99, 0.96	0.97, 0.93	0.99, 0.96	0.98, 0.95	0.98, 0.95	0.90, 0.86
H19	2.04	2.05	2.08	2.05	2.05	1.99
H20	3.94	3.96	3.98	3.94	3.95	3.91

Crystal Structure Determination of 4. Single crystals of **4** were grown via vapor diffusion of dichloromethane and toluene. Crystals grew as very thin, colorless plates. A single plate was selected for data collection, mounted in Paratone-N oil on the end of a glass fiber, and placed in the N_2 cold stream of a Bruker Kappa APEX2 diffractometer, equipped with a CuKα IμS microsource (MX optics). SADABS-2008/1 (Bruker,2008) was used for absorption correction. wR2(int) was 0.1139 before and 0.0644 after correction. The ratio of minimum to maximum transmission was 0.7481. The λ/2 correction factor was 0.0015.

Solvent Treatment Details. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. Only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 1359.2 $Å^3$ [16.8%]. Total electron count / cell = 323.9.

Crystal Data. $C_{22}H_{38}N_2O_7$, M =442.54, triclinic, a = 20.5447(15) Å, b = 20.5837(16) Å, c = 23.010(2) Å, α = 109.756(5)°, β = 90.293(5)°, γ = 116.210(5)°, U = 8077.7(11) $Å^3$, T = 100.01, space group P1 (no. 1), Z = 12, μ(CuKα) = 0.665, 47508 reflections measured, 30860 unique (R_{int} = 0.0874, solvent masked data) which were used in all calculations. The structure was solved via Dual Space methods (XM, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122) and refined with SHELXL (XL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122). The final R1 [I>2σ(I)] = 10.07%. The absolute configuration was assigned on the basis of known stereocenters based on the 38952 crystal structure and is supported by the calculated absolute structure parameter (Flack = -0.1(2)) and the Bijvoet Pair Analysis which gives Hooft y = 0.15(16).

Structure notes. The asymmetric unit contains twelve independent molecules of **4**. Molecule 1 is shown in Figure 2. The remaining molecules, which adopt a range of conformations, are

labeled identically, with letters A-K appended. The crystal structure presented here was obtained after many attempts at crystallization and crystals grew as very thin plates that did not diffract to high resolution. While we are confident of the general connectivity and the relative and absolute stereochemical assignments, the metric data should not be used to support precise distances or angles.

Crystal Structure Determination of 5. Single crystals of **5** were grown via slow evaporation from tetrahydrofuran solution. Crystals grew as colorless plates. A single plate was selected for data collection, mounted in Paratone-N oil on the end of a glass fiber, and placed in the N_2 cold stream of a Bruker Kappa APEX2 diffractometer, equipped with a CuKα IμS microsource (MX optics). SADABS-2008/1 (Bruker,2008) was used for absorption correction. wR2(int) was 0.0627 before and 0.0472 after correction. The ratio of minimum to maximum transmission was 0.9202. The λ/2 correction factor was 0.0015.

Solvent Treatment Details. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. Only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 1426.3 Å3 [24.7%]. Total electron count / cell = 224.9.

Crystal Data. $C_{22}H_{38}N_2O_7$, M =442.54, orthorhombic, a = 10.7860(2) Å, b = 19.7586(4) Å, c = 27.0501(5) Å, U = 5764.82(19) Å^3, T = 100.0, space group $P2_12_12_1$ (no. 19), Z = 8, μ(CuKα) = 0.621, 37798 reflections measured, 9930 unique (R_{int} = 0.0394, solvent masked data) which were used in all calculations. The structure was solved via Dual Space methods (XM, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122) and refined with SHELXL (XL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122). The final R1 [I>2σ(I)] = 4.07 %. The absolute configuration was

assigned on the basis of the calculated absolute structure parameter (Flack = 0.00(13)) and is confirmed by the Bijvoet Pair analysis which gives Hooft y = 0.04(6).

Inhibition of MetAP-2 and HUVEC proliferation by acid degradants. Compounds **4 - 8** were tested for their ability to inhibit methionine-AMC hydrolysis in pH 7.5 HEPES buffer as described previously[i]. To evaluate the pH dependence of inhibition by **6**, the standard assay buffer (20 mM HEPES pH 7.5, 0.1 M KCl, 10% glycerol, 0.1 mM $CoSO_4$, 1x complete protease inhibitors) was compared with buffer in which 20 mM MES, pH 6.15, replaced HEPES. Inhibition of HUVEC proliferation following the same protocol as previously[i]. Direct measurements of the stability of **6** were performed by diluting 1 mg/mL solutions tenfold into 3 buffers (20 mM MES, 0.1 M KCl, pH 6.15; 50 mM phosphate, pH 6.8; 20 mM HEPES, 0.1 M KCl, pH 7.5), and incubating at 30ºC for eight hours. Aliquots were removed at 0, 1, 2, 4, and 8 hour timepoints and levels of **6** and **3** were quantitated from peak areas by LCMS, using a Thermo LTQ-XL mass spectrometer and a formic acid / acetonitrile gradient.

Stability of 6 in rat plasma. Standards of compounds **3** and **6** were prepared at concentrations of 1, 5, 10, 50, 100, 500, and 1000 ng/mL in rat plasma (Valley Biomedical). Additionally, two standards of PPI-4021 in solvent (μL 95%water/5% CH_3CN) were prepared at 5 and 500 ng/mL. Duplicate aliquots (100 μL) of each standard were placed in a well of a polypropylene deep-well 96 well plate and refrigerated at 4°C for 1 hour. The samples were each treated with 100 μL octadeuterated **3** as an internal standard (30 ng/mL in 95% water:5% CH_3CN) and vortexed, then quenched with 400 μL CH_3CN and vortexed. The samples were centrifuged (3500 rpm, 10 min, 15°C) and 400 μL of supernatant was transferred to a fresh well-plate. The samples were

evaporated to dryness with N_2 (ca. 60 min, 55°C) and the residue was reconstituted in 100 μL 95%water/5% CH_3CN with vortexing. The plate was covered with a CapMat piercable cover for analysis by HPLC/MS/MS.

A milder sample preparation, incorporating no incubation time, was employed using the following procedure to evaluate concentrations of **6** in rat plasma. No more than 1 min processing time was allowed for analyte stock solution (2 μL) and deuterated **3** internal standard solution (200 μL) to be added to the blank plasma (198 μL) in an Eppendorf tube, vortexed and quenched with CH_3CN (800 μL). The procedure was repeated in triplicate; then the samples were centrifuged (14K, 10 min, ambient temperature). An aliquot of the supernatant (20 μL) was diluted with 180 μL water in a siliconized sample vial insert. The samples were vortexed for analysis.

HPLC/MS/MS analysis of the samples was performed using Shimadzu HPLC pumps and a CTC Pal HTS autosampler coupled to an Applied Biosystems API 4000 mass spectrometer. Sample injections (40 μL) were made onto a Clipeus C_8 (2.1 x 30 mm) column at a 400 μL/min flowrate with the following HPLC program (Mobile Phase A = 85:5:10 water: CH_3CN:(25 mM ammonium acetate, pH 3.5), Mobile Phase B =90:10 CH_3CN:(25 mM ammonium acetate, pH 3.5)): 1) 0.5 minute isocratic at 80% A:20% B; 2) 3.0 minute linear gradient to 10% A:90% B; 3) 0.5 minute isocratic at 10% A:90% B; 4) 0.1 minute linear gradient to 80% A:20% B; 5) 0.6 min isocratic at 80% A:20% B. The mass spectrometer was operated with multiple reaction monitoring data acquisition switching between transitions for **3** (m/z 442.5→375.4), **6** (m/z 478.5→429.4) and deuterated **3** (m/z 450.5→383.4). Data processing was performed using Analyst 1.2 software provided with the mass spectrometer.

Table S2: Average concentrations of 3 found in plasma and solvent standards of 6 and 3 controls

Parent Compound	Theoretical Parent Concentration (ng/mL)	Detected Concentration of **3** (ng/mL)
3* t = 1 h (plasma)	1	1.02
	5	4.81
	10	9.52
	50	51.6
	100	97.7
	500	545
	1000	1030
6* t = 1 h (solvent)	5	0.118
	500	2.61
6* t = 1 h (plasma)	1	1.15
	5	5.62
	10	11.8
	50	61.3
	100	128
	500	653
	1000	1270
6 t = 1 min (plasma)	1000	71.4

* average value, n = 2

Table S2 lists the average concentration of **3** found in each sample of **6** standard. Compound **6** reverted quantitatively to **3** *ex-vivo* in rat plasma within 1 hour at 4°C, while solvent standards demonstrated less than 3% reversion at concentrations of 5 or 500 ng/mL under identical

experimental conditions. Significant levels of reversion were still observed (≤15%) after reducing the sample processing time to 1 min. Thus, **6** rapidly reverted to **3** in plasma, even under mild sample handling conditions.

Determination of *in vivo* MetAP2 inhibition.

Species and dosing. All animals were maintained following to the Praecis Pharmaceutical Institutional Animal Care and Use Committee (IACUC) guidelines, in accordance with the Guide for the Care and Use of Laboratory Animals as adopted by the US National Institutes of Health. Male Sprague-Dawley rats (200-225 g) were purchased from Charles River Laboratories (Wilmington, MA) 5 days before the study start. Food (Harlan 2018 18% Protein Rodent Diet) and water were available at libitum. Compounds **3-8** were formulated in 11% HPCD / WFI, with or without 10 mM NH_4OAc, pH 5, to inhibit recyclization of HCl adducts prior to administration. Dosing was performed according to the study design below, using 25G butterfly infusion sets and 5 cc syringes for IV administration and 18G feeding needles with 3 cc syringes for PO administration, respectively.

Group	**Treatment**	**Route**	**Conc (mg/ml)**	**Dose vol. (mL / kg)**	**Dose (mg / kg)**	**N =**
1	vehicle	PO	0	5	0	3
2	**3**	PO	0.6	5	3	3
3	**4**	PO	0.6	5	3	3
4	**5**	PO	0.6	5	3	3
5	**6**	PO	0.3	10	3	3
6	**7**	PO	0.6	5	3	3
7	**8**	PO	0.6	5	3	3

Sample collection and preparation. Blood was collected from the jugular vein of each conscious rat (~500 uL) 2 - 4 h following administration. Approximately 24 h following compound administration, animals were anesthetized with Isoflurane inhalant anesthetic, and blood was collected via cardiac puncture prior to euthanizing animals with an overdose of CO_2. Following euthanasia, liver and thymus were collected from each animal. Immediately following the initial collection of blood, samples were placed into microtainers containing EDTA. Samples were briefly placed on a tilt table, then centrifuged at 6000 g for 8 min in an Eppendorf centrifuge (Brinkmann Inc., Westbury, NY). Plasma (supernatant) was pipetted into 1.2 silanized Eppendorf tubes (Corning, Corning, NY) and stored at -80°C until analysis. Immediately following the 24 h collection, ~ 0.5 mL of each sample was placed in microtainers containing EDTA, and processed as described above. The remaining blood samples, ~ 5 mL / rat, were placed into 5 mL tubes containing EDTA (Becton-Dickinson), pooled by group into 50 mL conical tubes, and placed on ice until analyzed for free MetAP2 content. Organs were immediately frozen with liquid nitrogen and stored at -80°C until analysis.

Plasma sample analysis and free MetAP2 levels. Plasma samples were thawed at room temperature for determination of plasma drug levels. Two hundred μL of each plasma sample was transferred to a microcentrifuge tube to which 100 μL of a 5 ng / mL solution of **3**-*d*8 was added as an internal standard. Standard curve samples were prepared for each analyte in blank rat plasma (points: 0.05, 0.2, 2, 5, 20 ng / mL). Protein was precipitated by adding 0.5 mL acetonitrile and vortexing. The tubes were then centrifuged at 14,000 rpm for 10 min at room temperature in a tabletop microcentrifuge. The resulting supernatants were transferred to clean microcentrifuge tubes and dried under nitrogen for 30 min at 50°C. The samples were then reconstituted with water to ~ 100 μL followed by vortexing and centrifugation. The resulting

supernatants were transferred to LC autosampler vials, and 40 μL was injected into a Clipeus C8 HPLC column and separated by ~4.5 min gradient elution. LC/MS/MS analysis was achieved using a Sciex 4000 triple quadropole mass spectrometer using multiple reaction monitoring data acquisition including transitions appropriate for each analyst. Quantitation was performed with Analyst 2.1 software (PE Sciex). Determination of free MetAP2 content in plasma and homogenized tissue samples was performed by ELISA methods as described previously.[ii]

Table S3. Plasma exposure data as determined by LC/MS/MS.

Rat #	Compound Dosed	Dose	Exposure (ng/mL)[a] 2h[b]	24h
1			0.94	BLQ
2	**3**	3.0 mg / kg PO	1	BLQ
3			1.2	0.05
4			11.5	1.5
5	**4**	3.0 mg / kg PO	8.1	0.52
6			8.5	0.13
7			15.5	0.56
8	**5**	3.0 mg / kg PO	11.1	0.08
9			17.1	0.93
10			0.12	BLQ
11	**6**[c]	3.0 mg / kg PO	0.16	BLQ
12			0.15	BLQ
13			6.1	BLQ
14	**7**[d]	3.0 mg / kg PO	4	BLQ
15			3	BLQ
16			1.7	BLQ
17	**8**	3.0 mg / kg PO	2.3	BLQ
18			2.2	BLQ

[a]Limit of quantitation: 0.05 – 0.1 ng/mL for all compounds except **8** (0.2 ng/mL)

[b]4h for compound **6**

[c]Quantitated as **3** only; no parent **6** detected

[d]Quantitated as **8** only; no parent **7** detected

References

[i]Arico-Muendel, C. C.; Benjamin, D. R.; Caiazzo, T. M.; Centrella, P. A.; Contonio, B. D.; Cook, C. M.; Doyle, E. G.; Hannig, G.; Labenski, M. T.; Searle, L. L.; Lind, K.; Morgan, B. A.; Olson, G.; Paradise, C. L; Self, C.; Skinner, S. R.; Sluboski, B.; Svendsen, J. L.; Thompson, C. D.; Westlin, W., White, K. F. Carbamate analogues of fumagillin as potent, targeted inhibitors of methionine aminopeptidase-2. *J. Med. Chem*. **2009**, *52*, 8047 – 8056.

[ii]Bernier, S. G.; Lazarus, D. D; Clark, E.; Doyle, B.; Labenski, M. T.; Thompson, C. D.; Westlin, W. F.; Hannig, G. A methionine aminopeptidase-2 inhibitor, PPI-2458, for the treatment of rheumatoid arthritis. *Proc. Natl. Acad. Sci. U.S.A.* **2004**, *101*, 10768 – 10773.

CIF File for Compound **4**

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O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H.
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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.

 Each crystallographically unique molecule was refined such that
chemically
 equivalent bonds were restrained to be equivalent to those in Molecule 1.

 Global rigid bond (esds = 0.004 0.008) and similarity (esds = 0.01 0.02)
 restraints were applied to keep displacement parameters reasonable.
 Despite these restraints, there are still elongated ellipsoids which
indicate
 disorder that was not modeled.

 Regions of diffuse residual electron density could not be modeled as
solvent
 molecules.  The electronic contributions of these disordered solvents
were
 removed from the data via the solvent-masking procedure in Olex2.

 Several hydrogen bond donors lack appropriate acceptors.  It is possible
that
 the acceptors would be found on solvent molecules that were removed.

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H13F H 0.1558 0.5842 0.4944 0.222 Uiso 1 1 calc R . .
C14A C -0.0130(8) 0.4660(15) 0.4251(10) 0.203(10) Uani 1 1 d DU . .
H14D H -0.0253 0.5053 0.4531 0.305 Uiso 1 1 calc R . .
H14E H -0.0231 0.4252 0.4417 0.305 Uiso 1 1 calc R . .
H14F H -0.0431 0.4425 0.3832 0.305 Uiso 1 1 calc R . .
C15A C -0.0552(4) 0.5255(7) 0.2400(6) 0.068(3) Uani 1 1 d DU . .
H15D H -0.0630 0.5266 0.2823 0.101 Uiso 1 1 calc R . .
H15E H -0.0751 0.4711 0.2105 0.101 Uiso 1 1 calc R . .
H15F H -0.0804 0.5504 0.2270 0.101 Uiso 1 1 calc R . .
C16A C -0.0218(6) 0.3304(5) 0.1453(7) 0.078(4) Uani 1 1 d DU . .
H16D H -0.0082 0.3103 0.1048 0.117 Uiso 1 1 calc R . .
H16E H -0.0743 0.3162 0.1388 0.117 Uiso 1 1 calc R . .
H16F H -0.0125 0.3077 0.1735 0.117 Uiso 1 1 calc R . .
C17A C 0.1469(4) 0.4137(4) 0.0954(5) 0.046(2) Uani 1 1 d DU . .
C18A C 0.2436(4) 0.3980(5) 0.1413(4) 0.0381(17) Uani 1 1 d DU . .
H18A H 0.2148 0.3430 0.1102 0.046 Uiso 1 1 calc R . .
C19A C 0.3227(4) 0.4346(5) 0.1291(4) 0.050(2) Uani 1 1 d DU . .
C20A C 0.2440(5) 0.3989(6) 0.2085(4) 0.050(2) Uani 1 1 d DU . .
H20A H 0.2703 0.4547 0.2387 0.060 Uiso 1 1 calc R . .
C21A C 0.2835(7) 0.3568(8) 0.2211(6) 0.080(4) Uani 1 1 d DU . .
H21D H 0.2532 0.3003 0.1983 0.120 Uiso 1 1 calc R . .
H21E H 0.2919 0.3683 0.2662 0.120 Uiso 1 1 calc R . .
H21F H 0.3310 0.3745 0.2069 0.120 Uiso 1 1 calc R . .
C22A C 0.1627(5) 0.3623(7) 0.2186(5) 0.066(3) Uani 1 1 d DU . .
H22D H 0.1432 0.3990 0.2225 0.100 Uiso 1 1 calc R . .
H22E H 0.1608 0.3513 0.2569 0.100 Uiso 1 1 calc R . .
H22F H 0.1328 0.3135 0.1825 0.100 Uiso 1 1 calc R . .
O1B O 0.6998(4) 0.0691(4) 0.1434(4) 0.0719(19) Uani 1 1 d DU . .
O2B O 0.7341(5) 0.0788(6) 0.0245(5) 0.101(3) Uani 1 1 d DU . .
H2OB H 0.7315 0.0356 0.0022 0.151 Uiso 1 1 calc R . .
O3B O 0.6116(3) 0.1314(5) 0.2041(4) 0.060(2) Uani 1 1 d DU . .
H3OB H 0.5934 0.1211 0.1674 0.091 Uiso 1 1 calc R . .
O4B O 0.7168(4) 0.2788(4) 0.1158(4) 0.079(2) Uani 1 1 d DU . .
O5B O 0.5814(4) 0.1746(4) 0.0300(4) 0.0691(18) Uani 1 1 d DU . .
O6B O 0.6033(4) 0.2955(5) 0.0346(5) 0.080(3) Uani 1 1 d DU . .
O7B O 0.3681(3) 0.1852(4) 0.0920(4) 0.065(2) Uani 1 1 d DU . .
N1B N 0.5171(4) 0.2259(5) 0.0813(4) 0.0553(19) Uani 1 1 d DU . .
H1NB H 0.4976 0.1831 0.0896 0.066 Uiso 1 1 calc R . .
N2B N 0.3870(5) 0.2642(6) 0.0389(5) 0.080(3) Uani 1 1 d DU . .
H2NE H 0.3408 0.2387 0.0193 0.096 Uiso 1 1 calc R . .
H2NF H 0.4190 0.3051 0.0317 0.096 Uiso 1 1 calc R . .
C1B C 0.7185(4) 0.1506(5) 0.1539(4) 0.0684(19) Uani 1 1 d DU . .
C2B C 0.6750(5) 0.1434(5) 0.0949(4) 0.0680(19) Uani 1 1 d DU . .
H2B H 0.6253 0.1361 0.1043 0.082 Uiso 1 1 calc R . .
C3B C 0.7047(5) 0.2081(5) 0.0684(4) 0.072(2) Uani 1 1 d DU . .
H3B H 0.7530 0.2141 0.0561 0.086 Uiso 1 1 calc R . .
C4B C 0.6505(5) 0.1822(6) 0.0095(4) 0.079(2) Uani 1 1 d DU . .
H4B H 0.6693 0.2221 -0.0101 0.095 Uiso 1 1 calc R . .
C5B C 0.6290(7) 0.1003(6) -0.0396(4) 0.084(3) Uani 1 1 d DU . .
H5BA H 0.6715 0.1017 -0.0601 0.101 Uiso 1 1 calc R . .
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H5BB H 0.5880 0.0854 -0.0723 0.101 Uiso 1 1 calc R . .
C6B C 0.6050(6) 0.0384(6) -0.0100(5) 0.093(3) Uani 1 1 d DU . .
H6BA H 0.5575 0.0300 0.0041 0.111 Uiso 1 1 calc R . .
H6BB H 0.5981 -0.0120 -0.0416 0.111 Uiso 1 1 calc R . .
C7B C 0.6634(5) 0.0659(5) 0.0450(4) 0.080(2) Uani 1 1 d DU . .
C8B C 0.6494(5) 0.0162(5) 0.0840(4) 0.072(2) Uani 1 1 d DU . .
H8BA H 0.5976 -0.0050 0.0903 0.087 Uiso 1 1 calc R . .
H8BB H 0.6599 -0.0280 0.0633 0.087 Uiso 1 1 calc R . .
C9B C 0.6898(4) 0.1781(5) 0.2147(4) 0.068(2) Uani 1 1 d DU . .
H9B H 0.7109 0.1662 0.2466 0.082 Uiso 1 1 calc R . .
C10B C 0.7101(6) 0.2640(5) 0.2445(5) 0.070(2) Uani 1 1 d DU . .
H10E H 0.7639 0.2956 0.2479 0.084 Uiso 1 1 calc R . .
H10F H 0.6847 0.2764 0.2164 0.084 Uiso 1 1 calc R . .
C11B C 0.6910(6) 0.2878(6) 0.3077(5) 0.073(3) Uani 1 1 d DU . .
H11B H 0.6600 0.2460 0.3197 0.087 Uiso 1 1 calc R . .
C12B C 0.7104(7) 0.3564(6) 0.3483(5) 0.085(3) Uani 1 1 d DU . .
C13B C 0.7543(9) 0.4278(7) 0.3322(8) 0.124(6) Uani 1 1 d DU . .
H13G H 0.8023 0.4608 0.3605 0.185 Uiso 1 1 calc R . .
H13H H 0.7272 0.4577 0.3371 0.185 Uiso 1 1 calc R . .
H13I H 0.7618 0.4109 0.2887 0.185 Uiso 1 1 calc R . .
C14B C 0.6893(8) 0.3744(9) 0.4131(5) 0.102(4) Uani 1 1 d DU . .
H14G H 0.6535 0.3256 0.4167 0.153 Uiso 1 1 calc R . .
H14H H 0.6674 0.4094 0.4190 0.153 Uiso 1 1 calc R . .
H14I H 0.7335 0.3998 0.4454 0.153 Uiso 1 1 calc R . .
C15B C 0.8020(4) 0.1963(7) 0.1623(6) 0.080(4) Uani 1 1 d DU . .
H15G H 0.8251 0.1823 0.1901 0.120 Uiso 1 1 calc R . .
H15H H 0.8176 0.2525 0.1809 0.120 Uiso 1 1 calc R . .
H15I H 0.8170 0.1836 0.1213 0.120 Uiso 1 1 calc R . .
C16B C 0.7626(7) 0.3482(7) 0.1032(8) 0.104(4) Uani 1 1 d DU . .
H16G H 0.7346 0.3513 0.0706 0.156 Uiso 1 1 calc R . .
H16H H 0.8064 0.3453 0.0889 0.156 Uiso 1 1 calc R . .
H16I H 0.7778 0.3948 0.1417 0.156 Uiso 1 1 calc R . .
C17B C 0.5694(5) 0.2364(5) 0.0466(5) 0.060(2) Uani 1 1 d DU . .
C18B C 0.4910(4) 0.2834(5) 0.1061(4) 0.056(2) Uani 1 1 d DU . .
H18B H 0.5169 0.3272 0.0912 0.067 Uiso 1 1 calc R . .
C19B C 0.4083(4) 0.2412(6) 0.0789(5) 0.059(2) Uani 1 1 d DU . .
C20B C 0.5042(5) 0.3166(6) 0.1783(4) 0.066(2) Uani 1 1 d DU . .
H20B H 0.4816 0.2719 0.1926 0.080 Uiso 1 1 calc R . .
C21B C 0.4675(7) 0.3675(7) 0.2017(7) 0.089(4) Uani 1 1 d DU . .
H21G H 0.4834 0.4069 0.1827 0.134 Uiso 1 1 calc R . .
H21H H 0.4815 0.3937 0.2475 0.134 Uiso 1 1 calc R . .
H21I H 0.4138 0.3350 0.1899 0.134 Uiso 1 1 calc R . .
C22B C 0.5880(5) 0.3621(8) 0.2047(7) 0.092(4) Uani 1 1 d DU . .
H22G H 0.6074 0.3250 0.1987 0.138 Uiso 1 1 calc R . .
H22H H 0.5967 0.3934 0.2496 0.138 Uiso 1 1 calc R . .
H22I H 0.6130 0.3967 0.1824 0.138 Uiso 1 1 calc R . .
O1C O 0.4782(3) 0.1202(3) 0.2609(3) 0.0418(14) Uani 1 1 d DU . .
O2C O 0.3882(3) 0.1511(4) 0.3427(3) 0.0452(16) Uani 1 1 d DU . .
H2OC H 0.4181 0.1814 0.3767 0.068 Uiso 1 1 calc R . .
O3C O 0.4870(3) 0.1216(4) 0.1450(3) 0.0392(16) Uani 1 1 d DU . .
H3OC H 0.4985 0.1597 0.1791 0.059 Uiso 1 1 calc R . .
O4C O 0.2465(3) 0.0260(4) 0.1731(3) 0.0547(18) Uani 1 1 d DU . .
O5C O 0.2661(3) 0.1724(4) 0.1972(3) 0.0475(16) Uani 1 1 d DU . .
O6C O 0.1416(3) 0.1102(5) 0.1661(4) 0.075(2) Uani 1 1 d DU . .
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O7C O 0.2294(3) 0.2305(4) 0.0200(4) 0.0537(19) Uani 1 1 d DU . .
N1C N 0.2216(4) 0.1503(5) 0.1024(3) 0.055(2) Uani 1 1 d DU . .
H1NC H 0.2683 0.1786 0.1017 0.066 Uiso 1 1 calc R . .
N2C N 0.1112(4) 0.1946(5) 0.0320(4) 0.054(2) Uani 1 1 d DU . .
H2NG H 0.1123 0.2352 0.0263 0.064 Uiso 1 1 calc R . .
H2NH H 0.0706 0.1606 0.0391 0.064 Uiso 1 1 calc R . .
C1C C 0.4080(4) 0.0710(4) 0.2157(3) 0.0409(16) Uani 1 1 d DU . .
C2C C 0.3681(3) 0.1221(4) 0.2311(4) 0.0390(17) Uani 1 1 d DU . .
H2C H 0.3769 0.1481 0.2001 0.047 Uiso 1 1 calc R . .
C3C C 0.2854(3) 0.0854(4) 0.2319(4) 0.0471(19) Uani 1 1 d DU . .
H3C H 0.2758 0.0616 0.2643 0.057 Uiso 1 1 calc R . .
C4C C 0.2608(4) 0.1485(5) 0.2499(4) 0.0518(18) Uani 1 1 d DU . .
H4C H 0.2081 0.1252 0.2554 0.062 Uiso 1 1 calc R . .
C5C C 0.3075(4) 0.2207(5) 0.3087(4) 0.053(2) Uani 1 1 d DU . .
H5CA H 0.2953 0.2074 0.3461 0.063 Uiso 1 1 calc R . .
H5CB H 0.2945 0.2624 0.3112 0.063 Uiso 1 1 calc R . .
C6C C 0.3914(4) 0.2528(5) 0.3105(5) 0.053(2) Uani 1 1 d DU . .
H6CA H 0.4066 0.2779 0.2795 0.063 Uiso 1 1 calc R . .
H6CB H 0.4186 0.2927 0.3528 0.063 Uiso 1 1 calc R . .
C7C C 0.4093(4) 0.1860(4) 0.2953(4) 0.0452(16) Uani 1 1 d DU . .
C8C C 0.4875(4) 0.1996(4) 0.2895(5) 0.044(2) Uani 1 1 d DU . .
H8CA H 0.5082 0.2294 0.2624 0.053 Uiso 1 1 calc R . .
H8CB H 0.5201 0.2281 0.3312 0.053 Uiso 1 1 calc R . .
C9C C 0.4284(4) 0.0526(5) 0.1493(3) 0.047(2) Uani 1 1 d DU . .
H9C H 0.4482 0.0149 0.1442 0.057 Uiso 1 1 calc R . .
C10C C 0.3675(5) 0.0161(6) 0.0924(4) 0.054(2) Uani 1 1 d DU . .
H10G H 0.3232 -0.0266 0.0977 0.065 Uiso 1 1 calc R . .
H10H H 0.3541 0.0562 0.0909 0.065 Uiso 1 1 calc R . .
C11C C 0.3888(6) -0.0158(6) 0.0322(4) 0.071(3) Uani 1 1 d DU . .
H11C H 0.4227 0.0223 0.0179 0.085 Uiso 1 1 calc R . .
C12C C 0.3684(8) -0.0868(6) -0.0036(5) 0.086(3) Uani 1 1 d DU . .
C13C C 0.3248(12) -0.1524(8) 0.0184(9) 0.146(7) Uani 1 1 d DU . .
H13J H 0.3199 -0.1304 0.0621 0.218 Uiso 1 1 calc R . .
H13K H 0.3504 -0.1835 0.0153 0.218 Uiso 1 1 calc R . .
H13L H 0.2756 -0.1859 -0.0081 0.218 Uiso 1 1 calc R . .
C14C C 0.3998(10) -0.1073(10) -0.0632(7) 0.136(7) Uani 1 1 d DU . .
H14J H 0.4213 -0.0621 -0.0757 0.204 Uiso 1 1 calc R . .
H14K H 0.3602 -0.1518 -0.0970 0.204 Uiso 1 1 calc R . .
H14L H 0.4380 -0.1210 -0.0552 0.204 Uiso 1 1 calc R . .
C15C C 0.3703(5) -0.0044(5) 0.2276(5) 0.045(2) Uani 1 1 d DU . .
H15J H 0.4049 -0.0252 0.2277 0.067 Uiso 1 1 calc R . .
H15K H 0.3271 -0.0428 0.1945 0.067 Uiso 1 1 calc R . .
H15L H 0.3546 0.0063 0.2685 0.067 Uiso 1 1 calc R . .
C16C C 0.1735(4) -0.0310(6) 0.1735(7) 0.073(4) Uani 1 1 d DU . .
H16J H 0.1499 -0.0690 0.1306 0.109 Uiso 1 1 calc R . .
H16K H 0.1441 -0.0045 0.1899 0.109 Uiso 1 1 calc R . .
H16L H 0.1769 -0.0581 0.2002 0.109 Uiso 1 1 calc R . .
C17C C 0.2043(4) 0.1403(6) 0.1552(4) 0.050(2) Uani 1 1 d DU . .
C18C C 0.1675(5) 0.1171(5) 0.0452(4) 0.056(2) Uani 1 1 d DU . .
H18C H 0.1172 0.0873 0.0533 0.067 Uiso 1 1 calc R . .
C19C C 0.1704(4) 0.1846(5) 0.0299(5) 0.055(2) Uani 1 1 d DU . .
C20C C 0.1823(6) 0.0618(5) -0.0112(4) 0.070(3) Uani 1 1 d DU . .
H20C H 0.2328 0.0935 -0.0180 0.084 Uiso 1 1 calc R . .
C21C C 0.1298(6) 0.0334(7) -0.0705(5) 0.076(3) Uani 1 1 d DU . .
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H21J H 0.0795 0.0010 -0.0661 0.113 Uiso 1 1 calc R . .
H21K H 0.1435 0.0023 -0.1058 0.113 Uiso 1 1 calc R . .
H21L H 0.1322 0.0784 -0.0781 0.113 Uiso 1 1 calc R . .
C22C C 0.1849(7) -0.0034(6) 0.0058(7) 0.089(4) Uani 1 1 d DU . .
H22J H 0.2305 0.0186 0.0355 0.133 Uiso 1 1 calc R . .
H22K H 0.1835 -0.0444 -0.0324 0.133 Uiso 1 1 calc R . .
H22L H 0.1423 -0.0259 0.0250 0.133 Uiso 1 1 calc R . .
O1D O 0.6951(3) 1.0714(3) 0.4900(3) 0.0407(14) Uani 1 1 d DU . .
O2D O 0.7014(3) 0.9382(4) 0.4163(3) 0.0381(15) Uani 1 1 d DU . .
H2OD H 0.7248 0.9175 0.3943 0.057 Uiso 1 1 calc R . .
O3D O 0.7205(3) 1.1433(3) 0.6159(3) 0.0373(15) Uani 1 1 d DU . .
H3OD H 0.7304 1.1766 0.5994 0.056 Uiso 1 1 calc R . .
O4D O 0.6087(3) 0.8790(3) 0.5632(3) 0.0341(14) Uani 1 1 d DU . .
O5D O 0.7438(3) 0.8937(3) 0.5857(3) 0.0365(14) Uani 1 1 d DU . .
O6D O 0.6810(4) 0.7782(3) 0.5988(3) 0.0472(17) Uani 1 1 d DU . .
O7D O 0.8303(3) 0.9505(4) 0.7965(3) 0.0481(17) Uani 1 1 d DU . .
N1D N 0.7307(4) 0.8941(4) 0.6805(3) 0.0400(17) Uani 1 1 d DU . .
H1D H 0.7530 0.9453 0.6918 0.048 Uiso 1 1 calc R . .
N2D N 0.7926(5) 0.8229(5) 0.7710(4) 0.055(2) Uani 1 1 d DU . .
H2NI H 0.8330 0.8323 0.7932 0.066 Uiso 1 1 calc R . .
H2NJ H 0.7582 0.7743 0.7504 0.066 Uiso 1 1 calc R . .
C1D C 0.6509(3) 1.0210(4) 0.5229(3) 0.0362(15) Uani 1 1 d DU . .
C2D C 0.6939(4) 0.9770(4) 0.5275(4) 0.0319(15) Uani 1 1 d DU . .
H2D H 0.7258 1.0054 0.5702 0.038 Uiso 1 1 calc R . .
C3D C 0.6534(4) 0.8903(4) 0.5168(4) 0.0315(15) Uani 1 1 d DU . .
H3D H 0.6214 0.8600 0.4742 0.038 Uiso 1 1 calc R . .
C4D C 0.7098(4) 0.8610(5) 0.5208(3) 0.0339(16) Uani 1 1 d DU . .
H4D H 0.6823 0.8028 0.5074 0.041 Uiso 1 1 calc R . .
C5D C 0.7694(4) 0.8805(5) 0.4803(4) 0.0390(19) Uani 1 1 d DU . .
H5DA H 0.8083 0.8688 0.4920 0.047 Uiso 1 1 calc R . .
H5DB H 0.7473 0.8477 0.4355 0.047 Uiso 1 1 calc R . .
C6D C 0.8038(4) 0.9673(5) 0.4898(5) 0.0418(19) Uani 1 1 d DU . .
H6DA H 0.8326 1.0001 0.5330 0.050 Uiso 1 1 calc R . .
H6DB H 0.8380 0.9777 0.4601 0.050 Uiso 1 1 calc R . .
C7D C 0.7451(4) 0.9885(4) 0.4795(3) 0.0389(15) Uani 1 1 d DU . .
C8D C 0.7663(4) 1.0723(4) 0.4881(5) 0.0416(19) Uani 1 1 d DU . .
H8DA H 0.8017 1.1102 0.5277 0.050 Uiso 1 1 calc R . .
H8DB H 0.7877 1.0848 0.4524 0.050 Uiso 1 1 calc R . .
C9D C 0.6487(4) 1.0783(4) 0.5859(3) 0.0348(17) Uani 1 1 d DU . .
H9D H 0.6171 1.1001 0.5761 0.042 Uiso 1 1 calc R . .
C10D C 0.6167(5) 1.0432(5) 0.6344(4) 0.046(2) Uani 1 1 d DU . .
H10I H 0.5746 0.9903 0.6124 0.055 Uiso 1 1 calc R . .
H10J H 0.6547 1.0374 0.6555 0.055 Uiso 1 1 calc R . .
C11D C 0.5912(6) 1.0914(6) 0.6827(4) 0.056(2) Uani 1 1 d DU . .
H11D H 0.5602 1.1063 0.6657 0.068 Uiso 1 1 calc R . .
C12D C 0.6028(7) 1.1166(8) 0.7424(4) 0.080(3) Uani 1 1 d DU . .
C13D C 0.6524(8) 1.1006(10) 0.7782(6) 0.105(4) Uani 1 1 d DU . .
H13M H 0.6227 1.0524 0.7853 0.157 Uiso 1 1 calc R . .
H13N H 0.6768 1.1444 0.8187 0.157 Uiso 1 1 calc R . .
H13O H 0.6897 1.0947 0.7537 0.157 Uiso 1 1 calc R . .
C14D C 0.5698(10) 1.1644(10) 0.7856(6) 0.116(5) Uani 1 1 d DU . .
H14M H 0.5550 1.1902 0.7634 0.173 Uiso 1 1 calc R . .
H14N H 0.6067 1.2040 0.8233 0.173 Uiso 1 1 calc R . .
H14O H 0.5265 1.1295 0.7978 0.173 Uiso 1 1 calc R . .
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C15D C 0.5746(4) 0.9689(5) 0.4817(5) 0.046(2) Uani 1 1 d DU . .
H15M H 0.5554 1.0016 0.4737 0.069 Uiso 1 1 calc R . .
H15N H 0.5413 0.9375 0.5033 0.069 Uiso 1 1 calc R . .
H15O H 0.5779 0.9342 0.4418 0.069 Uiso 1 1 calc R . .
C16D C 0.5468(4) 0.8016(4) 0.5424(5) 0.034(2) Uani 1 1 d DU . .
H16M H 0.5132 0.7941 0.5075 0.051 Uiso 1 1 calc R . .
H16N H 0.5205 0.7954 0.5772 0.051 Uiso 1 1 calc R . .
H16O H 0.5644 0.7627 0.5284 0.051 Uiso 1 1 calc R . .
C17D C 0.7169(5) 0.8504(4) 0.6199(3) 0.0343(18) Uani 1 1 d DU . .
C18D C 0.7114(4) 0.8629(6) 0.7296(3) 0.0455(17) Uani 1 1 d DU . .
H18D H 0.6808 0.8047 0.7094 0.055 Uiso 1 1 calc R . .
C19D C 0.7834(4) 0.8820(5) 0.7684(4) 0.049(2) Uani 1 1 d DU . .
C20D C 0.6675(5) 0.8965(7) 0.7736(4) 0.059(2) Uani 1 1 d DU . .
H20D H 0.6979 0.9548 0.7918 0.071 Uiso 1 1 calc R . .
C21D C 0.6529(6) 0.8690(7) 0.8274(5) 0.063(3) Uani 1 1 d DU . .
H21M H 0.6227 0.8120 0.8108 0.095 Uiso 1 1 calc R . .
H21N H 0.6266 0.8933 0.8543 0.095 Uiso 1 1 calc R . .
H21O H 0.6999 0.8838 0.8519 0.095 Uiso 1 1 calc R . .
C22D C 0.5949(5) 0.8765(8) 0.7347(6) 0.073(3) Uani 1 1 d DU . .
H22M H 0.6062 0.8985 0.7022 0.109 Uiso 1 1 calc R . .
H22N H 0.5676 0.8986 0.7624 0.109 Uiso 1 1 calc R . .
H22O H 0.5648 0.8195 0.7149 0.109 Uiso 1 1 calc R . .
O1E O 0.1981(3) 0.7162(4) 0.7055(3) 0.0633(18) Uani 1 1 d DU . .
O2E O 0.1468(5) 0.6919(5) 0.8160(4) 0.074(2) Uani 1 1 d DU . .
H2OE H 0.1799 0.7005 0.8435 0.111 Uiso 1 1 calc R . .
O3E O 0.1523(4) 0.7928(4) 0.6494(4) 0.0538(19) Uani 1 1 d DU . .
H3E H 0.1551 0.8176 0.6876 0.081 Uiso 1 1 calc R . .
O4E O -0.0244(3) 0.6999(4) 0.7272(3) 0.0594(18) Uani 1 1 d DU . .
O5E O 0.0564(3) 0.8506(4) 0.8229(3) 0.0556(16) Uani 1 1 d DU . .
O6E O -0.0604(4) 0.8346(4) 0.8183(4) 0.060(2) Uani 1 1 d DU . .
O7E O 0.0802(4) 1.0680(4) 0.7741(4) 0.059(2) Uani 1 1 d DU . .
N1E N 0.0270(4) 0.9144(4) 0.7785(4) 0.0501(18) Uani 1 1 d DU . .
H1NE H 0.0731 0.9317 0.7729 0.060 Uiso 1 1 calc R . .
N2E N -0.0106(4) 1.0639(5) 0.8296(4) 0.059(3) Uani 1 1 d DU . .
H2EK H 0.0113 1.1150 0.8500 0.070 Uiso 1 1 calc R . .
H2EL H -0.0534 1.0343 0.8372 0.070 Uiso 1 1 calc R . .
C1E C 0.1183(4) 0.6915(4) 0.6930(3) 0.0570(17) Uani 1 1 d DU . .
C2E C 0.1055(4) 0.7439(5) 0.7529(3) 0.0529(18) Uani 1 1 d DU . .
H2E H 0.1172 0.7939 0.7475 0.064 Uiso 1 1 calc R . .
C3E C 0.0310(4) 0.7170(5) 0.7747(4) 0.056(2) Uani 1 1 d DU . .
H5 H 0.0190 0.6683 0.7824 0.067 Uiso 1 1 calc R . .
C4E C 0.0368(5) 0.7808(5) 0.8366(4) 0.0581(19) Uani 1 1 d DU . .
H4E H -0.0113 0.7644 0.8518 0.070 Uiso 1 1 calc R . .
C5E C 0.0989(5) 0.8001(7) 0.8865(4) 0.062(2) Uani 1 1 d DU . .
H5EA H 0.0874 0.7534 0.8965 0.074 Uiso 1 1 calc R . .
H5EB H 0.1027 0.8425 0.9255 0.074 Uiso 1 1 calc R . .
C6E C 0.1735(5) 0.8262(6) 0.8630(4) 0.063(2) Uani 1 1 d DU . .
H6EA H 0.1867 0.8748 0.8556 0.076 Uiso 1 1 calc R . .
H6EB H 0.2130 0.8371 0.8953 0.076 Uiso 1 1 calc R . .
C7E C 0.1670(4) 0.7628(5) 0.8033(4) 0.0594(18) Uani 1 1 d DU . .
C8E C 0.2310(4) 0.7754(6) 0.7682(4) 0.066(2) Uani 1 1 d DU . .
H8EA H 0.2539 0.8285 0.7672 0.079 Uiso 1 1 calc R . .
H8EB H 0.2690 0.7684 0.7881 0.079 Uiso 1 1 calc R . .
C9E C 0.1100(4) 0.7106(5) 0.6351(4) 0.055(2) Uani 1 1 d DU . .
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H9E H 0.1319 0.6843 0.6027 0.067 Uiso 1 1 calc R . .
C10E C 0.0315(4) 0.6825(6) 0.6044(4) 0.056(2) Uani 1 1 d DU . .
H10K H 0.0005 0.6278 0.6004 0.067 Uiso 1 1 calc R . .
H10L H 0.0113 0.7148 0.6321 0.067 Uiso 1 1 calc R . .
C11E C 0.0264(5) 0.6865(7) 0.5417(4) 0.061(2) Uani 1 1 d DU . .
H11E H 0.0726 0.7090 0.5292 0.073 Uiso 1 1 calc R . .
C12E C -0.0291(5) 0.6649(7) 0.5015(5) 0.068(3) Uani 1 1 d DU . .
C13E C -0.1043(5) 0.6287(9) 0.5188(6) 0.084(4) Uani 1 1 d DU . .
H13P H -0.0983 0.6343 0.5628 0.126 Uiso 1 1 calc R . .
H13Q H -0.1314 0.5731 0.4917 0.126 Uiso 1 1 calc R . .
H13R H -0.1318 0.6554 0.5131 0.126 Uiso 1 1 calc R . .
C14E C -0.0278(8) 0.6683(9) 0.4363(5) 0.090(4) Uani 1 1 d DU . .
H14P H 0.0234 0.6971 0.4317 0.135 Uiso 1 1 calc R . .
H14Q H -0.0554 0.6950 0.4308 0.135 Uiso 1 1 calc R . .
H14R H -0.0505 0.6150 0.4043 0.135 Uiso 1 1 calc R . .
C15E C 0.0771(6) 0.6044(5) 0.6793(6) 0.063(3) Uani 1 1 d DU . .
H15P H 0.1113 0.5824 0.6700 0.094 Uiso 1 1 calc R . .
H15Q H 0.0371 0.5786 0.6431 0.094 Uiso 1 1 calc R . .
H15R H 0.0564 0.5961 0.7160 0.094 Uiso 1 1 calc R . .
C16E C -0.0987(5) 0.6579(7) 0.7366(6) 0.068(3) Uani 1 1 d DU . .
H16P H -0.1340 0.6443 0.7003 0.101 Uiso 1 1 calc R . .
H16Q H -0.1073 0.6910 0.7746 0.101 Uiso 1 1 calc R . .
H16R H -0.1053 0.6100 0.7415 0.101 Uiso 1 1 calc R . .
C17E C 0.0020(4) 0.8638(6) 0.8064(5) 0.053(2) Uani 1 1 d DU . .
C18E C -0.0175(4) 0.9428(4) 0.7565(4) 0.0463(18) Uani 1 1 d DU . .
H18E H -0.0665 0.9218 0.7696 0.056 Uiso 1 1 calc R . .
C19E C 0.0210(4) 1.0316(4) 0.7876(5) 0.053(2) Uani 1 1 d DU . .
C20E C -0.0301(5) 0.9156(5) 0.6841(4) 0.054(2) Uani 1 1 d DU . .
H20E H 0.0189 0.9338 0.6706 0.065 Uiso 1 1 calc R . .
C21E C -0.0716(6) 0.9519(7) 0.6640(6) 0.072(3) Uani 1 1 d DU . .
H21P H -0.1165 0.9405 0.6821 0.108 Uiso 1 1 calc R . .
H21Q H -0.0848 0.9300 0.6181 0.108 Uiso 1 1 calc R . .
H21R H -0.0403 1.0087 0.6788 0.108 Uiso 1 1 calc R . .
C22E C -0.0731(6) 0.8243(5) 0.6540(5) 0.064(3) Uani 1 1 d DU . .
H22P H -0.0492 0.8027 0.6734 0.096 Uiso 1 1 calc R . .
H22Q H -0.0729 0.8066 0.6088 0.096 Uiso 1 1 calc R . .
H22R H -0.1241 0.8062 0.6610 0.096 Uiso 1 1 calc R . .
O1F O 0.6785(4) 0.6665(4) 0.6851(3) 0.0709(19) Uani 1 1 d DU . .
O2F O 0.5881(4) 0.6260(4) 0.5721(4) 0.059(2) Uani 1 1 d DU . .
H2OF H 0.6164 0.6739 0.5815 0.089 Uiso 1 1 calc R . .
O3F O 0.5874(7) 0.5001(5) 0.7331(5) 0.126(4) Uani 1 1 d DU . .
H3OF H 0.5515 0.5043 0.7477 0.189 Uiso 1 1 calc R . .
O4F O 0.4827(5) 0.4322(5) 0.6220(4) 0.092(3) Uani 1 1 d DU . .
O5F O 0.5442(3) 0.3798(3) 0.5222(3) 0.0545(17) Uani 1 1 d DU . .
O6F O 0.4432(3) 0.2727(4) 0.4586(3) 0.0531(19) Uani 1 1 d DU . .
O7F O 0.5967(3) 0.1503(4) 0.4592(3) 0.0429(17) Uani 1 1 d DU . .
N1F N 0.5353(4) 0.2639(4) 0.5047(4) 0.0446(18) Uani 1 1 d DU . .
H1NF H 0.5808 0.2899 0.5259 0.054 Uiso 1 1 calc R . .
N2F N 0.5096(4) 0.1139(4) 0.3784(3) 0.0352(18) Uani 1 1 d DU . .
H2NM H 0.5309 0.0929 0.3505 0.042 Uiso 1 1 calc R . .
H2NN H 0.4684 0.1130 0.3662 0.042 Uiso 1 1 calc R . .
C1F C 0.6120(5) 0.5966(5) 0.6840(4) 0.074(2) Uani 1 1 d DU . .
C2F C 0.5940(4) 0.5361(4) 0.6164(4) 0.059(2) Uani 1 1 d DU . .
H2F H 0.6200 0.5048 0.6158 0.070 Uiso 1 1 calc R . .
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C3F C 0.5133(5) 0.4790(5) 0.5859(4) 0.070(2) Uani 1 1 d DU . .
H3F H 0.4857 0.5086 0.5854 0.084 Uiso 1 1 calc R . .
C4F C 0.5101(5) 0.4280(5) 0.5184(4) 0.0627(19) Uani 1 1 d DU . .
H4F H 0.4577 0.3936 0.4963 0.075 Uiso 1 1 calc R . .
C5F C 0.5541(5) 0.4758(5) 0.4811(4) 0.060(2) Uani 1 1 d DU . .
H5FA H 0.5275 0.5018 0.4711 0.072 Uiso 1 1 calc R . .
H5FB H 0.5566 0.4397 0.4408 0.072 Uiso 1 1 calc R . .
C6F C 0.6333(5) 0.5385(5) 0.5152(4) 0.056(2) Uani 1 1 d DU . .
H6FA H 0.6634 0.5129 0.5185 0.067 Uiso 1 1 calc R . .
H6FB H 0.6562 0.5718 0.4910 0.067 Uiso 1 1 calc R . .
C7F C 0.6312(4) 0.5875(4) 0.5793(3) 0.0502(17) Uani 1 1 d DU . .
C8F C 0.7022(4) 0.6474(6) 0.6252(4) 0.068(2) Uani 1 1 d DU . .
H8FA H 0.7361 0.6252 0.6257 0.082 Uiso 1 1 calc R . .
H8FB H 0.7273 0.6943 0.6145 0.082 Uiso 1 1 calc R . .
C9F C 0.6405(7) 0.5737(6) 0.7328(5) 0.116(3) Uani 1 1 d DU . .
H9F H 0.6850 0.5684 0.7201 0.139 Uiso 1 1 calc R . .
C10F C 0.6636(12) 0.6336(8) 0.8000(6) 0.151(5) Uani 1 1 d DU . .
H10N H 0.6997 0.6855 0.8005 0.181 Uiso 1 1 calc R . .
H10M H 0.6198 0.6378 0.8145 0.181 Uiso 1 1 calc R . .
C11F C 0.6967(12) 0.6136(11) 0.8442(8) 0.180(5) Uani 1 1 d DU . .
H11F H 0.6659 0.5647 0.8472 0.215 Uiso 1 1 calc R . .
C12F C 0.7607(12) 0.6523(12) 0.8789(10) 0.197(6) Uani 1 1 d DU . .
C13F C 0.8054(15) 0.7390(12) 0.8919(12) 0.206(9) Uani 1 1 d DU . .
H13S H 0.7997 0.7481 0.8535 0.308 Uiso 1 1 calc R . .
H13T H 0.8575 0.7564 0.9059 0.308 Uiso 1 1 calc R . .
H13U H 0.7876 0.7685 0.9248 0.308 Uiso 1 1 calc R . .
C14F C 0.7751(17) 0.6274(15) 0.9314(11) 0.239(10) Uani 1 1 d DU . .
H14S H 0.7453 0.5706 0.9185 0.358 Uiso 1 1 calc R . .
H14T H 0.7617 0.6538 0.9698 0.358 Uiso 1 1 calc R . .
H14U H 0.8275 0.6418 0.9396 0.358 Uiso 1 1 calc R . .
C15F C 0.5549(7) 0.6231(8) 0.7037(7) 0.099(4) Uani 1 1 d DU . .
H15S H 0.5795 0.6773 0.7341 0.148 Uiso 1 1 calc R . .
H15T H 0.5204 0.5894 0.7230 0.148 Uiso 1 1 calc R . .
H15U H 0.5279 0.6199 0.6667 0.148 Uiso 1 1 calc R . .
C16F C 0.4046(6) 0.3794(7) 0.6011(8) 0.119(6) Uani 1 1 d DU . .
H16S H 0.3943 0.3514 0.5555 0.179 Uiso 1 1 calc R . .
H16T H 0.3772 0.4094 0.6120 0.179 Uiso 1 1 calc R . .
H16U H 0.3892 0.3417 0.6217 0.179 Uiso 1 1 calc R . .
C17F C 0.5028(4) 0.3028(4) 0.4930(4) 0.0411(19) Uani 1 1 d DU . .
C18F C 0.4964(5) 0.1789(4) 0.4830(4) 0.0411(18) Uani 1 1 d DU . .
H18F H 0.4470 0.1602 0.4584 0.049 Uiso 1 1 calc R . .
C19F C 0.5390(4) 0.1465(5) 0.4381(3) 0.0325(17) Uani 1 1 d DU . .
C20F C 0.4835(5) 0.1489(5) 0.5370(4) 0.045(2) Uani 1 1 d DU . .
H20F H 0.5328 0.1644 0.5599 0.054 Uiso 1 1 calc R . .
C21F C 0.4398(6) 0.0609(5) 0.5122(5) 0.055(3) Uani 1 1 d DU . .
H21S H 0.3880 0.0448 0.4981 0.082 Uiso 1 1 calc R . .
H21T H 0.4435 0.0425 0.5455 0.082 Uiso 1 1 calc R . .
H21U H 0.4596 0.0384 0.4767 0.082 Uiso 1 1 calc R . .
C22F C 0.4464(6) 0.1894(6) 0.5836(5) 0.054(3) Uani 1 1 d DU . .
H22S H 0.4652 0.2433 0.5862 0.081 Uiso 1 1 calc R . .
H22T H 0.4576 0.1897 0.6252 0.081 Uiso 1 1 calc R . .
H22U H 0.3929 0.1607 0.5689 0.081 Uiso 1 1 calc R . .
O1G O 0.7465(4) 0.5971(5) 0.1726(4) 0.0647(18) Uani 1 1 d DU . .
O2G O 0.7619(3) 0.7240(4) 0.2806(4) 0.059(2) Uani 1 1 d DU . .
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H2OG H 0.7180 0.6929 0.2622 0.088 Uiso 1 1 calc R . .
O3G O 0.9252(4) 0.6700(7) 0.1205(4) 0.086(3) Uani 1 1 d DU . .
H3OG H 0.9429 0.7100 0.1540 0.129 Uiso 1 1 calc R . .
O4G O 0.9667(4) 0.8037(5) 0.2245(4) 0.077(2) Uani 1 1 d DU . .
O5G O 0.9959(3) 0.7826(4) 0.3328(4) 0.0517(17) Uani 1 1 d DU . .
O6G O 1.0840(3) 0.8994(4) 0.4023(4) 0.0474(18) Uani 1 1 d DU . .
O7G O 1.2081(3) 0.7468(4) 0.4016(3) 0.0398(16) Uani 1 1 d DU . .
N1G N 1.1076(4) 0.7991(5) 0.3553(4) 0.0426(18) Uani 1 1 d DU . .
H1NG H 1.0879 0.7488 0.3323 0.051 Uiso 1 1 calc R . .
N2G N 1.2234(4) 0.8535(5) 0.4830(4) 0.0386(19) Uani 1 1 d DU . .
H2NO H 1.2347 0.8372 0.5104 0.046 Uiso 1 1 calc R . .
H2NP H 1.2225 0.8984 0.4959 0.046 Uiso 1 1 calc R . .
C1G C 0.8167(5) 0.6620(7) 0.1708(5) 0.069(2) Uani 1 1 d DU . .
C2G C 0.8616(5) 0.7021(6) 0.2383(5) 0.060(2) Uani 1 1 d DU . .
H2G H 0.8917 0.6756 0.2405 0.072 Uiso 1 1 calc R . .
C3G C 0.9129(5) 0.7901(7) 0.2662(5) 0.065(2) Uani 1 1 d DU . .
H3G H 0.8840 0.8180 0.2645 0.078 Uiso 1 1 calc R . .
C4G C 0.9471(5) 0.8165(7) 0.3341(5) 0.0581(19) Uani 1 1 d DU . .
H4G H 0.9752 0.8749 0.3539 0.070 Uiso 1 1 calc R . .
C5G C 0.8892(5) 0.7843(6) 0.3720(5) 0.058(2) Uani 1 1 d DU . .
H5GA H 0.9150 0.7950 0.4132 0.070 Uiso 1 1 calc R . .
H5GB H 0.8606 0.8136 0.3801 0.070 Uiso 1 1 calc R . .
C6G C 0.8354(5) 0.6980(6) 0.3426(5) 0.053(2) Uani 1 1 d DU . .
H6GA H 0.8613 0.6669 0.3411 0.064 Uiso 1 1 calc R . .
H6GB H 0.7962 0.6843 0.3678 0.064 Uiso 1 1 calc R . .
C7G C 0.8024(5) 0.6801(6) 0.2777(5) 0.0512(18) Uani 1 1 d DU . .
C8G C 0.7532(6) 0.5946(6) 0.2347(5) 0.061(2) Uani 1 1 d DU . .
H8GA H 0.7764 0.5618 0.2359 0.073 Uiso 1 1 calc R . .
H8GB H 0.7043 0.5736 0.2471 0.073 Uiso 1 1 calc R . .
C9G C 0.8538(6) 0.6172(8) 0.1238(5) 0.080(3) Uani 1 1 d DU . .
H9G H 0.8590 0.5811 0.1413 0.096 Uiso 1 1 calc R . .
C10G C 0.8087(7) 0.5672(8) 0.0564(6) 0.086(3) Uani 1 1 d DU . .
H10O H 0.7557 0.5443 0.0592 0.104 Uiso 1 1 calc R . .
H10P H 0.8175 0.6028 0.0338 0.104 Uiso 1 1 calc R . .
C11G C 0.8236(9) 0.5008(9) 0.0162(7) 0.104(4) Uani 1 1 d DU . .
H11G H 0.8745 0.5149 0.0213 0.125 Uiso 1 1 calc R . .
C12G C 0.7833(8) 0.4309(9) -0.0226(7) 0.101(3) Uani 1 1 d DU . .
C13G C 0.8099(11) 0.3719(11) -0.0529(9) 0.130(5) Uani 1 1 d DU . .
H13V H 0.8304 0.3803 -0.0896 0.195 Uiso 1 1 calc R . .
H13W H 0.7684 0.3189 -0.0661 0.195 Uiso 1 1 calc R . .
H13X H 0.8481 0.3782 -0.0226 0.195 Uiso 1 1 calc R . .
C14G C 0.6994(8) 0.3950(12) -0.0435(9) 0.124(5) Uani 1 1 d DU . .
H14V H 0.6734 0.3540 -0.0271 0.187 Uiso 1 1 calc R . .
H14W H 0.6870 0.3724 -0.0895 0.187 Uiso 1 1 calc R . .
H14X H 0.6844 0.4359 -0.0273 0.187 Uiso 1 1 calc R . .
C15G C 0.7955(7) 0.7093(8) 0.1449(6) 0.068(3) Uani 1 1 d DU . .
H15V H 0.7426 0.6804 0.1275 0.102 Uiso 1 1 calc R . .
H15W H 0.8234 0.7192 0.1117 0.102 Uiso 1 1 calc R . .
H15X H 0.8068 0.7593 0.1786 0.102 Uiso 1 1 calc R . .
C16G C 1.0117(7) 0.8825(8) 0.2363(8) 0.098(4) Uani 1 1 d DU . .
H16V H 0.9942 0.8966 0.2051 0.147 Uiso 1 1 calc R . .
H16W H 1.0625 0.8921 0.2337 0.147 Uiso 1 1 calc R . .
H16X H 1.0100 0.9143 0.2784 0.147 Uiso 1 1 calc R . .
C17G C 1.0627(4) 0.8325(5) 0.3680(5) 0.0341(18) Uani 1 1 d DU . .
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C18G C 1.1874(4) 0.8427(6) 0.3782(4) 0.0371(17) Uani 1 1 d DU . .
H18G H 1.1996 0.8982 0.4034 0.045 Uiso 1 1 calc R . .
C19G C 1.2079(5) 0.8109(5) 0.4232(4) 0.0337(18) Uani 1 1 d DU . .
C20G C 1.2306(5) 0.8436(6) 0.3248(5) 0.043(2) Uani 1 1 d DU . .
H20G H 1.2206 0.7886 0.3010 0.051 Uiso 1 1 calc R . .
C21G C 1.3137(5) 0.8928(6) 0.3498(6) 0.052(3) Uani 1 1 d DU . .
H21V H 1.3289 0.9474 0.3561 0.078 Uiso 1 1 calc R . .
H21W H 1.3401 0.8728 0.3195 0.078 Uiso 1 1 calc R . .
H21X H 1.3252 0.8898 0.3899 0.078 Uiso 1 1 calc R . .
C22G C 1.2044(6) 0.8692(7) 0.2799(5) 0.052(3) Uani 1 1 d DU . .
H22V H 1.1505 0.8387 0.2676 0.078 Uiso 1 1 calc R . .
H22W H 1.2270 0.8608 0.2425 0.078 Uiso 1 1 calc R . .
H22X H 1.2185 0.9249 0.3003 0.078 Uiso 1 1 calc R . .
O1H O 0.1848(3) -0.0859(3) 0.5995(3) 0.0463(15) Uani 1 1 d DU . .
O2H O 0.1760(3) -0.0141(4) 0.5190(3) 0.0426(16) Uani 1 1 d DU . .
H2OH H 0.1507 -0.0206 0.4868 0.064 Uiso 1 1 calc R . .
O3H O 0.1528(3) -0.0648(4) 0.7159(3) 0.0422(16) Uani 1 1 d DU . .
H3OH H 0.1411 -0.1106 0.6911 0.063 Uiso 1 1 calc R . .
O4H O 0.2629(3) 0.1697(3) 0.6914(3) 0.0542(18) Uani 1 1 d DU . .
O5H O 0.1222(3) 0.1445(3) 0.6703(3) 0.0538(18) Uani 1 1 d DU . .
O6H O 0.1752(4) 0.2763(4) 0.7016(4) 0.060(2) Uani 1 1 d DU . .
O7H O 0.0153(3) 0.2248(4) 0.8431(3) 0.0484(18) Uani 1 1 d DU . .
N1H N 0.1233(4) 0.2141(4) 0.7672(3) 0.0503(19) Uani 1 1 d DU . .
H1NH H 0.0999 0.1679 0.7699 0.060 Uiso 1 1 calc R . .
N2H N 0.0539(5) 0.3388(5) 0.8308(5) 0.059(2) Uani 1 1 d DU . .
H2NQ H 0.0117 0.3393 0.8362 0.071 Uiso 1 1 calc R . .
H2NR H 0.0898 0.3774 0.8236 0.071 Uiso 1 1 calc R . .
C1H C 0.2241(4) -0.0045(4) 0.6451(3) 0.0447(16) Uani 1 1 d DU . .
C2H C 0.1788(4) 0.0337(4) 0.6320(4) 0.0433(17) Uani 1 1 d DU . .
H2H H 0.1454 0.0333 0.6635 0.052 Uiso 1 1 calc R . .
C3H C 0.2174(4) 0.1165(4) 0.6326(4) 0.0449(18) Uani 1 1 d DU . .
H3H H 0.2492 0.1174 0.5998 0.054 Uiso 1 1 calc R . .
C4H C 0.1590(4) 0.1378(5) 0.6157(4) 0.0519(18) Uani 1 1 d DU . .
H4H H 0.1836 0.1894 0.6108 0.062 Uiso 1 1 calc R . .
C5H C 0.0999(5) 0.0767(5) 0.5580(4) 0.053(2) Uani 1 1 d DU . .
H5HA H 0.1214 0.0782 0.5198 0.063 Uiso 1 1 calc R . .
H5HB H 0.0594 0.0903 0.5569 0.063 Uiso 1 1 calc R . .
C6H C 0.0676(4) -0.0068(5) 0.5569(5) 0.050(2) Uani 1 1 d DU . .
H6HA H 0.0373 -0.0122 0.5899 0.060 Uiso 1 1 calc R . .
H6HB H 0.0358 -0.0450 0.5157 0.060 Uiso 1 1 calc R . .
C7H C 0.1304(4) -0.0224(4) 0.5682(3) 0.0456(16) Uani 1 1 d DU . .
C8H C 0.1134(4) -0.1004(4) 0.5719(4) 0.0402(18) Uani 1 1 d DU . .
H8HA H 0.0764 -0.1144 0.5989 0.048 Uiso 1 1 calc R . .
H8HB H 0.0951 -0.1428 0.5297 0.048 Uiso 1 1 calc R . .
C9H C 0.2248(4) -0.0115(5) 0.7094(3) 0.048(2) Uani 1 1 d DU . .
H9H H 0.2578 -0.0350 0.7114 0.057 Uiso 1 1 calc R . .
C10H C 0.2529(6) 0.0630(5) 0.7682(4) 0.066(3) Uani 1 1 d DU . .
H10Q H 0.2946 0.1060 0.7607 0.079 Uiso 1 1 calc R . .
H10R H 0.2131 0.0777 0.7765 0.079 Uiso 1 1 calc R . .
C11H C 0.2779(6) 0.0536(8) 0.8242(5) 0.083(3) Uani 1 1 d DU . .
H11H H 0.2415 0.0118 0.8334 0.099 Uiso 1 1 calc R . .
C12H C 0.3391(6) 0.0915(8) 0.8617(6) 0.100(4) Uani 1 1 d DU . .
C13H C 0.3961(9) 0.1692(10) 0.8603(10) 0.147(7) Uani 1 1 d DU . .
H13Y H 0.3765 0.1805 0.8281 0.220 Uiso 1 1 calc R . .
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H13Z H 0.4413 0.1663 0.8504 0.220 Uiso 1 1 calc R . .
H13 H 0.4072 0.2110 0.9014 0.220 Uiso 1 1 calc R . .
C14H C 0.3540(9) 0.0721(10) 0.9175(7) 0.113(5) Uani 1 1 d DU . .
H14Y H 0.3524 0.1098 0.9564 0.170 Uiso 1 1 calc R . .
H14Z H 0.4028 0.0748 0.9199 0.170 Uiso 1 1 calc R . .
H14 H 0.3163 0.0192 0.9118 0.170 Uiso 1 1 calc R . .
C15H C 0.3022(4) 0.0306(6) 0.6312(5) 0.052(3) Uani 1 1 d DU . .
H15Y H 0.3255 -0.0010 0.6342 0.078 Uiso 1 1 calc R . .
H15Z H 0.3312 0.0843 0.6619 0.078 Uiso 1 1 calc R . .
H151 H 0.2999 0.0310 0.5888 0.078 Uiso 1 1 calc R . .
C16H C 0.3200(6) 0.2425(5) 0.6905(6) 0.074(4) Uani 1 1 d DU . .
H16Y H 0.3513 0.2316 0.6608 0.111 Uiso 1 1 calc R . .
H16Z H 0.3501 0.2755 0.7326 0.111 Uiso 1 1 calc R . .
H161 H 0.2972 0.2696 0.6776 0.111 Uiso 1 1 calc R . .
C17H C 0.1431(5) 0.2168(4) 0.7129(4) 0.049(2) Uani 1 1 d DU . .
C18H C 0.1378(4) 0.2829(5) 0.8228(4) 0.051(2) Uani 1 1 d DU . .
H18H H 0.1689 0.3308 0.8140 0.062 Uiso 1 1 calc R . .
C19H C 0.0632(4) 0.2802(5) 0.8333(5) 0.046(2) Uani 1 1 d DU . .
C20H C 0.1782(5) 0.2874(6) 0.8820(4) 0.060(2) Uani 1 1 d DU . .
H20H H 0.1445 0.2406 0.8911 0.072 Uiso 1 1 calc R . .
C21H C 0.1908(7) 0.3585(7) 0.9387(4) 0.067(3) Uani 1 1 d DU . .
H21Y H 0.2227 0.4060 0.9314 0.100 Uiso 1 1 calc R . .
H21Z H 0.2147 0.3584 0.9757 0.100 Uiso 1 1 calc R . .
H211 H 0.1434 0.3573 0.9459 0.100 Uiso 1 1 calc R . .
C22H C 0.2501(5) 0.2821(8) 0.8714(6) 0.081(4) Uani 1 1 d DU . .
H22Y H 0.2434 0.2462 0.8284 0.122 Uiso 1 1 calc R . .
H22Z H 0.2621 0.2626 0.9011 0.122 Uiso 1 1 calc R . .
H221 H 0.2904 0.3341 0.8781 0.122 Uiso 1 1 calc R . .
O1I O 0.6633(4) 0.3587(5) 0.6050(4) 0.0757(19) Uani 1 1 d DU . .
O2I O 0.7244(6) 0.4712(5) 0.7326(5) 0.101(3) Uani 1 1 d DU . .
H2OI H 0.7080 0.4868 0.7648 0.152 Uiso 1 1 calc R . .
O3I O 0.7025(4) 0.2369(4) 0.5611(4) 0.061(2) Uani 1 1 d DU . .
H3OI H 0.6825 0.2420 0.5930 0.092 Uiso 1 1 calc R . .
O4I O 0.8778(3) 0.3942(4) 0.6839(4) 0.0646(19) Uani 1 1 d DU . .
O5I O 0.7978(4) 0.3113(4) 0.7596(3) 0.0569(17) Uani 1 1 d DU . .
O6I O 0.9098(4) 0.3351(4) 0.8006(4) 0.064(2) Uani 1 1 d DU . .
O7I O 0.7775(4) 0.0493(4) 0.6947(4) 0.057(2) Uani 1 1 d DU . .
N1I N 0.8274(4) 0.2168(4) 0.7288(3) 0.0392(17) Uani 1 1 d DU . .
H1NI H 0.7809 0.1878 0.7098 0.047 Uiso 1 1 calc R . .
N2I N 0.8701(4) 0.0967(5) 0.7741(4) 0.055(2) Uani 1 1 d DU . .
H2NS H 0.8501 0.0530 0.7810 0.066 Uiso 1 1 calc R . .
H2NT H 0.9122 0.1360 0.7974 0.066 Uiso 1 1 calc R . .
C1I C 0.7414(4) 0.3772(5) 0.6139(4) 0.0709(19) Uani 1 1 d DU . .
C2I C 0.7530(4) 0.3686(6) 0.6763(4) 0.0650(19) Uani 1 1 d DU . .
H2I H 0.7360 0.3116 0.6655 0.078 Uiso 1 1 calc R . .
C3I C 0.8280(4) 0.4116(6) 0.7191(4) 0.066(2) Uani 1 1 d DU . .
H3I H 0.8452 0.4689 0.7318 0.079 Uiso 1 1 calc R . .
C4I C 0.8198(5) 0.3941(5) 0.7788(4) 0.068(2) Uani 1 1 d DU . .
H4I H 0.8684 0.4256 0.8081 0.082 Uiso 1 1 calc R . .
C5I C 0.7602(6) 0.4082(8) 0.8135(4) 0.085(3) Uani 1 1 d DU . .
H5IA H 0.7544 0.3895 0.8485 0.102 Uiso 1 1 calc R . .
H5IB H 0.7754 0.4649 0.8313 0.102 Uiso 1 1 calc R . .
C6I C 0.6864(5) 0.3639(7) 0.7673(5) 0.083(3) Uani 1 1 d DU . .
H6IA H 0.6682 0.3069 0.7536 0.100 Uiso 1 1 calc R . .
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H6IB H 0.6493 0.3765 0.7886 0.100 Uiso 1 1 calc R . .
C7I C 0.6959(5) 0.3864(5) 0.7114(4) 0.081(2) Uani 1 1 d DU . .
C8I C 0.6305(5) 0.3455(7) 0.6583(4) 0.079(3) Uani 1 1 d DU . .
H8IA H 0.6029 0.2888 0.6498 0.095 Uiso 1 1 calc R . .
H8IB H 0.5965 0.3683 0.6683 0.095 Uiso 1 1 calc R . .
C9I C 0.7430(5) 0.3122(4) 0.5562(5) 0.069(2) Uani 1 1 d DU . .
H9I H 0.7161 0.3101 0.5187 0.082 Uiso 1 1 calc R . .
C10I C 0.8190(5) 0.3230(7) 0.5420(6) 0.080(3) Uani 1 1 d DU . .
H10S H 0.8505 0.3777 0.5458 0.096 Uiso 1 1 calc R . .
H10T H 0.8431 0.3128 0.5727 0.096 Uiso 1 1 calc R . .
C11I C 0.8111(7) 0.2686(8) 0.4777(6) 0.105(4) Uani 1 1 d DU . .
H11I H 0.7623 0.2425 0.4545 0.126 Uiso 1 1 calc R . .
C12I C 0.8543(8) 0.2487(12) 0.4464(7) 0.143(5) Uani 1 1 d DU . .
C13I C 0.9311(9) 0.2760(15) 0.4791(10) 0.177(8) Uani 1 1 d DU . .
H132 H 0.9676 0.3122 0.4626 0.266 Uiso 1 1 calc R . .
H133 H 0.9395 0.2308 0.4714 0.266 Uiso 1 1 calc R . .
H134 H 0.9359 0.3027 0.5243 0.266 Uiso 1 1 calc R . .
C14I C 0.8328(10) 0.1960(14) 0.3769(7) 0.190(10) Uani 1 1 d DU . .
H142 H 0.8299 0.1455 0.3721 0.285 Uiso 1 1 calc R . .
H143 H 0.8700 0.2209 0.3542 0.285 Uiso 1 1 calc R . .
H144 H 0.7847 0.1875 0.3599 0.285 Uiso 1 1 calc R . .
C15I C 0.7864(7) 0.4580(5) 0.6123(7) 0.094(4) Uani 1 1 d DU . .
H152 H 0.7676 0.4593 0.5737 0.140 Uiso 1 1 calc R . .
H153 H 0.8382 0.4698 0.6133 0.140 Uiso 1 1 calc R . .
H154 H 0.7825 0.4971 0.6488 0.140 Uiso 1 1 calc R . .
C16I C 0.9547(5) 0.4435(8) 0.7112(7) 0.089(4) Uani 1 1 d DU . .
H162 H 0.9839 0.4218 0.6861 0.134 Uiso 1 1 calc R . .
H163 H 0.9629 0.4463 0.7542 0.134 Uiso 1 1 calc R . .
H164 H 0.9699 0.4962 0.7120 0.134 Uiso 1 1 calc R . .
C17I C 0.8502(4) 0.2907(4) 0.7647(5) 0.045(2) Uani 1 1 d DU . .
C18I C 0.8761(4) 0.1809(4) 0.7191(4) 0.0435(17) Uani 1 1 d DU . .
H18I H 0.9223 0.2164 0.7514 0.052 Uiso 1 1 calc R . .
C19I C 0.8368(4) 0.1033(4) 0.7286(4) 0.045(2) Uani 1 1 d DU . .
C20I C 0.8968(5) 0.1669(5) 0.6531(4) 0.049(2) Uani 1 1 d DU . .
H20I H 0.8505 0.1311 0.6209 0.058 Uiso 1 1 calc R . .
C21I C 0.9469(6) 0.1293(7) 0.6441(6) 0.074(3) Uani 1 1 d DU . .
H212 H 0.9944 0.1660 0.6726 0.111 Uiso 1 1 calc R . .
H213 H 0.9548 0.1159 0.6006 0.111 Uiso 1 1 calc R . .
H214 H 0.9238 0.0817 0.6533 0.111 Uiso 1 1 calc R . .
C22I C 0.9355(7) 0.2461(6) 0.6440(6) 0.067(3) Uani 1 1 d DU . .
H222 H 0.9048 0.2724 0.6537 0.101 Uiso 1 1 calc R . .
H223 H 0.9425 0.2363 0.6003 0.101 Uiso 1 1 calc R . .
H224 H 0.9836 0.2795 0.6721 0.101 Uiso 1 1 calc R . .
O1J O 0.1572(3) 0.4554(3) 0.7900(3) 0.0556(17) Uani 1 1 d DU . .
O2J O 0.2659(4) 0.4330(5) 0.7212(5) 0.072(2) Uani 1 1 d DU . .
H2OJ H 0.2394 0.3846 0.7111 0.108 Uiso 1 1 calc R . .
O3J O 0.2447(4) 0.6672(4) 0.8740(4) 0.067(2) Uani 1 1 d DU . .
H3OJ H 0.2851 0.6703 0.8644 0.100 Uiso 1 1 calc R . .
O4J O 0.3553(4) 0.6733(4) 0.8061(4) 0.0661(19) Uani 1 1 d DU . .
O5J O 0.3139(4) 0.6454(4) 0.6822(3) 0.0550(16) Uani 1 1 d DU . .
O6J O 0.4069(4) 0.6921(4) 0.6301(4) 0.055(2) Uani 1 1 d DU . .
O7J O 0.2370(3) 0.7728(4) 0.5611(3) 0.0456(17) Uani 1 1 d DU . .
N1J N 0.3141(4) 0.7242(4) 0.6364(4) 0.0463(18) Uani 1 1 d DU . .
H1NJ H 0.2710 0.7154 0.6476 0.056 Uiso 1 1 calc R . .
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N2J N 0.2967(4) 0.7248(5) 0.4922(3) 0.046(2) Uani 1 1 d DU . .
H2NU H 0.2641 0.7120 0.4599 0.055 Uiso 1 1 calc R . .
H2NV H 0.3345 0.7154 0.4859 0.055 Uiso 1 1 calc R . .
C1J C 0.2230(4) 0.5332(4) 0.8158(3) 0.0528(17) Uani 1 1 d DU . .
C2J C 0.2511(4) 0.5486(4) 0.7572(4) 0.0542(19) Uani 1 1 d DU . .
H2J H 0.2251 0.5744 0.7449 0.065 Uiso 1 1 calc R . .
C3J C 0.3333(4) 0.5977(5) 0.7599(4) 0.060(2) Uani 1 1 d DU . .
H3J H 0.3613 0.5738 0.7725 0.072 Uiso 1 1 calc R . .
C4J C 0.3445(5) 0.5982(5) 0.6941(4) 0.0566(19) Uani 1 1 d DU . .
H4J H 0.3987 0.6246 0.6944 0.068 Uiso 1 1 calc R . .
C5J C 0.3105(5) 0.5180(5) 0.6415(5) 0.066(2) Uani 1 1 d DU . .
H5JA H 0.3378 0.4900 0.6457 0.079 Uiso 1 1 calc R . .
H5JB H 0.3152 0.5241 0.6006 0.079 Uiso 1 1 calc R . .
C6J C 0.2284(5) 0.4689(6) 0.6424(4) 0.064(2) Uani 1 1 d DU . .
H6JA H 0.1993 0.4925 0.6322 0.077 Uiso 1 1 calc R . .
H6JB H 0.2091 0.4151 0.6107 0.077 Uiso 1 1 calc R . .
C7J C 0.2212(4) 0.4667(4) 0.7068(4) 0.0570(18) Uani 1 1 d DU . .
C8J C 0.1455(4) 0.4275(5) 0.7220(4) 0.055(2) Uani 1 1 d DU . .
H8JA H 0.1116 0.4425 0.7059 0.066 Uiso 1 1 calc R . .
H8JB H 0.1244 0.3699 0.7032 0.066 Uiso 1 1 calc R . .
C9J C 0.1892(5) 0.5873(4) 0.8492(4) 0.059(2) Uani 1 1 d DU . .
H9J H 0.1516 0.5812 0.8173 0.071 Uiso 1 1 calc R . .
C10J C 0.1521(7) 0.5709(6) 0.9036(5) 0.072(3) Uani 1 1 d DU . .
H10U H 0.1093 0.5178 0.8869 0.086 Uiso 1 1 calc R . .
H10V H 0.1874 0.5711 0.9331 0.086 Uiso 1 1 calc R . .
C11J C 0.1262(6) 0.6274(6) 0.9392(5) 0.071(3) Uani 1 1 d DU . .
H11J H 0.1645 0.6783 0.9637 0.085 Uiso 1 1 calc R . .
C12J C 0.0608(5) 0.6187(6) 0.9422(6) 0.074(3) Uani 1 1 d DU . .
C13J C -0.0064(7) 0.5404(7) 0.9069(8) 0.117(6) Uani 1 1 d DU . .
H135 H 0.0092 0.5047 0.8781 0.176 Uiso 1 1 calc R . .
H136 H -0.0403 0.5477 0.8829 0.176 Uiso 1 1 calc R . .
H137 H -0.0313 0.5181 0.9369 0.176 Uiso 1 1 calc R . .
C14J C 0.0420(7) 0.6814(7) 0.9845(7) 0.091(4) Uani 1 1 d DU . .
H145 H 0.0857 0.7231 1.0161 0.137 Uiso 1 1 calc R . .
H146 H 0.0019 0.6577 1.0056 0.137 Uiso 1 1 calc R . .
H147 H 0.0264 0.7034 0.9589 0.137 Uiso 1 1 calc R . .
C15J C 0.2768(6) 0.5330(7) 0.8603(5) 0.069(3) Uani 1 1 d DU . .
H155 H 0.2545 0.5243 0.8963 0.104 Uiso 1 1 calc R . .
H156 H 0.3218 0.5835 0.8749 0.104 Uiso 1 1 calc R . .
H157 H 0.2891 0.4911 0.8385 0.104 Uiso 1 1 calc R . .
C16J C 0.4342(5) 0.7261(8) 0.8210(9) 0.110(5) Uani 1 1 d DU . .
H165 H 0.4470 0.7553 0.7932 0.165 Uiso 1 1 calc R . .
H166 H 0.4611 0.6958 0.8150 0.165 Uiso 1 1 calc R . .
H167 H 0.4476 0.7628 0.8648 0.165 Uiso 1 1 calc R . .
C17J C 0.3487(5) 0.6869(6) 0.6482(5) 0.0493(19) Uani 1 1 d DU . .
C18J C 0.3466(4) 0.7795(4) 0.6053(4) 0.0434(18) Uani 1 1 d DU . .
H18J H 0.3890 0.7733 0.5880 0.052 Uiso 1 1 calc R . .
C19J C 0.2891(4) 0.7582(5) 0.5497(3) 0.045(2) Uani 1 1 d DU . .
C20J C 0.3762(5) 0.8666(4) 0.6494(4) 0.054(2) Uani 1 1 d DU . .
H20J H 0.3345 0.8750 0.6660 0.065 Uiso 1 1 calc R . .
C21J C 0.4100(6) 0.9164(6) 0.6114(6) 0.065(3) Uani 1 1 d DU . .
H215 H 0.4633 0.9342 0.6166 0.098 Uiso 1 1 calc R . .
H216 H 0.4012 0.9619 0.6259 0.098 Uiso 1 1 calc R . .
H217 H 0.3876 0.8854 0.5669 0.098 Uiso 1 1 calc R . .
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C22J C 0.4349(7) 0.8885(8) 0.7046(5) 0.084(4) Uani 1 1 d DU . .
H225 H 0.4170 0.8474 0.7217 0.126 Uiso 1 1 calc R . .
H226 H 0.4439 0.9382 0.7375 0.126 Uiso 1 1 calc R . .
H227 H 0.4808 0.8939 0.6896 0.126 Uiso 1 1 calc R . .
O1K O 0.9817(3) 0.0960(4) 0.0720(3) 0.0545(16) Uani 1 1 d DU . .
O2K O 0.9937(4) 0.0145(5) 0.1472(5) 0.078(3) Uani 1 1 d DU . .
H2OK H 1.0282 0.0367 0.1781 0.118 Uiso 1 1 calc R . .
O3K O 0.7903(3) -0.0250(5) -0.0132(4) 0.073(2) Uani 1 1 d DU . .
H3OK H 0.7869 -0.0609 -0.0019 0.110 Uiso 1 1 calc R . .
O4K O 0.7756(4) -0.1139(5) 0.0572(4) 0.084(2) Uani 1 1 d DU . .
O5K O 0.7660(3) -0.0346(4) 0.1768(4) 0.0607(17) Uani 1 1 d DU . .
O6K O 0.7081(4) -0.1084(4) 0.2321(4) 0.060(2) Uani 1 1 d DU . .
O7K O 0.6109(4) 0.0799(4) 0.2988(3) 0.0443(17) Uani 1 1 d DU . .
N1K N 0.6739(4) -0.0227(5) 0.2203(4) 0.0488(18) Uani 1 1 d DU . .
H1NK H 0.6846 0.0149 0.2062 0.059 Uiso 1 1 calc R . .
N2K N 0.6429(4) 0.0400(5) 0.3659(3) 0.0412(19) Uani 1 1 d DU . .
H2NW H 0.6478 0.0816 0.3976 0.049 Uiso 1 1 calc R . .
H2NX H 0.6514 0.0048 0.3730 0.049 Uiso 1 1 calc R . .
C1K C 0.9127(4) 0.0213(4) 0.0460(3) 0.0565(18) Uani 1 1 d DU . .
C2K C 0.8825(4) 0.0099(5) 0.1049(4) 0.057(2) Uani 1 1 d DU . .
H2K H 0.8508 0.0362 0.1153 0.069 Uiso 1 1 calc R . .
C3K C 0.8381(4) -0.0720(5) 0.1050(4) 0.066(2) Uani 1 1 d DU . .
H3K H 0.8693 -0.0990 0.0958 0.080 Uiso 1 1 calc R . .
C4K C 0.8189(4) -0.0657(6) 0.1703(4) 0.063(2) Uani 1 1 d DU . .
H4K H 0.7945 -0.1190 0.1720 0.075 Uiso 1 1 calc R . .
C5K C 0.8838(5) -0.0109(6) 0.2247(5) 0.068(2) Uani 1 1 d DU . .
H5KA H 0.9153 -0.0358 0.2254 0.082 Uiso 1 1 calc R . .
H5KB H 0.8649 -0.0029 0.2646 0.082 Uiso 1 1 calc R . .
C6K C 0.9309(5) 0.0690(5) 0.2203(4) 0.070(2) Uani 1 1 d DU . .
H6KA H 0.9029 0.0989 0.2281 0.084 Uiso 1 1 calc R . .
H6KB H 0.9763 0.0993 0.2527 0.084 Uiso 1 1 calc R . .
C7K C 0.9507(4) 0.0573(5) 0.1564(4) 0.0611(18) Uani 1 1 d DU . .
C8K C 0.9919(5) 0.1281(5) 0.1394(4) 0.057(2) Uani 1 1 d DU . .
H8KA H 0.9709 0.1647 0.1536 0.068 Uiso 1 1 calc R . .
H8KB H 1.0449 0.1562 0.1584 0.068 Uiso 1 1 calc R . .
C9K C 0.8643(4) 0.0381(6) 0.0078(4) 0.062(2) Uani 1 1 d DU . .
H9K H 0.8611 0.0847 0.0373 0.074 Uiso 1 1 calc R . .
C10K C 0.8925(6) 0.0580(7) -0.0479(5) 0.071(2) Uani 1 1 d DU . .
H10W H 0.9445 0.0995 -0.0343 0.086 Uiso 1 1 calc R . .
H10X H 0.8912 0.0111 -0.0804 0.086 Uiso 1 1 calc R . .
C11K C 0.8490(6) 0.0852(6) -0.0763(6) 0.077(3) Uani 1 1 d DU . .
H11K H 0.8022 0.0450 -0.1006 0.092 Uiso 1 1 calc R . .
C12K C 0.8645(6) 0.1537(6) -0.0732(6) 0.077(3) Uani 1 1 d DU . .
C13K C 0.9342(6) 0.2257(7) -0.0338(7) 0.102(5) Uani 1 1 d DU . .
H138 H 0.9243 0.2500 0.0074 0.152 Uiso 1 1 calc R . .
H139 H 0.9512 0.2630 -0.0548 0.152 Uiso 1 1 calc R . .
H130 H 0.9724 0.2110 -0.0282 0.152 Uiso 1 1 calc R . .
C14K C 0.8102(7) 0.1686(9) -0.1061(7) 0.094(4) Uani 1 1 d DU . .
H148 H 0.7732 0.1191 -0.1381 0.141 Uiso 1 1 calc R . .
H149 H 0.8372 0.2054 -0.1261 0.141 Uiso 1 1 calc R . .
H140 H 0.7856 0.1907 -0.0750 0.141 Uiso 1 1 calc R . .
C15K C 0.9321(6) -0.0410(6) 0.0066(6) 0.073(3) Uani 1 1 d DU . .
H158 H 0.9567 -0.0258 -0.0265 0.109 Uiso 1 1 calc R . .
H159 H 0.8869 -0.0910 -0.0124 0.109 Uiso 1 1 calc R . .
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 H150 H 0.9652 -0.0464 0.0333 0.109 Uiso 1 1 calc R . .
 C16K C 0.7323(8) -0.1965(6) 0.0438(9) 0.119(5) Uani 1 1 d DU . .
 H168 H 0.7593 -0.2240 0.0226 0.179 Uiso 1 1 calc R . .
 H169 H 0.6852 -0.2170 0.0165 0.179 Uiso 1 1 calc R . .
 H160 H 0.7229 -0.2045 0.0832 0.179 Uiso 1 1 calc R . .
 C17K C 0.7144(5) -0.0602(6) 0.2102(6) 0.057(2) Uani 1 1 d DU . .
 C18K C 0.6128(4) -0.0423(5) 0.2539(3) 0.0432(19) Uani 1 1 d DU . .
 H18K H 0.6140 -0.0798 0.2718 0.052 Uiso 1 1 calc R . .
 C19K C 0.6229(4) 0.0305(4) 0.3086(3) 0.0360(18) Uani 1 1 d DU . .
 C20K C 0.5355(4) -0.0826(5) 0.2112(4) 0.048(2) Uani 1 1 d DU . .
 H20K H 0.5308 -0.0461 0.1940 0.058 Uiso 1 1 calc R . .
 C21K C 0.4781(5) -0.1047(6) 0.2522(5) 0.060(3) Uani 1 1 d DU . .
 H218 H 0.4856 -0.1376 0.2710 0.089 Uiso 1 1 calc R . .
 H219 H 0.4286 -0.1336 0.2264 0.089 Uiso 1 1 calc R . .
 H210 H 0.4831 -0.0571 0.2855 0.089 Uiso 1 1 calc R . .
 C22K C 0.5254(7) -0.1577(6) 0.1572(5) 0.076(4) Uani 1 1 d DU . .
 H228 H 0.5609 -0.1435 0.1297 0.115 Uiso 1 1 calc R . .
 H229 H 0.4751 -0.1858 0.1329 0.115 Uiso 1 1 calc R . .
 H220 H 0.5336 -0.1913 0.1747 0.115 Uiso 1 1 calc R . .

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 0.034(3) 0.036(3) 0.054(4) 0.019(3) 0.020(3) 0.022(3)
 O2 0.022(3) 0.033(4) 0.051(4) 0.019(3) 0.006(3) -0.002(3)
 O3 0.025(3) 0.045(3) 0.042(4) 0.021(3) 0.015(3) 0.018(3)
 O4 0.018(3) 0.035(3) 0.053(4) 0.025(3) 0.009(3) 0.009(2)
 O5 0.024(3) 0.039(3) 0.055(3) 0.025(3) 0.022(3) 0.013(3)
 O6 0.015(3) 0.061(5) 0.059(5) 0.029(4) 0.011(3) 0.017(3)
 O7 0.041(3) 0.061(4) 0.059(5) 0.022(4) 0.014(3) 0.021(3)
 N1 0.024(4) 0.048(4) 0.053(3) 0.019(3) 0.016(3) 0.019(3)
 N2 0.029(4) 0.068(6) 0.093(7) 0.040(6) 0.028(5) 0.019(4)
 C1 0.028(3) 0.035(3) 0.054(4) 0.024(3) 0.016(3) 0.017(3)
 C2 0.023(3) 0.035(4) 0.054(4) 0.023(3) 0.014(3) 0.015(3)
 C3 0.020(3) 0.041(4) 0.048(4) 0.025(3) 0.008(3) 0.016(3)
 C4 0.031(4) 0.041(4) 0.053(4) 0.024(3) 0.018(3) 0.023(3)
 C5 0.042(4) 0.044(5) 0.052(5) 0.026(4) 0.019(4) 0.024(4)
 C6 0.041(4) 0.047(4) 0.042(5) 0.026(4) 0.018(4) 0.021(3)
 C7 0.030(3) 0.042(4) 0.050(4) 0.024(3) 0.008(3) 0.013(3)
 C8 0.030(3) 0.035(4) 0.052(5) 0.024(4) 0.014(3) 0.012(3)
 C9 0.023(4) 0.043(4) 0.055(4) 0.023(4) 0.012(3) 0.016(3)
 C10 0.023(4) 0.062(5) 0.057(5) 0.033(4) 0.007(3) 0.008(4)
 C11 0.038(5) 0.072(6) 0.068(5) 0.046(5) 0.001(4) 0.006(5)
 C12 0.063(6) 0.093(7) 0.067(5) 0.055(5) 0.001(5) 0.001(5)
 C13 0.114(11) 0.109(11) 0.063(9) 0.033(8) 0.002(8) 0.023(8)
 C14 0.106(10) 0.150(12) 0.081(9) 0.070(9) -0.023(8) 0.020(9)
 C15 0.021(5) 0.042(4) 0.065(7) 0.016(4) 0.001(4) 0.016(4)
 C16 0.013(4) 0.050(6) 0.066(7) 0.028(5) 0.005(4) 0.003(3)
 C17 0.018(3) 0.039(4) 0.053(4) 0.023(4) 0.017(3) 0.017(3)
```

C18 0.041(4) 0.053(4) 0.053(4) 0.029(3) 0.019(3) 0.018(3)
C19 0.031(4) 0.050(4) 0.057(5) 0.035(4) 0.030(4) 0.015(3)
C20 0.061(5) 0.059(5) 0.060(5) 0.031(4) 0.021(4) 0.032(5)
C21 0.072(8) 0.085(8) 0.077(8) 0.056(7) 0.034(6) 0.031(7)
C22 0.115(10) 0.057(6) 0.072(8) 0.030(5) 0.005(7) 0.044(7)
O1A 0.037(3) 0.070(4) 0.086(4) 0.017(3) 0.016(3) 0.039(3)
O2A 0.056(4) 0.082(6) 0.108(7) 0.026(5) -0.008(4) 0.040(4)
O3A 0.032(3) 0.058(5) 0.083(6) 0.012(4) 0.012(4) 0.030(3)
O4A 0.020(3) 0.054(3) 0.078(5) 0.031(3) 0.001(3) 0.004(3)
O5A 0.027(3) 0.052(3) 0.057(4) 0.019(3) 0.005(3) 0.019(3)
O6A 0.030(4) 0.047(3) 0.074(5) 0.013(4) -0.013(3) 0.018(3)
O7A 0.029(4) 0.065(5) 0.086(6) -0.005(4) 0.005(4) 0.027(3)
N1A 0.025(3) 0.034(4) 0.050(4) 0.010(3) 0.005(3) 0.015(3)
N2A 0.022(4) 0.070(6) 0.074(7) -0.008(5) -0.005(4) 0.009(5)
C1A 0.041(3) 0.067(4) 0.076(4) 0.019(4) 0.012(3) 0.030(4)
C2A 0.037(4) 0.062(3) 0.076(4) 0.025(3) 0.011(3) 0.032(4)
C3A 0.028(4) 0.062(4) 0.074(5) 0.024(3) 0.004(3) 0.025(4)
C4A 0.037(3) 0.070(4) 0.065(4) 0.024(4) -0.001(3) 0.029(4)
C5A 0.049(5) 0.081(5) 0.074(5) 0.032(4) 0.003(4) 0.038(5)
C6A 0.060(5) 0.083(5) 0.072(5) 0.032(4) -0.007(4) 0.042(5)
C7A 0.055(4) 0.072(4) 0.079(4) 0.026(3) -0.005(4) 0.039(4)
C8A 0.052(5) 0.068(4) 0.080(5) 0.027(3) 0.002(4) 0.040(4)
C9A 0.040(3) 0.063(5) 0.073(5) 0.020(4) 0.016(4) 0.029(4)
C10A 0.063(6) 0.065(5) 0.081(6) 0.026(5) 0.025(5) 0.031(5)
C11A 0.101(7) 0.072(6) 0.090(6) 0.037(5) 0.019(5) 0.037(6)
C12A 0.153(9) 0.092(8) 0.094(7) 0.043(7) 0.018(6) 0.006(8)
C13A 0.209(13) 0.091(11) 0.077(10) 0.030(9) 0.005(9) 0.017(12)
C14A 0.164(10) 0.156(15) 0.150(14) 0.039(13) 0.042(10) -0.027(13)
C15A 0.041(4) 0.086(7) 0.070(8) 0.018(7) 0.011(5) 0.033(5)
C16A 0.035(6) 0.054(4) 0.120(10) 0.026(6) 0.020(6) 0.005(5)
C17A 0.021(4) 0.045(4) 0.063(5) 0.018(4) 0.006(3) 0.011(3)
C18A 0.026(3) 0.036(4) 0.048(4) 0.004(4) -0.002(3) 0.019(3)
C19A 0.029(4) 0.051(5) 0.064(5) 0.018(4) 0.002(4) 0.017(3)
C20A 0.050(4) 0.038(5) 0.063(5) 0.022(4) 0.005(4) 0.019(4)
C21A 0.105(8) 0.068(8) 0.091(9) 0.038(7) 0.005(7) 0.055(7)
C22A 0.051(5) 0.056(7) 0.054(7) 0.017(6) 0.002(5) -0.003(5)
O1B 0.038(4) 0.104(4) 0.126(5) 0.084(4) 0.039(3) 0.047(3)
O2B 0.099(5) 0.139(8) 0.143(9) 0.098(7) 0.084(5) 0.088(6)
O3B 0.017(3) 0.103(5) 0.089(6) 0.063(5) 0.015(3) 0.031(3)
O4B 0.050(4) 0.093(4) 0.127(6) 0.083(4) 0.042(4) 0.032(4)
O5B 0.075(4) 0.102(4) 0.086(5) 0.065(4) 0.045(3) 0.066(4)
O6B 0.060(5) 0.095(6) 0.139(8) 0.084(6) 0.048(5) 0.051(5)
O7B 0.030(4) 0.053(5) 0.134(7) 0.058(5) 0.013(4) 0.022(3)
N1B 0.038(4) 0.068(5) 0.093(5) 0.059(4) 0.027(3) 0.031(3)
N2B 0.050(5) 0.072(7) 0.157(10) 0.074(7) 0.018(5) 0.039(5)
C1B 0.038(3) 0.105(4) 0.119(5) 0.086(4) 0.035(3) 0.049(4)
C2B 0.053(4) 0.111(4) 0.110(5) 0.086(4) 0.048(3) 0.064(4)
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C5B 0.096(6) 0.123(6) 0.095(6) 0.071(4) 0.056(5) 0.082(5)
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C7B 0.073(4) 0.117(5) 0.112(5) 0.080(4) 0.050(4) 0.067(4)
C8B 0.051(5) 0.108(5) 0.116(6) 0.079(4) 0.045(4) 0.059(4)
C9B 0.025(3) 0.097(5) 0.112(5) 0.068(5) 0.023(4) 0.031(4)

C10B 0.033(5) 0.091(4) 0.111(6) 0.074(5) 0.023(4) 0.023(4)
C11B 0.045(5) 0.079(5) 0.102(6) 0.055(5) 0.008(5) 0.021(5)
C12B 0.054(6) 0.085(6) 0.110(7) 0.039(5) -0.020(6) 0.026(6)
C13B 0.086(10) 0.070(7) 0.146(12) 0.032(8) -0.048(9) -0.013(8)
C14B 0.092(9) 0.109(10) 0.098(8) 0.021(7) -0.030(7) 0.055(8)
C15B 0.043(4) 0.097(8) 0.144(11) 0.085(8) 0.042(5) 0.039(5)
C16B 0.053(8) 0.113(7) 0.189(13) 0.118(8) 0.035(8) 0.031(7)
C17B 0.053(5) 0.090(5) 0.085(6) 0.066(4) 0.030(4) 0.049(4)
C18B 0.035(3) 0.061(5) 0.100(5) 0.058(4) 0.028(4) 0.026(3)
C19B 0.035(4) 0.059(5) 0.110(6) 0.053(5) 0.025(4) 0.027(4)
C20B 0.062(5) 0.066(6) 0.100(5) 0.058(5) 0.023(5) 0.034(4)
C21B 0.099(8) 0.061(8) 0.132(10) 0.053(7) 0.047(8) 0.045(7)
C22B 0.078(6) 0.101(10) 0.113(9) 0.064(8) -0.005(6) 0.039(7)
O1C 0.019(3) 0.048(3) 0.060(4) 0.023(3) 0.004(2) 0.015(3)
O2C 0.030(4) 0.048(4) 0.055(4) 0.021(4) -0.004(3) 0.014(3)
O3C 0.033(3) 0.044(4) 0.042(4) 0.023(3) 0.009(3) 0.015(3)
O4C 0.013(3) 0.059(4) 0.074(4) 0.028(3) 0.004(3) 0.000(3)
O5C 0.022(3) 0.046(4) 0.080(4) 0.032(3) 0.004(3) 0.015(3)
O6C 0.024(3) 0.091(6) 0.111(7) 0.044(5) 0.004(4) 0.024(4)
O7C 0.034(3) 0.053(4) 0.068(5) 0.023(4) 0.003(4) 0.016(3)
N1C 0.028(4) 0.050(4) 0.082(4) 0.028(4) -0.007(3) 0.011(4)
N2C 0.021(4) 0.057(6) 0.080(7) 0.039(5) -0.010(4) 0.006(4)
C1C 0.020(3) 0.043(3) 0.059(4) 0.025(3) 0.007(3) 0.011(3)
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C4C 0.024(4) 0.059(4) 0.074(4) 0.033(3) 0.008(3) 0.014(3)
C5C 0.037(4) 0.055(5) 0.076(5) 0.033(4) 0.000(4) 0.024(4)
C6C 0.036(4) 0.048(4) 0.074(6) 0.024(4) 0.002(4) 0.020(4)
C7C 0.028(3) 0.044(4) 0.065(4) 0.024(3) 0.003(3) 0.015(3)
C8C 0.022(3) 0.047(4) 0.053(5) 0.015(4) -0.005(3) 0.012(3)
C9C 0.034(4) 0.046(4) 0.059(4) 0.027(4) 0.009(3) 0.011(3)
C10C 0.039(4) 0.062(5) 0.060(4) 0.035(4) 0.008(3) 0.014(4)
C11C 0.054(6) 0.078(5) 0.065(5) 0.024(5) 0.006(4) 0.021(5)
C12C 0.081(7) 0.082(6) 0.083(7) 0.023(5) 0.011(5) 0.034(6)
C13C 0.167(14) 0.076(8) 0.122(12) 0.025(9) 0.021(10) 0.006(10)
C14C 0.113(11) 0.141(13) 0.092(10) -0.002(9) 0.024(8) 0.043(10)
C15C 0.028(5) 0.042(5) 0.067(7) 0.027(5) 0.024(5) 0.014(4)
C16C 0.015(4) 0.061(7) 0.130(10) 0.055(7) -0.008(5) -0.006(4)
C17C 0.028(3) 0.045(5) 0.088(5) 0.034(4) -0.001(3) 0.019(4)
C18C 0.031(4) 0.050(4) 0.077(4) 0.021(4) -0.009(3) 0.014(4)
C19C 0.030(4) 0.051(5) 0.077(6) 0.027(4) -0.003(4) 0.010(4)
C20C 0.037(5) 0.056(5) 0.094(6) 0.009(4) -0.004(4) 0.017(5)
C21C 0.042(6) 0.072(8) 0.088(7) -0.010(6) -0.003(5) 0.037(6)
C22C 0.054(7) 0.052(7) 0.138(11) 0.023(7) 0.004(7) 0.018(6)
O1D 0.034(3) 0.040(3) 0.055(4) 0.032(3) 0.001(3) 0.013(3)
O2D 0.030(3) 0.053(4) 0.043(3) 0.028(3) 0.010(3) 0.021(3)
O3D 0.033(3) 0.040(4) 0.049(4) 0.029(3) 0.000(3) 0.017(3)
O4D 0.026(3) 0.035(3) 0.042(4) 0.021(3) 0.012(2) 0.010(2)
O5D 0.039(3) 0.041(3) 0.044(3) 0.029(3) 0.007(3) 0.022(3)
O6D 0.062(5) 0.033(3) 0.060(5) 0.025(3) 0.022(4) 0.028(3)
O7D 0.033(4) 0.058(4) 0.064(5) 0.032(4) 0.017(3) 0.025(3)
N1D 0.040(4) 0.035(4) 0.052(3) 0.021(3) 0.007(3) 0.021(3)
N2D 0.048(5) 0.049(5) 0.059(6) 0.025(5) -0.005(4) 0.014(4)
C1D 0.024(3) 0.037(4) 0.053(4) 0.024(3) 0.008(3) 0.014(3)

C2D 0.023(3) 0.035(3) 0.046(4) 0.026(3) 0.009(3) 0.013(3)
C3D 0.022(3) 0.034(3) 0.041(4) 0.023(3) 0.010(3) 0.009(3)
C4D 0.033(4) 0.035(4) 0.042(3) 0.022(3) 0.010(3) 0.017(3)
C5D 0.027(4) 0.046(4) 0.041(4) 0.021(4) 0.006(3) 0.012(4)
C6D 0.019(4) 0.051(4) 0.052(5) 0.028(4) 0.008(3) 0.007(3)
C7D 0.028(4) 0.047(4) 0.047(4) 0.031(3) 0.012(3) 0.012(3)
C8D 0.028(4) 0.049(4) 0.051(5) 0.034(4) 0.014(4) 0.010(3)
C9D 0.023(3) 0.040(4) 0.053(4) 0.024(3) 0.008(3) 0.020(3)
C10D 0.045(5) 0.041(5) 0.058(5) 0.022(4) 0.021(4) 0.024(4)
C11D 0.071(6) 0.058(5) 0.051(4) 0.021(5) 0.025(4) 0.038(5)
C12D 0.089(7) 0.093(7) 0.052(5) 0.026(5) 0.033(5) 0.039(5)
C13D 0.101(10) 0.128(12) 0.063(9) 0.036(8) 0.006(7) 0.036(8)
C14D 0.150(12) 0.111(11) 0.065(9) 0.008(8) 0.048(8) 0.063(9)
C15D 0.031(4) 0.037(6) 0.066(7) 0.017(5) 0.000(4) 0.015(4)
C16D 0.022(4) 0.032(4) 0.055(7) 0.025(5) 0.010(4) 0.014(3)
C17D 0.038(4) 0.035(3) 0.048(4) 0.028(3) 0.009(4) 0.024(4)
C18D 0.045(4) 0.053(4) 0.051(4) 0.025(3) 0.012(3) 0.030(3)
C19D 0.041(4) 0.060(4) 0.053(5) 0.032(5) 0.010(4) 0.023(4)
C20D 0.047(5) 0.071(6) 0.064(5) 0.022(4) 0.017(4) 0.034(4)
C21D 0.054(7) 0.068(7) 0.074(7) 0.027(6) 0.030(5) 0.033(6)
C22D 0.052(6) 0.094(9) 0.085(8) 0.032(7) 0.016(5) 0.046(7)
O1E 0.059(3) 0.072(4) 0.087(4) 0.041(3) 0.034(3) 0.046(3)
O2E 0.089(6) 0.094(5) 0.087(7) 0.064(5) 0.036(5) 0.060(5)
O3E 0.068(4) 0.047(3) 0.070(5) 0.030(4) 0.034(4) 0.040(3)
O4E 0.049(3) 0.059(4) 0.088(5) 0.040(4) 0.024(3) 0.032(3)
O5E 0.050(3) 0.066(4) 0.070(4) 0.037(3) 0.024(3) 0.035(3)
O6E 0.050(4) 0.063(5) 0.085(6) 0.033(4) 0.029(4) 0.038(4)
O7E 0.049(4) 0.039(4) 0.092(6) 0.028(4) 0.031(4) 0.020(3)
N1E 0.033(4) 0.049(4) 0.076(5) 0.027(4) 0.009(3) 0.024(3)
N2E 0.036(5) 0.038(5) 0.104(8) 0.026(5) 0.025(5) 0.020(4)
C1E 0.059(3) 0.059(4) 0.080(4) 0.040(3) 0.029(3) 0.041(4)
C2E 0.053(3) 0.064(4) 0.071(4) 0.044(3) 0.029(3) 0.038(4)
C3E 0.052(3) 0.061(4) 0.079(5) 0.045(4) 0.029(3) 0.033(4)
C4E 0.047(4) 0.069(4) 0.082(5) 0.041(3) 0.023(3) 0.037(4)
C5E 0.054(4) 0.078(6) 0.079(5) 0.038(4) 0.024(3) 0.047(4)
C6E 0.051(4) 0.081(5) 0.078(5) 0.040(4) 0.018(4) 0.040(5)
C7E 0.058(4) 0.077(4) 0.074(4) 0.048(3) 0.028(3) 0.043(4)
C8E 0.061(4) 0.082(6) 0.081(5) 0.045(4) 0.028(3) 0.043(4)
C9E 0.062(4) 0.053(4) 0.073(5) 0.036(4) 0.037(4) 0.036(4)
C10E 0.063(4) 0.060(5) 0.080(5) 0.044(5) 0.039(4) 0.044(4)
C11E 0.065(5) 0.061(5) 0.083(6) 0.044(5) 0.032(4) 0.039(5)
C12E 0.065(5) 0.064(6) 0.095(6) 0.047(6) 0.024(4) 0.034(5)
C13E 0.059(6) 0.087(9) 0.076(9) 0.028(8) 0.006(6) 0.012(7)
C14E 0.096(9) 0.087(9) 0.093(8) 0.046(8) 0.025(6) 0.038(8)
C15E 0.066(6) 0.062(4) 0.090(8) 0.048(5) 0.029(6) 0.041(5)
C16E 0.056(5) 0.059(7) 0.099(9) 0.031(7) 0.034(6) 0.034(5)
C17E 0.043(4) 0.055(5) 0.070(5) 0.030(4) 0.013(4) 0.025(4)
C18E 0.026(4) 0.040(3) 0.077(4) 0.026(3) 0.008(4) 0.017(3)
C19E 0.033(4) 0.038(4) 0.084(6) 0.019(4) 0.012(4) 0.016(3)
C20E 0.033(5) 0.059(4) 0.076(4) 0.024(4) 0.006(4) 0.027(4)
C21E 0.049(7) 0.086(8) 0.094(9) 0.042(7) -0.004(6) 0.036(6)
C22E 0.056(7) 0.062(5) 0.069(7) 0.030(5) -0.001(6) 0.019(5)
O1F 0.086(4) 0.066(4) 0.078(4) 0.040(3) 0.005(3) 0.042(3)
O2F 0.053(4) 0.044(4) 0.097(6) 0.040(4) 0.008(4) 0.027(4)

O3F 0.239(12) 0.090(5) 0.082(7) 0.057(5) 0.061(7) 0.086(6)
O4F 0.098(5) 0.057(5) 0.137(6) 0.048(4) 0.073(5) 0.042(4)
O5F 0.048(4) 0.040(3) 0.084(5) 0.024(3) 0.009(3) 0.028(3)
O6F 0.035(4) 0.045(4) 0.084(6) 0.024(4) 0.009(3) 0.024(3)
O7F 0.033(4) 0.039(4) 0.057(5) 0.014(4) 0.006(3) 0.021(3)
N1F 0.033(4) 0.036(3) 0.069(5) 0.024(3) 0.010(3) 0.018(3)
N2F 0.031(4) 0.045(5) 0.046(4) 0.024(4) 0.009(3) 0.027(4)
C1F 0.111(5) 0.059(4) 0.084(4) 0.043(3) 0.030(4) 0.055(3)
C2F 0.070(4) 0.048(4) 0.086(4) 0.042(3) 0.028(4) 0.039(3)
C3F 0.066(4) 0.041(4) 0.117(5) 0.038(3) 0.042(4) 0.031(3)
C4F 0.058(4) 0.042(4) 0.102(5) 0.034(3) 0.015(4) 0.030(3)
C5F 0.057(5) 0.042(5) 0.086(5) 0.025(4) 0.009(4) 0.028(4)
C6F 0.054(4) 0.042(5) 0.080(5) 0.031(4) 0.020(4) 0.023(4)
C7F 0.047(4) 0.046(4) 0.078(4) 0.036(3) 0.020(3) 0.029(3)
C8F 0.065(5) 0.060(5) 0.085(5) 0.035(4) 0.006(4) 0.029(4)
C9F 0.195(8) 0.085(6) 0.097(5) 0.057(5) 0.012(6) 0.074(5)
C10F 0.239(10) 0.115(7) 0.105(6) 0.044(6) -0.012(7) 0.088(8)
C11F 0.267(12) 0.149(9) 0.126(8) 0.048(7) -0.033(8) 0.105(9)
C12F 0.274(13) 0.175(10) 0.137(10) 0.040(9) -0.043(9) 0.117(10)
C13F 0.252(18) 0.185(12) 0.157(16) 0.049(13) -0.020(15) 0.096(12)
C14F 0.34(2) 0.217(16) 0.136(15) 0.054(13) -0.057(14) 0.127(17)
C15F 0.124(8) 0.088(9) 0.113(10) 0.047(8) 0.060(8) 0.067(7)
C16F 0.097(6) 0.059(8) 0.195(14) 0.046(9) 0.106(8) 0.032(6)
C17F 0.037(4) 0.040(3) 0.057(5) 0.024(4) 0.014(3) 0.023(3)
C18F 0.035(4) 0.038(3) 0.055(4) 0.026(3) 0.020(3) 0.016(3)
C19F 0.036(4) 0.031(4) 0.041(4) 0.025(4) 0.013(3) 0.016(4)
C20F 0.042(5) 0.050(4) 0.063(5) 0.035(4) 0.030(4) 0.027(4)
C21F 0.057(7) 0.050(4) 0.080(8) 0.043(5) 0.036(6) 0.030(5)
C22F 0.063(7) 0.061(6) 0.064(7) 0.037(6) 0.036(5) 0.040(6)
O1G 0.041(3) 0.081(4) 0.084(4) 0.034(4) 0.029(3) 0.037(3)
O2G 0.019(3) 0.054(4) 0.113(6) 0.038(5) 0.021(4) 0.021(3)
O3G 0.051(4) 0.167(9) 0.076(6) 0.068(6) 0.037(4) 0.066(4)
O4G 0.024(4) 0.117(5) 0.129(5) 0.094(5) 0.027(3) 0.032(4)
O5G 0.018(3) 0.048(4) 0.092(5) 0.031(3) 0.008(3) 0.015(2)
O6G 0.008(3) 0.043(3) 0.096(6) 0.027(4) 0.002(3) 0.016(3)
O7G 0.032(4) 0.049(4) 0.048(4) 0.018(3) 0.007(3) 0.028(3)
N1G 0.016(3) 0.051(4) 0.061(5) 0.021(4) 0.010(3) 0.016(3)
N2G 0.036(5) 0.039(5) 0.053(4) 0.026(4) 0.019(4) 0.021(4)
C1G 0.048(4) 0.097(5) 0.082(4) 0.050(4) 0.029(3) 0.039(3)
C2G 0.026(4) 0.087(4) 0.088(4) 0.051(4) 0.026(3) 0.030(3)
C3G 0.022(4) 0.089(4) 0.110(5) 0.065(4) 0.022(3) 0.027(3)
C4G 0.016(4) 0.068(4) 0.105(4) 0.045(4) 0.018(3) 0.023(3)
C5G 0.027(4) 0.065(5) 0.094(5) 0.044(4) 0.016(4) 0.021(4)
C6G 0.022(4) 0.066(5) 0.084(5) 0.038(4) 0.024(4) 0.023(3)
C7G 0.024(4) 0.065(4) 0.084(4) 0.040(4) 0.025(3) 0.028(3)
C8G 0.041(5) 0.065(4) 0.087(5) 0.033(4) 0.027(4) 0.030(4)
C9G 0.058(5) 0.132(6) 0.084(5) 0.061(5) 0.039(4) 0.059(4)
C10G 0.070(5) 0.144(7) 0.083(5) 0.057(5) 0.043(4) 0.071(5)
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C12G 0.116(7) 0.142(8) 0.096(8) 0.066(6) 0.031(6) 0.087(7)
C13G 0.149(12) 0.147(11) 0.138(13) 0.065(9) 0.067(10) 0.097(10)
C14G 0.116(8) 0.166(13) 0.108(12) 0.053(10) 0.026(8) 0.080(9)
C15G 0.064(7) 0.088(8) 0.059(7) 0.032(6) 0.014(6) 0.039(6)
C16G 0.037(7) 0.119(7) 0.163(12) 0.095(9) 0.030(7) 0.027(6)

C17G 0.018(3) 0.038(4) 0.058(5) 0.033(3) 0.009(3) 0.012(3)
C18G 0.018(3) 0.044(4) 0.053(4) 0.029(4) 0.010(3) 0.010(3)
C19G 0.019(4) 0.040(4) 0.050(4) 0.025(3) 0.015(4) 0.015(4)
C20G 0.031(3) 0.053(5) 0.052(5) 0.033(4) 0.013(3) 0.016(4)
C21G 0.030(4) 0.048(6) 0.078(8) 0.026(6) 0.020(4) 0.017(5)
C22G 0.050(6) 0.056(7) 0.065(7) 0.042(6) 0.015(5) 0.024(5)
O1H 0.039(3) 0.047(3) 0.061(4) 0.027(3) 0.018(3) 0.021(3)
O2H 0.046(4) 0.044(4) 0.042(4) 0.013(4) 0.012(3) 0.027(4)
O3H 0.036(3) 0.043(4) 0.057(5) 0.022(4) 0.027(3) 0.024(3)
O4H 0.056(4) 0.031(3) 0.065(4) 0.015(3) 0.021(3) 0.013(3)
O5H 0.041(4) 0.034(3) 0.075(4) 0.008(3) 0.027(3) 0.017(3)
O6H 0.057(5) 0.044(4) 0.086(6) 0.031(4) 0.020(4) 0.027(4)
O7H 0.026(3) 0.043(4) 0.073(5) 0.024(4) 0.012(3) 0.012(3)
N1H 0.044(4) 0.038(4) 0.071(4) 0.018(3) 0.021(4) 0.023(4)
N2H 0.044(5) 0.040(5) 0.091(7) 0.020(5) 0.012(5) 0.022(4)
C1H 0.038(3) 0.042(3) 0.066(4) 0.027(3) 0.020(3) 0.023(3)
C2H 0.043(4) 0.040(3) 0.052(4) 0.020(3) 0.015(3) 0.023(3)
C3H 0.045(4) 0.037(3) 0.058(4) 0.021(3) 0.024(3) 0.022(3)
C4H 0.052(4) 0.043(4) 0.070(4) 0.022(4) 0.027(3) 0.030(3)
C5H 0.051(5) 0.056(4) 0.064(5) 0.027(4) 0.025(3) 0.033(4)
C6H 0.041(4) 0.055(4) 0.060(5) 0.024(4) 0.016(4) 0.025(4)
C7H 0.037(4) 0.052(4) 0.051(4) 0.021(3) 0.016(3) 0.022(3)
C8H 0.032(4) 0.045(4) 0.047(5) 0.011(3) 0.026(3) 0.026(3)
C9H 0.032(4) 0.059(5) 0.067(4) 0.032(3) 0.023(4) 0.027(3)
C10H 0.051(5) 0.072(5) 0.065(5) 0.031(4) 0.030(4) 0.018(4)
C11H 0.075(6) 0.097(7) 0.068(6) 0.040(5) 0.028(4) 0.026(5)
C12H 0.073(6) 0.129(8) 0.092(7) 0.047(6) 0.024(5) 0.039(6)
C13H 0.082(10) 0.162(13) 0.155(14) 0.080(11) 0.003(10) 0.009(8)
C14H 0.106(10) 0.145(12) 0.093(10) 0.046(9) 0.017(8) 0.062(10)
C15H 0.044(4) 0.043(6) 0.072(7) 0.022(5) 0.029(5) 0.023(4)
C16H 0.066(7) 0.032(5) 0.101(9) 0.016(6) 0.035(6) 0.010(4)
C17H 0.045(5) 0.035(3) 0.072(5) 0.016(3) 0.019(4) 0.026(4)
C18H 0.034(4) 0.047(4) 0.066(4) 0.013(3) 0.014(4) 0.019(4)
C19H 0.031(4) 0.032(4) 0.067(6) 0.014(4) 0.015(4) 0.013(3)
C20H 0.038(4) 0.053(5) 0.075(5) 0.023(4) 0.006(4) 0.012(4)
C21H 0.064(7) 0.074(7) 0.066(6) 0.020(5) -0.015(6) 0.040(6)
C22H 0.038(6) 0.079(9) 0.092(9) 0.002(7) -0.009(6) 0.022(6)
O1I 0.076(4) 0.067(4) 0.096(5) 0.031(4) -0.008(3) 0.043(4)
O2I 0.138(8) 0.086(4) 0.092(7) -0.001(5) -0.009(6) 0.089(5)
O3I 0.065(5) 0.043(4) 0.085(6) 0.034(4) 0.005(4) 0.025(4)
O4I 0.054(3) 0.043(4) 0.087(5) 0.021(4) 0.002(3) 0.018(3)
O5I 0.055(4) 0.050(3) 0.074(5) 0.023(3) 0.000(3) 0.033(3)
O6I 0.052(4) 0.049(4) 0.078(6) 0.008(4) -0.019(3) 0.026(4)
O7I 0.053(4) 0.035(4) 0.072(5) 0.018(4) -0.008(3) 0.014(3)
N1I 0.031(4) 0.037(3) 0.048(4) 0.016(3) -0.001(3) 0.015(3)
N2I 0.045(5) 0.055(6) 0.067(6) 0.036(5) 0.005(4) 0.016(5)
C1I 0.072(4) 0.048(4) 0.104(5) 0.032(4) 0.001(4) 0.035(4)
C2I 0.071(4) 0.042(4) 0.092(4) 0.020(4) 0.004(3) 0.039(4)
C3I 0.071(4) 0.037(4) 0.092(5) 0.019(4) 0.003(3) 0.032(4)
C4I 0.077(4) 0.054(4) 0.082(5) 0.014(4) 0.007(4) 0.047(4)
C5I 0.089(5) 0.090(6) 0.082(6) 0.006(5) 0.004(4) 0.066(5)
C6I 0.086(5) 0.098(6) 0.079(5) 0.011(5) 0.008(4) 0.072(5)
C7I 0.085(4) 0.081(4) 0.088(5) 0.013(4) 0.000(3) 0.062(4)
C8I 0.081(5) 0.078(5) 0.094(6) 0.025(5) -0.001(4) 0.056(5)

C9I 0.069(5) 0.050(4) 0.098(5) 0.042(4) 0.017(4) 0.028(4)
C10I 0.075(5) 0.074(6) 0.108(7) 0.053(5) 0.029(5) 0.035(5)
C11I 0.088(7) 0.102(8) 0.107(7) 0.048(6) 0.038(6) 0.024(6)
C12I 0.094(7) 0.142(9) 0.126(9) 0.018(7) 0.041(6) 0.023(7)
C13I 0.119(10) 0.185(16) 0.184(15) 0.039(14) 0.021(10) 0.058(12)
C14I 0.116(12) 0.175(16) 0.136(11) -0.007(11) 0.052(9) -0.001(12)
C15I 0.106(8) 0.049(5) 0.120(11) 0.039(6) -0.007(8) 0.027(6)
C16I 0.052(4) 0.072(8) 0.137(11) 0.066(8) -0.004(6) 0.004(6)
C17I 0.039(4) 0.035(4) 0.063(5) 0.023(4) -0.002(4) 0.016(3)
C18I 0.037(4) 0.038(4) 0.051(4) 0.014(3) 0.002(3) 0.017(3)
C19I 0.041(5) 0.038(4) 0.056(5) 0.016(4) 0.001(3) 0.019(3)
C20I 0.035(5) 0.052(5) 0.053(5) 0.018(4) 0.005(4) 0.016(4)
C21I 0.059(7) 0.091(8) 0.082(9) 0.027(7) 0.020(6) 0.048(6)
C22I 0.065(7) 0.052(6) 0.065(8) 0.021(6) 0.028(6) 0.012(6)
O1J 0.046(3) 0.042(3) 0.080(4) 0.028(3) 0.016(3) 0.017(3)
O2J 0.048(4) 0.058(5) 0.127(7) 0.047(5) 0.020(5) 0.031(4)
O3J 0.066(5) 0.049(3) 0.101(7) 0.032(4) 0.019(4) 0.037(3)
O4J 0.058(4) 0.045(3) 0.091(5) 0.039(3) 0.007(4) 0.011(3)
O5J 0.051(4) 0.054(4) 0.083(5) 0.040(3) 0.019(3) 0.033(3)
O6J 0.048(4) 0.063(5) 0.079(6) 0.030(4) 0.026(4) 0.043(4)
O7J 0.030(3) 0.060(5) 0.061(5) 0.034(4) 0.021(3) 0.025(3)
N1J 0.041(4) 0.059(4) 0.066(5) 0.038(4) 0.026(4) 0.035(3)
N2J 0.022(4) 0.052(5) 0.055(4) 0.024(4) 0.016(4) 0.008(4)
C1J 0.049(4) 0.041(3) 0.078(4) 0.030(3) 0.010(3) 0.025(3)
C2J 0.050(4) 0.042(3) 0.082(4) 0.036(3) 0.011(3) 0.022(3)
C3J 0.052(4) 0.051(4) 0.093(5) 0.040(3) 0.017(4) 0.028(3)
C4J 0.053(4) 0.048(4) 0.094(5) 0.039(3) 0.027(4) 0.036(3)
C5J 0.056(4) 0.061(5) 0.093(5) 0.031(4) 0.018(5) 0.036(4)
C6J 0.059(4) 0.057(5) 0.088(5) 0.030(4) 0.023(4) 0.035(4)
C7J 0.050(4) 0.048(4) 0.088(4) 0.029(3) 0.022(4) 0.033(3)
C8J 0.049(4) 0.041(4) 0.081(4) 0.021(4) 0.017(4) 0.027(4)
C9J 0.070(5) 0.046(4) 0.084(5) 0.034(4) 0.015(4) 0.038(3)
C10J 0.083(6) 0.057(5) 0.082(6) 0.029(5) 0.023(4) 0.036(4)
C11J 0.076(5) 0.061(5) 0.081(6) 0.030(5) 0.023(5) 0.035(4)
C12J 0.067(5) 0.059(5) 0.096(7) 0.039(5) 0.017(5) 0.024(4)
C13J 0.084(7) 0.091(8) 0.120(12) 0.021(8) 0.006(9) 0.009(6)
C14J 0.062(8) 0.081(8) 0.123(11) 0.037(7) 0.036(7) 0.029(6)
C15J 0.068(7) 0.064(7) 0.091(8) 0.043(7) 0.001(5) 0.033(5)
C16J 0.062(5) 0.079(8) 0.151(13) 0.038(8) 0.003(8) 0.006(6)
C17J 0.041(4) 0.060(5) 0.071(5) 0.036(4) 0.021(4) 0.035(4)
C18J 0.036(4) 0.053(4) 0.061(4) 0.033(3) 0.022(3) 0.029(4)
C19J 0.033(4) 0.057(5) 0.056(4) 0.034(4) 0.025(3) 0.022(4)
C20J 0.036(5) 0.053(4) 0.078(6) 0.026(4) 0.010(4) 0.024(4)
C21J 0.041(6) 0.059(6) 0.112(9) 0.043(6) 0.028(6) 0.029(6)
C22J 0.070(8) 0.077(8) 0.089(8) 0.012(6) -0.013(6) 0.037(7)
O1K 0.039(3) 0.056(4) 0.077(4) 0.032(3) 0.018(3) 0.025(3)
O2K 0.038(4) 0.090(6) 0.150(8) 0.077(6) 0.039(4) 0.042(4)
O3K 0.039(3) 0.086(6) 0.087(6) 0.019(5) 0.018(4) 0.032(3)
O4K 0.039(4) 0.082(5) 0.110(5) 0.031(5) 0.017(3) 0.014(4)
O5K 0.046(4) 0.070(4) 0.097(5) 0.048(4) 0.026(3) 0.041(3)
O6K 0.035(4) 0.061(5) 0.110(6) 0.054(5) 0.021(4) 0.029(4)
O7K 0.048(4) 0.048(4) 0.051(4) 0.035(4) 0.021(3) 0.023(3)
N1K 0.045(4) 0.057(4) 0.068(5) 0.038(4) 0.022(3) 0.034(3)
N2K 0.047(5) 0.046(5) 0.037(4) 0.024(4) 0.019(4) 0.022(4)

```
 C1K 0.037(4) 0.058(4) 0.081(4) 0.023(3) 0.021(3) 0.030(3)
 C2K 0.031(4) 0.066(4) 0.089(4) 0.036(4) 0.023(3) 0.030(3)
 C3K 0.031(4) 0.071(4) 0.104(5) 0.039(4) 0.026(3) 0.025(3)
 C4K 0.037(4) 0.072(5) 0.106(5) 0.049(4) 0.026(3) 0.037(3)
 C5K 0.048(5) 0.082(5) 0.105(5) 0.055(5) 0.020(4) 0.040(4)
 C6K 0.046(5) 0.082(5) 0.097(5) 0.050(5) 0.015(4) 0.032(4)
 C7K 0.042(4) 0.069(4) 0.096(4) 0.049(4) 0.015(3) 0.033(3)
 C8K 0.042(5) 0.059(5) 0.078(4) 0.034(4) 0.013(4) 0.025(4)
 C9K 0.045(4) 0.068(5) 0.074(5) 0.021(4) 0.015(4) 0.033(3)
 C10K 0.051(5) 0.086(6) 0.066(6) 0.020(5) 0.009(4) 0.029(4)
 C11K 0.061(6) 0.083(5) 0.071(6) 0.028(5) 0.003(5) 0.023(5)
 C12K 0.060(5) 0.078(6) 0.078(7) 0.023(6) 0.019(5) 0.025(5)
 C13K 0.055(7) 0.092(8) 0.113(11) 0.008(8) 0.024(6) 0.020(6)
 C14K 0.094(8) 0.095(9) 0.092(10) 0.016(8) 0.018(7) 0.057(8)
 C15K 0.058(7) 0.051(6) 0.119(9) 0.032(6) 0.051(7) 0.033(5)
 C16K 0.066(9) 0.087(6) 0.164(13) 0.046(9) 0.003(8) 0.004(7)
 C17K 0.046(4) 0.065(5) 0.089(6) 0.046(4) 0.021(4) 0.037(4)
 C18K 0.035(3) 0.052(4) 0.050(4) 0.022(3) 0.012(3) 0.025(3)
 C19K 0.026(4) 0.042(4) 0.042(4) 0.028(3) 0.013(4) 0.008(4)
 C20K 0.044(4) 0.051(5) 0.055(5) 0.019(4) 0.006(3) 0.028(4)
 C21K 0.035(5) 0.039(6) 0.089(8) 0.024(6) 0.014(5) 0.005(5)
 C22K 0.083(8) 0.067(7) 0.060(7) 0.002(5) -0.010(6) 0.036(7)

_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_
  _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 1.468(7) . ?
 O1 C8 1.453(7) . ?
 O2 H2O 0.8400 . ?
 O2 C7 1.469(7) . ?
 O3 H3O 0.8400 . ?
 O3 C9 1.435(7) . ?
 O4 C3 1.426(7) . ?
 O4 C16 1.438(7) . ?
 O5 C4 1.444(7) . ?
 O5 C17 1.329(6) . ?
 O6 C17 1.223(7) . ?
 O7 C19 1.230(7) . ?
 N1 H1N 0.8800 . ?
 N1 C17 1.328(7) . ?
 N1 C18 1.450(7) . ?
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N2 H2NA 0.8800 . ?
N2 H2NB 0.8800 . ?
N2 C19 1.323(7) . ?
C1 C2 1.548(7) . ?
C1 C9 1.549(7) . ?
C1 C15 1.517(8) . ?
C2 H2 1.0000 . ?
C2 C3 1.525(7) . ?
C2 C7 1.530(7) . ?
C3 H3 1.0000 . ?
C3 C4 1.541(7) . ?
C4 H4 1.0000 . ?
C4 C5 1.516(7) . ?
C5 H5A 0.9900 . ?
C5 H5B 0.9900 . ?
C5 C6 1.533(8) . ?
C6 H6A 0.9900 . ?
C6 H6B 0.9900 . ?
C6 C7 1.494(7) . ?
C7 C8 1.526(7) . ?
C8 H8A 0.9900 . ?
C8 H8B 0.9900 . ?
C9 H9 1.0000 . ?
C9 C10 1.525(8) . ?
C10 H10A 0.9900 . ?
C10 H10B 0.9900 . ?
C10 C11 1.485(8) . ?
C11 H11 0.9500 . ?
C11 C12 1.276(8) . ?
C12 C13 1.509(9) . ?
C12 C14 1.535(9) . ?
C13 H13A 0.9800 . ?
C13 H13B 0.9800 . ?
C13 H13C 0.9800 . ?
C14 H14A 0.9800 . ?
C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
C15 H15A 0.9800 . ?
C15 H15B 0.9800 . ?
C15 H15C 0.9800 . ?
C16 H16A 0.9800 . ?
C16 H16B 0.9800 . ?
C16 H16C 0.9800 . ?
C18 H18 1.0000 . ?
C18 C19 1.533(7) . ?
C18 C20 1.547(8) . ?
C20 H20 1.0000 . ?
C20 C21 1.518(8) . ?
C20 C22 1.532(8) . ?
C21 H21A 0.9800 . ?
C21 H21B 0.9800 . ?
C21 H21C 0.9800 . ?
C22 H22A 0.9800 . ?
C22 H22B 0.9800 . ?
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C22 H22C 0.9800 . ?
O1A C1A 1.473(8) . ?
O1A C8A 1.451(8) . ?
O2A H2OA 0.8400 . ?
O2A C7A 1.470(8) . ?
O3A H3OA 0.8400 . ?
O3A C9A 1.445(8) . ?
O4A C3A 1.413(8) . ?
O4A C16A 1.436(8) . ?
O5A C4A 1.447(7) . ?
O5A C17A 1.324(7) . ?
O6A C17A 1.224(7) . ?
O7A C19A 1.231(7) . ?
N1A H1NA 0.8800 . ?
N1A C17A 1.332(7) . ?
N1A C18A 1.469(7) . ?
N2A H2NC 0.8800 . ?
N2A H2ND 0.8800 . ?
N2A C19A 1.324(8) . ?
C1A C2A 1.534(8) . ?
C1A C9A 1.550(8) . ?
C1A C15A 1.522(8) . ?
C2A H2A 1.0000 . ?
C2A C3A 1.526(8) . ?
C2A C7A 1.529(8) . ?
C3A H3A 1.0000 . ?
C3A C4A 1.531(8) . ?
C4A H4A 1.0000 . ?
C4A C5A 1.535(8) . ?
C5A H5AA 0.9900 . ?
C5A H5AB 0.9900 . ?
C5A C6A 1.543(9) . ?
C6A H6AA 0.9900 . ?
C6A H6AB 0.9900 . ?
C6A C7A 1.496(8) . ?
C7A C8A 1.514(8) . ?
C8A H8AA 0.9900 . ?
C8A H8AB 0.9900 . ?
C9A H9A 1.0000 . ?
C9A C10A 1.537(8) . ?
C10A H10C 0.9900 . ?
C10A H10D 0.9900 . ?
C10A C11A 1.482(9) . ?
C11A H11A 0.9500 . ?
C11A C12A 1.267(9) . ?
C12A C13A 1.513(10) . ?
C12A C14A 1.537(10) . ?
C13A H13D 0.9800 . ?
C13A H13E 0.9800 . ?
C13A H13F 0.9800 . ?
C14A H14D 0.9800 . ?
C14A H14E 0.9800 . ?
C14A H14F 0.9800 . ?
C15A H15D 0.9800 . ?
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C15A H15E 0.9800 . ?
C15A H15F 0.9800 . ?
C16A H16D 0.9800 . ?
C16A H16E 0.9800 . ?
C16A H16F 0.9800 . ?
C18A H18A 1.0000 . ?
C18A C19A 1.534(8) . ?
C18A C20A 1.541(8) . ?
C20A H20A 1.0000 . ?
C20A C21A 1.509(8) . ?
C20A C22A 1.557(8) . ?
C21A H21D 0.9800 . ?
C21A H21E 0.9800 . ?
C21A H21F 0.9800 . ?
C22A H22D 0.9800 . ?
C22A H22E 0.9800 . ?
C22A H22F 0.9800 . ?
O1B C1B 1.476(8) . ?
O1B C8B 1.453(8) . ?
O2B H2OB 0.8400 . ?
O2B C7B 1.469(8) . ?
O3B H3OB 0.8400 . ?
O3B C9B 1.429(7) . ?
O4B C3B 1.406(8) . ?
O4B C16B 1.449(8) . ?
O5B C4B 1.457(8) . ?
O5B C17B 1.333(7) . ?
O6B C17B 1.234(7) . ?
O7B C19B 1.224(7) . ?
N1B H1NB 0.8800 . ?
N1B C17B 1.327(7) . ?
N1B C18B 1.457(8) . ?
N2B H2NE 0.8800 . ?
N2B H2NF 0.8800 . ?
N2B C19B 1.318(8) . ?
C1B C2B 1.549(8) . ?
C1B C9B 1.547(8) . ?
C1B C15B 1.520(8) . ?
C2B H2B 1.0000 . ?
C2B C3B 1.532(8) . ?
C2B C7B 1.532(8) . ?
C3B H3B 1.0000 . ?
C3B C4B 1.528(8) . ?
C4B H4B 1.0000 . ?
C4B C5B 1.537(9) . ?
C5B H5BA 0.9900 . ?
C5B H5BB 0.9900 . ?
C5B C6B 1.538(9) . ?
C6B H6BA 0.9900 . ?
C6B H6BB 0.9900 . ?
C6B C7B 1.504(8) . ?
C7B C8B 1.515(8) . ?
C8B H8BA 0.9900 . ?
C8B H8BB 0.9900 . ?
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C9B H9B 1.0000 . ?
C9B C10B 1.515(8) . ?
C10B H10E 0.9900 . ?
C10B H10F 0.9900 . ?
C10B C11B 1.484(9) . ?
C11B H11B 0.9500 . ?
C11B C12B 1.279(9) . ?
C12B C13B 1.520(10) . ?
C12B C14B 1.524(10) . ?
C13B H13G 0.9800 . ?
C13B H13H 0.9800 . ?
C13B H13I 0.9800 . ?
C14B H14G 0.9800 . ?
C14B H14H 0.9800 . ?
C14B H14I 0.9800 . ?
C15B H15G 0.9800 . ?
C15B H15H 0.9800 . ?
C15B H15I 0.9800 . ?
C16B H16G 0.9800 . ?
C16B H16H 0.9800 . ?
C16B H16I 0.9800 . ?
C18B H18B 1.0000 . ?
C18B C19B 1.533(8) . ?
C18B C20B 1.539(8) . ?
C20B H20B 1.0000 . ?
C20B C21B 1.508(9) . ?
C20B C22B 1.546(9) . ?
C21B H21G 0.9800 . ?
C21B H21H 0.9800 . ?
C21B H21I 0.9800 . ?
C22B H22G 0.9800 . ?
C22B H22H 0.9800 . ?
C22B H22I 0.9800 . ?
O1C C1C 1.474(7) . ?
O1C C8C 1.461(7) . ?
O2C H2OC 0.8400 . ?
O2C C7C 1.468(8) . ?
O3C H3OC 0.8400 . ?
O3C C9C 1.436(7) . ?
O4C C3C 1.404(7) . ?
O4C C16C 1.441(7) . ?
O5C C4C 1.442(7) . ?
O5C C17C 1.341(7) . ?
O6C C17C 1.230(7) . ?
O7C C19C 1.245(7) . ?
N1C H1NC 0.8800 . ?
N1C C17C 1.324(7) . ?
N1C C18C 1.462(8) . ?
N2C H2NG 0.8800 . ?
N2C H2NH 0.8800 . ?
N2C C19C 1.319(8) . ?
C1C C2C 1.553(8) . ?
C1C C9C 1.552(8) . ?
C1C C15C 1.522(8) . ?
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C2C H2C 1.0000 . ?
C2C C3C 1.528(8) . ?
C2C C7C 1.523(8) . ?
C3C H3C 1.0000 . ?
C3C C4C 1.526(8) . ?
C4C H4C 1.0000 . ?
C4C C5C 1.527(8) . ?
C5C H5CA 0.9900 . ?
C5C H5CB 0.9900 . ?
C5C C6C 1.544(8) . ?
C6C H6CA 0.9900 . ?
C6C H6CB 0.9900 . ?
C6C C7C 1.507(8) . ?
C7C C8C 1.518(8) . ?
C8C H8CA 0.9900 . ?
C8C H8CB 0.9900 . ?
C9C H9C 1.0000 . ?
C9C C10C 1.526(8) . ?
C10C H10G 0.9900 . ?
C10C H10H 0.9900 . ?
C10C C11C 1.480(9) . ?
C11C H11C 0.9500 . ?
C11C C12C 1.277(9) . ?
C12C C13C 1.509(10) . ?
C12C C14C 1.527(10) . ?
C13C H13J 0.9800 . ?
C13C H13K 0.9800 . ?
C13C H13L 0.9800 . ?
C14C H14J 0.9800 . ?
C14C H14K 0.9800 . ?
C14C H14L 0.9800 . ?
C15C H15J 0.9800 . ?
C15C H15K 0.9800 . ?
C15C H15L 0.9800 . ?
C16C H16J 0.9800 . ?
C16C H16K 0.9800 . ?
C16C H16L 0.9800 . ?
C18C H18C 1.0000 . ?
C18C C19C 1.522(8) . ?
C18C C20C 1.544(8) . ?
C20C H20C 1.0000 . ?
C20C C21C 1.501(9) . ?
C20C C22C 1.541(9) . ?
C21C H21J 0.9800 . ?
C21C H21K 0.9800 . ?
C21C H21L 0.9800 . ?
C22C H22J 0.9800 . ?
C22C H22K 0.9800 . ?
C22C H22L 0.9800 . ?
O1D C1D 1.478(7) . ?
O1D C8D 1.457(7) . ?
O2D H2OD 0.8400 . ?
O2D C7D 1.464(7) . ?
O3D H3OD 0.8400 . ?
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O3D C9D 1.436(7) . ?
O4D C3D 1.424(7) . ?
O4D C16D 1.441(7) . ?
O5D C4D 1.437(7) . ?
O5D C17D 1.329(7) . ?
O6D C17D 1.236(7) . ?
O7D C19D 1.229(7) . ?
N1D H1D 0.8800 . ?
N1D C17D 1.326(7) . ?
N1D C18D 1.454(7) . ?
N2D H2NI 0.8800 . ?
N2D H2NJ 0.8800 . ?
N2D C19D 1.329(8) . ?
C1D C2D 1.543(7) . ?
C1D C9D 1.544(8) . ?
C1D C15D 1.523(8) . ?
C2D H2D 1.0000 . ?
C2D C3D 1.526(8) . ?
C2D C7D 1.535(8) . ?
C3D H3D 1.0000 . ?
C3D C4D 1.539(8) . ?
C4D H4D 1.0000 . ?
C4D C5D 1.535(8) . ?
C5D H5DA 0.9900 . ?
C5D H5DB 0.9900 . ?
C5D C6D 1.535(8) . ?
C6D H6DA 0.9900 . ?
C6D H6DB 0.9900 . ?
C6D C7D 1.495(8) . ?
C7D C8D 1.519(8) . ?
C8D H8DA 0.9900 . ?
C8D H8DB 0.9900 . ?
C9D H9D 1.0000 . ?
C9D C10D 1.526(8) . ?
C10D H10I 0.9900 . ?
C10D H10J 0.9900 . ?
C10D C11D 1.489(8) . ?
C11D H11D 0.9500 . ?
C11D C12D 1.272(9) . ?
C12D C13D 1.515(10) . ?
C12D C14D 1.533(10) . ?
C13D H13M 0.9800 . ?
C13D H13N 0.9800 . ?
C13D H13O 0.9800 . ?
C14D H14M 0.9800 . ?
C14D H14N 0.9800 . ?
C14D H14O 0.9800 . ?
C15D H15M 0.9800 . ?
C15D H15N 0.9800 . ?
C15D H15O 0.9800 . ?
C16D H16M 0.9800 . ?
C16D H16N 0.9800 . ?
C16D H16O 0.9800 . ?
C18D H18D 1.0000 . ?
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C18D C19D 1.543(8) . ?
C18D C20D 1.551(8) . ?
C20D H20D 1.0000 . ?
C20D C21D 1.507(9) . ?
C20D C22D 1.546(9) . ?
C21D H21M 0.9800 . ?
C21D H21N 0.9800 . ?
C21D H21O 0.9800 . ?
C22D H22M 0.9800 . ?
C22D H22N 0.9800 . ?
C22D H22O 0.9800 . ?
O1E C1E 1.480(7) . ?
O1E C8E 1.447(8) . ?
O2E H2OE 0.8400 . ?
O2E C7E 1.465(8) . ?
O3E H3E 0.8400 . ?
O3E C9E 1.431(8) . ?
O4E C3E 1.410(8) . ?
O4E C16E 1.446(8) . ?
O5E C4E 1.457(8) . ?
O5E C17E 1.342(7) . ?
O6E C17E 1.231(7) . ?
O7E C19E 1.222(7) . ?
N1E H1NE 0.8800 . ?
N1E C17E 1.321(7) . ?
N1E C18E 1.450(7) . ?
N2E H2EK 0.8800 . ?
N2E H2EL 0.8800 . ?
N2E C19E 1.322(8) . ?
C1E C2E 1.543(8) . ?
C1E C9E 1.540(8) . ?
C1E C15E 1.518(8) . ?
C2E H2E 1.0000 . ?
C2E C3E 1.533(8) . ?
C2E C7E 1.529(8) . ?
C3E H5 1.0000 . ?
C3E C4E 1.536(8) . ?
C4E H4E 1.0000 . ?
C4E C5E 1.528(8) . ?
C5E H5EA 0.9900 . ?
C5E H5EB 0.9900 . ?
C5E C6E 1.552(8) . ?
C6E H6EA 0.9900 . ?
C6E H6EB 0.9900 . ?
C6E C7E 1.497(8) . ?
C7E C8E 1.515(8) . ?
C8E H8EA 0.9900 . ?
C8E H8EB 0.9900 . ?
C9E H9E 1.0000 . ?
C9E C10E 1.523(8) . ?
C10E H10K 0.9900 . ?
C10E H10L 0.9900 . ?
C10E C11E 1.477(9) . ?
C11E H11E 0.9500 . ?
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C11E C12E 1.273(9) . ?
C12E C13E 1.513(9) . ?
C12E C14E 1.525(9) . ?
C13E H13P 0.9800 . ?
C13E H13Q 0.9800 . ?
C13E H13R 0.9800 . ?
C14E H14P 0.9800 . ?
C14E H14Q 0.9800 . ?
C14E H14R 0.9800 . ?
C15E H15P 0.9800 . ?
C15E H15Q 0.9800 . ?
C15E H15R 0.9800 . ?
C16E H16P 0.9800 . ?
C16E H16Q 0.9800 . ?
C16E H16R 0.9800 . ?
C18E H18E 1.0000 . ?
C18E C19E 1.520(8) . ?
C18E C20E 1.546(8) . ?
C20E H20E 1.0000 . ?
C20E C21E 1.514(8) . ?
C20E C22E 1.562(9) . ?
C21E H21P 0.9800 . ?
C21E H21Q 0.9800 . ?
C21E H21R 0.9800 . ?
C22E H22P 0.9800 . ?
C22E H22Q 0.9800 . ?
C22E H22R 0.9800 . ?
O1F C1F 1.475(8) . ?
O1F C8F 1.450(8) . ?
O2F H2OF 0.8400 . ?
O2F C7F 1.463(7) . ?
O3F H3OF 0.8400 . ?
O3F C9F 1.425(9) . ?
O4F C3F 1.423(8) . ?
O4F C16F 1.444(9) . ?
O5F C4F 1.465(8) . ?
O5F C17F 1.331(7) . ?
O6F C17F 1.224(7) . ?
O7F C19F 1.237(7) . ?
N1F H1NF 0.8800 . ?
N1F C17F 1.334(7) . ?
N1F C18F 1.456(7) . ?
N2F H2NM 0.8800 . ?
N2F H2NN 0.8800 . ?
N2F C19F 1.308(7) . ?
C1F C2F 1.543(8) . ?
C1F C9F 1.555(8) . ?
C1F C15F 1.511(8) . ?
C2F H2F 1.0000 . ?
C2F C3F 1.528(8) . ?
C2F C7F 1.530(8) . ?
C3F H3F 1.0000 . ?
C3F C4F 1.534(8) . ?
C4F H4F 1.0000 . ?
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C4F C5F 1.523(8) . ?
C5F H5FA 0.9900 . ?
C5F H5FB 0.9900 . ?
C5F C6F 1.541(8) . ?
C6F H6FA 0.9900 . ?
C6F H6FB 0.9900 . ?
C6F C7F 1.492(8) . ?
C7F C8F 1.510(8) . ?
C8F H8FA 0.9900 . ?
C8F H8FB 0.9900 . ?
C9F H9F 1.0000 . ?
C9F C10F 1.524(9) . ?
C10F H10N 0.9900 . ?
C10F H10M 0.9900 . ?
C10F C11F 1.481(10) . ?
C11F H11F 0.9500 . ?
C11F C12F 1.279(10) . ?
C12F C13F 1.518(11) . ?
C12F C14F 1.538(10) . ?
C13F H13S 0.9800 . ?
C13F H13T 0.9800 . ?
C13F H13U 0.9800 . ?
C14F H14S 0.9800 . ?
C14F H14T 0.9800 . ?
C14F H14U 0.9800 . ?
C15F H15S 0.9800 . ?
C15F H15T 0.9800 . ?
C15F H15U 0.9800 . ?
C16F H16S 0.9800 . ?
C16F H16T 0.9800 . ?
C16F H16U 0.9800 . ?
C18F H18F 1.0000 . ?
C18F C19F 1.530(8) . ?
C18F C20F 1.541(8) . ?
C20F H20F 1.0000 . ?
C20F C21F 1.507(8) . ?
C20F C22F 1.545(8) . ?
C21F H21S 0.9800 . ?
C21F H21T 0.9800 . ?
C21F H21U 0.9800 . ?
C22F H22S 0.9800 . ?
C22F H22T 0.9800 . ?
C22F H22U 0.9800 . ?
O1G C1G 1.483(11) . ?
O1G C8G 1.456(12) . ?
O2G H2OG 0.8400 . ?
O2G C7G 1.462(11) . ?
O3G H3OG 0.8400 . ?
O3G C9G 1.410(12) . ?
O4G C3G 1.463(11) . ?
O4G C16G 1.391(13) . ?
O5G C4G 1.448(11) . ?
O5G C17G 1.333(10) . ?
O6G C17G 1.200(10) . ?
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O7G C19G 1.245(10) . ?
N1G H1NG 0.8800 . ?
N1G C17G 1.357(10) . ?
N1G C18G 1.462(10) . ?
N2G H2NO 0.8800 . ?
N2G H2NP 0.8800 . ?
N2G C19G 1.302(10) . ?
C1G C2G 1.546(13) . ?
C1G C9G 1.598(13) . ?
C1G C15G 1.503(13) . ?
C2G H2G 1.0000 . ?
C2G C3G 1.526(13) . ?
C2G C7G 1.520(11) . ?
C3G H3G 1.0000 . ?
C3G C4G 1.517(13) . ?
C4G H4G 1.0000 . ?
C4G C5G 1.524(12) . ?
C5G H5GA 0.9900 . ?
C5G H5GB 0.9900 . ?
C5G C6G 1.510(13) . ?
C6G H6GA 0.9900 . ?
C6G H6GB 0.9900 . ?
C6G C7G 1.491(12) . ?
C7G C8G 1.529(12) . ?
C8G H8GA 0.9900 . ?
C8G H8GB 0.9900 . ?
C9G H9G 1.0000 . ?
C9G C10G 1.546(14) . ?
C10G H10O 0.9900 . ?
C10G H10P 0.9900 . ?
C10G C11G 1.527(15) . ?
C11G H11G 0.9500 . ?
C11G C12G 1.276(15) . ?
C12G C13G 1.508(16) . ?
C12G C14G 1.541(16) . ?
C13G H13V 0.9800 . ?
C13G H13W 0.9800 . ?
C13G H13X 0.9800 . ?
C14G H14V 0.9800 . ?
C14G H14W 0.9800 . ?
C14G H14X 0.9800 . ?
C15G H15V 0.9800 . ?
C15G H15W 0.9800 . ?
C15G H15X 0.9800 . ?
C16G H16V 0.9800 . ?
C16G H16W 0.9800 . ?
C16G H16X 0.9800 . ?
C18G H18G 1.0000 . ?
C18G C19G 1.541(11) . ?
C18G C20G 1.519(11) . ?
C20G H20G 1.0000 . ?
C20G C21G 1.530(12) . ?
C20G C22G 1.499(12) . ?
C21G H21V 0.9800 . ?
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C21G H21W 0.9800 . ?
C21G H21X 0.9800 . ?
C22G H22V 0.9800 . ?
C22G H22W 0.9800 . ?
C22G H22X 0.9800 . ?
O1H C1H 1.472(7) . ?
O1H C8H 1.455(7) . ?
O2H H2OH 0.8400 . ?
O2H C7H 1.479(7) . ?
O3H H3OH 0.8400 . ?
O3H C9H 1.447(7) . ?
O4H C3H 1.409(7) . ?
O4H C16H 1.446(8) . ?
O5H C4H 1.469(7) . ?
O5H C17H 1.344(7) . ?
O6H C17H 1.226(7) . ?
O7H C19H 1.226(7) . ?
N1H H1NH 0.8800 . ?
N1H C17H 1.328(7) . ?
N1H C18H 1.459(8) . ?
N2H H2NQ 0.8800 . ?
N2H H2NR 0.8800 . ?
N2H C19H 1.323(8) . ?
C1H C2H 1.542(8) . ?
C1H C9H 1.535(8) . ?
C1H C15H 1.528(8) . ?
C2H H2H 1.0000 . ?
C2H C3H 1.523(8) . ?
C2H C7H 1.519(8) . ?
C3H H3H 1.0000 . ?
C3H C4H 1.537(8) . ?
C4H H4H 1.0000 . ?
C4H C5H 1.524(8) . ?
C5H H5HA 0.9900 . ?
C5H H5HB 0.9900 . ?
C5H C6H 1.536(8) . ?
C6H H6HA 0.9900 . ?
C6H H6HB 0.9900 . ?
C6H C7H 1.500(8) . ?
C7H C8H 1.518(8) . ?
C8H H8HA 0.9900 . ?
C8H H8HB 0.9900 . ?
C9H H9H 1.0000 . ?
C9H C10H 1.523(8) . ?
C10H H10Q 0.9900 . ?
C10H H10R 0.9900 . ?
C10H C11H 1.487(9) . ?
C11H H11H 0.9500 . ?
C11H C12H 1.266(9) . ?
C12H C13H 1.521(10) . ?
C12H C14H 1.533(10) . ?
C13H H13Y 0.9800 . ?
C13H H13Z 0.9800 . ?
C13H H13 0.9800 . ?
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C14H H14Y 0.9800 . ?
C14H H14Z 0.9800 . ?
C14H H14 0.9800 . ?
C15H H15Y 0.9800 . ?
C15H H15Z 0.9800 . ?
C15H H151 0.9800 . ?
C16H H16Y 0.9800 . ?
C16H H16Z 0.9800 . ?
C16H H161 0.9800 . ?
C18H H18H 1.0000 . ?
C18H C19H 1.532(8) . ?
C18H C20H 1.546(8) . ?
C20H H20H 1.0000 . ?
C20H C21H 1.510(9) . ?
C20H C22H 1.544(9) . ?
C21H H21Y 0.9800 . ?
C21H H21Z 0.9800 . ?
C21H H211 0.9800 . ?
C22H H22Y 0.9800 . ?
C22H H22Z 0.9800 . ?
C22H H221 0.9800 . ?
O1I C1I 1.471(8) . ?
O1I C8I 1.450(8) . ?
O2I H2OI 0.8400 . ?
O2I C7I 1.465(8) . ?
O3I H3OI 0.8400 . ?
O3I C9I 1.444(8) . ?
O4I C3I 1.403(8) . ?
O4I C16I 1.438(8) . ?
O5I C4I 1.453(8) . ?
O5I C17I 1.339(7) . ?
O6I C17I 1.228(7) . ?
O7I C19I 1.239(7) . ?
N1I H1NI 0.8800 . ?
N1I C17I 1.315(7) . ?
N1I C18I 1.464(7) . ?
N2I H2NS 0.8800 . ?
N2I H2NT 0.8800 . ?
N2I C19I 1.323(8) . ?
C1I C2I 1.534(8) . ?
C1I C9I 1.547(8) . ?
C1I C15I 1.519(8) . ?
C2I H2I 1.0000 . ?
C2I C3I 1.523(8) . ?
C2I C7I 1.534(8) . ?
C3I H3I 1.0000 . ?
C3I C4I 1.525(8) . ?
C4I H4I 1.0000 . ?
C4I C5I 1.545(8) . ?
C5I H5IA 0.9900 . ?
C5I H5IB 0.9900 . ?
C5I C6I 1.538(9) . ?
C6I H6IA 0.9900 . ?
C6I H6IB 0.9900 . ?
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C6I C7I 1.494(8) . ?
C7I C8I 1.515(8) . ?
C8I H8IA 0.9900 . ?
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C12I C13I 1.512(10) . ?
C12I C14I 1.525(10) . ?
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C13I H133 0.9800 . ?
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C14I H142 0.9800 . ?
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C15I H152 0.9800 . ?
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C15I H154 0.9800 . ?
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C16I H163 0.9800 . ?
C16I H164 0.9800 . ?
C18I H18I 1.0000 . ?
C18I C19I 1.533(8) . ?
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O2J H2OJ 0.8400 . ?
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O6J C17J 1.239(7) . ?
O7J C19J 1.240(7) . ?
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N1J C18J 1.460(7) . ?
N2J H2NU 0.8800 . ?
N2J H2NV 0.8800 . ?
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C1J C9J 1.557(8) . ?
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C2J H2J 1.0000 . ?
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C2J C7J 1.523(8) . ?
C3J H3J 1.0000 . ?
C3J C4J 1.537(8) . ?
C4J H4J 1.0000 . ?
C4J C5J 1.517(8) . ?
C5J H5JA 0.9900 . ?
C5J H5JB 0.9900 . ?
C5J C6J 1.542(8) . ?
C6J H6JA 0.9900 . ?
C6J H6JB 0.9900 . ?
C6J C7J 1.503(8) . ?
C7J C8J 1.509(8) . ?
C8J H8JA 0.9900 . ?
C8J H8JB 0.9900 . ?
C9J H9J 1.0000 . ?
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C11J C12J 1.281(9) . ?
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C22J H227 0.9800 . ?
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  _geom_angle_atom_site_label_3
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 C7 O2 H2O 109.5 . . ?
 C9 O3 H3O 109.5 . . ?
 C3 O4 C16 112.9(6) . . ?
 C17 O5 C4 117.3(6) . . ?
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 C17 N1 C18 124.3(6) . . ?
 C18 N1 H1N 117.8 . . ?
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 C19 N2 H2NA 120.0 . . ?
 C19 N2 H2NB 120.0 . . ?
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 O1 C1 C9 105.3(5) . . ?
 O1 C1 C15 106.5(6) . . ?
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 O4 C3 H3 109.6 . . ?
 O4 C3 C4 109.8(5) . . ?
 C2 C3 H3 109.6 . . ?
 C2 C3 C4 109.0(5) . . ?
 C4 C3 H3 109.6 . . ?
 O5 C4 C3 106.7(6) . . ?
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C5 C4 C3 115.7(5) . . ?
C5 C4 H4 108.7 . . ?
C4 C5 H5A 108.9 . . ?
C4 C5 H5B 108.9 . . ?
C4 C5 C6 113.2(6) . . ?
H5A C5 H5B 107.8 . . ?
C6 C5 H5A 108.9 . . ?
C6 C5 H5B 108.9 . . ?
C5 C6 H6A 109.7 . . ?
C5 C6 H6B 109.7 . . ?
H6A C6 H6B 108.2 . . ?
C7 C6 C5 110.0(6) . . ?
C7 C6 H6A 109.7 . . ?
C7 C6 H6B 109.7 . . ?
O2 C7 C2 109.5(6) . . ?
O2 C7 C6 110.1(6) . . ?
O2 C7 C8 105.9(6) . . ?
C6 C7 C2 110.8(6) . . ?
C6 C7 C8 118.9(6) . . ?
C8 C7 C2 101.0(5) . . ?
O1 C8 C7 101.8(5) . . ?
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O1 C8 H8B 111.4 . . ?
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C7 C8 H8B 111.4 . . ?
H8A C8 H8B 109.3 . . ?
O3 C9 C1 110.8(5) . . ?
O3 C9 H9 106.6 . . ?
O3 C9 C10 107.8(6) . . ?
C1 C9 H9 106.6 . . ?
C10 C9 C1 117.8(6) . . ?
C10 C9 H9 106.6 . . ?
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C9 C10 H10B 108.6 . . ?
H10A C10 H10B 107.6 . . ?
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C11 C10 H10A 108.6 . . ?
C11 C10 H10B 108.6 . . ?
C10 C11 H11 113.9 . . ?
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C12 C11 H11 113.9 . . ?
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C11 C12 C14 122.1(9) . . ?
C13 C12 C14 114.9(9) . . ?
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C12 C13 H13B 109.5 . . ?
C12 C13 H13C 109.5 . . ?
H13A C13 H13B 109.5 . . ?
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H13B C13 H13C 109.5 . . ?
C12 C14 H14A 109.5 . . ?
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C12 C14 H14C 109.5 . . ?
H14A C14 H14B 109.5 . . ?
H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
C1 C15 H15A 109.5 . . ?
C1 C15 H15B 109.5 . . ?
C1 C15 H15C 109.5 . . ?
H15A C15 H15B 109.5 . . ?
H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
O4 C16 H16A 109.5 . . ?
O4 C16 H16B 109.5 . . ?
O4 C16 H16C 109.5 . . ?
H16A C16 H16B 109.5 . . ?
H16A C16 H16C 109.5 . . ?
H16B C16 H16C 109.5 . . ?
O6 C17 O5 125.0(6) . . ?
O6 C17 N1 124.6(6) . . ?
N1 C17 O5 110.5(6) . . ?
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N1 C18 C19 109.0(6) . . ?
N1 C18 C20 111.5(6) . . ?
C19 C18 H18 108.6 . . ?
C19 C18 C20 110.3(6) . . ?
C20 C18 H18 108.6 . . ?
O7 C19 N2 121.3(7) . . ?
O7 C19 C18 120.2(7) . . ?
N2 C19 C18 118.4(7) . . ?
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C21 C20 C22 112.2(8) . . ?
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C20 C21 H21B 109.5 . . ?
C20 C21 H21C 109.5 . . ?
H21A C21 H21B 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
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C20 C22 H22B 109.5 . . ?
C20 C22 H22C 109.5 . . ?
H22A C22 H22B 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?
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C9A O3A H3OA 109.5 . . ?
C3A O4A C16A 116.0(8) . . ?
C17A O5A C4A 119.0(6) . . ?
C17A N1A H1NA 119.5 . . ?
C17A N1A C18A 121.1(6) . . ?
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O1A C1A C9A 105.8(6) . . ?
O1A C1A C15A 106.5(7) . . ?
C2A C1A C9A 115.0(6) . . ?
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C7A C2A H2A 106.3 . . ?
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O4A C3A H3A 108.0 . . ?
O4A C3A C4A 116.3(6) . . ?
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O2A C7A C6A 108.8(7) . . ?
O2A C7A C8A 108.2(7) . . ?
C6A C7A C2A 113.1(6) . . ?
C6A C7A C8A 118.7(7) . . ?
C8A C7A C2A 100.8(6) . . ?
O1A C8A C7A 102.8(6) . . ?
O1A C8A H8AA 111.2 . . ?
O1A C8A H8AB 111.2 . . ?
C7A C8A H8AA 111.2 . . ?
C7A C8A H8AB 111.2 . . ?
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O3A C9A H9A 107.8 . . ?
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H10C C10A H10D 108.1 . . ?
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C11A C10A H10D 109.5 . . ?
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C12A C11A H11A 113.8 . . ?
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C11A C12A C14A 124.1(11) . . ?
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O4A C16A H16F 109.5 . . ?
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H16D C16A H16F 109.5 . . ?
H16E C16A H16F 109.5 . . ?
O5A C17A N1A 110.1(6) . . ?
O6A C17A O5A 123.8(7) . . ?
O6A C17A N1A 126.1(7) . . ?
N1A C18A H18A 109.9 . . ?
N1A C18A C19A 105.6(6) . . ?
N1A C18A C20A 110.9(6) . . ?
C19A C18A H18A 109.9 . . ?
C19A C18A C20A 110.5(6) . . ?
C20A C18A H18A 109.9 . . ?
O7A C19A N2A 123.2(7) . . ?
O7A C19A C18A 120.0(7) . . ?
N2A C19A C18A 116.8(7) . . ?
C18A C20A H20A 108.3 . . ?
C18A C20A C22A 108.2(7) . . ?
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C21A C20A C18A 112.2(7) . . ?
C21A C20A H20A 108.3 . . ?
C21A C20A C22A 111.5(8) . . ?
C22A C20A H20A 108.3 . . ?
C20A C21A H21D 109.5 . . ?
C20A C21A H21E 109.5 . . ?
C20A C21A H21F 109.5 . . ?
H21D C21A H21E 109.5 . . ?
H21D C21A H21F 109.5 . . ?
H21E C21A H21F 109.5 . . ?
C20A C22A H22D 109.5 . . ?
C20A C22A H22E 109.5 . . ?
C20A C22A H22F 109.5 . . ?
H22D C22A H22E 109.5 . . ?
H22D C22A H22F 109.5 . . ?
H22E C22A H22F 109.5 . . ?
C8B O1B C1B 110.0(6) . . ?
C7B O2B H2OB 109.5 . . ?
C9B O3B H3OB 109.5 . . ?
C3B O4B C16B 114.6(9) . . ?
C17B O5B C4B 118.6(7) . . ?
C17B N1B H1NB 119.2 . . ?
C17B N1B C18B 121.6(7) . . ?
C18B N1B H1NB 119.2 . . ?
H2NE N2B H2NF 120.0 . . ?
C19B N2B H2NE 120.0 . . ?
C19B N2B H2NF 120.0 . . ?
O1B C1B C2B 104.0(6) . . ?
O1B C1B C9B 104.2(6) . . ?
O1B C1B C15B 107.3(7) . . ?
C9B C1B C2B 113.0(6) . . ?
C15B C1B C2B 115.0(7) . . ?
C15B C1B C9B 112.1(7) . . ?
C1B C2B H2B 106.9 . . ?
C3B C2B C1B 121.3(7) . . ?
C3B C2B H2B 106.9 . . ?
C7B C2B C1B 103.7(5) . . ?
C7B C2B H2B 106.9 . . ?
C7B C2B C3B 110.2(6) . . ?
O4B C3B C2B 108.8(7) . . ?
O4B C3B H3B 108.4 . . ?
O4B C3B C4B 114.2(7) . . ?
C2B C3B H3B 108.4 . . ?
C4B C3B C2B 108.4(6) . . ?
C4B C3B H3B 108.4 . . ?
O5B C4B C3B 106.1(7) . . ?
O5B C4B H4B 110.5 . . ?
O5B C4B C5B 103.6(7) . . ?
C3B C4B H4B 110.5 . . ?
C3B C4B C5B 115.3(7) . . ?
C5B C4B H4B 110.5 . . ?
C4B C5B H5BA 109.2 . . ?
C4B C5B H5BB 109.2 . . ?
C4B C5B C6B 111.9(8) . . ?
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H5BA C5B H5BB 107.9 . . ?
C6B C5B H5BA 109.2 . . ?
C6B C5B H5BB 109.2 . . ?
C5B C6B H6BA 109.8 . . ?
C5B C6B H6BB 109.8 . . ?
H6BA C6B H6BB 108.3 . . ?
C7B C6B C5B 109.3(7) . . ?
C7B C6B H6BA 109.8 . . ?
C7B C6B H6BB 109.8 . . ?
O2B C7B C2B 107.6(7) . . ?
O2B C7B C6B 110.1(8) . . ?
O2B C7B C8B 107.6(7) . . ?
C6B C7B C2B 111.0(7) . . ?
C6B C7B C8B 118.6(7) . . ?
C8B C7B C2B 101.2(6) . . ?
O1B C8B C7B 104.8(6) . . ?
O1B C8B H8BA 110.8 . . ?
O1B C8B H8BB 110.8 . . ?
C7B C8B H8BA 110.8 . . ?
C7B C8B H8BB 110.8 . . ?
H8BA C8B H8BB 108.9 . . ?
O3B C9B C1B 109.2(6) . . ?
O3B C9B H9B 106.4 . . ?
O3B C9B C10B 109.7(7) . . ?
C1B C9B H9B 106.4 . . ?
C10B C9B C1B 118.1(7) . . ?
C10B C9B H9B 106.4 . . ?
C9B C10B H10E 108.6 . . ?
C9B C10B H10F 108.6 . . ?
H10E C10B H10F 107.6 . . ?
C11B C10B C9B 114.5(7) . . ?
C11B C10B H10E 108.6 . . ?
C11B C10B H10F 108.6 . . ?
C10B C11B H11B 115.3 . . ?
C12B C11B C10B 129.4(9) . . ?
C12B C11B H11B 115.3 . . ?
C11B C12B C13B 120.2(10) . . ?
C11B C12B C14B 125.1(10) . . ?
C13B C12B C14B 114.7(10) . . ?
C12B C13B H13G 109.5 . . ?
C12B C13B H13H 109.5 . . ?
C12B C13B H13I 109.5 . . ?
H13G C13B H13H 109.5 . . ?
H13G C13B H13I 109.5 . . ?
H13H C13B H13I 109.5 . . ?
C12B C14B H14G 109.5 . . ?
C12B C14B H14H 109.5 . . ?
C12B C14B H14I 109.5 . . ?
H14G C14B H14H 109.5 . . ?
H14G C14B H14I 109.5 . . ?
H14H C14B H14I 109.5 . . ?
C1B C15B H15G 109.5 . . ?
C1B C15B H15H 109.5 . . ?
C1B C15B H15I 109.5 . . ?
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H15G C15B H15H 109.5 . . ?
H15G C15B H15I 109.5 . . ?
H15H C15B H15I 109.5 . . ?
O4B C16B H16G 109.5 . . ?
O4B C16B H16H 109.5 . . ?
O4B C16B H16I 109.5 . . ?
H16G C16B H16H 109.5 . . ?
H16G C16B H16I 109.5 . . ?
H16H C16B H16I 109.5 . . ?
O6B C17B O5B 126.3(7) . . ?
O6B C17B N1B 125.1(8) . . ?
N1B C17B O5B 108.5(6) . . ?
N1B C18B H18B 109.3 . . ?
N1B C18B C19B 106.3(7) . . ?
N1B C18B C20B 111.9(7) . . ?
C19B C18B H18B 109.3 . . ?
C19B C18B C20B 110.6(7) . . ?
C20B C18B H18B 109.3 . . ?
O7B C19B N2B 124.9(8) . . ?
O7B C19B C18B 117.9(7) . . ?
N2B C19B C18B 116.9(7) . . ?
C18B C20B H20B 108.4 . . ?
C18B C20B C22B 109.7(8) . . ?
C21B C20B C18B 110.1(8) . . ?
C21B C20B H20B 108.4 . . ?
C21B C20B C22B 111.7(9) . . ?
C22B C20B H20B 108.4 . . ?
C20B C21B H21G 109.5 . . ?
C20B C21B H21H 109.5 . . ?
C20B C21B H21I 109.5 . . ?
H21G C21B H21H 109.5 . . ?
H21G C21B H21I 109.5 . . ?
H21H C21B H21I 109.5 . . ?
C20B C22B H22G 109.5 . . ?
C20B C22B H22H 109.5 . . ?
C20B C22B H22I 109.5 . . ?
H22G C22B H22H 109.5 . . ?
H22G C22B H22I 109.5 . . ?
H22H C22B H22I 109.5 . . ?
C8C O1C C1C 108.5(5) . . ?
C7C O2C H2OC 109.5 . . ?
C9C O3C H3OC 109.5 . . ?
C3C O4C C16C 115.0(7) . . ?
C17C O5C C4C 117.7(6) . . ?
C17C N1C H1NC 118.1 . . ?
C17C N1C C18C 123.9(7) . . ?
C18C N1C H1NC 118.1 . . ?
H2NG N2C H2NH 120.0 . . ?
C19C N2C H2NG 120.0 . . ?
C19C N2C H2NH 120.0 . . ?
O1C C1C C2C 103.7(5) . . ?
O1C C1C C9C 106.5(5) . . ?
O1C C1C C15C 105.8(6) . . ?
C9C C1C C2C 115.5(6) . . ?
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C15C C1C C2C 115.3(6) . . ?
C15C C1C C9C 109.0(6) . . ?
C1C C2C H2C 107.2 . . ?
C3C C2C C1C 120.6(6) . . ?
C3C C2C H2C 107.2 . . ?
C7C C2C C1C 105.2(5) . . ?
C7C C2C H2C 107.2 . . ?
C7C C2C C3C 108.9(6) . . ?
O4C C3C C2C 109.7(6) . . ?
O4C C3C H3C 108.4 . . ?
O4C C3C C4C 111.9(6) . . ?
C2C C3C H3C 108.4 . . ?
C4C C3C C2C 109.9(6) . . ?
C4C C3C H3C 108.4 . . ?
O5C C4C C3C 105.5(6) . . ?
O5C C4C H4C 109.3 . . ?
O5C C4C C5C 108.4(7) . . ?
C3C C4C H4C 109.3 . . ?
C3C C4C C5C 115.0(6) . . ?
C5C C4C H4C 109.3 . . ?
C4C C5C H5CA 108.8 . . ?
C4C C5C H5CB 108.8 . . ?
C4C C5C C6C 113.7(7) . . ?
H5CA C5C H5CB 107.7 . . ?
C6C C5C H5CA 108.8 . . ?
C6C C5C H5CB 108.8 . . ?
C5C C6C H6CA 109.9 . . ?
C5C C6C H6CB 109.9 . . ?
H6CA C6C H6CB 108.3 . . ?
C7C C6C C5C 108.8(6) . . ?
C7C C6C H6CA 109.9 . . ?
C7C C6C H6CB 109.9 . . ?
O2C C7C C2C 108.0(6) . . ?
O2C C7C C6C 109.0(6) . . ?
O2C C7C C8C 106.2(6) . . ?
C6C C7C C2C 112.4(6) . . ?
C6C C7C C8C 120.4(6) . . ?
C8C C7C C2C 100.0(5) . . ?
O1C C8C C7C 103.0(5) . . ?
O1C C8C H8CA 111.2 . . ?
O1C C8C H8CB 111.2 . . ?
C7C C8C H8CA 111.2 . . ?
C7C C8C H8CB 111.2 . . ?
H8CA C8C H8CB 109.1 . . ?
O3C C9C C1C 110.6(6) . . ?
O3C C9C H9C 106.7 . . ?
O3C C9C C10C 107.3(6) . . ?
C1C C9C H9C 106.7 . . ?
C10C C9C C1C 118.4(6) . . ?
C10C C9C H9C 106.7 . . ?
C9C C10C H10G 108.9 . . ?
C9C C10C H10H 108.9 . . ?
H10G C10C H10H 107.7 . . ?
C11C C10C C9C 113.3(7) . . ?
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C11C C10C H10G 108.9 . . ?
C11C C10C H10H 108.9 . . ?
C10C C11C H11C 115.1 . . ?
C12C C11C C10C 129.8(10) . . ?
C12C C11C H11C 115.1 . . ?
C11C C12C C13C 120.5(10) . . ?
C11C C12C C14C 121.4(10) . . ?
C13C C12C C14C 117.0(10) . . ?
C12C C13C H13J 109.5 . . ?
C12C C13C H13K 109.5 . . ?
C12C C13C H13L 109.5 . . ?
H13J C13C H13K 109.5 . . ?
H13J C13C H13L 109.5 . . ?
H13K C13C H13L 109.5 . . ?
C12C C14C H14J 109.5 . . ?
C12C C14C H14K 109.5 . . ?
C12C C14C H14L 109.5 . . ?
H14J C14C H14K 109.5 . . ?
H14J C14C H14L 109.5 . . ?
H14K C14C H14L 109.5 . . ?
C1C C15C H15J 109.5 . . ?
C1C C15C H15K 109.5 . . ?
C1C C15C H15L 109.5 . . ?
H15J C15C H15K 109.5 . . ?
H15J C15C H15L 109.5 . . ?
H15K C15C H15L 109.5 . . ?
O4C C16C H16J 109.5 . . ?
O4C C16C H16K 109.5 . . ?
O4C C16C H16L 109.5 . . ?
H16J C16C H16K 109.5 . . ?
H16J C16C H16L 109.5 . . ?
H16K C16C H16L 109.5 . . ?
O6C C17C O5C 124.2(7) . . ?
O6C C17C N1C 126.0(7) . . ?
N1C C17C O5C 109.7(6) . . ?
N1C C18C H18C 108.9 . . ?
N1C C18C C19C 107.9(7) . . ?
N1C C18C C20C 112.7(7) . . ?
C19C C18C H18C 108.9 . . ?
C19C C18C C20C 109.6(7) . . ?
C20C C18C H18C 108.9 . . ?
O7C C19C N2C 123.0(7) . . ?
O7C C19C C18C 118.9(7) . . ?
N2C C19C C18C 117.9(7) . . ?
C18C C20C H20C 106.7 . . ?
C21C C20C C18C 111.8(7) . . ?
C21C C20C H20C 106.7 . . ?
C21C C20C C22C 114.8(8) . . ?
C22C C20C C18C 109.8(8) . . ?
C22C C20C H20C 106.7 . . ?
C20C C21C H21J 109.5 . . ?
C20C C21C H21K 109.5 . . ?
C20C C21C H21L 109.5 . . ?
H21J C21C H21K 109.5 . . ?
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H21J C21C H21L 109.5 . . ?
H21K C21C H21L 109.5 . . ?
C20C C22C H22J 109.5 . . ?
C20C C22C H22K 109.5 . . ?
C20C C22C H22L 109.5 . . ?
H22J C22C H22K 109.5 . . ?
H22J C22C H22L 109.5 . . ?
H22K C22C H22L 109.5 . . ?
C8D O1D C1D 109.8(5) . . ?
C7D O2D H2OD 109.5 . . ?
C9D O3D H3OD 109.5 . . ?
C3D O4D C16D 112.8(6) . . ?
C17D O5D C4D 118.1(6) . . ?
C17D N1D H1D 118.0 . . ?
C17D N1D C18D 124.1(7) . . ?
C18D N1D H1D 118.0 . . ?
H2NI N2D H2NJ 120.0 . . ?
C19D N2D H2NI 120.0 . . ?
C19D N2D H2NJ 120.0 . . ?
O1D C1D C2D 103.3(5) . . ?
O1D C1D C9D 104.7(5) . . ?
O1D C1D C15D 105.8(6) . . ?
C2D C1D C9D 115.8(6) . . ?
C15D C1D C2D 114.4(6) . . ?
C15D C1D C9D 111.4(6) . . ?
C1D C2D H2D 107.4 . . ?
C3D C2D C1D 120.8(6) . . ?
C3D C2D H2D 107.4 . . ?
C3D C2D C7D 108.9(5) . . ?
C7D C2D C1D 104.3(5) . . ?
C7D C2D H2D 107.4 . . ?
O4D C3D C2D 109.7(6) . . ?
O4D C3D H3D 109.3 . . ?
O4D C3D C4D 109.6(5) . . ?
C2D C3D H3D 109.3 . . ?
C2D C3D C4D 109.6(5) . . ?
C4D C3D H3D 109.3 . . ?
O5D C4D C3D 107.3(6) . . ?
O5D C4D H4D 108.0 . . ?
O5D C4D C5D 109.8(6) . . ?
C3D C4D H4D 108.0 . . ?
C5D C4D C3D 115.4(5) . . ?
C5D C4D H4D 108.0 . . ?
C4D C5D H5DA 109.6 . . ?
C4D C5D H5DB 109.6 . . ?
H5DA C5D H5DB 108.1 . . ?
C6D C5D C4D 110.4(6) . . ?
C6D C5D H5DA 109.6 . . ?
C6D C5D H5DB 109.6 . . ?
C5D C6D H6DA 109.5 . . ?
C5D C6D H6DB 109.5 . . ?
H6DA C6D H6DB 108.1 . . ?
C7D C6D C5D 110.5(6) . . ?
C7D C6D H6DA 109.5 . . ?
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C7D C6D H6DB 109.5 . . ?
O2D C7D C2D 108.8(6) . . ?
O2D C7D C6D 109.2(6) . . ?
O2D C7D C8D 107.3(6) . . ?
C6D C7D C2D 110.4(6) . . ?
C6D C7D C8D 119.8(6) . . ?
C8D C7D C2D 100.7(5) . . ?
O1D C8D C7D 101.4(5) . . ?
O1D C8D H8DA 111.5 . . ?
O1D C8D H8DB 111.5 . . ?
C7D C8D H8DA 111.5 . . ?
C7D C8D H8DB 111.5 . . ?
H8DA C8D H8DB 109.3 . . ?
O3D C9D C1D 112.0(5) . . ?
O3D C9D H9D 107.0 . . ?
O3D C9D C10D 107.3(6) . . ?
C1D C9D H9D 107.0 . . ?
C10D C9D C1D 116.1(6) . . ?
C10D C9D H9D 107.0 . . ?
C9D C10D H10I 108.9 . . ?
C9D C10D H10J 108.9 . . ?
H10I C10D H10J 107.8 . . ?
C11D C10D C9D 113.2(7) . . ?
C11D C10D H10I 108.9 . . ?
C11D C10D H10J 108.9 . . ?
C10D C11D H11D 113.7 . . ?
C12D C11D C10D 132.5(9) . . ?
C12D C11D H11D 113.7 . . ?
C11D C12D C13D 121.4(9) . . ?
C11D C12D C14D 125.7(10) . . ?
C13D C12D C14D 112.9(9) . . ?
C12D C13D H13M 109.5 . . ?
C12D C13D H13N 109.5 . . ?
C12D C13D H13O 109.5 . . ?
H13M C13D H13N 109.5 . . ?
H13M C13D H13O 109.5 . . ?
H13N C13D H13O 109.5 . . ?
C12D C14D H14M 109.5 . . ?
C12D C14D H14N 109.5 . . ?
C12D C14D H14O 109.5 . . ?
H14M C14D H14N 109.5 . . ?
H14M C14D H14O 109.5 . . ?
H14N C14D H14O 109.5 . . ?
C1D C15D H15M 109.5 . . ?
C1D C15D H15N 109.5 . . ?
C1D C15D H15O 109.5 . . ?
H15M C15D H15N 109.5 . . ?
H15M C15D H15O 109.5 . . ?
H15N C15D H15O 109.5 . . ?
O4D C16D H16M 109.5 . . ?
O4D C16D H16N 109.5 . . ?
O4D C16D H16O 109.5 . . ?
H16M C16D H16N 109.5 . . ?
H16M C16D H16O 109.5 . . ?
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H16N C16D H16O 109.5 . . ?
O6D C17D O5D 125.3(7) . . ?
O6D C17D N1D 122.9(6) . . ?
N1D C17D O5D 111.8(6) . . ?
N1D C18D H18D 108.7 . . ?
N1D C18D C19D 108.1(6) . . ?
N1D C18D C20D 113.1(6) . . ?
C19D C18D H18D 108.7 . . ?
C19D C18D C20D 109.5(6) . . ?
C20D C18D H18D 108.7 . . ?
O7D C19D N2D 121.7(7) . . ?
O7D C19D C18D 119.9(7) . . ?
N2D C19D C18D 118.3(7) . . ?
C18D C20D H20D 107.7 . . ?
C21D C20D C18D 112.9(7) . . ?
C21D C20D H20D 107.7 . . ?
C21D C20D C22D 111.2(8) . . ?
C22D C20D C18D 109.5(7) . . ?
C22D C20D H20D 107.7 . . ?
C20D C21D H21M 109.5 . . ?
C20D C21D H21N 109.5 . . ?
C20D C21D H21O 109.5 . . ?
H21M C21D H21N 109.5 . . ?
H21M C21D H21O 109.5 . . ?
H21N C21D H21O 109.5 . . ?
C20D C22D H22M 109.5 . . ?
C20D C22D H22N 109.5 . . ?
C20D C22D H22O 109.5 . . ?
H22M C22D H22N 109.5 . . ?
H22M C22D H22O 109.5 . . ?
H22N C22D H22O 109.5 . . ?
C8E O1E C1E 109.9(6) . . ?
C7E O2E H2OE 109.5 . . ?
C9E O3E H3E 109.5 . . ?
C3E O4E C16E 114.2(7) . . ?
C17E O5E C4E 118.5(6) . . ?
C17E N1E H1NE 118.3 . . ?
C17E N1E C18E 123.5(7) . . ?
C18E N1E H1NE 118.3 . . ?
H2EK N2E H2EL 120.0 . . ?
C19E N2E H2EK 120.0 . . ?
C19E N2E H2EL 120.0 . . ?
O1E C1E C2E 104.2(5) . . ?
O1E C1E C9E 102.9(6) . . ?
O1E C1E C15E 107.4(7) . . ?
C9E C1E C2E 113.2(6) . . ?
C15E C1E C2E 115.2(7) . . ?
C15E C1E C9E 112.6(7) . . ?
C1E C2E H2E 106.8 . . ?
C3E C2E C1E 121.8(7) . . ?
C3E C2E H2E 106.8 . . ?
C7E C2E C1E 102.6(5) . . ?
C7E C2E H2E 106.8 . . ?
C7E C2E C3E 111.0(6) . . ?
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O4E C3E C2E 109.5(6) . . ?
O4E C3E H5 108.6 . . ?
O4E C3E C4E 112.0(6) . . ?
C2E C3E H5 108.6 . . ?
C2E C3E C4E 109.3(6) . . ?
C4E C3E H5 108.6 . . ?
O5E C4E C3E 106.1(6) . . ?
O5E C4E H4E 110.7 . . ?
O5E C4E C5E 107.6(7) . . ?
C3E C4E H4E 110.7 . . ?
C5E C4E C3E 110.9(6) . . ?
C5E C4E H4E 110.7 . . ?
C4E C5E H5EA 109.5 . . ?
C4E C5E H5EB 109.5 . . ?
C4E C5E C6E 110.6(7) . . ?
H5EA C5E H5EB 108.1 . . ?
C6E C5E H5EA 109.5 . . ?
C6E C5E H5EB 109.5 . . ?
C5E C6E H6EA 109.8 . . ?
C5E C6E H6EB 109.8 . . ?
H6EA C6E H6EB 108.2 . . ?
C7E C6E C5E 109.5(7) . . ?
C7E C6E H6EA 109.8 . . ?
C7E C6E H6EB 109.8 . . ?
O2E C7E C2E 107.3(7) . . ?
O2E C7E C6E 108.1(7) . . ?
O2E C7E C8E 108.2(7) . . ?
C6E C7E C2E 110.9(6) . . ?
C6E C7E C8E 120.3(7) . . ?
C8E C7E C2E 101.4(6) . . ?
O1E C8E C7E 104.4(6) . . ?
O1E C8E H8EA 110.9 . . ?
O1E C8E H8EB 110.9 . . ?
C7E C8E H8EA 110.9 . . ?
C7E C8E H8EB 110.9 . . ?
H8EA C8E H8EB 108.9 . . ?
O3E C9E C1E 110.7(6) . . ?
O3E C9E H9E 106.6 . . ?
O3E C9E C10E 109.1(7) . . ?
C1E C9E H9E 106.6 . . ?
C10E C9E C1E 116.6(6) . . ?
C10E C9E H9E 106.6 . . ?
C9E C10E H10K 108.9 . . ?
C9E C10E H10L 108.9 . . ?
H10K C10E H10L 107.7 . . ?
C11E C10E C9E 113.6(7) . . ?
C11E C10E H10K 108.9 . . ?
C11E C10E H10L 108.9 . . ?
C10E C11E H11E 114.4 . . ?
C12E C11E C10E 131.3(9) . . ?
C12E C11E H11E 114.4 . . ?
C11E C12E C13E 116.7(8) . . ?
C11E C12E C14E 126.5(9) . . ?
C13E C12E C14E 116.6(9) . . ?
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C12E C13E H13P 109.5 . . ?
C12E C13E H13Q 109.5 . . ?
C12E C13E H13R 109.5 . . ?
H13P C13E H13Q 109.5 . . ?
H13P C13E H13R 109.5 . . ?
H13Q C13E H13R 109.5 . . ?
C12E C14E H14P 109.5 . . ?
C12E C14E H14Q 109.5 . . ?
C12E C14E H14R 109.5 . . ?
H14P C14E H14Q 109.5 . . ?
H14P C14E H14R 109.5 . . ?
H14Q C14E H14R 109.5 . . ?
C1E C15E H15P 109.5 . . ?
C1E C15E H15Q 109.5 . . ?
C1E C15E H15R 109.5 . . ?
H15P C15E H15Q 109.5 . . ?
H15P C15E H15R 109.5 . . ?
H15Q C15E H15R 109.5 . . ?
O4E C16E H16P 109.5 . . ?
O4E C16E H16Q 109.5 . . ?
O4E C16E H16R 109.5 . . ?
H16P C16E H16Q 109.5 . . ?
H16P C16E H16R 109.5 . . ?
H16Q C16E H16R 109.5 . . ?
O6E C17E O5E 123.9(7) . . ?
O6E C17E N1E 126.4(7) . . ?
N1E C17E O5E 109.6(6) . . ?
N1E C18E H18E 108.6 . . ?
N1E C18E C19E 108.4(7) . . ?
N1E C18E C20E 111.4(6) . . ?
C19E C18E H18E 108.6 . . ?
C19E C18E C20E 111.1(7) . . ?
C20E C18E H18E 108.6 . . ?
O7E C19E N2E 124.5(7) . . ?
O7E C19E C18E 118.0(7) . . ?
N2E C19E C18E 117.5(7) . . ?
C18E C20E H20E 108.8 . . ?
C18E C20E C22E 109.4(7) . . ?
C21E C20E C18E 109.3(7) . . ?
C21E C20E H20E 108.8 . . ?
C21E C20E C22E 111.6(8) . . ?
C22E C20E H20E 108.8 . . ?
C20E C21E H21P 109.5 . . ?
C20E C21E H21Q 109.5 . . ?
C20E C21E H21R 109.5 . . ?
H21P C21E H21Q 109.5 . . ?
H21P C21E H21R 109.5 . . ?
H21Q C21E H21R 109.5 . . ?
C20E C22E H22P 109.5 . . ?
C20E C22E H22Q 109.5 . . ?
C20E C22E H22R 109.5 . . ?
H22P C22E H22Q 109.5 . . ?
H22P C22E H22R 109.5 . . ?
H22Q C22E H22R 109.5 . . ?
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C8F O1F C1F 108.5(6) . . ?
C7F O2F H2OF 109.5 . . ?
C9F O3F H3OF 109.5 . . ?
C3F O4F C16F 113.7(9) . . ?
C17F O5F C4F 116.1(6) . . ?
C17F N1F H1NF 119.6 . . ?
C17F N1F C18F 120.8(7) . . ?
C18F N1F H1NF 119.6 . . ?
H2NM N2F H2NN 120.0 . . ?
C19F N2F H2NM 120.0 . . ?
C19F N2F H2NN 120.0 . . ?
O1F C1F C2F 104.5(6) . . ?
O1F C1F C9F 102.3(7) . . ?
O1F C1F C15F 106.0(7) . . ?
C2F C1F C9F 112.1(7) . . ?
C15F C1F C2F 116.3(8) . . ?
C15F C1F C9F 113.9(8) . . ?
C1F C2F H2F 107.9 . . ?
C3F C2F C1F 118.9(7) . . ?
C3F C2F H2F 107.9 . . ?
C3F C2F C7F 110.8(6) . . ?
C7F C2F C1F 102.9(5) . . ?
C7F C2F H2F 107.9 . . ?
O4F C3F C2F 107.8(7) . . ?
O4F C3F H3F 109.9 . . ?
O4F C3F C4F 110.6(7) . . ?
C2F C3F H3F 109.9 . . ?
C2F C3F C4F 108.7(6) . . ?
C4F C3F H3F 109.9 . . ?
O5F C4F C3F 107.5(7) . . ?
O5F C4F H4F 109.9 . . ?
O5F C4F C5F 106.7(7) . . ?
C3F C4F H4F 109.9 . . ?
C5F C4F C3F 112.8(6) . . ?
C5F C4F H4F 109.9 . . ?
C4F C5F H5FA 108.7 . . ?
C4F C5F H5FB 108.7 . . ?
C4F C5F C6F 114.1(7) . . ?
H5FA C5F H5FB 107.6 . . ?
C6F C5F H5FA 108.7 . . ?
C6F C5F H5FB 108.7 . . ?
C5F C6F H6FA 109.8 . . ?
C5F C6F H6FB 109.8 . . ?
H6FA C6F H6FB 108.2 . . ?
C7F C6F C5F 109.5(7) . . ?
C7F C6F H6FA 109.8 . . ?
C7F C6F H6FB 109.8 . . ?
O2F C7F C2F 109.1(6) . . ?
O2F C7F C6F 107.9(6) . . ?
O2F C7F C8F 109.2(7) . . ?
C6F C7F C2F 110.2(6) . . ?
C6F C7F C8F 120.0(7) . . ?
C8F C7F C2F 99.9(6) . . ?
O1F C8F C7F 103.7(6) . . ?
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O1F C8F H8FA 111.0 . . ?
O1F C8F H8FB 111.0 . . ?
C7F C8F H8FA 111.0 . . ?
C7F C8F H8FB 111.0 . . ?
H8FA C8F H8FB 109.0 . . ?
O3F C9F C1F 112.0(8) . . ?
O3F C9F H9F 107.4 . . ?
O3F C9F C10F 107.9(10) . . ?
C1F C9F H9F 107.4 . . ?
C10F C9F C1F 114.5(8) . . ?
C10F C9F H9F 107.4 . . ?
C9F C10F H10N 109.0 . . ?
C9F C10F H10M 109.0 . . ?
H10N C10F H10M 107.8 . . ?
C11F C10F C9F 113.0(11) . . ?
C11F C10F H10N 109.0 . . ?
C11F C10F H10M 109.0 . . ?
C10F C11F H11F 115.2 . . ?
C12F C11F C10F 129.5(14) . . ?
C12F C11F H11F 115.2 . . ?
C11F C12F C13F 119.0(13) . . ?
C11F C12F C14F 118.6(14) . . ?
C13F C12F C14F 115.1(12) . . ?
C12F C13F H13S 109.5 . . ?
C12F C13F H13T 109.5 . . ?
C12F C13F H13U 109.5 . . ?
H13S C13F H13T 109.5 . . ?
H13S C13F H13U 109.5 . . ?
H13T C13F H13U 109.5 . . ?
C12F C14F H14S 109.5 . . ?
C12F C14F H14T 109.5 . . ?
C12F C14F H14U 109.5 . . ?
H14S C14F H14T 109.5 . . ?
H14S C14F H14U 109.5 . . ?
H14T C14F H14U 109.5 . . ?
C1F C15F H15S 109.5 . . ?
C1F C15F H15T 109.5 . . ?
C1F C15F H15U 109.5 . . ?
H15S C15F H15T 109.5 . . ?
H15S C15F H15U 109.5 . . ?
H15T C15F H15U 109.5 . . ?
O4F C16F H16S 109.5 . . ?
O4F C16F H16T 109.5 . . ?
O4F C16F H16U 109.5 . . ?
H16S C16F H16T 109.5 . . ?
H16S C16F H16U 109.5 . . ?
H16T C16F H16U 109.5 . . ?
O5F C17F N1F 111.6(6) . . ?
O6F C17F O5F 123.3(7) . . ?
O6F C17F N1F 125.1(7) . . ?
N1F C18F H18F 107.7 . . ?
N1F C18F C19F 108.3(6) . . ?
N1F C18F C20F 113.1(6) . . ?
C19F C18F H18F 107.7 . . ?
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C19F C18F C20F 112.1(6) . . ?
C20F C18F H18F 107.7 . . ?
O7F C19F N2F 124.1(7) . . ?
O7F C19F C18F 119.9(7) . . ?
N2F C19F C18F 116.0(7) . . ?
C18F C20F H20F 107.9 . . ?
C18F C20F C22F 109.4(6) . . ?
C21F C20F C18F 111.1(7) . . ?
C21F C20F H20F 107.9 . . ?
C21F C20F C22F 112.7(7) . . ?
C22F C20F H20F 107.9 . . ?
C20F C21F H21S 109.5 . . ?
C20F C21F H21T 109.5 . . ?
C20F C21F H21U 109.5 . . ?
H21S C21F H21T 109.5 . . ?
H21S C21F H21U 109.5 . . ?
H21T C21F H21U 109.5 . . ?
C20F C22F H22S 109.5 . . ?
C20F C22F H22T 109.5 . . ?
C20F C22F H22U 109.5 . . ?
H22S C22F H22T 109.5 . . ?
H22S C22F H22U 109.5 . . ?
H22T C22F H22U 109.5 . . ?
C8G O1G C1G 107.1(7) . . ?
C7G O2G H2OG 109.5 . . ?
C9G O3G H3OG 109.5 . . ?
C16G O4G C3G 113.5(10) . . ?
C17G O5G C4G 114.5(7) . . ?
C17G N1G H1NG 118.4 . . ?
C17G N1G C18G 123.1(8) . . ?
C18G N1G H1NG 118.4 . . ?
H2NO N2G H2NP 120.0 . . ?
C19G N2G H2NO 120.0 . . ?
C19G N2G H2NP 120.0 . . ?
O1G C1G C2G 105.2(7) . . ?
O1G C1G C9G 103.0(8) . . ?
O1G C1G C15G 106.2(8) . . ?
C2G C1G C9G 110.2(8) . . ?
C15G C1G C2G 118.2(10) . . ?
C15G C1G C9G 112.5(9) . . ?
C1G C2G H2G 107.5 . . ?
C3G C2G C1G 120.7(9) . . ?
C3G C2G H2G 107.5 . . ?
C7G C2G C1G 103.0(7) . . ?
C7G C2G H2G 107.5 . . ?
C7G C2G C3G 110.0(8) . . ?
O4G C3G C2G 104.7(9) . . ?
O4G C3G H3G 109.0 . . ?
O4G C3G C4G 114.0(8) . . ?
C2G C3G H3G 109.0 . . ?
C4G C3G C2G 111.0(8) . . ?
C4G C3G H3G 109.0 . . ?
O5G C4G C3G 106.4(8) . . ?
O5G C4G H4G 110.6 . . ?
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O5G C4G C5G 106.7(8) . . ?
C3G C4G H4G 110.6 . . ?
C3G C4G C5G 111.7(8) . . ?
C5G C4G H4G 110.6 . . ?
C4G C5G H5GA 108.2 . . ?
C4G C5G H5GB 108.2 . . ?
H5GA C5G H5GB 107.4 . . ?
C6G C5G C4G 116.2(9) . . ?
C6G C5G H5GA 108.2 . . ?
C6G C5G H5GB 108.2 . . ?
C5G C6G H6GA 110.0 . . ?
C5G C6G H6GB 110.0 . . ?
H6GA C6G H6GB 108.4 . . ?
C7G C6G C5G 108.4(9) . . ?
C7G C6G H6GA 110.0 . . ?
C7G C6G H6GB 110.0 . . ?
O2G C7G C2G 109.0(8) . . ?
O2G C7G C6G 109.4(8) . . ?
O2G C7G C8G 108.9(7) . . ?
C2G C7G C8G 99.1(8) . . ?
C6G C7G C2G 111.1(8) . . ?
C6G C7G C8G 118.7(8) . . ?
O1G C8G C7G 103.9(8) . . ?
O1G C8G H8GA 111.0 . . ?
O1G C8G H8GB 111.0 . . ?
C7G C8G H8GA 111.0 . . ?
C7G C8G H8GB 111.0 . . ?
H8GA C8G H8GB 109.0 . . ?
O3G C9G C1G 111.2(10) . . ?
O3G C9G H9G 107.4 . . ?
O3G C9G C10G 108.5(9) . . ?
C1G C9G H9G 107.4 . . ?
C10G C9G C1G 114.7(9) . . ?
C10G C9G H9G 107.4 . . ?
C9G C10G H10O 107.9 . . ?
C9G C10G H10P 107.9 . . ?
H10O C10G H10P 107.2 . . ?
C11G C10G C9G 117.7(11) . . ?
C11G C10G H10O 107.9 . . ?
C11G C10G H10P 107.9 . . ?
C10G C11G H11G 112.6 . . ?
C12G C11G C10G 134.7(14) . . ?
C12G C11G H11G 112.6 . . ?
C11G C12G C13G 125.5(15) . . ?
C11G C12G C14G 123.5(14) . . ?
C13G C12G C14G 111.0(14) . . ?
C12G C13G H13V 109.5 . . ?
C12G C13G H13W 109.5 . . ?
C12G C13G H13X 109.5 . . ?
H13V C13G H13W 109.5 . . ?
H13V C13G H13X 109.5 . . ?
H13W C13G H13X 109.5 . . ?
C12G C14G H14V 109.5 . . ?
C12G C14G H14W 109.5 . . ?
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C12G C14G H14X 109.5 . . ?
H14V C14G H14W 109.5 . . ?
H14V C14G H14X 109.5 . . ?
H14W C14G H14X 109.5 . . ?
C1G C15G H15V 109.5 . . ?
C1G C15G H15W 109.5 . . ?
C1G C15G H15X 109.5 . . ?
H15V C15G H15W 109.5 . . ?
H15V C15G H15X 109.5 . . ?
H15W C15G H15X 109.5 . . ?
O4G C16G H16V 109.5 . . ?
O4G C16G H16W 109.5 . . ?
O4G C16G H16X 109.5 . . ?
H16V C16G H16W 109.5 . . ?
H16V C16G H16X 109.5 . . ?
H16W C16G H16X 109.5 . . ?
O5G C17G N1G 109.7(8) . . ?
O6G C17G O5G 127.0(8) . . ?
O6G C17G N1G 123.0(8) . . ?
N1G C18G H18G 107.2 . . ?
N1G C18G C19G 109.3(7) . . ?
N1G C18G C20G 112.1(7) . . ?
C19G C18G H18G 107.2 . . ?
C20G C18G H18G 107.2 . . ?
C20G C18G C19G 113.6(7) . . ?
O7G C19G N2G 123.4(8) . . ?
O7G C19G C18G 119.7(8) . . ?
N2G C19G C18G 116.9(8) . . ?
C18G C20G H20G 107.2 . . ?
C18G C20G C21G 111.3(8) . . ?
C21G C20G H20G 107.2 . . ?
C22G C20G C18G 111.2(8) . . ?
C22G C20G H20G 107.2 . . ?
C22G C20G C21G 112.4(8) . . ?
C20G C21G H21V 109.5 . . ?
C20G C21G H21W 109.5 . . ?
C20G C21G H21X 109.5 . . ?
H21V C21G H21W 109.5 . . ?
H21V C21G H21X 109.5 . . ?
H21W C21G H21X 109.5 . . ?
C20G C22G H22V 109.5 . . ?
C20G C22G H22W 109.5 . . ?
C20G C22G H22X 109.5 . . ?
H22V C22G H22W 109.5 . . ?
H22V C22G H22X 109.5 . . ?
H22W C22G H22X 109.5 . . ?
C8H O1H C1H 108.6(5) . . ?
C7H O2H H2OH 109.5 . . ?
C9H O3H H3OH 109.5 . . ?
C3H O4H C16H 114.2(7) . . ?
C17H O5H C4H 117.3(6) . . ?
C17H N1H H1NH 118.0 . . ?
C17H N1H C18H 124.0(7) . . ?
C18H N1H H1NH 118.0 . . ?
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H2NQ N2H H2NR 120.0 . . ?
C19H N2H H2NQ 120.0 . . ?
C19H N2H H2NR 120.0 . . ?
O1H C1H C2H 104.2(5) . . ?
O1H C1H C9H 104.6(5) . . ?
O1H C1H C15H 106.6(6) . . ?
C9H C1H C2H 116.0(6) . . ?
C15H C1H C2H 113.2(6) . . ?
C15H C1H C9H 111.0(6) . . ?
C1H C2H H2H 107.2 . . ?
C3H C2H C1H 120.5(6) . . ?
C3H C2H H2H 107.2 . . ?
C7H C2H C1H 104.7(5) . . ?
C7H C2H H2H 107.2 . . ?
C7H C2H C3H 109.4(6) . . ?
O4H C3H C2H 110.4(6) . . ?
O4H C3H H3H 108.4 . . ?
O4H C3H C4H 112.1(6) . . ?
C2H C3H H3H 108.4 . . ?
C2H C3H C4H 109.1(6) . . ?
C4H C3H H3H 108.4 . . ?
O5H C4H C3H 103.8(6) . . ?
O5H C4H H4H 110.0 . . ?
O5H C4H C5H 107.4(6) . . ?
C3H C4H H4H 110.0 . . ?
C5H C4H C3H 115.6(6) . . ?
C5H C4H H4H 110.0 . . ?
C4H C5H H5HA 108.9 . . ?
C4H C5H H5HB 108.9 . . ?
C4H C5H C6H 113.3(7) . . ?
H5HA C5H H5HB 107.7 . . ?
C6H C5H H5HA 108.9 . . ?
C6H C5H H5HB 108.9 . . ?
C5H C6H H6HA 110.0 . . ?
C5H C6H H6HB 110.0 . . ?
H6HA C6H H6HB 108.4 . . ?
C7H C6H C5H 108.4(6) . . ?
C7H C6H H6HA 110.0 . . ?
C7H C6H H6HB 110.0 . . ?
O2H C7H C2H 108.9(6) . . ?
O2H C7H C6H 110.1(6) . . ?
O2H C7H C8H 106.3(6) . . ?
C6H C7H C2H 111.1(6) . . ?
C6H C7H C8H 118.9(6) . . ?
C8H C7H C2H 100.7(5) . . ?
O1H C8H C7H 102.7(5) . . ?
O1H C8H H8HA 111.2 . . ?
O1H C8H H8HB 111.2 . . ?
C7H C8H H8HA 111.2 . . ?
C7H C8H H8HB 111.2 . . ?
H8HA C8H H8HB 109.1 . . ?
O3H C9H C1H 112.1(6) . . ?
O3H C9H H9H 106.5 . . ?
O3H C9H C10H 106.4(6) . . ?
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C1H C9H H9H 106.5 . . ?
C10H C9H C1H 118.3(7) . . ?
C10H C9H H9H 106.5 . . ?
C9H C10H H10Q 109.2 . . ?
C9H C10H H10R 109.2 . . ?
H10Q C10H H10R 107.9 . . ?
C11H C10H C9H 112.2(8) . . ?
C11H C10H H10Q 109.2 . . ?
C11H C10H H10R 109.2 . . ?
C10H C11H H11H 114.3 . . ?
C12H C11H C10H 131.4(10) . . ?
C12H C11H H11H 114.3 . . ?
C11H C12H C13H 119.1(10) . . ?
C11H C12H C14H 123.3(10) . . ?
C13H C12H C14H 116.5(10) . . ?
C12H C13H H13Y 109.5 . . ?
C12H C13H H13Z 109.5 . . ?
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H14Y C14H H14 109.5 . . ?
H14Z C14H H14 109.5 . . ?
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C1H C15H H15Z 109.5 . . ?
C1H C15H H151 109.5 . . ?
H15Y C15H H15Z 109.5 . . ?
H15Y C15H H151 109.5 . . ?
H15Z C15H H151 109.5 . . ?
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H16Y C16H H161 109.5 . . ?
H16Z C16H H161 109.5 . . ?
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N1H C17H O5H 110.8(6) . . ?
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N1H C18H C19H 107.1(6) . . ?
N1H C18H C20H 113.2(7) . . ?
C19H C18H H18H 108.6 . . ?
C19H C18H C20H 110.6(7) . . ?
C20H C18H H18H 108.6 . . ?
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O7H C19H C18H 119.8(7) . . ?
N2H C19H C18H 117.1(7) . . ?
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C21H C20H C18H 111.7(7) . . ?
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O4I C3I C4I 116.7(7) . . ?
C2I C3I H3I 107.3 . . ?
C2I C3I C4I 109.7(7) . . ?
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 O2A H2OA O3G 0.84 1.99 2.797(13) 161.6 1_455
 O3A H3OA O7G 0.84 1.87 2.663(10) 157.1 1_455
 N1A H1NA O3 0.88 2.13 2.853(9) 139.4 .
 N2A H2ND O7C 0.88 2.04 2.882(11) 158.8 .
 O2B H2OB O3K 0.84 2.04 2.754(12) 141.9 .
 O3B H3OB O3C 0.84 2.25 2.786(9) 122.0 .
 N1B H1NB O3C 0.88 2.03 2.846(9) 153.5 .
 N2B H2NE O7C 0.88 2.22 2.991(11) 146.2 .
 N2B H2NF O7 0.88 2.11 2.923(12) 152.4 .
 O2C H2OC O6F 0.84 2.02 2.759(10) 146.2 .
 N1C H1NC O7B 0.88 2.01 2.802(10) 148.6 .
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 N2C H2NG O6A 0.88 2.14 2.933(11) 149.6 .
 N2C H2NH O1K 0.88 2.06 2.927(10) 169.6 1_455
 O3D H3OD O3I 0.84 2.00 2.777(9) 152.5 1_565
 N1D H1D O7I 0.88 1.95 2.794(10) 161.4 1_565
 N2D H2NJ O1F 0.88 2.09 2.958(11) 167.6 .
 O2E H2OE O3J 0.84 1.96 2.724(11) 149.7 .
 O3E H3E O3H 0.84 2.31 2.806(9) 118.5 1_565
 N1E H1NE O3H 0.88 2.10 2.901(9) 151.8 1_565
 N2E H2EL O7D 0.88 2.19 2.958(10) 145.2 1_455
 O2F H2OF O6D 0.84 1.85 2.691(9) 177.1 .
 N1F H1NF O1I 0.88 2.07 2.901(10) 156.1 .
 N2F H2NM O7K 0.88 2.09 2.939(9) 161.0 .
 O2G H2OG O6 0.84 1.92 2.686(8) 151.1 .
 O3G H3OG O4G 0.84 1.91 2.734(15) 168.1 .
 N1G H1NG O1A 0.88 2.13 2.945(11) 154.8 1_655
 N2G H2NO O7J 0.88 2.05 2.914(10) 165.1 1_655
 O2H H2OH O6G 0.84 2.05 2.775(10) 144.9 1_445
 O3H H3OH O3E 0.84 2.01 2.806(9) 157.4 1_545
 N1H H1NH O7E 0.88 1.95 2.798(10) 161.2 1_545
 N2H H2NR O1J 0.88 2.00 2.861(10) 167.9 .
 N1I H1NI O3D 0.88 2.16 2.865(9) 136.4 1_545
 N2I H2NS O7D 0.88 2.12 2.979(10) 164.9 1_545
 N2I H2NT O7H 0.88 2.05 2.924(10) 173.6 1_655
 O2J H2OJ O6H 0.84 1.96 2.789(10) 170.8 .
 O3J H3OJ O4J 0.84 1.97 2.746(11) 153.0 .
 N1J H1NJ O1E 0.88 2.01 2.846(9) 157.9 .
 O3K H3OK O4K 0.84 1.97 2.754(13) 155.7 .
 N1K H1NK O1B 0.88 2.05 2.891(10) 159.3 .

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 O1 C1 C9 C10 -169.6(7) . . . . ?
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 O3 C9 C10 C11 73.4(10) . . . . ?
 O4 C3 C4 O5 -48.3(7) . . . . ?
 O4 C3 C4 C5 -168.8(7) . . . . ?
 O5 C4 C5 C6 -74.8(8) . . . . ?
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 N1 C18 C19 N2 -117.1(9) . . . . ?
 N1 C18 C20 C21 -178.5(8) . . . . ?
 N1 C18 C20 C22 59.0(10) . . . . ?
 C1 O1 C8 C7 34.4(8) . . . . ?
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C1 C2 C7 C6 164.6(6) . . . . ?
C1 C2 C7 C8 37.6(7) . . . . ?
C1 C9 C10 C11 -160.4(8) . . . . ?
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C2 C1 C9 C10 -56.0(9) . . . . ?
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C2 C3 C4 C5 -49.1(9) . . . . ?
C2 C7 C8 O1 -43.9(7) . . . . ?
C3 C2 C7 O2 55.5(7) . . . . ?
C3 C2 C7 C6 -66.1(8) . . . . ?
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C4 O5 C17 N1 -157.4(7) . . . . ?
C4 C5 C6 C7 -48.9(10) . . . . ?
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C5 C6 C7 C2 60.2(8) . . . . ?
C5 C6 C7 C8 176.6(7) . . . . ?
C6 C7 C8 O1 -165.3(7) . . . . ?
C7 C2 C3 O4 177.7(6) . . . . ?
C7 C2 C3 C4 57.7(7) . . . . ?
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C8 O1 C1 C9 109.4(7) . . . . ?
C8 O1 C1 C15 -131.0(7) . . . . ?
C9 C1 C2 C3 106.5(7) . . . . ?
C9 C1 C2 C7 -131.8(6) . . . . ?
C9 C10 C11 C12 -131.4(13) . . . . ?
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C17 O5 C4 C5 -139.0(7) . . . . ?
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C17 N1 C18 C20 -123.9(9) . . . . ?
C18 N1 C17 O5 -176.5(7) . . . . ?
C18 N1 C17 O6 4.8(14) . . . . ?
C19 C18 C20 C21 -57.2(10) . . . . ?
C19 C18 C20 C22 -179.7(8) . . . . ?
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C20 C18 C19 N2 120.1(9) . . . . ?
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O1A C1A C2A C7A -23.3(8) . . . . ?
O1A C1A C9A O3A -67.6(8) . . . . ?
O1A C1A C9A C10A 170.2(7) . . . . ?
O2A C7A C8A O1A 72.6(8) . . . . ?
O3A C9A C10A C11A 69.1(11) . . . . ?
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O5A C4A C5A C6A -66.9(9) . . . . ?
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N1A C18A C20A C21A -174.1(8) . . . . ?
N1A C18A C20A C22A 62.5(9) . . . . ?
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C1A C2A C7A C6A 166.7(7) . . . . ?
C1A C2A C7A C8A 38.9(8) . . . . ?
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C3A C2A C7A O2A 58.7(8) . . . . ?
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C3A C2A C7A C8A 171.5(7) . . . . ?
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C4A O5A C17A N1A -160.5(7) . . . . ?
C4A C5A C6A C7A -51.9(10) . . . . ?
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C8A O1A C1A C2A -2.0(8) . . . . ?
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C8A O1A C1A C15A -124.1(8) . . . . ?
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C9A C10A C11A C12A 127.0(19) . . . . ?
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C19A C18A C20A C22A 179.2(8) . . . . ?
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O1B C1B C9B C10B 171.2(8) . . . . ?
O2B C7B C8B O1B 74.2(9) . . . . ?
O3B C9B C10B C11B 63.6(12) . . . . ?
O4B C3B C4B O5B -58.8(9) . . . . ?
O4B C3B C4B C5B -172.8(7) . . . . ?
O5B C4B C5B C6B -65.8(10) . . . . ?
N1B C18B C19B O7B 61.4(12) . . . . ?
N1B C18B C19B N2B -113.1(11) . . . . ?
N1B C18B C20B C21B -172.5(8) . . . . ?
N1B C18B C20B C22B 64.1(10) . . . . ?
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C1B C2B C3B C4B 178.2(7) . . . . ?
C1B C2B C7B O2B -74.8(8) . . . . ?
C1B C2B C7B C6B 164.7(7) . . . . ?
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C3B C4B C5B C6B 49.7(11) . . . . ?
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C6B C7B C8B O1B -160.1(8) . . . . ?
C7B C2B C3B O4B -178.3(7) . . . . ?
C7B C2B C3B C4B 56.9(9) . . . . ?
C8B O1B C1B C2B -0.2(8) . . . . ?
C8B O1B C1B C9B 118.5(7) . . . . ?
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C9B C1B C2B C3B 99.3(9) . . . . ?
C9B C1B C2B C7B -136.3(7) . . . . ?
C9B C10B C11B C12B 168.4(13) . . . . ?
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C15B C1B C9B O3B -178.3(8) . . . . ?
C15B C1B C9B C10B 55.5(11) . . . . ?
C16B O4B C3B C2B 164.3(8) . . . . ?
C16B O4B C3B C4B -74.4(11) . . . . ?
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C18B N1B C17B O6B 3.8(18) . . . . ?
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C20B C18B C19B O7B -60.3(12) . . . . ?
C20B C18B C19B N2B 125.2(10) . . . . ?
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O1C C1C C2C C7C -15.4(7) . . . . ?
O1C C1C C9C O3C -43.9(8) . . . . ?
O1C C1C C9C C10C -168.2(7) . . . . ?
O2C C7C C8C O1C 68.3(8) . . . . ?
O3C C9C C10C C11C 67.7(10) . . . . ?
O4C C3C C4C O5C -52.5(8) . . . . ?
O4C C3C C4C C5C -171.9(7) . . . . ?
O5C C4C C5C C6C -71.5(9) . . . . ?
N1C C18C C19C O7C 59.9(12) . . . . ?
N1C C18C C19C N2C -115.5(10) . . . . ?
N1C C18C C20C C21C -175.6(9) . . . . ?
N1C C18C C20C C22C 55.9(10) . . . . ?
C1C O1C C8C C7C 36.4(8) . . . . ?
C1C C2C C3C O4C -58.0(9) . . . . ?
C1C C2C C3C C4C 178.6(6) . . . . ?
C1C C2C C7C O2C -74.7(6) . . . . ?
C1C C2C C7C C6C 165.0(6) . . . . ?
C1C C2C C7C C8C 36.2(7) . . . . ?
C1C C9C C10C C11C -166.4(8) . . . . ?
C2C C1C C9C O3C 70.6(8) . . . . ?
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C3C C2C C7C C8C 166.7(6) . . . . ?
C3C C4C C5C C6C 46.3(10) . . . . ?
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C4C O5C C17C N1C -162.2(7) . . . . ?
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C5C C6C C7C O2C -61.0(9) . . . . ?
C5C C6C C7C C2C 58.7(9) . . . . ?
C5C C6C C7C C8C 176.0(8) . . . . ?
C6C C7C C8C O1C -167.5(7) . . . . ?
C7C C2C C3C O4C -179.6(6) . . . . ?
C7C C2C C3C C4C 57.0(8) . . . . ?
C8C O1C C1C C2C -12.9(7) . . . . ?
C8C O1C C1C C9C 109.4(7) . . . . ?
C8C O1C C1C C15C -134.7(7) . . . . ?
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C9C C10C C11C C12C 106.6(16) . . . . ?
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O1D C1D C2D C7D -16.6(7) . . . . ?
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O1D C1D C9D C10D -170.7(6) . . . . ?
O2D C7D C8D O1D 69.1(7) . . . . ?
O3D C9D C10D C11D 74.7(10) . . . . ?
O4D C3D C4D O5D -48.4(7) . . . . ?
O4D C3D C4D C5D -171.2(6) . . . . ?
O5D C4D C5D C6D -73.1(8) . . . . ?
N1D C18D C19D O7D 60.8(11) . . . . ?
N1D C18D C19D N2D -119.8(9) . . . . ?
N1D C18D C20D C21D -175.4(8) . . . . ?
N1D C18D C20D C22D 60.1(11) . . . . ?
C1D O1D C8D C7D 36.3(8) . . . . ?
C1D C2D C3D O4D -62.7(9) . . . . ?
C1D C2D C3D C4D 177.0(6) . . . . ?
C1D C2D C7D O2D -74.7(6) . . . . ?
C1D C2D C7D C6D 165.4(6) . . . . ?
C1D C2D C7D C8D 37.8(7) . . . . ?
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C2D C1D C9D O3D 66.0(7) . . . . ?
C2D C1D C9D C10D -57.6(8) . . . . ?
C2D C3D C4D O5D 72.0(7) . . . . ?
C2D C3D C4D C5D -50.8(9) . . . . ?
C2D C7D C8D O1D -44.7(7) . . . . ?
C3D C2D C7D O2D 55.5(7) . . . . ?
C3D C2D C7D C6D -64.3(8) . . . . ?
C3D C2D C7D C8D 168.1(6) . . . . ?
C3D C4D C5D C6D 48.3(9) . . . . ?
C4D O5D C17D O6D 22.7(12) . . . . ?
C4D O5D C17D N1D -154.8(7) . . . . ?
C4D C5D C6D C7D -52.9(9) . . . . ?
C5D C6D C7D O2D -57.4(8) . . . . ?
C5D C6D C7D C2D 62.2(9) . . . . ?
C5D C6D C7D C8D 178.4(7) . . . . ?
C6D C7D C8D O1D -165.8(7) . . . . ?
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C7D C2D C3D O4D 176.8(6) . . . . ?
C7D C2D C3D C4D 56.5(8) . . . . ?
C8D O1D C1D C2D -12.3(8) . . . . ?
C8D O1D C1D C9D 109.4(7) . . . . ?
C8D O1D C1D C15D -132.8(7) . . . . ?
C9D C1D C2D C3D 106.8(7) . . . . ?
C9D C1D C2D C7D -130.5(6) . . . . ?
C9D C10D C11D C12D -130.5(14) . . . . ?
C10D C11D C12D C13D 2(2) . . . . ?
C10D C11D C12D C14D -178.1(13) . . . . ?
C15D C1D C2D C3D -24.9(9) . . . . ?
C15D C1D C2D C7D 97.9(7) . . . . ?
C15D C1D C9D O3D -160.9(6) . . . . ?
C15D C1D C9D C10D 75.5(9) . . . . ?
C16D O4D C3D C2D 154.5(6) . . . . ?
C16D O4D C3D C4D -85.2(8) . . . . ?
C17D O5D C4D C3D 95.9(7) . . . . ?
C17D O5D C4D C5D -138.0(7) . . . . ?
C17D N1D C18D C19D 110.3(9) . . . . ?
C17D N1D C18D C20D -128.3(9) . . . . ?
C18D N1D C17D O5D -176.6(7) . . . . ?
C18D N1D C17D O6D 5.7(13) . . . . ?
C19D C18D C20D C21D -54.8(11) . . . . ?
C19D C18D C20D C22D -179.3(8) . . . . ?
C20D C18D C19D O7D -62.8(11) . . . . ?
C20D C18D C19D N2D 116.6(10) . . . . ?
O1E C1E C2E C3E -151.6(7) . . . . ?
O1E C1E C2E C7E -26.8(7) . . . . ?
O1E C1E C9E O3E -62.0(8) . . . . ?
O1E C1E C9E C10E 172.5(7) . . . . ?
O2E C7E C8E O1E 73.7(9) . . . . ?
O3E C9E C10E C11E 67.0(11) . . . . ?
O4E C3E C4E O5E -61.6(8) . . . . ?
O4E C3E C4E C5E -178.1(7) . . . . ?
O5E C4E C5E C6E -58.4(10) . . . . ?
N1E C18E C19E O7E 66.2(11) . . . . ?
N1E C18E C19E N2E -110.9(10) . . . . ?
N1E C18E C20E C21E -175.6(8) . . . . ?
N1E C18E C20E C22E 61.9(9) . . . . ?
C1E O1E C8E C7E 22.9(9) . . . . ?
C1E C2E C3E O4E -58.9(10) . . . . ?
C1E C2E C3E C4E 178.1(6) . . . . ?
C1E C2E C7E O2E -73.3(7) . . . . ?
C1E C2E C7E C6E 168.9(7) . . . . ?
C1E C2E C7E C8E 40.1(8) . . . . ?
C1E C9E C10E C11E -166.7(8) . . . . ?
C2E C1E C9E O3E 49.8(9) . . . . ?
C2E C1E C9E C10E -75.7(9) . . . . ?
C2E C3E C4E O5E 60.0(8) . . . . ?
C2E C3E C4E C5E -56.6(9) . . . . ?
C2E C7E C8E O1E -39.0(9) . . . . ?
C3E C2E C7E O2E 58.4(8) . . . . ?
C3E C2E C7E C6E -59.4(9) . . . . ?
C3E C2E C7E C8E 171.8(7) . . . . ?
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C3E C4E C5E C6E 57.2(10) . . . . ?
C4E O5E C17E O6E 21.1(16) . . . . ?
C4E O5E C17E N1E -161.6(8) . . . . ?
C4E C5E C6E C7E -57.8(11) . . . . ?
C5E C6E C7E O2E -58.9(9) . . . . ?
C5E C6E C7E C2E 58.5(9) . . . . ?
C5E C6E C7E C8E 176.3(8) . . . . ?
C6E C7E C8E O1E -161.6(8) . . . . ?
C7E C2E C3E O4E -179.8(7) . . . . ?
C7E C2E C3E C4E 57.1(9) . . . . ?
C8E O1E C1E C2E 2.7(9) . . . . ?
C8E O1E C1E C9E 121.0(7) . . . . ?
C8E O1E C1E C15E -120.0(8) . . . . ?
C9E C1E C2E C3E 97.4(8) . . . . ?
C9E C1E C2E C7E -137.8(6) . . . . ?
C9E C10E C11E C12E 176.2(13) . . . . ?
C10E C11E C12E C13E 0(2) . . . . ?
C10E C11E C12E C14E -176.7(12) . . . . ?
C15E C1E C2E C3E -34.3(10) . . . . ?
C15E C1E C2E C7E 90.5(8) . . . . ?
C15E C1E C9E O3E -177.3(7) . . . . ?
C15E C1E C9E C10E 57.2(10) . . . . ?
C16E O4E C3E C2E 167.0(8) . . . . ?
C16E O4E C3E C4E -71.5(10) . . . . ?
C17E O5E C4E C3E 92.9(9) . . . . ?
C17E O5E C4E C5E -148.3(8) . . . . ?
C17E N1E C18E C19E 123.0(10) . . . . ?
C17E N1E C18E C20E -114.5(10) . . . . ?
C18E N1E C17E O5E -178.1(8) . . . . ?
C18E N1E C17E O6E -0.9(18) . . . . ?
C19E C18E C20E C21E -54.7(10) . . . . ?
C19E C18E C20E C22E -177.2(7) . . . . ?
C20E C18E C19E O7E -56.5(12) . . . . ?
C20E C18E C19E N2E 126.5(10) . . . . ?
O1F C1F C2F C3F -145.8(7) . . . . ?
O1F C1F C2F C7F -23.0(8) . . . . ?
O1F C1F C9F O3F -171.7(10) . . . . ?
O1F C1F C9F C10F 65.1(13) . . . . ?
O2F C7F C8F O1F 70.1(9) . . . . ?
O3F C9F C10F C11F 59.9(19) . . . . ?
O4F C3F C4F O5F -52.5(9) . . . . ?
O4F C3F C4F C5F -169.8(8) . . . . ?
O5F C4F C5F C6F -68.4(9) . . . . ?
N1F C18F C19F O7F 76.0(9) . . . . ?
N1F C18F C19F N2F -105.9(8) . . . . ?
N1F C18F C20F C21F 177.2(7) . . . . ?
N1F C18F C20F C22F 52.2(10) . . . . ?
C1F O1F C8F C7F 31.1(9) . . . . ?
C1F C2F C3F O4F -62.4(9) . . . . ?
C1F C2F C3F C4F 177.6(6) . . . . ?
C1F C2F C7F O2F -73.8(7) . . . . ?
C1F C2F C7F C6F 167.9(7) . . . . ?
C1F C2F C7F C8F 40.7(8) . . . . ?
C1F C9F C10F C11F -174.7(15) . . . . ?
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C2F C1F C9F O3F -60.2(12) . . . . ?
C2F C1F C9F C10F 176.6(12) . . . . ?
C2F C3F C4F O5F 65.7(8) . . . . ?
C2F C3F C4F C5F -51.6(9) . . . . ?
C2F C7F C8F O1F -44.3(8) . . . . ?
C3F C2F C7F O2F 54.3(8) . . . . ?
C3F C2F C7F C6F -64.0(8) . . . . ?
C3F C2F C7F C8F 168.8(7) . . . . ?
C3F C4F C5F C6F 49.4(10) . . . . ?
C4F O5F C17F O6F 8.5(14) . . . . ?
C4F O5F C17F N1F -173.2(7) . . . . ?
C4F C5F C6F C7F -51.8(10) . . . . ?
C5F C6F C7F O2F -61.1(9) . . . . ?
C5F C6F C7F C2F 57.9(9) . . . . ?
C5F C6F C7F C8F 173.0(8) . . . . ?
C6F C7F C8F O1F -164.6(7) . . . . ?
C7F C2F C3F O4F 178.8(7) . . . . ?
C7F C2F C3F C4F 58.8(8) . . . . ?
C8F O1F C1F C2F -4.7(9) . . . . ?
C8F O1F C1F C9F 112.3(8) . . . . ?
C8F O1F C1F C15F -128.1(9) . . . . ?
C9F C1F C2F C3F 104.1(9) . . . . ?
C9F C1F C2F C7F -133.0(8) . . . . ?
C9F C10F C11F C12F 121(3) . . . . ?
C10F C11F C12F C13F 17(4) . . . . ?
C10F C11F C12F C14F 166(2) . . . . ?
C15F C1F C2F C3F -29.3(10) . . . . ?
C15F C1F C2F C7F 93.5(9) . . . . ?
C15F C1F C9F O3F 74.4(12) . . . . ?
C15F C1F C9F C10F -48.8(15) . . . . ?
C16F O4F C3F C2F 175.3(9) . . . . ?
C16F O4F C3F C4F -65.9(11) . . . . ?
C17F O5F C4F C3F 123.9(8) . . . . ?
C17F O5F C4F C5F -114.8(9) . . . . ?
C17F N1F C18F C19F 118.8(9) . . . . ?
C17F N1F C18F C20F -116.3(9) . . . . ?
C18F N1F C17F O5F 173.5(7) . . . . ?
C18F N1F C17F O6F -8.2(14) . . . . ?
C19F C18F C20F C21F -60.0(9) . . . . ?
C19F C18F C20F C22F 175.0(8) . . . . ?
C20F C18F C19F O7F -49.5(10) . . . . ?
C20F C18F C19F N2F 128.5(8) . . . . ?
O1G C1G C2G C3G -146.5(8) . . . . ?
O1G C1G C2G C7G -23.5(10) . . . . ?
O1G C1G C9G O3G -174.7(9) . . . . ?
O1G C1G C9G C10G 61.7(12) . . . . ?
O2G C7G C8G O1G 68.0(9) . . . . ?
O3G C9G C10G C11G 77.2(15) . . . . ?
O4G C3G C4G O5G -50.5(11) . . . . ?
O4G C3G C4G C5G -166.6(9) . . . . ?
O5G C4G C5G C6G -68.1(11) . . . . ?
N1G C18G C19G O7G 74.6(10) . . . . ?
N1G C18G C19G N2G -104.5(9) . . . . ?
N1G C18G C20G C21G 177.2(8) . . . . ?
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N1G C18G C20G C22G 51.1(11) . . . . ?
C1G O1G C8G C7G 32.2(9) . . . . ?
C1G C2G C3G O4G -60.2(11) . . . . ?
C1G C2G C3G C4G 176.4(8) . . . . ?
C1G C2G C7G O2G -72.3(10) . . . . ?
C1G C2G C7G C6G 167.1(9) . . . . ?
C1G C2G C7G C8G 41.4(10) . . . . ?
C1G C9G C10G C11G -157.9(12) . . . . ?
C2G C1G C9G O3G -63.0(12) . . . . ?
C2G C1G C9G C10G 173.5(10) . . . . ?
C2G C3G C4G O5G 67.4(9) . . . . ?
C2G C3G C4G C5G -48.7(11) . . . . ?
C2G C7G C8G O1G -45.8(9) . . . . ?
C3G C2G C7G O2G 57.6(10) . . . . ?
C3G C2G C7G C6G -63.1(11) . . . . ?
C3G C2G C7G C8G 171.3(8) . . . . ?
C3G C4G C5G C6G 47.9(12) . . . . ?
C4G O5G C17G O6G 4.6(14) . . . . ?
C4G O5G C17G N1G -169.6(7) . . . . ?
C4G C5G C6G C7G -51.9(11) . . . . ?
C5G C6G C7G O2G -61.8(9) . . . . ?
C5G C6G C7G C2G 58.6(11) . . . . ?
C5G C6G C7G C8G 172.4(8) . . . . ?
C6G C7G C8G O1G -166.0(7) . . . . ?
C7G C2G C3G O4G -179.8(8) . . . . ?
C7G C2G C3G C4G 56.8(11) . . . . ?
C8G O1G C1G C2G -5.3(10) . . . . ?
C8G O1G C1G C9G 110.1(9) . . . . ?
C8G O1G C1G C15G -131.5(9) . . . . ?
C9G C1G C2G C3G 103.1(11) . . . . ?
C9G C1G C2G C7G -133.9(9) . . . . ?
C9G C10G C11G C12G 140(2) . . . . ?
C10G C11G C12G C13G -173.7(17) . . . . ?
C10G C11G C12G C14G 5(3) . . . . ?
C15G C1G C2G C3G -28.2(13) . . . . ?
C15G C1G C2G C7G 94.8(10) . . . . ?
C15G C1G C9G O3G 71.3(12) . . . . ?
C15G C1G C9G C10G -52.2(14) . . . . ?
C16G O4G C3G C2G 170.3(9) . . . . ?
C16G O4G C3G C4G -68.2(12) . . . . ?
C17G O5G C4G C3G 132.6(8) . . . . ?
C17G O5G C4G C5G -108.0(9) . . . . ?
C17G N1G C18G C19G 116.1(10) . . . . ?
C17G N1G C18G C20G -117.0(10) . . . . ?
C18G N1G C17G O5G 169.5(8) . . . . ?
C18G N1G C17G O6G -5.0(14) . . . . ?
C19G C18G C20G C21G -58.2(11) . . . . ?
C19G C18G C20G C22G 175.7(8) . . . . ?
C20G C18G C19G O7G -51.5(11) . . . . ?
C20G C18G C19G N2G 129.5(9) . . . . ?
O1H C1H C2H C3H -139.2(7) . . . . ?
O1H C1H C2H C7H -15.7(7) . . . . ?
O1H C1H C9H O3H -47.8(8) . . . . ?
O1H C1H C9H C10H -172.2(7) . . . . ?
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O2H C7H C8H O1H 70.1(7) . . . . ?
O3H C9H C10H C11H 75.0(10) . . . . ?
O4H C3H C4H O5H -53.4(8) . . . . ?
O4H C3H C4H C5H -170.6(7) . . . . ?
O5H C4H C5H C6H -69.3(9) . . . . ?
N1H C18H C19H O7H 60.8(11) . . . . ?
N1H C18H C19H N2H -118.7(10) . . . . ?
N1H C18H C20H C21H -178.8(8) . . . . ?
N1H C18H C20H C22H 54.2(11) . . . . ?
C1H O1H C8H C7H 35.4(7) . . . . ?
C1H C2H C3H O4H -58.6(9) . . . . ?
C1H C2H C3H C4H 177.8(6) . . . . ?
C1H C2H C7H O2H -75.4(7) . . . . ?
C1H C2H C7H C6H 163.0(6) . . . . ?
C1H C2H C7H C8H 36.1(7) . . . . ?
C1H C9H C10H C11H -157.9(8) . . . . ?
C2H C1H C9H O3H 66.4(8) . . . . ?
C2H C1H C9H C10H -58.0(9) . . . . ?
C2H C3H C4H O5H 69.1(7) . . . . ?
C2H C3H C4H C5H -48.1(9) . . . . ?
C2H C7H C8H O1H -43.5(7) . . . . ?
C3H C2H C7H O2H 55.0(7) . . . . ?
C3H C2H C7H C6H -66.5(8) . . . . ?
C3H C2H C7H C8H 166.5(6) . . . . ?
C3H C4H C5H C6H 45.9(10) . . . . ?
C4H O5H C17H O6H 19.8(14) . . . . ?
C4H O5H C17H N1H -161.1(7) . . . . ?
C4H C5H C6H C7H -50.4(10) . . . . ?
C5H C6H C7H O2H -59.4(9) . . . . ?
C5H C6H C7H C2H 61.4(9) . . . . ?
C5H C6H C7H C8H 177.6(7) . . . . ?
C6H C7H C8H O1H -165.1(7) . . . . ?
C7H C2H C3H O4H -179.8(6) . . . . ?
C7H C2H C3H C4H 56.6(8) . . . . ?
C8H O1H C1H C2H -12.2(7) . . . . ?
C8H O1H C1H C9H 110.1(6) . . . . ?
C8H O1H C1H C15H -132.2(7) . . . . ?
C9H C1H C2H C3H 106.4(8) . . . . ?
C9H C1H C2H C7H -130.1(6) . . . . ?
C9H C10H C11H C12H 123.6(17) . . . . ?
C10H C11H C12H C13H 13(3) . . . . ?
C10H C11H C12H C14H -179.9(14) . . . . ?
C15H C1H C2H C3H -23.8(10) . . . . ?
C15H C1H C2H C7H 99.8(8) . . . . ?
C15H C1H C9H O3H -162.5(7) . . . . ?
C15H C1H C9H C10H 73.2(9) . . . . ?
C16H O4H C3H C2H 159.7(8) . . . . ?
C16H O4H C3H C4H -78.5(10) . . . . ?
C17H O5H C4H C3H 99.5(8) . . . . ?
C17H O5H C4H C5H -137.7(8) . . . . ?
C17H N1H C18H C19H 111.4(10) . . . . ?
C17H N1H C18H C20H -126.5(10) . . . . ?
C18H N1H C17H O5H -179.7(7) . . . . ?
C18H N1H C17H O6H -0.7(16) . . . . ?
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C19H C18H C20H C21H -58.7(10) . . . . ?
C19H C18H C20H C22H 174.3(8) . . . . ?
C20H C18H C19H O7H -63.0(11) . . . . ?
C20H C18H C19H N2H 117.5(10) . . . . ?
O1I C1I C2I C3I -154.3(8) . . . . ?
O1I C1I C2I C7I -27.3(8) . . . . ?
O1I C1I C9I O3I -67.9(9) . . . . ?
O1I C1I C9I C10I 167.0(8) . . . . ?
O2I C7I C8I O1I 74.0(10) . . . . ?
O3I C9I C10I C11I 69.1(13) . . . . ?
O4I C3I C4I O5I -57.3(10) . . . . ?
O4I C3I C4I C5I -175.5(8) . . . . ?
O5I C4I C5I C6I -65.2(11) . . . . ?
N1I C18I C19I O7I 61.5(11) . . . . ?
N1I C18I C19I N2I -119.5(9) . . . . ?
N1I C18I C20I C21I -179.7(8) . . . . ?
N1I C18I C20I C22I 58.5(10) . . . . ?
C1I O1I C8I C7I 21.5(10) . . . . ?
C1I C2I C3I O4I -55.0(10) . . . . ?
C1I C2I C3I C4I 176.7(7) . . . . ?
C1I C2I C7I O2I -74.0(8) . . . . ?
C1I C2I C7I C6I 167.2(8) . . . . ?
C1I C2I C7I C8I 39.9(8) . . . . ?
C1I C9I C10I C11I -165.1(10) . . . . ?
C2I C1I C9I O3I 42.4(10) . . . . ?
C2I C1I C9I C10I -82.7(10) . . . . ?
C2I C3I C4I O5I 66.1(8) . . . . ?
C2I C3I C4I C5I -52.0(10) . . . . ?
C2I C7I C8I O1I -37.3(9) . . . . ?
C3I C2I C7I O2I 60.0(9) . . . . ?
C3I C2I C7I C6I -58.7(10) . . . . ?
C3I C2I C7I C8I 173.9(8) . . . . ?
C3I C4I C5I C6I 52.7(12) . . . . ?
C4I O5I C17I O6I 22.5(14) . . . . ?
C4I O5I C17I N1I -160.4(8) . . . . ?
C4I C5I C6I C7I -54.5(12) . . . . ?
C5I C6I C7I O2I -57.9(10) . . . . ?
C5I C6I C7I C2I 59.1(10) . . . . ?
C5I C6I C7I C8I 176.3(8) . . . . ?
C6I C7I C8I O1I -160.3(9) . . . . ?
C7I C2I C3I O4I -178.8(7) . . . . ?
C7I C2I C3I C4I 52.9(9) . . . . ?
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;

The solvent masking procedure as implemented in Olex2 was used to remove
the
electronic contribution of solvent molecules from the refinement.  Only
the
atoms used in the refinement model are reported in the formula here.

Total solvent accessible volume / cell = 1359.2 Ang^3^ [16.8%]
Total electron count / cell = 323.9

;
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_vrf_THETM01_38593
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: Despite long exposure times, no significant intensity was
observed
beyond approximately 1.0 Ang. resolution.
;
_vrf_PLAT023_38593
;
PROBLEM: Resolution (too) Low [sin(theta)/Lambda < 0.6]..      50.51 Deg.
RESPONSE: Despite long exposure times, no significant intensity was
observed
beyond approximately 1.0 Ang. resolution.
;
_vrf_PLAT213_38593
;
PROBLEM: Atom O48#            has ADP max/min Ratio .....        8.0 prola
RESPONSE: Indicative of disorder that was not modeled by splitting atomic
positions.
;
_vrf_PLAT414_38593
;
PROBLEM: Short Intra D-H..H-X       H3OB   ..  H2B     ..       1.66 Ang.
RESPONSE: All hydrogen atoms were refined with riding models.  Due to the
poor
quality of data, these short H-H distances should be considered with care.
;
_vrf_PLAT417_38593
;
```

```
PROBLEM: Short Inter D-H..H-D       H3E    ..  H3OH    ..       1.60 Ang.
RESPONSE: All hydrogen atoms were refined with riding models.  Due to the
poor
quality of data, these short H-H distances should be considered with care.
;
_vrf_PLAT602_38593
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure        !
RESPONSE: The solvent-masking procedure in Olex2 was used to remove
electronic
contributions from disordered solvent molecules.
;
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CIF File for Compound **5**

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2-methyl-propyl]carbamate

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wR2(int) was 0.0627 before and 0.0472 after correction.
The Ratio of minimum to maximum transmission is 0.9202.
The \l/2 correction factor is 0.0015.
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O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H.
Puschmann,
OLEX2: a complete structure solution, refinement and analysis program.
J. Appl. Cryst. (2009). 42, 339-341.
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O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H.
Puschmann,
OLEX2: a complete structure solution, refinement and analysis program.
J. Appl. Cryst. (2009). 42, 339-341.
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XL, G.M. Sheldrick, Acta Cryst.
(2008). A64, 112-122
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(2008). A64, 112-122
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 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.
 Coordinates and displacement parameters for the Hydrogen atoms on N2A
were
 freely refined, but the N-H distances subjected to similarity restraints
 (SADI).

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 H3 H 0.332(3) 0.5888(14) 0.2258(11) 0.063(9) Uiso 1 1 d . . .
 O4 O 0.26752(15) 0.58001(8) 0.42165(5) 0.0421(4) Uani 1 1 d . . .
 O5 O 0.36939(12) 0.44800(8) 0.42549(5) 0.0350(3) Uani 1 1 d . . .
 O6 O 0.37996(14) 0.47595(8) 0.50691(5) 0.0446(4) Uani 1 1 d . . .
 O7 O 0.79057(15) 0.40055(9) 0.47206(5) 0.0471(4) Uani 1 1 d . . .
 N1 N 0.55317(16) 0.46200(10) 0.46017(6) 0.0363(4) Uani 1 1 d . . .
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H1 H 0.5825(19) 0.4563(10) 0.4328(8) 0.026(5) Uiso 1 1 d . . .
N2 N 0.76542(19) 0.41653(11) 0.55356(7) 0.0402(4) Uani 1 1 d . . .
H2B H 0.731(2) 0.4364(11) 0.5724(9) 0.032(7) Uiso 1 1 d . . .
H2C H 0.818(2) 0.3843(11) 0.5564(7) 0.025(5) Uiso 1 1 d . . .
C1 C 0.18367(17) 0.58054(11) 0.31209(7) 0.0314(4) Uani 1 1 d . . .
C2 C 0.24956(17) 0.52582(10) 0.34426(6) 0.0278(4) Uani 1 1 d . . .
H2D H 0.3408 0.5348 0.3435 0.033 Uiso 1 1 calc R . .
C3 C 0.20705(18) 0.52415(11) 0.39874(7) 0.0351(5) Uani 1 1 d . . .
H3B H 0.1155 0.5320 0.3999 0.042 Uiso 1 1 calc R . .
C4 C 0.23551(18) 0.45747(11) 0.42425(7) 0.0361(5) Uani 1 1 d . . .
H4 H 0.2028 0.4588 0.4588 0.043 Uiso 1 1 calc R . .
C5 C 0.17802(19) 0.39883(12) 0.39707(7) 0.0385(5) Uani 1 1 d . . .
H5A H 0.0871 0.4051 0.3953 0.046 Uiso 1 1 calc R . .
H5B H 0.1948 0.3563 0.4152 0.046 Uiso 1 1 calc R . .
C6 C 0.23109(19) 0.39374(11) 0.34474(7) 0.0354(5) Uani 1 1 d . . .
H6A H 0.3189 0.3794 0.3469 0.042 Uiso 1 1 calc R . .
H6B H 0.1854 0.3582 0.3265 0.042 Uiso 1 1 calc R . .
C7 C 0.22418(17) 0.45940(11) 0.31540(7) 0.0313(4) Uani 1 1 d . . .
C8 C 0.09919(18) 0.47499(11) 0.29304(7) 0.0338(4) Uani 1 1 d . . .
H8A H 0.0801 0.4436 0.2655 0.041 Uiso 1 1 calc R . .
H8B H 0.0327 0.4719 0.3182 0.041 Uiso 1 1 calc R . .
C9 C 0.09055(18) 0.62653(11) 0.33895(7) 0.0346(5) Uani 1 1 d . . .
H9A H 0.0597 0.6610 0.3160 0.052 Uiso 1 1 calc R . .
H9B H 0.1316 0.6486 0.3669 0.052 Uiso 1 1 calc R . .
H9C H 0.0210 0.5993 0.3510 0.052 Uiso 1 1 calc R . .
C10 C 0.27522(17) 0.62490(10) 0.28253(7) 0.0308(4) Uani 1 1 d . . .
H10 H 0.2260 0.6535 0.2591 0.037 Uiso 1 1 calc R . .
C11 C 0.35141(18) 0.67208(11) 0.31529(8) 0.0371(5) Uani 1 1 d . . .
H11C H 0.2948 0.7040 0.3322 0.045 Uiso 1 1 calc R . .
H11D H 0.3938 0.6450 0.3410 0.045 Uiso 1 1 calc R . .
C12 C 0.44645(19) 0.71160(10) 0.28689(8) 0.0363(5) Uani 1 1 d . . .
H12 H 0.4385 0.7125 0.2519 0.044 Uiso 1 1 calc R . .
C13 C 0.54099(19) 0.74554(10) 0.30660(8) 0.0391(5) Uani 1 1 d . . .
C14 C 0.6312(2) 0.78395(12) 0.27481(10) 0.0495(6) Uani 1 1 d . . .
H14D H 0.6118 0.7761 0.2399 0.074 Uiso 1 1 calc R . .
H14E H 0.7157 0.7683 0.2817 0.074 Uiso 1 1 calc R . .
H14F H 0.6249 0.8324 0.2821 0.074 Uiso 1 1 calc R . .
C15 C 0.5658(2) 0.74736(13) 0.36152(9) 0.0543(6) Uani 1 1 d . . .
H15D H 0.5448 0.7922 0.3745 0.081 Uiso 1 1 calc R . .
H15E H 0.6537 0.7381 0.3676 0.081 Uiso 1 1 calc R . .
H15F H 0.5151 0.7130 0.3780 0.081 Uiso 1 1 calc R . .
C16 C 0.2062(3) 0.60319(15) 0.46531(8) 0.0606(7) Uani 1 1 d . . .
H16D H 0.1205 0.6154 0.4573 0.091 Uiso 1 1 calc R . .
H16E H 0.2497 0.6429 0.4784 0.091 Uiso 1 1 calc R . .
H16F H 0.2065 0.5671 0.4902 0.091 Uiso 1 1 calc R . .
C17 C 0.43182(19) 0.46415(11) 0.46739(7) 0.0347(5) Uani 1 1 d . . .
C18 C 0.64203(19) 0.48467(11) 0.49727(7) 0.0350(5) Uani 1 1 d . . .
H18 H 0.5962 0.4931 0.5288 0.042 Uiso 1 1 calc R . .
C19 C 0.73673(19) 0.42995(11) 0.50648(7) 0.0347(5) Uani 1 1 d . . .
C20 C 0.7031(2) 0.55138(13) 0.48099(8) 0.0447(5) Uani 1 1 d . . .
H20 H 0.7384 0.5443 0.4472 0.054 Uiso 1 1 calc R . .
C21 C 0.6072(3) 0.60798(14) 0.47750(10) 0.0651(8) Uani 1 1 d . . .
H21D H 0.5780 0.6196 0.5107 0.098 Uiso 1 1 calc R . .
H21E H 0.5371 0.5928 0.4573 0.098 Uiso 1 1 calc R . .
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H21F H 0.6451 0.6479 0.4622 0.098 Uiso 1 1 calc R . .
C22 C 0.8095(3) 0.57129(15) 0.51518(9) 0.0605(7) Uani 1 1 d . . .
H22D H 0.7773 0.5792 0.5486 0.091 Uiso 1 1 calc R . .
H22E H 0.8487 0.6127 0.5028 0.091 Uiso 1 1 calc R . .
H22F H 0.8708 0.5347 0.5161 0.091 Uiso 1 1 calc R . .
O1A O 0.88798(11) 0.54285(7) 0.85609(4) 0.0291(3) Uani 1 1 d . . .
O2A O 0.68510(12) 0.45343(8) 0.85254(5) 0.0318(3) Uani 1 1 d . . .
H2A H 0.661(2) 0.4915(12) 0.8679(8) 0.038(6) Uiso 1 1 d . . .
O3A O 0.64386(12) 0.58352(7) 0.87849(5) 0.0335(3) Uani 1 1 d . . .
H3A H 0.657(2) 0.5863(13) 0.9086(10) 0.049(7) Uiso 1 1 d . . .
O4A O 0.73205(14) 0.58985(8) 0.71159(5) 0.0399(3) Uani 1 1 d . . .
O5A O 0.62801(11) 0.45831(7) 0.70477(4) 0.0331(3) Uani 1 1 d . . .
O6A O 0.61223(12) 0.48754(7) 0.62356(5) 0.0344(3) Uani 1 1 d . . .
O7A O 0.20904(15) 0.39260(10) 0.66033(5) 0.0566(5) Uani 1 1 d . . .
N1A N 0.44311(15) 0.46416(9) 0.67056(6) 0.0324(4) Uani 1 1 d . . .
H1A H 0.420(2) 0.4542(11) 0.7001(9) 0.039(6) Uiso 1 1 d . . .
N2A N 0.2564(3) 0.39583(19) 0.58038(8) 0.1030(14) Uani 1 1 d D . .
H2AA H 0.210(3) 0.3611(13) 0.5749(11) 0.076(10) Uiso 1 1 d D . .
H2AB H 0.275(4) 0.4200(18) 0.5556(12) 0.116(14) Uiso 1 1 d D . .
C1A C 0.81741(16) 0.58365(10) 0.82087(7) 0.0268(4) Uani 1 1 d . . .
C2A C 0.75024(16) 0.53067(10) 0.78714(6) 0.0261(4) Uani 1 1 d . . .
H2AC H 0.6593 0.5404 0.7884 0.031 Uiso 1 1 calc R . .
C3A C 0.79128(17) 0.53322(10) 0.73242(6) 0.0312(4) Uani 1 1 d . . .
H3AA H 0.8829 0.5408 0.7313 0.037 Uiso 1 1 calc R . .
C4A C 0.76160(18) 0.46786(11) 0.70475(7) 0.0371(5) Uani 1 1 d . . .
H4A H 0.7925 0.4710 0.6700 0.044 Uiso 1 1 calc R . .
C5A C 0.81867(19) 0.40755(11) 0.73000(8) 0.0377(5) Uani 1 1 d . . .
H5AA H 0.9096 0.4138 0.7323 0.045 Uiso 1 1 calc R . .
H5AB H 0.8025 0.3663 0.7102 0.045 Uiso 1 1 calc R . .
C6A C 0.76454(18) 0.39883(10) 0.78176(7) 0.0355(5) Uani 1 1 d . . .
H6AA H 0.8091 0.3617 0.7987 0.043 Uiso 1 1 calc R . .
H6AB H 0.6765 0.3853 0.7788 0.043 Uiso 1 1 calc R . .
C7A C 0.77273(16) 0.46263(10) 0.81349(7) 0.0291(4) Uani 1 1 d . . .
C8A C 0.89885(17) 0.47612(10) 0.83596(7) 0.0309(4) Uani 1 1 d . . .
H8AA H 0.9180 0.4428 0.8622 0.037 Uiso 1 1 calc R . .
H8AB H 0.9646 0.4743 0.8105 0.037 Uiso 1 1 calc R . .
C9A C 0.91115(18) 0.62936(10) 0.79536(7) 0.0329(4) Uani 1 1 d . . .
H9AA H 0.9396 0.6641 0.8186 0.049 Uiso 1 1 calc R . .
H9AB H 0.8722 0.6511 0.7667 0.049 Uiso 1 1 calc R . .
H9AC H 0.9821 0.6023 0.7843 0.049 Uiso 1 1 calc R . .
C10A C 0.72936(18) 0.62609(10) 0.85250(7) 0.0312(4) Uani 1 1 d . . .
H10A H 0.7799 0.6513 0.8774 0.037 Uiso 1 1 calc R . .
C11A C 0.6544(2) 0.67786(12) 0.82251(7) 0.0396(5) Uani 1 1 d . . .
H11A H 0.7121 0.7093 0.8057 0.048 Uiso 1 1 calc R . .
H11B H 0.6063 0.6539 0.7967 0.048 Uiso 1 1 calc R . .
C12A C 0.5673(2) 0.71769(11) 0.85446(8) 0.0424(5) Uani 1 1 d . . .
H12A H 0.5733 0.7111 0.8892 0.051 Uiso 1 1 calc R . .
C13A C 0.48290(19) 0.76117(11) 0.83871(8) 0.0382(5) Uani 1 1 d . . .
C14A C 0.3991(3) 0.79720(14) 0.87457(11) 0.0672(8) Uani 1 1 d . . .
H14A H 0.4146 0.8460 0.8729 0.101 Uiso 1 1 calc R . .
H14B H 0.4157 0.7810 0.9082 0.101 Uiso 1 1 calc R . .
H14C H 0.3124 0.7881 0.8660 0.101 Uiso 1 1 calc R . .
C15A C 0.4651(2) 0.77800(14) 0.78603(9) 0.0556(7) Uani 1 1 d . . .
H15A H 0.3807 0.7659 0.7760 0.083 Uiso 1 1 calc R . .
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 H15B H 0.5249 0.7526 0.7660 0.083 Uiso 1 1 calc R . .
 H15C H 0.4780 0.8266 0.7811 0.083 Uiso 1 1 calc R . .
 C16A C 0.7902(3) 0.61580(13) 0.66828(8) 0.0525(6) Uani 1 1 d . . .
 H16A H 0.7858 0.5820 0.6419 0.079 Uiso 1 1 calc R . .
 H16B H 0.8772 0.6261 0.6755 0.079 Uiso 1 1 calc R . .
 H16C H 0.7476 0.6571 0.6577 0.079 Uiso 1 1 calc R . .
 C17A C 0.56518(18) 0.47209(10) 0.66312(7) 0.0302(4) Uani 1 1 d . . .
 C18A C 0.35153(18) 0.47893(11) 0.63247(7) 0.0345(5) Uani 1 1 d . . .
 H18A H 0.3962 0.4872 0.6006 0.041 Uiso 1 1 calc R . .
 C19A C 0.2673(2) 0.41808(13) 0.62578(7) 0.0453(6) Uani 1 1 d . . .
 C20A C 0.2779(2) 0.54300(14) 0.64568(8) 0.0549(7) Uani 1 1 d . . .
 H20A H 0.2451 0.5376 0.6800 0.066 Uiso 1 1 calc R . .
 C21A C 0.3626(4) 0.60436(14) 0.64490(11) 0.0794(10) Uani 1 1 d . . .
 H21A H 0.4334 0.5964 0.6668 0.119 Uiso 1 1 calc R . .
 H21B H 0.3166 0.6442 0.6563 0.119 Uiso 1 1 calc R . .
 H21C H 0.3923 0.6120 0.6111 0.119 Uiso 1 1 calc R . .
 C22A C 0.1666(3) 0.5515(2) 0.61039(10) 0.0907(13) Uani 1 1 d . . .
 H22A H 0.1967 0.5552 0.5763 0.136 Uiso 1 1 calc R . .
 H22B H 0.1207 0.5926 0.6192 0.136 Uiso 1 1 calc R . .
 H22C H 0.1118 0.5121 0.6133 0.136 Uiso 1 1 calc R . .

loop_
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  _atom_site_aniso_U_13
  _atom_site_aniso_U_12
 O1 0.0236(6) 0.0448(8) 0.0259(6) 0.0005(6) -0.0045(5) -0.0028(6)
 O2 0.0308(7) 0.0423(8) 0.0240(7) -0.0035(6) 0.0041(5) -0.0010(6)
 O3 0.0245(7) 0.0459(9) 0.0266(7) -0.0013(6) -0.0014(6) -0.0049(6)
 O4 0.0502(9) 0.0523(9) 0.0238(7) -0.0071(6) -0.0042(7) 0.0018(8)
 O5 0.0272(7) 0.0561(9) 0.0218(6) 0.0017(6) -0.0009(5) 0.0018(6)
 O6 0.0396(8) 0.0736(11) 0.0207(7) -0.0009(7) 0.0057(6) -0.0026(8)
 O7 0.0518(9) 0.0630(11) 0.0264(7) -0.0033(7) 0.0058(7) 0.0180(8)
 N1 0.0344(9) 0.0550(12) 0.0194(8) -0.0016(8) -0.0002(7) 0.0009(8)
 N2 0.0426(11) 0.0529(12) 0.0250(10) 0.0006(9) 0.0023(9) 0.0124(10)
 C1 0.0246(9) 0.0444(12) 0.0253(10) -0.0004(9) -0.0032(8) 0.0008(9)
 C2 0.0198(8) 0.0397(11) 0.0238(9) 0.0009(8) 0.0016(7) -0.0015(8)
 C3 0.0282(10) 0.0520(13) 0.0250(10) -0.0038(9) -0.0012(8) 0.0030(9)
 C4 0.0299(10) 0.0556(13) 0.0229(9) 0.0044(9) 0.0029(8) 0.0018(10)
 C5 0.0316(10) 0.0514(14) 0.0325(11) 0.0083(9) -0.0026(9) -0.0018(10)
 C6 0.0306(10) 0.0440(12) 0.0314(10) 0.0032(9) -0.0018(8) -0.0057(9)
 C7 0.0237(9) 0.0453(12) 0.0250(9) -0.0033(9) 0.0000(7) -0.0021(9)
 C8 0.0277(9) 0.0472(12) 0.0265(9) -0.0027(9) -0.0031(8) -0.0069(9)
 C9 0.0257(9) 0.0489(12) 0.0293(10) -0.0045(9) -0.0002(8) 0.0012(9)
 C10 0.0238(9) 0.0395(11) 0.0292(10) 0.0036(8) -0.0026(8) 0.0025(8)
 C11 0.0306(10) 0.0436(12) 0.0372(11) 0.0028(9) -0.0041(9) -0.0048(9)
 C12 0.0353(10) 0.0357(11) 0.0380(11) 0.0086(9) -0.0023(9) 0.0047(9)
 C13 0.0310(10) 0.0342(12) 0.0521(13) 0.0061(10) -0.0057(10) 0.0017(9)
 C14 0.0315(11) 0.0425(13) 0.0745(16) 0.0137(12) -0.0052(11) -0.0008(10)
 C15 0.0545(14) 0.0512(15) 0.0573(15) 0.0029(12) -0.0150(12) -0.0089(12)
 C16 0.0787(19) 0.0691(18) 0.0341(12) -0.0142(12) 0.0042(12) 0.0125(15)
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 C17 0.0381(11) 0.0466(12) 0.0194(9) 0.0007(9) -0.0014(8) 0.0044(10)
 C18 0.0364(10) 0.0483(12) 0.0205(9) -0.0026(9) -0.0021(8) 0.0016(9)
 C19 0.0357(10) 0.0445(12) 0.0239(10) 0.0011(8) 0.0017(9) -0.0003(9)
 C20 0.0491(13) 0.0553(15) 0.0296(10) -0.0017(10) -0.0022(10) -0.0051(12)
 C21 0.098(2) 0.0476(15) 0.0502(14) -0.0073(12) -0.0025(15) -0.0068(15)
 C22 0.0647(16) 0.0701(18) 0.0467(14) 0.0036(12) -0.0112(13) -0.0251(14)
 O1A 0.0250(6) 0.0369(7) 0.0253(6) 0.0028(6) -0.0039(5) 0.0013(6)
 O2A 0.0265(6) 0.0427(9) 0.0262(7) 0.0045(6) 0.0021(5) -0.0001(6)
 O3A 0.0277(7) 0.0486(9) 0.0242(7) -0.0005(6) -0.0005(6) 0.0001(6)
 O4A 0.0424(8) 0.0510(9) 0.0264(7) 0.0074(6) -0.0046(6) -0.0040(7)
 O5A 0.0255(6) 0.0510(8) 0.0227(6) -0.0038(6) -0.0012(5) -0.0065(6)
 O6A 0.0328(7) 0.0476(8) 0.0229(7) -0.0005(6) 0.0020(6) -0.0051(6)
 O7A 0.0469(9) 0.0916(13) 0.0314(8) -0.0052(8) 0.0061(7) -0.0238(9)
 N1A 0.0261(8) 0.0509(11) 0.0203(8) -0.0003(7) 0.0010(7) -0.0015(8)
 N2A 0.132(3) 0.152(3) 0.0255(12) -0.0139(14) 0.0097(14) -0.103(3)
 C1A 0.0214(9) 0.0365(11) 0.0224(9) 0.0033(8) -0.0058(7) 0.0030(8)
 C2A 0.0183(8) 0.0381(11) 0.0220(9) 0.0007(8) -0.0009(7) 0.0017(8)
 C3A 0.0264(9) 0.0444(12) 0.0228(9) 0.0021(8) 0.0024(7) -0.0040(9)
 C4A 0.0253(9) 0.0586(14) 0.0273(10) -0.0063(9) 0.0058(8) -0.0052(10)
 C5A 0.0316(10) 0.0450(13) 0.0365(11) -0.0115(10) -0.0049(9) 0.0004(9)
 C6A 0.0279(10) 0.0381(11) 0.0405(11) -0.0048(9) -0.0038(9) -0.0020(9)
 C7A 0.0216(9) 0.0402(11) 0.0255(9) -0.0024(8) -0.0008(7) 0.0010(8)
 C8A 0.0244(9) 0.0388(11) 0.0295(10) 0.0021(8) -0.0014(8) 0.0006(8)
 C9A 0.0303(10) 0.0380(11) 0.0304(10) -0.0007(8) -0.0006(8) -0.0060(8)
 C10A 0.0316(10) 0.0408(11) 0.0213(9) -0.0019(8) -0.0015(8) -0.0010(9)
 C11A 0.0422(12) 0.0492(13) 0.0274(10) 0.0017(9) 0.0032(9) 0.0150(10)
 C12A 0.0524(13) 0.0434(13) 0.0314(11) 0.0043(9) 0.0085(10) 0.0110(11)
 C13A 0.0326(10) 0.0357(11) 0.0464(12) 0.0065(9) 0.0100(10) 0.0045(9)
 C14A 0.0689(17) 0.0474(15) 0.085(2) 0.0169(14) 0.0362(16) 0.0214(13)
 C15A 0.0487(14) 0.0623(16) 0.0559(15) 0.0053(12) -0.0006(12) 0.0271(12)
 C16A 0.0677(16) 0.0643(16) 0.0256(11) 0.0087(10) -0.0010(11) -0.0229(13)
 C17A 0.0315(10) 0.0351(11) 0.0241(10) -0.0067(8) 0.0038(8) -0.0037(8)
 C18A 0.0318(10) 0.0543(13) 0.0175(9) 0.0022(9) 0.0024(8) 0.0032(9)
 C19A 0.0376(11) 0.0738(16) 0.0243(11) 0.0038(10) -0.0010(9) -0.0106(11)
 C20A 0.0587(15) 0.0745(18) 0.0314(11) 0.0070(12) 0.0073(11) 0.0261(14)
 C21A 0.121(3) 0.0470(16) 0.0697(19) 0.0049(14) 0.0267(19) 0.0115(18)
 C22A 0.077(2) 0.149(3) 0.0455(16) 0.0101(18) -0.0039(15) 0.060(2)

_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.
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O1 C1 1.454(2) . ?
O1 C8 1.431(2) . ?
O2 H2 0.93(3) . ?
O2 C7 1.437(2) . ?
O3 H3 0.82(3) . ?
O3 C10 1.422(2) . ?
O4 C3 1.424(3) . ?
O4 C16 1.429(3) . ?
O5 C4 1.456(2) . ?
O5 C17 1.356(2) . ?
O6 C17 1.229(2) . ?
O7 C19 1.242(2) . ?
N1 H1 0.81(2) . ?
N1 C17 1.324(3) . ?
N1 C18 1.458(3) . ?
N2 H2B 0.74(2) . ?
N2 H2C 0.86(2) . ?
N2 C19 1.337(3) . ?
C1 C2 1.559(3) . ?
C1 C9 1.537(3) . ?
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C15 H15E 0.9800 . ?
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C6A H6AB 0.9900 . ?
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C8A H8AB 0.9900 . ?
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 C17 O5 C4 118.76(15) . . ?
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 C17 N1 C18 122.58(17) . . ?
 C18 N1 H1 114.4(15) . . ?
 H2B N2 H2C 132(2) . . ?
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 C19 N2 H2C 112.7(14) . . ?
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O5 C4 H4 109.4 . . ?
O5 C4 C5 108.71(17) . . ?
C3 C4 H4 109.4 . . ?
C5 C4 C3 111.24(16) . . ?
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C4 C5 H5B 109.6 . . ?
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C5 C6 H6B 108.7 . . ?
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H15D C15 H15F 109.5 . . ?
H15E C15 H15F 109.5 . . ?
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O4 C16 H16F 109.5 . . ?
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H16D C16 H16F 109.5 . . ?
H16E C16 H16F 109.5 . . ?
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O6 C17 N1 125.76(18) . . ?
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N1 C18 C20 110.36(16) . . ?
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O7 C19 C18 121.90(17) . . ?
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C20 C21 H21E 109.5 . . ?
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C17A N1A C18A 122.42(17) . . ?
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H15B C15A H15C 109.5 . . ?
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O4A C16A H16C 109.5 . . ?
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 N1 H1 O1A 0.81(2) 2.10(2) 2.888(2) 163(2) 2_664
 N2 H2B O6A 0.74(2) 2.14(2) 2.878(3) 173(2) .
 O2A H2A O3A 0.90(2) 1.85(2) 2.701(2) 158(2) .
 O3A H3A O7 0.83(3) 1.83(3) 2.6470(19) 170(3) 2_665
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O2 C7 C8 O1 -71.78(19) . . . . ?
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O4 C3 C4 O5 -56.1(2) . . . . ?
O4 C3 C4 C5 -175.84(16) . . . . ?
O5 C4 C5 C6 -58.1(2) . . . . ?
N1 C18 C19 O7 48.3(3) . . . . ?
N1 C18 C19 N2 -135.0(2) . . . . ?
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C18 N1 C17 O6 -10.5(4) . . . . ?
C19 C18 C20 C21 -173.66(18) . . . . ?
C19 C18 C20 C22 -49.3(3) . . . . ?
C20 C18 C19 O7 -74.5(3) . . . . ?
C20 C18 C19 N2 102.2(2) . . . . ?
O1A C1A C2A C3A -116.23(16) . . . . ?
O1A C1A C2A C7A 9.90(17) . . . . ?
O1A C1A C10A O3A -63.68(18) . . . . ?
O1A C1A C10A C11A 174.63(16) . . . . ?
O2A C7A C8A O1A -71.26(18) . . . . ?
O3A C10A C11A C12A 55.8(2) . . . . ?
O4A C3A C4A O5A -57.7(2) . . . . ?
O4A C3A C4A C5A -175.89(15) . . . . ?
O5A C4A C5A C6A -56.0(2) . . . . ?
N1A C18A C19A O7A 55.5(3) . . . . ?
N1A C18A C19A N2A -127.1(3) . . . . ?
N1A C18A C20A C21A 65.9(2) . . . . ?
N1A C18A C20A C22A -170.1(2) . . . . ?
C1A O1A C8A C7A -40.27(17) . . . . ?
C1A C2A C3A O4A -76.76(18) . . . . ?
C1A C2A C3A C4A 159.85(15) . . . . ?
C1A C2A C7A O2A 82.19(16) . . . . ?
C1A C2A C7A C6A -156.93(15) . . . . ?
C1A C2A C7A C8A -32.16(16) . . . . ?
C1A C10A C11A C12A 178.92(18) . . . . ?
C2A C1A C10A O3A 50.24(19) . . . . ?
C2A C1A C10A C11A -71.4(2) . . . . ?
C2A C3A C4A O5A 62.1(2) . . . . ?
C2A C3A C4A C5A -56.0(2) . . . . ?
C2A C7A C8A O1A 44.42(16) . . . . ?
C3A C2A C7A O2A -152.59(15) . . . . ?
C3A C2A C7A C6A -31.7(2) . . . . ?
C3A C2A C7A C8A 93.06(17) . . . . ?
C3A C4A C5A C6A 62.7(2) . . . . ?
C4A O5A C17A O6A 5.6(3) . . . . ?
C4A O5A C17A N1A -176.55(17) . . . . ?
C4A C5A C6A C7A -53.2(2) . . . . ?
C5A C6A C7A O2A 161.49(16) . . . . ?
C5A C6A C7A C2A 38.2(2) . . . . ?
C5A C6A C7A C8A -78.6(2) . . . . ?
C6A C7A C8A O1A 170.42(16) . . . . ?
C7A C2A C3A O4A 163.31(14) . . . . ?
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 C7A C2A C3A C4A 39.9(2) . . . . ?
 C8A O1A C1A C2A 18.30(17) . . . . ?
 C8A O1A C1A C9A -104.94(16) . . . . ?
 C8A O1A C1A C10A 138.59(15) . . . . ?
 C9A C1A C2A C3A 0.3(2) . . . . ?
 C9A C1A C2A C7A 126.41(16) . . . . ?
 C9A C1A C10A O3A -177.47(14) . . . . ?
 C9A C1A C10A C11A 60.8(2) . . . . ?
 C10A C1A C2A C3A 129.53(17) . . . . ?
 C10A C1A C2A C7A -104.35(17) . . . . ?
 C10A C11A C12A C13A -173.2(2) . . . . ?
 C11A C12A C13A C14A 178.9(2) . . . . ?
 C11A C12A C13A C15A -1.7(4) . . . . ?
 C16A O4A C3A C2A 157.93(16) . . . . ?
 C16A O4A C3A C4A -78.7(2) . . . . ?
 C17A O5A C4A C3A 103.52(19) . . . . ?
 C17A O5A C4A C5A -136.06(17) . . . . ?
 C17A N1A C18A C19A 127.5(2) . . . . ?
 C17A N1A C18A C20A -109.0(2) . . . . ?
 C18A N1A C17A O5A 176.86(17) . . . . ?
 C18A N1A C17A O6A -5.3(3) . . . . ?
 C19A C18A C20A C21A -172.0(2) . . . . ?
 C19A C18A C20A C22A -48.0(3) . . . . ?
 C20A C18A C19A O7A -67.3(3) . . . . ?
 C20A C18A C19A N2A 110.1(3) . . . . ?


loop_
  _smtbx_masks_void_nr
  _smtbx_masks_void_average_x
  _smtbx_masks_void_average_y
  _smtbx_masks_void_average_z
  _smtbx_masks_void_volume
  _smtbx_masks_void_count_electrons
  _smtbx_masks_void_content
 1 -0.281 -0.250 0.000 378.4 128.1 ?
 2 0.192 0.250 0.000 334.7 21.3 ?
 3 -0.727 0.250 0.500 378.4 128.1 ?
 4 0.321 0.750 0.500 334.7 21.3 ?

_local_nu_authors                 'Dr. Amy A. Sarjeant'
_local_nu_crystal_method          'slow evaporation'
_local_nu_crystal_solvent         tetrahydrofuran
_local_nu_labbook_chem            N23696-3-B1
_local_nu_labbook_crystalization  NUGSK01_040
_local_nu_labbook_xray            NUGSK01_040
_local_nu_project_code            '16841, 17768'
_local_nu_project_name            unknown
_local_nu_quality_factor          2
_local_nu_refine_ls_disord_occ    'freely refined'
_local_nu_refine_ls_disord_u      'freely refined, with restraints'
_local_nu_refine_ls_disord_xyz    'freely refined with distance
restraints'
_local_nu_refine_ls_h_carbon_u    riding
```

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_local_nu_refine_ls_h_carbon_xyz  riding
_local_nu_refine_ls_h_hetero_u    'freely refined'
_local_nu_refine_ls_h_hetero_xyz  'freely refined'
_local_nu_refine_ls_nonh_u        anisotropic
_local_nu_refine_ls_nonh_xyz      'freely refined'
_local_nunumber                   GSK2974844A
_local_xraynumber                 38592


_vrf_PLAT601_38592
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of .        339 A**3
RESPONSE: The solvent-masking procedure in Olex2 was used to remove
electronic
contributions from disordered solvent molecules.
;
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