STUDY OF HYDROGEN BONDING INTERACTIONS VIA X-RAY ANALYSIS

by

Olga Gorlova

A Dissertation submitted to the

Graduate School-Newark

Rutgers, The State University of New Jersey

in partial fulfillment of the requirements

for the degree of

Master of Science

Graduate Program in Chemistry

written under the direction of

Dr. Roger A. Lalancette

and approved by

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Newark, New Jersey

May 2012

ABSTRACT

X-ray diffraction is a useful method for studying the absolute structure of a molecule or complex in crystalline form. Analysis and determination by this technique provides information on atomic positions within the molecule as well as bond lengths, angles, unit cell, space group and symmetry. We used X-ray analysis to study hydrogen-bonding interactions in a number of molecules. A hydrogen bond occurs between a hydrogen atom covalently bonded to a first row electronegative atom and weakly bonded to another first-row electronegative atom having at least one lone pair of electrons. Hydrogen-bonding interactions affect the coordination and complexation of molecular compounds. In this paper, we examine a structural anomaly of a far-too-short hydrogen bond in $H_5O_2^+$cation and describe the various methods employed to resolve this issue. We also investigate intra- and inter-molecular hydrogen bonding in an oligosaccharide, as well as sulfate ion coordination due to hydrogen bonding in two different macrocycles.

ACKNOWLEDGEMENTS

I would like to express my sincerest gratitude to Professor Lalancette. His enthusiasm, dedication, and ability to explain things clearly and simply made for a wonderful research experience.

I would also like to thank Ruveda, Stortz and S. Ranganathan for providing me with crystal samples and relevant information

Lastly, I would like to thank the Rutgers Chemistry Department, specifically Professor Piotr Piotrowiak, for encouraging me to pursue a graduate education and guiding me throughout my educational endeavors.

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INTRODUCTION:

X-Ray Diffraction for Structural Analysis and Determination

General Information

The typical procedure for this type of analysis is:

A) Crystallization of the material to be studied

The crystallization of the material is generally achieved through slow solvent evaporation, although there are many other techniques. Quality crystals are required for X-ray analysis. X-ray crystallography works through the scattering of X-ray waves via the electrons of the atoms in a crystal. An X-ray strikes the electrons and produces a wave which emanates from those electrons; this diffraction produces an array specific to each crystal and can therefore be used to analyze the absolute structure of the desired compound

Growing crystals optimal for X-ray crystallography may seem difficult in many circumstances. As the solvent evaporates, crystals may grow on the sides of a beaker, making them small, or grown together and not ideal for X-ray crystallography. The solution may be too dilute causing similar problems in crystal growth. Agitation of the sample even in the early stages may disturb the formation of 'good' crystals. Twinning of the crystals may occur, which may not be evident until a large amount of data have already been collected. All of these factors need to be taken into account during crystal growth for they hinder the production of crystals adequate for X-ray crystallography.

B) Data Collection

Once a quality crystal of a material to be studied is formed, it is chosen to be < 0.5 mm in the longest dimension (or cut to be this size) and mounted on a Cryoloop® with

Paratone-N® (this is a long-chain hydrocarbon which is used just to hold the crystal on the loop). The mounted crystal is then centered on the diffractometer and, ideally, put under a stream of dry nitrogen gas to lower and then maintain the crystal temperature at 100K. The low temperature slows the thermal motion of the atoms and allows for a better and a more detailed data set to be collected.

Data are then collected on a Bruker SMART ApexII area-detector diffractometer and the structure is solved using SHELXTL V5.[1,2] Atoms are detected by diffraction of electromagnetic radiation. The radiation source used is CuKα and many reflections are measured for each crystal. The X-rays interact with each atom's electrons and produce various distinct diffraction patterns. These patterns are called reflections and are collected on a CCD detector. Data are collected at many positions and angles, leading to the determination of the unit cell, the space group, and the symmetry between the molecules.

C) Solving the Structure

The data collected by the diffractometer is used to "solve" the structure. The end product then determines bond distances, bond angles, and intermolecular interactions of the molecules within the structure. Usually an absorption correction is applied[3], which allows for the determination of the absolute configuration of the molecule (Flack[4]).

D) Refinement

The structure is then least-squared-refined in order to determine the optimal atom positions, distances and angles. The ultimate goal becomes solving a structure with an R-factor below 5% and the GOOF, Goodness-Of-Fit, close to 1. These are some of the

parameters which we use to indicate the molecules' positions within the cell and which tell us whether the structure has solved properly.

CHAPTER 1: K[cis-dinitrocobalt(III)(N,N-glycinato)$_2$] $\cdot$ H_2O

Introduction

The synthesis for the compound K[cis-dinitrocobalt(III)(N,N-glycinato)$_2$] $\cdot$ H_2O was initially published in 1966 by Matsuoka, et al.[5], but this group did not study the crystal structure of the complex. Bernal repeated Matsuoka's synthesis with the idea that amine carboxylate ligands have a pronounced tendency to trap hydronium cations in their crystal lattices; and since the structure of this species was not known, it was possible that it contained one of these hydronium ions: H_3O^+, $H_5O_2^+$, $H_7O_3^+$or $H_9O_4^+$. Bernal had been successful in finding some of these hydronium ions before.[6-9] From Matsuoka's preparation, Bernal did not isolate the expected complex, but obtained $K^+(H_9O_4^+)$[cis-dinitrocobalt(III)(trans–N,N–glycinato)$_2$]$^-$ ^{2} crystals; this complex was found to contain the trapped hydronium ion, $H_9O_4^+$. In subsequent syntheses of the same compound, Bernal found that two different species of crystals formed in the same preparation: deepred hexagonal rods (the complex above with the hydronium ion), and dark yellow-brown crystals, which are Matsuoka's complex, as reported, determined later by Lalancette.[10]

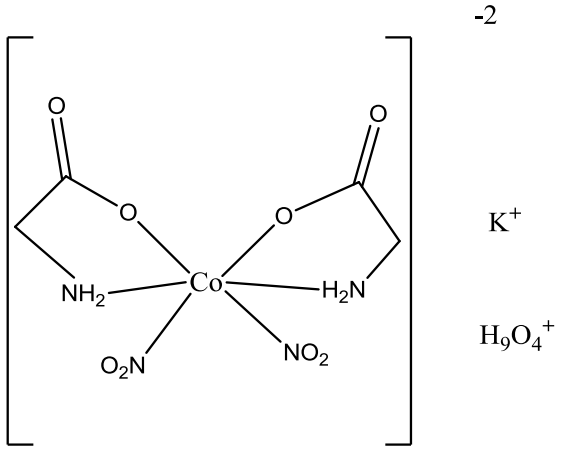

Diagram 1. ChemDraw Representation of $K^+(H_9O_4^+)$[cis-dinitrocobalt (III) (trans – N,N– glycinato)$_2$]$^{-2}$

The study of these trapped hydronium ions has proven to be difficult due to various issues that arise with the data collections from the crystals. Analysis of Bernal's reported crystal structure data raised concern about the nature of the trapped hydronium ion. The distance between two oxygens of the $H_5O_2^+$ portion of the $H_9O_4^+$ (we can think of this $H_9O_4^+$ as being $H_5O_2^+ + 2H_2O$) in this complex $K^+(H_9O_4^+)$[cis-dinitrocobalt(III)(trans–N,N–glycinato)$_2$]$^{-2}$ was found to be in the range of ~1.33 to 1.61Å. These values are significantly less than the generally encountered ~2.7 to 3.0 Å range between two oxygen atoms linked by a hydrogen bond. In fact, it is an impossibly short O···O distance. Recently, a structure containing a $H_5O_2^+$cation was reported to have an O···O bond length of 2.445(10) Å, but this is still notably closer to the normal O···O range.[11]

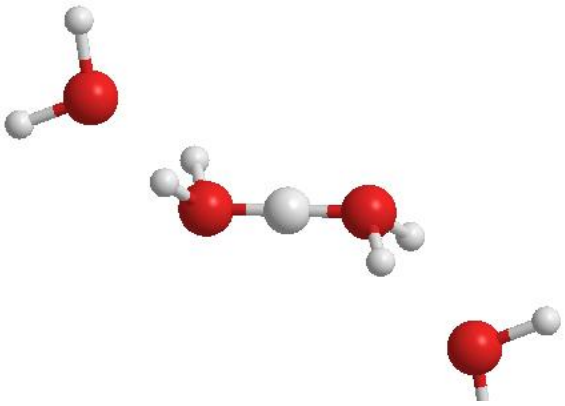

Diagram 2. Chem3D representation of the $H_9O_4^+$ as $H_5O_2^+ + 2H_2O$.

In order to resolve this discrepancy, we repeated Bernal's work and wished to collect data at 100K rather than at room temperature to be able to better assess this extremely short O···O bond distance. Since Ivan Bernal's original data were not available, we prepared our own crystals for X-ray analysis following the original preparation by Matsuoka. This report provides a summary of our methods, data and results, and compares them to those of published data to provide further insight on the species trapped in $K^+(H_9O_4^+)$[cis-dinitrocobalt(III)(trans–N,N–glycinato)$_2$]$^{-2}$. The CDC reference code for

this compound (as published by Bernal) is OBATAM, which I will use to refer to this compound from here on.

Experimental Procedure for making OBATAM

The original preparation given by Matsuoka, et al. is as follows:

To 40 g of $Co(II)Cl_2 . 6H_2O$ dissolved in 50 mL H_2O were added, in the following order:

1) KNO_2 (50g) in 70 mL H_2O

2) Glycine (20g) in 150 mL H_2O

In order to oxidize the resulting dark brown solution ($Co^{2+} \rightarrow Co^{3+}$), air was bubbled through the solution for three hours. Then, 100 mL of EtOH were added and this solution was refrigerated overnight. The yellow-brown crystals that were in the solution were then filtered, washed with EtOH and recrystallized from hot H_2O. The liquid was decanted and the crystals were dried by heating at 105 °C.

Our multiple preparations were exactly as above, but later on, scaled down by a factor of 10. In attempting to resolve the hydronium cation concern, we altered the preparation as well as the crystallization techniques by varying solvents and crystallization processes. This is discussed in further detail in the following section.

$Co(II)Cl_2 \cdot 6H_2O$ dissolved in H_2O was a dark magenta solution prior to the addition of the KNO_2 solution which turned the mixture into a wine-red opaque color. Upon addition of glycine, the solution turned brown and effervesced, producing a pungent odor. We initially thought that Cl_2 was given off, and subsequent preparations sparked further interest in the species given off, which is also discussed next.

RESULTS / DISCUSSION

After some initial difficulty with the production of quality crystals, OBATAM was crystallized for X-ray analysis. Two types of crystals were formed from the reaction mixture. There were long dark-red hexagonal rods and flat orange octagonal plates. The rods proved to be easier for X-ray analysis as they were less likely to crystallize in layers, and produced crystals of better quality and clarity.

Optimal X-ray analysis requires data collection at lower temperatures, such as 100K. As we placed the mounted crystal under the cold nitrogen stream at 100K, we saw the crystal crack. This made it unsuitable for X-ray analysis. Consequently, we had to settle for a room temperature data collection since the crystals were cracking below 273K. The cell dimensions collected at room temperature were a = 19.991(2) Å, b = 15.4261(19)Å, c = 8.1439(11)Å with $\beta = 101.818(8)^{O}$, which are identical to those reported by Bernal.[9] With that being so, our data also gave a hydrogen bond ($OH^{\cdots}O$) distance in the hydronium ion which was too short to be plausible. Acknowledging that single crystal X-ray diffraction comes with several of its own common concerns, we took into account factors such as crystal

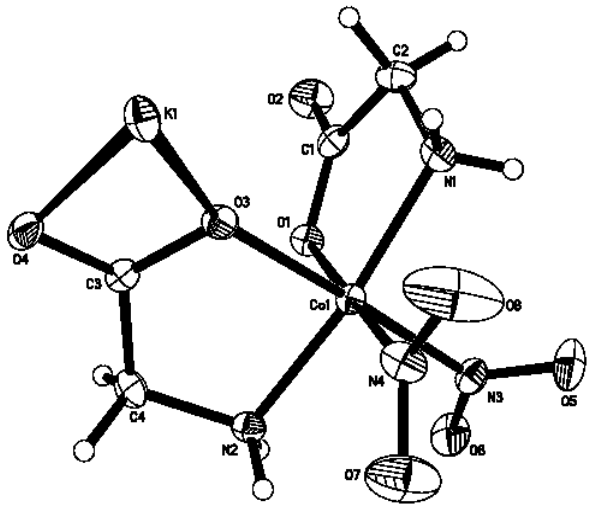

Fig. 1. ORTEP Representation of the asymmetric unit of cis-dinitrocobalt(III)(trans-N,N-glycinato)$_2^-$ ^{2} anion with numbering scheme. Displacement ellipsoids are drawn at 30% probability level for non-H atoms.

twinning and molecular disorder. These potential anomalies were ruled out with subsequent data sets which provided identical results to the first data set. To resolve the problem at hand, we had to figure out ways of collecting low temperature data without having the crystal crack and to consider the possibility that we may not be dealing with a trapped hydronium ion at all but possibly another species.

We proposed that at low temperatures, the $H_5O_2^+$ species was causing the cracking of the crystal lattice in the presence of the surrounding water molecules. Introducing these crystals to low temperatures could be causing a solid-state phase transition in which the water molecules formed an aggregate of a greater volume. As a result, the unit cell would increase in size and the stress from the combined actions of all the unit cells would cause the crystals to fracture along weaker points within the lattice. Data at high temperatures could still be taken; however it always gave the same results and did not explain the close proximity of the oxygen in the $H_5O_2^+$ cation.

Analysis of the crystals' thermal properties allowed us to find the specific transition at which the crystals were cracking. Differential Scanning Calorimetry (DSC)shows a specific transition at ≈ -40°C or 233K (see Figure 2A, 2B)[12]

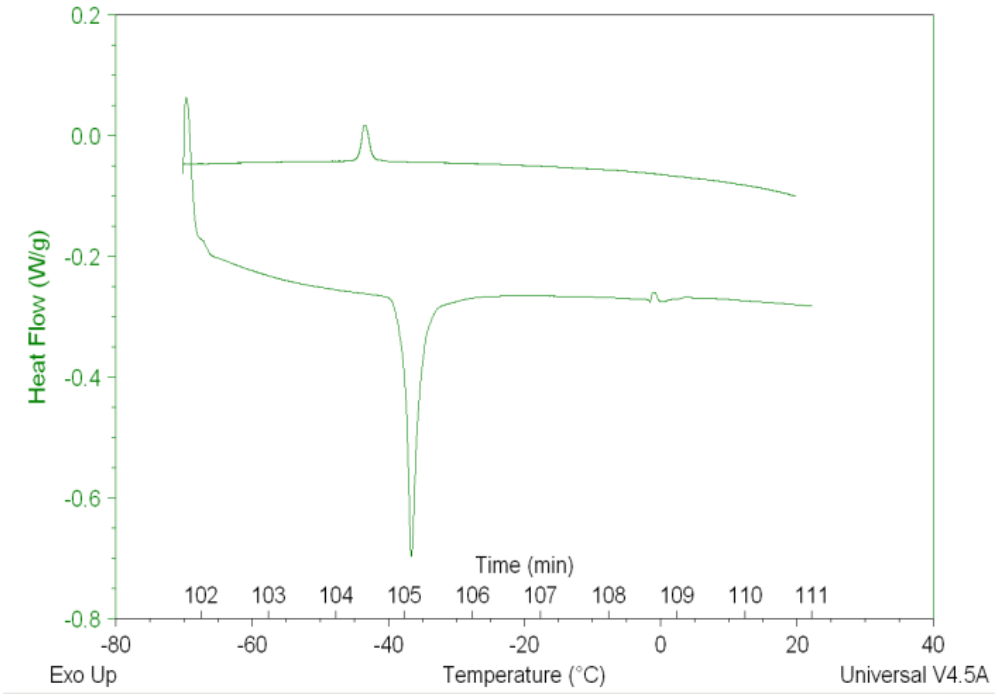

Fig. 2A. DSC trace showing the transition at ≈ -40°C. The upper trace is a cooling curve (blown up in Figure 2B). The endotherm is demonstrated by the peak pointing up. The lower trace is a heating curve, showing the exotherm (peak pointing down) when the solid state phase transition occurs on heating.

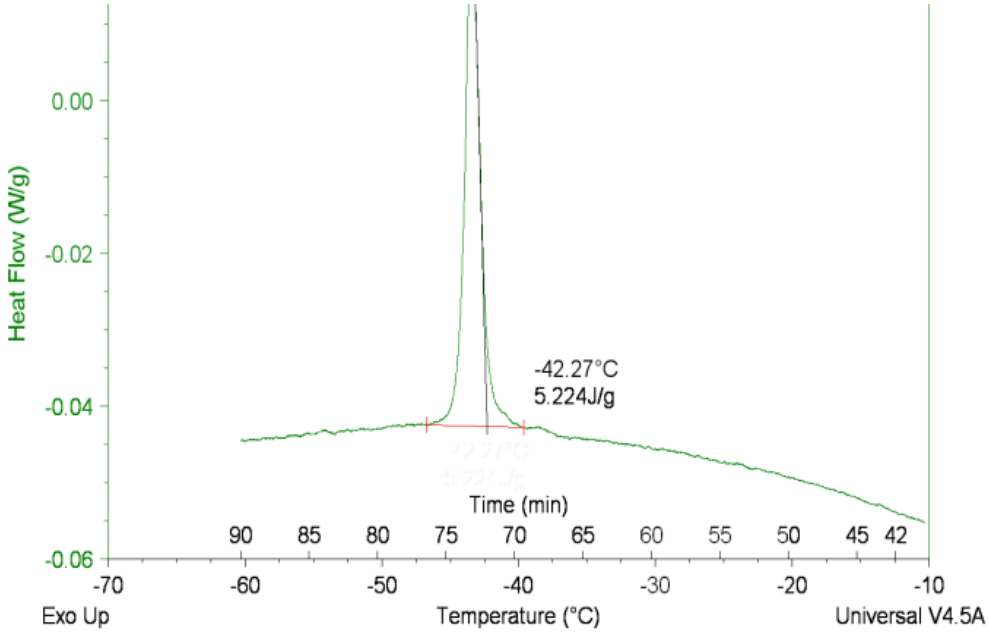

Fig. 2B. DSC trace showing solid state phase transition at ≈ -40°C of the complex. This is enlarged from Figure 2A.

The solid-state phase transition was the biggest obstacle in acquiring the low temperature data set required to understand the dilemma of the short oxygen – oxygen distance. We employed a variety of techniques to help us solve the problem. A few simple methods were tried. The crystal temperature was lowered very slowly so that there would be minimal immediate strain on the lattice during the cooling, but this proved unsuccessful as the crystal ultimately cracked once the temperature was below the solid phase transition. We also placed a mounted crystal in a freezer for 72 hrs to anneal it, but this did not yield much success because again, as the temperature of the crystal was lowered below its solid state transition, it cracked. A method commonly used by protein crystallographers was also attempted without much success. This method consists of coating the crystals in mixtures of various ratios of PEG (polyethylene glycol) and in this case glycine (a component of the complex), and then flash-freezing the mounted crystal in liquid nitrogen. This also did not protect the crystal from cracking.

Also, to grow better crystals, we tried a new technique prior to crystallization. Choosing between various possible silanes, diphenylchlorosilane was used to coat the inside walls of several beakers in preparation for crystallization. The silane coating is very hydrophobic and does not allow many small crystals to grow in various nucleation sites on the walls of the beaker. With the silane, as the solvent evaporates from the beaker, it leaves a more and more concentrated solution at the bottom of the beaker, which ultimately crystallizes into larger and better crystals. Consequently, the crystals which form are larger, brighter and clearer. Experimenting with diphenylchlorosilane, the coating on some beakers was “neat” and in some the silane was diluted with water in approximately a 1:1 ratio. The beakers with dilute diphenylchlorosilane produced optimal

crystals. Further experimentation included the filtering of the desired compound through a syringe filter and implementing the diphenylcholorosilane for better crystals. This technique was used with some preparations of OBATAM and resulted in many more suitable crystals for X-ray analysis. Although there were more quality crystals, these crystals were identical to those in the previous batches in that they cracked at low temperatures.

We chose to prepare a new batch of OBATAM where we would oven-dry half of the crystals, as per original preparation, and air-dry the other half. This yielded different cells but did not provide additional insight on the nature of the trapped hydronium ion in the crystal lattice of OBATAM. We prepared a fresh solution and split it into quarters. One quarter was allowed to crystallize as per the original preparation, while the others were a) not refrigerated and not washed in any alcohol, b) refrigerated and not washed in alcohol and c) refrigerated and washed in methanol instead of ethanol. None of these provided any new information.

At this point, we attempted to crystallize OBATAM out of other solvents, instead of water. Solvents interact with solvated complexes and may affect the nature of the species trapped in a crystal lattice. From a fresh batch of OBATAM, we isolated several crystals to see their behavior in varying solvents. We did not find OBATAM to dissolve in any of the following common solvents: cyclohexane, choloroform, dichloromethane, methyl-isobutyl ketone, benzene, acetone, ethyl acetate, 100% and 95% ethyl alcohol, THF and acetonitrile. Ultimately, the original method of crystallizing in H_2O yielded optimal results.

While preparing the complex, there was a notable amount of effervescence which was accompanied by a pungent odor, specifically after the addition of glycine to the mixture of $Co(II)Cl_2 \cdot 6H_2O$ and KNO_2. Analysis of this gas by GC/MS showed that it was in fact a mixture of NO_2 and NO gas being evolved during the reaction. This provides the possibility that our initially proposed $H_5O_2^+$ cation may in fact be a disordered N=O with one of the surrounding waters being protonated to account for the charge. Another possibility would be a disordered NO^+. The expected bond distance for N=O is 1.15 Å; disorder would be responsible for the longer length of our bond in the experimental data. Since we proposed that it may not be a hydronium ion altogether, another possibility is a trapped hydrogen peroxide in the crystal lattice. We were not able to draw any conclusive results to verify this hypothesis, even though the O···O bond distance in peroxide is close to what we see.

Continuing to collect data sets on the original crystals, we proposed to alter the preparation another way: by bubbling nitrogen gas through the solution instead of air and slow the oxidation process. This preparation, hopefully, will allow us to gather OBATAM crystals and collect data at 100K without the crystals cracking. OBATAM remains a work in progress, with hopes of being able to explain the very short oxygen-to-oxygen bond length discrepancy.

CHAPTER 2: HYDROGEN BONDING

Introduction

Hydrogen bonding is an interaction where a hydrogen atom, covalently bonded to a first row electronegative atom (either N, O or F) [the Donor atom], is weakly bonded to another first-row electronegative atom (the Acceptor atom) having at least one lone pair of electrons. This interaction creates a dipole because the electronegative element covalently bonded to the hydrogen attracts the electron density away from it; this results in a bond which has both a partially negative and a partially positive charged end. In the presence of other electronegative atoms, the positive end will be attracted to the electronegative atom forming a hydrogen bond. This bond is relatively strong, about 10% as strong as a regular covalent bond. Hydrogen bonding can be both intra- and inter-molecular and is commonly responsible for many chemical and physical properties of the overall molecule.

Studying the nature of hydrogen bonding modes between molecules elucidates their influence within a particular molecular structure. X-ray analysis allows optimal study of the hydrogen bonding schematics in the crystalline state of a specific complex. In the crystalline state, the hydrogen bond is less flexible and dynamic than in solution. Since it is now fixed and rigid, it is much easier to determine. We studied several complexes with notable hydrogen bonding which will be further discussed below.

6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside

This sugar molecule (an oligosaccharide) was synthesized by our collaborators in Argentina. The purpose of solving its structure was to gain knowledge about the hydrogen bonding interactions in the compound in order to explain its glycosylation regioselectivity. This is deemed important since there has been a huge attempt to synthesize various carbohydrate oligomers in order to understand their stereo- and regio-chemical properties. Since these factors are difficult to predict, Colombo, Rúveda and Stortz required the crystal structure to compare it to their theoretical calculations to verify and to rationalize their results.[13] The specific compound studied by X-ray analysis was chosen from a group of similar compounds because it purportedly had an intramolecular hydrogen bond which was crucial in explaining the reactivity of a specific OH group in glycosylation reactions. The structural findings of this study might help to provide more insight into the geometry of other sugar acceptors as well as to rationalize their reactivity. Looking at the structure of the molecule, there are two potential hydrogen-bonding interactions involving the two different hydroxyl groups on the oligosaccharide ring.

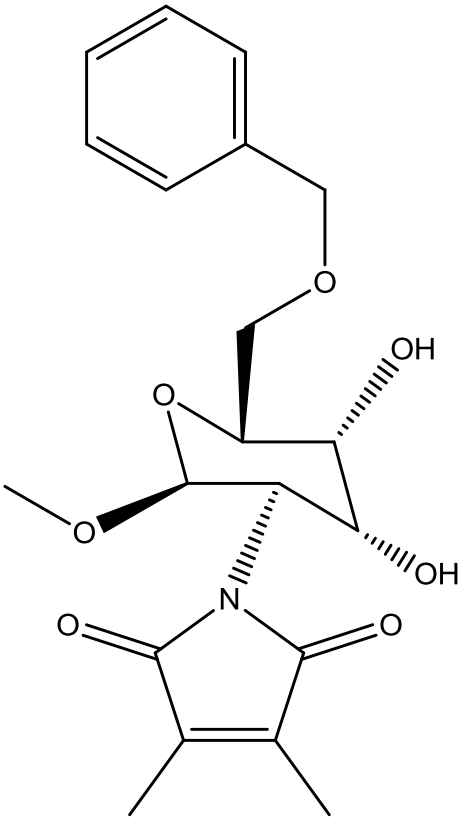

Diagram 3. ChemDraw Representation of the structure of 6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside

Crystal and molecular structure details

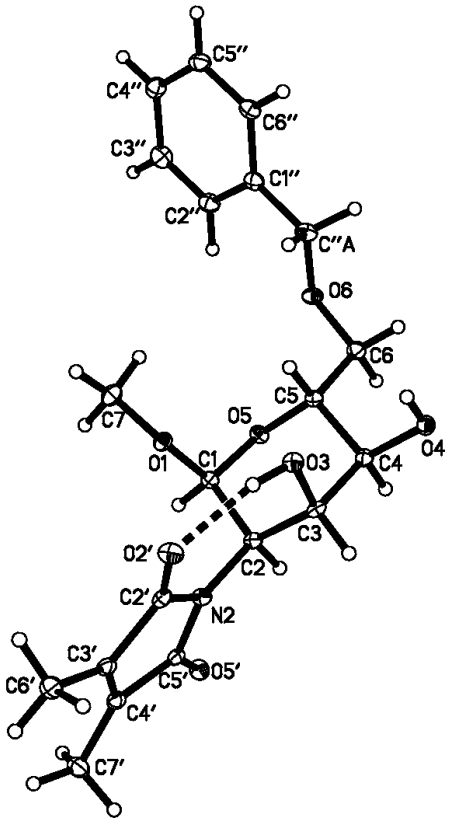

Fig. 3. ORTEP Representation of showing the asymmetric unit of 6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside with the numbering scheme. Displacement ellipsoids are drawn out at 30% probability level for non-H atoms.

The X-ray crystal structure revealed two hydrogen bonding interactions: an intra- and an inter-molecular hydrogen bond. A strong intramolecular hydrogen bond between O3 and O2' was observed (see Figure 3). The numbering scheme for the molecule is shown in this figure. The H3···O2' bond distance is 1.84(2) Å and the hydrogen bond distance (O3-H3···O2') is 2.6797(15) Å; the O3-H3-O2' bond angle is 164.9(19)º. These distances and angles demonstrate that this is a relatively strong hydrogen bond. Colombo, Rúveda and Stortz also analyzed many similar molecules by DFT calculation methods.[13] For this particular structure, the calculated H···O distance ranges from 1.723 to 1.787Å (DFT calculations) and is 1.860 Å from MM3 calculations. The shorter H···O distance found from the X-ray measurement (compared to the MM3 value) can be attributed to a small increase in the hydrogen bond strength due to packing forces. The intramolecular hydrogen bond (O3-H3···O2') was almost identical between the experimental X-ray results [2.6797(15) Å] and the calculated values from the DFT calculations (2.679-2.719 Å**)**, but smaller than the 2.728 Å from the MM3 calculations.

A second hydrogen bond, intermolecular and weaker, was also observed between O4 and O5’ of a neighboring molecule. Although this bond is still strong [its O···O distance is 2.8396(14)Å], it is weaker than the first one. In order for this intramolecular hydrogen bond to occur, the N-dimethylmaleoyl (DMM) group has to tilt with respect to the C2-H2 bond. Details of the structure determination are given in Table 1, whereas the thermal ellipsoid plot with atom numbering and hydrogen bonds is shown in Figure 3.

Additionally, puckering parameters, found by Colombo, Ruveda and Stortz from DFT and MM3 calculation, help in the determination of the degree of planarity between the rings, in this case the phenyl and the DMM. Table 2 shows the crystal structure assessment of these same dihedral angles between rings. These values correspond closely with the calculated puckering parameters found by Colombo, Ruveda and Stortz (0.561-0.572 Å, 5.1-5.6º). Additional information from the data collected from the crystal diffraction is provided below. The structural findings of this study may help to provide more insight into the geometry of other sugar acceptors as well as to rationalize their reactivity (Figure 3).

Table 1. Crystal data and structure refinement for 6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside

Crystal data	
$C_{20}H_{25}NO_7$	V = 1909.76 (12) Å^3
Mr = 391.41	Z = 4
Orthorhombic, P212121	Cu $K\alpha$ radiation, λ = 1.54178 Å
a = 10.0296 (4) Å	μ = 0.86 mm−1
b = 11.9099 (4) Å	T = 100 K
c = 15.9877 (5) Å	0.49 × 0.44 × 0.21 mm
Data collection	
Bruker SMART CCD Apex-II area-detector Diffractometer	3388 independent reflections
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)	3360 reflections with $I > 2\sigma(I)$
Tmin = 0.679, Tmax = 0.838	Rint = 0.047
16476 measured reflections	
Refinement	
$R[F2 > 2\sigma(F2)]$ = 0.028	H-atom parameters constrained
$wR(F2)$ = 0.074	Δρmax = 0.20 e Å^{-3}
S = 1.07	Δρmin = −0.16 e Å^{-3}
3388 reflections	Absolute structure: Flack (1983), 1419 Friedel pairs
259 parameters	Flack parameter: 0.02 (13)
0 restraints	

Table 2. Select Crystal Geometries for 6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside

Bond lengths (Å)		**Bond angles (º)**	
C1-O1	1.3964 (17)	C1-C2-C3	113.48(11)
C2-N2	1.4686(17)	C5-O5-C1	114.2(1)
C3-O3	1.4189(17)	C1-O1-C7	112.7(1)
C4-O4	1.4173(17)	O1-C1-O5	113.76(11)
C5-O5	1.4400(17)	C2-C3-O3	116.49(12)
O5-C1	1.4128(16)	C6-O6-C"A	112.58(11)
O1-C7	1.4293(17)	C2-N2-C2'	130.65(11)
C1-C2	1.5337(18)	N2-C2'-O'	126.89(13)
C5-C6	1.5185(18)		
Atomic distances (Å)		**Torsion angles (º)**	
H(O)3-O2'	1.838	O5-C1-O1-C7	68.37(14)
O3-O2'	2.6797(15)	C1-C2-N2-C2'	-85.41(17)
Puckering parameters		C2-C3-O3-H	42.3
Sugar Q (Å)	0.577	C3-C4-O4-H	-62.4
Sugar θ (º)	5.7	O5-C5-C6-O6	63.10(15)
DMM Q (pm)	0.17	C5-C6-O6-C"A	84.19(15)
Phenyl Q (pm)	1.55	C6-O6-C"A-C1"	-174.39(11)
		O6-C"A-C1"-C2"	14.41(19)

CHAPTER 3: SULFATE ANION HYDROGEN BONDING INTERACTIONS

Introduction

Recent interest in the selective binding of sulfate anions has stemmed from their affect on biological and environmental systems. Sulfate ions have also been found to affect the way the immune system recognizes gram-negative bacteria, known to cause septic shock and death. The drugs currently available to treat these bacteria sometimes have unpleasant side effects.[14-16] Consequently, isolating the sulfate ions has been a major research goal.

These anion receptors, SO_4^{-2}, have proven difficult to study due to the solvation effects resulting from their complementary cations, often variations of tert-butyl ammonium ion (TBA). Determining the crystal structure of these coordinating complexes serves to further explain the behavior of the sulfate ion, its relationship to its counterion and to the complex as a whole. Previous studies have demonstrated interesting coordination through N-H···O hydrogen bonds. [14-16] We have elucidated two new structures both with coordinating sulfate ions hydrogen bonded to a number of nitrogen atoms through N-H···O interactions.

The complexes were synthesized by S. Ranganathan and coworkers.[17] It can be difficult to solve structures with TBA ions due to their disorder. These ions are usually disordered and are difficult to refine, even at 100K. It is thought that the TBA ion is responsible for the packing in the complex. We suggested to our collaborators that they should use another counterion, such as tetramethylammonium or Ph_4As^+ (tetraphenylarsonium). Due to limited results, no viable crystalline products were isolated

from these experiments, so we solved the structures of the two sulfate-coordinating complexes that they had made, the details of which are below.

$C_{20}H_{20}N_8O_8 \cdot 2(C_{16}H_{36}N)^{+} \cdot SO_4^{-2}$:

A urea-based macrocycle for sulfate ion binding

The first structure we examined was a complex consisting of a symmetrical chain containing eight nitrogens, two from NO_2 groups, and the remaining six nitrogens being hydrogen bonded to the oxygens of two different coordinating sulfate ions. For each chain, nitrogens 2, 3, 4 hydrogen bond to one sulfate ion, while nitrogens 5, 6, 7 hydrogen bond to the sulfate ion in the adjacent symmetry-related molecule (Diagram 4). In other words, this produces a second chain by symmetry through the coordinating sulfate anion. As a result, the sulfates and 'nitrogen chains' further coordinate into a long chain-like complex which is then sustained by surrounding TBA cations (two for each sulfate). For clarity we have omitted the TBA molecules from the figure and diagram below.

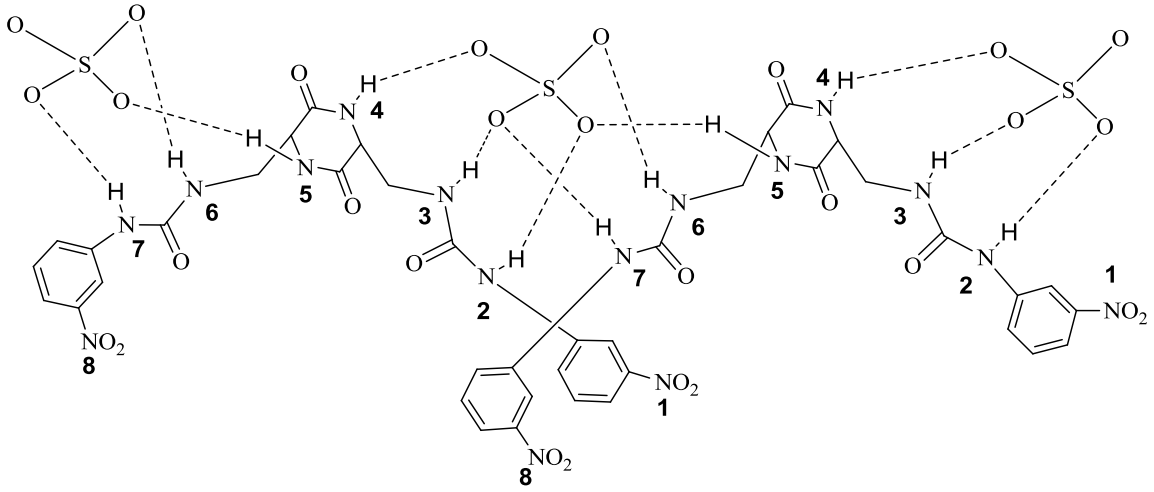

Diagram 4. ChemDraw Representation of the six N-H···O hydrogen bonds to each sulfate and the six to each macrocycle are shown with dotted lines.

As we grow the structure, we see the effects of the coordinating sulfate anions. The crystal data from this structure show that all of the sulfates coordinate and connect identically to each subsequent molecule. There was difficulty in the refinement of this structure due to the counter TBA cations. We collected 9772 independent reflections and were only able to refine it to an R-factor = 11.4% (crystal data can be found in Table 4). Although this R-factor is relatively high, it was enough for us to easily determine the structure of the coordinating hydrogen bonds to the sulfate anion (Figures 4 and 5).

The two disordered TBA cations lead to the relatively high R-factor. The unique building block of the cell (one macrocycle and one sulfate ion) is numbered completely below (Figure 4). Figure 5 shows a partial packing diagram. The relevant information about the N-H···O bonds are found in Table 3.

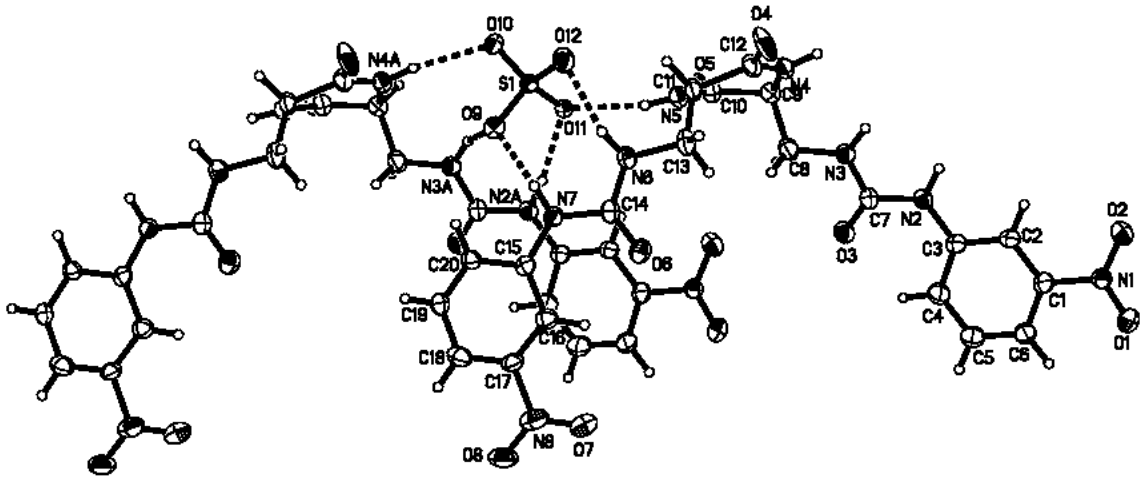

Fig. 4. ORTEP representation of the unique building block with its symmetry-generated macrocycle is shown above with the respective hydrogen bonds as dotted lines. Displacement ellipsoids are drawn at 30% probability level for non-H atoms.

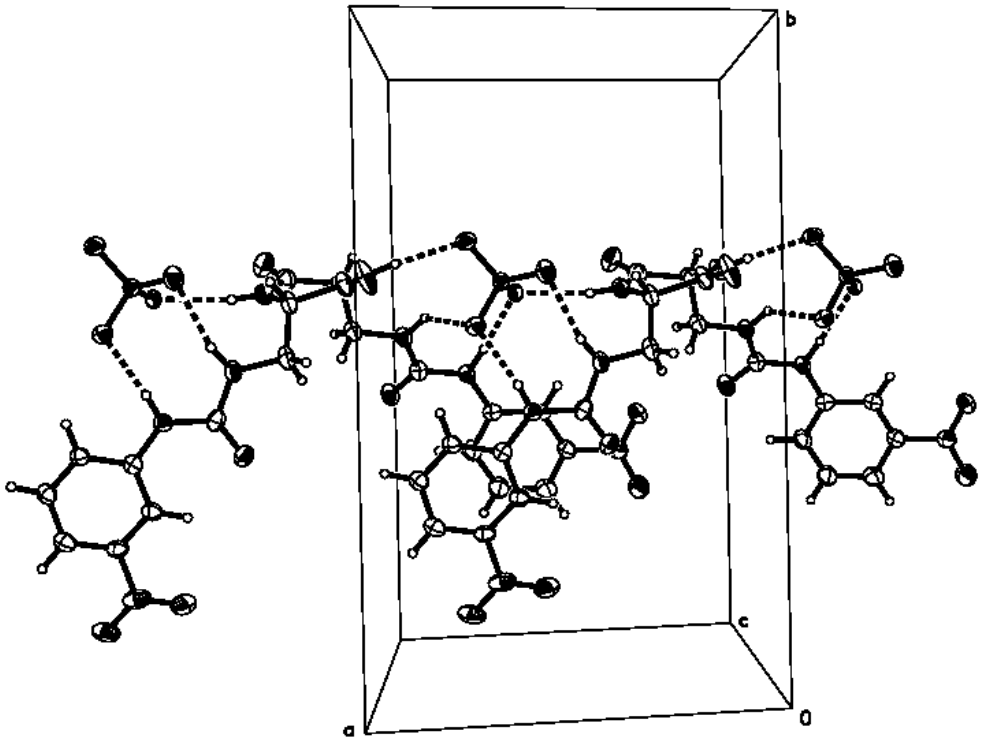

Fig. 5. ORTEP representation showing three molecules generated by translation along the *a* cell dimension. The TBA counterions found in the empty volume in the cell have been omitted for clarity. Displacement ellipsoids are drawn at 30% probability level for non-H atoms.

Table 3. Crystal Structure Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N2A—H2A···O11Ai	0.88	2.02	2.886 (6)	141
N3A—H3A···O9Ai	0.88	2.20	2.884 (7)	134
N4A—H4A···O10Ai	0.88	2.11	2.963 (7)	165
N5A—H5A···O11A	0.88	2.09	2.963 (7)	169
N6A—H6A···O12A	0.88	2.06	2.912 (8)	163
N7A—H7A···O9A	0.88	1.98	2.805 (7)	156

Table 4. Crystal data and structure refinement for $C_{20}H_{20}N_8O_8 \cdot 2(C_{16}H_{36}N)^{+} \cdot SO_4^{-2}$

Crystal data

$C_{20}H_{20}N_8O_8 \cdot 2(C_{16}H_{36}N) \cdot SO_4$	V = 2898.46 (6) Å^3
Mr = 1081.42	Z = 2
Monoclinic, $P21$	Cu $K\alpha$ radiation, λ = 1.54178 Å
a = 10.0504 (1) Å	μ = 1.04 mm−1
b = 16.1550 (2) Å	T = 100 K
c = 18.4676 (2) Å	0.24 × 0.18 × 0.17 mm
β = 104.840 (1)°	

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer	9771 independent reflections
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)	8713 reflections with $I > 2\sigma(I)$
Tmin = 0.790, Tmax = 0.844	Rint = 0.026
29334 measured reflections	

Refinement

$R[F2 > 2\sigma(F2)]$ = 0.114	H-atom parameters constrained
$wR(F2)$ = 0.317	Δρmax = 1.48 e Å^{-3}
S = 1.12	Δρmin = −0.83 e Å^{-3}
9771 reflections	Absolute structure: Flack (1983), 4388 Friedel pairs
370 parameters	Flack parameter: 0.05 (4)
33 restraints	

$C_{20}H_{20}N_8O_6S_2 \cdot 2(C_{16}H_{36}N)^+ \cdot SO_4^{-2} \cdot H_2O$:

A thiourea-based macrocycle for sulfate ion binding

This structure was more difficult to solve and analyze than the previous one. It has two thiourea moieties in its backbone chain instead of two ureas. This yields a more intricate structure. Each cell has four independent complexes, each with its own sulfate. In other words, each asymmetric unit has four of the structures shown below (Diagram 5), but with varying hydrogen-bonding connectivity to its own sulfate. Each of these interactions varies by the torsion and connectivity of the N-H···O bonds from each respective molecule.

Each of the pair of macrocycles is produced by symmetry through the sulfate ion. In Figure 6, chain 'AA' is generated from chain 'A' by a translation along the *a* cell dimension (chain AA is identical to chain A, but is one cell away in the *a* cell dimension).

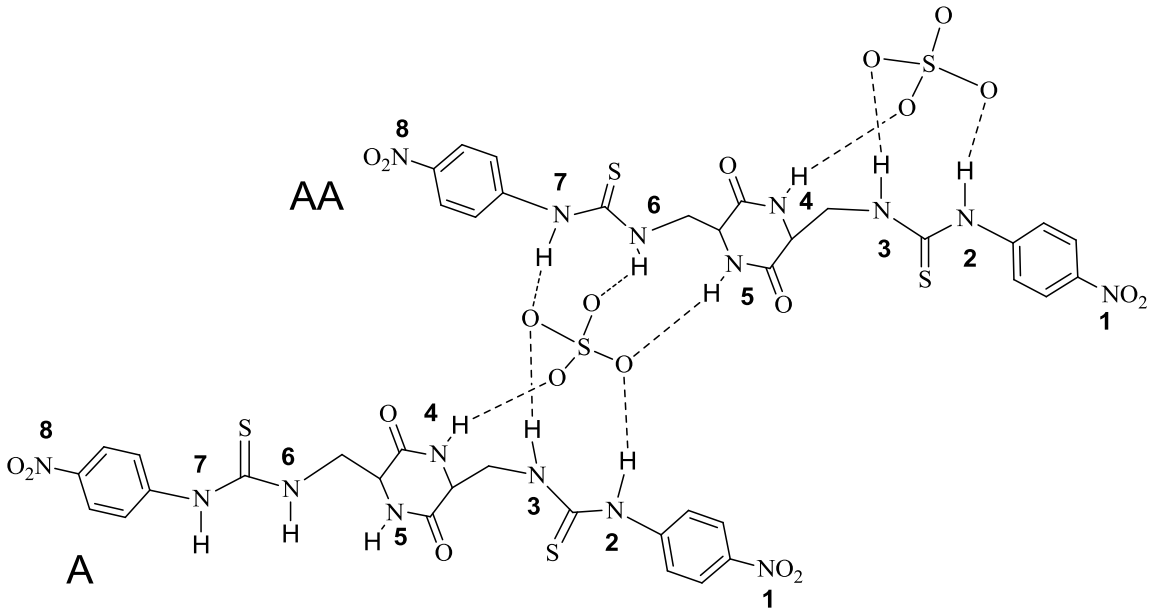

Diagram 5. ChemDraw representation of the symmetry-generated macrocycle pair across a coordinating sulfate ion.

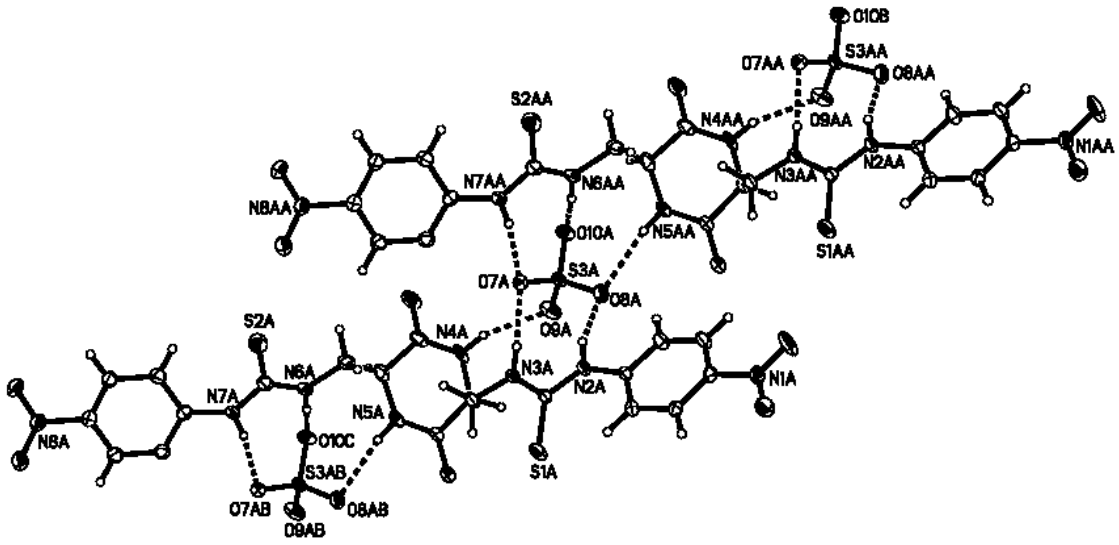

Fig. 6. ORTEP representation of the symmetry-generated macrocycle pair across coordinating sulfate ion. Displacement ellipsoids are drawn at 30% probability level for non-H atoms.

Depicted in the figures above, each original macrocyle hydrogen bonds only through N2, N3 and N4 to its coordinating sulfate anion, while the symmetry-generated unit hydrogen bonds through its N5, N6 and N7. This is similar to the relationship in the previous structure, with the significant difference that we are no longer producing one long complex chain of coordinating sulfates between molecules, but rather four different chains each with their own sulfates. As a result, we found that each asymmetric unit has four independent receptors, four sulfates and eight TBA counter ions (Figure 6). To the best of our knowledge, this is the greatest amount of reported sulfate ions to have been found trapped in this sort of structure. Again, the counter TBA cations have made it difficult to refine the structure very well. The final R-factor was 7.6%. Additional crystal data information can be found in Table 7.

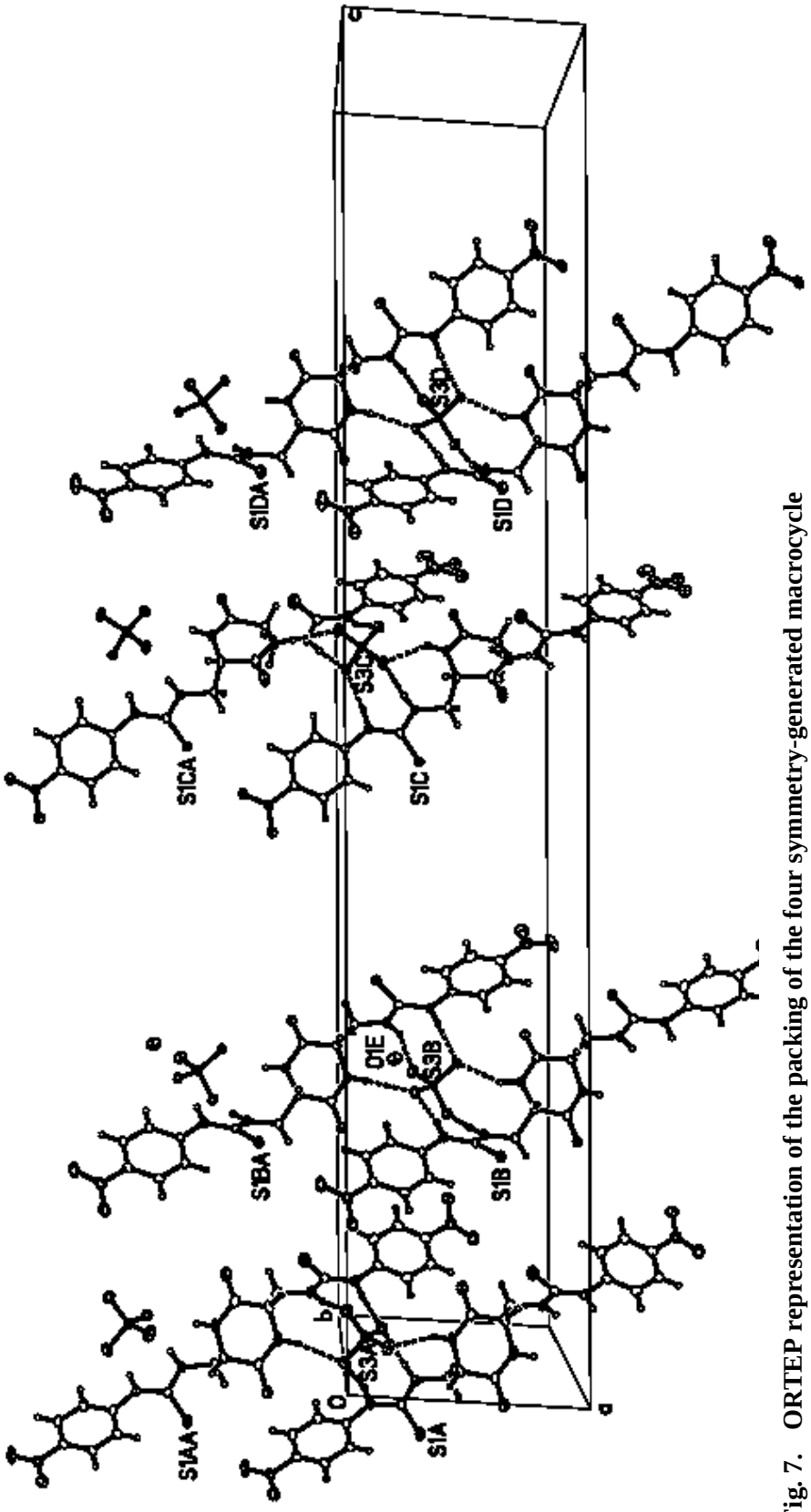

Fig. 7. ORTEP representation of the packing of the four symmetry-generated macrocycle pairs in the unit cell, with omitted TBA ions for clarity. Displacement ellipsoids are drawn at 30% probability level for non-H atoms.

We determined that each of the macrocycle pairs in the asymmetric unit has an individual hydrogen-bonding connectivity to its respective coordinating sulfate ion. The relationships listed below (Table 5) show the hydrogen-bond connectivity of each macrocycle pair; further details about the hydrogen-bond geometries are listed in Table 6.

Table 5. Hydrogen-bond connectivities for each of the macrocycle pairs in the asymmetric unit. Bold hydrogen-bonding interactions emphasize the connectivity variance between subsequent molecules of the unit cell.

MoleculeA:	**Molecule B:**	**Molecule C:**	**Molecule D:**
N2A···O8A	N2B···O8B	N2C···O8C	N2D···O8D
N3A···O7A	N3B···O7B	N3C···O7C	N3D···O7D
N4A···O9A	N4B···O9B	N4C···O7C	**N4D···O10D**
N5AA···O8A	N5BA···O8B	**N5CA···O10C**	**N5DA···O8D**
N6AA···O10A	N6BA···O10B	**N6CA···O8C**	**N6DA···O10D**
N7AA···O7A	**N7BA···O9B**	N7CA···O9C	N7DA···O9D

Table 6. Hydrogen-bond geometries (Å, º).

D—H···A	**D—H**	**H···A**	**D···A**	**D—H···A**
N2A—H2A···O8A	0.88	2.04	2.884 (6)	159
N3A—H3A···O7A	0.88	1.92	2.796 (6)	177
N4A—H4AA···O9A	0.88	2.15	2.990 (6)	159
N5A—H5AA···O8Ai	0.88	2.20	3.057 (6)	164
N6A—H6A···O10Ai	0.88	1.94	2.788 (6)	163
N7A—H7A···O7Ai	0.88	1.92	2.785 (6)	169
N2B—H2B···O8B	0.88	1.98	2.852 (5)	171
N3B—H3B···O7B	0.88	1.85	2.712 (5)	167
N4B—H4BA···O9B	0.88	2.07	2.883 (5)	154
N5B—H5BA···O8Bi	0.88	2.35	3.012 (5)	133
N6B—H6B···O10Bi	0.88	1.93	2.750 (6)	154
N7B—H7B···O9Bi	0.88	2.01	2.861 (5)	164
N2C—H2C···O8C	0.88	1.88	2.752 (5)	168
N3C—H3C···O7C	0.88	1.90	2.781 (5)	174
N4C—H4CA···O7C	0.88	2.40	3.092 (5)	136
N5C—H5CB···O10Ci	0.88	2.00	2.867 (5)	167
N6C—H6C···O8Ci	0.88	1.93	2.795 (5)	167

N7C—H7C···O9Ci	0.88	2.04	2.885 (6)	160
N2D—H2D···O8D	0.88	2.08	2.955 (5)	172
N3D—H3D···O7D	0.88	1.92	2.751 (6)	157
N4D—H4DA···O10D	0.88	2.08	2.887 (6)	152
N5D—H5DA···O8Di	0.88	2.07	2.895 (5)	156
N6D—H6D···O10Di	0.88	2.03	2.896 (5)	169
N7D—H7D···O9Di	0.88	1.83	2.699 (6)	167

Symmetry code: (i) x+1, y, z.

Table 7. Crystal data and structure refinement for $4(C_{20}H_{20}N_8O_6S_2) \cdot 8(C_{16}H_{36}N)^{+} \cdot 4(SO_4)^{-2} \cdot H_2O$

Crystal data

$4(C_{20}H_{20}N_8O_6S_2)\cdot8(C_{16}H_{36}N)\cdot4(SO_4)\cdot O$
Mr = 4470.16
Monoclinic, *P*21
a = 10.2409 (1) Å
b = 19.8608 (2) Å
c = 58.5086 (6) Å
β = 93.857 (1)°
V = 11873.3 (2) Å^3
Z = 2
Cu *K*α radiation, λ = 1.54178 Å
μ = 1.65 mm−1
T = 100 K
0.29 × 0.17 × 0.14 mm

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer
Absorption correction: Multi-scan *SADABS* (Sheldrick, 2008a)
*T*min = 0.646, *T*max = 0.802
105825 measured reflections
39531 independent reflections
34782 reflections with $I > 2\sigma(I)$
*R*int = 0.058

Refinement

R[*F*2 > 2σ(*F*2)] = 0.076
wR(*F*2) = 0.203
S = 1.05
39531 reflections
2580 parameters
1 restraint
H-atom parameters constrained
Δρmax = 2.01 e Å−3
Δρmin = −0.64 e Å−3
Absolute structure: Flack (1983), 15878 Friedel pairs
Flack parameter: 0.020 (12)

CONCLUSIONS

Optimal X-ray analysis for structural determination requires clear single crystals and data collection at low temperatures, such as 100K. This approach allowed us to successfully solve the crystal structures and examine the hydrogen-bonding interactions in an oligosaccharide and in two different sulfate-anion-coordinated macrocycle complexes. We also used X-ray analysis attempting to resolve a structural anomaly of far-too-short hydrogen bond found in a species trapped within a crystal lattice.

The crystal structure of the oligosaccharide, 6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside, determined two hydrogen-bonding interactions, an intra- and inter-molecular hydrogen bond. The determined intramolecular hydrogen bond measuring 2.6797(15) Å and a weaker intermolecular hydrogen bond measuring 2.8396(14) Å. These structural findings serve to explain the reactivity of the hydroxyl (-OH) group in glycosylation reactions of 6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside and, potentially, other sugar receptors.

Selective binding of the sulfate anions has sparked recent interest in various biological and environmental fields. We determined the crystal structure of two sulfate-anion-coordinating complexes. In the first, a urea-based macrocycle coordinated into a symmetrical chain linked through N-H···O hydrogen bonds to two sulfate anions, one on each end of the macrocycle. The chain of macrocycles was produced by symmetry through these coordinating sulfate anions. Each subsequent macrocycle and sulfate anion was connected identically to the previous. The second sulfate-anion-coordinating complex contained a thiourea-based macrocycle. The unit cell contained four independent complexes, each of which had unique N-H···O hydrogen bonding to its

symmetry produced macrocycle pair. TBA cations sustain the structure of both sulfate anion complexes.

OBATAM remains a work in progress. The X-ray results consistently determine a trapped species with the short bond. We continue to look for new methods in order to resolve this structural anomaly.

APPENDICES

Appendix 1.
Supplementary Data for
6-O-benzyl-2-deoxy-2-dimethylmaleimido-α-d-allopyranoside

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.57911 (10)	0.59104 (8)	0.04968 (5)	0.0174 (2)
O3	0.56029 (10)	0.79001 (9)	−0.06066 (6)	0.0181 (2)
H3	0.5868 (19)	0.7342 (17)	−0.0906 (12)	0.027*
O4	0.42996 (11)	0.96080 (8)	0.01424 (6)	0.0198 (2)
H4	0.513 (2)	0.9609 (16)	0.0062 (12)	0.030*
O5	0.41786 (10)	0.69035 (8)	0.12684 (6)	0.0171 (2)
O6	0.50907 (11)	0.83289 (9)	0.25841 (6)	0.0194 (2)
C1	0.44365 (14)	0.61193 (12)	0.06253 (8)	0.0160 (3)
H1A	0.3998	0.5394	0.0780	0.019*
C2	0.38168 (13)	0.65327 (11)	−0.01959 (8)	0.0154 (3)
H2A	0.2839	0.6581	−0.0080	0.019*
C3	0.42314 (14)	0.77286 (12)	−0.04304 (8)	0.0160 (3)
H3A	0.3690	0.7984	−0.0920	0.019*
C4	0.39286 (14)	0.84847 (12)	0.03202 (8)	0.0170 (3)
H4A	0.2947	0.8464	0.0428	0.020*
C5	0.46489 (14)	0.80215 (12)	0.10935 (8)	0.0167 (3)
H5A	0.5631	0.8002	0.0986	0.020*
C6	0.43711 (15)	0.87192 (12)	0.18692 (9)	0.0194 (3)
H6A	0.4618	0.9510	0.1757	0.023*
H6B	0.3404	0.8697	0.1992	0.023*
C7	0.63931 (15)	0.53248 (13)	0.11797 (9)	0.0229 (3)
H7A	0.6372	0.5799	0.1680	0.034*
H7B	0.7320	0.5145	0.1040	0.034*
H7C	0.5900	0.4629	0.1287	0.034*
C"A	0.64039 (15)	0.87601 (13)	0.26195 (9)	0.0208 (3)
H"A	0.6371	0.9585	0.2695	0.025*
H"B	0.6869	0.8601	0.2086	0.025*
N2	0.39429 (11)	0.56872 (10)	−0.08599 (7)	0.0160 (3)
O2'	0.59673 (10)	0.60469 (9)	−0.15291 (6)	0.0228 (2)
O5'	0.19590 (10)	0.47926 (9)	−0.05569 (6)	0.0211 (2)
C2'	0.49823 (14)	0.54699 (12)	−0.14126 (8)	0.0168 (3)

C3'	0.46490 (15)	0.44076 (12)	−0.18662 (8)	0.0186 (3)
C4'	0.34778 (15)	0.40327 (13)	−0.15926 (8)	0.0187 (3)
C5'	0.29897 (14)	0.48340 (12)	−0.09431 (8)	0.0161 (3)
C6'	0.55690 (16)	0.39520 (14)	−0.25151 (9)	0.0242 (3)
H6'A	0.5243	0.3220	−0.2705	0.036*
H6'B	0.6463	0.3866	−0.2276	0.036*
H6'C	0.5606	0.4471	−0.2990	0.036*
C7'	0.26891 (16)	0.30240 (14)	−0.18345 (10)	0.0259 (3)
H7'A	0.1896	0.3259	−0.2147	0.039*
H7'B	0.2416	0.2617	−0.1330	0.039*
H7'C	0.3237	0.2532	−0.2186	0.039*
C1"	0.71655 (16)	0.82376 (13)	0.33336 (9)	0.0202 (3)
C2"	0.67269 (15)	0.72830 (13)	0.37498 (10)	0.0235 (3)
H2"	0.5886	0.6966	0.3612	0.028*
C3"	0.75084 (17)	0.67871 (14)	0.43657 (10)	0.0278 (4)
H3"	0.7199	0.6135	0.4647	0.033*
C4"	0.87367 (17)	0.72427 (14)	0.45697 (9)	0.0255 (3)
H4"	0.9276	0.6897	0.4985	0.031*
C5"	0.91785 (16)	0.82053 (13)	0.41656 (9)	0.0243 (3)
H5"	1.0018	0.8523	0.4305	0.029*
C6"	0.83866 (16)	0.86995 (13)	0.35574 (9)	0.0219 (3)
H6"	0.8684	0.9365	0.3289	0.026*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0179 (5)	0.0200 (5)	0.0144 (4)	0.0017 (4)	−0.0003 (4)	0.0024 (4)
O3	0.0159 (5)	0.0214 (5)	0.0170 (4)	−0.0013 (4)	0.0032 (4)	0.0000 (4)
O4	0.0171 (5)	0.0169 (5)	0.0253 (5)	0.0000 (4)	−0.0011 (4)	0.0015 (4)
O5	0.0210 (5)	0.0175 (5)	0.0128 (4)	−0.0019 (4)	0.0028 (4)	−0.0006 (3)
O6	0.0188 (5)	0.0248 (5)	0.0146 (4)	−0.0032 (4)	−0.0003 (4)	−0.0016 (4)
C1	0.0173 (7)	0.0165 (7)	0.0144 (6)	−0.0008 (5)	0.0015 (5)	−0.0004 (5)
C2	0.0125 (6)	0.0195 (7)	0.0143 (6)	−0.0001 (5)	0.0013 (5)	−0.0022 (5)
C3	0.0133 (6)	0.0213 (7)	0.0134 (6)	0.0005 (5)	−0.0022 (5)	0.0020 (5)
C4	0.0141 (6)	0.0172 (7)	0.0197 (7)	−0.0008 (5)	0.0008 (6)	0.0010 (5)
C5	0.0155 (7)	0.0180 (7)	0.0165 (6)	−0.0012 (5)	−0.0003 (5)	−0.0006 (5)
C6	0.0197 (7)	0.0216 (7)	0.0169 (6)	0.0009 (6)	−0.0001 (6)	−0.0022 (5)
C7	0.0233 (7)	0.0253 (7)	0.0202 (7)	0.0019 (6)	−0.0015 (6)	0.0051 (6)

C"A	0.0210 (7)	0.0238 (7)	0.0177 (7)	−0.0059 (6)	0.0018 (6)	−0.0005 (5)
N2	0.0136 (5)	0.0206 (6)	0.0136 (5)	−0.0013 (5)	0.0019 (4)	−0.0016 (4)
O2'	0.0175 (5)	0.0309 (6)	0.0201 (5)	−0.0037 (5)	0.0048 (4)	−0.0046 (4)
O5'	0.0177 (5)	0.0214 (5)	0.0241 (5)	−0.0017 (4)	0.0041 (4)	−0.0011 (4)
C2'	0.0141 (7)	0.0238 (7)	0.0126 (6)	0.0042 (6)	−0.0002 (5)	0.0015 (5)
C3'	0.0194 (7)	0.0231 (7)	0.0132 (6)	0.0042 (6)	−0.0032 (5)	−0.0011 (5)
C4'	0.0197 (7)	0.0214 (7)	0.0151 (6)	0.0030 (6)	−0.0027 (5)	0.0001 (5)
C5'	0.0149 (6)	0.0176 (7)	0.0157 (6)	0.0012 (6)	−0.0032 (6)	0.0026 (5)
C6'	0.0248 (8)	0.0308 (8)	0.0169 (6)	0.0053 (7)	0.0025 (6)	−0.0058 (6)
C7'	0.0264 (8)	0.0251 (8)	0.0263 (7)	−0.0010 (7)	0.0007 (7)	−0.0081 (6)
C1"	0.0211 (7)	0.0227 (7)	0.0167 (6)	−0.0004 (6)	0.0027 (6)	−0.0047 (5)
C2"	0.0212 (8)	0.0255 (8)	0.0239 (7)	−0.0038 (6)	0.0026 (6)	−0.0021 (6)
C3"	0.0320 (9)	0.0263 (9)	0.0253 (8)	−0.0032 (7)	0.0039 (7)	0.0030 (6)
C4"	0.0281 (8)	0.0288 (8)	0.0195 (7)	0.0040 (7)	−0.0020 (6)	−0.0009 (6)
C5"	0.0217 (7)	0.0282 (9)	0.0230 (7)	−0.0013 (7)	−0.0011 (6)	−0.0065 (6)
C6"	0.0240 (8)	0.0210 (7)	0.0208 (7)	−0.0045 (6)	0.0022 (6)	−0.0013 (6)

Geometric parameters (Å, º)

O1—C1	1.3964 (17)	C"A—H"B	0.9900
O1—C7	1.4293 (17)	N2—C2'	1.3909 (18)
O3—C3	1.4189 (17)	N2—C5'	1.4015 (18)
O3—H3	0.86 (2)	O2'—C2'	1.2177 (18)
O4—C4	1.4173 (17)	O5'—C5'	1.2051 (18)
O4—H4	0.85 (2)	C2'—C3'	1.496 (2)
O5—C1	1.4128 (16)	C3'—C4'	1.331 (2)
O5—C5	1.4400 (17)	C3'—C6'	1.491 (2)
O6—C"A	1.4149 (18)	C4'—C7'	1.489 (2)
O6—C6	1.4294 (17)	C4'—C5'	1.493 (2)
C1—C2	1.5337 (18)	C6'—H6'A	0.9800
C1—H1A	1.0000	C6'—H6'B	0.9800
C2—N2	1.4686 (17)	C6'—H6'C	0.9800
C2—C3	1.5305 (19)	C7'—H7'A	0.9800
C2—H2A	1.0000	C7'—H7'B	0.9800
C3—C4	1.5308 (18)	C7'—H7'C	0.9800
C3—H3A	1.0000	C1"—C2"	1.389 (2)
C4—C5	1.5345 (19)	C1"—C6"	1.389 (2)
C4—H4A	1.0000	C2"—C3"	1.390 (2)

C5—C6	1.5185 (18)	C2"—H2"	0.9500
C5—H5A	1.0000	C3"—C4"	1.385 (2)
C6—H6A	0.9900	C3"—H3"	0.9500
C6—H6B	0.9900	C4"—C5"	1.389 (2)
C7—H7A	0.9800	C4"—H4"	0.9500
C7—H7B	0.9800	C5"—C6"	1.387 (2)
C7—H7C	0.9800	C5"—H5"	0.9500
C"A—C1"	1.508 (2)	C6"—H6"	0.9500
C"A—H"A	0.9900		
C1—O1—C7	112.68 (10)	C1"—C"A—H"A	109.5
C3—O3—H3	107.3 (13)	O6—C"A—H"B	109.5
C4—O4—H4	107.0 (13)	C1"—C"A—H"B	109.5
C1—O5—C5	114.20 (10)	H"A—C"A—H"B	108.1
C"A—O6—C6	112.58 (11)	C2'—N2—C5'	108.42 (11)
O1—C1—O5	113.76 (11)	C2'—N2—C2	130.65 (11)
O1—C1—C2	109.00 (10)	C5'—N2—C2	120.46 (11)
O5—C1—C2	109.67 (11)	O2'—C2'—N2	126.89 (13)
O1—C1—H1A	108.1	O2'—C2'—C3'	125.75 (13)
O5—C1—H1A	108.1	N2—C2'—C3'	107.33 (12)
C2—C1—H1A	108.1	C4'—C3'—C6'	130.77 (14)
N2—C2—C3	115.95 (11)	C4'—C3'—C2'	108.77 (12)
N2—C2—C1	111.33 (11)	C6'—C3'—C2'	120.46 (13)
C3—C2—C1	113.48 (11)	C3'—C4'—C7'	130.86 (14)
N2—C2—H2A	104.9	C3'—C4'—C5'	107.67 (13)
C3—C2—H2A	104.9	C7'—C4'—C5'	121.47 (13)
C1—C2—H2A	104.9	O5'—C5'—N2	124.49 (13)
O3—C3—C2	116.49 (12)	O5'—C5'—C4'	127.69 (13)
O3—C3—C4	105.26 (11)	N2—C5'—C4'	107.81 (12)
C2—C3—C4	107.55 (10)	C3'—C6'—H6'A	109.5
O3—C3—H3A	109.1	C3'—C6'—H6'B	109.5
C2—C3—H3A	109.1	H6'A—C6'—H6'B	109.5
C4—C3—H3A	109.1	C3'—C6'—H6'C	109.5
O4—C4—C3	110.24 (11)	H6'A—C6'—H6'C	109.5
O4—C4—C5	112.17 (11)	H6'B—C6'—H6'C	109.5
C3—C4—C5	109.07 (11)	C4'—C7'—H7'A	109.5
O4—C4—H4A	108.4	C4'—C7'—H7'B	109.5
C3—C4—H4A	108.4	H7'A—C7'—H7'B	109.5
C5—C4—H4A	108.4	C4'—C7'—H7'C	109.5

O5—C5—C6	106.70 (11)	H7'A—C7'—H7'C	109.5
O5—C5—C4	109.55 (11)	H7'B—C7'—H7'C	109.5
C6—C5—C4	112.02 (12)	C2"—C1"—C6"	118.68 (15)
O5—C5—H5A	109.5	C2"—C1"—C"A	122.69 (14)
C6—C5—H5A	109.5	C6"—C1"—C"A	118.56 (14)
C4—C5—H5A	109.5	C1"—C2"—C3"	120.56 (15)
O6—C6—C5	112.49 (12)	C1"—C2"—H2"	119.7
O6—C6—H6A	109.1	C3"—C2"—H2"	119.7
C5—C6—H6A	109.1	C4"—C3"—C2"	120.12 (16)
O6—C6—H6B	109.1	C4"—C3"—H3"	119.9
C5—C6—H6B	109.1	C2"—C3"—H3"	119.9
H6A—C6—H6B	107.8	C3"—C4"—C5"	119.85 (15)
O1—C7—H7A	109.5	C3"—C4"—H4"	120.1
O1—C7—H7B	109.5	C5"—C4"—H4"	120.1
H7A—C7—H7B	109.5	C6"—C5"—C4"	119.60 (15)
O1—C7—H7C	109.5	C6"—C5"—H5"	120.2
H7A—C7—H7C	109.5	C4"—C5"—H5"	120.2
H7B—C7—H7C	109.5	C5"—C6"—C1"	121.16 (15)
O6—C"A—C1"	110.61 (12)	C5"—C6"—H6"	119.4
O6—C"A—H"A	109.5	C1"—C6"—H6"	119.4
C7—O1—C1—O5	68.37 (14)	C5'—N2—C2'—O2'	177.89 (14)
C7—O1—C1—C2	−168.92 (11)	C2—N2—C2'—O2'	−10.1 (2)
C5—O5—C1—O1	65.39 (14)	C5'—N2—C2'—C3'	−0.17 (14)
C5—O5—C1—C2	−56.96 (14)	C2—N2—C2'—C3'	171.80 (12)
O1—C1—C2—N2	60.72 (14)	O2'—C2'—C3'—C4'	−177.90 (13)
O5—C1—C2—N2	−174.14 (10)	N2—C2'—C3'—C4'	0.19 (15)
O1—C1—C2—C3	−72.27 (14)	O2'—C2'—C3'—C6'	1.3 (2)
O5—C1—C2—C3	52.88 (15)	N2—C2'—C3'—C6'	179.35 (12)
N2—C2—C3—O3	−66.30 (15)	C6'—C3'—C4'—C7'	0.6 (3)
C1—C2—C3—O3	64.43 (15)	C2'—C3'—C4'—C7'	179.68 (15)
N2—C2—C3—C4	175.92 (11)	C6'—C3'—C4'—C5'	−179.17 (14)
C1—C2—C3—C4	−53.35 (14)	C2'—C3'—C4'—C5'	−0.13 (15)
O3—C3—C4—O4	54.84 (14)	C2'—N2—C5'—O5'	−178.83 (13)
C2—C3—C4—O4	179.67 (11)	C2—N2—C5'—O5'	8.2 (2)
O3—C3—C4—C5	−68.73 (13)	C2'—N2—C5'—C4'	0.09 (14)
C2—C3—C4—C5	56.10 (14)	C2—N2—C5'—C4'	−172.85 (11)
C1—O5—C5—C6	−176.25 (11)	C3'—C4'—C5'—O5'	178.91 (14)
C1—O5—C5—C4	62.29 (14)	C7'—C4'—C5'—O5'	−0.9 (2)

O4—C4—C5—O5	176.90 (10)	C3'—C4'—C5'—N2	0.03 (15)
C3—C4—C5—O5	−60.68 (14)	C7'—C4'—C5'—N2	−179.81 (13)
O4—C4—C5—C6	58.71 (15)	O6—C"A—C1"—C2"	14.41 (19)
C3—C4—C5—C6	−178.88 (11)	O6—C"A—C1"—C6"	−168.74 (13)
C"A—O6—C6—C5	84.19 (15)	C6"—C1"—C2"—C3"	−1.3 (2)
O5—C5—C6—O6	63.10 (15)	C"A—C1"—C2"—C3"	175.52 (14)
C4—C5—C6—O6	−177.02 (11)	C1"—C2"—C3"—C4"	0.0 (2)
C6—O6—C"A—C1"	−174.39 (11)	C2"—C3"—C4"—C5"	0.9 (2)
C3—C2—N2—C2'	46.33 (19)	C3"—C4"—C5"—C6"	−0.3 (2)
C1—C2—N2—C2'	−85.41 (17)	C4"—C5"—C6"—C1"	−1.1 (2)
C3—C2—N2—C5'	−142.51 (12)	C2"—C1"—C6"—C5"	1.9 (2)
C1—C2—N2—C5'	85.75 (14)	C"A—C1"—C6"—C5"	−175.07 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2′	0.86 (2)	1.84 (2)	2.6797 (15)	164.9 (19)
O4—H4···O5′^{i}	0.85 (2)	2.12 (2)	2.8396 (14)	142.9 (18)

Symmetry code: (i) *x*+1/2, −*y*+3/2, −*z*.

Appendix 2.
Supplementary Data for
$C_{20}H_{20}N_8O_8 \cdot 2(C_{16}H_{36}N)^+ \cdot SO_4^{-2}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.67639 (13)	0.63247 (16)	0.72382 (7)	0.0358 (3)
O1A	−0.7121 (6)	0.2676 (4)	0.8458 (4)	0.0735 (17)
O2A	−0.7115 (5)	0.3984 (4)	0.8281 (3)	0.0592 (13)
O3A	0.0083 (5)	0.4410 (3)	0.9325 (3)	0.0508 (12)
O4A	0.0377 (5)	0.6406 (5)	0.6103 (3)	0.081 (2)
O5A	0.3524 (6)	0.6709 (4)	0.8847 (3)	0.0644 (14)
O6A	0.3827 (5)	0.3537 (3)	0.6853 (3)	0.0496 (11)
O7A	0.5667 (8)	0.1075 (4)	0.7579 (5)	0.087 (2)
O8A	0.7803 (7)	0.0647 (4)	0.7835 (3)	0.0700 (16)
O9A	0.7496 (5)	0.5578 (3)	0.7049 (2)	0.0435 (10)
O10A	0.7724 (5)	0.7016 (3)	0.7341 (3)	0.0485 (11)
O11A	0.6368 (4)	0.6140 (3)	0.7939 (2)	0.0368 (9)
O12A	0.5512 (5)	0.6461 (4)	0.6625 (3)	0.0554 (13)
N1A	−0.6536 (6)	0.3339 (4)	0.8480 (3)	0.0436 (12)
N2A	−0.2175 (5)	0.4745 (3)	0.8748 (3)	0.0366 (11)
H2A	−0.2678	0.5172	0.8544	0.044*
N3A	−0.0410 (5)	0.5417 (4)	0.8439 (3)	0.0416 (12)
H3A	−0.1042	0.5736	0.8154	0.050*
N4A	0.0537 (5)	0.6462 (4)	0.7346 (3)	0.0504 (14)
H4A	−0.0314	0.6647	0.7254	0.061*
N5A	0.3336 (6)	0.6184 (4)	0.7683 (3)	0.0475 (13)
H5A	0.4232	0.6108	0.7786	0.057*
N6A	0.4030 (5)	0.4928 (4)	0.6700 (3)	0.0472 (13)
H6A	0.4582	0.5326	0.6631	0.057*
N7A	0.5953 (5)	0.4114 (3)	0.6933 (3)	0.0385 (11)
H7A	0.6343	0.4572	0.6830	0.046*
N8A	0.6918 (8)	0.1193 (4)	0.7660 (4)	0.0630 (18)
C1A	−0.5032 (7)	0.3369 (4)	0.8791 (4)	0.0425 (14)
C2A	−0.4313 (7)	0.4047 (4)	0.8661 (3)	0.0376 (13)
H2AA	−0.4785	0.4507	0.8394	0.045*
C3A	−0.2884 (7)	0.4059 (4)	0.8922 (3)	0.0382 (13)

C4A	−0.2252 (8)	0.3377 (5)	0.9335 (4)	0.0530 (17)
H4AA	−0.1283	0.3379	0.9538	0.064*
C5A	−0.3016 (8)	0.2690 (6)	0.9457 (5)	0.064 (2)
H5AA	−0.2549	0.2235	0.9736	0.077*
C6A	−0.4411 (8)	0.2656 (5)	0.9188 (5)	0.0583 (19)
H6AA	−0.4932	0.2187	0.9261	0.070*
C7A	−0.0781 (6)	0.4823 (4)	0.8862 (3)	0.0397 (13)
C8A	0.1024 (7)	0.5531 (5)	0.8453 (4)	0.0467 (15)
H8A	0.1315	0.5082	0.8163	0.056*
H8B	0.1589	0.5492	0.8977	0.056*
C9A	0.1282 (6)	0.6349 (5)	0.8134 (4)	0.0486 (15)
H9A	0.0979	0.6794	0.8433	0.058*
C10A	0.2810 (7)	0.6436 (5)	0.8237 (4)	0.0517 (17)
C11A	0.2548 (6)	0.6028 (5)	0.6927 (4)	0.0461 (15)
H11A	0.2982	0.6367	0.6596	0.055*
C12A	0.1034 (6)	0.6311 (6)	0.6763 (4)	0.0548 (18)
C13A	0.2607 (7)	0.5124 (5)	0.6678 (4)	0.0502 (16)
H13A	0.2270	0.4751	0.7018	0.060*
H13B	0.2017	0.5049	0.6164	0.060*
C14A	0.4533 (7)	0.4133 (5)	0.6827 (3)	0.0428 (14)
C15A	0.6824 (6)	0.3441 (4)	0.7186 (3)	0.0367 (13)
C16A	0.6382 (7)	0.2652 (4)	0.7324 (4)	0.0429 (14)
H16A	0.5434	0.2535	0.7265	0.051*
C17A	0.7371 (8)	0.2043 (4)	0.7550 (4)	0.0440 (15)
C18A	0.8784 (8)	0.2177 (5)	0.7676 (4)	0.0522 (17)
H18A	0.9433	0.1742	0.7822	0.063*
C19A	0.9190 (7)	0.2985 (4)	0.7575 (4)	0.0449 (15)
H19A	1.0142	0.3117	0.7688	0.054*
C20A	0.8237 (7)	0.3592 (4)	0.7316 (3)	0.0405 (13)
H20A	0.8541	0.4128	0.7223	0.049*
N1	0.2827	0.3553	0.1077	0.040
N2	0.3400	0.1744	0.5221	0.072
C1	0.3079	0.4424	0.0861	0.069
H11	0.3359	0.4753	0.1327	0.083*
H12	0.2190	0.4651	0.0567	0.083*
C2	0.4130	0.4572	0.0419	0.072
H21	0.4961	0.4239	0.0642	0.086*
H22	0.3750	0.4374	−0.0100	0.086*

C3	0.4547	0.5467	0.0395	0.070
H31	0.4867	0.5664	0.0918	0.084*
H32	0.3709	0.5786	0.0156	0.084*
C4	0.5640	0.5688	−0.0001	0.096
H41	0.5230	0.5705	−0.0543	0.144*
H42	0.6372	0.5272	0.0112	0.144*
H43	0.6026	0.6232	0.0171	0.144*
C5	0.2303	0.3088	0.0356	0.066
H51	0.3049	0.3067	0.0096	0.079*
H52	0.1536	0.3409	0.0035	0.079*
C6	0.1804	0.2216	0.0417	0.075
H61	0.2592	0.1854	0.0651	0.091*
H62	0.1148	0.2209	0.0736	0.091*
C7	0.1105	0.1900	−0.0355	0.083
H71	0.1806	0.1848	−0.0644	0.100*
H72	0.0428	0.2320	−0.0610	0.100*
C8	0.0373	0.1080	−0.0384	0.088
H81	−0.0389	0.1136	−0.0145	0.132*
H82	0.1021	0.0661	−0.0117	0.132*
H83	0.0012	0.0911	−0.0907	0.132*
C9	0.4125	0.3154	0.1526	0.062
H91	0.4732	0.3049	0.1190	0.074*
H92	0.3886	0.2611	0.1706	0.074*
C10	0.4926	0.3644	0.2192	0.064
H101	0.5333	0.4135	0.2010	0.077*
H102	0.4284	0.3844	0.2480	0.077*
C11	0.6059	0.3152	0.2705	0.099
H111	0.6598	0.2875	0.2395	0.118*
H112	0.5628	0.2712	0.2942	0.118*
C12	0.7046	0.3627	0.3318	0.150*
H121	0.7841	0.3804	0.3141	0.225*
H122	0.7358	0.3271	0.3759	0.225*
H123	0.6580	0.4115	0.3452	0.225*
C13	0.1821	0.3585	0.1552	0.064
H131	0.2103	0.4040	0.1918	0.077*
H132	0.1907	0.3062	0.1841	0.077*
C14	0.0321	0.3706	0.1160	0.083
H141	−0.0057	0.3179	0.0919	0.099*

H142	0.0243	0.4126	0.0761	0.099*
C15	−0.0528	0.3980	0.1683	0.115
H151	−0.0385	0.3588	0.2108	0.138*
H152	−0.0211	0.4533	0.1887	0.138*
C16	−0.2041	0.4020	0.1293	0.186
H161	−0.2424	0.3459	0.1232	0.280*
H162	−0.2164	0.4276	0.0799	0.280*
H163	−0.2519	0.4350	0.1593	0.280*
C17	0.2794	0.2327	0.4590	0.092*
H171	0.1802	0.2194	0.4409	0.111*
H172	0.3220	0.2198	0.4175	0.111*
C18	0.2913	0.3250	0.4720	0.150*
H181	0.3879	0.3433	0.4797	0.180*
H182	0.2592	0.3404	0.5166	0.180*
C19	0.2008	0.3639	0.4021	0.150*
H191	0.2082	0.3335	0.3568	0.180*
H192	0.1033	0.3644	0.4041	0.180*
C20	0.2559	0.4509	0.4023	0.150*
H201	0.2913	0.4590	0.3581	0.225*
H202	0.3303	0.4595	0.4477	0.225*
H203	0.1818	0.4906	0.4013	0.225*
C21	0.3206	0.0880	0.4912	0.085
H211	0.4017	0.0583	0.5220	0.102*
H212	0.3391	0.0941	0.4413	0.102*
C22	0.2091	0.0230	0.4777	0.150*
H221	0.1410	0.0352	0.4298	0.180*
H222	0.1610	0.0264	0.5181	0.180*
C23	0.2620	−0.0641	0.4748	0.150*
H231	0.3162	−0.0735	0.4377	0.180*
H232	0.3051	−0.0895	0.5239	0.180*
C24	0.1088	−0.0775	0.4462	0.150*
H241	0.0603	−0.0260	0.4510	0.225*
H242	0.0795	−0.1211	0.4756	0.225*
H243	0.0872	−0.0940	0.3934	0.225*
C25	0.2701	0.1866	0.5840	0.085*
H251	0.1722	0.1966	0.5584	0.102*
H252	0.3060	0.2398	0.6076	0.102*
C26	0.2676	0.1295	0.6483	0.150*

H261	0.3552	0.1311	0.6879	0.180*
H262	0.2465	0.0717	0.6315	0.180*
C27	0.1509	0.1689	0.6737	0.150*
H271	0.1709	0.2248	0.6958	0.180*
H272	0.0603	0.1666	0.6366	0.180*
C28	0.1776	0.0990	0.7299	0.150*
H281	0.1623	0.1184	0.7773	0.225*
H282	0.2731	0.0802	0.7381	0.225*
H283	0.1150	0.0530	0.7106	0.225*
C29	0.4895	0.1924	0.5559	0.113
H291	0.5242	0.1511	0.5959	0.136*
H292	0.4958	0.2473	0.5804	0.136*
C30	0.5859	0.1928	0.5053	0.150
H301	0.5574	0.2389	0.4693	0.180*
H302	0.5696	0.1409	0.4758	0.180*
C31	0.7395	0.2004	0.5378	0.150*
H311	0.7859	0.2255	0.5019	0.180*
H312	0.7625	0.2321	0.5852	0.180*
C32	0.7729	0.1095	0.5502	0.150*
H321	0.8524	0.0959	0.5308	0.225*
H322	0.6935	0.0764	0.5239	0.225*
H323	0.7946	0.0972	0.6039	0.225*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0316 (6)	0.0390 (7)	0.0351 (6)	0.0004 (6)	0.0056 (5)	0.0053 (6)
O1A	0.052 (3)	0.067 (4)	0.111 (5)	0.000 (3)	0.039 (3)	0.021 (3)
O2A	0.045 (3)	0.055 (3)	0.079 (4)	0.012 (2)	0.018 (3)	0.002 (3)
O3A	0.041 (2)	0.063 (3)	0.046 (2)	0.010 (2)	0.008 (2)	0.019 (2)
O4A	0.051 (3)	0.141 (6)	0.056 (3)	0.048 (4)	0.021 (2)	0.036 (4)
O5A	0.053 (3)	0.080 (4)	0.063 (3)	−0.016 (3)	0.021 (3)	−0.020 (3)
O6A	0.045 (2)	0.052 (3)	0.052 (3)	−0.009 (2)	0.011 (2)	−0.006 (2)
O7A	0.086 (4)	0.047 (3)	0.138 (6)	−0.010 (3)	0.048 (4)	0.008 (3)
O8A	0.100 (5)	0.041 (3)	0.077 (4)	0.013 (3)	0.037 (3)	0.016 (3)
O9A	0.048 (2)	0.041 (2)	0.044 (2)	−0.0043 (19)	0.0147 (19)	−0.0030 (19)
O10A	0.054 (3)	0.039 (2)	0.059 (3)	−0.003 (2)	0.026 (2)	0.003 (2)
O11A	0.0309 (18)	0.040 (2)	0.040 (2)	0.0028 (16)	0.0103 (16)	0.0079 (17)

O12A	0.045 (2)	0.068 (4)	0.052 (3)	0.006 (2)	0.011 (2)	0.013 (2)
N1A	0.047 (3)	0.043 (3)	0.050 (3)	0.002 (3)	0.029 (2)	0.004 (2)
N2A	0.036 (2)	0.042 (3)	0.031 (2)	0.006 (2)	0.0063 (19)	0.008 (2)
N3A	0.035 (3)	0.049 (3)	0.038 (3)	0.007 (2)	0.006 (2)	0.013 (2)
N4A	0.036 (3)	0.058 (4)	0.062 (3)	0.013 (3)	0.019 (2)	0.018 (3)
N5A	0.041 (3)	0.050 (3)	0.054 (3)	0.007 (3)	0.016 (2)	0.005 (3)
N6A	0.032 (3)	0.055 (3)	0.052 (3)	0.005 (2)	0.006 (2)	0.003 (3)
N7A	0.041 (3)	0.037 (3)	0.039 (3)	0.001 (2)	0.014 (2)	0.000 (2)
N8A	0.101 (5)	0.044 (4)	0.054 (3)	−0.012 (4)	0.037 (4)	−0.003 (3)
C1A	0.045 (3)	0.047 (4)	0.043 (3)	0.005 (3)	0.024 (3)	0.000 (3)
C2A	0.049 (3)	0.038 (3)	0.033 (3)	0.004 (3)	0.024 (3)	0.001 (2)
C3A	0.050 (3)	0.039 (3)	0.031 (3)	−0.001 (3)	0.021 (2)	−0.002 (2)
C4A	0.048 (4)	0.055 (4)	0.053 (4)	0.008 (3)	0.006 (3)	0.017 (3)
C5A	0.053 (4)	0.060 (5)	0.075 (5)	0.002 (4)	0.008 (4)	0.028 (4)
C6A	0.062 (4)	0.053 (4)	0.064 (5)	0.005 (4)	0.023 (4)	0.023 (4)
C7A	0.039 (3)	0.054 (4)	0.025 (2)	0.002 (3)	0.007 (2)	0.002 (3)
C8A	0.039 (3)	0.053 (4)	0.050 (4)	0.009 (3)	0.014 (3)	0.005 (3)
C9A	0.045 (3)	0.048 (4)	0.058 (4)	0.011 (3)	0.021 (3)	0.007 (3)
C10A	0.047 (3)	0.055 (4)	0.057 (4)	0.003 (3)	0.020 (3)	0.003 (3)
C11A	0.032 (3)	0.061 (4)	0.046 (3)	0.010 (3)	0.012 (3)	0.018 (3)
C12A	0.038 (3)	0.073 (5)	0.056 (4)	0.019 (4)	0.017 (3)	0.035 (4)
C13A	0.035 (3)	0.066 (5)	0.052 (4)	0.009 (3)	0.014 (3)	0.012 (3)
C14A	0.040 (3)	0.053 (4)	0.036 (3)	−0.009 (3)	0.010 (3)	−0.006 (3)
C15A	0.043 (3)	0.042 (3)	0.028 (2)	0.001 (3)	0.015 (2)	0.002 (2)
C16A	0.051 (4)	0.039 (3)	0.042 (3)	0.002 (3)	0.016 (3)	−0.003 (3)
C17A	0.059 (4)	0.034 (3)	0.044 (3)	−0.002 (3)	0.022 (3)	0.006 (3)
C18A	0.060 (4)	0.043 (4)	0.054 (4)	0.011 (3)	0.017 (3)	0.007 (3)
C19A	0.047 (3)	0.049 (4)	0.042 (3)	0.005 (3)	0.018 (3)	0.002 (3)
C20A	0.048 (3)	0.038 (3)	0.042 (3)	0.001 (3)	0.022 (3)	−0.003 (3)
N1	0.032	0.046	0.041	0.010	0.010	0.003
N2	0.056	0.112	0.041	−0.010	−0.004	−0.017
C1	0.065	0.068	0.071	0.003	0.012	0.012
C2	0.055	0.067	0.092	0.004	0.016	0.005
C3	0.069	0.072	0.078	0.003	0.034	0.009
C4	0.090	0.076	0.128	−0.014	0.037	−0.021
C5	0.060	0.076	0.062	−0.004	0.019	0.009
C6	0.046	0.068	0.105	−0.002	0.005	−0.036
C7	0.077	0.101	0.069	0.026	0.014	0.023

C8	0.072	0.101	0.086	−0.031	0.011	−0.029
C9	0.052	0.067	0.058	0.006	−0.002	0.001
C10	0.061	0.076	0.048	−0.010	0.001	0.001
C11	0.071	0.107	0.095	−0.015	−0.021	0.034
C13	0.061	0.070	0.066	0.011	0.026	0.011
C14	0.049	0.109	0.094	0.013	0.027	−0.004
C15	0.057	0.154	0.146	0.016	0.049	0.036
C16	0.079	0.312	0.195	0.091	0.084	0.090
C21	0.047	0.139	0.079	−0.013	0.038	−0.045
C29	0.095	0.127	0.099	−0.054	−0.009	−0.004
C30	0.076	0.236	0.126	−0.028	0.003	−0.074

Geometric parameters (Å, º)

S1A—O10A	1.455 (5)	C5—H51	0.9900
S1A—O12A	1.477 (5)	C5—H52	0.9900
S1A—O11A	1.479 (4)	C6—C7	1.5088
S1A—O9A	1.500 (5)	C6—H61	0.9900
O1A—N1A	1.218 (8)	C6—H62	0.9900
O2A—N1A	1.203 (7)	C7—C8	1.5097
O3A—C7A	1.245 (8)	C7—H71	0.9900
O4A—C12A	1.237 (9)	C7—H72	0.9900
O5A—C10A	1.251 (9)	C8—H81	0.9800
O6A—C14A	1.204 (8)	C8—H82	0.9800
O7A—N8A	1.243 (10)	C8—H83	0.9800
O8A—N8A	1.235 (9)	C9—C10	1.5093
N1A—C1A	1.473 (9)	C9—H91	0.9900
N2A—C7A	1.368 (8)	C9—H92	0.9900
N2A—C3A	1.400 (8)	C10—C11	1.5083
N2A—H2A	0.8800	C10—H101	0.9900
N3A—C7A	1.349 (8)	C10—H102	0.9900
N3A—C8A	1.447 (8)	C11—C12	1.5092
N3A—H3A	0.8800	C11—H111	0.9900
N4A—C12A	1.321 (9)	C11—H112	0.9900
N4A—C9A	1.467 (9)	C12—H121	0.9800
N4A—H4A	0.8800	C12—H122	0.9800
N5A—C10A	1.331 (9)	C12—H123	0.9800
N5A—C11A	1.440 (9)	C13—C14	1.5090

N5A—H5A	0.8800	C13—H131	0.9900
N6A—C14A	1.378 (9)	C13—H132	0.9900
N6A—C13A	1.455 (8)	C14—C15	1.5092
N6A—H6A	0.8800	C14—H141	0.9900
N7A—C14A	1.391 (8)	C14—H142	0.9900
N7A—C15A	1.400 (8)	C15—C16	1.5086
N7A—H7A	0.8800	C15—H151	0.9900
N8A—C17A	1.478 (9)	C15—H152	0.9900
C1A—C2A	1.367 (9)	C16—H161	0.9800
C1A—C6A	1.421 (10)	C16—H162	0.9800
C2A—C3A	1.393 (9)	C16—H163	0.9800
C2A—H2AA	0.9500	C17—C18	1.5103
C3A—C4A	1.397 (10)	C17—H171	0.9900
C4A—C5A	1.399 (11)	C17—H172	0.9900
C4A—H4AA	0.9500	C18—C19	1.5117
C5A—C6A	1.363 (11)	C18—H181	0.9900
C5A—H5AA	0.9500	C18—H182	0.9900
C6A—H6AA	0.9500	C19—C20	1.5097
C8A—C9A	1.497 (10)	C19—H191	0.9900
C8A—H8A	0.9900	C19—H192	0.9900
C8A—H8B	0.9900	C20—H201	0.9800
C9A—C10A	1.505 (9)	C20—H202	0.9800
C9A—H9A	1.0000	C20—H203	0.9800
C11A—C13A	1.538 (11)	C21—C22	1.5095
C11A—C12A	1.543 (8)	C21—H211	0.9900
C11A—H11A	1.0000	C21—H212	0.9900
C13A—H13A	0.9900	C22—C23	1.5100
C13A—H13B	0.9900	C22—H221	0.9900
C15A—C16A	1.395 (9)	C22—H222	0.9900
C15A—C20A	1.399 (9)	C23—C24	1.5097
C16A—C17A	1.384 (10)	C23—H231	0.9900
C16A—H16A	0.9500	C23—H232	0.9900
C17A—C18A	1.396 (11)	C24—H241	0.9800
C18A—C19A	1.394 (10)	C24—H242	0.9800
C18A—H18A	0.9500	C24—H243	0.9800
C19A—C20A	1.368 (9)	C25—C26	1.5100
C19A—H19A	0.9500	C25—H251	0.9900
C20A—H20A	0.9500	C25—H252	0.9900

N1—C13	1.4994	C26—C27	1.5114
N1—C9	1.5006	C26—H261	0.9900
N1—C5	1.5011	C26—H262	0.9900
N1—C1	1.5011	C27—C28	1.5093
N2—C25	1.4994	C27—H271	0.9900
N2—C29	1.4999	C27—H272	0.9900
N2—C17	1.5011	C28—H281	0.9800
N2—C21	1.5014	C28—H282	0.9800
C1—C2	1.5099	C28—H283	0.9800
C1—H11	0.9900	C29—C30	1.5097
C1—H12	0.9900	C29—H291	0.9900
C2—C3	1.5090	C29—H292	0.9900
C2—H21	0.9900	C30—C31	1.5115
C2—H22	0.9900	C30—H301	0.9900
C3—C4	1.5094	C30—H302	0.9900
C3—H31	0.9900	C31—C32	1.5101
C3—H32	0.9900	C31—H311	0.9900
C4—H41	0.9800	C31—H312	0.9900
C4—H42	0.9800	C32—H321	0.9800
C4—H43	0.9800	C32—H322	0.9800
C5—C6	1.5091	C32—H323	0.9800
O10A—S1A—O12A	113.1 (3)	C6—C7—H72	108.3
O10A—S1A—O11A	110.9 (3)	C8—C7—H72	108.3
O12A—S1A—O11A	109.5 (3)	H71—C7—H72	107.4
O10A—S1A—O9A	107.4 (3)	C7—C8—H81	109.5
O12A—S1A—O9A	108.3 (3)	C7—C8—H82	109.5
O11A—S1A—O9A	107.4 (2)	H81—C8—H82	109.5
O2A—N1A—O1A	124.0 (6)	C7—C8—H83	109.5
O2A—N1A—C1A	117.3 (6)	H81—C8—H83	109.5
O1A—N1A—C1A	118.7 (6)	H82—C8—H83	109.5
C7A—N2A—C3A	126.8 (5)	N1—C9—C10	115.6
C7A—N2A—H2A	116.6	N1—C9—H91	108.4
C3A—N2A—H2A	116.6	C10—C9—H91	108.4
C7A—N3A—C8A	120.1 (5)	N1—C9—H92	108.4
C7A—N3A—H3A	119.9	C10—C9—H92	108.4
C8A—N3A—H3A	119.9	H91—C9—H92	107.4
C12A—N4A—C9A	125.6 (5)	C11—C10—C9	113.3
C12A—N4A—H4A	117.2	C11—C10—H101	108.9

C9A—N4A—H4A	117.2	C9—C10—H101	108.9
C10A—N5A—C11A	124.8 (6)	C11—C10—H102	108.9
C10A—N5A—H5A	117.6	C9—C10—H102	108.9
C11A—N5A—H5A	117.6	H101—C10—H102	107.7
C14A—N6A—C13A	121.5 (6)	C10—C11—C12	116.7
C14A—N6A—H6A	119.3	C10—C11—H111	108.1
C13A—N6A—H6A	119.3	C12—C11—H111	108.1
C14A—N7A—C15A	126.5 (6)	C10—C11—H112	108.1
C14A—N7A—H7A	116.7	C12—C11—H112	108.1
C15A—N7A—H7A	116.7	H111—C11—H112	107.3
O8A—N8A—O7A	124.1 (7)	C11—C12—H121	109.5
O8A—N8A—C17A	118.2 (7)	C11—C12—H122	109.5
O7A—N8A—C17A	117.7 (7)	H121—C12—H122	109.5
C2A—C1A—C6A	123.9 (6)	C11—C12—H123	109.5
C2A—C1A—N1A	119.6 (6)	H121—C12—H123	109.5
C6A—C1A—N1A	116.5 (6)	H122—C12—H123	109.5
C1A—C2A—C3A	119.7 (6)	N1—C13—C14	117.6
C1A—C2A—H2AA	120.1	N1—C13—H131	107.9
C3A—C2A—H2AA	120.1	C14—C13—H131	107.9
C2A—C3A—C4A	117.5 (6)	N1—C13—H132	107.9
C2A—C3A—N2A	118.2 (5)	C14—C13—H132	107.9
C4A—C3A—N2A	124.3 (6)	H131—C13—H132	107.2
C3A—C4A—C5A	121.4 (7)	C13—C14—C15	112.9
C3A—C4A—H4AA	119.3	C13—C14—H141	109.0
C5A—C4A—H4AA	119.3	C15—C14—H141	109.0
C6A—C5A—C4A	121.9 (7)	C13—C14—H142	109.0
C6A—C5A—H5AA	119.0	C15—C14—H142	109.0
C4A—C5A—H5AA	119.0	H141—C14—H142	107.8
C5A—C6A—C1A	115.5 (7)	C16—C15—C14	111.9
C5A—C6A—H6AA	122.3	C16—C15—H151	109.2
C1A—C6A—H6AA	122.3	C14—C15—H151	109.2
O3A—C7A—N3A	122.1 (6)	C16—C15—H152	109.2
O3A—C7A—N2A	124.3 (6)	C14—C15—H152	109.2
N3A—C7A—N2A	113.6 (5)	H151—C15—H152	107.9
N3A—C8A—C9A	112.2 (5)	C15—C16—H161	109.5
N3A—C8A—H8A	109.2	C15—C16—H162	109.5
C9A—C8A—H8A	109.2	H161—C16—H162	109.5
N3A—C8A—H8B	109.2	C15—C16—H163	109.5

C9A—C8A—H8B	109.2	H161—C16—H163	109.5
H8A—C8A—H8B	107.9	H162—C16—H163	109.5
N4A—C9A—C8A	113.9 (6)	N2—C17—C18	119.7
N4A—C9A—C10A	111.1 (5)	N2—C17—H171	107.4
C8A—C9A—C10A	107.8 (6)	C18—C17—H171	107.4
N4A—C9A—H9A	108.0	N2—C17—H172	107.4
C8A—C9A—H9A	108.0	C18—C17—H172	107.4
C10A—C9A—H9A	108.0	H171—C17—H172	106.9
O5A—C10A—N5A	123.4 (6)	C17—C18—C19	105.6
O5A—C10A—C9A	118.6 (6)	C17—C18—H181	110.6
N5A—C10A—C9A	117.9 (6)	C19—C18—H181	110.6
N5A—C11A—C13A	113.7 (5)	C17—C18—H182	110.6
N5A—C11A—C12A	114.1 (6)	C19—C18—H182	110.6
C13A—C11A—C12A	109.5 (6)	H181—C18—H182	108.8
N5A—C11A—H11A	106.3	C20—C19—C18	104.2
C13A—C11A—H11A	106.3	C20—C19—H191	110.9
C12A—C11A—H11A	106.3	C18—C19—H191	110.9
O4A—C12A—N4A	124.2 (6)	C20—C19—H192	110.9
O4A—C12A—C11A	118.7 (6)	C18—C19—H192	110.9
N4A—C12A—C11A	117.0 (6)	H191—C19—H192	108.9
N6A—C13A—C11A	108.1 (6)	C19—C20—H201	109.5
N6A—C13A—H13A	110.1	C19—C20—H202	109.5
C11A—C13A—H13A	110.1	H201—C20—H202	109.5
N6A—C13A—H13B	110.1	C19—C20—H203	109.5
C11A—C13A—H13B	110.1	H201—C20—H203	109.5
H13A—C13A—H13B	108.4	H202—C20—H203	109.5
O6A—C14A—N6A	123.9 (6)	N2—C21—C22	136.7
O6A—C14A—N7A	124.9 (6)	N2—C21—H211	103.0
N6A—C14A—N7A	111.2 (6)	C22—C21—H211	103.0
C16A—C15A—C20A	119.0 (6)	N2—C21—H212	103.0
C16A—C15A—N7A	124.8 (6)	C22—C21—H212	103.0
C20A—C15A—N7A	116.2 (6)	H211—C21—H212	105.1
C17A—C16A—C15A	117.8 (6)	C21—C22—C23	113.6
C17A—C16A—H16A	121.1	C21—C22—H221	108.8
C15A—C16A—H16A	121.1	C23—C22—H221	108.8
C16A—C17A—C18A	124.2 (6)	C21—C22—H222	108.8
C16A—C17A—N8A	118.6 (7)	C23—C22—H222	108.8
C18A—C17A—N8A	117.2 (6)	H221—C22—H222	107.7

C19A—C18A—C17A	116.3 (6)	C24—C23—C22	79.0
C19A—C18A—H18A	121.9	C24—C23—H231	115.4
C17A—C18A—H18A	121.9	C22—C23—H231	115.4
C20A—C19A—C18A	121.0 (7)	C24—C23—H232	115.4
C20A—C19A—H19A	119.5	C22—C23—H232	115.4
C18A—C19A—H19A	119.5	H231—C23—H232	112.4
C19A—C20A—C15A	121.6 (6)	C23—C24—H241	109.5
C19A—C20A—H20A	119.2	C23—C24—H242	109.5
C15A—C20A—H20A	119.2	H241—C24—H242	109.5
C13—N1—C9	108.2	C23—C24—H243	109.5
C13—N1—C5	113.6	H241—C24—H243	109.5
C9—N1—C5	109.5	H242—C24—H243	109.5
C13—N1—C1	108.0	N2—C25—C26	128.7
C9—N1—C1	111.5	N2—C25—H251	105.1
C5—N1—C1	106.1	C26—C25—H251	105.1
C25—N2—C29	105.8	N2—C25—H252	105.1
C25—N2—C17	109.5	C26—C25—H252	105.1
C29—N2—C17	111.4	H251—C25—H252	105.9
C25—N2—C21	111.8	C25—C26—C27	99.1
C29—N2—C21	110.9	C25—C26—H261	112.0
C17—N2—C21	107.5	C27—C26—H261	112.0
N1—C1—C2	118.8	C25—C26—H262	112.0
N1—C1—H11	107.6	C27—C26—H262	112.0
C2—C1—H11	107.6	H261—C26—H262	109.6
N1—C1—H12	107.6	C28—C27—C26	83.2
C2—C1—H12	107.6	C28—C27—H271	114.8
H11—C1—H12	107.0	C26—C27—H271	114.8
C3—C2—C1	114.0	C28—C27—H272	114.8
C3—C2—H21	108.8	C26—C27—H272	114.8
C1—C2—H21	108.8	H271—C27—H272	111.8
C3—C2—H22	108.8	C27—C28—H281	109.5
C1—C2—H22	108.8	C27—C28—H282	109.5
H21—C2—H22	107.6	H281—C28—H282	109.5
C2—C3—C4	119.0	C27—C28—H283	109.5
C2—C3—H31	107.6	H281—C28—H283	109.5
C4—C3—H31	107.6	H282—C28—H283	109.5
C2—C3—H32	107.6	N2—C29—C30	118.4
C4—C3—H32	107.6	N2—C29—H291	107.7

H31—C3—H32	107.0	C30—C29—H291	107.7
C3—C4—H41	109.5	N2—C29—H292	107.7
C3—C4—H42	109.5	C30—C29—H292	107.7
H41—C4—H42	109.5	H291—C29—H292	107.1
C3—C4—H43	109.5	C29—C30—C31	120.5
H41—C4—H43	109.5	C29—C30—H301	107.2
H42—C4—H43	109.5	C31—C30—H301	107.2
N1—C5—C6	116.7	C29—C30—H302	107.2
N1—C5—H51	108.1	C31—C30—H302	107.2
C6—C5—H51	108.1	H301—C30—H302	106.8
N1—C5—H52	108.1	C32—C31—C30	98.4
C6—C5—H52	108.1	C32—C31—H311	112.1
H51—C5—H52	107.3	C30—C31—H311	112.1
C7—C6—C5	109.2	C32—C31—H312	112.1
C7—C6—H61	109.8	C30—C31—H312	112.1
C5—C6—H61	109.8	H311—C31—H312	109.7
C7—C6—H62	109.8	C31—C32—H321	109.5
C5—C6—H62	109.8	C31—C32—H322	109.5
H61—C6—H62	108.3	H321—C32—H322	109.5
C6—C7—C8	115.7	C31—C32—H323	109.5
C6—C7—H71	108.3	H321—C32—H323	109.5
C8—C7—H71	108.3	H322—C32—H323	109.5
O2A—N1A—C1A—C2A	−17.7 (8)	C15A—C16A—C17A—N8A	−176.8 (5)
O1A—N1A—C1A—C2A	164.2 (6)	O8A—N8A—C17A—C16A	177.5 (6)
O2A—N1A—C1A—C6A	165.1 (6)	O7A—N8A—C17A—C16A	−3.6 (10)
O1A—N1A—C1A—C6A	−13.0 (9)	O8A—N8A—C17A—C18A	−1.9 (9)
C6A—C1A—C2A—C3A	0.3 (10)	O7A—N8A—C17A—C18A	177.0 (7)
N1A—C1A—C2A—C3A	−176.8 (5)	C16A—C17A—C18A—C19A	1.2 (10)
C1A—C2A—C3A—C4A	−2.3 (9)	N8A—C17A—C18A—C19A	−179.5 (6)
C1A—C2A—C3A—N2A	177.0 (5)	C17A—C18A—C19A—C20A	−4.4 (10)
C7A—N2A—C3A—C2A	−170.4 (5)	C18A—C19A—C20A—C15A	3.9 (10)

C7A—N2A—C3A—C4A	8.9 (9)	C16A—C15A—C20A—C19A	0.0 (9)
C2A—C3A—C4A—C5A	2.6 (11)	N7A—C15A—C20A—C19A	179.0 (5)
N2A—C3A—C4A—C5A	−176.7 (7)	C13—N1—C1—C2	176.1
C3A—C4A—C5A—C6A	−0.8 (14)	C9—N1—C1—C2	57.4
C4A—C5A—C6A—C1A	−1.3 (13)	C5—N1—C1—C2	−61.8
C2A—C1A—C6A—C5A	1.6 (11)	N1—C1—C2—C3	−166.0
N1A—C1A—C6A—C5A	178.7 (7)	C1—C2—C3—C4	177.3
C8A—N3A—C7A—O3A	6.9 (10)	C13—N1—C5—C6	−54.3
C8A—N3A—C7A—N2A	−175.2 (6)	C9—N1—C5—C6	66.7
C3A—N2A—C7A—O3A	−22.2 (10)	C1—N1—C5—C6	−172.8
C3A—N2A—C7A—N3A	160.0 (5)	N1—C5—C6—C7	170.7
C7A—N3A—C8A—C9A	−163.7 (6)	C5—C6—C7—C8	−171.8
C12A—N4A—C9A—C8A	−94.8 (8)	C13—N1—C9—C10	−67.3
C12A—N4A—C9A—C10A	27.1 (11)	C5—N1—C9—C10	168.5
N3A—C8A—C9A—N4A	−61.2 (7)	C1—N1—C9—C10	51.3
N3A—C8A—C9A—C10A	175.1 (6)	N1—C9—C10—C11	168.8
C11A—N5A—C10A—O5A	−166.6 (7)	C9—C10—C11—C12	170.9
C11A—N5A—C10A—C9A	16.2 (11)	C9—N1—C13—C14	−161.2
N4A—C9A—C10A—O5A	149.5 (7)	C5—N1—C13—C14	−39.5
C8A—C9A—C10A—O5A	−85.1 (9)	C1—N1—C13—C14	78.0
N4A—C9A—C10A—N5A	−33.1 (10)	N1—C13—C14—C15	−162.9
C8A—C9A—C10A—N5A	92.3 (8)	C13—C14—C15—C16	−174.7

C10A—N5A—C11A—C13A	−117.2 (7)	C25—N2—C17—C18	62.1
C10A—N5A—C11A—C12A	9.4 (10)	C29—N2—C17—C18	−54.5
C9A—N4A—C12A—O4A	179.4 (9)	C21—N2—C17—C18	−176.3
C9A—N4A—C12A—C11A	−2.9 (12)	N2—C17—C18—C19	−171.0
N5A—C11A—C12A—O4A	161.4 (8)	C17—C18—C19—C20	−158.2
C13A—C11A—C12A—O4A	−69.8 (10)	C25—N2—C21—C22	34.2
N5A—C11A—C12A—N4A	−16.4 (10)	C29—N2—C21—C22	152.1
C13A—C11A—C12A—N4A	112.3 (8)	C17—N2—C21—C22	−85.9
C14A—N6A—C13A—C11A	151.6 (6)	N2—C21—C22—C23	−156.3
N5A—C11A—C13A—N6A	−62.1 (7)	C21—C22—C23—C24	−168.6
C12A—C11A—C13A—N6A	168.9 (5)	C29—N2—C25—C26	−77.5
C13A—N6A—C14A—O6A	7.8 (10)	C17—N2—C25—C26	162.3
C13A—N6A—C14A—N7A	−171.2 (6)	C21—N2—C25—C26	43.4
C15A—N7A—C14A—O6A	−9.5 (10)	N2—C25—C26—C27	−165.3
C15A—N7A—C14A—N6A	169.5 (5)	C25—C26—C27—C28	178.3
C14A—N7A—C15A—C16A	4.8 (9)	C25—N2—C29—C30	−174.7
C14A—N7A—C15A—C20A	−174.1 (5)	C17—N2—C29—C30	−55.8
C20A—C15A—C16A—C17A	−3.1 (8)	C21—N2—C29—C30	63.9
N7A—C15A—C16A—C17A	178.0 (6)	N2—C29—C30—C31	−172.7
C15A—C16A—C17A—C18A	2.6 (10)	C29—C30—C31—C32	88.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*A*···O11*A*^{i}	0.88	2.02	2.886 (6)	170
N3*A*—H3*A*···O9*A*^{i}	0.88	2.20	2.884 (7)	134
N4*A*—H4*A*···O10*A*^{i}	0.88	2.11	2.963 (7)	165
N5*A*—H5*A*···O11*A*	0.88	2.09	2.963 (7)	169
N6*A*—H6*A*···O12*A*	0.88	2.06	2.912 (8)	163
N7*A*—H7*A*···O9*A*	0.88	1.98	2.805 (7)	156

Symmetry code: (i) *x*−1, *y*, *z*.

Appendix 3.
Supplementary Data for
$C_{20}H_{20}N_8O_8 \cdot 2(C_{16}H_{36}N)^+ \cdot SO_4^{-2} \cdot H_2O$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1A	0.32594 (12)	0.31933 (7)	−0.04743 (2)	0.0415 (3)	
S2A	0.83114 (15)	0.42579 (8)	0.07347 (3)	0.0488 (3)	
O1A	−0.3052 (4)	0.3816 (3)	−0.10340 (7)	0.0498 (11)	
O2A	−0.4275 (4)	0.3297 (3)	−0.08116 (9)	0.0679 (16)	
O3A	0.4979 (4)	0.2153 (3)	0.07036 (7)	0.0652 (15)	
O4A	0.6694 (4)	0.1895 (3)	−0.01361 (7)	0.0512 (11)	
O5A	1.4700 (4)	0.5249 (3)	0.12249 (8)	0.0609 (13)	
O6A	1.5803 (4)	0.4983 (3)	0.09400 (8)	0.0555 (11)	
N1A	−0.3205 (4)	0.3491 (2)	−0.08610 (7)	0.0347 (9)	
N2A	0.1101 (4)	0.2895 (2)	−0.02470 (7)	0.0264 (8)	
H2A	0.0832	0.2732	−0.0118	0.032*	
N3A	0.3038 (4)	0.2823 (3)	−0.00463 (7)	0.0366 (10)	
H3A	0.2558	0.2762	0.0071	0.044*	
N4A	0.4532 (4)	0.1997 (3)	0.03231 (8)	0.0450 (12)	
H4AA	0.3751	0.1837	0.0347	0.054*	
N5A	0.7146 (4)	0.2098 (2)	0.02447 (8)	0.0363 (10)	
H5AA	0.7987	0.2048	0.0227	0.044*	
N6A	0.8565 (4)	0.3052 (3)	0.05592 (8)	0.0389 (10)	
H6A	0.9049	0.2720	0.0512	0.047*	
N7A	1.0491 (4)	0.3563 (2)	0.06336 (7)	0.0317 (9)	
H7A	1.0756	0.3241	0.0544	0.038*	
N8A	1.4800 (5)	0.4968 (3)	0.10439 (8)	0.0418 (11)	
C1A	−0.2060 (5)	0.3334 (3)	−0.07049 (8)	0.0317 (10)	
C2A	−0.0855 (5)	0.3550 (3)	−0.07576 (8)	0.0328 (10)	
H2AA	−0.0762	0.3796	−0.0895	0.039*	
C3A	0.0235 (5)	0.3414 (3)	−0.06127 (8)	0.0324 (10)	
H3AA	0.1073	0.3574	−0.0647	0.039*	
C4A	0.0084 (4)	0.3037 (2)	−0.04136 (8)	0.0249 (9)	
C5A	−0.1141 (5)	0.2806 (3)	−0.03693 (9)	0.0338 (11)	
H5AB	−0.1236	0.2541	−0.0236	0.041*	
C6A	−0.2236 (5)	0.2946 (3)	−0.05119 (9)	0.0363 (11)	

H6AA	−0.3076	0.2784	−0.0479	0.044*
C7A	0.2431 (4)	0.2962 (2)	−0.02476 (8)	0.0248 (9)
C8A	0.4459 (5)	0.2766 (3)	−0.00070 (9)	0.0395 (13)
H8AA	0.4780	0.3121	0.0101	0.047*
H8AB	0.4870	0.2840	−0.0153	0.047*
C9A	0.4864 (5)	0.2089 (3)	0.00881 (9)	0.0329 (10)
H9AA	0.4392	0.1737	−0.0008	0.039*
C10A	0.5343 (5)	0.2141 (4)	0.05070 (9)	0.0446 (14)
C11A	0.6784 (5)	0.2263 (3)	0.04731 (9)	0.0400 (13)
H11A	0.7295	0.1956	0.0581	0.048*
C12A	0.6336 (5)	0.2015 (3)	0.00570 (9)	0.0350 (11)
C13A	0.7124 (5)	0.2962 (3)	0.05443 (10)	0.0425 (13)
H13A	0.6715	0.3284	0.0432	0.051*
H13B	0.6780	0.3057	0.0695	0.051*
C14A	0.9164 (5)	0.3600 (3)	0.06398 (8)	0.0366 (12)
C15A	1.1515 (5)	0.3937 (3)	0.07416 (8)	0.0310 (10)
C16A	1.1358 (5)	0.4398 (3)	0.09174 (9)	0.0356 (11)
H16A	1.0514	0.4485	0.0969	0.043*
C17A	1.2456 (5)	0.4731 (3)	0.10170 (9)	0.0362 (11)
H17A	1.2365	0.5042	0.1139	0.043*
C18A	1.3649 (5)	0.4610 (3)	0.09394 (9)	0.0337 (11)
C19A	1.3834 (5)	0.4156 (3)	0.07651 (9)	0.0380 (11)
H19A	1.4681	0.4081	0.0713	0.046*
C20A	1.2771 (5)	0.3818 (3)	0.06692 (9)	0.0352 (11)
H20A	1.2886	0.3497	0.0552	0.042*
S1B	0.63984 (11)	0.04233 (7)	0.17621 (2)	0.0302 (2)
S2B	1.13412 (11)	0.17652 (8)	0.295955 (19)	0.0343 (3)
O1B	0.0187 (4)	−0.0854 (2)	0.12719 (7)	0.0491 (10)
O2B	−0.1075 (4)	−0.0474 (3)	0.15231 (9)	0.0584 (13)
O3B	0.9869 (3)	0.1958 (2)	0.18455 (5)	0.0353 (8)
O4B	0.7791 (3)	0.28120 (18)	0.25977 (5)	0.0288 (7)
O5B	1.7274 (5)	0.0184 (2)	0.34104 (7)	0.0542 (11)
O6B	1.8641 (5)	0.0963 (3)	0.33270 (9)	0.0633 (13)
N1B	0.0001 (4)	−0.0503 (2)	0.14386 (8)	0.0351 (9)
N2B	0.4107 (4)	0.10232 (18)	0.18570 (6)	0.0218 (7)
H2B	0.3816	0.1309	0.1957	0.026*
N3B	0.5866 (3)	0.1695 (2)	0.18659 (6)	0.0241 (7)
H3B	0.5300	0.2002	0.1904	0.029*

N4B	0.7510 (3)	0.2260 (2)	0.22570 (6)	0.0231 (7)
H4BA	0.6672	0.2361	0.2244	0.028*
N5B	1.0146 (3)	0.2307 (2)	0.22138 (6)	0.0266 (8)
H5BA	1.0917	0.2481	0.2191	0.032*
N6B	1.1846 (4)	0.2625 (2)	0.26308 (6)	0.0274 (8)
H6B	1.2402	0.2827	0.2545	0.033*
N7B	1.3641 (4)	0.2063 (2)	0.27727 (6)	0.0268 (8)
H7B	1.3982	0.2265	0.2657	0.032*
N8B	1.7546 (5)	0.0709 (3)	0.33152 (8)	0.0422 (11)
C1B	0.1078 (4)	−0.0114 (2)	0.15471 (8)	0.0262 (9)
C2B	0.0825 (4)	0.0377 (3)	0.17085 (8)	0.0288 (10)
H2BA	−0.0044	0.0467	0.1747	0.035*
C3B	0.1862 (4)	0.0726 (2)	0.18099 (7)	0.0243 (9)
H3BA	0.1703	0.1061	0.1920	0.029*
C4B	0.3166 (4)	0.0600 (2)	0.17546 (7)	0.0195 (8)
C5B	0.3378 (4)	0.0093 (2)	0.15954 (8)	0.0253 (9)
H5BB	0.4247	−0.0011	0.1560	0.030*
C6B	0.2352 (5)	−0.0257 (2)	0.14895 (8)	0.0268 (9)
H6BA	0.2506	−0.0592	0.1378	0.032*
C7B	0.5426 (4)	0.1067 (2)	0.18273 (7)	0.0221 (8)
C8B	0.7219 (4)	0.1902 (2)	0.18495 (7)	0.0244 (9)
H8BA	0.7234	0.2376	0.1797	0.029*
H8BB	0.7618	0.1622	0.1733	0.029*
C9B	0.8047 (4)	0.1842 (2)	0.20765 (7)	0.0224 (8)
H9BA	0.8046	0.1361	0.2127	0.027*
C10B	0.9451 (4)	0.2045 (2)	0.20350 (7)	0.0255 (9)
C11B	0.9694 (4)	0.2319 (2)	0.24466 (7)	0.0243 (9)
H11B	0.9819	0.1860	0.2515	0.029*
C12B	0.8239 (4)	0.2492 (2)	0.24404 (7)	0.0227 (9)
C13B	1.0468 (4)	0.2815 (2)	0.25977 (8)	0.0256 (9)
H13C	1.0400	0.3268	0.2527	0.031*
H13D	1.0087	0.2838	0.2749	0.031*
C14B	1.2320 (5)	0.2168 (3)	0.27821 (7)	0.0275 (9)
C15B	1.4543 (4)	0.1698 (3)	0.29110 (7)	0.0282 (10)
C16B	1.4234 (5)	0.1187 (4)	0.30633 (10)	0.0456 (14)
H16B	1.3346	0.1064	0.3077	0.055*
C17B	1.5219 (6)	0.0858 (3)	0.31948 (10)	0.0463 (14)
H17B	1.5011	0.0508	0.3297	0.056*

C18B	1.6506 (5)	0.1048 (3)	0.31752 (8)	0.0342 (11)	
C19B	1.6848 (5)	0.1550 (3)	0.30228 (8)	0.0324 (11)	
H19B	1.7739	0.1668	0.3010	0.039*	
C20B	1.5857 (4)	0.1872 (3)	0.28901 (8)	0.0292 (10)	
H20B	1.6072	0.2212	0.2785	0.035*	
S1C	0.33195 (11)	0.32502 (7)	0.460327 (18)	0.0322 (3)	
S2C	0.79551 (15)	0.46213 (10)	0.57845 (3)	0.0546 (4)	
O1C	−0.3033 (4)	0.3328 (3)	0.39980 (7)	0.0641 (15)	
O2C	−0.4270 (4)	0.3318 (3)	0.42764 (7)	0.0628 (15)	
O3C	0.6678 (4)	0.1524 (2)	0.51338 (8)	0.0450 (10)	
O4C	0.4838 (3)	0.3253 (3)	0.57347 (6)	0.0487 (11)	
O5C	1.5139 (9)	0.5468 (4)	0.61816 (16)	0.0431 (19)*	0.50
O5CA	1.5435 (9)	0.5425 (5)	0.60879 (17)	0.046 (2)*	0.50
O6C	1.3888 (6)	0.6155 (3)	0.62412 (8)	0.0708 (16)	
N1C	−0.3193 (4)	0.3296 (3)	0.42018 (7)	0.0407 (11)	
N2C	0.1138 (4)	0.2920 (2)	0.48245 (6)	0.0236 (7)	
H2C	0.0892	0.2843	0.4963	0.028*	
N3C	0.3081 (3)	0.2563 (2)	0.49853 (6)	0.0250 (8)	
H3C	0.2598	0.2371	0.5086	0.030*	
N4C	0.4437 (4)	0.2517 (2)	0.54425 (6)	0.0310 (9)	
H4CA	0.3610	0.2492	0.5474	0.037*	
N5C	0.7076 (4)	0.2292 (2)	0.54160 (7)	0.0307 (9)	
H5CB	0.7883	0.2145	0.5442	0.037*	
N6C	0.8497 (4)	0.3681 (2)	0.54805 (7)	0.0276 (8)	
H6C	0.9055	0.3476	0.5396	0.033*	
N7C	1.0282 (4)	0.4047 (2)	0.56854 (7)	0.0292 (8)	
H7C	1.0624	0.3691	0.5623	0.035*	
N8C	1.4184 (6)	0.5638 (3)	0.61448 (10)	0.0571 (16)	
C1C	−0.2070 (5)	0.3218 (3)	0.43640 (8)	0.0292 (10)	
C2C	−0.0829 (5)	0.3296 (3)	0.42854 (8)	0.0321 (10)	
H2CA	−0.0732	0.3407	0.4129	0.039*	
C3C	0.0260 (5)	0.3213 (3)	0.44337 (8)	0.0283 (9)	
H3CA	0.1109	0.3273	0.4381	0.034*	
C4C	0.0117 (4)	0.3042 (2)	0.46634 (7)	0.0209 (8)	
C5C	−0.1143 (5)	0.2975 (2)	0.47381 (8)	0.0267 (9)	
H5CC	−0.1248	0.2870	0.4894	0.032*	
C6C	−0.2241 (5)	0.3060 (3)	0.45902 (8)	0.0277 (9)	
H6CA	−0.3094	0.3010	0.4643	0.033*	

C7C	0.2469 (4)	0.2898 (2)	0.48071 (7)	0.0245 (9)
C8C	0.4505 (4)	0.2503 (3)	0.50194 (8)	0.0288 (10)
H8CA	0.4912	0.2956	0.5022	0.035*
H8CB	0.4851	0.2243	0.4892	0.035*
C9C	0.4827 (4)	0.2144 (2)	0.52465 (8)	0.0268 (9)
H9CA	0.4328	0.1710	0.5242	0.032*
C10C	0.6309 (5)	0.1963 (3)	0.52627 (9)	0.0323 (10)
C11C	0.7098 (4)	0.3549 (3)	0.54377 (8)	0.0284 (10)
H11C	0.6881	0.3531	0.5270	0.034*
H11D	0.6596	0.3924	0.5501	0.034*
C12C	0.6688 (4)	0.2883 (3)	0.55465 (7)	0.0283 (10)
H12A	0.7157	0.2855	0.5702	0.034*
C13C	0.5236 (5)	0.2903 (3)	0.55808 (8)	0.0326 (11)
C14C	0.8956 (5)	0.4106 (3)	0.56456 (8)	0.0324 (10)
C15C	1.1197 (5)	0.4464 (3)	0.58107 (7)	0.0294 (10)
C16C	1.2505 (5)	0.4304 (3)	0.57847 (9)	0.0376 (12)
H16C	1.2717	0.3936	0.5691	0.045*
C17C	1.3501 (6)	0.4683 (3)	0.58957 (10)	0.0433 (14)
H17C	1.4394	0.4573	0.5881	0.052*
C18C	1.3160 (6)	0.5219 (3)	0.60271 (9)	0.0434 (14)
C19C	1.1875 (6)	0.5377 (3)	0.60609 (9)	0.0460 (14)
H19C	1.1672	0.5742	0.6157	0.055*
C20C	1.0875 (6)	0.4991 (3)	0.59512 (10)	0.0469 (14)
H20C	0.9984	0.5091	0.5973	0.056*
S1D	0.65701 (11)	0.04342 (7)	0.66179 (2)	0.0327 (2)
S2D	1.15854 (12)	0.13189 (8)	0.79518 (2)	0.0370 (3)
O1D	−0.0934 (4)	−0.0458 (3)	0.64083 (10)	0.0710 (17)
O2D	0.0355 (4)	−0.0964 (2)	0.61889 (7)	0.0432 (9)
O3D	0.8006 (3)	0.2281 (2)	0.75739 (6)	0.0328 (7)
O4D	1.0072 (3)	0.1782 (2)	0.67925 (6)	0.0354 (8)
O5D	1.7877 (4)	0.0839 (2)	0.85737 (7)	0.0498 (11)
O6D	1.9164 (4)	0.1028 (3)	0.83044 (7)	0.0542 (12)
N1D	0.0146 (4)	−0.0548 (2)	0.63353 (8)	0.0357 (10)
N2D	0.4281 (4)	0.0967 (2)	0.67503 (6)	0.0241 (7)
H2D	0.3990	0.1234	0.6855	0.029*
N3D	0.6060 (3)	0.16356 (19)	0.67891 (7)	0.0244 (8)
H3D	0.5492	0.1933	0.6834	0.029*
N4D	0.7728 (3)	0.1902 (2)	0.72115 (6)	0.0255 (8)

H4DA	0.6891	0.2004	0.7209	0.031*
N5D	1.0378 (3)	0.1894 (2)	0.71756 (6)	0.0256 (8)
H5DA	1.1199	0.2011	0.7164	0.031*
N6D	1.3844 (4)	0.1585 (2)	0.77489 (6)	0.0270 (8)
H6D	1.4125	0.1646	0.7612	0.032*
N7D	1.2045 (4)	0.2125 (2)	0.76022 (6)	0.0269 (8)
H7D	1.2596	0.2303	0.7510	0.032*
N8D	1.8077 (5)	0.0979 (2)	0.83724 (7)	0.0370 (10)
C1D	0.1251 (4)	−0.0161 (2)	0.64367 (8)	0.0261 (9)
C2D	0.2521 (5)	−0.0364 (2)	0.63995 (8)	0.0263 (9)
H2DA	0.2670	−0.0741	0.6305	0.032*
C3D	0.3569 (5)	−0.0007 (2)	0.65031 (8)	0.0257 (9)
H3DA	0.4442	−0.0142	0.6482	0.031*
C4D	0.3330 (4)	0.0555 (2)	0.66398 (7)	0.0235 (9)
C5D	0.2038 (4)	0.0745 (2)	0.66697 (7)	0.0245 (9)
H5DB	0.1878	0.1128	0.6761	0.029*
C6D	0.0989 (5)	0.0390 (3)	0.65701 (8)	0.0285 (9)
H6DA	0.0115	0.0520	0.6593	0.034*
C7D	0.5614 (4)	0.1022 (2)	0.67210 (7)	0.0237 (9)
C8D	0.7421 (4)	0.1828 (2)	0.67924 (7)	0.0243 (9)
H8DA	0.7481	0.2324	0.6780	0.029*
H8DB	0.7811	0.1630	0.6657	0.029*
C9D	0.8204 (4)	0.1599 (2)	0.70082 (7)	0.0235 (9)
H9DA	0.8118	0.1099	0.7021	0.028*
C10D	0.9650 (4)	0.1768 (2)	0.69844 (8)	0.0264 (9)
C11D	0.9900 (4)	0.1850 (2)	0.74057 (8)	0.0257 (9)
H11E	1.0012	0.1377	0.7462	0.031*
C12D	0.8458 (4)	0.2036 (3)	0.74017 (7)	0.0265 (9)
C13D	1.0677 (4)	0.2321 (3)	0.75700 (8)	0.0278 (9)
H13E	1.0621	0.2786	0.7509	0.033*
H13F	1.0285	0.2318	0.7720	0.033*
C14D	1.2529 (4)	0.1690 (2)	0.77623 (7)	0.0266 (9)
C15D	1.4817 (4)	0.1396 (2)	0.79158 (7)	0.0246 (9)
C16D	1.4631 (5)	0.1112 (3)	0.81262 (8)	0.0295 (10)
H16D	1.3772	0.1012	0.8168	0.035*
C17D	1.5708 (5)	0.0972 (3)	0.82777 (8)	0.0323 (10)
H17D	1.5586	0.0780	0.8423	0.039*
C18D	1.6944 (5)	0.1114 (3)	0.82146 (8)	0.0295 (10)

C19D	1.7155 (5)	0.1386 (2)	0.80009 (8)	0.0286 (10)
H19D	1.8018	0.1471	0.7958	0.034*
C20D	1.6104 (4)	0.1527 (2)	0.78549 (7)	0.0263 (9)
H20D	1.6237	0.1717	0.7709	0.032*
S3A	0.08587 (11)	0.20117 (7)	0.030562 (19)	0.0293 (2)
O7A	0.1591 (4)	0.2656 (2)	0.03384 (7)	0.0448 (9)
O8A	−0.0043 (4)	0.2094 (2)	0.00990 (7)	0.0432 (9)
O9A	0.1783 (4)	0.1484 (3)	0.02708 (9)	0.0567 (11)
O10A	0.0050 (4)	0.1896 (2)	0.04995 (6)	0.0412 (9)
S3B	0.38028 (9)	0.26004 (6)	0.218359 (16)	0.0202 (2)
O7B	0.4411 (3)	0.27795 (17)	0.19699 (5)	0.0295 (7)
O8B	0.2968 (3)	0.19980 (17)	0.21414 (5)	0.0278 (7)
O9B	0.4829 (3)	0.24532 (19)	0.23641 (5)	0.0302 (7)
O10B	0.2992 (4)	0.31600 (18)	0.22596 (6)	0.0361 (8)
S3C	0.08075 (9)	0.23797 (6)	0.542838 (17)	0.0229 (2)
O7C	0.1701 (3)	0.19145 (18)	0.53147 (6)	0.0329 (7)
O8C	0.0177 (3)	0.28447 (18)	0.52519 (5)	0.0283 (7)
O9C	0.1575 (3)	0.2793 (2)	0.55960 (6)	0.0364 (8)
O10C	−0.0218 (3)	0.20067 (19)	0.55344 (6)	0.0350 (8)
S3D	0.41241 (10)	0.23394 (6)	0.718085 (16)	0.0226 (2)
O7D	0.4853 (3)	0.26740 (18)	0.70040 (6)	0.0329 (7)
O8D	0.3102 (3)	0.19008 (17)	0.70714 (5)	0.0269 (7)
O9D	0.3516 (3)	0.28466 (18)	0.73249 (6)	0.0314 (7)
O10D	0.5032 (3)	0.1911 (2)	0.73274 (5)	0.0331 (8)
N1E	0.7666	0.7106	0.1210	0.031
N1F	0.3880	0.9151	0.2337	0.024
N1G	0.2148	0.2165	0.3806	0.024
N1H	0.0047	0.0212	0.5096	0.053
N1I	0.2472	0.2806	0.6348	0.057
N1J	0.4350	0.9499	0.7402	0.024
N1K	0.8992	0.0092	0.9990	0.052
N1L	0.2231	0.2295	0.1273	0.040
C1E	0.9067	0.7276	0.1171	0.038
H1EA	0.9070	0.7653	0.1061	0.045*
H1EB	0.9465	0.6882	0.1098	0.045*
C2E	0.9926	0.7467	0.1381	0.049
H2EA	0.9880	0.7112	0.1499	0.059*
H2EB	0.9610	0.7893	0.1445	0.059*

C3E	1.1330	0.7551	0.1318	0.063
H3EA	1.1354	0.7875	0.1190	0.076*
H3EB	1.1658	0.7113	0.1265	0.076*
C4E	1.2236	0.7802	0.1520	0.077
H4EA	1.3128	0.7848	0.1471	0.116*
H4EB	1.2231	0.7479	0.1647	0.116*
H4EC	1.1928	0.8241	0.1571	0.116*
C5E	0.7600	0.6498	0.1372	0.036
H5EA	0.7962	0.6636	0.1526	0.043*
H5EB	0.6669	0.6380	0.1385	0.043*
C6E	0.8318	0.5872	0.1302	0.033
H6EA	0.9263	0.5973	0.1298	0.040*
H6EB	0.7984	0.5732	0.1147	0.040*
C7E	0.8128	0.5303	0.1471	0.038
H7EA	0.7198	0.5163	0.1461	0.046*
H7EB	0.8359	0.5461	0.1629	0.046*
C8E	0.8996	0.4701	0.1416	0.047
H8EA	0.8872	0.4337	0.1526	0.070*
H8EB	0.9916	0.4840	0.1427	0.070*
H8EC	0.8755	0.4540	0.1260	0.070*
C9E	0.6950	0.6928	0.0977	0.041
H9EA	0.7082	0.7301	0.0869	0.049*
H9EB	0.7362	0.6521	0.0916	0.049*
C10E	0.5517	0.6804	0.0984	0.053
H10E	0.5077	0.7216	0.1034	0.064*
H10F	0.5362	0.6440	0.1094	0.064*
C11E	0.4945	0.6598	0.0740	0.064
H11F	0.5061	0.6975	0.0633	0.077*
H11G	0.5439	0.6207	0.0687	0.077*
C12E	0.3531	0.6421	0.0737	0.086
H12B	0.3215	0.6294	0.0581	0.128*
H12C	0.3034	0.6810	0.0786	0.128*
H12D	0.3412	0.6042	0.0841	0.128*
C13E	0.7016	0.7697	0.1314	0.034
H13G	0.7462	0.7783	0.1466	0.040*
H13U	0.6100	0.7571	0.1338	0.040*
C14E	0.6996	0.8344	0.1180	0.034
H14A	0.6619	0.8260	0.1022	0.041*

H14B	0.7904	0.8507	0.1170	0.041*
C15E	0.6195	0.8883	0.1292	0.040
H15A	0.6580	0.8975	0.1448	0.048*
H15B	0.5289	0.8719	0.1304	0.048*
C16E	0.6169	0.9532	0.1151	0.045
H16E	0.5647	0.9872	0.1226	0.068*
H16F	0.5778	0.9442	0.0997	0.068*
H16G	0.7064	0.9699	0.1142	0.068*
C1F	0.2573	0.9299	0.2213	0.030
H1FA	0.2719	0.9429	0.2053	0.036*
H1FB	0.2175	0.9689	0.2287	0.036*
C2F	0.1591	0.8705	0.2208	0.034
H2FA	0.1995	0.8302	0.2143	0.040*
H2FB	0.1371	0.8597	0.2366	0.040*
C3F	0.0347	0.8891	0.2064	0.038
H3FA	−0.0209	0.8485	0.2043	0.045*
H3FB	0.0588	0.9038	0.1910	0.045*
C4F	−0.0442	0.9448	0.2170	0.049
H4FA	−0.1226	0.9544	0.2070	0.074*
H4FB	0.0094	0.9855	0.2187	0.074*
H4FC	−0.0701	0.9301	0.2320	0.074*
C5F	0.4586	0.8584	0.2227	0.025
H5FA	0.4123	0.8158	0.2256	0.030*
H5FB	0.5478	0.8548	0.2302	0.030*
C6F	0.4700	0.8651	0.1969	0.027
H6FA	0.5064	0.9098	0.1935	0.032*
H6FB	0.3820	0.8616	0.1889	0.032*
C7F	0.5584	0.8102	0.1883	0.032
H7FA	0.5434	0.8067	0.1715	0.039*
H7FB	0.5340	0.7665	0.1950	0.039*
C8F	0.7038	0.8231	0.1943	0.040
H8FA	0.7554	0.7862	0.1884	0.060*
H8FB	0.7199	0.8256	0.2110	0.060*
H8FC	0.7294	0.8657	0.1874	0.060*
C9F	0.4662	0.9802	0.2326	0.029
H9FA	0.4773	0.9904	0.2163	0.035*
H9FB	0.4133	1.0170	0.2387	0.035*
C10F	0.5997	0.9816	0.2452	0.040

H10G	0.6605	0.9523	0.2373	0.048*
H10H	0.5936	0.9644	0.2610	0.048*
C11F	0.6514	1.0534	0.2461	0.041
H11H	0.6510	1.0709	0.2302	0.049*
H11I	0.5911	1.0817	0.2545	0.049*
C12F	0.7863	1.0603	0.2572	0.045
H12E	0.8131	1.1076	0.2570	0.068*
H12F	0.8473	1.0332	0.2488	0.068*
H12G	0.7872	1.0445	0.2731	0.068*
C13F	0.3735	0.8939	0.2586	0.029
H13H	0.3205	0.8522	0.2587	0.034*
H13I	0.4613	0.8832	0.2658	0.034*
C14F	0.3097	0.9468	0.2731	0.044
H14C	0.2175	0.9533	0.2674	0.053*
H14D	0.3559	0.9903	0.2719	0.053*
C15F	0.3147	0.9250	0.2984	0.049
H15C	0.2854	0.8778	0.2999	0.059*
H15D	0.2595	0.9545	0.3074	0.059*
C16F	0.4681	0.9330	0.3066	0.150*
H16H	0.4817	0.9201	0.3228	0.225*
H16I	0.4948	0.9799	0.3048	0.225*
H16J	0.5205	0.9038	0.2973	0.225*
C1G	0.0717	0.2368	0.3774	0.028
H1GA	0.0175	0.1974	0.3810	0.034*
H1GB	0.0550	0.2725	0.3886	0.034*
C2G	0.0261	0.2619	0.3537	0.032
H2GA	0.0546	0.2300	0.3420	0.039*
H2GB	0.0667	0.3062	0.3509	0.039*
C3G	−0.1233	0.2688	0.3512	0.041
H3GA	−0.1637	0.2236	0.3517	0.049*
H3GB	−0.1530	0.2953	0.3643	0.049*
C4G	−0.1675	0.3035	0.3289	0.048
H4GA	−0.2631	0.3075	0.3277	0.072*
H4GB	−0.1395	0.2769	0.3160	0.072*
H4GC	−0.1284	0.3485	0.3285	0.072*
C6G	0.2960	0.3381	0.3890	0.027
H6GA	0.2049	0.3551	0.3882	0.032*
H6GB	0.3221	0.3276	0.4052	0.032*

C5G	0.3032	0.2740	0.3745	0.025
H5GA	0.2817	0.2861	0.3583	0.029*
H5GB	0.3947	0.2576	0.3757	0.029*
C7G	0.3854	0.3912	0.3804	0.030
H7GA	0.3533	0.4048	0.3648	0.036*
H7GB	0.4741	0.3720	0.3796	0.036*
C8G	0.3933	0.4528	0.3957	0.051
H8GA	0.4520	0.4861	0.3894	0.076*
H8GB	0.4272	0.4399	0.4111	0.076*
H8GC	0.3058	0.4724	0.3964	0.076*
C9G	0.2422	0.1575	0.3648	0.024
H9GA	0.2303	0.1732	0.3488	0.029*
H9GB	0.3350	0.1441	0.3677	0.029*
C10G	0.1575	0.0960	0.3674	0.030
H10I	0.0641	0.1091	0.3657	0.036*
H10J	0.1753	0.0767	0.3829	0.036*
C11G	0.1851	0.0429	0.3494	0.035
H11J	0.1658	0.0622	0.3339	0.042*
H11K	0.2790	0.0308	0.3508	0.042*
C12G	0.1046	−0.0193	0.3518	0.042
H12H	0.1246	−0.0518	0.3399	0.063*
H12I	0.0114	−0.0076	0.3501	0.063*
H12J	0.1249	−0.0391	0.3670	0.063*
C13G	0.2406	0.1953	0.4056	0.027
H13J	0.2040	0.2301	0.4154	0.033*
H13K	0.1927	0.1528	0.4080	0.033*
C14G	0.3839	0.1847	0.4133	0.042
H14E	0.4261	0.1566	0.4019	0.050*
H14F	0.4292	0.2288	0.4142	0.050*
C15G	0.3974	0.1505	0.4366	0.042
H15E	0.3604	0.1044	0.4354	0.051*
H15F	0.3482	0.1761	0.4477	0.051*
C16G	0.5441	0.1469	0.4451	0.059
H16K	0.5526	0.1246	0.4601	0.089*
H16L	0.5800	0.1925	0.4465	0.089*
H16M	0.5923	0.1212	0.4341	0.089*
C1H	0.0218	0.0789	0.4935	0.049
H1HA	0.0885	0.1099	0.5006	0.058*

H1HB	−0.0618	0.1040	0.4916	0.058*
C2H	0.0630	0.0591	0.4695	0.053
H2HA	0.1556	0.0443	0.4707	0.064*
H2HB	0.0088	0.0208	0.4636	0.064*
C3H	0.0470	0.1184	0.4528	0.055
H3HA	0.0918	0.1583	0.4598	0.066*
H3HB	0.0899	0.1071	0.4386	0.066*
C4H	−0.0955	0.1358	0.4467	0.064
H4HA	−0.1003	0.1739	0.4360	0.096*
H4HB	−0.1381	0.1479	0.4606	0.096*
H4HC	−0.1400	0.0968	0.4394	0.096*
C5H	−0.0928	−0.0299	0.5001	0.067
H5HA	−0.1090	−0.0629	0.5123	0.080*
H5HB	−0.0539	−0.0546	0.4875	0.080*
C6H	−0.2263	0.0002	0.4909	0.064
H6HA	−0.2624	0.0288	0.5028	0.077*
H6HB	−0.2133	0.0287	0.4773	0.077*
C7H	−0.3209	−0.0553	0.4843	0.091*
H7HA	−0.2768	−0.0884	0.4748	0.110*
H7HB	−0.3445	−0.0786	0.4984	0.110*
C8H	−0.4323	−0.0343	0.4726	0.111*
H8HA	−0.4885	−0.0732	0.4688	0.166*
H8HB	−0.4103	−0.0117	0.4585	0.166*
H8HC	−0.4786	−0.0027	0.4821	0.166*
C9H	−0.0385	0.0519	0.5313	0.047
H9HA	−0.1231	0.0750	0.5278	0.056*
H9HB	0.0262	0.0865	0.5366	0.056*
C10H	−0.0545	0.0018	0.5509	0.081
H10K	0.0281	−0.0235	0.5542	0.097*
H10L	−0.1246	−0.0309	0.5464	0.097*
C11H	−0.0900	0.0413	0.5727	0.101
H11L	−0.1401	0.0132	0.5830	0.121*
H11M	−0.1392	0.0831	0.5688	0.121*
C12H	0.0543	0.0566	0.5833	0.150*
H12K	0.0496	0.0825	0.5975	0.225*
H12L	0.1018	0.0826	0.5723	0.225*
H12M	0.1002	0.0140	0.5867	0.225*
C13H	0.1361	−0.0182	0.5132	0.071

H13L	0.1230	−0.0561	0.5238	0.085*
H13V	0.1566	−0.0378	0.4983	0.085*
C14H	0.2543	0.0222	0.5226	0.074
H14G	0.2320	0.0470	0.5364	0.089*
H14H	0.2787	0.0555	0.5110	0.089*
C15H	0.3711	−0.0255	0.5285	0.095*
H15G	0.3481	−0.0562	0.5410	0.114*
H15H	0.3869	−0.0533	0.5150	0.114*
C16H	0.4948	0.0113	0.5360	0.107*
H16N	0.5654	−0.0212	0.5394	0.160*
H16O	0.4809	0.0379	0.5497	0.160*
H16P	0.5189	0.0414	0.5237	0.160*
C1I	0.3032	0.2137	0.6313	0.069
H1IA	0.2369	0.1794	0.6347	0.083*
H1IB	0.3789	0.2075	0.6425	0.083*
C2I	0.3481	0.2003	0.6074	0.089
H2IA	0.2771	0.2125	0.5959	0.106*
H2IB	0.4249	0.2289	0.6049	0.106*
C3I	0.3842	0.1271	0.6045	0.126*
H3IA	0.4425	0.1123	0.6177	0.151*
H3IB	0.3041	0.0990	0.6040	0.151*
C4I	0.4463	0.1187	0.5847	0.150*
H4IA	0.4705	0.0713	0.5830	0.225*
H4IB	0.5254	0.1466	0.5852	0.225*
H4IC	0.3875	0.1323	0.5716	0.225*
C5I	0.2156	0.2846	0.6595	0.052
H5IA	0.1453	0.2519	0.6621	0.062*
H5IB	0.2940	0.2709	0.6692	0.062*
C6I	0.1736	0.3518	0.6670	0.082*
H6IA	0.0976	0.3671	0.6570	0.099*
H6IB	0.2456	0.3845	0.6656	0.099*
C7I	0.1364	0.3500	0.6917	0.067
H7IA	0.0540	0.3243	0.6925	0.080*
H7IB	0.2055	0.3259	0.7011	0.080*
C8I	0.1188	0.4181	0.7016	0.103*
H8IA	0.0949	0.4138	0.7175	0.155*
H8IB	0.0491	0.4419	0.6926	0.155*
H8IC	0.2007	0.4434	0.7012	0.155*

C9I	0.1239	0.2921	0.6191	0.050
H9IA	0.0881	0.3372	0.6224	0.060*
H9IB	0.1478	0.2920	0.6030	0.060*
C10I	0.0178	0.2394	0.6219	0.073
H10M	0.0512	0.1944	0.6180	0.088*
H10N	−0.0052	0.2383	0.6381	0.088*
C11I	−0.1018	0.2556	0.6067	0.079*
H11N	−0.0783	0.2589	0.5906	0.095*
H11O	−0.1383	0.2994	0.6112	0.095*
C12I	−0.2056	0.1992	0.6089	0.094*
H12N	−0.2847	0.2103	0.5993	0.141*
H12O	−0.2274	0.1956	0.6249	0.141*
H12P	−0.1701	0.1562	0.6040	0.141*
C13I	0.3479	0.3341	0.6288	0.088*
H13M	0.3193	0.3788	0.6340	0.105*
H13N	0.3530	0.3359	0.6119	0.105*
C14I	0.4885	0.3173	0.6406	0.139*
H14I	0.5088	0.2691	0.6384	0.167*
H14J	0.4897	0.3264	0.6572	0.167*
C15I	0.5953	0.3630	0.6292	0.101*
H15I	0.5924	0.3550	0.6125	0.121*
H15J	0.5770	0.4112	0.6318	0.121*
C16I	0.7211	0.3458	0.6395	0.150*
H16Q	0.7874	0.3752	0.6334	0.225*
H16R	0.7408	0.2988	0.6359	0.225*
H16S	0.7215	0.3515	0.6561	0.225*
C1J	0.3174	0.9907	0.7311	0.027
H1JA	0.3002	1.0260	0.7425	0.033*
H1JB	0.3398	1.0137	0.7169	0.033*
C2J	0.1928	0.9507	0.7260	0.031
H2JA	0.1681	0.9280	0.7402	0.037*
H2JB	0.2080	0.9156	0.7145	0.037*
C3J	0.0818	0.9964	0.7171	0.033
H3JA	0.0551	1.0254	0.7297	0.040*
H3JB	0.1137	1.0261	0.7051	0.040*
C4J	−0.0366	0.9576	0.7072	0.037
H4JA	−0.1049	0.9893	0.7017	0.055*
H4JB	−0.0700	0.9289	0.7191	0.055*

H4JC	−0.0113	0.9295	0.6945	0.055*
C5J	0.4108	0.9159	0.7630	0.025
H5JA	0.3348	0.8853	0.7605	0.029*
H5JB	0.4879	0.8879	0.7677	0.029*
C6J	0.3850	0.9636	0.7827	0.035
H6JA	0.3157	0.9962	0.7777	0.042*
H6JB	0.4655	0.9891	0.7873	0.042*
C7J	0.3417	0.9220	0.8030	0.036
H7JA	0.3990	0.8820	0.8051	0.043*
H7JB	0.3525	0.9494	0.8171	0.043*
C8J	0.1988	0.8987	0.7995	0.046
H8JA	0.1758	0.8725	0.8129	0.069*
H8JB	0.1879	0.8708	0.7857	0.069*
H8JC	0.1414	0.9382	0.7978	0.069*
C9J	0.4657	0.8930	0.7241	0.026
H9JA	0.3979	0.8577	0.7250	0.031*
H9JB	0.5507	0.8728	0.7295	0.031*
C10J	0.4724	0.9137	0.6988	0.030
H10O	0.3831	0.9230	0.6920	0.037*
H10P	0.5246	0.9555	0.6979	0.037*
C11J	0.5348	0.8579	0.6853	0.032
H11P	0.5004	0.8139	0.6902	0.038*
H11Q	0.5083	0.8637	0.6688	0.038*
C12J	0.6835	0.8564	0.6884	0.035
H12Q	0.7168	0.8194	0.6793	0.052*
H12R	0.7107	0.8496	0.7046	0.052*
H12S	0.7187	0.8992	0.6832	0.052*
C13J	0.5488	0.9995	0.7431	0.028
H13O	0.5680	1.0167	0.7278	0.034*
H13P	0.5208	1.0383	0.7522	0.034*
C15J	0.7852	1.0222	0.7547	0.034
H15K	0.7549	1.0659	0.7605	0.041*
H15L	0.8107	1.0291	0.7389	0.041*
C14J	0.6738	0.9711	0.7546	0.040
H14K	0.6989	0.9299	0.7465	0.048*
H14L	0.6585	0.9584	0.7706	0.048*
C16J	0.9042	0.9981	0.7698	0.043
H16T	0.9740	1.0318	0.7696	0.064*

H16U	0.9354	0.9553	0.7638	0.064*
H16V	0.8793	0.9918	0.7855	0.064*
C1K	1.0107	−0.0406	1.0010	0.067
H1KA	0.9846	−0.0782	1.0108	0.080*
H1KB	1.0217	−0.0594	0.9856	0.080*
C2K	1.1411	−0.0152	1.0104	0.079
H2KA	1.1326	0.0031	1.0260	0.095*
H2KB	1.1700	0.0218	1.0006	0.095*
C3K	1.2417	−0.0700	1.0114	0.106
H3KA	1.2635	−0.0813	0.9957	0.127*
H3KB	1.2040	−0.1108	1.0182	0.127*
C4K	1.3734	−0.0499	1.0262	0.144*
H4KA	1.4358	−0.0874	1.0262	0.216*
H4KB	1.3531	−0.0402	1.0420	0.216*
H4KC	1.4120	−0.0099	1.0196	0.216*
C5K	0.7775	−0.0272	0.9903	0.063
H5KA	0.7582	−0.0629	1.0013	0.076*
H5KB	0.7942	−0.0494	0.9756	0.076*
C6K	0.6585	0.0178	0.9866	0.090*
H6KA	0.6731	0.0528	0.9750	0.108*
H6KB	0.6380	0.0400	1.0010	0.108*
C7K	0.5455	−0.0305	0.9780	0.106*
H7KA	0.5245	−0.0625	0.9902	0.128*
H7KB	0.5696	−0.0562	0.9644	0.128*
C8K	0.4266	0.0177	0.9717	0.128*
H8KA	0.3512	−0.0090	0.9658	0.192*
H8KB	0.4505	0.0498	0.9600	0.192*
H8KC	0.4040	0.0422	0.9854	0.192*
C9K	0.8797	0.0425	1.0223	0.055
H9KA	0.9548	0.0728	1.0261	0.066*
H9KB	0.7999	0.0708	1.0207	0.066*
C10K	0.8672	−0.0045	1.0414	0.071
H10Q	0.9542	−0.0239	1.0460	0.085*
H10R	0.8083	−0.0418	1.0364	0.085*
C11K	0.8128	0.0303	1.0624	0.070
H11R	0.8579	0.0740	1.0651	0.084*
H11S	0.8307	0.0019	1.0761	0.084*
C12K	0.6596	0.0427	1.0585	0.089

H12T	0.6280	0.0655	1.0719	0.133*
H12U	0.6147	−0.0006	1.0563	0.133*
H12V	0.6418	0.0709	1.0449	0.133*
C13K	0.9312	0.0674	0.9832	0.047
H13Q	0.8596	0.1009	0.9833	0.057*
H13R	1.0121	0.0896	0.9897	0.057*
C14K	0.9504	0.0488	0.9585	0.049
H14M	0.8661	0.0333	0.9510	0.059*
H14N	1.0138	0.0112	0.9581	0.059*
C15K	1.0007	0.1090	0.9454	0.061
H15M	0.9956	0.0982	0.9288	0.073*
H15N	0.9430	0.1481	0.9476	0.073*
C16K	1.1342	0.1275	0.9525	0.078
H16W	1.1607	0.1662	0.9435	0.117*
H16X	1.1925	0.0894	0.9500	0.117*
H16Y	1.1399	0.1393	0.9688	0.117*
C1L	0.2022	0.2551	0.1521	0.071
H1LA	0.1529	0.2204	0.1601	0.085*
H1LB	0.2890	0.2597	0.1605	0.085*
C2L	0.1307	0.3213	0.1536	0.098
H2LA	0.0359	0.3109	0.1529	0.117*
H2LB	0.1466	0.3471	0.1396	0.117*
C3L	0.1596	0.3680	0.1739	0.106*
H3LA	0.0828	0.3976	0.1752	0.127*
H3LB	0.1687	0.3402	0.1880	0.127*
C4L	0.2723	0.4092	0.1733	0.082*
H4LA	0.2821	0.4361	0.1874	0.122*
H4LB	0.2629	0.4392	0.1600	0.122*
H4LC	0.3498	0.3807	0.1722	0.122*
C5L	0.3250	0.2762	0.1174	0.047
H5LA	0.3307	0.2655	0.1010	0.057*
H5LB	0.2940	0.3233	0.1184	0.057*
C6L	0.4614	0.2715	0.1293	0.051
H6LA	0.4991	0.2268	0.1262	0.062*
H6LB	0.4548	0.2753	0.1461	0.062*
C7L	0.5538	0.3268	0.1214	0.067
H7LA	0.5708	0.3188	0.1052	0.080*
H7LB	0.5100	0.3710	0.1223	0.080*

C8L	0.6791	0.3290	0.1351	0.069
H8LA	0.7337	0.3649	0.1294	0.103*
H8LB	0.7240	0.2857	0.1340	0.103*
H8LC	0.6631	0.3378	0.1512	0.103*
C9L	0.2747	0.1599	0.1287	0.077
H9LA	0.2066	0.1313	0.1350	0.092*
H9LB	0.3508	0.1599	0.1401	0.092*
C10L	0.3173	0.1258	0.1070	0.099*
H10S	0.3417	0.1606	0.0960	0.119*
H10T	0.3955	0.0977	0.1109	0.119*
C11L	0.2136	0.0838	0.0964	0.109*
H11T	0.1408	0.1119	0.0897	0.131*
H11U	0.1792	0.0527	0.1077	0.131*
C12L	0.2848	0.0405	0.0757	0.110*
H12W	0.2195	0.0116	0.0675	0.165*
H12X	0.3558	0.0126	0.0826	0.165*
H12Y	0.3203	0.0722	0.0648	0.165*
C13L	0.0984	0.2370	0.1129	0.044
H13S	0.1132	0.2242	0.0969	0.052*
H13T	0.0712	0.2848	0.1129	0.052*
C14L	−0.0150	0.1921	0.1218	0.041
H14O	0.0150	0.1449	0.1236	0.050*
H14P	−0.0396	0.2088	0.1369	0.050*
C15L	−0.1335	0.1954	0.1044	0.055
H15O	−0.1082	0.1798	0.0892	0.065*
H15P	−0.1644	0.2425	0.1028	0.065*
C16L	−0.2447	0.1505	0.1125	0.061
H16Z	−0.3204	0.1530	0.1014	0.091*
H17E	−0.2698	0.1663	0.1275	0.091*
H17F	−0.2142	0.1038	0.1139	0.091*
O1E	0.2049	0.0905	0.2413	0.044

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0240 (6)	0.0577 (8)	0.0434 (7)	−0.0014 (5)	0.0060 (5)	0.0191 (6)
S2A	0.0392 (7)	0.0472 (8)	0.0598 (9)	0.0087 (6)	0.0008 (6)	−0.0038 (6)
O1A	0.036 (2)	0.076 (3)	0.037 (2)	0.003 (2)	−0.0021 (16)	0.023 (2)

O2A	0.019 (2)	0.114 (4)	0.069 (3)	−0.009 (2)	−0.0038 (19)	0.047 (3)
O3A	0.032 (2)	0.125 (5)	0.038 (2)	−0.002 (2)	0.0023 (17)	0.028 (3)
O4A	0.0262 (19)	0.079 (3)	0.049 (2)	−0.0071 (19)	0.0059 (16)	−0.016 (2)
O5A	0.046 (3)	0.091 (4)	0.046 (2)	−0.008 (2)	−0.0008 (19)	−0.032 (2)
O6A	0.036 (2)	0.066 (3)	0.064 (3)	−0.007 (2)	0.004 (2)	−0.023 (2)
N1A	0.025 (2)	0.042 (2)	0.037 (2)	0.0044 (18)	−0.0053 (17)	−0.0008 (18)
N2A	0.0180 (18)	0.032 (2)	0.0294 (19)	−0.0009 (15)	0.0006 (14)	0.0063 (15)
N3A	0.020 (2)	0.065 (3)	0.0253 (19)	−0.0008 (19)	0.0016 (15)	0.0005 (19)
N4A	0.0106 (18)	0.074 (3)	0.050 (3)	−0.0017 (19)	−0.0037 (17)	0.025 (2)
N5A	0.0163 (19)	0.045 (3)	0.048 (2)	0.0043 (17)	0.0040 (17)	0.002 (2)
N6A	0.023 (2)	0.057 (3)	0.038 (2)	0.0042 (19)	0.0092 (17)	−0.010 (2)
N7A	0.027 (2)	0.040 (2)	0.0286 (19)	−0.0060 (17)	0.0070 (16)	0.0004 (17)
N8A	0.033 (2)	0.050 (3)	0.042 (2)	0.002 (2)	−0.0016 (19)	−0.013 (2)
C1A	0.022 (2)	0.043 (3)	0.029 (2)	0.007 (2)	−0.0042 (18)	−0.003 (2)
C2A	0.029 (3)	0.045 (3)	0.024 (2)	−0.005 (2)	−0.0023 (18)	0.0015 (19)
C3A	0.025 (2)	0.041 (3)	0.031 (2)	−0.004 (2)	−0.0010 (18)	−0.002 (2)
C4A	0.019 (2)	0.025 (2)	0.030 (2)	0.0009 (17)	0.0026 (17)	−0.0008 (17)
C5A	0.025 (2)	0.039 (3)	0.037 (2)	0.002 (2)	−0.0010 (19)	0.015 (2)
C6A	0.018 (2)	0.048 (3)	0.043 (3)	0.001 (2)	0.0025 (19)	0.010 (2)
C7A	0.021 (2)	0.025 (2)	0.029 (2)	−0.0013 (17)	0.0026 (17)	−0.0014 (17)
C8A	0.020 (2)	0.065 (4)	0.034 (2)	−0.009 (2)	0.0011 (19)	0.011 (2)
C9A	0.018 (2)	0.037 (3)	0.043 (3)	−0.0038 (19)	−0.0022 (19)	−0.007 (2)
C10A	0.028 (3)	0.071 (4)	0.035 (3)	0.004 (3)	0.008 (2)	0.024 (3)
C11A	0.020 (2)	0.059 (4)	0.040 (3)	0.003 (2)	−0.008 (2)	0.020 (2)
C12A	0.019 (2)	0.048 (3)	0.038 (3)	−0.001 (2)	0.0041 (19)	−0.003 (2)
C13A	0.031 (3)	0.058 (4)	0.040 (3)	0.008 (2)	0.007 (2)	−0.001 (2)
C14A	0.030 (3)	0.056 (3)	0.023 (2)	−0.001 (2)	0.0010 (18)	0.010 (2)
C15A	0.035 (3)	0.033 (3)	0.024 (2)	0.001 (2)	−0.0011 (18)	0.0031 (18)
C16A	0.032 (3)	0.036 (3)	0.040 (3)	0.001 (2)	0.007 (2)	0.000 (2)
C17A	0.036 (3)	0.039 (3)	0.033 (2)	−0.001 (2)	−0.002 (2)	−0.004 (2)
C18A	0.036 (3)	0.031 (2)	0.034 (2)	−0.001 (2)	−0.001 (2)	0.001 (2)
C19A	0.029 (3)	0.049 (3)	0.036 (3)	0.005 (2)	0.002 (2)	−0.003 (2)
C20A	0.038 (3)	0.035 (3)	0.033 (2)	−0.002 (2)	0.005 (2)	0.000 (2)
S1B	0.0209 (5)	0.0306 (6)	0.0388 (6)	0.0033 (4)	−0.0008 (4)	−0.0073 (5)
S2B	0.0227 (6)	0.0544 (8)	0.0261 (5)	0.0002 (5)	0.0038 (4)	0.0043 (5)
O1B	0.032 (2)	0.059 (3)	0.056 (2)	−0.0124 (18)	−0.0003 (17)	−0.028 (2)
O2B	0.025 (2)	0.077 (3)	0.072 (3)	−0.014 (2)	0.0002 (19)	−0.034 (3)
O3B	0.0228 (17)	0.058 (2)	0.0250 (16)	−0.0055 (15)	0.0036 (13)	0.0010 (15)

O4B	0.0206 (16)	0.0357 (18)	0.0301 (16)	0.0001 (13)	0.0018 (12)	−0.0087 (13)
O5B	0.056 (3)	0.057 (3)	0.049 (2)	0.024 (2)	−0.002 (2)	0.013 (2)
O6B	0.050 (3)	0.056 (3)	0.079 (3)	0.007 (2)	−0.033 (2)	0.005 (2)
N1B	0.029 (2)	0.035 (2)	0.040 (2)	−0.0058 (18)	−0.0033 (18)	−0.0076 (19)
N2B	0.0190 (18)	0.0196 (17)	0.0268 (18)	0.0002 (14)	0.0012 (14)	−0.0015 (14)
N3B	0.0133 (17)	0.029 (2)	0.0305 (18)	−0.0028 (14)	0.0020 (13)	−0.0029 (15)
N4B	0.0144 (17)	0.033 (2)	0.0220 (16)	−0.0024 (14)	−0.0005 (13)	0.0004 (14)
N5B	0.0125 (17)	0.042 (2)	0.0254 (17)	−0.0047 (15)	0.0000 (13)	−0.0027 (16)
N6B	0.0166 (18)	0.039 (2)	0.0264 (18)	0.0016 (15)	−0.0007 (14)	−0.0030 (16)
N7B	0.0176 (18)	0.041 (2)	0.0221 (17)	0.0008 (16)	0.0026 (13)	0.0010 (16)
N8B	0.040 (3)	0.052 (3)	0.033 (2)	0.025 (2)	−0.0034 (19)	0.001 (2)
C1B	0.024 (2)	0.025 (2)	0.029 (2)	−0.0048 (18)	−0.0033 (17)	0.0002 (17)
C2B	0.017 (2)	0.035 (3)	0.033 (2)	0.0026 (18)	−0.0002 (17)	−0.0016 (19)
C3B	0.023 (2)	0.023 (2)	0.026 (2)	−0.0011 (17)	0.0012 (16)	−0.0044 (17)
C4B	0.016 (2)	0.019 (2)	0.0229 (19)	−0.0028 (15)	−0.0021 (15)	0.0058 (15)
C5B	0.019 (2)	0.026 (2)	0.031 (2)	0.0035 (17)	0.0003 (17)	−0.0003 (17)
C6B	0.031 (2)	0.025 (2)	0.023 (2)	−0.0018 (18)	−0.0008 (17)	0.0010 (17)
C7B	0.021 (2)	0.023 (2)	0.0209 (19)	−0.0008 (16)	−0.0024 (15)	0.0016 (16)
C8B	0.017 (2)	0.029 (2)	0.027 (2)	−0.0051 (17)	−0.0010 (16)	0.0032 (17)
C9B	0.019 (2)	0.024 (2)	0.024 (2)	−0.0024 (16)	0.0002 (16)	0.0028 (16)
C10B	0.020 (2)	0.030 (2)	0.027 (2)	0.0038 (17)	0.0008 (16)	0.0050 (18)
C11B	0.022 (2)	0.027 (2)	0.024 (2)	0.0031 (17)	0.0028 (16)	0.0003 (17)
C12B	0.016 (2)	0.025 (2)	0.028 (2)	−0.0002 (16)	0.0015 (16)	−0.0012 (17)
C13B	0.020 (2)	0.030 (2)	0.027 (2)	0.0018 (17)	0.0022 (16)	−0.0038 (17)
C14B	0.024 (2)	0.037 (3)	0.021 (2)	0.0019 (18)	−0.0015 (16)	−0.0051 (17)
C15B	0.024 (2)	0.042 (3)	0.0185 (19)	0.0034 (19)	−0.0014 (16)	−0.0047 (18)
C16B	0.024 (3)	0.071 (4)	0.043 (3)	0.006 (2)	0.010 (2)	0.019 (3)
C17B	0.041 (3)	0.061 (4)	0.039 (3)	0.016 (3)	0.012 (2)	0.021 (3)
C18B	0.038 (3)	0.036 (3)	0.027 (2)	0.013 (2)	−0.002 (2)	−0.0043 (19)
C19B	0.022 (2)	0.041 (3)	0.034 (2)	0.005 (2)	−0.0070 (19)	−0.005 (2)
C20B	0.022 (2)	0.032 (2)	0.033 (2)	0.0070 (18)	−0.0028 (18)	0.0000 (19)
S1C	0.0240 (5)	0.0503 (7)	0.0222 (5)	−0.0087 (5)	0.0014 (4)	0.0010 (5)
S2C	0.0381 (8)	0.0642 (10)	0.0615 (9)	0.0017 (7)	0.0031 (7)	−0.0334 (8)
O1C	0.029 (2)	0.133 (5)	0.030 (2)	0.011 (2)	−0.0002 (16)	0.006 (2)
O2C	0.022 (2)	0.130 (5)	0.036 (2)	0.004 (2)	−0.0012 (16)	0.019 (2)
O3C	0.0238 (18)	0.042 (2)	0.068 (3)	0.0022 (16)	−0.0047 (17)	−0.0134 (19)
O4C	0.0192 (17)	0.100 (3)	0.0273 (17)	0.0008 (19)	0.0014 (13)	−0.020 (2)
O6C	0.091 (4)	0.077 (4)	0.045 (2)	−0.059 (3)	0.003 (2)	−0.012 (2)

N1C	0.023 (2)	0.075 (3)	0.024 (2)	0.011 (2)	−0.0027 (16)	0.007 (2)
N2C	0.0212 (18)	0.032 (2)	0.0179 (16)	−0.0007 (15)	0.0009 (13)	−0.0018 (14)
N3C	0.0150 (17)	0.039 (2)	0.0210 (16)	−0.0005 (15)	−0.0006 (13)	−0.0017 (15)
N4C	0.0117 (17)	0.055 (3)	0.0262 (18)	−0.0038 (17)	0.0027 (14)	−0.0003 (17)
N5C	0.0127 (17)	0.029 (2)	0.049 (2)	−0.0023 (15)	−0.0065 (16)	0.0056 (18)
N6C	0.0152 (18)	0.036 (2)	0.0312 (19)	−0.0027 (15)	0.0014 (14)	−0.0055 (16)
N7C	0.027 (2)	0.030 (2)	0.0307 (19)	−0.0062 (16)	−0.0013 (16)	−0.0058 (16)
N8C	0.057 (4)	0.053 (3)	0.057 (3)	−0.035 (3)	−0.023 (3)	0.019 (3)
C1C	0.024 (2)	0.039 (3)	0.024 (2)	0.0106 (19)	−0.0037 (17)	0.0036 (19)
C2C	0.028 (2)	0.048 (3)	0.021 (2)	0.008 (2)	−0.0007 (17)	0.004 (2)
C3C	0.023 (2)	0.038 (3)	0.024 (2)	0.0042 (19)	0.0015 (17)	0.0030 (18)
C4C	0.020 (2)	0.022 (2)	0.0207 (19)	0.0014 (16)	−0.0023 (15)	−0.0021 (15)
C5C	0.026 (2)	0.028 (2)	0.026 (2)	0.0019 (18)	−0.0009 (17)	−0.0013 (17)
C6C	0.021 (2)	0.037 (3)	0.025 (2)	0.0012 (18)	0.0037 (17)	0.0013 (18)
C7C	0.020 (2)	0.029 (2)	0.024 (2)	−0.0008 (17)	−0.0010 (16)	−0.0073 (17)
C8C	0.015 (2)	0.044 (3)	0.027 (2)	−0.0020 (18)	0.0011 (16)	−0.0026 (19)
C9C	0.013 (2)	0.031 (2)	0.036 (2)	−0.0014 (16)	−0.0007 (17)	0.0001 (18)
C10C	0.019 (2)	0.032 (3)	0.046 (3)	0.0000 (19)	−0.0023 (19)	0.000 (2)
C11C	0.018 (2)	0.035 (3)	0.032 (2)	0.0037 (18)	−0.0037 (17)	−0.0034 (19)
C12C	0.017 (2)	0.044 (3)	0.023 (2)	−0.0012 (18)	−0.0039 (16)	0.0034 (19)
C13C	0.020 (2)	0.057 (3)	0.020 (2)	−0.005 (2)	−0.0004 (17)	−0.001 (2)
C14C	0.028 (2)	0.038 (3)	0.031 (2)	−0.007 (2)	0.0013 (19)	0.003 (2)
C15C	0.028 (2)	0.041 (3)	0.0179 (19)	−0.014 (2)	−0.0057 (17)	0.0064 (18)
C16C	0.033 (3)	0.044 (3)	0.034 (3)	−0.012 (2)	−0.006 (2)	0.013 (2)
C17C	0.031 (3)	0.050 (3)	0.047 (3)	−0.018 (2)	−0.014 (2)	0.018 (3)
C18C	0.058 (4)	0.041 (3)	0.028 (2)	−0.026 (3)	−0.012 (2)	0.009 (2)
C19C	0.052 (4)	0.052 (3)	0.034 (3)	−0.026 (3)	0.002 (2)	−0.007 (2)
C20C	0.043 (3)	0.063 (4)	0.036 (3)	−0.016 (3)	0.004 (2)	−0.013 (3)
S1D	0.0215 (5)	0.0298 (6)	0.0467 (7)	0.0005 (4)	0.0007 (5)	−0.0087 (5)
S2D	0.0246 (6)	0.0539 (8)	0.0325 (6)	−0.0065 (5)	0.0026 (5)	0.0064 (5)
O1D	0.027 (2)	0.082 (4)	0.103 (4)	−0.020 (2)	0.004 (2)	−0.057 (3)
O2D	0.033 (2)	0.041 (2)	0.056 (2)	−0.0104 (16)	−0.0038 (17)	−0.0194 (18)
O3D	0.0205 (16)	0.047 (2)	0.0308 (16)	−0.0027 (14)	0.0036 (12)	−0.0086 (15)
O4D	0.0149 (15)	0.062 (2)	0.0289 (16)	−0.0037 (15)	0.0012 (12)	−0.0063 (16)
O5D	0.044 (2)	0.068 (3)	0.035 (2)	−0.008 (2)	−0.0099 (17)	0.0184 (19)
O6D	0.027 (2)	0.092 (4)	0.042 (2)	0.010 (2)	−0.0087 (17)	0.014 (2)
N1D	0.025 (2)	0.039 (2)	0.043 (2)	−0.0069 (18)	−0.0016 (17)	−0.0141 (19)
N2D	0.0174 (18)	0.0270 (19)	0.0274 (18)	−0.0044 (14)	−0.0024 (14)	−0.0038 (15)

N3D	0.0144 (17)	0.0232 (19)	0.0348 (19)	−0.0019 (14)	−0.0037 (14)	−0.0005 (15)
N4D	0.0123 (17)	0.036 (2)	0.0282 (18)	0.0013 (14)	0.0007 (14)	0.0043 (15)
N5D	0.0131 (17)	0.040 (2)	0.0231 (17)	−0.0008 (15)	−0.0028 (13)	−0.0062 (15)
N6D	0.0199 (19)	0.041 (2)	0.0196 (17)	−0.0025 (16)	0.0002 (14)	0.0020 (15)
N7D	0.0176 (18)	0.040 (2)	0.0229 (17)	0.0008 (15)	0.0030 (13)	−0.0017 (15)
N8D	0.039 (3)	0.042 (2)	0.029 (2)	−0.0025 (19)	−0.0108 (18)	0.0067 (18)
C1D	0.023 (2)	0.028 (2)	0.027 (2)	−0.0109 (18)	−0.0028 (17)	−0.0028 (17)
C2D	0.027 (2)	0.024 (2)	0.027 (2)	−0.0038 (18)	−0.0030 (17)	0.0000 (17)
C3D	0.029 (2)	0.019 (2)	0.028 (2)	−0.0010 (17)	−0.0007 (17)	0.0034 (16)
C4D	0.020 (2)	0.025 (2)	0.025 (2)	−0.0063 (16)	−0.0042 (16)	0.0061 (16)
C5D	0.020 (2)	0.029 (2)	0.024 (2)	−0.0008 (17)	0.0007 (16)	−0.0025 (17)
C6D	0.020 (2)	0.034 (2)	0.032 (2)	−0.0035 (19)	0.0032 (17)	−0.0061 (19)
C7D	0.018 (2)	0.029 (2)	0.023 (2)	0.0001 (17)	−0.0044 (16)	0.0003 (17)
C8D	0.018 (2)	0.028 (2)	0.026 (2)	−0.0083 (17)	−0.0033 (16)	0.0033 (17)
C9D	0.016 (2)	0.028 (2)	0.027 (2)	−0.0023 (16)	−0.0014 (16)	0.0016 (17)
C10D	0.017 (2)	0.032 (2)	0.029 (2)	−0.0033 (17)	−0.0007 (16)	−0.0056 (18)
C11D	0.020 (2)	0.027 (2)	0.030 (2)	−0.0007 (17)	−0.0002 (17)	−0.0033 (17)
C12D	0.019 (2)	0.034 (2)	0.026 (2)	−0.0034 (18)	0.0027 (16)	−0.0023 (18)
C13D	0.020 (2)	0.035 (2)	0.027 (2)	0.0009 (18)	−0.0025 (17)	0.0015 (19)
C14D	0.023 (2)	0.032 (2)	0.025 (2)	−0.0034 (18)	−0.0009 (17)	−0.0044 (18)
C15D	0.026 (2)	0.024 (2)	0.024 (2)	−0.0023 (17)	−0.0029 (17)	0.0000 (16)
C16D	0.026 (2)	0.033 (3)	0.030 (2)	−0.0046 (19)	0.0054 (18)	−0.0044 (19)
C17D	0.035 (3)	0.035 (3)	0.026 (2)	−0.002 (2)	−0.0036 (19)	0.0025 (19)
C18D	0.026 (2)	0.036 (3)	0.025 (2)	0.0022 (19)	−0.0064 (18)	0.0002 (18)
C19D	0.029 (2)	0.032 (2)	0.025 (2)	0.0010 (19)	0.0015 (18)	−0.0007 (18)
C20D	0.025 (2)	0.034 (2)	0.0195 (19)	0.0018 (18)	−0.0020 (16)	−0.0024 (17)
S3A	0.0179 (5)	0.0386 (6)	0.0315 (5)	0.0021 (4)	0.0022 (4)	0.0085 (5)
O7A	0.035 (2)	0.063 (3)	0.0377 (19)	−0.0136 (18)	0.0083 (15)	−0.0130 (18)
O8A	0.034 (2)	0.054 (2)	0.0400 (19)	−0.0089 (17)	−0.0048 (16)	0.0065 (17)
O9A	0.039 (2)	0.058 (3)	0.075 (3)	0.004 (2)	0.020 (2)	0.002 (2)
O10A	0.038 (2)	0.049 (2)	0.0383 (19)	0.0046 (17)	0.0120 (15)	0.0148 (16)
S3B	0.0144 (5)	0.0240 (5)	0.0221 (4)	−0.0022 (4)	0.0001 (4)	−0.0008 (4)
O7B	0.0271 (17)	0.0317 (17)	0.0303 (16)	0.0010 (13)	0.0070 (13)	0.0048 (13)
O8B	0.0190 (15)	0.0306 (17)	0.0341 (16)	−0.0070 (13)	0.0049 (12)	−0.0060 (13)
O9B	0.0173 (15)	0.047 (2)	0.0261 (15)	−0.0030 (14)	−0.0028 (12)	0.0070 (14)
O10B	0.039 (2)	0.0296 (18)	0.0408 (19)	0.0093 (15)	0.0107 (15)	0.0021 (14)
S3C	0.0129 (4)	0.0313 (5)	0.0243 (5)	−0.0013 (4)	−0.0011 (4)	0.0046 (4)
O7C	0.0203 (16)	0.0338 (19)	0.0452 (19)	0.0013 (13)	0.0077 (13)	0.0014 (15)

O8C	0.0251 (16)	0.0416 (19)	0.0182 (14)	0.0095 (14)	0.0012 (11)	0.0019 (13)
O9C	0.0278 (18)	0.047 (2)	0.0331 (17)	−0.0050 (15)	−0.0070 (14)	−0.0034 (15)
O10C	0.0170 (16)	0.0387 (19)	0.050 (2)	0.0015 (14)	0.0064 (14)	0.0138 (16)
S3D	0.0146 (5)	0.0329 (5)	0.0201 (4)	−0.0021 (4)	−0.0011 (3)	−0.0010 (4)
O7D	0.0263 (17)	0.0346 (18)	0.0384 (18)	0.0014 (14)	0.0079 (14)	0.0052 (14)
O8D	0.0145 (14)	0.0376 (18)	0.0282 (15)	−0.0001 (13)	−0.0024 (11)	−0.0065 (13)
O9D	0.0260 (17)	0.0331 (18)	0.0352 (17)	−0.0005 (14)	0.0038 (13)	−0.0072 (14)
O10D	0.0184 (15)	0.054 (2)	0.0271 (15)	0.0047 (15)	−0.0020 (12)	0.0074 (15)
N1E	0.027	0.043	0.023	−0.007	−0.005	0.002
N1F	0.022	0.025	0.024	−0.003	0.002	0.001
N1G	0.025	0.026	0.020	0.010	0.002	0.001
N1H	0.072	0.026	0.063	−0.001	0.019	−0.002
N1I	0.051	0.065	0.054	−0.003	−0.016	0.042
N1J	0.023	0.022	0.028	0.000	−0.001	0.002
N1K	0.068	0.047	0.042	−0.017	0.014	−0.004
N1L	0.032	0.057	0.032	0.005	0.007	0.017
C1E	0.025	0.053	0.036	−0.006	0.005	0.013
C2E	0.030	0.055	0.060	−0.020	−0.015	0.022
C3E	0.031	0.069	0.086	−0.011	−0.012	0.024
C4E	0.045	0.058	0.122	−0.024	−0.043	0.035
C5E	0.029	0.055	0.023	−0.016	−0.002	0.000
C6E	0.026	0.046	0.027	−0.012	−0.001	0.004
C7E	0.037	0.050	0.027	−0.018	−0.003	0.004
C8E	0.044	0.053	0.042	−0.005	0.000	0.009
C9E	0.049	0.052	0.020	−0.001	−0.011	−0.005
C10E	0.050	0.061	0.045	−0.016	−0.020	−0.004
C11E	0.085	0.051	0.051	−0.011	−0.041	−0.009
C12E	0.090	0.063	0.095	−0.036	−0.058	0.018
C13E	0.029	0.039	0.032	−0.009	0.001	−0.010
C14E	0.030	0.042	0.031	−0.011	−0.001	−0.003
C15E	0.027	0.049	0.043	−0.007	0.004	−0.003
C16E	0.046	0.052	0.038	−0.005	0.003	0.002
C1F	0.025	0.032	0.033	0.003	0.001	0.006
C2F	0.033	0.032	0.036	−0.001	0.000	0.003
C3F	0.025	0.039	0.050	−0.001	0.002	0.003
C4F	0.027	0.051	0.070	0.009	0.007	−0.006
C5F	0.026	0.024	0.026	0.002	0.002	0.004
C6F	0.028	0.031	0.022	−0.001	0.000	−0.001

C7F	0.037	0.030	0.030	0.003	0.005	0.000
C8F	0.034	0.051	0.034	0.005	0.005	0.004
C9F	0.034	0.025	0.030	0.002	0.010	0.003
C10F	0.038	0.032	0.052	−0.013	0.005	−0.008
C11F	0.053	0.037	0.032	−0.014	0.003	−0.002
C12F	0.043	0.042	0.051	−0.016	0.005	−0.008
C13F	0.040	0.025	0.022	0.005	0.008	0.008
C14F	0.063	0.033	0.037	0.005	0.016	0.005
C15F	0.080	0.033	0.036	0.000	0.020	−0.001
C1G	0.016	0.039	0.030	0.004	0.003	0.000
C2G	0.025	0.037	0.035	0.010	−0.003	−0.005
C3G	0.027	0.044	0.052	0.009	−0.003	−0.012
C4G	0.037	0.047	0.057	0.009	−0.020	−0.004
C6G	0.022	0.030	0.028	0.004	0.000	0.002
C5G	0.022	0.034	0.018	0.006	0.004	0.006
C7G	0.023	0.038	0.028	−0.001	−0.002	0.008
C8G	0.061	0.046	0.046	−0.022	0.005	−0.005
C9G	0.024	0.029	0.018	0.011	0.003	0.000
C10G	0.029	0.034	0.027	0.006	0.001	−0.005
C11G	0.034	0.036	0.036	0.006	0.005	−0.011
C12G	0.044	0.042	0.041	0.009	0.003	−0.008
C13G	0.038	0.026	0.018	0.007	0.007	0.004
C14G	0.042	0.057	0.025	0.022	−0.005	0.007
C15G	0.062	0.033	0.030	0.008	−0.009	0.008
C16G	0.081	0.057	0.036	0.025	−0.024	−0.001
C1H	0.062	0.031	0.054	0.000	0.017	−0.001
C2H	0.072	0.029	0.061	0.003	0.023	−0.004
C3H	0.063	0.036	0.067	−0.007	0.019	0.003
C4H	0.098	0.029	0.064	0.009	−0.007	−0.009
C5H	0.108	0.029	0.066	−0.015	0.019	−0.004
C6H	0.103	0.047	0.043	−0.040	0.009	−0.001
C9H	0.050	0.034	0.057	−0.007	0.017	−0.006
C10H	0.098	0.068	0.080	0.005	0.031	0.021
C11H	0.142	0.103	0.061	−0.045	0.034	0.005
C13H	0.099	0.032	0.085	0.017	0.031	0.015
C14H	0.078	0.040	0.105	0.016	0.014	0.015
C1I	0.042	0.088	0.079	0.022	0.012	0.054
C2I	0.078	0.112	0.076	0.036	0.005	0.056

C5I	0.052	0.044	0.056	−0.011	−0.025	0.028
C7I	0.079	0.050	0.068	0.007	−0.027	0.015
C9I	0.053	0.047	0.047	0.020	−0.018	0.009
C10I	0.064	0.084	0.067	0.000	−0.023	0.004
C1J	0.026	0.025	0.030	0.003	0.001	0.003
C2J	0.025	0.025	0.042	0.004	0.000	0.001
C3J	0.025	0.035	0.039	0.000	0.001	0.007
C4J	0.025	0.045	0.039	0.002	−0.005	0.001
C5J	0.027	0.024	0.023	0.000	0.005	0.003
C6J	0.048	0.029	0.028	0.002	0.001	−0.003
C7J	0.045	0.038	0.026	0.005	0.007	−0.002
C8J	0.049	0.046	0.046	0.003	0.016	0.000
C9J	0.027	0.026	0.025	0.000	0.004	0.001
C10J	0.028	0.033	0.030	−0.002	0.000	0.003
C11J	0.037	0.027	0.030	−0.001	0.001	0.005
C12J	0.036	0.046	0.022	−0.001	0.005	0.002
C13J	0.031	0.018	0.034	−0.005	−0.004	−0.001
C15J	0.026	0.037	0.039	−0.002	0.001	−0.005
C14J	0.036	0.033	0.049	−0.002	−0.007	0.013
C16J	0.025	0.055	0.048	−0.008	−0.004	0.000
C1K	0.100	0.049	0.053	−0.008	0.023	0.005
C2K	0.058	0.107	0.074	0.013	0.020	−0.027
C3K	0.098	0.079	0.136	−0.011	−0.025	0.057
C5K	0.076	0.068	0.047	−0.038	0.008	−0.004
C9K	0.074	0.050	0.043	−0.016	0.015	0.000
C10K	0.094	0.083	0.038	0.004	0.018	0.008
C11K	0.085	0.090	0.037	−0.004	0.030	0.002
C12K	0.108	0.092	0.067	−0.008	0.012	0.017
C13K	0.061	0.037	0.045	−0.016	0.014	−0.001
C14K	0.065	0.047	0.037	−0.013	0.006	−0.001
C15K	0.081	0.048	0.054	0.001	0.010	0.017
C16K	0.087	0.053	0.099	0.006	0.040	0.011
C1L	0.044	0.136	0.032	−0.021	−0.002	0.030
C2L	0.118	0.084	0.098	−0.033	0.062	−0.043
C5L	0.042	0.052	0.050	−0.004	0.014	0.012
C6L	0.039	0.056	0.060	0.003	0.012	0.018
C7L	0.061	0.067	0.074	−0.008	0.011	0.034
C8L	0.077	0.065	0.064	−0.021	0.004	0.005

C9L	0.044	0.072	0.116	0.011	0.020	0.047
C13L	0.039	0.057	0.035	0.006	−0.002	0.011
C14L	0.035	0.060	0.028	0.003	−0.002	0.006
C15L	0.038	0.083	0.042	0.004	0.000	0.006
C16L	0.042	0.084	0.054	−0.002	−0.006	−0.007
O1E	0.061	0.030	0.043	0.002	0.009	−0.003

Geometric parameters (Å, º)

S1A—C7A	1.686 (5)	C2F—C3F	1.5257
S2A—C14A	1.686 (6)	C2F—H2FA	0.9900
O1A—N1A	1.220 (6)	C2F—H2FB	0.9900
O2A—N1A	1.214 (6)	C3F—C4F	1.5265
O3A—C10A	1.233 (7)	C3F—H3FA	0.9900
O4A—C12A	1.234 (7)	C3F—H3FB	0.9900
O5A—N8A	1.208 (6)	C4F—H4FA	0.9800
O6A—N8A	1.228 (7)	C4F—H4FB	0.9800
N1A—C1A	1.471 (6)	C4F—H4FC	0.9800
N2A—C7A	1.368 (6)	C5F—C6F	1.5228
N2A—C4A	1.407 (6)	C5F—H5FA	0.9900
N2A—H2A	0.8800	C5F—H5FB	0.9900
N3A—C7A	1.323 (6)	C6F—C7F	1.5248
N3A—C8A	1.462 (6)	C6F—H6FA	0.9900
N3A—H3A	0.8800	C6F—H6FB	0.9900
N4A—C10A	1.345 (8)	C7F—C8F	1.5279
N4A—C9A	1.450 (7)	C7F—H7FA	0.9900
N4A—H4AA	0.8800	C7F—H7FB	0.9900
N5A—C12A	1.342 (7)	C8F—H8FA	0.9800
N5A—C11A	1.448 (7)	C8F—H8FB	0.9800
N5A—H5AA	0.8800	C8F—H8FC	0.9800
N6A—C14A	1.322 (8)	C9F—C10F	1.5096
N6A—C13A	1.483 (7)	C9F—H9FA	0.9900
N6A—H6A	0.8800	C9F—H9FB	0.9900
N7A—C14A	1.364 (7)	C10F—C11F	1.5199
N7A—C15A	1.401 (7)	C10F—H10G	0.9900
N7A—H7A	0.8800	C10F—H10H	0.9900
N8A—C18A	1.474 (7)	C11F—C12F	1.4942
C1A—C2A	1.362 (7)	C11F—H11H	0.9900

C1A—C6A	1.388 (8)	C11F—H11I	0.9900
C2A—C3A	1.382 (7)	C12F—H12E	0.9800
C2A—H2AA	0.9500	C12F—H12F	0.9800
C3A—C4A	1.402 (7)	C12F—H12G	0.9800
C3A—H3AA	0.9500	C13F—C14F	1.5258
C4A—C5A	1.377 (7)	C13F—H13H	0.9900
C5A—C6A	1.380 (7)	C13F—H13I	0.9900
C5A—H5AB	0.9500	C14F—C15F	1.5377
C6A—H6AA	0.9500	C14F—H14C	0.9900
C8A—C9A	1.503 (8)	C14F—H14D	0.9900
C8A—H8AA	0.9900	C15F—C16F	1.6195
C8A—H8AB	0.9900	C15F—H15C	0.9900
C9A—C12A	1.538 (7)	C15F—H15D	0.9900
C9A—H9AA	1.0000	C16F—H16H	0.9800
C10A—C11A	1.522 (7)	C16F—H16I	0.9800
C11A—C13A	1.485 (9)	C16F—H16J	0.9800
C11A—H11A	1.0000	C1G—C2G	1.5193
C13A—H13A	0.9900	C1G—H1GA	0.9900
C13A—H13B	0.9900	C1G—H1GB	0.9900
C15A—C16A	1.395 (7)	C2G—C3G	1.5328
C15A—C20A	1.401 (8)	C2G—H2GA	0.9900
C16A—C17A	1.397 (7)	C2G—H2GB	0.9900
C16A—H16A	0.9500	C3G—C4G	1.5206
C17A—C18A	1.353 (8)	C3G—H3GA	0.9900
C17A—H17A	0.9500	C3G—H3GB	0.9900
C18A—C19A	1.384 (8)	C4G—H4GA	0.9800
C19A—C20A	1.367 (8)	C4G—H4GB	0.9800
C19A—H19A	0.9500	C4G—H4GC	0.9800
C20A—H20A	0.9500	C6G—C7G	1.5060
S1B—C7B	1.680 (5)	C6G—C5G	1.5351
S2B—C14B	1.692 (5)	C6G—H6GA	0.9900
O1B—N1B	1.224 (6)	C6G—H6GB	0.9900
O2B—N1B	1.239 (6)	C5G—H5GA	0.9900
O3B—C10B	1.228 (6)	C5G—H5GB	0.9900
O4B—C12B	1.232 (6)	C7G—C8G	1.5136
O5B—N8B	1.222 (7)	C7G—H7GA	0.9900
O6B—N8B	1.228 (7)	C7G—H7GB	0.9900
N1B—C1B	1.458 (6)	C8G—H8GA	0.9800

N2B—C7B	1.376 (6)	C8G—H8GB	0.9800
N2B—C4B	1.384 (5)	C8G—H8GC	0.9800
N2B—H2B	0.8800	C9G—C10G	1.5125
N3B—C7B	1.340 (6)	C9G—H9GA	0.9900
N3B—C8B	1.455 (5)	C9G—H9GB	0.9900
N3B—H3B	0.8800	C10G—C11G	1.5329
N4B—C12B	1.347 (6)	C10G—H10I	0.9900
N4B—C9B	1.477 (6)	C10G—H10J	0.9900
N4B—H4BA	0.8800	C11G—C12G	1.4967
N5B—C10B	1.331 (6)	C11G—H11J	0.9900
N5B—C11B	1.468 (5)	C11G—H11K	0.9900
N5B—H5BA	0.8800	C12G—H12H	0.9800
N6B—C14B	1.337 (6)	C12G—H12I	0.9800
N6B—C13B	1.460 (6)	C12G—H12J	0.9800
N6B—H6B	0.8800	C13G—C14G	1.5217
N7B—C14B	1.374 (6)	C13G—H13J	0.9900
N7B—C15B	1.389 (6)	C13G—H13K	0.9900
N7B—H7B	0.8800	C14G—C15G	1.5203
N8B—C18B	1.463 (6)	C14G—H14E	0.9900
C1B—C2B	1.394 (7)	C14G—H14F	0.9900
C1B—C6B	1.399 (7)	C15G—C16G	1.5520
C2B—C3B	1.369 (6)	C15G—H15E	0.9900
C2B—H2BA	0.9500	C15G—H15F	0.9900
C3B—C4B	1.417 (6)	C16G—H16K	0.9800
C3B—H3BA	0.9500	C16G—H16L	0.9800
C4B—C5B	1.399 (6)	C16G—H16M	0.9800
C5B—C6B	1.372 (6)	C1H—C2H	1.5428
C5B—H5BB	0.9500	C1H—H1HA	0.9900
C6B—H6BA	0.9500	C1H—H1HB	0.9900
C8B—C9B	1.531 (6)	C2H—C3H	1.5316
C8B—H8BA	0.9900	C2H—H2HA	0.9900
C8B—H8BB	0.9900	C2H—H2HB	0.9900
C9B—C10B	1.529 (6)	C3H—C4H	1.5194
C9B—H9BA	1.0000	C3H—H3HA	0.9900
C11B—C13B	1.511 (6)	C3H—H3HB	0.9900
C11B—C12B	1.528 (6)	C4H—H4HA	0.9800
C11B—H11B	1.0000	C4H—H4HB	0.9800
C13B—H13C	0.9900	C4H—H4HC	0.9800

C13B—H13D	0.9900	C5H—C6H	1.5555
C15B—C16B	1.401 (8)	C5H—H5HA	0.9900
C15B—C20B	1.403 (7)	C5H—H5HB	0.9900
C16B—C17B	1.390 (8)	C6H—C7H	1.4991
C16B—H16B	0.9500	C6H—H6HA	0.9900
C17B—C18B	1.383 (8)	C6H—H6HB	0.9900
C17B—H17B	0.9500	C7H—C8H	1.3564
C18B—C19B	1.398 (8)	C7H—H7HA	0.9900
C19B—C20B	1.392 (6)	C7H—H7HB	0.9900
C19B—H19B	0.9500	C8H—H8HA	0.9800
C20B—H20B	0.9500	C8H—H8HB	0.9800
S1C—C7C	1.676 (5)	C8H—H8HC	0.9800
S2C—C14C	1.694 (6)	C9H—C10H	1.5349
O1C—N1C	1.217 (6)	C9H—H9HA	0.9900
O2C—N1C	1.214 (6)	C9H—H9HB	0.9900
O3C—C10C	1.229 (7)	C10H—C11H	1.5621
O4C—C13C	1.229 (7)	C10H—H10K	0.9900
O5C—O5CA	0.650 (10)	C10H—H10L	0.9900
O5C—N8C	1.044 (10)	C11H—C12H	1.5932
O5CA—N8C	1.410 (12)	C11H—H11L	0.9900
O6C—N8C	1.219 (9)	C11H—H11M	0.9900
N1C—C1C	1.449 (6)	C12H—H12K	0.9800
N2C—C7C	1.374 (6)	C12H—H12L	0.9800
N2C—C4C	1.381 (5)	C12H—H12M	0.9800
N2C—H2C	0.8800	C13H—C14H	1.5242
N3C—C7C	1.355 (6)	C13H—H13L	0.9900
N3C—C8C	1.463 (5)	C13H—H13V	0.9900
N3C—H3C	0.8800	C14H—C15H	1.5487
N4C—C13C	1.350 (7)	C14H—H14G	0.9900
N4C—C9C	1.445 (6)	C14H—H14H	0.9900
N4C—H4CA	0.8800	C15H—C16H	1.5018
N5C—C10C	1.325 (6)	C15H—H15G	0.9900
N5C—C12C	1.470 (7)	C15H—H15H	0.9900
N5C—H5CB	0.8800	C16H—H16N	0.9800
N6C—C14C	1.344 (6)	C16H—H16O	0.9800
N6C—C11C	1.461 (6)	C16H—H16P	0.9800
N6C—H6C	0.8800	C1I—C2I	1.5220
N7C—C14C	1.367 (6)	C1I—H1IA	0.9900

N7C—C15C	1.418 (6)	C1I—H1IB	0.9900
N7C—H7C	0.8800	C2I—C3I	1.5135
N8C—C18C	1.473 (7)	C2I—H2IA	0.9900
C1C—C6C	1.383 (7)	C2I—H2IB	0.9900
C1C—C2C	1.389 (7)	C3I—C4I	1.3721
C2C—C3C	1.376 (6)	C3I—H3IA	0.9900
C2C—H2CA	0.9500	C3I—H3IB	0.9900
C3C—C4C	1.404 (6)	C4I—H4IA	0.9800
C3C—H3CA	0.9500	C4I—H4IB	0.9800
C4C—C5C	1.396 (7)	C4I—H4IC	0.9800
C5C—C6C	1.382 (6)	C5I—C6I	1.4791
C5C—H5CC	0.9500	C5I—H5IA	0.9900
C6C—H6CA	0.9500	C5I—H5IB	0.9900
C8C—C9C	1.525 (6)	C6I—C7I	1.5217
C8C—H8CA	0.9900	C6I—H6IA	0.9900
C8C—H8CB	0.9900	C6I—H6IB	0.9900
C9C—C10C	1.557 (6)	C7I—C8I	1.4851
C9C—H9CA	1.0000	C7I—H7IA	0.9900
C11C—C12C	1.538 (7)	C7I—H7IB	0.9900
C11C—H11C	0.9900	C8I—H8IA	0.9800
C11C—H11D	0.9900	C8I—H8IB	0.9800
C12C—C13C	1.514 (7)	C8I—H8IC	0.9800
C12C—H12A	1.0000	C9I—C10I	1.5255
C15C—C20C	1.386 (9)	C9I—H9IA	0.9900
C15C—C16C	1.394 (8)	C9I—H9IB	0.9900
C16C—C17C	1.392 (7)	C10I—C11I	1.5006
C16C—H16C	0.9500	C10I—H10M	0.9900
C17C—C18C	1.372 (10)	C10I—H10N	0.9900
C17C—H17C	0.9500	C11I—C12I	1.5553
C18C—C19C	1.380 (10)	C11I—H11N	0.9900
C19C—C20C	1.399 (8)	C11I—H11O	0.9900
C19C—H19C	0.9500	C12I—H12N	0.9800
C20C—H20C	0.9500	C12I—H12O	0.9800
S1D—C7D	1.663 (5)	C12I—H12P	0.9800
S2D—C14D	1.689 (5)	C13I—C14I	1.5895
O1D—N1D	1.225 (6)	C13I—H13M	0.9900
O2D—N1D	1.220 (6)	C13I—H13N	0.9900
O3D—C12D	1.236 (6)	C14I—C15I	1.6003

O4D—C10D	1.230 (6)	C14I—H14I	0.9900
O5D—N8D	1.240 (6)	C14I—H14J	0.9900
O6D—N8D	1.211 (6)	C15I—C16I	1.4250
N1D—C1D	1.460 (6)	C15I—H15I	0.9900
N2D—C7D	1.392 (6)	C15I—H15J	0.9900
N2D—C4D	1.397 (6)	C16I—H16Q	0.9800
N2D—H2D	0.8800	C16I—H16R	0.9800
N3D—C7D	1.351 (6)	C16I—H16S	0.9800
N3D—C8D	1.444 (5)	C1J—C2J	1.5165
N3D—H3D	0.8800	C1J—H1JA	0.9900
N4D—C12D	1.326 (6)	C1J—H1JB	0.9900
N4D—C9D	1.447 (6)	C2J—C3J	1.5218
N4D—H4DA	0.8800	C2J—H2JA	0.9900
N5D—C10D	1.326 (6)	C2J—H2JB	0.9900
N5D—C11D	1.466 (6)	C3J—C4J	1.5176
N5D—H5DA	0.8800	C3J—H3JA	0.9900
N6D—C14D	1.370 (6)	C3J—H3JB	0.9900
N6D—C15D	1.399 (6)	C4J—H4JA	0.9800
N6D—H6D	0.8800	C4J—H4JB	0.9800
N7D—C14D	1.344 (6)	C4J—H4JC	0.9800
N7D—C13D	1.454 (6)	C5J—C6J	1.5282
N7D—H7D	0.8800	C5J—H5JA	0.9900
N8D—C18D	1.459 (6)	C5J—H5JB	0.9900
C1D—C6D	1.380 (7)	C6J—C7J	1.5359
C1D—C2D	1.393 (7)	C6J—H6JA	0.9900
C2D—C3D	1.391 (6)	C6J—H6JB	0.9900
C2D—H2DA	0.9500	C7J—C8J	1.5354
C3D—C4D	1.404 (7)	C7J—H7JA	0.9900
C3D—H3DA	0.9500	C7J—H7JB	0.9900
C4D—C5D	1.397 (6)	C8J—H8JA	0.9800
C5D—C6D	1.381 (6)	C8J—H8JB	0.9800
C5D—H5DB	0.9500	C8J—H8JC	0.9800
C6D—H6DA	0.9500	C9J—C10J	1.5398
C8D—C9D	1.519 (6)	C9J—H9JA	0.9900
C8D—H8DA	0.9900	C9J—H9JB	0.9900
C8D—H8DB	0.9900	C10J—C11J	1.5271
C9D—C10D	1.534 (6)	C10J—H10O	0.9900
C9D—H9DA	1.0000	C10J—H10P	0.9900

C11D—C12D	1.521 (6)	C11J—C12J	1.5216
C11D—C13D	1.526 (6)	C11J—H11P	0.9900
C11D—H11E	1.0000	C11J—H11Q	0.9900
C13D—H13E	0.9900	C12J—H12Q	0.9800
C13D—H13F	0.9900	C12J—H12R	0.9800
C15D—C16D	1.379 (7)	C12J—H12S	0.9800
C15D—C20D	1.412 (7)	C13J—C14J	1.5148
C16D—C17D	1.396 (7)	C13J—H13O	0.9900
C16D—H16D	0.9500	C13J—H13P	0.9900
C17D—C18D	1.371 (7)	C15J—C14J	1.5273
C17D—H17D	0.9500	C15J—C16J	1.5313
C18D—C19D	1.392 (7)	C15J—H15K	0.9900
C19D—C20D	1.357 (6)	C15J—H15L	0.9900
C19D—H19D	0.9500	C14J—H14K	0.9900
C20D—H20D	0.9500	C14J—H14L	0.9900
S3A—O9A	1.436 (5)	C16J—H16T	0.9800
S3A—O10A	1.467 (4)	C16J—H16U	0.9800
S3A—O8A	1.480 (4)	C16J—H16V	0.9800
S3A—O7A	1.489 (4)	C1K—C2K	1.4973
S3B—O9B	1.468 (3)	C1K—H1KA	0.9900
S3B—O10B	1.474 (4)	C1K—H1KB	0.9900
S3B—O7B	1.478 (3)	C2K—C3K	1.4979
S3B—O8B	1.481 (3)	C2K—H2KA	0.9900
S3C—O10C	1.457 (3)	C2K—H2KB	0.9900
S3C—O9C	1.466 (4)	C3K—C4K	1.6036
S3C—O7C	1.488 (4)	C3K—H3KA	0.9900
S3C—O8C	1.499 (3)	C3K—H3KB	0.9900
S3D—O7D	1.474 (4)	C4K—H4KA	0.9800
S3D—O8D	1.475 (3)	C4K—H4KB	0.9800
S3D—O9D	1.478 (4)	C4K—H4KC	0.9800
S3D—O10D	1.488 (3)	C5K—C6K	1.5162
N1E—C13E	1.4981	C5K—H5KA	0.9900
N1E—C1E	1.5053	C5K—H5KB	0.9900
N1E—C5E	1.5413	C6K—C7K	1.5589
N1E—C9E	1.5416	C6K—H6KA	0.9900
N1F—C1F	1.5080	C6K—H6KB	0.9900
N1F—C5F	1.5080	C7K—C8K	1.5723
N1F—C9F	1.5234	C7K—H7KA	0.9900

N1F—C13F	1.5347	C7K—H7KB	0.9900
N1G—C5G	1.5143	C8K—H8KA	0.9800
N1G—C1G	1.5196	C8K—H8KB	0.9800
N1G—C13G	1.5235	C8K—H8KC	0.9800
N1G—C9G	1.5319	C9K—C10K	1.4716
N1H—C9H	1.4995	C9K—H9KA	0.9900
N1H—C1H	1.5023	C9K—H9KB	0.9900
N1H—C5H	1.5052	C10K—C11K	1.5426
N1H—C13H	1.5586	C10K—H10Q	0.9900
N1I—C1I	1.4662	C10K—H10R	0.9900
N1I—C5I	1.5044	C11K—C12K	1.5895
N1I—C9I	1.5260	C11K—H11R	0.9900
N1I—C13I	1.5382	C11K—H11S	0.9900
N1J—C1J	1.5170	C12K—H12T	0.9800
N1J—C9J	1.5180	C12K—H12U	0.9800
N1J—C13J	1.5270	C12K—H12V	0.9800
N1J—C5J	1.5315	C13K—C14K	1.5169
N1K—C5K	1.5003	C13K—H13Q	0.9900
N1K—C1K	1.5093	C13K—H13R	0.9900
N1K—C13K	1.5267	C14K—C15K	1.5311
N1K—C9K	1.5405	C14K—H14M	0.9900
N1L—C9L	1.4794	C14K—H14N	0.9900
N1L—C13L	1.4869	C15K—C16K	1.4496
N1L—C5L	1.5371	C15K—H15M	0.9900
N1L—C1L	1.5697	C15K—H15N	0.9900
C1E—C2E	1.5111	C16K—H16W	0.9800
C1E—H1EA	0.9900	C16K—H16X	0.9800
C1E—H1EB	0.9900	C16K—H16Y	0.9800
C2E—C3E	1.5169	C1L—C2L	1.5089
C2E—H2EA	0.9900	C1L—H1LA	0.9900
C2E—H2EB	0.9900	C1L—H1LB	0.9900
C3E—C4E	1.5345	C2L—C3L	1.5196
C3E—H3EA	0.9900	C2L—H2LA	0.9900
C3E—H3EB	0.9900	C2L—H2LB	0.9900
C4E—H4EA	0.9800	C3L—C4L	1.4166
C4E—H4EB	0.9800	C3L—H3LA	0.9900
C4E—H4EC	0.9800	C3L—H3LB	0.9900
C5E—C6E	1.5132	C4L—H4LA	0.9800

C5E—H5EA	0.9900	C4L—H4LB	0.9800
C5E—H5EB	0.9900	C4L—H4LC	0.9800
C6E—C7E	1.5205	C5L—C6L	1.5215
C6E—H6EA	0.9900	C5L—H5LA	0.9900
C6E—H6EB	0.9900	C5L—H5LB	0.9900
C7E—C8E	1.5384	C6L—C7L	1.5404
C7E—H7EA	0.9900	C6L—H6LA	0.9900
C7E—H7EB	0.9900	C6L—H6LB	0.9900
C8E—H8EA	0.9800	C7L—C8L	1.4677
C8E—H8EB	0.9800	C7L—H7LA	0.9900
C8E—H8EC	0.9800	C7L—H7LB	0.9900
C9E—C10E	1.4912	C8L—H8LA	0.9800
C9E—H9EA	0.9900	C8L—H8LB	0.9800
C9E—H9EB	0.9900	C8L—H8LC	0.9800
C10E—C11E	1.5580	C9L—C10L	1.5296
C10E—H10E	0.9900	C9L—H9LA	0.9900
C10E—H10F	0.9900	C9L—H9LB	0.9900
C11E—C12E	1.4890	C10L—C11L	1.4560
C11E—H11F	0.9900	C10L—H10S	0.9900
C11E—H11G	0.9900	C10L—H10T	0.9900
C12E—H12B	0.9800	C11L—C12L	1.6901
C12E—H12C	0.9800	C11L—H11T	0.9900
C12E—H12D	0.9800	C11L—H11U	0.9900
C13E—C14E	1.5036	C12L—H12W	0.9800
C13E—H13G	0.9900	C12L—H12X	0.9800
C13E—H13U	0.9900	C12L—H12Y	0.9800
C14E—C15E	1.5236	C13L—C14L	1.5790
C14E—H14A	0.9900	C13L—H13S	0.9900
C14E—H14B	0.9900	C13L—H13T	0.9900
C15E—C16E	1.5269	C14L—C15L	1.5320
C15E—H15A	0.9900	C14L—H14O	0.9900
C15E—H15B	0.9900	C14L—H14P	0.9900
C16E—H16E	0.9800	C15L—C16L	1.5460
C16E—H16F	0.9800	C15L—H15O	0.9900
C16E—H16G	0.9800	C15L—H15P	0.9900
C1F—C2F	1.5487	C16L—H16Z	0.9800
C1F—H1FA	0.9900	C16L—H17E	0.9800
C1F—H1FB	0.9900	C16L—H17F	0.9800

O1E···O8B	2.884 (3)		
O2A—N1A—C1A—C2A	−179.7 (6)	C4D—C5D—C6D—C1D	−0.6 (7)
O1A—N1A—C1A—C2A	−0.5 (8)	C8D—N3D—C7D—N2D	176.1 (4)
O2A—N1A—C1A—C6A	2.7 (8)	C8D—N3D—C7D—S1D	−3.9 (6)
O1A—N1A—C1A—C6A	−178.0 (5)	C4D—N2D—C7D—N3D	155.4 (4)
C6A—C1A—C2A—C3A	−3.1 (8)	C4D—N2D—C7D—S1D	−24.6 (7)
N1A—C1A—C2A—C3A	179.4 (5)	C7D—N3D—C8D—C9D	−83.4 (5)
C1A—C2A—C3A—C4A	1.5 (8)	C12D—N4D—C9D—C8D	−150.3 (4)
C2A—C3A—C4A—C5A	0.7 (8)	C12D—N4D—C9D—C10D	−28.7 (6)
C2A—C3A—C4A—N2A	−176.6 (5)	N3D—C8D—C9D—N4D	−62.0 (5)
C7A—N2A—C4A—C5A	169.8 (5)	N3D—C8D—C9D—C10D	174.7 (4)
C7A—N2A—C4A—C3A	−12.8 (8)	C11D—N5D—C10D—O4D	−177.3 (5)
C3A—C4A—C5A—C6A	−1.5 (8)	C11D—N5D—C10D—C9D	3.0 (7)
N2A—C4A—C5A—C6A	176.0 (5)	N4D—C9D—C10D—O4D	−152.6 (4)
C4A—C5A—C6A—C1A	0.0 (9)	C8D—C9D—C10D—O4D	−29.1 (6)
C2A—C1A—C6A—C5A	2.3 (8)	N4D—C9D—C10D—N5D	27.2 (6)
N1A—C1A—C6A—C5A	179.8 (5)	C8D—C9D—C10D—N5D	150.6 (4)
C8A—N3A—C7A—N2A	171.4 (5)	C10D—N5D—C11D—C12D	−32.0 (6)
C8A—N3A—C7A—S1A	−8.6 (8)	C10D—N5D—C11D—C13D	−152.9 (5)
C4A—N2A—C7A—N3A	174.4 (5)	C9D—N4D—C12D—O3D	−178.2 (4)
C4A—N2A—C7A—S1A	−5.6 (8)	C9D—N4D—C12D—C11D	−0.6 (7)
C7A—N3A—C8A—	−122.0 (6)	N5D—C11D—C12D—	−151.9 (4)

C9A		O3D	
C10A—N4A—C9A—C8A	−92.2 (7)	C13D—C11D—C12D—O3D	−30.1 (6)
C10A—N4A—C9A—C12A	29.3 (8)	N5D—C11D—C12D—N4D	30.4 (6)
N3A—C8A—C9A—N4A	−70.8 (5)	C13D—C11D—C12D—N4D	152.2 (4)
N3A—C8A—C9A—C12A	164.1 (4)	C14D—N7D—C13D—C11D	−88.9 (5)
C9A—N4A—C10A—O3A	169.0 (6)	N5D—C11D—C13D—N7D	−64.5 (5)
C9A—N4A—C10A—C11A	−13.8 (9)	C12D—C11D—C13D—N7D	173.6 (4)
C12A—N5A—C11A—C13A	−107.9 (6)	C13D—N7D—C14D—N6D	178.2 (4)
C12A—N5A—C11A—C10A	17.0 (8)	C13D—N7D—C14D—S2D	−0.8 (6)
O3A—C10A—C11A—N5A	167.8 (6)	C15D—N6D—C14D—N7D	153.3 (5)
N4A—C10A—C11A—N5A	−9.5 (8)	C15D—N6D—C14D—S2D	−27.7 (7)
O3A—C10A—C11A—C13A	−64.8 (7)	C14D—N6D—C15D—C16D	17.0 (8)
N4A—C10A—C11A—C13A	117.8 (6)	C14D—N6D—C15D—C20D	−162.4 (5)
C11A—N5A—C12A—O4A	177.7 (6)	N6D—C15D—C16D—C17D	−177.9 (5)
C11A—N5A—C12A—C9A	−1.1 (8)	C20D—C15D—C16D—C17D	1.5 (7)
N4A—C9A—C12A—O4A	159.9 (5)	C15D—C16D—C17D—C18D	−0.6 (8)
C8A—C9A—C12A—O4A	−75.2 (6)	C16D—C17D—C18D—C19D	−1.0 (8)
N4A—C9A—C12A—N5A	−21.2 (7)	C16D—C17D—C18D—N8D	179.1 (5)
C8A—C9A—C12A—N5A	103.7 (6)	O6D—N8D—C18D—C17D	170.9 (5)
C14A—N6A—C13A—C11A	−173.1 (5)	O5D—N8D—C18D—C17D	−11.3 (8)
N5A—C11A—C13A—N6A	−64.5 (6)	O6D—N8D—C18D—C19D	−9.0 (8)
C10A—C11A—C13A—	168.3 (4)	O5D—N8D—C18D—	168.8 (5)

N6A		C19D	
C13A—N6A—C14A—N7A	−179.4 (5)	C17D—C18D—C19D—C20D	1.6 (8)
C13A—N6A—C14A—S2A	0.1 (7)	N8D—C18D—C19D—C20D	−178.5 (4)
C15A—N7A—C14A—N6A	−164.0 (5)	C18D—C19D—C20D—C15D	−0.6 (7)
C15A—N7A—C14A—S2A	16.6 (8)	C16D—C15D—C20D—C19D	−0.9 (7)
C14A—N7A—C15A—C16A	10.7 (8)	N6D—C15D—C20D—C19D	178.6 (4)
C14A—N7A—C15A—C20A	−171.1 (5)	C13E—N1E—C1E—C2E	59.6
N7A—C15A—C16A—C17A	178.3 (5)	C5E—N1E—C1E—C2E	−60.6
C20A—C15A—C16A—C17A	0.1 (8)	C9E—N1E—C1E—C2E	179.8
C15A—C16A—C17A—C18A	1.0 (8)	N1E—C1E—C2E—C3E	174.1
C16A—C17A—C18A—C19A	−0.9 (8)	C1E—C2E—C3E—C4E	175.2
C16A—C17A—C18A—N8A	179.4 (5)	C13E—N1E—C5E—C6E	−174.9
O5A—N8A—C18A—C17A	15.2 (8)	C1E—N1E—C5E—C6E	−54.1
O6A—N8A—C18A—C17A	−162.6 (6)	C9E—N1E—C5E—C6E	65.2
O5A—N8A—C18A—C19A	−164.4 (6)	N1E—C5E—C6E—C7E	−177.6
O6A—N8A—C18A—C19A	17.7 (8)	C5E—C6E—C7E—C8E	−173.0
C17A—C18A—C19A—C20A	−0.3 (8)	C13E—N1E—C9E—C10E	−54.8
N8A—C18A—C19A—C20A	179.4 (5)	C1E—N1E—C9E—C10E	−175.1
C18A—C19A—C20A—C15A	1.4 (8)	C5E—N1E—C9E—C10E	64.5
C16A—C15A—C20A—C19A	−1.4 (8)	N1E—C9E—C10E—C11E	−177.4
N7A—C15A—C20A—C19A	−179.6 (5)	C9E—C10E—C11E—C12E	176.2
O1B—N1B—C1B—C2B	168.3 (5)	C1E—N1E—C13E—	58.3

O2B—N1B—C1B—C2B	−13.1 (7)	C14E	
O1B—N1B—C1B—C6B	−13.3 (7)	C5E—N1E—C13E—C14E	179.4
O2B—N1B—C1B—C6B	165.4 (5)	C9E—N1E—C13E—C14E	−61.2
C6B—C1B—C2B—C3B	0.5 (7)	N1E—C13E—C14E—C15E	174.4
N1B—C1B—C2B—C3B	179.0 (4)	C13E—C14E—C15E—C16E	−179.1
C1B—C2B—C3B—C4B	0.1 (7)	C5F—N1F—C1F—C2F	61.4
C7B—N2B—C4B—C5B	1.7 (7)	C9F—N1F—C1F—C2F	−178.6
C7B—N2B—C4B—C3B	−174.8 (4)	C13F—N1F—C1F—C2F	−57.8
C2B—C3B—C4B—N2B	175.4 (4)	N1F—C1F—C2F—C3F	−175.7
C2B—C3B—C4B—C5B	−1.5 (7)	C1F—C2F—C3F—C4F	−67.2
N2B—C4B—C5B—C6B	−174.1 (4)	C1F—N1F—C5F—C6F	50.9
C3B—C4B—C5B—C6B	2.3 (6)	C9F—N1F—C5F—C6F	−66.3
C4B—C5B—C6B—C1B	−1.8 (7)	C13F—N1F—C5F—C6F	173.3
C2B—C1B—C6B—C5B	0.3 (7)	N1F—C5F—C6F—C7F	172.3
N1B—C1B—C6B—C5B	−178.1 (4)	C5F—C6F—C7F—C8F	−75.7
C8B—N3B—C7B—N2B	179.7 (4)	C1F—N1F—C9F—C10F	175.9
C8B—N3B—C7B—S1B	2.0 (6)	C5F—N1F—C9F—C10F	−63.0
C4B—N2B—C7B—N3B	150.8 (4)	C13F—N1F—C9F—C10F	54.6
C4B—N2B—C7B—S1B	−31.6 (6)	N1F—C9F—C10F—C11F	−169.3
C7B—N3B—C8B—C9B	−90.9 (5)	C9F—C10F—C11F—C12F	−177.1
C12B—N4B—C9B—C10B	−34.6 (6)	C1F—N1F—C13F—C14F	−60.4
C12B—N4B—C9B—C8B	−155.6 (4)	C5F—N1F—C13F—C14F	177.1
N3B—C8B—C9B—N4B	−59.5 (5)	C9F—N1F—C13F—C14F	57.1
N3B—C8B—C9B—C10B	177.7 (4)	N1F—C13F—C14F—C15F	−172.9
C11B—N5B—C10B—O3B	−171.1 (4)	C13F—C14F—C15F—C16F	71.5
C11B—N5B—C10B—C9B	8.4 (7)	C5G—N1G—C1G—C2G	56.1
		C13G—N1G—C1G—C2G	178.2

N4B—C9B—C10B—O3B	−151.9 (4)	C9G—N1G—C1G—C2G	−62.4
C8B—C9B—C10B—O3B	−29.0 (6)	N1G—C1G—C2G—C3G	170.0
N4B—C9B—C10B—N5B	28.6 (5)	C1G—C2G—C3G—C4G	171.7
C8B—C9B—C10B—N5B	151.5 (4)	C1G—N1G—C5G—C6G	62.2
C10B—N5B—C11B—C13B	−163.2 (4)	C13G—N1G—C5G—C6G	−57.3
C10B—N5B—C11B—C12B	−40.6 (6)	C9G—N1G—C5G—C6G	−177.7
C9B—N4B—C12B—O4B	−176.2 (4)	C7G—C6G—C5G—N1G	−178.1
C9B—N4B—C12B—C11B	2.3 (6)	C5G—C6G—C7G—C8G	−173.8
N5B—C11B—C12B—O4B	−147.5 (4)	C5G—N1G—C9G—C10G	−176.8
C13B—C11B—C12B—O4B	−24.0 (6)	C1G—N1G—C9G—C10G	−56.0
N5B—C11B—C12B—N4B	33.8 (5)	C13G—N1G—C9G—C10G	61.7
C13B—C11B—C12B—N4B	157.4 (4)	N1G—C9G—C10G—C11G	174.9
C14B—N6B—C13B—C11B	−81.4 (5)	C9G—C10G—C11G—C12G	178.9
N5B—C11B—C13B—N6B	−63.8 (5)	C5G—N1G—C13G—C14G	−48.1
C12B—C11B—C13B—N6B	173.3 (4)	C1G—N1G—C13G—C14G	−169.9
C13B—N6B—C14B—N7B	177.5 (4)	C9G—N1G—C13G—C14G	70.7
C13B—N6B—C14B—S2B	−1.5 (6)	N1G—C13G—C14G—C15G	−168.6
C15B—N7B—C14B—N6B	171.9 (5)	C13G—C14G—C15G—C16G	−174.4
C15B—N7B—C14B—S2B	−9.1 (8)	C9H—N1H—C1H—C2H	−178.5
C14B—N7B—C15B—C16B	19.1 (9)	C5H—N1H—C1H—C2H	−56.8
C14B—N7B—C15B—C20B	−161.2 (5)	C13H—N1H—C1H—C2H	59.2

N7B—C15B—C16B—C17B	−179.6 (5)	N1H—C1H—C2H—C3H	166.8
C20B—C15B—C16B—C17B	0.7 (9)	C1H—C2H—C3H—C4H	−69.7
C15B—C16B—C17B—C18B	0.7 (10)	C9H—N1H—C5H—C6H	68.3
C16B—C17B—C18B—C19B	−1.5 (9)	C1H—N1H—C5H—C6H	−50.4
C16B—C17B—C18B—N8B	179.3 (5)	C13H—N1H—C5H—C6H	−169.1
O5B—N8B—C18B—C17B	14.3 (7)	N1H—C5H—C6H—C7H	−173.5
O6B—N8B—C18B—C17B	−166.8 (6)	C5H—C6H—C7H—C8H	−169.7
O5B—N8B—C18B—C19B	−164.9 (5)	C1H—N1H—C9H—C10H	−176.7
O6B—N8B—C18B—C19B	14.0 (7)	C5H—N1H—C9H—C10H	60.7
C17B—C18B—C19B—C20B	1.0 (8)	C13H—N1H—C9H—C10H	−56.9
N8B—C18B—C19B—C20B	−179.9 (4)	N1H—C9H—C10H—C11H	176.1
C18B—C19B—C20B—C15B	0.5 (7)	C9H—C10H—C11H—C12H	−88.4
N7B—C15B—C20B—C19B	178.9 (4)	C9H—N1H—C13H—C14H	−59.5
C16B—C15B—C20B—C19B	−1.3 (8)	C1H—N1H—C13H—C14H	58.4
O5CA—O5C—N8C—O6C	−125.8 (15)	C5H—N1H—C13H—C14H	179.3
O5CA—O5C—N8C—C18C	67.5 (17)	N1H—C13H—C14H—C15H	171.5
O5C—O5CA—N8C—O6C	68.6 (17)	C13H—C14H—C15H—C16H	175.0
O5C—O5CA—N8C—C18C	−124.0 (15)	C5I—N1I—C1I—C2I	−177.3
O2C—N1C—C1C—C6C	10.8 (9)	C9I—N1I—C1I—C2I	62.1
O1C—N1C—C1C—C6C	−168.3 (6)	C13I—N1I—C1I—C2I	−56.2
O2C—N1C—C1C—C2C	−170.2 (6)	N1I—C1I—C2I—C3I	−171.1
O1C—N1C—C1C—C2C	10.6 (9)	C1I—C2I—C3I—C4I	−169.0
C6C—C1C—C2C—C3C	0.2 (8)	C1I—N1I—C5I—C6I	172.6

N1C—C1C—C2C—C3C	−178.7 (5)	C9I—N1I—C5I—C6I	−65.9
C1C—C2C—C3C—C4C	0.8 (8)	C13I—N1I—C5I—C6I	53.6
C7C—N2C—C4C—C5C	175.4 (5)	N1I—C5I—C6I—C7I	176.7
C7C—N2C—C4C—C3C	−3.6 (8)	C5I—C6I—C7I—C8I	168.7
C2C—C3C—C4C—N2C	177.3 (5)	C1I—N1I—C9I—C10I	56.8
C2C—C3C—C4C—C5C	−1.7 (7)	C5I—N1I—C9I—C10I	−61.9
N2C—C4C—C5C—C6C	−177.5 (4)	C13I—N1I—C9I—C10I	175.9
C3C—C4C—C5C—C6C	1.5 (7)	N1I—C9I—C10I—C11I	177.9
C4C—C5C—C6C—C1C	−0.5 (7)	C9I—C10I—C11I—C12I	177.1
C2C—C1C—C6C—C5C	−0.4 (8)	C1I—N1I—C13I—C14I	−47.7
N1C—C1C—C6C—C5C	178.6 (5)	C5I—N1I—C13I—C14I	70.3
C8C—N3C—C7C—N2C	−175.5 (4)	C9I—N1I—C13I—C14I	−168.6
C8C—N3C—C7C—S1C	2.5 (6)	N1I—C13I—C14I—C15I	166.4
C4C—N2C—C7C—N3C	−160.8 (4)	C13I—C14I—C15I—C16I	−178.2
C4C—N2C—C7C—S1C	21.4 (7)	C9J—N1J—C1J—C2J	56.4
C7C—N3C—C8C—C9C	175.4 (4)	C13J—N1J—C1J—C2J	177.8
C13C—N4C—C9C—C8C	−98.8 (5)	C5J—N1J—C1J—C2J	−61.5
C13C—N4C—C9C—C10C	24.9 (7)	N1J—C1J—C2J—C3J	−179.9
N3C—C8C—C9C—N4C	−64.0 (5)	C1J—C2J—C3J—C4J	168.3
N3C—C8C—C9C—C10C	169.8 (4)	C1J—N1J—C5J—C6J	−61.5
C12C—N5C—C10C—O3C	170.4 (5)	C9J—N1J—C5J—C6J	176.7
C12C—N5C—C10C—C9C	−10.1 (7)	C13J—N1J—C5J—C6J	56.4
N4C—C9C—C10C—O3C	163.9 (5)	N1J—C5J—C6J—C7J	171.2
C8C—C9C—C10C—O3C	−69.7 (6)	C5J—C6J—C7J—C8J	−77.0
N4C—C9C—C10C—N5C	−15.7 (6)	C1J—N1J—C9J—C10J	49.2
C8C—C9C—C10C—N5C	110.7 (5)	C13J—N1J—C9J—C10J	−69.2
C14C—N6C—C11C—C12C	−100.1 (5)	C5J—N1J—C9J—C10J	170.8
C10C—N5C—C12C—C13C	27.5 (7)	N1J—C9J—C10J—C11J	166.6

C10C—N5C—C12C—C11C	−96.9 (5)	C9J—C10J—C11J—C12J	−80.0
N6C—C11C—C12C—N5C	−76.0 (5)	C1J—N1J—C13J—C14J	173.3
N6C—C11C—C12C—C13C	157.6 (4)	C9J—N1J—C13J—C14J	−64.8
C9C—N4C—C13C—O4C	174.1 (5)	C5J—N1J—C13J—C14J	52.0
C9C—N4C—C13C—C12C	−7.5 (7)	N1J—C13J—C14J—C15J	174.5
N5C—C12C—C13C—O4C	160.4 (5)	C16J—C15J—C14J—C13J	170.5
C11C—C12C—C13C—O4C	−73.7 (6)	C5K—N1K—C1K—C2K	−177.4
N5C—C12C—C13C—N4C	−18.1 (6)	C13K—N1K—C1K—C2K	59.9
C11C—C12C—C13C—N4C	107.9 (5)	C9K—N1K—C1K—C2K	−55.8
C11C—N6C—C14C—N7C	167.6 (4)	N1K—C1K—C2K—C3K	179.9
C11C—N6C—C14C—S2C	−10.9 (7)	C1K—C2K—C3K—C4K	−167.6
C15C—N7C—C14C—N6C	167.3 (4)	C1K—N1K—C5K—C6K	−177.8
C15C—N7C—C14C—S2C	−14.3 (8)	C13K—N1K—C5K—C6K	−55.7
C14C—N7C—C15C—C20C	10.1 (8)	C9K—N1K—C5K—C6K	60.5
C14C—N7C—C15C—C16C	−170.2 (5)	N1K—C5K—C6K—C7K	−179.2
C20C—C15C—C16C—C17C	−1.4 (8)	C5K—C6K—C7K—C8K	−174.2
N7C—C15C—C16C—C17C	178.9 (4)	C5K—N1K—C9K—C10K	68.5
C15C—C16C—C17C—C18C	−1.1 (8)	C1K—N1K—C9K—C10K	−51.8
C16C—C17C—C18C—C19C	2.9 (8)	C13K—N1K—C9K—C10K	−171.1
C16C—C17C—C18C—N8C	−179.2 (5)	N1K—C9K—C10K—C11K	−165.1
O5C—N8C—C18C—C17C	−21.6 (10)	C9K—C10K—C11K—C12K	76.0

O6C—N8C—C18C—C17C	172.2 (5)	C5K—N1K—C13K—C14K	−57.9
O5CA—N8C—C18C—C17C	3.6 (8)	C1K—N1K—C13K—C14K	62.9
O5C—N8C—C18C—C19C	156.5 (9)	C9K—N1K—C13K—C14K	−177.8
O6C—N8C—C18C—C19C	−9.8 (8)	N1K—C13K—C14K—C15K	−172.0
O5CA—N8C—C18C—C19C	−178.4 (6)	C13K—C14K—C15K—C16K	69.7
C17C—C18C—C19C—C20C	−2.3 (9)	C9L—N1L—C1L—C2L	−171.0
N8C—C18C—C19C—C20C	179.8 (5)	C13L—N1L—C1L—C2L	−45.6
C16C—C15C—C20C—C19C	2.0 (8)	C5L—N1L—C1L—C2L	70.7
N7C—C15C—C20C—C19C	−178.3 (5)	N1L—C1L—C2L—C3L	−149.7
C18C—C19C—C20C—C15C	−0.3 (9)	C1L—C2L—C3L—C4L	80.6
O2D—N1D—C1D—C6D	168.4 (5)	C9L—N1L—C5L—C6L	−51.1
O1D—N1D—C1D—C6D	−14.6 (8)	C13L—N1L—C5L—C6L	−176.5
O2D—N1D—C1D—C2D	−12.7 (7)	C1L—N1L—C5L—C6L	66.5
O1D—N1D—C1D—C2D	164.2 (6)	N1L—C5L—C6L—C7L	−171.0
C6D—C1D—C2D—C3D	1.0 (7)	C5L—C6L—C7L—C8L	171.5
N1D—C1D—C2D—C3D	−177.8 (4)	C13L—N1L—C9L—C10L	64.3
C1D—C2D—C3D—C4D	−1.0 (7)	C5L—N1L—C9L—C10L	−57.1
C7D—N2D—C4D—C5D	−164.6 (4)	C1L—N1L—C9L—C10L	−173.6
C7D—N2D—C4D—C3D	14.3 (7)	N1L—C9L—C10L—C11L	−95.9
C2D—C3D—C4D—N2D	−178.7 (4)	C9L—C10L—C11L—C12L	−170.8
C2D—C3D—C4D—C5D	0.1 (6)	C9L—N1L—C13L—C14L	58.7
N2D—C4D—C5D—	179.6 (4)	C5L—N1L—C13L—	−178.8

C6D		C14L	
C3D—C4D—C5D—C6D	0.7 (7)	C1L—N1L—C13L—C14L	−63.2
C2D—C1D—C6D—C5D	−0.2 (7)	N1L—C13L—C14L—C15L	−172.5
N1D—C1D—C6D—C5D	178.6 (4)	C13L—C14L—C15L—C16L	178.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*A*···O8*A*	0.88	2.04	2.884 (6)	159
N3*A*—H3*A*···O7*A*	0.88	1.92	2.796 (6)	177
N4*A*—H4*AA*···O9*A*	0.88	2.15	2.990 (6)	159
N5*A*—H5*AA*···O8*A*^{i}	0.88	2.20	3.057 (6)	164
N6*A*—H6*A*···O10*A*^{i}	0.88	1.94	2.788 (6)	163
N7*A*—H7*A*···O7*A*^{i}	0.88	1.92	2.785 (6)	169
N2*B*—H2*B*···O8*B*	0.88	1.98	2.852 (5)	171
N3*B*—H3*B*···O7*B*	0.88	1.85	2.712 (5)	167
N4*B*—H4*BA*···O9*B*	0.88	2.07	2.883 (5)	154
N5*B*—H5*BA*···O8*B*^{i}	0.88	2.35	3.012 (5)	133
N6*B*—H6*B*···O10*B*^{i}	0.88	1.93	2.750 (5)	154
N7*B*—H7*B*···O9*B*^{i}	0.88	2.01	2.861 (5)	164
N2*C*—H2*C*···O8*C*	0.88	1.88	2.752 (5)	168
N3*C*—H3*C*···O7*C*	0.88	1.90	2.781 (5)	174
N4*C*—H4*CA*···O7*C*	0.88	2.40	3.092 (5)	136
N5*C*—H5*CB*···O10*C*^{i}	0.88	2.00	2.867 (5)	167
N6*C*—H6*C*···O8*C*^{i}	0.88	1.93	2.795 (5)	167
N7*C*—H7*C*···O9*C*^{i}	0.88	2.04	2.885 (6)	160
N2*D*—H2*D*···O8*D*	0.88	2.08	2.955 (5)	172
N3*D*—H3*D*···O7*D*	0.88	1.92	2.751 (5)	158
N4*D*—H4*DA*···O10*D*	0.88	2.08	2.887 (5)	152
N5*D*—H5*DA*···O8*D*^{i}	0.88	2.07	2.895 (5)	156
N6*D*—H6*D*···O10*D*^{i}	0.88	2.03	2.896 (5)	169
N7*D*—H7*D*···O9*D*^{i}	0.88	1.83	2.699 (5)	167

Symmetry code: (i) *x*+1, *y*, *z*.

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Olga Gorlova

1990	Born on July 5 in Nikolaev, Ukraine
2004-2008	Graduated Fort Lee High School, Fort Lee, NJ
2006-2010`	Research Assistant at St. Luke's Roosevelt Hospital and New York Obesity Research Center, New York, NY
2008	Edward J. Bloustein D.S.P. Newark Chancellor Scholarship Rutgers Scarlet Scholarship Thomas J. Watson Memorial Scholarship
2008-2012	Attended Rutgers University – Newark Bachelors of Arts in Chemistry 01/12
2009	Ochner, Christopher, Eva Conceição, and Olga Gorlova. Appetite and Nutritional Assessment: The Validity of Nutritional Assessment: Current Status. 3rd Quarter. Nova Publishers, 2009. 189-196. Print.
2010	Ochner, Christopher, Wu J, Gorlova O, Carnell S, Geliebter A. Causal Factors, Diagnostic Criteria and Treatment of Binge Eating Disorder. In Columbus F, ed. Eating Disorders: Causes, Diagnosis and Treatments. New York, NY: Nova Science Publishers, 2010: in press. Anna and Bernard Z. Senkowski. Undergraduate Chemistry. Scholarship Award Phi Beta Kappa Honors Society National Collegiate Honor Society
2010-2012	Graduate Work Rutgers University – Newark
2011-2012	Teaching Assistant General Chemistry Laboratory at Rutgers University – Newark
2011-2012	Kaplan SAT Instructor
2012	Colombo M.I., Rúveda, E. A., Gorlova O., Lalancette R.A., Stortz, C. A. (2012). *Carbohydr. Res.* Accepted.