Electronic supplementary information

Supramolecular Aluminium-based Molecular Catalyst for Water Oxidation into H_2O_2 in Saline Water

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X-ray Structural data of [AlTPyP(OH)(OH_2)](H_2O)$_3$@TMbCD (1:2)

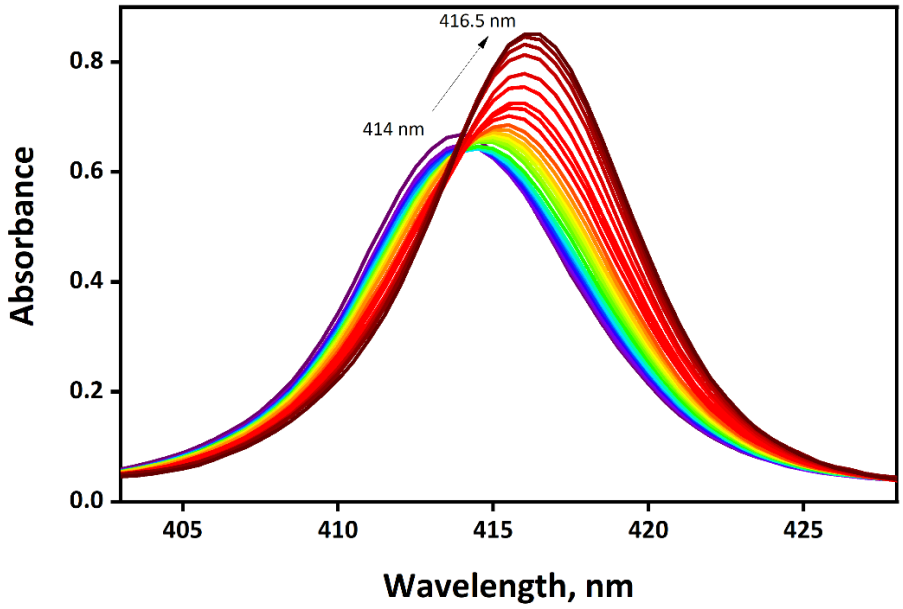

Figure S1. UV-Vis spectral changes in accordance with host-guest complex formation on 1:1 complex of AlTPyP@TMβCD (6.45 x 10^{-7}M) in water upon addition of TMβCD (0 – 4.78 x 10^{-5} M).

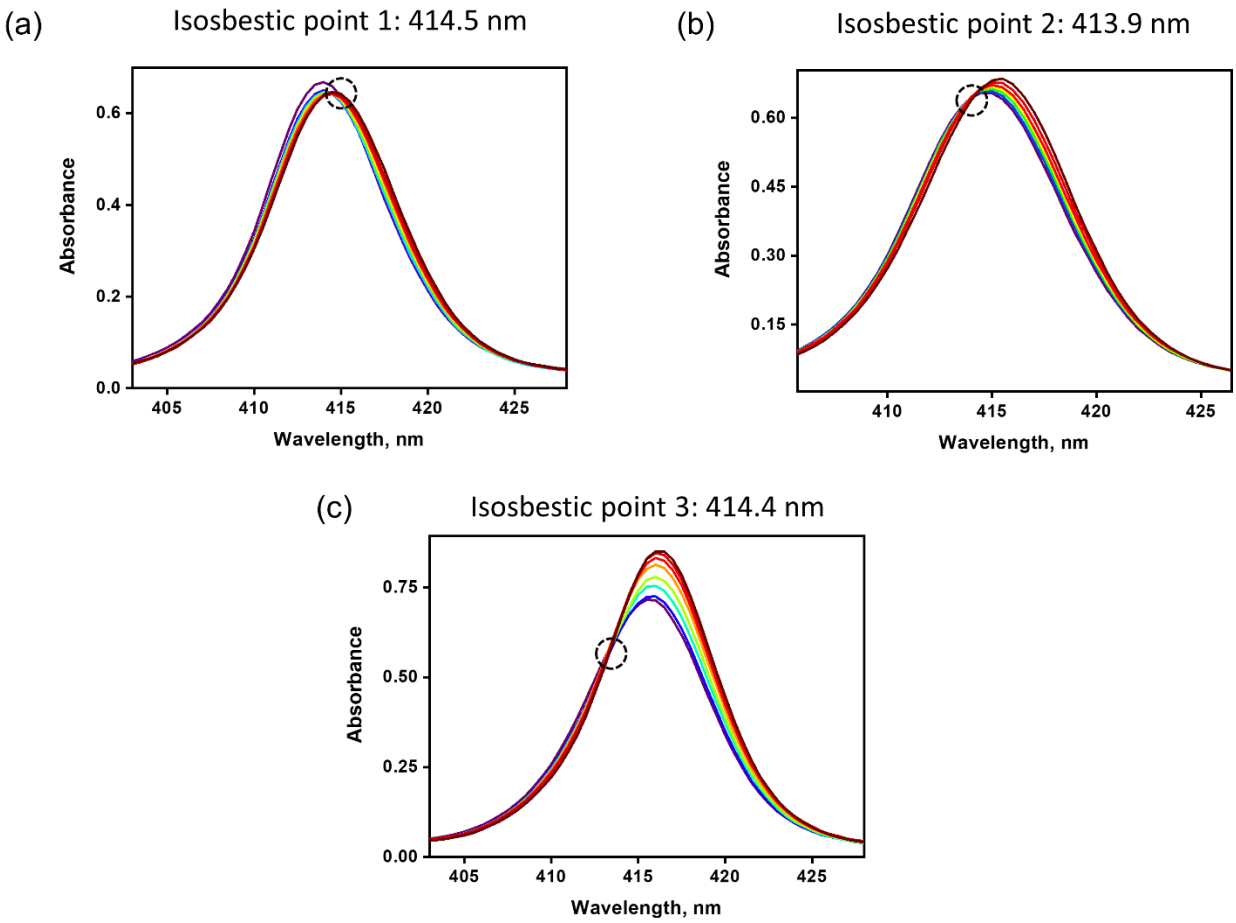

Figure S2. Three isosbestic points formed during the stepwise process of host-guest complex formation starting from 1:1 complex of AlTPyP@TMβCD.

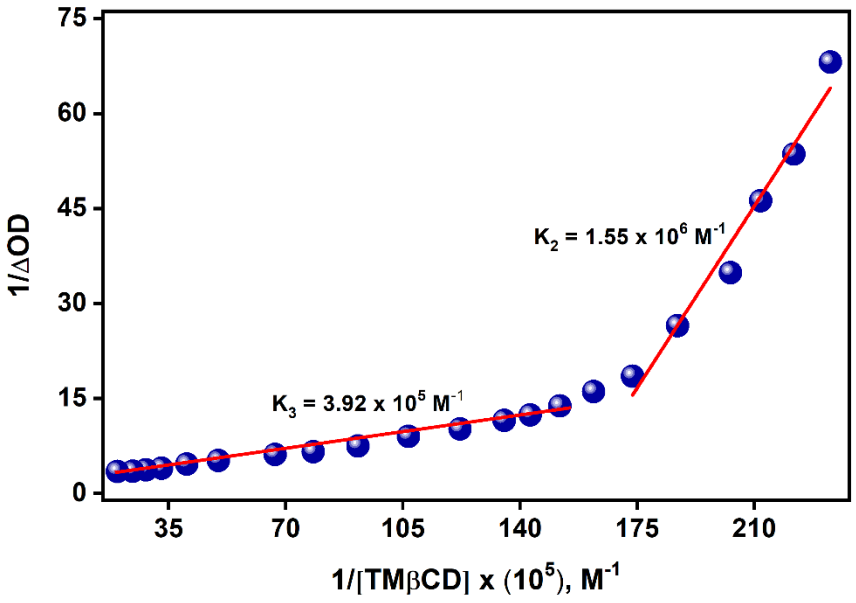

Figure S3. Estimation of association constant (K) using the Benesi-Hilderbrand treatment. The difference absorbance at 416 nm (ΔOD) was monitored for AlTPyP@TMβCD (1: 1) (6.45×10^{-7}M) in water upon addition of TMβCD (0 – 4.78×10^{-5} M).

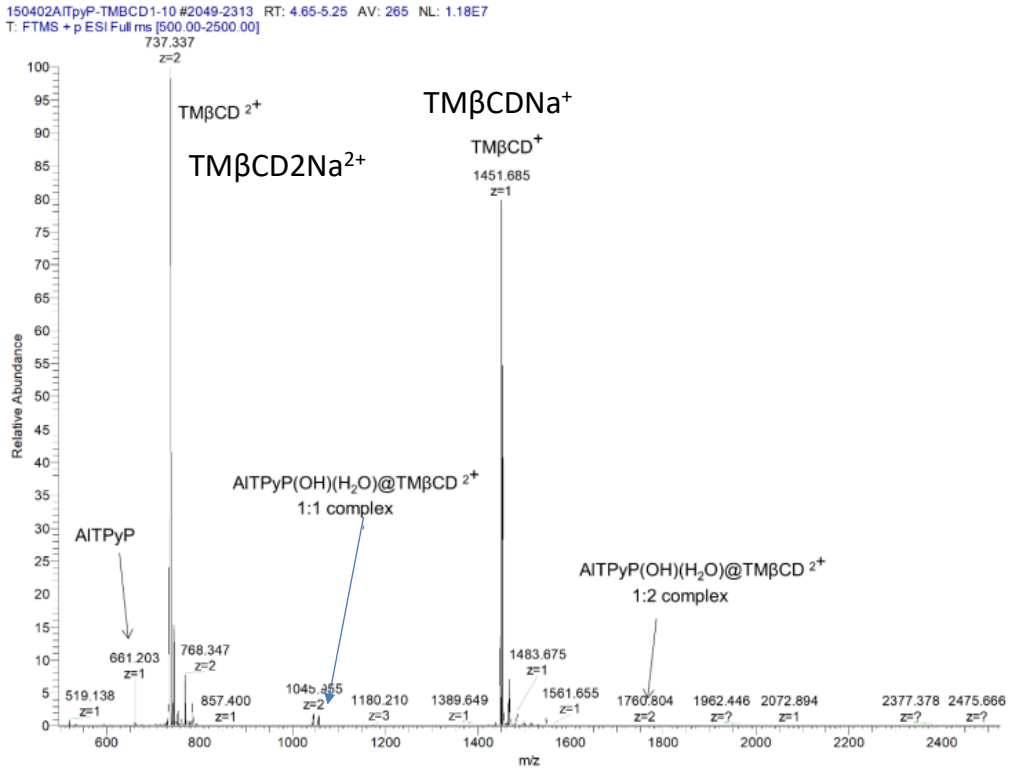

Figure S4. HRMS spectra analysis of 1:1 and 1:2 host-guest complex of AlTPyP@TMβCD.

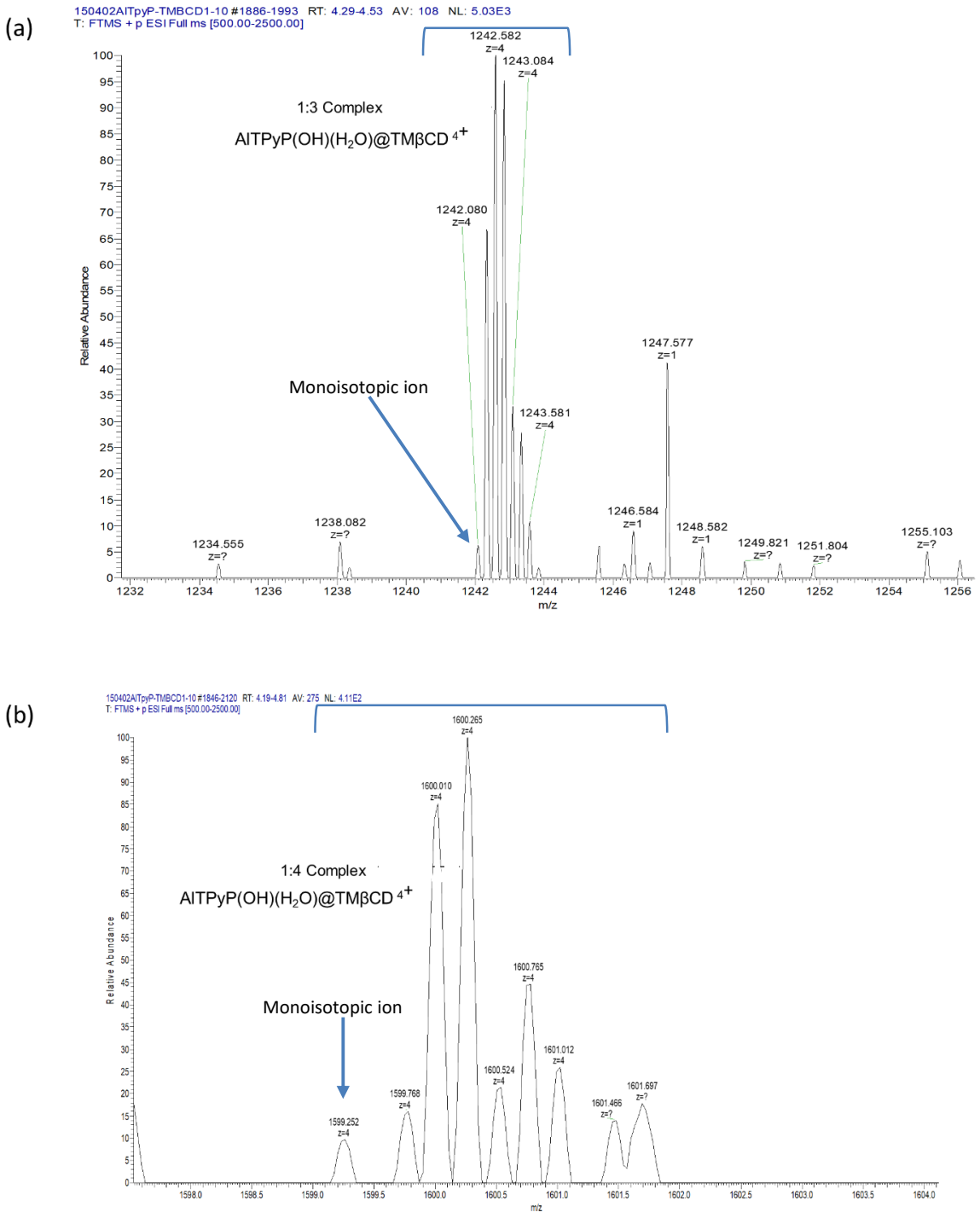

Figure S5. HRMS spectra analysis of host-guest complex of AlTPyP@TMβCD; 1:3 complex (a) and 1:4 complex (b). The absence of the 2nd ion peak for 1:4 complex might be due to the low signal intensity.

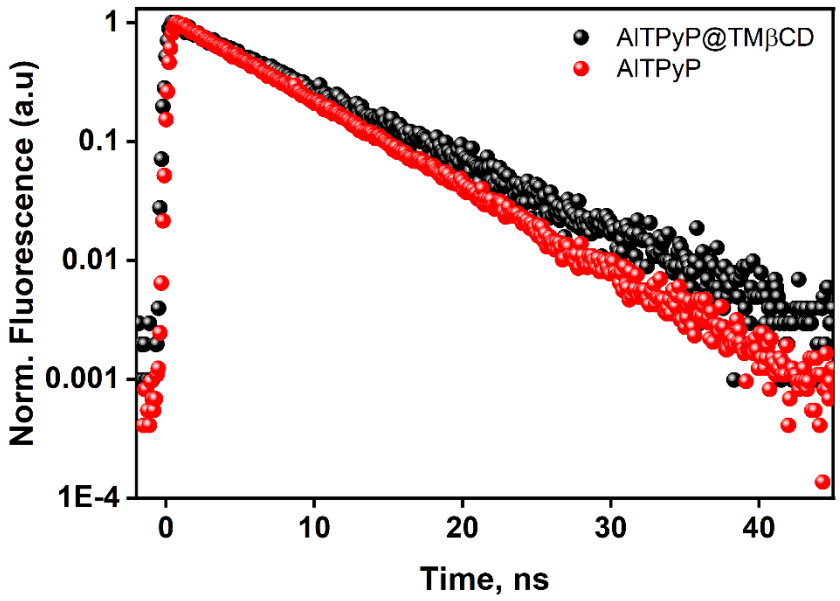

Figure S6. Comparison of decay profile of fluorescence of AlTPyP (red) in MeOH/ H_2O (9/1, v/v) and AlTPyP@TMβCD (1: 4) ([Al(III)TPyP] 1.27 x 10^{-7} M, [TMβCD] = 6.05 x 10^{-5} M) in water. The fluorescence decay profiles were well fitted with single exponential function upon excitation with λ_{ex} = 416 nm.

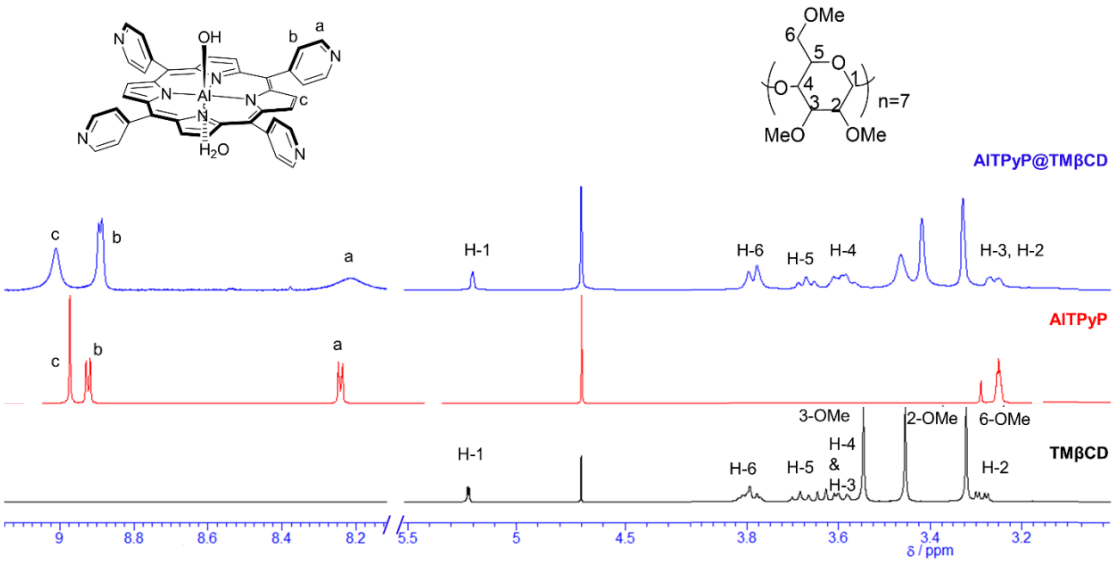

Figure S7. Representative ^{1}H NMR spectra of TMβCD (in D_2O), AlTPyP (in MeOD), and AlTPyP@TMβCD (1:4) (in D_2O).

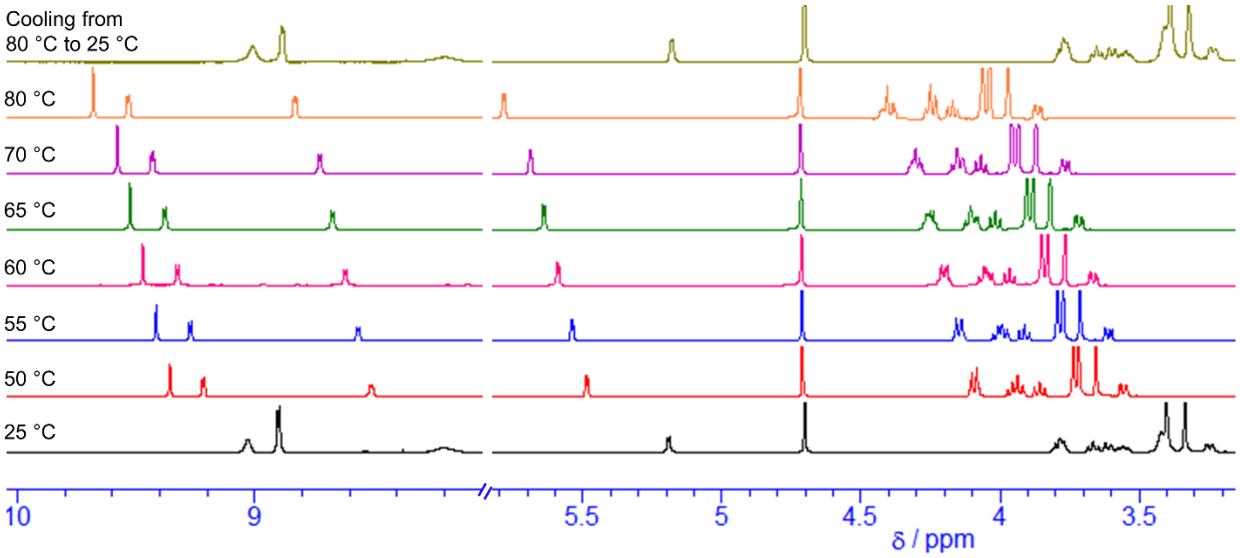

Figure S8. Varying temperature NMR (VT-NMR) monitoring of guest-host complex of AlTPyP@TMβCD (1:4).

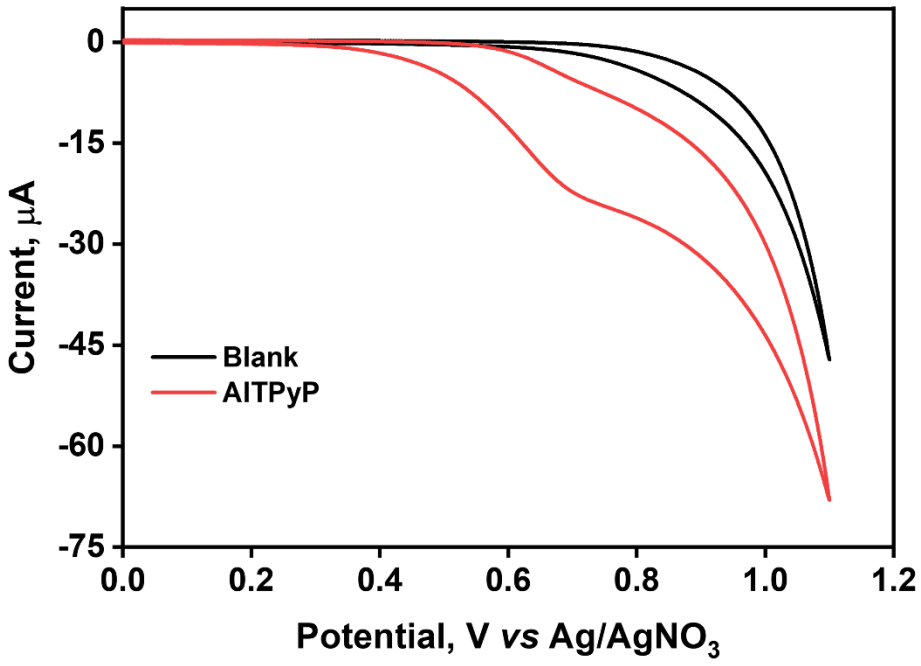

Figure S9. Cyclic voltammogram of AlTPyP (0.2 mM) in DMF/H_2O (8/2, v/v/) with WE: BDD, RE: Ag/ANO_3, CE: Pt coil.

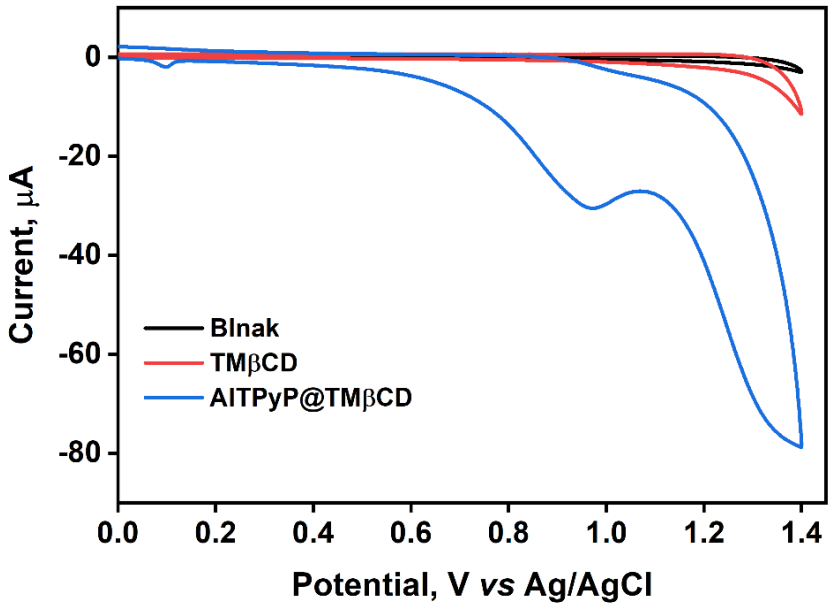

Figure S10. Cyclic voltammogram of AlTPyP@TMβCD (1:1) (1.25 x 10^{-4} M) and TMβCD in water, WE: BDD, RE: Ag/AgCl, CE: Pt coil.

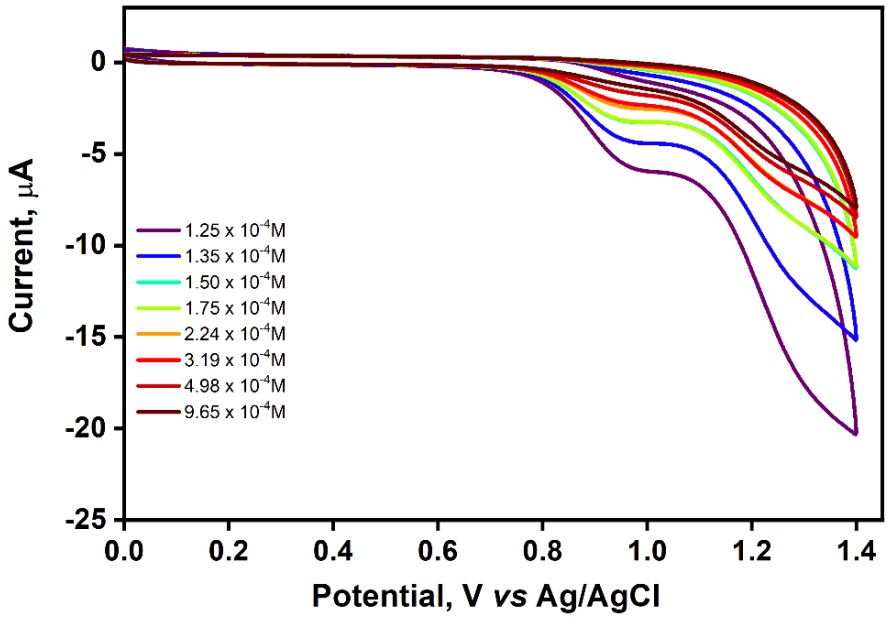

Figure S11. Titrating cyclic voltammogram starting from AlTPyP@TMβCD (1:1) (1.25 x 10^{-4} M) upon addition of TMβCD (1.25x10^{-4} - 9.65 x 10^{-4}M) in water, WE: BDD, RE: Ag/AgCl, CE: Pt coil.

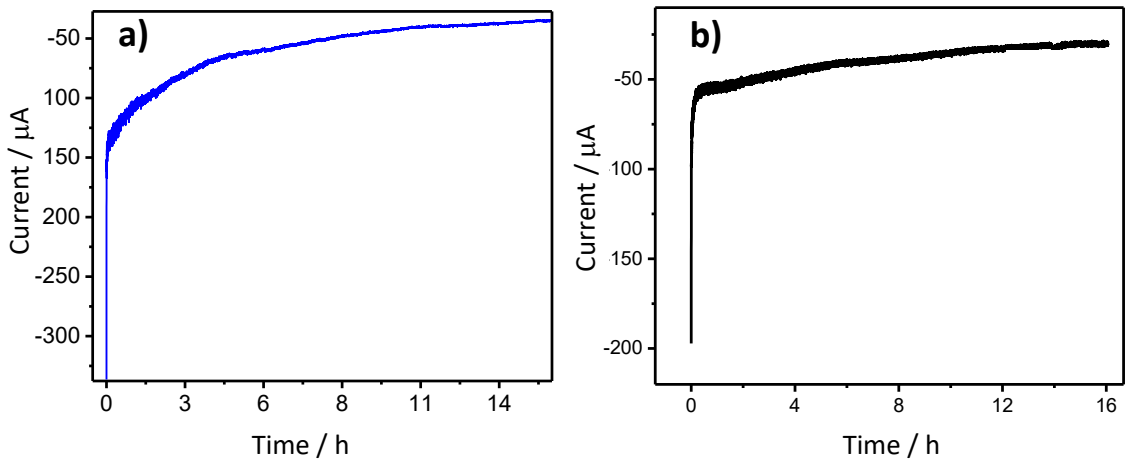

Figure S12. I-T curve in the controlled potential electrolysis catalysed by AlTPyP@TMβCD (1:4) at pH 9.7 (NaCl (0.1M) + $NaHCO_3$ (0.1M)) (a) and pH 12.5 (NaCl (0.1 M) + NaOH)

X-ray Structural data of [AlTPyP(OH)(OH_2)](H_2O)$_3$@TMbCD (1:2)

Experimental

Data Collection

A purple block crystal of $C_{166}H_{256}AlN_8O_{74}$ having approximate dimensions of 0.250 x 0.250 x 0.250 mm was mounted in a loop. All measurements were made on a Rigaku R-AXIS RAPID 191R diffractometer using filtered Mo-Kα radiation.

The crystal-to-detector distance was 191.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a = 16.9295(7) Å α = 99.007(7)^o
b = 17.4527(8) Å β = 112.736(8)^o
c = 17.615(2) Å γ = 102.562(8)^o
V = 4514.9(6) Å^3

For Z = 1 and F.W. = 3574.84, the calculated density is 1.315 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P1 (#1)

The data were collected at a temperature of -100 $\pm$ 1^{o}C to a maximum 2θ value of 55.0^o. A total of 44 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 5.0^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 10.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 160.0^o in 5.0^o step, at χ=45.0^o and ϕ = 180.0^o. The exposure rate was 10.0 [sec./^{o}]. The crystal-to-detector distance was 191.00 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 44255 reflections that were collected, 33620 were unique (R_{int} = 0.0566); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 1.074 cm^{-1}. An empirical

absorption correction was applied which resulted in transmission factors ranging from 0.704 to 0.973. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[2] on F^2 was based on 33572 observed reflections and 2280 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0793$$

$$wR2 = [\; \Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2]^{1/2} = 0.1885$$

The standard deviation of an observation of unit weight[3] was 1.09. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.90 and -0.38 $e^-/Å^3$, respectively. The absolute structure was deduced based on Flack parameter, 0.0(5), refined using 12996 Friedel pairs.[4]

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL-97[10].

References

(1) SIR2004: M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, R. Spagna (2005)

(2) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(3) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(4) Flack, H. D. (1983), Acta Cryst. A39, 876-881.

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

(10) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{166}H_{256}AlN_8O_{74}$
Formula Weight	3574.84
Crystal Color, Habit	purple, block
Crystal Dimensions	0.250 X 0.250 X 0.250 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 16.9295(7) Å b = 17.4527(8) Å c = 17.615(2) Å α = 99.007(7) ^{o} β = 112.736(8) ^{o} γ = 102.562(8) ^{o} V = 4514.9(6) Å^3
Space Group	P1 (#1)
Z value	1
D_{calc}	1.315 g/cm^3
F_{000}	1913.00
μ(MoKα)	1.074 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID 191R
Radiation	MoKα (λ = 0.71075 Å)
Voltage, Current	45kV, 55mA
Temperature	-100.0^{o}C
Detector Aperture	458 x 382 mm
Data Images	44 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{o}
Exposure Rate	10.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 160.0^{o}
Exposure Rate	10.0 sec./^{o}
Detector Position	191.00 mm
Pixel Size	0.100 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 44255 Unique: 33572 (R_{int} = 0.0566) Friedel pairs: 12996
Corrections	Lorentz-polarization Absorption (trans. factors: 0.704 - 0.973)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.1000 \cdot P)^2 + 0.0000 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	33572
No. Variables	2280
Reflection/Parameter Ratio	14.72
Residuals: R1 (I>2.00σ(I))	0.0793
Residuals: R (All reflections)	0.1167
Residuals: wR2 (All reflections)	0.1885
Goodness of Fit Indicator	1.088
Flack Parameter (Friedel pairs = 12996)	0.0(5)
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.90 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.38 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Al1	0.9441(2)	0.3289(2)	0.8456(2)	4.55(6)	1
O10	1.0018(3)	0.2567(3)	0.8915(3)	2.92(9)	1
O11	0.8820(5)	0.4158(5)	0.7878(6)	7.5(2)	1
O58	1.3504(3)	0.5189(3)	1.4249(3)	2.85(9)	1
O59	1.3075(3)	0.4395(3)	1.2880(3)	2.48(8)	1
O60	1.2154(5)	0.3121(3)	1.3247(4)	5.0(2)	1
O62	1.0879(4)	0.3898(3)	1.3519(3)	3.15(9)	1
O64	1.3348(4)	0.6610(3)	1.5330(4)	3.9(1)	1
O72	1.5041(3)	0.4601(3)	1.2407(3)	2.50(8)	1
O73	1.4240(3)	0.4609(3)	1.0989(3)	2.12(7)	1
O74	1.3420(4)	0.2918(3)	1.0550(3)	2.89(9)	1
O76	1.2534(3)	0.2924(3)	1.1585(3)	3.12(9)	1
O78	1.5353(4)	0.5047(3)	1.4149(3)	3.21(9)	1
O86	1.5276(3)	0.6321(3)	1.0358(3)	2.49(8)	1
O87	1.3917(3)	0.6128(3)	0.9166(3)	2.06(7)	1
O88	1.4155(3)	0.4760(3)	0.8303(3)	2.80(8)	1
O90	1.4473(3)	0.3846(3)	0.9546(3)	2.17(7)	1
O92	1.6330(4)	0.6253(3)	1.2003(4)	3.9(1)	1
O100	1.3351(3)	0.8049(3)	0.9170(3)	2.58(8)	1
O101	1.1849(3)	0.7241(3)	0.8497(3)	2.67(8)	1
O102	1.2002(3)	0.6998(3)	0.6913(3)	3.20(9)	1
O104	1.3356(3)	0.6202(3)	0.7426(3)	2.87(9)	1
O106	1.5216(4)	0.8180(3)	1.0173(3)	3.7(1)	1
O114	1.0265(3)	0.8175(3)	0.8936(3)	2.41(8)	1
O115	0.9734(3)	0.7101(3)	0.9423(3)	2.48(8)	1
O116	0.8745(3)	0.6115(3)	0.7713(4)	3.4(1)	1
O118	1.0124(4)	0.6218(3)	0.7200(3)	3.08(9)	1
O120	1.1639(3)	0.9226(3)	0.8711(4)	3.4(1)	1
O128	0.9611(4)	0.7848(3)	1.1438(4)	3.6(1)	1
O129	0.9730(3)	0.6647(3)	1.1852(3)	2.95(9)	1
O130	0.7943(4)	0.5843(4)	1.0686(4)	4.7(2)	1
O133	0.8039(3)	0.6064(3)	0.9174(4)	3.6(1)	1
O135	0.9849(5)	0.9039(4)	1.0539(4)	6.1(2)	1
O143	1.1571(3)	0.6982(3)	1.3953(3)	2.77(8)	1
O144	1.1308(3)	0.5573(3)	1.3587(3)	2.47(8)	1
O145	0.9882(3)	0.5394(3)	1.4110(3)	3.16(9)	1
O147	0.8821(3)	0.6015(3)	1.2813(3)	3.28(9)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
O149	1.2411(4)	0.7771(3)	1.2976(4)	4.2(1)	1
O157	0.6035(3)	-0.1295(3)	0.8330(3)	2.49(8)	1
O158	0.5659(3)	-0.0092(3)	0.8193(3)	2.16(7)	1
O159	0.6886(3)	0.0667(3)	0.9918(3)	3.00(9)	1
O161	0.8457(3)	0.0470(3)	0.9816(3)	2.78(9)	1
O163	0.7006(4)	-0.2425(3)	0.8122(5)	4.6(2)	1
O171	0.3553(3)	-0.0373(3)	0.6330(3)	2.56(8)	1
O172	0.4087(3)	0.1025(3)	0.6534(3)	2.64(8)	1
O173	0.3419(3)	0.1244(3)	0.7830(3)	2.58(8)	1
O175	0.4625(3)	0.0577(3)	0.8943(3)	2.54(8)	1
O177	0.4641(4)	-0.1478(3)	0.5814(4)	3.8(1)	1
O185	0.3393(3)	0.1790(3)	0.4620(3)	2.64(8)	1
O186	0.4855(3)	0.2501(3)	0.4898(3)	2.53(8)	1
O187	0.4924(4)	0.3682(3)	0.6247(3)	3.5(1)	1
O189	0.4361(3)	0.2732(3)	0.7177(3)	2.70(8)	1
O191	0.2112(4)	0.0459(4)	0.4577(4)	3.9(1)	1
O199	0.5079(3)	0.2406(3)	0.2881(3)	2.52(8)	1
O200	0.6459(3)	0.2172(3)	0.3539(3)	2.36(8)	1
O201	0.7248(4)	0.3891(3)	0.4351(5)	4.8(2)	1
O203	0.6370(4)	0.3865(3)	0.5389(4)	4.0(1)	1
O206	0.3497(4)	0.1108(4)	0.2328(4)	5.1(2)	1
O214	0.6756(3)	0.0302(3)	0.2553(3)	2.84(9)	1
O215	0.8040(3)	0.0519(3)	0.3825(3)	2.41(8)	1
O216	0.9003(4)	0.1675(4)	0.3235(4)	4.1(1)	1
O218	0.8030(3)	0.2788(3)	0.3295(3)	3.02(9)	1
O220	0.5197(4)	0.0486(5)	0.1511(4)	5.6(2)	1
O228	0.8098(3)	-0.1315(3)	0.4604(3)	2.59(8)	1
O229	0.8958(3)	-0.0477(3)	0.5983(3)	2.44(8)	1
O230	1.0502(3)	-0.0239(3)	0.5638(3)	2.86(9)	1
O232	0.9830(3)	0.0503(3)	0.4291(3)	2.61(8)	1
O234	0.6303(4)	-0.1631(3)	0.3943(4)	4.0(1)	1
O242	0.8578(3)	-0.1463(3)	0.7574(3)	2.24(8)	1
O243	0.8111(3)	-0.0430(3)	0.8132(3)	2.06(7)	1
O244	0.9868(3)	0.0600(3)	0.8937(3)	2.93(9)	1
O246	1.0353(3)	0.0554(3)	0.7577(3)	2.66(8)	1
O248	0.8713(4)	-0.2438(3)	0.6173(3)	2.98(9)	1
O250	1.1753(5)	0.2679(6)	0.9058(5)	7.4(2)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
O251	0.685(4)	0.355(3)	0.742(4)	12(2)	1/4
O252	0.856(1)	0.450(1)	0.627(1)	11.7(4)	3/4
N2	0.8213(3)	0.2663(3)	0.8289(3)	1.83(9)	1
N3	0.9624(3)	0.3982(3)	0.9573(3)	2.04(9)	1
N4	1.0580(3)	0.4025(3)	0.8565(3)	1.79(8)	1
N5	0.9117(3)	0.2775(3)	0.7239(3)	1.87(9)	1
N6	0.6710(4)	0.3234(4)	1.1131(5)	3.7(2)	1
N7	1.3250(4)	0.7103(4)	1.1754(4)	3.5(2)	1
N8	1.2081(4)	0.3367(4)	0.5746(4)	3.1(1)	1
N9	0.5585(4)	-0.0243(4)	0.4811(5)	3.7(2)	1
C12	0.7594(4)	0.2014(4)	0.7595(4)	1.9(1)	1
C13	0.6863(4)	0.1645(4)	0.7777(5)	2.4(1)	1
C14	0.7032(4)	0.2067(4)	0.8556(4)	2.4(1)	1
C15	0.7862(4)	0.2707(4)	0.8874(4)	2.2(1)	1
C16	0.8238(4)	0.3287(4)	0.9648(4)	2.2(1)	1
C17	0.9062(4)	0.3898(4)	0.9969(4)	2.2(1)	1
C18	0.9427(4)	0.4524(4)	1.0739(4)	2.5(2)	1
C19	1.0212(5)	0.5001(4)	1.0825(4)	2.5(2)	1
C20	1.0338(4)	0.4663(4)	1.0108(4)	2.0(1)	1
C21	1.1092(4)	0.4982(4)	0.9978(4)	2.0(1)	1
C22	1.1202(4)	0.4666(4)	0.9256(4)	2.0(1)	1
C23	1.1991(4)	0.4953(4)	0.9127(4)	2.3(1)	1
C24	1.1847(4)	0.4510(4)	0.8377(4)	1.9(1)	1
C25	1.0964(4)	0.3937(4)	0.8009(4)	1.8(1)	1
C26	1.0530(4)	0.3409(4)	0.7185(4)	1.7(1)	1
C27	0.9644(4)	0.2894(4)	0.6812(4)	1.8(1)	1
C28	0.9195(4)	0.2360(4)	0.5967(4)	2.2(1)	1
C29	0.8400(4)	0.1907(4)	0.5873(4)	2.3(1)	1
C30	0.8348(4)	0.2147(4)	0.6658(4)	1.9(1)	1
C31	0.7637(4)	0.1778(4)	0.6836(4)	1.9(1)	1
C32	0.7716(4)	0.3269(4)	1.0174(4)	2.4(1)	1
C33	0.6946(5)	0.3494(4)	0.9915(5)	2.7(2)	1
C34	0.6456(5)	0.3462(5)	1.0406(5)	3.2(2)	1
C35	0.7471(5)	0.3029(5)	1.1377(5)	3.3(2)	1
C36	0.7987(5)	0.3036(4)	1.0922(5)	2.8(2)	1
C37	1.1818(4)	0.5713(4)	1.0614(4)	2.0(1)	1
C38	1.1950(6)	0.6451(5)	1.0422(5)	3.9(2)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C39	1.2669(6)	0.7117(5)	1.1014(5)	4.2(2)	1
C40	1.3099(5)	0.6394(5)	1.1955(5)	3.6(2)	1
C41	1.2400(5)	0.5697(4)	1.1416(5)	3.1(2)	1
C42	1.1053(4)	0.3398(4)	0.6670(4)	1.8(1)	1
C43	1.1813(4)	0.3134(4)	0.6943(4)	2.2(1)	1
C44	1.2308(5)	0.3140(4)	0.6477(5)	2.9(2)	1
C45	1.1344(5)	0.3610(4)	0.5485(4)	2.7(2)	1
C46	1.0827(4)	0.3643(4)	0.5920(4)	2.1(1)	1
C47	0.6896(4)	0.1074(4)	0.6145(4)	1.9(1)	1
C48	0.6874(5)	0.0290(4)	0.6167(5)	3.3(2)	1
C49	0.6221(5)	-0.0345(5)	0.5504(6)	4.3(2)	1
C50	0.5597(5)	0.0510(5)	0.4812(5)	3.7(2)	1
C51	0.6229(5)	0.1179(5)	0.5461(5)	3.5(2)	1
C52	1.3217(5)	0.4397(4)	1.3725(5)	2.9(2)	1
C53	1.2377(5)	0.3922(4)	1.3745(5)	3.0(2)	1
C54	1.1648(5)	0.4336(4)	1.3436(4)	2.7(2)	1
C55	1.1995(4)	0.5209(4)	1.3958(4)	2.3(1)	1
C56	1.2875(4)	0.5638(4)	1.3954(4)	2.4(1)	1
C57	1.3325(5)	0.6504(4)	1.4504(5)	3.0(2)	1
C61	1.1751(6)	0.2489(5)	1.3494(7)	5.6(3)	1
C63	1.0064(6)	0.3664(5)	1.2769(5)	3.9(2)	1
C65	1.4140(6)	0.6536(5)	1.5957(5)	4.0(2)	1
C66	1.4611(5)	0.4138(4)	1.1539(4)	2.2(1)	1
C67	1.3867(5)	0.3398(4)	1.1412(4)	2.3(1)	1
C68	1.3180(5)	0.3639(4)	1.1681(4)	2.3(1)	1
C69	1.3694(5)	0.4147(4)	1.2601(4)	2.5(2)	1
C70	1.4426(5)	0.4884(4)	1.2681(4)	2.5(1)	1
C71	1.4979(5)	0.5463(4)	1.3549(4)	2.7(2)	1
C75	1.3654(9)	0.2201(6)	1.0428(7)	6.3(3)	1
C77	1.1637(5)	0.2965(6)	1.1244(6)	4.2(2)	1
C79	1.5903(6)	0.5583(5)	1.4969(5)	4.1(2)	1
C80	1.4780(4)	0.6029(4)	0.9462(4)	2.2(1)	1
C81	1.4696(4)	0.5120(4)	0.9181(4)	2.0(1)	1
C82	1.4325(4)	0.4617(4)	0.9669(4)	2.1(1)	1
C83	1.4779(4)	0.5012(4)	1.0624(4)	2.1(1)	1
C84	1.4870(4)	0.5916(4)	1.0834(4)	2.2(1)	1
C85	1.5472(5)	0.6354(4)	1.1767(5)	2.7(2)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C89	1.4587(6)	0.4933(5)	0.7783(6)	3.9(2)	1
C91	1.3729(5)	0.3211(4)	0.8876(5)	2.6(2)	1
C93	1.6924(7)	0.6622(7)	1.2867(6)	5.9(3)	1
C94	1.2556(5)	0.7751(4)	0.8397(5)	2.5(1)	1
C95	1.2768(5)	0.7289(4)	0.7732(4)	2.5(1)	1
C96	1.3039(4)	0.6563(4)	0.7984(4)	2.2(1)	1
C97	1.3820(4)	0.6840(4)	0.8882(4)	2.0(1)	1
C98	1.3654(4)	0.7411(4)	0.9517(4)	2.1(1)	1
C99	1.4483(5)	0.7832(4)	1.0343(5)	2.8(2)	1
C103	1.1868(7)	0.7594(6)	0.6460(6)	5.4(2)	1
C105	1.2710(6)	0.5487(5)	0.6780(5)	3.9(2)	1
C107	1.6029(6)	0.8463(5)	1.0931(6)	5.3(2)	1
C108	0.9553(4)	0.7460(4)	0.8732(5)	2.4(1)	1
C109	0.9422(5)	0.6863(4)	0.7932(5)	2.6(2)	1
C110	1.0286(4)	0.6680(4)	0.8009(5)	2.4(1)	1
C111	1.1045(5)	0.7462(4)	0.8305(5)	2.4(1)	1
C112	1.1102(4)	0.8026(4)	0.9097(5)	2.4(1)	1
C113	1.1807(5)	0.8858(4)	0.9401(5)	2.9(2)	1
C117	0.7863(5)	0.6153(6)	0.7305(6)	4.5(2)	1
C119	1.030(2)	0.5498(6)	0.7159(7)	9.3(5)	1
C121	1.2294(6)	0.9990(5)	0.8941(8)	5.5(3)	1
C122	0.9154(5)	0.7110(5)	1.1512(5)	3.4(2)	1
C123	0.8407(5)	0.6597(5)	1.0639(5)	3.3(2)	1
C124	0.8770(5)	0.6449(5)	0.9988(5)	2.9(2)	1
C125	0.9291(5)	0.7256(4)	0.9954(5)	2.7(2)	1
C126	1.0007(5)	0.7763(5)	1.0849(5)	3.2(2)	1
C127	1.0463(6)	0.8612(5)	1.0886(6)	4.5(2)	1
C131	0.707(2)	0.561(2)	1.047(2)	4.5(4)	1/2
C132	0.714(2)	0.599(2)	1.081(2)	5.5(5)	1/2
C134	0.7889(8)	0.5222(5)	0.8893(7)	6.3(3)	1
C136	0.977(2)	0.9550(8)	1.113(1)	11.4(6)	1
C137	1.1252(5)	0.6243(4)	1.4119(4)	2.4(1)	1
C138	1.0260(5)	0.6101(4)	1.3918(5)	2.8(2)	1
C139	0.9720(4)	0.6051(4)	1.2990(5)	2.5(1)	1
C140	1.0133(5)	0.6799(4)	1.2754(5)	2.7(2)	1
C141	1.1148(5)	0.6976(4)	1.3073(5)	2.8(2)	1
C142	1.1597(5)	0.7781(4)	1.3003(5)	3.1(2)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C146	1.0183(6)	0.5471(6)	1.5002(5)	4.2(2)	1
C148	0.8207(5)	0.5200(5)	1.2418(6)	4.2(2)	1
C150	1.2877(6)	0.8514(5)	1.2904(6)	4.1(2)	1
C151	0.5961(4)	-0.0568(4)	0.8748(4)	2.2(1)	1
C152	0.6889(5)	-0.0076(4)	0.9455(4)	2.5(1)	1
C153	0.7584(4)	0.0122(4)	0.9109(4)	2.3(1)	1
C154	0.7587(4)	-0.0651(4)	0.8587(4)	2.1(1)	1
C155	0.6636(4)	-0.1170(4)	0.7937(4)	2.3(1)	1
C156	0.6597(5)	-0.2016(4)	0.7518(6)	3.5(2)	1
C160	0.6574(6)	0.0551(6)	1.0544(5)	4.3(2)	1
C162	0.8793(5)	0.1320(4)	0.9990(6)	4.0(2)	1
C164	0.6422(8)	-0.2933(8)	0.835(1)	8.6(4)	1
C165	0.3451(4)	0.0391(4)	0.6584(4)	2.3(1)	1
C166	0.3561(4)	0.0512(4)	0.7508(4)	2.3(1)	1
C167	0.4512(4)	0.0537(4)	0.8092(4)	1.8(1)	1
C168	0.4711(4)	-0.0229(4)	0.7769(4)	2.1(1)	1
C169	0.4432(4)	-0.0442(4)	0.6810(4)	2.2(1)	1
C170	0.4383(5)	-0.1321(4)	0.6485(5)	3.1(2)	1
C174	0.2518(5)	0.1255(5)	0.7439(5)	3.2(2)	1
C176	0.5046(5)	0.1377(5)	0.9494(5)	3.4(2)	1
C178	0.4002(6)	-0.1436(5)	0.5043(6)	4.1(2)	1
C179	0.4045(5)	0.2555(4)	0.4928(5)	2.7(2)	1
C180	0.4204(5)	0.2945(4)	0.5837(5)	2.7(2)	1
C181	0.4420(5)	0.2391(4)	0.6420(4)	2.4(1)	1
C182	0.3738(5)	0.1540(4)	0.5995(4)	2.3(1)	1
C183	0.3648(5)	0.1224(4)	0.5111(5)	2.7(2)	1
C184	0.2950(5)	0.0420(4)	0.4613(5)	3.0(2)	1
C188	0.4751(7)	0.4325(5)	0.5869(5)	4.2(2)	1
C190	0.5170(5)	0.2990(5)	0.7924(5)	3.5(2)	1
C192	0.1407(7)	-0.0199(8)	0.4010(9)	8.3(4)	1
C193	0.6029(4)	0.2736(4)	0.3237(5)	2.5(2)	1
C194	0.6319(5)	0.3480(4)	0.3993(5)	3.2(2)	1
C195	0.6085(5)	0.3199(4)	0.4674(5)	2.7(2)	1
C196	0.5080(5)	0.2816(4)	0.4280(4)	2.4(1)	1
C197	0.4744(4)	0.2120(4)	0.3452(4)	2.5(1)	1
C198	0.3734(5)	0.1817(5)	0.2960(5)	2.9(2)	1
C202	0.7463(8)	0.4537(7)	0.404(1)	8.7(4)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C204	0.6738(9)	0.3635(8)	0.6244(9)	5.4(3)	3/4
C205	0.718(2)	0.391(2)	0.608(2)	2.4(5)	1/4
C207	0.2553(6)	0.0799(7)	0.1844(8)	7.0(3)	1
C208	0.7699(5)	0.0548(5)	0.2960(4)	2.7(2)	1
C209	0.8053(4)	0.1404(5)	0.2902(5)	2.8(2)	1
C210	0.7757(4)	0.1995(4)	0.3390(4)	2.4(1)	1
C211	0.6736(4)	0.1719(4)	0.2997(4)	2.1(1)	1
C212	0.6350(4)	0.0813(4)	0.2914(4)	2.2(1)	1
C213	0.5352(5)	0.0467(5)	0.2342(5)	3.1(2)	1
C217	0.9313(7)	0.1302(7)	0.2667(8)	6.3(3)	1
C219	0.8812(5)	0.3317(5)	0.4021(5)	3.5(2)	1
C221	0.4286(7)	0.0152(7)	0.0936(7)	7.0(3)	1
C222	0.8959(4)	-0.1005(4)	0.5290(4)	2.2(1)	1
C223	0.9607(4)	-0.0548(4)	0.4994(4)	2.2(1)	1
C224	0.9313(4)	0.0148(4)	0.4678(4)	2.2(1)	1
C225	0.8326(4)	-0.0177(4)	0.4006(4)	2.3(1)	1
C226	0.7723(4)	-0.0684(4)	0.4321(5)	2.5(1)	1
C227	0.6776(5)	-0.1115(5)	0.3615(5)	3.3(2)	1
C231	1.0906(6)	-0.0846(5)	0.5843(6)	4.5(2)	1
C233	1.0515(5)	0.1248(4)	0.4819(5)	3.3(2)	1
C235	0.5362(5)	-0.1906(6)	0.3410(7)	5.1(2)	1
C236	0.8828(4)	-0.0761(4)	0.8253(4)	1.9(1)	1
C237	0.9641(4)	-0.0128(4)	0.8320(4)	2.3(1)	1
C238	0.9495(4)	0.0055(4)	0.7467(4)	2.2(1)	1
C239	0.9168(4)	-0.0717(4)	0.6766(4)	2.1(1)	1
C240	0.8347(4)	-0.1307(4)	0.6755(4)	2.2(1)	1
C241	0.7984(5)	-0.2121(4)	0.6094(5)	2.6(2)	1
C245	1.0608(8)	0.0752(7)	0.9670(8)	8.6(4)	1
C247	1.0306(5)	0.1229(4)	0.7225(5)	2.9(2)	1
C249	0.8470(6)	-0.3152(5)	0.5515(7)	4.7(2)	1

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H10A	1.2328	0.7712	0.6251	6.54	1
H10B	1.1913	0.8092	0.6840	6.54	1
H10C	1.1271	0.7390	0.5975	6.54	1
H10D	1.2965	0.5289	0.6403	4.68	1
H10E	1.2167	0.5619	0.6444	4.68	1
H10F	1.2555	0.5064	0.7049	4.68	1
H10G	1.6103	0.8023	1.1210	6.33	1
H10H	1.6013	0.8923	1.1317	6.33	1
H10I	1.6535	0.8640	1.0792	6.33	1
H11A	1.1777	0.9208	0.9883	3.48	1
H11B	1.2416	0.8794	0.9602	3.48	1
H11C	0.7739	0.6207	0.6728	5.45	1
H11D	0.7799	0.6625	0.7633	5.45	1
H11E	0.7436	0.5654	0.7271	5.45	1
H11F	1.0352	0.5334	0.7680	11.17	1
H11G	1.0862	0.5554	0.7107	11.17	1
H11H	0.9806	0.5084	0.6661	11.17	1
H12A	1.2884	0.9910	0.9074	6.63	1
H12B	1.2319	1.0348	0.9443	6.63	1
H12C	1.2132	1.0240	0.8464	6.63	1
H12D	1.0872	0.8912	1.1489	5.35	1
H12E	1.0833	0.8593	1.0569	5.35	1
H13	0.6355	0.1188	0.7413	2.88	1
H13A	0.7802	0.4956	0.9317	7.56	1
H13B	0.8409	0.5131	0.8820	7.56	1
H13C	0.7351	0.4994	0.8346	7.56	1
H13D	1.0287	1.0041	1.1390	13.70	1
H13E	0.9732	0.9284	1.1573	13.70	1
H13F	0.9216	0.9699	1.0865	13.70	1
H14	0.6666	0.1960	0.8846	2.89	1
H14A	1.1200	0.7894	1.2478	3.73	1
H14B	1.1712	0.8217	1.3500	3.73	1
H14C	1.0199	0.6007	1.5287	5.10	1
H14D	1.0788	0.5413	1.5242	5.10	1
H14E	0.9771	0.5044	1.5091	5.10	1
H14F	0.8438	0.4835	1.2755	4.99	1
H14G	0.8146	0.5015	1.1838	4.99	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H14H	0.7618	0.5197	1.2393	4.99	1
H15A	1.3008	0.8958	1.3393	4.98	1
H15B	1.2505	0.8625	1.2374	4.98	1
H15C	1.3442	0.8474	1.2895	4.98	1
H15D	0.5961	-0.2343	0.7157	4.19	1
H15E	0.6904	-0.1970	0.7141	4.19	1
H16A	0.6979	0.0338	1.0964	5.14	1
H16B	0.5967	0.0162	1.0269	5.14	1
H16C	0.6561	0.1073	1.0832	5.14	1
H16D	0.8416	0.1577	1.0178	4.77	1
H16E	0.8786	0.1463	0.9471	4.77	1
H16F	0.9411	0.1512	1.0441	4.77	1
H16G	0.5865	-0.3242	0.7844	10.27	1
H16H	0.6281	-0.2599	0.8758	10.27	1
H16I	0.6712	-0.3311	0.8624	10.27	1
H17A	0.4771	-0.1489	0.6971	3.77	1
H17B	0.3758	-0.1670	0.6287	3.77	1
H17C	0.2110	0.0725	0.7363	3.87	1
H17D	0.2389	0.1364	0.6881	3.87	1
H17E	0.2431	0.1683	0.7803	3.87	1
H17F	0.4737	0.1747	0.9228	4.06	1
H17G	0.5677	0.1557	0.9595	4.06	1
H17H	0.5014	0.1381	1.0038	4.06	1
H17I	0.4006	-0.0869	0.5076	4.88	1
H17J	0.3404	-0.1771	0.4935	4.88	1
H17K	0.4147	-0.1638	0.4578	4.88	1
H18	0.9164	0.4594	1.1124	3.04	1
H18A	0.2903	0.0278	0.4027	3.57	1
H18B	0.3124	-0.0009	0.4888	3.57	1
H18C	0.4153	0.4358	0.5786	4.98	1
H18D	0.4773	0.4220	0.5315	4.98	1
H18E	0.5206	0.4841	0.6244	4.98	1
H19	1.0606	0.5473	1.1278	3.04	1
H19A	0.5655	0.3292	0.7813	4.18	1
H19B	0.5310	0.2515	0.8108	4.18	1
H19C	0.5108	0.3345	0.8375	4.18	1
H19D	0.1513	-0.0699	0.4155	9.98	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H19E	0.1349	-0.0220	0.3431	9.98	1
H19F	0.0851	-0.0151	0.4037	9.98	1
H19G	0.3458	0.1704	0.3350	3.51	1
H19H	0.3514	0.2237	0.2697	3.51	1
H20A	0.7180	0.4942	0.4167	10.48	1
H20B	0.7246	0.4347	0.3419	10.48	1
H20C	0.8117	0.4785	0.4308	10.48	1
H20D	0.2327	0.1221	0.1606	8.42	1
H20E	0.2274	0.0637	0.2211	8.42	1
H20F	0.2405	0.0325	0.1377	8.42	1
H21A	0.5131	-0.0101	0.2359	3.68	1
H21B	0.5026	0.0792	0.2544	3.68	1
H21C	0.8915	0.1269	0.2077	7.58	1
H21D	0.9311	0.0752	0.2725	7.58	1
H21E	0.9926	0.1628	0.2810	7.58	1
H21F	0.9311	0.3087	0.4121	4.18	1
H21G	0.8689	0.3376	0.4524	4.18	1
H21H	0.8974	0.3852	0.3919	4.18	1
H22A	0.3945	0.0490	0.1079	8.42	1
H22B	0.4060	-0.0401	0.0973	8.42	1
H22C	0.4217	0.0133	0.0354	8.42	1
H22D	0.6467	-0.0711	0.3429	3.95	1
H22E	0.6803	-0.1439	0.3116	3.95	1
H23	1.2519	0.5383	0.9510	2.71	1
H23A	1.0886	-0.1174	0.5327	5.46	1
H23B	1.0582	-0.1197	0.6080	5.46	1
H23C	1.1534	-0.0591	0.6267	5.46	1
H23D	1.0847	0.1182	0.5387	4.02	1
H23E	1.0239	0.1681	0.4869	4.02	1
H23F	1.0929	0.1393	0.4564	4.02	1
H23G	0.5251	-0.2148	0.2823	6.12	1
H23H	0.5122	-0.1444	0.3422	6.12	1
H23I	0.5066	-0.2315	0.3616	6.12	1
H24	1.2256	0.4563	0.8126	2.26	1
H24A	0.7527	-0.2504	0.6186	3.17	1
H24B	0.7697	-0.2049	0.5513	3.17	1
H24C	1.0610	0.1175	1.0109	10.37	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H24D	1.1145	0.0939	0.9577	10.37	1
H24E	1.0610	0.0253	0.9859	10.37	1
H24F	1.0049	0.1039	0.6601	3.47	1
H24G	1.0911	0.1611	0.7445	3.47	1
H24H	0.9925	0.1504	0.7386	3.47	1
H24I	0.8196	-0.3044	0.4957	5.59	1
H24J	0.8038	-0.3596	0.5561	5.59	1
H24K	0.9008	-0.3309	0.5573	5.59	1
H28	0.9420	0.2332	0.5550	2.62	1
H29	0.7954	0.1502	0.5375	2.73	1
H33	0.6744	0.3670	0.9408	3.29	1
H34	0.5918	0.3610	1.0211	3.82	1
H35	0.7673	0.2870	1.1894	3.92	1
H36	0.8520	0.2881	1.1126	3.40	1
H38	1.1556	0.6506	0.9892	4.66	1
H39	1.2741	0.7620	1.0866	5.02	1
H40	1.3494	0.6366	1.2500	4.33	1
H41	1.2321	0.5212	1.1596	3.68	1
H43	1.1989	0.2952	0.7447	2.62	1
H44	1.2834	0.2975	0.6683	3.51	1
H45	1.1168	0.3770	0.4968	3.26	1
H46	1.0318	0.3831	0.5710	2.51	1
H48	0.7309	0.0186	0.6640	4.00	1
H49	0.6217	-0.0884	0.5534	5.14	1
H50	0.5146	0.0602	0.4340	4.49	1
H51	0.6200	0.1712	0.5432	4.17	1
H52	1.3694	0.4134	1.3964	3.54	1
H53	1.2513	0.3908	1.4347	3.55	1
H54	1.1478	0.4319	1.2822	3.26	1
H55	1.2096	0.5225	1.4559	2.75	1
H56	1.2757	0.5639	1.3352	2.87	1
H57A	1.3949	0.6683	1.4568	3.65	1
H57B	1.3002	0.6860	1.4210	3.65	1
H61A	1.1145	0.2504	1.3399	6.67	1
H61B	1.2111	0.2549	1.4102	6.67	1
H61C	1.1711	0.1967	1.3157	6.67	1
H63A	1.0155	0.3421	1.2281	4.71	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H63B	0.9868	0.4143	1.2675	4.71	1
H63C	0.9603	0.3264	1.2832	4.71	1
H65A	1.4667	0.6941	1.5998	4.75	1
H65B	1.4182	0.5988	1.5796	4.75	1
H65C	1.4119	0.6627	1.6511	4.75	1
H66	1.5063	0.3953	1.1388	2.58	1
H67	1.4143	0.3056	1.1779	2.77	1
H68	1.2881	0.3969	1.1312	2.74	1
H69	1.3981	0.3807	1.2963	3.00	1
H70	1.4133	0.5195	1.2283	2.97	1
H71A	1.5467	0.5884	1.3534	3.28	1
H71B	1.4598	0.5740	1.3719	3.28	1
H75A	1.3381	0.1816	1.0673	7.60	1
H75B	1.4309	0.2329	1.0711	7.60	1
H75C	1.3434	0.1958	0.9816	7.60	1
H77A	1.1470	0.3047	1.0671	4.99	1
H77B	1.1598	0.3421	1.1615	4.99	1
H77C	1.1227	0.2455	1.1210	4.99	1
H79A	1.5528	0.5800	1.5197	4.93	1
H79B	1.6336	0.6033	1.4932	4.93	1
H79C	1.6227	0.5288	1.5349	4.93	1
H80	1.5119	0.6340	0.9194	2.59	1
H81	1.5313	0.5081	0.9311	2.46	1
H82	1.3664	0.4536	0.9448	2.51	1
H83	1.5389	0.4940	1.0876	2.53	1
H84	1.4260	0.5984	1.0680	2.63	1
H85A	1.5527	0.6942	1.1863	3.28	1
H85B	1.5202	0.6133	1.2126	3.28	1
H89A	1.5187	0.4865	0.8030	4.63	1
H89B	1.4643	0.5495	0.7745	4.63	1
H89C	1.4233	0.4558	0.7210	4.63	1
H91A	1.3638	0.3321	0.8325	3.16	1
H91B	1.3186	0.3189	0.8960	3.16	1
H91C	1.3852	0.2688	0.8884	3.16	1
H93A	1.6773	0.6287	1.3218	7.12	1
H93B	1.6872	0.7164	1.3036	7.12	1
H93C	1.7542	0.6672	1.2951	7.12	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H94	1.2371	0.8222	0.8209	2.95	1
H95	1.3275	0.7662	0.7683	3.02	1
H96	1.2516	0.6153	0.7971	2.66	1
H97	1.4385	0.7124	0.8855	2.43	1
H98	1.3179	0.7086	0.9646	2.51	1
H99A	1.4370	0.8264	1.0685	3.42	1
H99B	1.4632	0.7435	1.0677	3.42	1
H108	0.8988	0.7610	0.8615	2.90	1
H109	0.9226	0.7119	0.7448	3.17	1
H110	1.0448	0.6353	0.8432	2.84	1
H111	1.0943	0.7741	0.7836	2.90	1
H112	1.1252	0.7754	0.9571	2.88	1
H122	0.8872	0.7236	1.1902	4.06	1
H123	0.7967	0.6905	1.0438	3.99	1
H124	0.9169	0.6097	1.0143	3.49	1
H125	0.8868	0.7567	0.9707	3.21	1
H126	1.0471	0.7479	1.1058	3.84	1
H137	1.1605	0.6272	1.4733	2.92	1
H138	1.0214	0.6581	1.4273	3.30	1
H139	0.9719	0.5549	1.2627	3.02	1
H140	1.0008	0.7284	1.3011	3.29	1
H141	1.1263	0.6538	1.2727	3.33	1
H151	0.5536	-0.0710	0.9007	2.65	1
H152	0.7084	-0.0411	0.9863	3.03	1
H153	0.7452	0.0512	0.8753	2.73	1
H154	0.7866	-0.0974	0.8976	2.55	1
H155	0.6406	-0.0887	0.7484	2.73	1
H165	0.2833	0.0390	0.6206	2.82	1
H166	0.3123	0.0039	0.7532	2.80	1
H167	0.4952	0.1026	0.8096	2.20	1
H168	0.4394	-0.0698	0.7912	2.54	1
H169	0.4884	-0.0070	0.6691	2.61	1
H179	0.3804	0.2908	0.4557	3.26	1
H180	0.3643	0.3064	0.5808	3.26	1
H181	0.5041	0.2357	0.6562	2.88	1
H182	0.3140	0.1556	0.5967	2.74	1
H183	0.4243	0.1183	0.5153	3.26	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H193	0.6205	0.2912	0.2796	3.05	1
H194	0.5980	0.3867	0.3786	3.80	1
H195	0.6388	0.2783	0.4857	3.22	1
H196	0.4781	0.3243	0.4135	2.86	1
H197	0.4968	0.1655	0.3607	2.95	1
H208	0.7911	0.0173	0.2648	3.26	1
H209	0.7790	0.1407	0.2288	3.32	1
H210	0.8012	0.2005	0.4008	2.93	1
H211	0.6493	0.1823	0.2420	2.54	1
H212	0.6461	0.0745	0.3496	2.70	1
H222	0.9160	-0.1469	0.5480	2.65	1
H223	0.9597	-0.0935	0.4505	2.68	1
H224	0.9373	0.0570	0.5169	2.66	1
H225	0.8286	-0.0520	0.3473	2.77	1
H226	0.7694	-0.0328	0.4806	2.95	1
H236	0.8996	-0.0925	0.8800	2.31	1
H237	1.0162	-0.0350	0.8501	2.77	1
H238	0.9047	0.0363	0.7317	2.61	1
H239	0.9657	-0.0977	0.6866	2.55	1
H240	0.7859	-0.1044	0.6638	2.64	1

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Al1	0.035(2)	0.070(2)	0.038(2)	-0.025(1)	0.026(1)	-0.033(2)
O10	0.030(3)	0.042(3)	0.026(3)	0.001(2)	0.010(2)	-0.001(2)
O11	0.084(5)	0.096(6)	0.095(6)	0.043(5)	0.021(5)	0.025(5)
O58	0.041(3)	0.045(3)	0.024(3)	0.022(3)	0.012(2)	0.006(2)
O59	0.041(3)	0.038(3)	0.022(3)	0.024(2)	0.013(2)	0.012(2)
O60	0.117(6)	0.036(3)	0.056(4)	0.024(3)	0.054(4)	0.012(3)
O62	0.050(3)	0.037(3)	0.026(3)	0.005(3)	0.014(3)	0.008(2)
O64	0.043(3)	0.046(3)	0.041(4)	0.007(3)	0.012(3)	-0.010(3)
O72	0.033(3)	0.035(3)	0.024(3)	0.016(2)	0.007(2)	0.009(2)
O73	0.031(3)	0.032(3)	0.025(3)	0.017(2)	0.014(2)	0.010(2)
O74	0.051(3)	0.036(3)	0.025(3)	0.023(3)	0.016(3)	0.004(2)
O76	0.043(3)	0.036(3)	0.037(3)	0.006(3)	0.021(3)	0.004(2)
O78	0.049(3)	0.042(3)	0.020(3)	0.017(3)	0.005(2)	0.003(2)
O86	0.028(3)	0.029(3)	0.033(3)	0.008(2)	0.010(2)	0.005(2)
O87	0.026(2)	0.026(2)	0.026(3)	0.010(2)	0.009(2)	0.008(2)
O88	0.050(3)	0.032(3)	0.026(3)	0.010(2)	0.021(3)	0.003(2)
O90	0.033(3)	0.024(2)	0.022(3)	0.014(2)	0.007(2)	0.002(2)
O92	0.036(3)	0.055(3)	0.031(3)	0.012(3)	-0.005(3)	-0.007(3)
O100	0.037(3)	0.022(2)	0.038(3)	0.013(2)	0.014(2)	0.007(2)
O101	0.030(3)	0.030(3)	0.049(3)	0.016(2)	0.018(3)	0.020(2)
O102	0.043(3)	0.038(3)	0.034(3)	0.014(3)	0.007(3)	0.015(3)
O104	0.042(3)	0.035(3)	0.030(3)	0.014(2)	0.013(2)	0.004(2)
O106	0.041(3)	0.039(3)	0.035(3)	-0.003(3)	0.004(3)	0.001(3)
O114	0.028(3)	0.028(3)	0.037(3)	0.012(2)	0.011(2)	0.015(2)
O115	0.031(3)	0.033(3)	0.038(3)	0.016(2)	0.017(2)	0.018(2)
O116	0.029(3)	0.034(3)	0.057(4)	0.003(2)	0.012(3)	0.011(3)
O118	0.051(3)	0.041(3)	0.030(3)	0.019(3)	0.019(3)	0.011(2)
O120	0.039(3)	0.033(3)	0.056(4)	0.006(3)	0.018(3)	0.019(3)
O128	0.059(4)	0.049(3)	0.041(3)	0.035(3)	0.023(3)	0.019(3)
O129	0.039(3)	0.050(3)	0.034(3)	0.024(3)	0.018(3)	0.019(3)
O130	0.030(3)	0.094(5)	0.062(4)	0.012(3)	0.027(3)	0.033(4)
O133	0.032(3)	0.055(4)	0.045(4)	0.009(3)	0.014(3)	0.018(3)
O135	0.115(6)	0.045(4)	0.055(5)	0.038(4)	0.011(4)	0.019(3)
O143	0.037(3)	0.029(3)	0.031(3)	0.008(2)	0.011(2)	-0.000(2)
O144	0.036(3)	0.030(3)	0.020(3)	0.010(2)	0.006(2)	0.002(2)
O145	0.047(3)	0.042(3)	0.030(3)	0.009(3)	0.017(3)	0.013(2)
O147	0.033(3)	0.056(3)	0.039(3)	0.018(3)	0.015(3)	0.017(3)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O149	0.056(4)	0.037(3)	0.071(4)	0.013(3)	0.035(3)	0.011(3)
O157	0.032(3)	0.030(3)	0.041(3)	0.014(2)	0.021(2)	0.013(2)
O158	0.025(2)	0.029(3)	0.033(3)	0.013(2)	0.013(2)	0.013(2)
O159	0.043(3)	0.043(3)	0.031(3)	0.019(3)	0.018(3)	0.003(2)
O161	0.031(3)	0.035(3)	0.031(3)	0.012(2)	0.006(2)	0.003(2)
O163	0.050(4)	0.026(3)	0.104(5)	0.014(3)	0.037(4)	0.018(3)
O171	0.030(3)	0.030(3)	0.026(3)	0.009(2)	0.004(2)	0.002(2)
O172	0.030(3)	0.039(3)	0.032(3)	0.016(2)	0.008(2)	0.019(2)
O173	0.028(3)	0.033(3)	0.037(3)	0.015(2)	0.011(2)	0.011(2)
O175	0.032(3)	0.041(3)	0.029(3)	0.016(2)	0.014(2)	0.015(2)
O177	0.044(3)	0.048(3)	0.051(4)	0.021(3)	0.021(3)	0.003(3)
O185	0.042(3)	0.040(3)	0.026(3)	0.022(3)	0.016(2)	0.016(2)
O186	0.039(3)	0.039(3)	0.024(3)	0.022(2)	0.012(2)	0.014(2)
O187	0.075(4)	0.032(3)	0.035(3)	0.025(3)	0.027(3)	0.015(3)
O189	0.042(3)	0.041(3)	0.020(3)	0.014(3)	0.014(2)	0.006(2)
O191	0.038(3)	0.056(4)	0.049(4)	0.017(3)	0.018(3)	-0.000(3)
O199	0.029(3)	0.048(3)	0.027(3)	0.017(2)	0.013(2)	0.022(2)
O200	0.031(3)	0.036(3)	0.029(3)	0.018(2)	0.014(2)	0.014(2)
O201	0.038(3)	0.038(3)	0.103(6)	0.007(3)	0.027(4)	0.023(3)
O203	0.052(3)	0.032(3)	0.049(4)	0.015(3)	0.009(3)	-0.006(3)
O206	0.036(3)	0.077(4)	0.052(4)	0.004(3)	0.011(3)	-0.016(3)
O214	0.034(3)	0.045(3)	0.022(3)	0.016(3)	0.006(2)	0.001(2)
O215	0.035(3)	0.037(3)	0.022(3)	0.018(2)	0.011(2)	0.008(2)
O216	0.031(3)	0.073(4)	0.064(4)	0.023(3)	0.026(3)	0.033(3)
O218	0.030(3)	0.043(3)	0.032(3)	0.001(2)	0.007(2)	0.016(3)
O220	0.049(4)	0.094(5)	0.047(4)	0.014(4)	0.006(3)	0.009(4)
O228	0.032(3)	0.029(3)	0.031(3)	0.006(2)	0.010(2)	0.006(2)
O229	0.040(3)	0.031(3)	0.027(3)	0.017(2)	0.016(2)	0.013(2)
O230	0.030(3)	0.029(3)	0.039(3)	0.012(2)	0.004(2)	0.009(2)
O232	0.031(3)	0.037(3)	0.037(3)	0.010(2)	0.019(2)	0.012(2)
O234	0.034(3)	0.046(3)	0.058(4)	-0.000(3)	0.017(3)	0.008(3)
O242	0.034(3)	0.026(2)	0.030(3)	0.013(2)	0.017(2)	0.009(2)
O243	0.028(3)	0.028(2)	0.029(3)	0.014(2)	0.014(2)	0.012(2)
O244	0.033(3)	0.038(3)	0.032(3)	0.011(2)	0.010(2)	-0.001(2)
O246	0.023(3)	0.035(3)	0.040(3)	0.007(2)	0.011(2)	0.016(2)
O248	0.048(3)	0.027(3)	0.041(3)	0.017(2)	0.021(3)	0.007(2)
O250	0.062(4)	0.147(7)	0.066(5)	0.045(5)	0.018(4)	0.026(5)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N2	0.020(3)	0.030(3)	0.016(3)	0.006(2)	0.007(2)	-0.001(2)
N3	0.017(3)	0.031(3)	0.017(3)	0.002(2)	0.003(2)	-0.005(2)
N4	0.017(3)	0.026(3)	0.016(3)	0.003(2)	0.004(2)	-0.003(2)
N5	0.022(3)	0.027(3)	0.020(3)	0.008(3)	0.007(2)	0.003(2)
N6	0.042(4)	0.054(4)	0.042(4)	-0.001(3)	0.030(3)	0.001(3)
N7	0.037(4)	0.040(4)	0.039(4)	-0.003(3)	0.014(3)	-0.007(3)
N8	0.043(4)	0.042(4)	0.032(4)	0.007(3)	0.022(3)	0.004(3)
N9	0.037(4)	0.036(4)	0.046(4)	0.003(3)	0.008(3)	-0.009(3)
C12	0.018(3)	0.025(3)	0.024(4)	0.004(3)	0.006(3)	0.005(3)
C13	0.020(3)	0.031(4)	0.033(4)	0.002(3)	0.010(3)	0.001(3)
C14	0.022(3)	0.039(4)	0.027(4)	0.003(3)	0.013(3)	0.004(3)
C15	0.023(3)	0.028(4)	0.031(4)	0.005(3)	0.014(3)	0.002(3)
C16	0.019(3)	0.036(4)	0.026(4)	0.005(3)	0.011(3)	-0.001(3)
C17	0.027(3)	0.038(4)	0.015(3)	0.009(3)	0.009(3)	-0.000(3)
C18	0.027(4)	0.039(4)	0.024(4)	0.004(3)	0.013(3)	-0.001(3)
C19	0.030(4)	0.030(4)	0.025(4)	0.004(3)	0.008(3)	-0.005(3)
C20	0.025(3)	0.031(3)	0.021(4)	0.011(3)	0.009(3)	0.003(3)
C21	0.028(3)	0.029(3)	0.016(3)	0.014(3)	0.005(3)	0.004(3)
C22	0.029(3)	0.021(3)	0.025(4)	0.011(3)	0.010(3)	0.003(3)
C23	0.019(3)	0.027(3)	0.032(4)	0.005(3)	0.005(3)	0.007(3)
C24	0.020(3)	0.026(3)	0.022(4)	0.005(3)	0.008(3)	0.004(3)
C25	0.025(3)	0.023(3)	0.018(3)	0.008(3)	0.008(3)	0.003(3)
C26	0.023(3)	0.024(3)	0.020(3)	0.013(3)	0.007(3)	0.008(3)
C27	0.021(3)	0.023(3)	0.022(4)	0.007(3)	0.006(3)	0.007(3)
C28	0.033(4)	0.032(4)	0.019(4)	0.010(3)	0.011(3)	0.009(3)
C29	0.029(4)	0.031(4)	0.016(4)	0.005(3)	0.004(3)	-0.000(3)
C30	0.022(3)	0.022(3)	0.017(3)	0.007(3)	0.001(3)	0.001(3)
C31	0.024(3)	0.019(3)	0.021(4)	0.003(3)	0.005(3)	0.000(3)
C32	0.023(3)	0.036(4)	0.025(4)	0.004(3)	0.008(3)	-0.004(3)
C33	0.029(4)	0.044(4)	0.021(4)	0.002(3)	0.009(3)	0.003(3)
C34	0.026(4)	0.052(5)	0.036(5)	0.011(4)	0.013(3)	-0.001(4)
C35	0.042(4)	0.047(5)	0.031(4)	0.007(4)	0.017(4)	0.006(4)
C36	0.030(4)	0.046(4)	0.025(4)	0.008(3)	0.010(3)	0.004(3)
C37	0.024(3)	0.025(3)	0.020(4)	0.005(3)	0.009(3)	-0.003(3)
C38	0.057(5)	0.036(4)	0.033(5)	0.001(4)	0.004(4)	0.009(4)
C39	0.083(6)	0.028(4)	0.035(5)	0.000(4)	0.022(5)	0.005(4)
C40	0.042(4)	0.039(4)	0.040(5)	0.016(4)	0.004(4)	0.003(4)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C41	0.039(4)	0.031(4)	0.036(4)	0.012(3)	0.006(4)	0.003(3)
C42	0.025(3)	0.020(3)	0.021(4)	0.006(3)	0.010(3)	0.001(3)
C43	0.029(4)	0.030(4)	0.028(4)	0.010(3)	0.015(3)	0.012(3)
C44	0.032(4)	0.044(4)	0.036(5)	0.013(3)	0.016(3)	0.006(4)
C45	0.036(4)	0.045(4)	0.022(4)	0.009(4)	0.014(3)	0.010(3)
C46	0.027(3)	0.025(3)	0.022(4)	0.006(3)	0.007(3)	0.005(3)
C47	0.024(3)	0.024(3)	0.022(4)	0.003(3)	0.011(3)	0.002(3)
C48	0.030(4)	0.031(4)	0.046(5)	0.012(3)	-0.001(4)	-0.000(4)
C49	0.045(5)	0.023(4)	0.068(6)	0.008(4)	0.004(4)	-0.002(4)
C50	0.037(4)	0.051(5)	0.030(4)	0.004(4)	-0.001(4)	0.003(4)
C51	0.044(4)	0.030(4)	0.035(5)	-0.002(3)	0.001(4)	0.009(3)
C52	0.054(5)	0.044(4)	0.025(4)	0.032(4)	0.020(4)	0.011(3)
C53	0.069(5)	0.029(4)	0.030(4)	0.026(4)	0.030(4)	0.015(3)
C54	0.045(4)	0.032(4)	0.020(4)	0.001(3)	0.014(3)	0.004(3)
C55	0.033(4)	0.030(4)	0.022(4)	0.015(3)	0.007(3)	0.007(3)
C56	0.036(4)	0.034(4)	0.021(4)	0.016(3)	0.010(3)	0.007(3)
C57	0.032(4)	0.037(4)	0.038(5)	0.005(3)	0.013(3)	0.003(3)
C61	0.057(6)	0.036(5)	0.098(8)	0.004(4)	0.016(5)	0.023(5)
C63	0.053(5)	0.047(5)	0.045(5)	0.004(4)	0.020(4)	0.019(4)
C65	0.056(5)	0.053(5)	0.029(5)	0.015(4)	0.011(4)	0.002(4)
C66	0.037(4)	0.029(3)	0.021(4)	0.022(3)	0.011(3)	0.009(3)
C67	0.043(4)	0.027(3)	0.024(4)	0.022(3)	0.014(3)	0.011(3)
C68	0.037(4)	0.030(4)	0.023(4)	0.014(3)	0.013(3)	0.009(3)
C69	0.050(4)	0.034(4)	0.017(4)	0.025(3)	0.013(3)	0.013(3)
C70	0.040(4)	0.038(4)	0.021(4)	0.026(3)	0.010(3)	0.011(3)
C71	0.036(4)	0.038(4)	0.025(4)	0.014(3)	0.008(3)	0.006(3)
C75	0.14(1)	0.049(5)	0.049(6)	0.050(6)	0.033(6)	0.007(5)
C77	0.044(5)	0.063(5)	0.042(5)	0.006(4)	0.022(4)	-0.001(4)
C79	0.051(5)	0.063(5)	0.025(4)	0.009(4)	0.004(4)	0.009(4)
C80	0.028(3)	0.028(3)	0.025(4)	0.007(3)	0.011(3)	0.007(3)
C81	0.027(3)	0.030(3)	0.026(4)	0.013(3)	0.015(3)	0.005(3)
C82	0.027(3)	0.027(3)	0.023(4)	0.013(3)	0.007(3)	0.007(3)
C83	0.028(3)	0.030(3)	0.020(4)	0.011(3)	0.008(3)	0.005(3)
C84	0.022(3)	0.027(3)	0.029(4)	0.006(3)	0.006(3)	0.006(3)
C85	0.039(4)	0.030(4)	0.028(4)	0.016(3)	0.007(3)	0.003(3)
C89	0.073(6)	0.053(5)	0.046(5)	0.031(4)	0.042(5)	0.018(4)
C91	0.043(4)	0.028(4)	0.027(4)	0.010(3)	0.016(3)	0.004(3)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C93	0.061(6)	0.087(7)	0.042(6)	0.026(6)	-0.005(5)	-0.012(5)
C94	0.036(4)	0.026(3)	0.035(4)	0.013(3)	0.015(3)	0.016(3)
C95	0.033(4)	0.036(4)	0.025(4)	0.010(3)	0.009(3)	0.011(3)
C96	0.032(4)	0.022(3)	0.025(4)	0.008(3)	0.007(3)	0.005(3)
C97	0.031(4)	0.021(3)	0.025(4)	0.010(3)	0.012(3)	0.008(3)
C98	0.031(4)	0.025(3)	0.027(4)	0.014(3)	0.013(3)	0.007(3)
C99	0.046(4)	0.031(4)	0.029(4)	0.016(3)	0.014(3)	0.001(3)
C103	0.080(7)	0.060(6)	0.049(6)	0.024(5)	0.003(5)	0.031(5)
C105	0.069(6)	0.039(4)	0.027(4)	0.012(4)	0.015(4)	-0.002(4)
C107	0.058(6)	0.046(5)	0.055(6)	-0.010(4)	-0.001(5)	0.007(4)
C108	0.026(4)	0.029(4)	0.036(4)	0.009(3)	0.011(3)	0.014(3)
C109	0.036(4)	0.034(4)	0.026(4)	0.009(3)	0.008(3)	0.016(3)
C110	0.032(4)	0.027(3)	0.034(4)	0.014(3)	0.012(3)	0.016(3)
C111	0.036(4)	0.030(4)	0.033(4)	0.015(3)	0.017(3)	0.017(3)
C112	0.028(4)	0.024(3)	0.035(4)	0.007(3)	0.008(3)	0.012(3)
C113	0.028(4)	0.034(4)	0.044(5)	0.012(3)	0.011(3)	0.007(3)
C117	0.030(4)	0.059(6)	0.060(6)	0.001(4)	0.005(4)	0.012(5)
C119	0.25(2)	0.042(6)	0.053(7)	0.060(8)	0.046(9)	0.008(5)
C121	0.064(6)	0.049(5)	0.110(9)	0.008(5)	0.052(6)	0.033(6)
C122	0.043(4)	0.067(5)	0.041(5)	0.037(4)	0.025(4)	0.028(4)
C123	0.031(4)	0.068(5)	0.043(5)	0.026(4)	0.021(4)	0.029(4)
C124	0.028(4)	0.045(4)	0.036(4)	0.014(3)	0.010(3)	0.015(4)
C125	0.035(4)	0.039(4)	0.037(4)	0.019(3)	0.017(3)	0.020(3)
C126	0.049(5)	0.043(4)	0.043(5)	0.023(4)	0.025(4)	0.023(4)
C127	0.066(6)	0.047(5)	0.044(5)	0.012(5)	0.013(5)	0.015(4)
C134	0.113(9)	0.041(5)	0.061(7)	-0.001(5)	0.024(6)	0.017(5)
C136	0.17(2)	0.082(9)	0.13(2)	0.08(1)	-0.00(1)	0.015(9)
C137	0.032(4)	0.028(4)	0.023(4)	0.007(3)	0.006(3)	0.003(3)
C138	0.039(4)	0.038(4)	0.027(4)	0.013(3)	0.016(3)	0.004(3)
C139	0.029(4)	0.043(4)	0.033(4)	0.018(3)	0.017(3)	0.013(3)
C140	0.038(4)	0.038(4)	0.031(4)	0.018(3)	0.015(3)	0.006(3)
C141	0.033(4)	0.037(4)	0.034(4)	0.013(3)	0.012(3)	0.008(3)
C142	0.042(4)	0.040(4)	0.041(5)	0.015(4)	0.020(4)	0.015(4)
C146	0.056(5)	0.063(5)	0.040(5)	0.013(4)	0.017(4)	0.023(4)
C148	0.036(4)	0.059(5)	0.060(6)	0.013(4)	0.019(4)	0.017(5)
C150	0.059(5)	0.037(4)	0.065(6)	0.009(4)	0.035(5)	0.007(4)
C151	0.027(3)	0.032(4)	0.031(4)	0.013(3)	0.016(3)	0.012(3)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C152	0.038(4)	0.034(4)	0.025(4)	0.019(3)	0.012(3)	0.007(3)
C153	0.029(4)	0.029(3)	0.022(4)	0.010(3)	0.004(3)	0.008(3)
C154	0.031(4)	0.028(3)	0.027(4)	0.014(3)	0.013(3)	0.012(3)
C155	0.032(4)	0.027(3)	0.027(4)	0.011(3)	0.011(3)	0.005(3)
C156	0.037(4)	0.032(4)	0.057(5)	0.007(3)	0.021(4)	-0.004(4)
C160	0.075(6)	0.069(6)	0.028(4)	0.038(5)	0.024(4)	0.010(4)
C162	0.032(4)	0.034(4)	0.062(6)	0.005(4)	0.007(4)	-0.005(4)
C164	0.075(8)	0.087(8)	0.21(2)	0.046(7)	0.072(9)	0.10(1)
C165	0.023(3)	0.034(4)	0.029(4)	0.010(3)	0.006(3)	0.010(3)
C166	0.032(4)	0.021(3)	0.036(4)	0.009(3)	0.013(3)	0.010(3)
C167	0.025(3)	0.029(3)	0.022(4)	0.012(3)	0.013(3)	0.011(3)
C168	0.020(3)	0.027(3)	0.033(4)	0.007(3)	0.011(3)	0.009(3)
C169	0.026(3)	0.025(3)	0.026(4)	0.005(3)	0.008(3)	0.006(3)
C170	0.040(4)	0.032(4)	0.043(5)	0.013(3)	0.016(4)	0.004(3)
C174	0.034(4)	0.054(5)	0.042(5)	0.027(4)	0.016(4)	0.013(4)
C176	0.054(5)	0.050(5)	0.028(4)	0.027(4)	0.016(4)	0.007(4)
C178	0.063(5)	0.043(5)	0.046(5)	0.020(4)	0.022(4)	0.005(4)
C179	0.048(4)	0.040(4)	0.029(4)	0.028(4)	0.019(4)	0.020(3)
C180	0.047(4)	0.034(4)	0.034(4)	0.021(4)	0.021(4)	0.017(3)
C181	0.039(4)	0.036(4)	0.023(4)	0.019(3)	0.016(3)	0.013(3)
C182	0.037(4)	0.031(4)	0.026(4)	0.017(3)	0.015(3)	0.015(3)
C183	0.043(4)	0.040(4)	0.031(4)	0.026(4)	0.017(3)	0.014(3)
C184	0.036(4)	0.044(4)	0.033(4)	0.017(4)	0.014(3)	0.005(3)
C188	0.099(7)	0.033(4)	0.036(5)	0.030(5)	0.033(5)	0.013(4)
C190	0.054(5)	0.050(5)	0.030(4)	0.022(4)	0.017(4)	0.011(4)
C192	0.047(6)	0.100(9)	0.12(1)	0.010(6)	0.025(6)	-0.052(8)
C193	0.024(3)	0.042(4)	0.039(4)	0.013(3)	0.016(3)	0.022(3)
C194	0.033(4)	0.027(4)	0.057(5)	0.009(3)	0.014(4)	0.015(4)
C195	0.038(4)	0.026(4)	0.032(4)	0.015(3)	0.008(3)	0.003(3)
C196	0.034(4)	0.032(4)	0.033(4)	0.021(3)	0.016(3)	0.014(3)
C197	0.031(4)	0.042(4)	0.025(4)	0.015(3)	0.013(3)	0.014(3)
C198	0.037(4)	0.047(4)	0.031(4)	0.012(4)	0.019(3)	0.010(4)
C202	0.067(7)	0.070(7)	0.22(2)	0.019(6)	0.072(9)	0.067(9)
C207	0.043(5)	0.099(8)	0.076(8)	-0.007(6)	0.011(5)	-0.027(6)
C208	0.037(4)	0.055(5)	0.015(4)	0.021(4)	0.012(3)	0.003(3)
C209	0.027(4)	0.058(5)	0.027(4)	0.020(4)	0.011(3)	0.021(4)
C210	0.033(4)	0.041(4)	0.020(4)	0.011(3)	0.010(3)	0.015(3)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C211	0.023(3)	0.035(4)	0.026(4)	0.011(3)	0.011(3)	0.014(3)
C212	0.027(3)	0.031(4)	0.024(4)	0.009(3)	0.009(3)	0.004(3)
C213	0.037(4)	0.049(5)	0.027(4)	0.012(4)	0.013(3)	0.005(3)
C217	0.079(7)	0.120(9)	0.099(9)	0.052(7)	0.076(7)	0.054(7)
C219	0.028(4)	0.054(5)	0.045(5)	0.005(4)	0.013(4)	0.015(4)
C221	0.070(7)	0.087(8)	0.061(7)	0.017(6)	-0.009(6)	0.001(6)
C222	0.036(4)	0.022(3)	0.026(4)	0.014(3)	0.012(3)	0.004(3)
C223	0.030(4)	0.029(4)	0.024(4)	0.010(3)	0.011(3)	0.004(3)
C224	0.032(4)	0.026(3)	0.025(4)	0.008(3)	0.013(3)	0.003(3)
C225	0.031(4)	0.033(4)	0.022(4)	0.014(3)	0.009(3)	0.006(3)
C226	0.027(4)	0.029(4)	0.030(4)	0.007(3)	0.008(3)	0.003(3)
C227	0.031(4)	0.041(4)	0.044(5)	0.007(3)	0.011(4)	0.006(4)
C231	0.042(5)	0.053(5)	0.073(7)	0.022(4)	0.013(5)	0.024(5)
C233	0.038(4)	0.032(4)	0.060(6)	0.007(4)	0.027(4)	0.013(4)
C235	0.037(5)	0.054(5)	0.078(7)	-0.004(4)	0.024(5)	-0.019(5)
C236	0.025(3)	0.027(3)	0.024(4)	0.013(3)	0.009(3)	0.011(3)
C237	0.025(3)	0.030(4)	0.027(4)	0.012(3)	0.005(3)	0.004(3)
C238	0.025(3)	0.026(3)	0.032(4)	0.012(3)	0.009(3)	0.013(3)
C239	0.028(3)	0.026(3)	0.031(4)	0.015(3)	0.012(3)	0.012(3)
C240	0.031(4)	0.033(4)	0.023(4)	0.016(3)	0.010(3)	0.012(3)
C241	0.039(4)	0.028(4)	0.030(4)	0.003(3)	0.015(3)	0.006(3)
C245	0.082(8)	0.068(7)	0.086(9)	0.035(6)	-0.043(7)	-0.031(6)
C247	0.037(4)	0.024(3)	0.044(5)	0.008(3)	0.014(4)	0.007(3)
C249	0.066(6)	0.038(5)	0.077(7)	0.012(4)	0.043(5)	0.001(4)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

Al(1)	O(10)	O(11)	N(2)	N(3)
N(4)	N(5)	N(6)	N(7)	N(8)
N(9)	C(12)	C(13)	C(14)	C(15)
C(16)	C(17)	C(18)	C(19)	C(20)
C(21)	C(22)	C(23)	C(24)	C(25)
C(26)	C(27)	C(28)	C(29)	C(30)
C(31)	C(32)	C(33)	C(34)	C(35)
C(36)	C(37)	C(38)	C(39)	C(40)
C(41)	C(42)	C(43)	C(44)	C(45)
C(46)	C(47)	C(48)	C(49)	C(50)
C(51)				

fragment: 2

O(58)	O(59)	O(60)	O(62)	O(64)
O(72)	O(73)	O(74)	O(76)	O(78)
O(86)	O(87)	O(88)	O(90)	O(92)
O(100)	O(101)	O(102)	O(104)	O(106)
O(114)	O(115)	O(116)	O(118)	O(120)
O(128)	O(129)	O(130)	O(133)	O(135)

Table 4. Fragment Analysis (continued)

O(143)	O(144)	O(145)	O(147)	O(149)
C(52)	C(53)	C(54)	C(55)	C(56)
C(57)	C(61)	C(63)	C(65)	C(66)
C(67)	C(68)	C(69)	C(70)	C(71)
C(75)	C(77)	C(79)	C(80)	C(81)
C(82)	C(83)	C(84)	C(85)	C(89)
C(91)	C(93)	C(94)	C(95)	C(96)
C(97)	C(98)	C(99)	C(103)	C(105)
C(107)	C(108)	C(109)	C(110)	C(111)
C(112)	C(113)	C(117)	C(119)	C(121)
C(122)	C(123)	C(124)	C(125)	C(126)
C(127)	C(131)	C(132)	C(134)	C(136)
C(137)	C(138)	C(139)	C(140)	C(141)
C(142)	C(146)	C(148)	C(150)	

fragment: 3

O(157)	O(158)	O(159)	O(161)	O(163)
O(171)	O(172)	O(173)	O(175)	O(177)
O(185)	O(186)	O(187)	O(189)	O(191)
O(199)	O(200)	O(201)	O(203)	O(206)

Table 4. Fragment Analysis (continued)

			O(214)	O(215)	O(216)
O(218)	O(220)				
O(228)	O(229)	O(230)	O(232)	O(234)	
O(242)	O(243)	O(244)	O(246)	O(248)	
C(151)	C(152)	C(153)	C(154)	C(155)	
C(156)	C(160)	C(162)	C(164)	C(165)	
C(166)	C(167)	C(168)	C(169)	C(170)	
C(174)	C(176)	C(178)	C(179)	C(180)	
C(181)	C(182)	C(183)	C(184)	C(188)	
C(190)	C(192)	C(193)	C(194)	C(195)	
C(196)	C(197)	C(198)	C(202)	C(204)	
C(205)	C(207)	C(208)	C(209)	C(210)	
C(211)	C(212)	C(213)	C(217)	C(219)	
C(221)	C(222)	C(223)	C(224)	C(225)	
C(226)	C(227)	C(231)	C(233)	C(235)	
C(236)	C(237)	C(238)	C(239)	C(240)	
C(241)	C(245)	C(247)	C(249)		

fragment: 4

O(250)

fragment: 5

Table 4. Fragment Analysis (continued)

	O(251)
fragment: 6	
	O(252)

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Al1	O10	1.855(6)	Al1	O11	2.189(10)
Al1	N2	2.010(6)	Al1	N3	2.011(6)
Al1	N4	1.991(6)	Al1	N5	1.995(6)
O58	C52	1.400(8)	O58	C56	1.442(9)
O59	C52	1.411(9)	O59	C69	1.434(11)
O60	C53	1.413(9)	O60	C61	1.389(13)
O62	C54	1.431(10)	O62	C63	1.412(8)
O64	C57	1.421(11)	O64	C65	1.418(10)
O72	C66	1.420(7)	O72	C70	1.449(10)
O73	C66	1.418(8)	O73	C83	1.435(9)
O74	C67	1.422(7)	O74	C75	1.401(13)
O76	C68	1.407(8)	O76	C77	1.424(10)
O78	C71	1.402(9)	O78	C79	1.410(8)
O86	C80	1.412(7)	O86	C84	1.447(10)
O87	C80	1.409(8)	O87	C97	1.430(8)
O88	C81	1.406(7)	O88	C89	1.406(13)
O90	C82	1.422(8)	O90	C91	1.429(6)
O92	C85	1.407(10)	O92	C93	1.404(9)
O100	C94	1.411(7)	O100	C98	1.449(8)
O101	C94	1.416(9)	O101	C111	1.424(9)
O102	C95	1.434(7)	O102	C103	1.411(12)
O104	C96	1.419(10)	O104	C105	1.431(7)
O106	C99	1.419(11)	O106	C107	1.414(9)
O114	C108	1.418(7)	O114	C112	1.424(9)
O115	C108	1.414(9)	O115	C125	1.438(11)
O116	C109	1.421(8)	O116	C117	1.407(10)
O118	C110	1.415(9)	O118	C119	1.348(14)
O120	C113	1.424(10)	O120	C121	1.419(10)
O128	C122	1.404(10)	O128	C126	1.443(12)
O129	C122	1.417(10)	O129	C140	1.418(9)
O130	C123	1.410(11)	O130	C131	1.32(2)
O130	C132	1.52(3)	O133	C124	1.416(7)
O133	C134	1.407(11)	O135	C127	1.413(13)
O135	C136	1.33(2)	O143	C137	1.407(9)
O143	C141	1.431(9)	O144	C55	1.431(9)
O144	C137	1.424(9)	O145	C138	1.416(10)
O145	C146	1.425(10)	O147	C139	1.415(9)

Table 5. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
O147	C148	1.441(9)	O149	C142	1.402(12)
O149	C150	1.416(11)	O157	C151	1.420(9)
O157	C155	1.434(10)	O158	C151	1.400(9)
O158	C168	1.428(7)	O159	C152	1.421(9)
O159	C160	1.416(12)	O161	C153	1.433(6)
O161	C162	1.404(8)	O163	C156	1.416(11)
O163	C164	1.406(18)	O171	C165	1.408(9)
O171	C169	1.442(8)	O172	C165	1.406(9)
O172	C182	1.458(9)	O173	C166	1.423(9)
O173	C174	1.417(9)	O175	C167	1.425(9)
O175	C176	1.418(8)	O177	C170	1.417(12)
O177	C178	1.397(10)	O185	C179	1.403(8)
O185	C183	1.439(9)	O186	C179	1.416(10)
O186	C196	1.432(10)	O187	C180	1.417(7)
O187	C188	1.419(10)	O189	C181	1.422(10)
O189	C190	1.401(8)	O191	C184	1.413(10)
O191	C192	1.366(10)	O199	C193	1.419(7)
O199	C197	1.433(10)	O200	C193	1.399(9)
O200	C211	1.425(9)	O201	C194	1.409(9)
O201	C202	1.371(17)	O203	C195	1.413(8)
O203	C204	1.546(17)	O203	C205	1.42(3)
O206	C198	1.392(9)	O206	C207	1.413(10)
O214	C208	1.403(8)	O214	C212	1.449(10)
O215	C208	1.419(8)	O215	C225	1.438(9)
O216	C209	1.417(8)	O216	C217	1.431(16)
O218	C210	1.419(9)	O218	C219	1.425(7)
O220	C213	1.390(11)	O220	C221	1.400(11)
O228	C222	1.403(7)	O228	C226	1.447(9)
O229	C222	1.411(9)	O229	C239	1.438(9)
O230	C223	1.413(7)	O230	C231	1.401(11)
O232	C224	1.404(10)	O232	C233	1.425(7)
O234	C227	1.412(11)	O234	C235	1.422(9)
O242	C236	1.426(7)	O242	C240	1.429(9)
O243	C154	1.441(10)	O243	C236	1.412(9)
O244	C237	1.405(8)	O244	C245	1.344(11)
O246	C238	1.445(8)	O246	C247	1.417(9)
O248	C241	1.426(10)	O248	C249	1.422(10)

Table 5. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
N2	C12	1.391(6)	N2	C15	1.374(10)
N3	C17	1.379(10)	N3	C20	1.381(6)
N4	C22	1.383(6)	N4	C25	1.377(10)
N5	C27	1.375(10)	N5	C30	1.393(6)
N6	C34	1.337(11)	N6	C35	1.339(11)
N7	C39	1.302(10)	N7	C40	1.338(11)
N8	C44	1.345(11)	N8	C45	1.341(10)
N9	C49	1.347(11)	N9	C50	1.310(11)
C12	C13	1.441(11)	C12	C31	1.371(10)
C13	C14	1.340(10)	C14	C15	1.432(8)
C15	C16	1.380(9)	C16	C17	1.399(8)
C16	C32	1.507(12)	C17	C18	1.418(9)
C18	C19	1.344(10)	C19	C20	1.421(11)
C20	C21	1.398(10)	C21	C22	1.401(11)
C21	C37	1.483(7)	C22	C23	1.437(11)
C23	C24	1.325(10)	C24	C25	1.433(8)
C25	C26	1.399(8)	C26	C27	1.399(8)
C26	C42	1.493(11)	C27	C28	1.430(8)
C28	C29	1.336(10)	C29	C30	1.423(10)
C30	C31	1.406(10)	C31	C47	1.499(7)
C32	C33	1.372(11)	C32	C36	1.376(11)
C33	C34	1.410(13)	C35	C36	1.395(13)
C37	C38	1.375(11)	C37	C41	1.385(9)
C38	C39	1.394(9)	C40	C41	1.388(8)
C42	C43	1.395(10)	C42	C46	1.390(10)
C43	C44	1.382(13)	C45	C46	1.372(12)
C47	C48	1.367(10)	C47	C51	1.368(10)
C48	C49	1.370(9)	C50	C51	1.381(9)
C52	C53	1.499(12)	C53	C54	1.526(11)
C54	C55	1.506(8)	C55	C56	1.519(10)
C56	C57	1.508(8)	C66	C67	1.513(9)
C67	C68	1.525(12)	C68	C69	1.516(8)
C69	C70	1.525(10)	C70	C71	1.495(8)
C80	C81	1.544(9)	C81	C82	1.523(11)
C82	C83	1.517(8)	C83	C84	1.523(9)
C84	C85	1.516(8)	C94	C95	1.518(12)
C95	C96	1.513(10)	C96	C97	1.532(8)

Table 5. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C97	C98	1.529(11)	C98	C99	1.505(8)
C108	C109	1.523(10)	C109	C110	1.523(11)
C110	C111	1.511(8)	C111	C112	1.533(11)
C112	C113	1.526(8)	C122	C123	1.529(9)
C123	C124	1.510(13)	C124	C125	1.514(11)
C125	C126	1.535(9)	C126	C127	1.494(11)
C131	C132	0.77(4)	C137	C138	1.529(11)
C138	C139	1.510(10)	C139	C140	1.538(11)
C140	C141	1.528(10)	C141	C142	1.493(11)
C151	C152	1.524(7)	C152	C153	1.523(12)
C153	C154	1.512(10)	C154	C155	1.529(7)
C155	C156	1.519(10)	C165	C166	1.540(11)
C166	C167	1.525(9)	C167	C168	1.527(10)
C168	C169	1.525(10)	C169	C170	1.524(10)
C179	C180	1.531(11)	C180	C181	1.516(11)
C181	C182	1.529(8)	C182	C183	1.505(11)
C183	C184	1.492(8)	C193	C194	1.542(10)
C194	C195	1.519(13)	C195	C196	1.508(9)
C196	C197	1.558(9)	C197	C198	1.508(9)
C204	C205	0.96(4)	C208	C209	1.518(11)
C209	C210	1.528(12)	C210	C211	1.518(9)
C211	C212	1.534(9)	C212	C213	1.511(8)
C222	C223	1.518(11)	C223	C224	1.513(10)
C224	C225	1.539(8)	C225	C226	1.526(11)
C226	C227	1.525(8)	C236	C237	1.517(9)
C237	C238	1.522(11)	C238	C239	1.507(8)
C239	C240	1.530(10)	C240	C241	1.517(8)

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C13	H13	0.950	C14	H14	0.950
C18	H18	0.950	C19	H19	0.950
C23	H23	0.950	C24	H24	0.950
C28	H28	0.950	C29	H29	0.950
C33	H33	0.950	C34	H34	0.950
C35	H35	0.950	C36	H36	0.950
C38	H38	0.950	C39	H39	0.950
C40	H40	0.950	C41	H41	0.950
C43	H43	0.950	C44	H44	0.950
C45	H45	0.950	C46	H46	0.950
C48	H48	0.950	C49	H49	0.950
C50	H50	0.950	C51	H51	0.950
C52	H52	1.000	C53	H53	1.000
C54	H54	1.000	C55	H55	1.000
C56	H56	1.000	C57	H57A	0.990
C57	H57B	0.990	C61	H61A	0.980
C61	H61B	0.980	C61	H61C	0.980
C63	H63A	0.980	C63	H63B	0.980
C63	H63C	0.980	C65	H65A	0.980
C65	H65B	0.980	C65	H65C	0.980
C66	H66	1.000	C67	H67	1.000
C68	H68	1.000	C69	H69	1.000
C70	H70	1.000	C71	H71A	0.990
C71	H71B	0.990	C75	H75A	0.980
C75	H75B	0.980	C75	H75C	0.980
C77	H77A	0.980	C77	H77B	0.980
C77	H77C	0.980	C79	H79A	0.980
C79	H79B	0.980	C79	H79C	0.980
C80	H80	1.000	C81	H81	1.000
C82	H82	1.000	C83	H83	1.000
C84	H84	1.000	C85	H85A	0.990
C85	H85B	0.990	C89	H89A	0.980
C89	H89B	0.980	C89	H89C	0.980
C91	H91A	0.980	C91	H91B	0.980
C91	H91C	0.980	C93	H93A	0.980
C93	H93B	0.980	C93	H93C	0.980
C94	H94	1.000	C95	H95	1.000

Table 6. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C96	H96	1.000	C97	H97	1.000
C98	H98	1.000	C99	H99A	0.990
C99	H99B	0.990	C103	H10A	0.980
C103	H10B	0.980	C103	H10C	0.980
C105	H10D	0.980	C105	H10E	0.980
C105	H10F	0.980	C107	H10G	0.980
C107	H10H	0.980	C107	H10I	0.980
C108	H108	1.000	C109	H109	1.000
C110	H110	1.000	C111	H111	1.000
C112	H112	1.000	C113	H11A	0.990
C113	H11B	0.990	C117	H11C	0.980
C117	H11D	0.980	C117	H11E	0.980
C119	H11F	0.980	C119	H11G	0.980
C119	H11H	0.980	C121	H12A	0.980
C121	H12B	0.980	C121	H12C	0.980
C122	H122	1.000	C123	H123	1.000
C124	H124	1.000	C125	H125	1.000
C126	H126	1.000	C127	H12D	0.990
C127	H12E	0.990	C134	H13A	0.980
C134	H13B	0.980	C134	H13C	0.980
C136	H13D	0.980	C136	H13E	0.980
C136	H13F	0.980	C137	H137	1.000
C138	H138	1.000	C139	H139	1.000
C140	H140	1.000	C141	H141	1.000
C142	H14A	0.990	C142	H14B	0.990
C146	H14C	0.980	C146	H14D	0.980
C146	H14E	0.980	C148	H14F	0.980
C148	H14G	0.980	C148	H14H	0.980
C150	H15A	0.980	C150	H15B	0.980
C150	H15C	0.980	C151	H151	1.000
C152	H152	1.000	C153	H153	1.000
C154	H154	1.000	C155	H155	1.000
C156	H15D	0.990	C156	H15E	0.990
C160	H16A	0.980	C160	H16B	0.980
C160	H16C	0.980	C162	H16D	0.980
C162	H16E	0.980	C162	H16F	0.980
C164	H16G	0.980	C164	H16H	0.980

Table 6. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C164	H16I	0.980	C165	H165	1.000
C166	H166	1.000	C167	H167	1.000
C168	H168	1.000	C169	H169	1.000
C170	H17A	0.990	C170	H17B	0.990
C174	H17C	0.980	C174	H17D	0.980
C174	H17E	0.980	C176	H17F	0.980
C176	H17G	0.980	C176	H17H	0.980
C178	H17I	0.980	C178	H17J	0.980
C178	H17K	0.980	C179	H179	1.000
C180	H180	1.000	C181	H181	1.000
C182	H182	1.000	C183	H183	1.000
C184	H18A	0.990	C184	H18B	0.990
C188	H18C	0.980	C188	H18D	0.980
C188	H18E	0.980	C190	H19A	0.980
C190	H19B	0.980	C190	H19C	0.980
C192	H19D	0.980	C192	H19E	0.980
C192	H19F	0.980	C193	H193	1.000
C194	H194	1.000	C195	H195	1.000
C196	H196	1.000	C197	H197	1.000
C198	H19G	0.990	C198	H19H	0.990
C202	H20A	0.980	C202	H20B	0.980
C202	H20C	0.980	C207	H20D	0.980
C207	H20E	0.980	C207	H20F	0.980
C208	H208	1.000	C209	H209	1.000
C210	H210	1.000	C211	H211	1.000
C212	H212	1.000	C213	H21A	0.990
C213	H21B	0.990	C217	H21C	0.980
C217	H21D	0.980	C217	H21E	0.980
C219	H21F	0.980	C219	H21G	0.980
C219	H21H	0.980	C221	H22A	0.980
C221	H22B	0.980	C221	H22C	0.980
C222	H222	1.000	C223	H223	1.000
C224	H224	1.000	C225	H225	1.000
C226	H226	1.000	C227	H22D	0.990
C227	H22E	0.990	C231	H23A	0.980
C231	H23B	0.980	C231	H23C	0.980
C233	H23D	0.980	C233	H23E	0.980

Table 6. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C233	H23F	0.980	C235	H23G	0.980
C235	H23H	0.980	C235	H23I	0.980
C236	H236	1.000	C237	H237	1.000
C238	H238	1.000	C239	H239	1.000
C240	H240	1.000	C241	H24A	0.990
C241	H24B	0.990	C245	H24C	0.980
C245	H24D	0.980	C245	H24E	0.980
C247	H24F	0.980	C247	H24G	0.980
C247	H24H	0.980	C249	H24I	0.980
C249	H24J	0.980	C249	H24K	0.980

Table 7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O10	Al1	O11	176.3(4)	O10	Al1	N2	96.0(3)
O10	Al1	N3	96.3(3)	O10	Al1	N4	91.9(3)
O10	Al1	N5	96.6(3)	O11	Al1	N2	87.1(3)
O11	Al1	N3	85.8(3)	O11	Al1	N4	85.0(3)
O11	Al1	N5	81.4(3)	N2	Al1	N3	88.8(3)
N2	Al1	N4	172.1(3)	N2	Al1	N5	89.7(3)
N3	Al1	N4	89.8(3)	N3	Al1	N5	167.1(3)
N4	Al1	N5	89.9(3)	C52	O58	C56	113.3(5)
C52	O59	C69	116.9(6)	C53	O60	C61	117.1(9)
C54	O62	C63	114.4(6)	C57	O64	C65	113.6(7)
C66	O72	C70	112.3(5)	C66	O73	C83	117.4(6)
C67	O74	C75	113.2(6)	C68	O76	C77	113.8(6)
C71	O78	C79	111.7(6)	C80	O86	C84	114.5(4)
C80	O87	C97	117.0(5)	C81	O88	C89	114.3(5)
C82	O90	C91	114.6(5)	C85	O92	C93	113.9(7)
C94	O100	C98	113.4(4)	C94	O101	C111	117.9(6)
C95	O102	C103	114.2(5)	C96	O104	C105	114.2(6)
C99	O106	C107	110.6(7)	C108	O114	C112	113.3(5)
C108	O115	C125	116.3(6)	C109	O116	C117	114.0(6)
C110	O118	C119	117.4(7)	C113	O120	C121	112.0(6)
C122	O128	C126	114.8(6)	C122	O129	C140	116.1(6)
C123	O130	C131	123.3(11)	C123	O130	C132	105.3(11)
C131	O130	C132	30.6(12)	C124	O133	C134	114.3(7)
C127	O135	C136	113.3(9)	C137	O143	C141	113.8(4)
C55	O144	C137	118.5(5)	C138	O145	C146	113.8(5)
C139	O147	C148	112.9(6)	C142	O149	C150	113.1(7)
C151	O157	C155	114.5(5)	C151	O158	C168	117.5(5)
C152	O159	C160	112.2(6)	C153	O161	C162	113.5(6)
C156	O163	C164	115.4(8)	C165	O171	C169	114.5(4)
C165	O172	C182	116.9(5)	C166	O173	C174	114.3(5)
C167	O175	C176	113.2(6)	C170	O177	C178	111.7(7)
C179	O185	C183	113.9(5)	C179	O186	C196	117.8(6)
C180	O187	C188	113.1(6)	C181	O189	C190	115.3(6)
C184	O191	C192	113.3(8)	C193	O199	C197	114.8(5)
C193	O200	C211	117.8(6)	C194	O201	C202	114.1(7)
C195	O203	C204	112.5(7)	C195	O203	C205	113.3(13)
C204	O203	C205	37.4(15)	C198	O206	C207	111.0(8)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C208	O214	C212	114.6(5)	C208	O215	C225	116.9(6)
C209	O216	C217	112.0(6)	C210	O218	C219	112.9(6)
C213	O220	C221	112.4(9)	C222	O228	C226	113.1(4)
C222	O229	C239	117.6(5)	C223	O230	C231	113.6(5)
C224	O232	C233	114.2(6)	C227	O234	C235	111.8(7)
C236	O242	C240	114.3(5)	C154	O243	C236	116.6(5)
C237	O244	C245	116.2(7)	C238	O246	C247	114.1(5)
C241	O248	C249	113.5(6)	Al1	N2	C12	126.2(5)
Al1	N2	C15	127.5(4)	C12	N2	C15	105.8(5)
Al1	N3	C17	128.2(4)	Al1	N3	C20	127.6(5)
C17	N3	C20	104.2(5)	Al1	N4	C22	127.5(5)
Al1	N4	C25	126.6(4)	C22	N4	C25	105.4(5)
Al1	N5	C27	127.7(3)	Al1	N5	C30	127.7(5)
C27	N5	C30	104.2(5)	C34	N6	C35	116.0(9)
C39	N7	C40	115.5(6)	C44	N8	C45	116.5(8)
C49	N9	C50	116.2(6)	N2	C12	C13	109.2(6)
N2	C12	C31	126.2(6)	C13	C12	C31	124.5(5)
C12	C13	C14	107.3(5)	C13	C14	C15	107.8(7)
N2	C15	C14	109.9(6)	N2	C15	C16	125.6(6)
C14	C15	C16	124.5(8)	C15	C16	C17	124.5(8)
C15	C16	C32	117.7(6)	C17	C16	C32	117.9(6)
N3	C17	C16	124.6(6)	N3	C17	C18	110.6(5)
C16	C17	C18	124.8(7)	C17	C18	C19	107.5(7)
C18	C19	C20	106.7(5)	N3	C20	C19	111.0(6)
N3	C20	C21	125.2(6)	C19	C20	C21	123.8(5)
C20	C21	C22	123.8(5)	C20	C21	C37	119.6(6)
C22	C21	C37	116.6(6)	N4	C22	C21	125.6(7)
N4	C22	C23	109.4(6)	C21	C22	C23	124.9(5)
C22	C23	C24	107.6(5)	C23	C24	C25	107.7(7)
N4	C25	C24	109.7(5)	N4	C25	C26	124.9(5)
C24	C25	C26	125.2(7)	C25	C26	C27	124.6(7)
C25	C26	C42	117.4(5)	C27	C26	C42	118.0(5)
N5	C27	C26	124.3(6)	N5	C27	C28	110.6(5)
C26	C27	C28	124.8(7)	C27	C28	C29	107.4(7)
C28	C29	C30	107.2(5)	N5	C30	C29	110.5(6)
N5	C30	C31	124.7(6)	C29	C30	C31	124.7(5)
C12	C31	C30	124.2(5)	C12	C31	C47	119.1(6)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C30	C31	C47	116.6(6)	C16	C32	C33	120.1(7)
C16	C32	C36	122.2(7)	C33	C32	C36	117.8(8)
C32	C33	C34	119.5(7)	N6	C34	C33	123.3(8)
N6	C35	C36	124.0(8)	C32	C36	C35	119.4(7)
C21	C37	C38	120.6(6)	C21	C37	C41	122.9(6)
C38	C37	C41	116.5(5)	C37	C38	C39	119.3(7)
N7	C39	C38	125.1(8)	N7	C40	C41	123.9(7)
C37	C41	C40	119.5(7)	C26	C42	C43	119.6(6)
C26	C42	C46	123.4(6)	C43	C42	C46	117.0(7)
C42	C43	C44	119.7(7)	N8	C44	C43	123.2(7)
N8	C45	C46	124.0(7)	C42	C46	C45	119.5(7)
C31	C47	C48	120.7(6)	C31	C47	C51	122.2(6)
C48	C47	C51	117.0(5)	C47	C48	C49	119.8(7)
N9	C49	C48	123.4(7)	N9	C50	C51	123.6(7)
C47	C51	C50	120.0(7)	O58	C52	O59	111.9(6)
O58	C52	C53	108.8(7)	O59	C52	C53	110.9(5)
O60	C53	C52	105.9(8)	O60	C53	C54	114.7(6)
C52	C53	C54	110.0(6)	O62	C54	C53	108.4(6)
O62	C54	C55	110.6(7)	C53	C54	C55	109.8(5)
O144	C55	C54	106.6(5)	O144	C55	C56	112.1(6)
C54	C55	C56	110.1(7)	O58	C56	C55	109.1(6)
O58	C56	C57	107.3(5)	C55	C56	C57	115.2(7)
O64	C57	C56	113.7(7)	O72	C66	O73	111.1(5)
O72	C66	C67	109.9(6)	O73	C66	C67	109.0(5)
O74	C67	C66	111.6(6)	O74	C67	C68	109.3(5)
C66	C67	C68	111.5(6)	O76	C68	C67	108.5(6)
O76	C68	C69	112.1(7)	C67	C68	C69	106.9(6)
O59	C69	C68	108.9(6)	O59	C69	C70	111.0(6)
C68	C69	C70	110.1(7)	O72	C70	C69	108.8(6)
O72	C70	C71	107.0(6)	C69	C70	C71	116.8(7)
O78	C71	C70	110.5(6)	O86	C80	O87	112.9(6)
O86	C80	C81	109.4(5)	O87	C80	C81	109.6(4)
O88	C81	C80	113.5(6)	O88	C81	C82	108.0(5)
C80	C81	C82	112.1(6)	O90	C82	C81	109.3(6)
O90	C82	C83	107.1(5)	C81	C82	C83	112.7(5)
O73	C83	C82	107.9(5)	O73	C83	C84	108.8(6)
C82	C83	C84	112.3(6)	O86	C84	C83	110.4(6)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O86	C84	C85	105.8(5)	C83	C84	C85	113.0(6)
O92	C85	C84	110.2(7)	O100	C94	O101	111.2(6)
O100	C94	C95	107.6(6)	O101	C94	C95	110.9(5)
O102	C95	C94	111.1(6)	O102	C95	C96	108.0(5)
C94	C95	C96	110.8(7)	O104	C96	C95	110.4(6)
O104	C96	C97	106.7(6)	C95	C96	C97	109.8(5)
O87	C97	C96	107.5(4)	O87	C97	C98	109.1(6)
C96	C97	C98	112.4(6)	O100	C98	C97	111.3(6)
O100	C98	C99	106.3(5)	C97	C98	C99	113.0(6)
O106	C99	C98	110.0(7)	O114	C108	O115	110.6(5)
O114	C108	C109	109.4(7)	O115	C108	C109	110.7(6)
O116	C109	C108	112.4(7)	O116	C109	C110	108.6(6)
C108	C109	C110	112.6(5)	O118	C110	C109	108.1(5)
O118	C110	C111	110.7(7)	C109	C110	C111	110.5(6)
O101	C111	C110	106.8(6)	O101	C111	C112	110.7(5)
C110	C111	C112	110.2(7)	O114	C112	C111	111.1(5)
O114	C112	C113	106.5(6)	C111	C112	C113	113.8(7)
O120	C113	C112	109.0(5)	O128	C122	O129	112.8(6)
O128	C122	C123	110.1(7)	O129	C122	C123	108.9(7)
O130	C123	C122	111.7(7)	O130	C123	C124	109.3(7)
C122	C123	C124	111.6(7)	O133	C124	C123	108.9(6)
O133	C124	C125	108.3(6)	C123	C124	C125	109.5(7)
O115	C125	C124	108.7(6)	O115	C125	C126	108.5(6)
C124	C125	C126	110.9(7)	O128	C126	C125	110.8(7)
O128	C126	C127	105.4(7)	C125	C126	C127	114.1(7)
O135	C127	C126	112.7(7)	O130	C131	C132	89(3)
O130	C132	C131	61(3)	O143	C137	O144	111.3(7)
O143	C137	C138	108.4(6)	O144	C137	C138	107.5(5)
O145	C138	C137	113.2(6)	O145	C138	C139	109.5(5)
C137	C138	C139	110.3(7)	O147	C139	C138	111.3(7)
O147	C139	C140	108.1(6)	C138	C139	C140	110.7(5)
O129	C140	C139	108.6(5)	O129	C140	C141	108.7(7)
C139	C140	C141	111.7(6)	O143	C141	C140	111.2(7)
O143	C141	C142	106.7(5)	C140	C141	C142	113.0(7)
O149	C142	C141	109.5(7)	O157	C151	O158	112.4(6)
O157	C151	C152	108.0(6)	O158	C151	C152	108.8(5)
O159	C152	C151	112.3(6)	O159	C152	C153	108.4(5)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C151	C152	C153	111.9(6)	O161	C153	C152	108.7(6)
O161	C153	C154	107.5(6)	C152	C153	C154	110.0(5)
O243	C154	C153	108.3(5)	O243	C154	C155	108.6(6)
C153	C154	C155	111.7(6)	O157	C155	C154	111.6(6)
O157	C155	C156	105.7(6)	C154	C155	C156	112.8(6)
O163	C156	C155	112.4(7)	O171	C165	O172	111.6(7)
O171	C165	C166	107.6(6)	O172	C165	C166	110.4(5)
O173	C166	C165	113.5(6)	O173	C166	C167	107.7(4)
C165	C166	C167	109.3(7)	O175	C167	C166	111.4(6)
O175	C167	C168	107.8(6)	C166	C167	C168	110.2(5)
O158	C168	C167	108.1(4)	O158	C168	C169	107.8(6)
C167	C168	C169	113.2(6)	O171	C169	C168	112.4(6)
O171	C169	C170	106.4(4)	C168	C169	C170	110.5(6)
O177	C170	C169	116.1(7)	O185	C179	O186	111.8(6)
O185	C179	C180	109.1(7)	O186	C179	C180	111.4(5)
O187	C180	C179	113.9(7)	O187	C180	C181	105.8(5)
C179	C180	C181	112.5(6)	O189	C181	C180	107.5(6)
O189	C181	C182	108.9(7)	C180	C181	C182	110.5(5)
O172	C182	C181	106.0(5)	O172	C182	C183	110.2(6)
C181	C182	C183	110.6(7)	O185	C183	C182	108.9(6)
O185	C183	C184	106.0(5)	C182	C183	C184	115.1(7)
O191	C184	C183	109.5(7)	O199	C193	O200	111.6(6)
O199	C193	C194	107.7(7)	O200	C193	C194	108.7(6)
O201	C194	C193	112.0(7)	O201	C194	C195	109.3(6)
C193	C194	C195	109.1(6)	O203	C195	C194	110.4(6)
O203	C195	C196	110.8(7)	C194	C195	C196	107.4(6)
O186	C196	C195	108.0(5)	O186	C196	C197	110.2(5)
C195	C196	C197	111.6(7)	O199	C197	C196	110.2(5)
O199	C197	C198	106.2(6)	C196	C197	C198	113.0(7)
O206	C198	C197	108.6(7)	O203	C204	C205	63.9(18)
O203	C205	C204	78.7(19)	O214	C208	O215	112.4(7)
O214	C208	C209	108.9(6)	O215	C208	C209	110.5(5)
O216	C209	C208	112.6(7)	O216	C209	C210	109.0(5)
C208	C209	C210	109.6(7)	O218	C210	C209	110.4(7)
O218	C210	C211	107.1(6)	C209	C210	C211	108.2(5)
O200	C211	C210	108.5(5)	O200	C211	C212	107.6(6)
C210	C211	C212	112.1(6)	O214	C212	C211	112.8(6)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O214	C212	C213	105.0(5)	C211	C212	C213	113.6(6)
O220	C213	C212	109.0(7)	O228	C222	O229	111.2(6)
O228	C222	C223	108.9(6)	O229	C222	C223	109.7(5)
O230	C223	C222	112.8(6)	O230	C223	C224	109.0(5)
C222	C223	C224	110.7(6)	O232	C224	C223	111.3(6)
O232	C224	C225	107.7(6)	C223	C224	C225	109.3(5)
O215	C225	C224	107.0(5)	O215	C225	C226	110.1(6)
C224	C225	C226	112.0(6)	O228	C226	C225	108.6(6)
O228	C226	C227	106.6(5)	C225	C226	C227	112.3(6)
O234	C227	C226	108.0(7)	O242	C236	O243	111.5(4)
O242	C236	C237	109.5(6)	O243	C236	C237	110.2(5)
O244	C237	C236	111.5(7)	O244	C237	C238	109.4(6)
C236	C237	C238	112.0(5)	O246	C238	C237	106.7(5)
O246	C238	C239	110.0(7)	C237	C238	C239	111.3(6)
O229	C239	C238	106.3(5)	O229	C239	C240	112.1(5)
C238	C239	C240	109.7(7)	O242	C240	C239	109.3(5)
O242	C240	C241	107.7(6)	C239	C240	C241	114.1(7)
O248	C241	C240	108.7(5)				

Table 8. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C12	C13	H13	126.4	C14	C13	H13	126.4
C13	C14	H14	126.1	C15	C14	H14	126.1
C17	C18	H18	126.2	C19	C18	H18	126.2
C18	C19	H19	126.7	C20	C19	H19	126.7
C22	C23	H23	126.2	C24	C23	H23	126.2
C23	C24	H24	126.1	C25	C24	H24	126.1
C27	C28	H28	126.3	C29	C28	H28	126.3
C28	C29	H29	126.4	C30	C29	H29	126.4
C32	C33	H33	120.3	C34	C33	H33	120.3
N6	C34	H34	118.3	C33	C34	H34	118.3
N6	C35	H35	118.0	C36	C35	H35	118.0
C32	C36	H36	120.3	C35	C36	H36	120.3
C37	C38	H38	120.3	C39	C38	H38	120.3
N7	C39	H39	117.5	C38	C39	H39	117.5
N7	C40	H40	118.0	C41	C40	H40	118.0
C37	C41	H41	120.2	C40	C41	H41	120.3
C42	C43	H43	120.2	C44	C43	H43	120.2
N8	C44	H44	118.4	C43	C44	H44	118.4
N8	C45	H45	118.0	C46	C45	H45	118.0
C42	C46	H46	120.3	C45	C46	H46	120.3
C47	C48	H48	120.1	C49	C48	H48	120.1
N9	C49	H49	118.3	C48	C49	H49	118.3
N9	C50	H50	118.2	C51	C50	H50	118.2
C47	C51	H51	120.0	C50	C51	H51	120.0
O58	C52	H52	108.4	O59	C52	H52	108.4
C53	C52	H52	108.4	O60	C53	H53	108.7
C52	C53	H53	108.7	C54	C53	H53	108.7
O62	C54	H54	109.3	C53	C54	H54	109.3
C55	C54	H54	109.3	O144	C55	H55	109.3
C54	C55	H55	109.3	C56	C55	H55	109.3
O58	C56	H56	108.3	C55	C56	H56	108.3
C57	C56	H56	108.4	O64	C57	H57A	108.8
O64	C57	H57B	108.8	C56	C57	H57A	108.8
C56	C57	H57B	108.8	H57A	C57	H57B	107.7
O60	C61	H61A	109.5	O60	C61	H61B	109.5
O60	C61	H61C	109.5	H61A	C61	H61B	109.5
H61A	C61	H61C	109.5	H61B	C61	H61C	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O62	C63	H63A	109.5	O62	C63	H63B	109.5
O62	C63	H63C	109.5	H63A	C63	H63B	109.5
H63A	C63	H63C	109.5	H63B	C63	H63C	109.5
O64	C65	H65A	109.5	O64	C65	H65B	109.5
O64	C65	H65C	109.5	H65A	C65	H65B	109.5
H65A	C65	H65C	109.5	H65B	C65	H65C	109.5
O72	C66	H66	108.9	O73	C66	H66	108.9
C67	C66	H66	108.9	O74	C67	H67	108.1
C66	C67	H67	108.1	C68	C67	H67	108.1
O76	C68	H68	109.8	C67	C68	H68	109.8
C69	C68	H68	109.8	O59	C69	H69	108.9
C68	C69	H69	108.9	C70	C69	H69	108.9
O72	C70	H70	108.0	C69	C70	H70	108.0
C71	C70	H70	108.0	O78	C71	H71A	109.5
O78	C71	H71B	109.6	C70	C71	H71A	109.5
C70	C71	H71B	109.6	H71A	C71	H71B	108.1
O74	C75	H75A	109.5	O74	C75	H75B	109.5
O74	C75	H75C	109.5	H75A	C75	H75B	109.5
H75A	C75	H75C	109.5	H75B	C75	H75C	109.5
O76	C77	H77A	109.5	O76	C77	H77B	109.5
O76	C77	H77C	109.5	H77A	C77	H77B	109.5
H77A	C77	H77C	109.5	H77B	C77	H77C	109.5
O78	C79	H79A	109.5	O78	C79	H79B	109.5
O78	C79	H79C	109.5	H79A	C79	H79B	109.5
H79A	C79	H79C	109.5	H79B	C79	H79C	109.5
O86	C80	H80	108.3	O87	C80	H80	108.3
C81	C80	H80	108.3	O88	C81	H81	107.7
C80	C81	H81	107.7	C82	C81	H81	107.7
O90	C82	H82	109.2	C81	C82	H82	109.2
C83	C82	H82	109.2	O73	C83	H83	109.3
C82	C83	H83	109.3	C84	C83	H83	109.3
O86	C84	H84	109.2	C83	C84	H84	109.2
C85	C84	H84	109.2	O92	C85	H85A	109.6
O92	C85	H85B	109.6	C84	C85	H85A	109.6
C84	C85	H85B	109.6	H85A	C85	H85B	108.2
O88	C89	H89A	109.5	O88	C89	H89B	109.5
O88	C89	H89C	109.5	H89A	C89	H89B	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H89A	C89	H89C	109.5	H89B	C89	H89C	109.5
O90	C91	H91A	109.5	O90	C91	H91B	109.5
O90	C91	H91C	109.5	H91A	C91	H91B	109.5
H91A	C91	H91C	109.5	H91B	C91	H91C	109.5
O92	C93	H93A	109.5	O92	C93	H93B	109.5
O92	C93	H93C	109.5	H93A	C93	H93B	109.5
H93A	C93	H93C	109.5	H93B	C93	H93C	109.5
O100	C94	H94	109.0	O101	C94	H94	109.0
C95	C94	H94	109.0	O102	C95	H95	108.9
C94	C95	H95	108.9	C96	C95	H95	109.0
O104	C96	H96	110.0	C95	C96	H96	110.0
C97	C96	H96	110.0	O87	C97	H97	109.3
C96	C97	H97	109.3	C98	C97	H97	109.3
O100	C98	H98	108.7	C97	C98	H98	108.7
C99	C98	H98	108.7	O106	C99	H99A	109.7
O106	C99	H99B	109.7	C98	C99	H99A	109.7
C98	C99	H99B	109.7	H99A	C99	H99B	108.2
O102	C103	H10A	109.5	O102	C103	H10B	109.5
O102	C103	H10C	109.5	H10A	C103	H10B	109.5
H10A	C103	H10C	109.5	H10B	C103	H10C	109.5
O104	C105	H10D	109.5	O104	C105	H10E	109.5
O104	C105	H10F	109.5	H10D	C105	H10E	109.5
H10D	C105	H10F	109.5	H10E	C105	H10F	109.5
O106	C107	H10G	109.5	O106	C107	H10H	109.5
O106	C107	H10I	109.5	H10G	C107	H10H	109.5
H10G	C107	H10I	109.5	H10H	C107	H10I	109.5
O114	C108	H108	108.7	O115	C108	H108	108.7
C109	C108	H108	108.7	O116	C109	H109	107.7
C108	C109	H109	107.7	C110	C109	H109	107.7
O118	C110	H110	109.2	C109	C110	H110	109.2
C111	C110	H110	109.2	O101	C111	H111	109.7
C110	C111	H111	109.7	C112	C111	H111	109.7
O114	C112	H112	108.5	C111	C112	H112	108.5
C113	C112	H112	108.5	O120	C113	H11A	109.9
O120	C113	H11B	109.9	C112	C113	H11A	109.9
C112	C113	H11B	109.9	H11A	C113	H11B	108.3
O116	C117	H11C	109.5	O116	C117	H11D	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O116	C117	H11E	109.5	H11C	C117	H11D	109.5
H11C	C117	H11E	109.5	H11D	C117	H11E	109.5
O118	C119	H11F	109.5	O118	C119	H11G	109.5
O118	C119	H11H	109.5	H11F	C119	H11G	109.5
H11F	C119	H11H	109.5	H11G	C119	H11H	109.5
O120	C121	H12A	109.5	O120	C121	H12B	109.5
O120	C121	H12C	109.5	H12A	C121	H12B	109.5
H12A	C121	H12C	109.5	H12B	C121	H12C	109.5
O128	C122	H122	108.3	O129	C122	H122	108.3
C123	C122	H122	108.3	O130	C123	H123	108.0
C122	C123	H123	108.0	C124	C123	H123	108.0
O133	C124	H124	110.0	C123	C124	H124	110.0
C125	C124	H124	110.0	O115	C125	H125	109.6
C124	C125	H125	109.5	C126	C125	H125	109.5
O128	C126	H126	108.8	C125	C126	H126	108.8
C127	C126	H126	108.8	O135	C127	H12D	109.0
O135	C127	H12E	109.0	C126	C127	H12D	109.1
C126	C127	H12E	109.1	H12D	C127	H12E	107.8
O133	C134	H13A	109.5	O133	C134	H13B	109.5
O133	C134	H13C	109.5	H13A	C134	H13B	109.5
H13A	C134	H13C	109.5	H13B	C134	H13C	109.5
O135	C136	H13D	109.5	O135	C136	H13E	109.5
O135	C136	H13F	109.5	H13D	C136	H13E	109.5
H13D	C136	H13F	109.5	H13E	C136	H13F	109.5
O143	C137	H137	109.8	O144	C137	H137	109.8
C138	C137	H137	109.9	O145	C138	H138	107.9
C137	C138	H138	107.9	C139	C138	H138	107.9
O147	C139	H139	108.9	C138	C139	H139	108.9
C140	C139	H139	108.9	O129	C140	H140	109.3
C139	C140	H140	109.2	C141	C140	H140	109.3
O143	C141	H141	108.6	C140	C141	H141	108.6
C142	C141	H141	108.6	O149	C142	H14A	109.8
O149	C142	H14B	109.8	C141	C142	H14A	109.8
C141	C142	H14B	109.8	H14A	C142	H14B	108.2
O145	C146	H14C	109.5	O145	C146	H14D	109.5
O145	C146	H14E	109.5	H14C	C146	H14D	109.5
H14C	C146	H14E	109.5	H14D	C146	H14E	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O147	C148	H14F	109.5	O147	C148	H14G	109.5
O147	C148	H14H	109.5	H14F	C148	H14G	109.5
H14F	C148	H14H	109.5	H14G	C148	H14H	109.5
O149	C150	H15A	109.5	O149	C150	H15B	109.5
O149	C150	H15C	109.5	H15A	C150	H15B	109.5
H15A	C150	H15C	109.5	H15B	C150	H15C	109.5
O157	C151	H151	109.2	O158	C151	H151	109.2
C152	C151	H151	109.2	O159	C152	H152	108.0
C151	C152	H152	108.0	C153	C152	H152	108.0
O161	C153	H153	110.2	C152	C153	H153	110.2
C154	C153	H153	110.2	O243	C154	H154	109.4
C153	C154	H154	109.4	C155	C154	H154	109.4
O157	C155	H155	108.8	C154	C155	H155	108.9
C156	C155	H155	108.9	O163	C156	H15D	109.1
O163	C156	H15E	109.1	C155	C156	H15D	109.1
C155	C156	H15E	109.1	H15D	C156	H15E	107.8
O159	C160	H16A	109.5	O159	C160	H16B	109.5
O159	C160	H16C	109.5	H16A	C160	H16B	109.5
H16A	C160	H16C	109.5	H16B	C160	H16C	109.5
O161	C162	H16D	109.5	O161	C162	H16E	109.5
O161	C162	H16F	109.5	H16D	C162	H16E	109.5
H16D	C162	H16F	109.5	H16E	C162	H16F	109.5
O163	C164	H16G	109.5	O163	C164	H16H	109.5
O163	C164	H16I	109.5	H16G	C164	H16H	109.5
H16G	C164	H16I	109.5	H16H	C164	H16I	109.5
O171	C165	H165	109.1	O172	C165	H165	109.1
C166	C165	H165	109.1	O173	C166	H166	108.8
C165	C166	H166	108.8	C167	C166	H166	108.8
O175	C167	H167	109.1	C166	C167	H167	109.2
C168	C167	H167	109.1	O158	C168	H168	109.2
C167	C168	H168	109.2	C169	C168	H168	109.2
O171	C169	H169	109.2	C168	C169	H169	109.2
C170	C169	H169	109.2	O177	C170	H17A	108.2
O177	C170	H17B	108.3	C169	C170	H17A	108.2
C169	C170	H17B	108.3	H17A	C170	H17B	107.4
O173	C174	H17C	109.5	O173	C174	H17D	109.5
O173	C174	H17E	109.5	H17C	C174	H17D	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H17C	C174	H17E	109.5	H17D	C174	H17E	109.5
O175	C176	H17F	109.5	O175	C176	H17G	109.5
O175	C176	H17H	109.5	H17F	C176	H17G	109.5
H17F	C176	H17H	109.5	H17G	C176	H17H	109.5
O177	C178	H17I	109.5	O177	C178	H17J	109.5
O177	C178	H17K	109.5	H17I	C178	H17J	109.5
H17I	C178	H17K	109.5	H17J	C178	H17K	109.5
O185	C179	H179	108.2	O186	C179	H179	108.2
C180	C179	H179	108.2	O187	C180	H180	108.2
C179	C180	H180	108.2	C181	C180	H180	108.1
O189	C181	H181	110.0	C180	C181	H181	110.0
C182	C181	H181	110.0	O172	C182	H182	110.0
C181	C182	H182	110.0	C183	C182	H182	110.0
O185	C183	H183	108.9	C182	C183	H183	108.9
C184	C183	H183	108.9	O191	C184	H18A	109.8
O191	C184	H18B	109.8	C183	C184	H18A	109.8
C183	C184	H18B	109.8	H18A	C184	H18B	108.2
O187	C188	H18C	109.5	O187	C188	H18D	109.5
O187	C188	H18E	109.5	H18C	C188	H18D	109.5
H18C	C188	H18E	109.5	H18D	C188	H18E	109.5
O189	C190	H19A	109.5	O189	C190	H19B	109.5
O189	C190	H19C	109.5	H19A	C190	H19B	109.5
H19A	C190	H19C	109.5	H19B	C190	H19C	109.5
O191	C192	H19D	109.5	O191	C192	H19E	109.5
O191	C192	H19F	109.5	H19D	C192	H19E	109.5
H19D	C192	H19F	109.5	H19E	C192	H19F	109.5
O199	C193	H193	109.6	O200	C193	H193	109.6
C194	C193	H193	109.6	O201	C194	H194	108.8
C193	C194	H194	108.8	C195	C194	H194	108.8
O203	C195	H195	109.4	C194	C195	H195	109.4
C196	C195	H195	109.4	O186	C196	H196	109.0
C195	C196	H196	109.0	C197	C196	H196	109.0
O199	C197	H197	109.1	C196	C197	H197	109.1
C198	C197	H197	109.1	O206	C198	H19G	110.0
O206	C198	H19H	110.0	C197	C198	H19G	110.0
C197	C198	H19H	110.0	H19G	C198	H19H	108.4
O201	C202	H20A	109.5	O201	C202	H20B	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O201	C202	H20C	109.5	H20A	C202	H20B	109.5
H20A	C202	H20C	109.5	H20B	C202	H20C	109.5
O206	C207	H20D	109.5	O206	C207	H20E	109.5
O206	C207	H20F	109.5	H20D	C207	H20E	109.5
H20D	C207	H20F	109.5	H20E	C207	H20F	109.5
O214	C208	H208	108.3	O215	C208	H208	108.3
C209	C208	H208	108.3	O216	C209	H209	108.5
C208	C209	H209	108.5	C210	C209	H209	108.5
O218	C210	H210	110.4	C209	C210	H210	110.4
C211	C210	H210	110.4	O200	C211	H211	109.5
C210	C211	H211	109.5	C212	C211	H211	109.5
O214	C212	H212	108.4	C211	C212	H212	108.4
C213	C212	H212	108.4	O220	C213	H21A	109.9
O220	C213	H21B	109.9	C212	C213	H21A	109.9
C212	C213	H21B	109.9	H21A	C213	H21B	108.3
O216	C217	H21C	109.5	O216	C217	H21D	109.5
O216	C217	H21E	109.5	H21C	C217	H21D	109.5
H21C	C217	H21E	109.5	H21D	C217	H21E	109.5
O218	C219	H21F	109.5	O218	C219	H21G	109.5
O218	C219	H21H	109.5	H21F	C219	H21G	109.5
H21F	C219	H21H	109.5	H21G	C219	H21H	109.5
O220	C221	H22A	109.5	O220	C221	H22B	109.5
O220	C221	H22C	109.5	H22A	C221	H22B	109.5
H22A	C221	H22C	109.5	H22B	C221	H22C	109.5
O228	C222	H222	109.0	O229	C222	H222	109.0
C223	C222	H222	109.0	O230	C223	H223	108.0
C222	C223	H223	108.0	C224	C223	H223	108.0
O232	C224	H224	109.5	C223	C224	H224	109.5
C225	C224	H224	109.5	O215	C225	H225	109.2
C224	C225	H225	109.2	C226	C225	H225	109.2
O228	C226	H226	109.7	C225	C226	H226	109.7
C227	C226	H226	109.8	O234	C227	H22D	110.1
O234	C227	H22E	110.1	C226	C227	H22D	110.1
C226	C227	H22E	110.1	H22D	C227	H22E	108.4
O230	C231	H23A	109.5	O230	C231	H23B	109.5
O230	C231	H23C	109.5	H23A	C231	H23B	109.5
H23A	C231	H23C	109.5	H23B	C231	H23C	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O232	C233	H23D	109.5	O232	C233	H23E	109.5
O232	C233	H23F	109.5	H23D	C233	H23E	109.5
H23D	C233	H23F	109.5	H23E	C233	H23F	109.5
O234	C235	H23G	109.5	O234	C235	H23H	109.5
O234	C235	H23I	109.5	H23G	C235	H23H	109.5
H23G	C235	H23I	109.5	H23H	C235	H23I	109.5
O242	C236	H236	108.5	O243	C236	H236	108.5
C237	C236	H236	108.5	O244	C237	H237	107.9
C236	C237	H237	107.9	C238	C237	H237	107.9
O246	C238	H238	109.6	C237	C238	H238	109.6
C239	C238	H238	109.6	O229	C239	H239	109.6
C238	C239	H239	109.6	C240	C239	H239	109.6
O242	C240	H240	108.5	C239	C240	H240	108.5
C241	C240	H240	108.5	O248	C241	H24A	110.0
O248	C241	H24B	110.0	C240	C241	H24A	110.0
C240	C241	H24B	110.0	H24A	C241	H24B	108.3
O244	C245	H24C	109.5	O244	C245	H24D	109.5
O244	C245	H24E	109.5	H24C	C245	H24D	109.5
H24C	C245	H24E	109.5	H24D	C245	H24E	109.5
O246	C247	H24F	109.5	O246	C247	H24G	109.5
O246	C247	H24H	109.5	H24F	C247	H24G	109.5
H24F	C247	H24H	109.5	H24G	C247	H24H	109.5
O248	C249	H24I	109.5	O248	C249	H24J	109.5
O248	C249	H24K	109.5	H24I	C249	H24J	109.5
H24I	C249	H24K	109.5	H24J	C249	H24K	109.5

Table 9. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O10	Al1	N2	C12	-83.9(5)	O10	Al1	N2	C15	86.3(5)
O10	Al1	N3	C17	-91.5(5)	O10	Al1	N3	C20	90.2(5)
O10	Al1	N4	C22	-89.6(5)	O10	Al1	N4	C25	81.8(5)
O10	Al1	N5	C27	-83.8(5)	O10	Al1	N5	C30	88.1(5)
O11	Al1	N2	C12	94.1(5)	O11	Al1	N2	C15	-95.6(5)
O11	Al1	N3	C17	91.6(5)	O11	Al1	N3	C20	-86.7(5)
O11	Al1	N4	C22	92.5(5)	O11	Al1	N4	C25	-96.2(5)
O11	Al1	N5	C27	93.0(5)	O11	Al1	N5	C30	-95.1(5)
N2	Al1	N3	C17	4.5(5)	N2	Al1	N3	C20	-173.9(5)
N3	Al1	N2	C12	179.9(4)	N3	Al1	N2	C15	-9.8(5)
N2	Al1	N5	C27	-179.9(5)	N2	Al1	N5	C30	-8.0(5)
N5	Al1	N2	C12	12.7(5)	N5	Al1	N2	C15	-177.0(5)
N3	Al1	N4	C22	6.7(5)	N3	Al1	N4	C25	178.0(4)
N4	Al1	N3	C17	176.7(5)	N4	Al1	N3	C20	-1.7(5)
N4	Al1	N5	C27	8.0(5)	N4	Al1	N5	C30	180.0(5)
N5	Al1	N4	C22	173.8(5)	N5	Al1	N4	C25	-14.8(5)
C52	O58	C56	C55	62.0(8)	C52	O58	C56	C57	-172.5(6)
C56	O58	C52	O59	59.2(9)	C56	O58	C52	C53	-63.8(7)
C52	O59	C69	C68	141.2(5)	C52	O59	C69	C70	-97.4(6)
C69	O59	C52	O58	110.6(6)	C69	O59	C52	C53	-127.6(6)
C61	O60	C53	C52	146.7(7)	C61	O60	C53	C54	-91.9(9)
C63	O62	C54	C53	-128.0(6)	C63	O62	C54	C55	111.5(6)
C65	O64	C57	C56	92.0(7)	C66	O72	C70	C69	61.6(6)
C66	O72	C70	C71	-171.4(5)	C70	O72	C66	O73	60.7(7)
C70	O72	C66	C67	-60.0(7)	C66	O73	C83	C82	112.7(5)
C66	O73	C83	C84	-125.3(5)	C83	O73	C66	O72	94.4(7)
C83	O73	C66	C67	-144.3(5)	C75	O74	C67	C66	105.0(8)
C75	O74	C67	C68	-131.2(8)	C77	O76	C68	C67	-139.4(6)
C77	O76	C68	C69	102.8(7)	C79	O78	C71	C70	178.1(7)
C80	O86	C84	C83	61.0(6)	C80	O86	C84	C85	-176.4(5)
C84	O86	C80	O87	60.9(7)	C84	O86	C80	C81	-61.4(7)
C80	O87	C97	C96	127.5(5)	C80	O87	C97	C98	-110.4(6)
C97	O87	C80	O86	95.3(7)	C97	O87	C80	C81	-142.6(5)
C89	O88	C81	C80	79.3(8)	C89	O88	C81	C82	-155.7(6)
C91	O90	C82	C81	-95.4(6)	C91	O90	C82	C83	142.2(6)
C93	O92	C85	C84	-178.3(7)	C94	O100	C98	C97	58.1(7)
C94	O100	C98	C99	-178.5(6)	C98	O100	C94	O101	57.1(8)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C98	O100	C94	C95	-64.6(7)
C94	O101	C111	C112	-89.3(7)
C111	O101	C94	C95	-118.4(6)
C103	O102	C95	C96	-158.5(7)
C105	O104	C96	C97	140.2(5)
C108	O114	C112	C111	61.8(7)
C112	O114	C108	O115	62.1(8)
C108	O115	C125	C124	124.7(5)
C125	O115	C108	O114	100.4(6)
C117	O116	C109	C108	78.2(8)
C119	O118	C110	C109	-125.1(10)
C121	O120	C113	C112	-177.6(7)
C122	O128	C126	C127	-179.0(5)
C126	O128	C122	C123	-58.0(8)
C122	O129	C140	C141	-127.8(6)
C140	O129	C122	C123	-147.9(6)
C131	O130	C123	C122	120.5(13)
C123	O130	C132	C131	131.1(16)
C132	O130	C123	C124	-142.8(10)
C132	O130	C131	C132	0(2)
C134	O133	C124	C125	138.1(8)
C137	O143	C141	C140	59.4(8)
C141	O143	C137	O144	53.8(7)
C55	O144	C137	O143	105.9(6)
C137	O144	C55	C54	152.8(5)
C146	O145	C138	C137	72.2(8)
C148	O147	C139	C138	-100.0(7)
C150	O149	C142	C141	179.6(6)
C151	O157	C155	C156	-178.9(4)
C155	O157	C151	C152	-60.9(7)
C151	O158	C168	C169	-122.9(6)
C168	O158	C151	C152	-149.7(5)
C160	O159	C152	C153	-155.0(5)
C162	O161	C153	C154	138.0(7)
C165	O171	C169	C168	54.9(7)
C169	O171	C165	O172	57.4(7)
C165	O172	C182	C181	147.0(6)
C94	O101	C111	C110	150.8(5)
C111	O101	C94	O100	121.8(6)
C103	O102	C95	C94	79.8(9)
C105	O104	C96	C95	-100.5(6)
C107	O106	C99	C98	-170.7(6)
C108	O114	C112	C113	-173.8(5)
C112	O114	C108	C109	-60.1(7)
C108	O115	C125	C126	-114.5(5)
C125	O115	C108	C109	-138.1(5)
C117	O116	C109	C110	-156.5(7)
C119	O118	C110	C111	113.8(10)
C122	O128	C126	C125	57.1(8)
C126	O128	C122	O129	63.9(7)
C122	O129	C140	C139	110.5(6)
C140	O129	C122	O128	89.6(8)
C123	O130	C131	C132	-60(3)
C131	O130	C123	C124	-115.5(13)
C132	O130	C123	C122	93.3(11)
C131	O130	C132	C131	-0(2)
C134	O133	C124	C123	-102.9(9)
C136	O135	C127	C126	100.7(11)
C137	O143	C141	C142	-177.0(6)
C141	O143	C137	C138	-64.3(7)
C55	O144	C137	C138	-135.5(5)
C137	O144	C55	C56	-86.6(7)
C146	O145	C138	C139	-164.2(7)
C148	O147	C139	C140	138.2(6)
C151	O157	C155	C154	58.1(6)
C155	O157	C151	O158	59.2(6)
C151	O158	C168	C167	114.5(6)
C168	O158	C151	O157	90.7(7)
C160	O159	C152	C151	80.8(7)
C162	O161	C153	C152	-103.0(7)
C164	O163	C156	C155	93.6(9)
C165	O171	C169	C170	175.9(6)
C169	O171	C165	C166	-63.8(7)
C165	O172	C182	C183	-93.3(7)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C182	O172	C165	O171	122.4(6)
C174	O173	C166	C165	68.7(8)
C176	O175	C167	C166	-98.8(6)
C178	O177	C170	C169	-71.8(7)
C179	O185	C183	C184	-171.0(6)
C183	O185	C179	C180	-61.4(8)
C179	O186	C196	C197	-94.4(6)
C196	O186	C179	C180	-128.6(5)
C188	O187	C180	C181	-168.8(7)
C190	O189	C181	C182	124.6(6)
C193	O199	C197	C196	55.9(7)
C197	O199	C193	O200	57.5(8)
C193	O200	C211	C210	111.3(5)
C211	O200	C193	O199	97.4(7)
C202	O201	C194	C193	95.1(10)
C195	O203	C204	C205	99.5(8)
C204	O203	C195	C196	98.8(9)
C205	O203	C195	C194	-101.6(15)
C204	O203	C205	C204	0.0(9)
C207	O206	C198	C197	-179.7(8)
C208	O214	C212	C213	176.2(5)
C212	O214	C208	C209	-59.9(7)
C208	O215	C225	C226	-114.7(6)
C225	O215	C208	C209	-138.1(6)
C217	O216	C209	C210	-163.1(8)
C219	O218	C210	C211	141.0(6)
C222	O228	C226	C225	62.0(7)
C226	O228	C222	O229	55.9(8)
C222	O229	C239	C238	156.9(5)
C239	O229	C222	O228	116.0(6)
C231	O230	C223	C222	69.7(9)
C233	O232	C224	C223	-101.4(6)
C235	O234	C227	C226	165.8(6)
C236	O242	C240	C241	-172.8(5)
C240	O242	C236	C237	-59.9(6)
C154	O243	C236	C237	-140.0(4)
C236	O243	C154	C155	-113.6(5)

atom1	atom2	atom3	atom4	angle
C182	O172	C165	C166	-118.0(6)
C174	O173	C166	C167	-170.3(6)
C176	O175	C167	C168	140.3(5)
C179	O185	C183	C182	64.7(8)
C183	O185	C179	O186	62.2(8)
C179	O186	C196	C195	143.6(5)
C196	O186	C179	O185	109.1(6)
C188	O187	C180	C179	67.1(9)
C190	O189	C181	C180	-115.7(6)
C192	O191	C184	C183	169.0(9)
C193	O199	C197	C198	178.6(5)
C197	O199	C193	C194	-61.7(7)
C193	O200	C211	C212	-127.2(5)
C211	O200	C193	C194	-144.0(5)
C202	O201	C194	C195	-143.9(10)
C204	O203	C195	C194	-142.4(8)
C195	O203	C205	C204	-96.9(17)
C205	O203	C195	C196	139.6(15)
C205	O203	C204	C205	-0.0(19)
C208	O214	C212	C211	52.0(7)
C212	O214	C208	O215	62.8(8)
C208	O215	C225	C224	123.4(6)
C225	O215	C208	O214	100.1(7)
C217	O216	C209	C208	75.1(9)
C219	O218	C210	C209	-101.5(6)
C221	O220	C213	C212	178.2(8)
C222	O228	C226	C227	-176.8(6)
C226	O228	C222	C223	-65.1(7)
C222	O229	C239	C240	-83.2(7)
C239	O229	C222	C223	-123.4(5)
C231	O230	C223	C224	-166.9(7)
C233	O232	C224	C225	138.8(5)
C236	O242	C240	C239	62.7(7)
C240	O242	C236	O243	62.3(7)
C154	O243	C236	O242	98.2(6)
C236	O243	C154	C153	124.9(4)
C245	O244	C237	C236	106.6(9)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C245	O244	C237	C238	-128.9(8)	C247	O246	C238	C237	-135.5(6)
C247	O246	C238	C239	103.7(6)	C249	O248	C241	C240	-172.6(7)
Al1	N2	C12	C13	170.5(4)	Al1	N2	C12	C31	-12.6(9)
Al1	N2	C15	C14	-170.1(4)	Al1	N2	C15	C16	10.9(10)
C12	N2	C15	C14	1.8(7)	C12	N2	C15	C16	-177.3(6)
C15	N2	C12	C13	-1.5(7)	C15	N2	C12	C31	175.4(6)
Al1	N3	C17	C16	0.5(10)	Al1	N3	C17	C18	-178.5(4)
Al1	N3	C20	C19	178.2(4)	Al1	N3	C20	C21	-2.4(9)
C17	N3	C20	C19	-0.5(7)	C17	N3	C20	C21	178.9(6)
C20	N3	C17	C16	179.2(6)	C20	N3	C17	C18	0.1(7)
Al1	N4	C22	C21	-8.3(9)	Al1	N4	C22	C23	170.9(4)
Al1	N4	C25	C24	-170.7(4)	Al1	N4	C25	C26	13.7(9)
C22	N4	C25	C24	2.2(7)	C22	N4	C25	C26	-173.4(6)
C25	N4	C22	C21	178.9(6)	C25	N4	C22	C23	-1.9(7)
Al1	N5	C27	C26	0.8(9)	Al1	N5	C27	C28	175.0(4)
Al1	N5	C30	C29	-175.3(4)	Al1	N5	C30	C31	2.1(9)
C27	N5	C30	C29	-1.9(7)	C27	N5	C30	C31	175.5(6)
C30	N5	C27	C26	-172.6(6)	C30	N5	C27	C28	1.5(7)
C34	N6	C35	C36	-0.7(9)	C35	N6	C34	C33	-0.1(9)
C39	N7	C40	C41	2.5(14)	C40	N7	C39	C38	-3.1(15)
C44	N8	C45	C46	0.5(8)	C45	N8	C44	C43	1.2(8)
C49	N9	C50	C51	1.8(14)	C50	N9	C49	C48	-2.5(15)
N2	C12	C13	C14	0.7(7)	N2	C12	C31	C30	2.7(10)
N2	C12	C31	C47	-178.5(5)	C13	C12	C31	C30	179.2(6)
C13	C12	C31	C47	-2.0(10)	C31	C12	C13	C14	-176.3(6)
C12	C13	C14	C15	0.4(8)	C13	C14	C15	N2	-1.4(8)
C13	C14	C15	C16	177.6(6)	N2	C15	C16	C17	-3.1(11)
N2	C15	C16	C32	175.7(6)	C14	C15	C16	C17	178.0(6)
C14	C15	C16	C32	-3.2(10)	C15	C16	C17	N3	-2.9(11)
C15	C16	C17	C18	176.0(6)	C15	C16	C32	C33	-70.8(8)
C15	C16	C32	C36	109.5(7)	C17	C16	C32	C33	108.0(6)
C17	C16	C32	C36	-71.7(8)	C32	C16	C17	N3	178.4(6)
C32	C16	C17	C18	-2.7(10)	N3	C17	C18	C19	0.3(8)
C16	C17	C18	C19	-178.8(6)	C17	C18	C19	C20	-0.6(8)
C18	C19	C20	N3	0.7(8)	C18	C19	C20	C21	-178.7(6)
N3	C20	C21	C22	3.0(11)	N3	C20	C21	C37	-179.1(6)
C19	C20	C21	C22	-177.7(6)	C19	C20	C21	C37	0.3(10)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C20	C21	C22	N4	2.6(11)	C20	C21	C22	C23	-176.4(6)
C20	C21	C37	C38	-109.3(8)	C20	C21	C37	C41	71.5(9)
C22	C21	C37	C38	68.8(9)	C22	C21	C37	C41	-110.4(8)
C37	C21	C22	N4	-175.4(6)	C37	C21	C22	C23	5.6(10)
N4	C22	C23	C24	0.9(7)	C21	C22	C23	C24	-179.9(6)
C22	C23	C24	C25	0.4(7)	C23	C24	C25	N4	-1.7(7)
C23	C24	C25	C26	173.9(6)	N4	C25	C26	C27	-0.2(10)
N4	C25	C26	C42	179.7(5)	C24	C25	C26	C27	-175.1(6)
C24	C25	C26	C42	4.7(9)	C25	C26	C27	N5	-7.4(10)
C25	C26	C27	C28	179.3(6)	C25	C26	C42	C43	64.3(7)
C25	C26	C42	C46	-115.5(6)	C27	C26	C42	C43	-115.9(6)
C27	C26	C42	C46	64.4(8)	C42	C26	C27	N5	172.7(5)
C42	C26	C27	C28	-0.6(9)	N5	C27	C28	C29	-0.7(7)
C26	C27	C28	C29	173.5(6)	C27	C28	C29	C30	-0.5(8)
C28	C29	C30	N5	1.5(8)	C28	C29	C30	C31	-175.9(6)
N5	C30	C31	C12	2.9(10)	N5	C30	C31	C47	-175.9(5)
C29	C30	C31	C12	179.9(6)	C29	C30	C31	C47	1.1(10)
C12	C31	C47	C48	-80.0(9)	C12	C31	C47	C51	101.4(8)
C30	C31	C47	C48	98.9(8)	C30	C31	C47	C51	-79.7(9)
C16	C32	C33	C34	179.0(5)	C16	C32	C36	C35	-179.7(5)
C33	C32	C36	C35	0.6(8)	C36	C32	C33	C34	-1.3(8)
C32	C33	C34	N6	1.1(9)	N6	C35	C36	C32	0.4(10)
C21	C37	C38	C39	-176.4(7)	C21	C37	C41	C40	175.8(7)
C38	C37	C41	C40	-3.4(12)	C41	C37	C38	C39	2.9(13)
C37	C38	C39	N7	0.5(17)	N7	C40	C41	C37	0.8(15)
C26	C42	C43	C44	-178.7(4)	C26	C42	C46	C45	-179.8(4)
C43	C42	C46	C45	0.5(7)	C46	C42	C43	C44	1.1(7)
C42	C43	C44	N8	-2.1(9)	N8	C45	C46	C42	-1.3(9)
C31	C47	C48	C49	-176.1(7)	C31	C47	C51	C50	175.5(7)
C48	C47	C51	C50	-3.1(13)	C51	C47	C48	C49	2.5(13)
C47	C48	C49	N9	0.3(15)	N9	C50	C51	C47	1.0(15)
O58	C52	C53	O60	-176.7(5)	O58	C52	C53	C54	58.9(7)
O59	C52	C53	O60	59.8(8)	O59	C52	C53	C54	-64.6(8)
O60	C53	C54	O62	64.7(9)	O60	C53	C54	C55	-174.3(7)
C52	C53	C54	O62	-176.0(5)	C52	C53	C54	C55	-55.1(8)
O62	C54	C55	O144	-65.2(7)	O62	C54	C55	C56	173.0(5)
C53	C54	C55	O144	175.2(6)	C53	C54	C55	C56	53.3(8)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O144	C55	C56	O58	-173.8(5)	O144	C55	C56	C57	65.5(7)
C54	C55	C56	O58	-55.3(7)	C54	C55	C56	C57	-176.1(5)
O58	C56	C57	O64	-76.5(8)	C55	C56	C57	O64	45.2(8)
O72	C66	C67	O74	-179.9(5)	O72	C66	C67	C68	57.6(7)
O73	C66	C67	O74	58.1(8)	O73	C66	C67	C68	-64.4(7)
O74	C67	C68	O76	59.0(7)	O74	C67	C68	C69	-180.0(5)
C66	C67	C68	O76	-177.2(5)	C66	C67	C68	C69	-56.2(7)
O76	C68	C69	O59	-61.8(7)	O76	C68	C69	C70	176.3(6)
C67	C68	C69	O59	179.5(5)	C67	C68	C69	C70	57.5(7)
O59	C69	C70	O72	178.9(4)	O59	C69	C70	C71	57.7(7)
C68	C69	C70	O72	-60.4(7)	C68	C69	C70	C71	178.3(6)
O72	C70	C71	O78	-68.5(8)	C69	C70	C71	O78	53.7(9)
O86	C80	C81	O88	175.6(6)	O86	C80	C81	C82	52.9(7)
O87	C80	C81	O88	51.4(8)	O87	C80	C81	C82	-71.4(6)
O88	C81	C82	O90	68.8(6)	O88	C81	C82	C83	-172.2(5)
C80	C81	C82	O90	-165.5(4)	C80	C81	C82	C83	-46.5(7)
O90	C82	C83	O73	-74.1(7)	O90	C82	C83	C84	166.0(5)
C81	C82	C83	O73	165.6(5)	C81	C82	C83	C84	45.8(8)
O73	C83	C84	O86	-170.2(4)	O73	C83	C84	C85	71.5(6)
C82	C83	C84	O86	-50.9(7)	C82	C83	C84	C85	-169.2(6)
O86	C84	C85	O92	-63.8(7)	C83	C84	C85	O92	57.0(8)
O100	C94	C95	O102	-177.2(5)	O100	C94	C95	C96	62.7(6)
O101	C94	C95	O102	60.9(7)	O101	C94	C95	C96	-59.2(6)
O102	C95	C96	O104	66.2(7)	O102	C95	C96	C97	-176.4(6)
C94	C95	C96	O104	-171.9(4)	C94	C95	C96	C97	-54.5(7)
O104	C96	C97	O87	-73.1(7)	O104	C96	C97	C98	166.9(5)
C95	C96	C97	O87	167.2(6)	C95	C96	C97	C98	47.2(8)
O87	C97	C98	O100	-167.0(4)	O87	C97	C98	C99	73.4(6)
C96	C97	C98	O100	-47.9(7)	C96	C97	C98	C99	-167.4(5)
O100	C98	C99	O106	-73.3(7)	C97	C98	C99	O106	49.0(8)
O114	C108	C109	O116	177.2(5)	O114	C108	C109	C110	54.2(7)
O115	C108	C109	O116	55.1(7)	O115	C108	C109	C110	-68.0(7)
O116	C109	C110	O118	62.9(7)	O116	C109	C110	C111	-175.9(5)
C108	C109	C110	O118	-171.9(6)	C108	C109	C110	C111	-50.7(8)
O118	C110	C111	O101	-69.9(7)	O118	C110	C111	C112	169.8(5)
C109	C110	C111	O101	170.4(6)	C109	C110	C111	C112	50.1(7)
O101	C111	C112	O114	-173.4(5)	O101	C111	C112	C113	66.4(7)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C110	C111	C112	O114	-55.5(7)
O114	C112	C113	O120	-67.7(8)
O128	C122	C123	O130	178.9(7)
O129	C122	C123	O130	54.8(9)
O130	C123	C124	O133	63.3(8)
C122	C123	C124	O133	-172.6(6)
O133	C124	C125	O115	-69.3(7)
C123	C124	C125	O115	172.1(5)
O115	C125	C126	O128	-172.6(5)
C124	C125	C126	O128	-53.3(9)
O128	C126	C127	O135	-68.1(8)
O130	C131	C132	O130	-0.0(3)
O143	C137	C138	C139	60.3(7)
O144	C137	C138	C139	-60.1(7)
O145	C138	C139	C140	-178.2(6)
C137	C138	C139	C140	-53.0(8)
O147	C139	C140	C141	169.7(5)
C138	C139	C140	C141	47.6(8)
O129	C140	C141	C142	71.0(7)
C139	C140	C141	C142	-169.1(6)
C140	C141	C142	O149	-156.9(6)
O157	C151	C152	C153	58.2(7)
O158	C151	C152	C153	-64.1(7)
O159	C152	C153	C154	-178.1(4)
C151	C152	C153	C154	-53.7(7)
O161	C153	C154	C155	167.1(5)
C152	C153	C154	C155	49.0(7)
O243	C154	C155	C156	71.1(7)
C153	C154	C155	C156	-169.5(6)
C154	C155	C156	O163	52.3(9)
O171	C165	C166	C167	63.4(6)
O172	C165	C166	C167	-58.6(7)
O173	C166	C167	C168	-179.0(5)
C165	C166	C167	C168	-55.3(7)
O175	C167	C168	C169	168.1(4)
C166	C167	C168	C169	46.4(8)
O158	C168	C169	C170	77.4(6)

atom1	atom2	atom3	atom4	angle
C110	C111	C112	C113	-175.7(5)
C111	C112	C113	O120	55.0(8)
O128	C122	C123	C124	56.2(9)
O129	C122	C123	C124	-67.9(9)
O130	C123	C124	C125	-178.4(5)
C122	C123	C124	C125	-54.4(8)
O133	C124	C125	C126	171.5(6)
C123	C124	C125	C126	52.8(8)
O115	C125	C126	C127	68.6(8)
C124	C125	C126	C127	-172.0(7)
C125	C126	C127	O135	53.7(11)
O143	C137	C138	O145	-176.6(5)
O144	C137	C138	O145	63.0(7)
O145	C138	C139	O147	61.6(8)
C137	C138	C139	O147	-173.1(5)
O147	C139	C140	O129	-70.4(7)
C138	C139	C140	O129	167.6(6)
O129	C140	C141	O143	-169.0(5)
C139	C140	C141	O143	-49.2(8)
O143	C141	C142	O149	80.6(8)
O157	C151	C152	O159	-179.6(6)
O158	C151	C152	O159	58.1(8)
O159	C152	C153	O161	64.5(6)
C151	C152	C153	O161	-171.1(5)
O161	C153	C154	O243	-73.3(6)
C152	C153	C154	O243	168.5(5)
O243	C154	C155	O157	-170.0(5)
C153	C154	C155	O157	-50.6(8)
O157	C155	C156	O163	-69.9(7)
O171	C165	C166	O173	-176.5(5)
O172	C165	C166	O173	61.6(7)
O173	C166	C167	O175	61.5(7)
C165	C166	C167	O175	-174.9(5)
O175	C167	C168	O158	-72.5(6)
C166	C167	C168	O158	165.7(6)
O158	C168	C169	O171	-164.0(4)
C167	C168	C169	O171	-44.5(7)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C167	C168	C169	C170	-163.1(5)
C168	C169	C170	O177	-145.2(6)
O185	C179	C180	C181	52.9(8)
O186	C179	C180	C181	-70.9(7)
O187	C180	C181	C182	-173.8(6)
C179	C180	C181	C182	-48.9(9)
O189	C181	C182	C183	168.9(5)
C180	C181	C182	C183	51.1(8)
O172	C182	C183	C184	67.1(7)
C181	C182	C183	C184	-175.9(6)
C182	C183	C184	O191	55.0(8)
O199	C193	C194	C195	63.4(7)
O200	C193	C194	C195	-57.7(7)
O201	C194	C195	C196	176.2(5)
C193	C194	C195	C196	-61.0(7)
O203	C195	C196	C197	175.8(5)
C194	C195	C196	C197	55.2(7)
O186	C196	C197	C198	69.6(7)
C195	C196	C197	C198	-170.4(6)
C196	C197	C198	O206	-169.2(6)
O214	C208	C209	O216	-175.0(6)
O215	C208	C209	O216	61.2(9)
O216	C209	C210	O218	60.4(7)
C208	C209	C210	O218	-176.0(4)
O218	C210	C211	O200	-71.5(7)
C209	C210	C211	O200	169.5(6)
O200	C211	C212	O214	-166.0(4)
C210	C211	C212	O214	-46.8(7)
O214	C212	C213	O220	-58.6(7)
O228	C222	C223	O230	-177.7(5)
O229	C222	C223	O230	60.4(7)
O230	C223	C224	O232	63.7(7)
C222	C223	C224	O232	-171.6(4)
O232	C224	C225	O215	-67.6(7)
C223	C224	C225	O215	171.4(6)
O215	C225	C226	O228	-172.5(4)
C224	C225	C226	O228	-53.6(7)
O171	C169	C170	O177	92.6(7)
O185	C179	C180	O187	173.3(6)
O186	C179	C180	O187	49.4(8)
O187	C180	C181	O189	67.5(8)
C179	C180	C181	O189	-167.6(5)
O189	C181	C182	O172	-71.6(7)
C180	C181	C182	O172	170.6(6)
O172	C182	C183	O185	-174.0(5)
C181	C182	C183	O185	-57.1(7)
O185	C183	C184	O191	-65.4(8)
O199	C193	C194	O201	-175.5(6)
O200	C193	C194	O201	63.4(8)
O201	C194	C195	O203	55.3(8)
C193	C194	C195	O203	178.1(5)
O203	C195	C196	O186	-63.0(7)
C194	C195	C196	O186	176.4(5)
O186	C196	C197	O199	-171.7(5)
C195	C196	C197	O199	-51.8(8)
O199	C197	C198	O206	69.8(7)
O203	C204	C205	O203	-0.0(3)
O214	C208	C209	C210	63.6(6)
O215	C208	C209	C210	-60.3(7)
O216	C209	C210	C211	177.2(6)
C208	C209	C210	C211	-59.2(7)
O218	C210	C211	C212	169.8(5)
C209	C210	C211	C212	50.8(8)
O200	C211	C212	C213	74.6(6)
C210	C211	C212	C213	-166.1(6)
C211	C212	C213	O220	65.1(8)
O228	C222	C223	C224	59.7(6)
O229	C222	C223	C224	-62.1(6)
O230	C223	C224	C225	-177.4(6)
C222	C223	C224	C225	-52.7(7)
O232	C224	C225	C226	171.7(5)
C223	C224	C225	C226	50.7(8)
O215	C225	C226	C227	69.9(6)
C224	C225	C226	C227	-171.2(5)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
O228	C226	C227	O234	55.1(8)
O242	C236	C237	O244	175.3(5)
O243	C236	C237	O244	52.3(7)
O244	C237	C238	O246	65.2(7)
C236	C237	C238	O246	-170.7(5)
O246	C238	C239	O229	-68.4(6)
C237	C238	C239	O229	173.6(5)
O229	C239	C240	O242	-174.7(5)
C238	C239	C240	O242	-56.9(7)
O242	C240	C241	O248	-71.8(7)
C225	C226	C227	O234	173.9(6)
O242	C236	C237	C238	52.3(7)
O243	C236	C237	C238	-70.6(7)
O244	C237	C238	C239	-174.8(5)
C236	C237	C238	C239	-50.7(8)
O246	C238	C239	C240	170.3(5)
C237	C238	C239	C240	52.2(7)
O229	C239	C240	C241	64.6(7)
C238	C239	C240	C241	-177.6(5)
C239	C240	C241	O248	49.8(8)

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Al1	C16	3.443(9)	Al1	C21	3.445(5)
Al1	C26	3.410(8)	Al1	C31	3.439(5)
O10	C25	3.511(9)	O11	C20	3.597(10)
O11	C27	3.522(12)	O11	C30	3.558(10)
O58	O60	3.559(6)	O58	O64	3.007(8)
O58	O78	3.261(9)	O58	C54	2.822(8)
O58	C65	3.149(9)	O58	C69	3.340(10)
O58	C71	3.167(11)	O59	O60	2.739(9)
O59	O76	2.857(6)	O59	O78	3.434(6)
O59	C54	2.924(11)	O59	C55	3.454(10)
O59	C56	2.815(9)	O59	C71	3.004(8)
O59	C77	3.185(8)	O60	O62	2.932(11)
O60	O76	3.215(10)	O60	C69	3.491(12)
O60	C77	3.240(12)	O62	O144	2.826(7)
O62	C61	3.134(12)	O64	O143	3.325(7)
O64	O144	3.460(6)	O64	C55	2.916(7)
O64	C137	3.207(8)	O72	O78	2.850(7)
O72	O92	3.562(8)	O72	C68	2.880(8)
O72	C83	3.216(9)	O72	C85	3.451(9)
O73	O74	2.812(6)	O73	O90	2.888(7)
O73	C68	2.929(10)	O73	C69	3.462(10)
O73	C70	2.823(9)	O73	C85	3.038(7)
O74	O76	2.774(9)	O74	O90	3.316(8)
O74	C91	3.282(10)	O76	C75	3.543(17)
O78	C52	3.283(10)	O78	C69	2.934(7)
O86	O92	2.792(7)	O86	O106	3.331(7)
O86	C82	2.860(7)	O86	C97	3.227(8)
O86	C99	3.208(9)	O86	C107	3.518(10)
O87	O88	2.815(7)	O87	O104	2.872(7)
O87	O106	3.519(6)	O87	C82	3.044(8)
O87	C83	3.524(8)	O87	C84	2.882(8)
O87	C99	3.059(8)	O88	O90	2.862(7)
O88	O104	3.411(7)	O88	C91	3.069(9)
O88	C105	3.484(10)	O90	C66	3.376(9)
O92	C83	2.905(6)	O100	O106	2.897(7)
O100	C96	2.868(8)	O100	C111	3.433(8)
O100	C113	3.352(10)	O101	O102	2.875(9)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
O101	O118	2.870(5)	O101	O120	3.535(7)
O101	C96	2.897(10)	O101	C97	3.391(9)
O101	C98	2.801(8)	O101	C113	3.044(9)
O101	C119	3.347(10)	O102	O104	2.860(8)
O102	O118	3.434(9)	O102	C105	3.138(11)
O102	C111	3.508(11)	O104	C80	3.570(8)
O104	C89	3.329(11)	O106	C80	3.579(8)
O106	C97	2.828(6)	O114	O120	2.831(8)
O114	O135	3.377(10)	O114	C110	2.868(8)
O114	C125	3.247(10)	O114	C127	3.267(12)
O115	O116	2.839(6)	O115	O133	2.867(7)
O115	O135	3.561(9)	O115	C110	3.022(10)
O115	C111	3.515(11)	O115	C112	2.826(9)
O115	C127	3.021(9)	O116	O118	2.793(9)
O116	O133	3.234(10)	O116	C119	3.45(2)
O116	C134	3.348(15)	O120	C94	3.362(10)
O120	C111	2.900(8)	O128	O135	2.855(10)
O128	C124	2.870(8)	O128	C136	3.075(16)
O128	C140	3.156(10)	O128	C142	3.468(9)
O129	O130	2.791(6)	O129	O147	2.882(9)
O129	C124	2.970(9)	O129	C125	3.522(10)
O129	C126	2.908(11)	O129	C142	3.014(7)
O130	O133	2.810(10)	O130	O147	3.389(9)
O130	C134	3.133(15)	O130	C148	3.319(13)
O133	C108	3.539(10)	O133	C117	3.220(13)
O133	C131	3.38(3)	O135	C125	2.932(9)
O143	O149	2.944(9)	O143	C55	3.325(9)
O143	C56	3.553(9)	O143	C57	3.091(10)
O143	C139	2.855(7)	O144	O145	2.874(8)
O144	C57	3.068(8)	O144	C63	3.273(8)
O144	C139	2.845(9)	O144	C140	3.356(9)
O144	C141	2.771(9)	O145	O147	2.842(8)
O145	C148	3.127(9)	O147	C122	3.334(11)
O147	C132	3.55(3)	O157	O163	2.893(8)
O157	C153	2.866(7)	O157	C164	3.071(15)
O157	C168	3.184(9)	O157	C170	3.355(8)
O158	O159	2.823(6)	O158	O175	2.892(8)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
O158	C153	2.930(8)	O158	C154	3.454(9)
O158	C155	2.854(9)	O158	C170	3.043(7)
O159	O161	2.825(8)	O159	O175	3.493(7)
O159	C162	3.128(11)	O159	C176	3.460(11)
O161	O243	2.899(7)	O161	O244	3.298(9)
O161	C236	3.557(9)	O163	O242	3.374(9)
O163	O243	3.570(7)	O163	C154	2.912(8)
O171	O177	3.197(9)	O171	C167	2.869(7)
O171	C178	3.128(12)	O171	C182	3.450(8)
O171	C184	3.412(10)	O172	O173	2.923(8)
O172	O189	2.882(7)	O172	O191	3.552(6)
O172	C167	2.871(9)	O172	C168	3.371(9)
O172	C169	2.820(8)	O172	C184	3.039(8)
O172	C190	3.505(8)	O173	O175	2.832(7)
O173	O189	3.341(8)	O173	C176	3.081(8)
O173	C182	3.572(10)	O175	C151	3.403(9)
O175	C160	3.429(10)	O185	O191	2.779(8)
O185	C181	2.842(7)	O185	C196	3.341(10)
O185	C198	3.198(10)	O186	O187	2.839(8)
O186	O203	2.825(7)	O186	C181	3.064(10)
O186	C182	3.546(10)	O186	C183	2.856(9)
O186	C188	3.444(10)	O186	C198	3.068(8)
O186	C204	3.105(12)	O187	O189	2.776(8)
O187	O203	3.324(10)	O187	C190	3.278(11)
O187	C204	3.091(18)	O191	C165	3.421(9)
O191	C182	2.885(7)	O199	O206	2.812(7)
O199	C195	2.871(8)	O199	C211	3.232(9)
O199	C213	3.547(10)	O200	O201	2.874(6)
O200	O218	2.863(8)	O200	C195	2.822(10)
O200	C196	3.385(10)	O200	C197	2.828(9)
O200	C213	3.061(7)	O201	O203	2.767(11)
O201	O218	3.288(9)	O201	C205	3.09(4)
O201	C219	3.242(12)	O203	C188	3.378(14)
O206	C213	3.550(11)	O206	C221	3.579(16)
O214	O220	2.691(8)	O214	C210	2.882(7)
O214	C225	3.270(8)	O214	C227	3.325(10)
O215	O216	2.889(9)	O215	O232	2.824(7)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
O215	C210	2.886(9)	O215	C211	3.444(9)
O215	C212	2.894(8)	O215	C227	3.042(9)
O216	O218	2.823(9)	O216	O232	3.166(8)
O216	C219	3.123(11)	O216	C233	3.294(10)
O218	C193	3.331(9)	O218	C202	3.598(15)
O220	C211	2.966(7)	O228	O234	2.689(7)
O228	O248	3.596(7)	O228	C224	2.857(8)
O228	C239	3.387(8)	O228	C241	3.215(10)
O229	O230	2.865(8)	O229	O246	2.854(5)
O229	O248	3.442(7)	O229	C224	2.900(10)
O229	C225	3.390(9)	O229	C226	2.772(8)
O229	C231	3.586(12)	O229	C241	3.057(8)
O229	C247	3.163(7)	O230	O232	2.850(7)
O230	C233	3.161(10)	O230	C239	3.593(10)
O232	C208	3.487(8)	O232	C217	3.277(15)
O242	O248	2.886(8)	O242	C154	3.250(10)
O242	C156	3.240(10)	O242	C238	2.838(8)
O243	O244	2.775(6)	O243	C156	3.039(8)
O243	C238	3.024(10)	O243	C239	3.547(10)
O243	C240	2.870(9)	O244	O246	2.813(9)
O244	C162	3.347(12)	O246	C245	3.494(15)
O248	C222	3.181(9)	O248	C239	2.845(7)
N2	C17	2.973(7)	N2	C30	2.984(9)
N3	C15	2.963(7)	N3	C22	2.974(10)
N4	C20	2.985(10)	N4	C27	2.981(7)
N5	C12	2.970(9)	N5	C25	2.972(7)
N6	C32	2.820(12)	N7	C37	2.819(7)
N8	C42	2.809(11)	N9	C47	2.790(7)
C12	C16	3.548(9)	C12	C48	3.245(9)
C12	C51	3.421(9)	C13	C16	3.564(8)
C13	C47	2.919(11)	C13	C48	3.406(11)
C14	C31	3.555(11)	C14	C32	2.895(9)
C14	C33	3.241(11)	C15	C31	3.538(10)
C15	C33	3.160(12)	C15	C36	3.478(11)
C16	C19	3.573(8)	C16	C20	3.537(9)
C17	C21	3.538(10)	C17	C33	3.457(11)
C17	C36	3.217(12)	C18	C21	3.559(11)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C18	C32	2.916(9)	C18	C36	3.302(11)
C19	C37	2.922(11)	C19	C41	3.309(10)
C20	C38	3.476(10)	C20	C41	3.240(8)
C21	C24	3.575(11)	C21	C25	3.559(10)
C22	C26	3.551(9)	C22	C38	3.131(9)
C22	C41	3.484(9)	C23	C26	3.571(7)
C23	C37	2.895(11)	C23	C38	3.221(11)
C24	C42	2.919(8)	C24	C43	3.174(10)
C25	C43	3.113(11)	C25	C46	3.543(10)
C26	C29	3.572(7)	C26	C30	3.540(8)
C27	C31	3.549(9)	C27	C43	3.515(10)
C27	C46	3.182(11)	C28	C31	3.573(11)
C28	C42	2.919(8)	C28	C46	3.193(10)
C29	C47	2.895(10)	C29	C51	3.358(11)
C30	C48	3.379(9)	C30	C51	3.251(8)
C33	C35	2.699(11)	C34	C36	2.706(11)
C38	C40	2.682(11)	C39	C41	2.675(12)
C43	C45	2.700(11)	C44	C46	2.711(11)
C48	C50	2.680(11)	C49	C51	2.669(11)
C52	C55	2.864(12)	C52	C61	3.553(12)
C52	C70	3.307(13)	C52	C71	3.307(12)
C53	C56	2.852(9)	C53	C63	3.503(12)
C53	C69	3.539(13)	C54	C61	3.281(12)
C55	C63	3.384(9)	C55	C138	3.594(11)
C56	C65	3.234(9)	C56	C137	3.246(11)
C57	C137	3.217(11)	C66	C69	2.856(12)
C66	C75	3.313(10)	C66	C82	3.404(10)
C66	C84	3.522(10)	C67	C70	2.845(9)
C67	C77	3.568(12)	C68	C75	3.509(15)
C69	C77	3.315(9)	C75	C91	3.504(14)
C80	C83	2.912(10)	C80	C89	3.120(12)
C80	C96	3.514(9)	C80	C98	3.395(10)
C80	C99	3.510(11)	C81	C84	2.896(10)
C81	C91	3.234(9)	C83	C91	3.582(8)
C89	C105	3.419(13)	C94	C97	2.885(10)
C94	C103	3.093(12)	C94	C112	3.238(12)
C94	C113	3.194(12)	C95	C98	2.862(9)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C95	C105	3.287(11)	C95	C111	3.490(12)
C97	C105	3.575(9)	C108	C111	2.901(12)
C108	C117	3.085(8)	C108	C124	3.498(12)
C108	C126	3.430(12)	C108	C127	3.544(11)
C109	C112	2.844(7)	C109	C119	3.436(19)
C111	C119	3.376(11)	C117	C134	3.438(16)
C122	C125	2.887(13)	C122	C131	3.485(17)
C122	C132	3.17(3)	C122	C139	3.385(12)
C122	C141	3.519(10)	C123	C126	2.864(11)
C123	C134	3.267(13)	C124	C131	3.40(3)
C124	C132	3.58(3)	C125	C134	3.543(10)
C126	C136	3.220(18)	C131	C134	3.59(3)
C131	C148	3.51(3)	C132	C148	3.39(3)
C137	C140	2.884(10)	C137	C146	3.047(14)
C138	C141	2.873(12)	C138	C148	3.280(9)
C140	C148	3.578(11)	C151	C154	2.905(11)
C151	C160	3.089(11)	C151	C167	3.412(10)
C151	C169	3.473(9)	C152	C155	2.854(10)
C152	C162	3.275(10)	C153	C236	3.496(11)
C154	C162	3.534(8)	C155	C164	3.250(16)
C155	C236	3.423(10)	C156	C236	3.531(9)
C160	C176	3.310(13)	C165	C168	2.889(10)
C165	C174	3.033(12)	C165	C183	3.256(12)
C165	C184	3.252(11)	C166	C169	2.878(11)
C166	C176	3.276(9)	C166	C182	3.508(11)
C168	C176	3.567(10)	C169	C178	3.039(11)
C179	C182	2.887(11)	C179	C188	2.996(10)
C179	C197	3.301(12)	C179	C198	3.294(11)
C180	C183	2.861(9)	C180	C190	3.378(11)
C180	C196	3.587(13)	C182	C190	3.479(8)
C193	C196	2.876(12)	C193	C202	3.227(12)
C193	C210	3.384(11)	C193	C212	3.510(10)
C194	C197	2.868(9)	C194	C205	3.28(3)
C195	C202	3.552(19)	C196	C204	3.331(13)
C196	C205	3.57(2)	C202	C219	3.449(17)
C208	C211	2.885(11)	C208	C217	3.033(16)
C208	C224	3.496(9)	C208	C226	3.457(11)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C208	C227	3.559(12)	C209	C212	2.853(11)
C209	C219	3.287(10)	C211	C219	3.556(8)
C217	C233	3.571(15)	C222	C225	2.860(10)
C222	C231	2.987(12)	C222	C240	3.204(11)
C222	C241	3.130(11)	C223	C226	2.880(10)
C223	C233	3.293(10)	C223	C239	3.518(11)
C225	C233	3.569(9)	C236	C239	2.901(11)
C236	C245	3.309(10)	C237	C240	2.868(7)
C237	C247	3.541(12)	C238	C245	3.459(13)
C239	C247	3.315(9)			

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O58	H53	2.561	O58	H54	3.204
O58	H55	2.655	O58	H57A	2.457
O58	H57B	3.212	O58	H65A	3.530
O58	H65B	2.526	O58	H69	3.486
O58	H71B	2.462	O58	H79A	3.016
O59	H53	3.245	O59	H54	2.639
O59	H56	2.447	O59	H68	2.616
O59	H70	2.664	O59	H71B	2.772
O59	H77B	2.601	O60	H52	2.504
O60	H54	2.667	O60	H63A	3.349
O60	H69	3.319	O60	H77B	2.831
O60	H77C	3.199	O62	H53	2.575
O62	H55	2.577	O62	H61A	2.561
O62	H61B	3.491	O64	H55	2.588
O64	H56	3.276	O64	H137	2.610
O72	H67	2.605	O72	H68	3.230
O72	H69	2.608	O72	H71A	2.505
O72	H71B	3.226	O72	H83	3.089
O72	H85B	2.770	O72	H93A	3.314
O73	H67	3.236	O73	H68	2.637
O73	H70	2.438	O73	H82	2.476
O73	H84	2.538	O73	H85B	2.769
O73	H91B	3.532	O74	H66	2.643
O74	H68	2.628	O74	H77A	3.443
O74	H91B	2.803	O74	H91C	3.274
O76	H67	2.562	O76	H69	2.619
O76	H75A	3.224	O78	H52	2.777
O78	H69	2.662	O78	H70	3.223
O86	H10G	2.866	O86	H81	2.643
O86	H82	3.328	O86	H83	2.726
O86	H85A	2.533	O86	H85B	3.228
O86	H97	3.201	O86	H99B	2.517
O87	H10F	3.464	O87	H81	3.248
O87	H82	2.869	O87	H84	2.567
O87	H89B	3.332	O87	H96	2.505
O87	H98	2.521	O87	H99B	2.857
O88	H10D	3.561	O88	H10F	2.977

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O88	H80	2.727	O88	H82	2.512
O88	H91A	2.484	O88	H91B	3.473
O90	H66	2.963	O90	H75C	3.576
O90	H81	2.500	O90	H83	2.458
O92	H83	2.506	O92	H84	3.249
O100	H11B	2.508	O100	H12A	3.519
O100	H95	2.545	O100	H96	3.298
O100	H97	2.771	O100	H99A	2.468
O100	H99B	3.219	O101	H10B	3.503
O101	H11B	2.798	O101	H11F	3.404
O101	H11G	3.147	O101	H95	3.265
O101	H96	2.632	O101	H98	2.480
O101	H110	2.485	O101	H112	2.596
O102	H10E	2.531	O102	H11G	2.976
O102	H94	2.637	O102	H96	2.563
O102	H111	3.185	O104	H80	3.307
O104	H89B	2.652	O104	H89C	3.540
O104	H95	2.561	O104	H97	2.467
O106	H80	3.336	O106	H97	2.402
O106	H98	3.241	O114	H11A	2.516
O114	H11B	3.223	O114	H12E	2.574
O114	H109	2.622	O114	H110	3.279
O114	H111	2.698	O114	H125	3.227
O115	H11D	3.372	O115	H12E	2.769
O115	H13B	3.411	O115	H109	3.251
O115	H110	2.795	O115	H112	2.466
O115	H124	2.550	O115	H126	2.561
O116	H11F	3.313	O116	H11H	3.582
O116	H13B	2.925	O116	H13C	3.369
O116	H108	2.689	O116	H110	2.566
O118	H109	2.513	O118	H111	2.551
O120	H94	2.587	O120	H111	2.549
O120	H112	3.252	O128	H12D	2.468
O128	H12E	3.197	O128	H13E	2.435
O128	H14A	2.579	O128	H123	2.620
O128	H124	3.257	O128	H125	2.724
O128	H140	2.967	O129	H14A	2.629

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O129	H14G	3.451	O129	H123	3.243
O129	H124	2.717	O129	H126	2.616
O129	H139	2.521	O129	H141	2.521
O130	H13A	2.547	O130	H14G	2.632
O130	H14H	3.564	O130	H122	2.660
O130	H124	2.586	O133	H11D	2.939
O133	H11E	3.013	O133	H108	3.316
O133	H123	2.528	O133	H125	2.518
O135	H108	3.433	O135	H125	2.567
O135	H126	3.261	O143	H14A	3.185
O143	H14B	2.409	O143	H55	3.579
O143	H57B	2.350	O143	H138	2.552
O143	H139	3.261	O143	H140	2.743
O144	H14D	3.389	O144	H54	2.517
O144	H56	2.623	O144	H57B	2.910
O144	H63B	2.797	O144	H138	3.235
O144	H139	2.551	O144	H141	2.430
O145	H14F	2.519	O145	H63B	3.060
O145	H137	2.667	O145	H139	2.584
O147	H122	2.867	O147	H138	2.580
O147	H140	2.519	O149	H57B	2.891
O149	H126	3.552	O149	H141	2.414
O157	H15D	2.479	O157	H15E	3.208
O157	H16G	3.292	O157	H16H	2.575
O157	H17A	2.427	O157	H152	2.575
O157	H153	3.294	O157	H154	2.746
O157	H168	3.044	O158	H16B	3.428
O158	H17A	2.665	O158	H17G	3.473
O158	H152	3.224	O158	H153	2.696
O158	H155	2.555	O158	H167	2.497
O158	H169	2.470	O159	H16D	2.552
O159	H17G	2.772	O159	H151	2.672
O159	H153	2.581	O161	H24C	3.386
O161	H152	2.533	O161	H154	2.477
O161	H236	3.290	O163	H154	2.510
O163	H155	3.278	O163	H236	3.420
O171	H17A	3.156	O171	H17B	2.356

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O171	H17I	2.686	O171	H17J	3.071
O171	H18B	2.581	O171	H166	2.545
O171	H167	3.265	O171	H168	2.810
O172	H17D	3.312	O172	H18B	2.784
O172	H19B	3.114	O172	H166	3.264
O172	H167	2.568	O172	H169	2.560
O172	H181	2.507	O172	H183	2.595
O173	H17F	2.457	O173	H19B	3.281
O173	H165	2.687	O173	H167	2.577
O173	H182	3.281	O175	H16B	2.878
O175	H16C	3.465	O175	H151	2.981
O175	H166	2.621	O175	H168	2.492
O177	H15D	3.371	O177	H155	3.092
O177	H169	2.544	O185	H18A	2.500
O185	H18B	3.207	O185	H19G	2.266
O185	H180	2.636	O185	H181	3.290
O185	H182	2.643	O185	H196	3.511
O186	H18D	3.022	O186	H19G	2.713
O186	H19H	3.547	O186	H180	3.266
O186	H181	2.881	O186	H183	2.492
O186	H195	2.566	O186	H197	2.606
O187	H19A	2.814	O187	H179	2.747
O187	H181	2.491	O187	H196	3.580
O189	H17D	3.453	O189	H180	2.471
O189	H182	2.532	O191	H165	2.683
O191	H182	2.544	O191	H183	3.228
O199	H19G	3.213	O199	H19H	2.485
O199	H21B	2.759	O199	H194	2.555
O199	H195	3.185	O199	H196	2.728
O199	H211	3.119	O200	H21B	2.759
O200	H21G	3.467	O200	H194	3.241
O200	H195	2.458	O200	H197	2.546
O200	H210	2.531	O200	H212	2.482
O201	H21G	2.705	O201	H21H	3.303
O201	H193	2.649	O201	H195	2.640
O203	H18D	2.863	O203	H18E	3.464
O203	H20A	3.533	O203	H194	2.641

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O203	H196	2.584	O206	H21B	2.660
O206	H22A	2.736	O206	H197	2.479
O214	H21A	2.557	O214	H21B	3.221
O214	H22D	2.608	O214	H22E	3.347
O214	H209	2.540	O214	H210	3.253
O214	H211	2.816	O214	H225	3.239
O215	H21D	3.411	O215	H22D	2.791
O215	H22E	3.339	O215	H23E	3.408
O215	H209	3.260	O215	H210	2.577
O215	H212	2.641	O215	H224	2.535
O215	H226	2.592	O216	H21F	2.529
O216	H23E	2.828	O216	H23F	3.392
O216	H208	2.631	O216	H210	2.637
O218	H20B	3.289	O218	H193	2.935
O218	H209	2.607	O218	H211	2.483
O220	H211	2.590	O220	H212	3.211
O228	H22D	3.248	O228	H22E	2.626
O228	H24B	2.404	O228	H24I	3.202
O228	H223	2.560	O228	H224	3.270
O228	H225	2.675	O229	H23B	3.221
O229	H24B	2.854	O229	H24F	2.648
O229	H24H	3.532	O229	H223	3.240
O229	H224	2.634	O229	H226	2.435
O229	H238	2.498	O229	H240	2.642
O230	H23D	2.569	O230	H24F	3.001
O230	H222	2.653	O230	H224	2.579
O230	H239	3.292	O232	H21D	2.690
O232	H21E	3.533	O232	H208	3.265
O232	H223	2.565	O232	H225	2.519
O234	H24B	3.175	O234	H226	2.618
O242	H15E	2.535	O242	H24A	2.507
O242	H24B	3.231	O242	H154	3.220
O242	H237	2.642	O242	H238	3.258
O242	H239	2.652	O243	H15E	2.798
O243	H16E	3.409	O243	H153	2.516
O243	H155	2.538	O243	H237	3.241
O243	H238	2.813	O243	H240	2.511

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O244	H16E	2.932	O244	H16F	3.309
O244	H24H	3.384	O244	H236	2.671
O244	H238	2.561	O246	H24D	3.143
O246	H237	2.498	O246	H239	2.558
O248	H23B	3.503	O248	H222	2.394
O248	H239	2.509	O248	H240	3.241
N2	H13	3.223	N2	H14	3.208
N3	H18	3.211	N3	H19	3.220
N4	H23	3.214	N4	H24	3.209
N5	H28	3.218	N5	H29	3.226
N6	H33	3.261	N6	H36	3.257
N7	H38	3.230	N7	H41	3.250
N8	H43	3.243	N8	H46	3.240
N9	H48	3.239	N9	H51	3.213
C12	H14	3.164	C12	H48	3.204
C12	H51	3.499	C13	H48	3.388
C14	H33	3.187	C15	H13	3.164
C15	H33	3.090	C16	H14	2.798
C16	H18	2.803	C16	H33	2.649
C16	H36	2.696	C17	H19	3.152
C17	H33	3.568	C17	H36	3.163
C18	H36	3.247	C19	H41	3.203
C20	H18	3.142	C20	H38	3.585
C20	H41	3.174	C21	H19	2.794
C21	H23	2.826	C21	H38	2.651
C21	H41	2.704	C22	H24	3.154
C22	H38	3.074	C23	H38	3.193
C24	H43	3.054	C25	H23	3.152
C25	H43	3.006	C26	H24	2.827
C26	H28	2.819	C26	H43	2.652
C26	H46	2.723	C27	H29	3.155
C27	H46	3.105	C28	H46	3.052
C29	H51	3.425	C30	H28	3.146
C30	H48	3.481	C30	H51	3.268
C31	H13	2.805	C31	H29	2.816
C31	H48	2.652	C31	H51	2.680
C32	H14	2.683	C32	H18	2.703

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C32	H34	3.248	C32	H35	3.237
C33	H14	2.848	C33	H18	3.425
C33	H36	3.218	C34	H35	3.128
C35	H34	3.130	C36	H14	3.406
C36	H18	2.877	C36	H33	3.219
C37	H19	2.718	C37	H23	2.693
C37	H39	3.232	C37	H40	3.242
C38	H19	3.483	C38	H23	2.832
C38	H41	3.215	C39	H23	3.588
C39	H40	3.092	C40	H39	3.094
C41	H19	2.884	C41	H23	3.407
C41	H38	3.217	C42	H24	2.718
C42	H28	2.719	C42	H44	3.250
C42	H45	3.234	C43	H24	2.734
C43	H46	3.243	C44	H24	3.557
C44	H45	3.141	C45	H28	3.577
C45	H44	3.143	C46	H24	3.553
C46	H28	2.700	C46	H43	3.242
C47	H13	2.719	C47	H29	2.686
C47	H49	3.215	C47	H50	3.226
C48	H13	3.009	C48	H29	3.312
C48	H51	3.199	C49	H50	3.119
C50	H49	3.113	C51	H13	3.359
C51	H29	2.919	C51	H48	3.199
C52	H54	2.713	C52	H55	3.245
C52	H56	2.554	C52	H69	2.455
C52	H71B	2.932	C52	H77B	3.513
C53	H55	2.725	C53	H56	3.167
C53	H61A	2.674	C53	H61B	2.562
C53	H61C	3.210	C53	H63A	3.453
C53	H69	3.515	C53	H77B	3.350
C54	H52	3.336	C54	H56	2.681
C54	H61A	3.108	C54	H63A	2.516
C54	H63B	2.699	C54	H63C	3.214
C54	H77B	3.312	C55	H53	2.698
C55	H57A	3.376	C55	H57B	2.878
C55	H63B	3.319	C55	H137	2.486

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C55	H141	3.518	C56	H52	3.224
C56	H53	3.186	C56	H54	2.724
C56	H65B	3.006	C56	H71B	3.072
C56	H137	3.253	C56	H141	3.600
C57	H55	2.743	C57	H65A	2.581
C57	H65B	2.598	C57	H65C	3.211
C57	H71B	3.364	C57	H137	3.042
C61	H52	3.578	C61	H53	2.450
C63	H54	2.377	C63	H61A	3.069
C63	H139	3.495	C65	H55	3.388
C65	H57A	2.404	C65	H57B	3.151
C65	H79A	3.489	C66	H68	2.739
C66	H69	3.164	C66	H70	2.547
C66	H75B	3.105	C66	H83	2.441
C66	H85B	3.279	C67	H69	2.633
C67	H70	3.121	C67	H75A	2.657
C67	H75B	2.485	C67	H75C	3.187
C68	H66	3.366	C68	H70	2.641
C68	H75A	3.544	C68	H77A	2.599
C68	H77B	2.577	C68	H77C	3.204
C69	H52	2.404	C69	H67	2.629
C69	H71A	3.401	C69	H71B	2.838
C69	H77B	3.131	C70	H52	3.277
C70	H66	3.239	C70	H67	3.176
C70	H68	2.702	C70	H85B	2.802
C71	H52	3.196	C71	H69	2.805
C71	H79A	2.604	C71	H79B	2.474
C71	H79C	3.165	C71	H85B	3.041
C71	H93A	3.370	C75	H66	3.161
C75	H67	2.325	C75	H91B	3.270
C75	H91C	3.089	C77	H54	3.491
C77	H68	2.378	C79	H52	3.588
C79	H71A	2.520	C79	H71B	2.548
C80	H82	2.858	C80	H83	3.352
C80	H84	2.621	C80	H89A	3.364
C80	H89B	2.925	C80	H97	2.426
C80	H99B	3.114	C81	H83	2.852

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C81	H84	3.246	C81	H89A	2.486
C81	H89B	2.684	C81	H89C	3.183
C81	H91A	3.053	C82	H66	3.296
C82	H80	3.384	C82	H84	2.794
C82	H91A	2.670	C82	H91B	2.563
C82	H91C	3.225	C83	H66	2.473
C83	H70	3.488	C83	H81	2.801
C83	H85A	3.379	C83	H85B	2.765
C84	H70	3.527	C84	H80	3.247
C84	H81	3.271	C84	H82	2.846
C84	H99B	2.805	C85	H10G	3.307
C85	H70	3.199	C85	H71A	3.344
C85	H83	2.654	C85	H93A	2.693
C85	H93B	2.463	C85	H93C	3.174
C85	H99B	3.075	C89	H10D	3.145
C89	H10F	3.249	C89	H80	2.902
C89	H81	2.431	C89	H91A	3.385
C91	H75C	3.011	C91	H81	3.501
C91	H82	2.416	C93	H71A	3.233
C93	H85A	2.585	C93	H85B	2.561
C94	H10B	2.747	C94	H11B	2.692
C94	H96	2.750	C94	H97	3.355
C94	H98	2.614	C94	H111	2.515
C94	H112	3.561	C95	H10A	2.692
C95	H10B	2.519	C95	H10C	3.215
C95	H10E	3.088	C95	H11G	3.571
C95	H97	2.798	C95	H98	3.262
C95	H111	3.414	C96	H10D	3.223
C96	H10E	2.589	C96	H10F	2.628
C96	H11G	3.316	C96	H80	3.485
C96	H94	3.352	C96	H98	2.826
C97	H80	2.440	C97	H95	2.718
C97	H99A	3.371	C97	H99B	2.821
C98	H11B	3.546	C98	H80	3.570
C98	H84	3.541	C98	H94	3.243
C98	H95	3.163	C98	H96	2.860
C99	H10G	2.483	C99	H10H	2.583

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C99	H10I	3.174	C99	H84	3.339
C99	H85A	3.399	C99	H97	2.642
C103	H10E	3.589	C103	H94	2.816
C103	H95	2.482	C103	H111	3.363
C105	H11G	3.416	C105	H89B	3.045
C105	H89C	3.247	C105	H96	2.409
C107	H85A	3.455	C107	H99A	2.605
C107	H99B	2.469	C108	H11D	2.735
C108	H12E	3.128	C108	H110	2.807
C108	H111	3.298	C108	H112	2.560
C108	H125	2.422	C109	H11C	2.661
C109	H11D	2.513	C109	H11E	3.200
C109	H11F	3.435	C109	H111	2.775
C109	H112	3.152	C110	H11F	2.369
C110	H11G	2.898	C110	H11H	3.084
C110	H108	3.379	C110	H112	2.708
C111	H11A	3.405	C111	H11B	2.812
C111	H11F	3.494	C111	H11G	3.533
C111	H94	2.428	C111	H109	2.727
C112	H12E	2.866	C112	H94	3.102
C112	H108	3.222	C112	H109	3.204
C112	H110	2.764	C113	H12A	2.592
C113	H12B	2.535	C113	H12C	3.197
C113	H12E	3.122	C113	H94	2.798
C113	H111	2.738	C117	H13B	3.385
C117	H13C	3.136	C117	H108	2.842
C117	H109	2.441	C119	H96	3.305
C119	H110	2.380	C121	H11A	2.588
C121	H11B	2.553	C121	H94	3.203
C122	H14A	3.069	C122	H124	2.771
C122	H125	3.279	C122	H126	2.635
C122	H140	2.401	C123	H13A	3.077
C123	H125	2.730	C123	H126	3.230
C124	H13A	2.560	C124	H13B	2.614
C124	H13C	3.203	C124	H108	3.463
C124	H122	3.358	C124	H126	2.751
C125	H12D	3.379	C125	H12E	2.794

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C125	H13B	3.597	C125	H108	2.422
C125	H112	3.591	C125	H123	2.677
C126	H13E	2.971	C126	H14A	2.735
C126	H108	3.572	C126	H122	3.240
C126	H123	3.188	C126	H124	2.779
C127	H11A	3.430	C127	H13D	2.632
C127	H13E	2.390	C127	H13F	3.124
C127	H14A	3.173	C127	H15B	3.429
C127	H112	3.402	C127	H125	2.697
C131	H13A	2.962	C131	H14G	2.909
C131	H14H	3.397	C131	H122	3.432
C131	H123	2.453	C132	H14G	2.975
C132	H14H	3.199	C132	H122	2.929
C132	H123	2.244	C134	H11D	3.541
C134	H11E	2.924	C134	H124	2.386
C136	H12D	2.315	C136	H12E	3.035
C136	H125	3.552	C137	H14C	3.219
C137	H14D	2.869	C137	H55	2.546
C137	H56	3.580	C137	H57B	2.855
C137	H139	2.734	C137	H140	3.339
C137	H141	2.590	C138	H14C	2.482
C138	H14D	2.723	C138	H14E	3.195
C138	H14F	3.054	C138	H63B	3.529
C138	H140	2.809	C138	H141	3.249
C139	H14F	2.532	C139	H14G	2.657
C139	H14H	3.210	C139	H63B	3.369
C139	H122	3.228	C139	H137	3.358
C139	H141	2.803	C140	H14A	2.572
C140	H14B	2.896	C140	H122	2.447
C140	H126	3.579	C140	H138	2.716
C141	H57B	3.073	C141	H126	3.599
C141	H137	3.233	C141	H138	3.165
C141	H139	2.823	C142	H12D	3.562
C142	H15A	2.560	C142	H15B	2.569
C142	H15C	3.186	C142	H57B	3.405
C142	H126	3.099	C142	H140	2.648
C146	H137	2.756	C146	H138	2.489

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C148	H139	2.363	C150	H14A	2.562
C150	H14B	2.568	C151	H16A	3.519
C151	H16B	2.775	C151	H17A	2.930
C151	H153	2.798	C151	H154	3.339
C151	H155	2.632	C151	H168	2.424
C152	H16A	2.578	C152	H16B	2.547
C152	H16C	3.196	C152	H16D	3.112
C152	H154	2.775	C152	H155	3.239
C153	H16D	2.621	C153	H16E	2.545
C153	H16F	3.209	C153	H151	3.379
C153	H155	2.785	C153	H236	3.455
C154	H15D	3.379	C154	H15E	2.801
C154	H16E	3.558	C154	H152	2.702
C154	H236	2.433	C155	H16G	3.522
C155	H16H	3.133	C155	H17A	2.820
C155	H151	3.249	C155	H152	3.164
C155	H153	2.825	C155	H236	3.579
C156	H16G	2.495	C156	H16H	2.730
C156	H16I	3.197	C156	H17A	3.246
C156	H24A	3.394	C156	H154	2.663
C156	H240	3.413	C160	H16D	3.582
C160	H17G	2.880	C160	H17H	3.181
C160	H151	2.835	C160	H152	2.407
C162	H24C	3.071	C162	H153	2.390
C164	H15D	2.424	C164	H15E	3.152
C164	H154	3.462	C165	H17C	3.179
C165	H17D	2.858	C165	H18B	2.760
C165	H167	2.720	C165	H168	3.384
C165	H169	2.666	C165	H182	2.512
C165	H183	3.599	C166	H17C	2.486
C166	H17D	2.734	C166	H17E	3.200
C166	H17F	3.036	C166	H168	2.818
C166	H169	3.338	C166	H182	3.438
C167	H17F	2.520	C167	H17G	2.652
C167	H17H	3.205	C167	H19B	3.414
C167	H151	3.305	C167	H165	3.362
C167	H169	2.878	C168	H17A	2.462

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C168	H17B	2.944	C168	H151	2.478
C168	H155	3.488	C168	H166	2.714
C169	H17I	2.784	C169	H17J	3.275
C169	H18B	3.559	C169	H155	3.396
C169	H165	3.246	C169	H166	3.144
C169	H167	2.851	C170	H15D	3.465
C170	H17I	2.607	C170	H17J	2.467
C170	H17K	3.168	C170	H155	3.032
C170	H168	2.569	C174	H165	2.738
C174	H166	2.550	C174	H182	3.226
C176	H16B	3.081	C176	H16C	2.955
C176	H19B	3.476	C176	H167	2.376
C178	H17A	3.158	C178	H17B	2.458
C178	H18B	3.162	C178	H169	3.044
C179	H18C	3.203	C179	H18D	2.756
C179	H19G	2.617	C179	H19H	3.596
C179	H181	2.839	C179	H182	3.277
C179	H183	2.559	C179	H196	2.483
C180	H18C	2.499	C180	H18D	2.666
C180	H18E	3.196	C180	H19A	3.256
C180	H182	2.788	C180	H183	3.147
C180	H196	3.569	C181	H19A	2.503
C181	H19B	2.712	C181	H19C	3.202
C181	H179	3.370	C181	H183	2.692
C182	H17D	3.217	C182	H18A	3.366
C182	H18B	2.784	C182	H19B	3.497
C182	H165	2.419	C182	H180	2.761
C183	H19G	3.253	C183	H165	3.131
C183	H179	3.227	C183	H180	3.256
C183	H181	2.782	C184	H17I	3.181
C184	H19D	2.511	C184	H19E	2.554
C184	H19F	3.163	C184	H19G	3.593
C184	H165	2.897	C184	H182	2.715
C188	H179	2.766	C188	H180	2.519
C188	H196	3.355	C190	H17F	3.562
C190	H167	3.441	C190	H181	2.385
C192	H18A	2.476	C192	H18B	2.627

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C192	H165	3.508	C193	H20B	2.990
C193	H21B	3.237	C193	H195	2.662
C193	H196	3.272	C193	H197	2.651
C193	H211	2.435	C194	H20A	2.553
C194	H20B	2.538	C194	H20C	3.169
C194	H196	2.661	C194	H197	3.285
C195	H18D	3.524	C195	H193	3.359
C195	H197	2.796	C196	H18D	3.081
C196	H19G	2.682	C196	H19H	2.838
C196	H179	2.423	C196	H194	2.599
C197	H21B	2.839	C197	H179	3.275
C197	H193	3.252	C197	H194	3.119
C197	H195	2.755	C198	H20D	2.490
C198	H20E	2.552	C198	H20F	3.154
C198	H21B	3.324	C198	H179	3.085
C198	H196	2.693	C202	H21G	3.185
C202	H21H	3.112	C202	H193	3.032
C202	H194	2.359	C204	H18D	3.547
C204	H181	3.519	C204	H195	2.427
C205	H195	2.362	C207	H19G	2.525
C207	H19H	2.521	C207	H22A	3.230
C208	H21C	3.193	C208	H21D	2.871
C208	H22D	3.125	C208	H22E	3.569
C208	H210	2.710	C208	H211	3.340
C208	H212	2.673	C208	H225	2.432
C209	H21C	2.444	C209	H21D	2.717
C209	H21E	3.179	C209	H21F	3.089
C209	H211	2.745	C209	H212	3.301
C210	H21F	2.577	C210	H21G	2.586
C210	H21H	3.207	C210	H193	3.284
C210	H208	3.348	C210	H212	2.824
C211	H21A	3.392	C211	H21B	2.723
C211	H193	2.464	C211	H197	3.538
C211	H209	2.640	C212	H22D	2.963
C212	H197	3.503	C212	H208	3.244
C212	H209	3.095	C212	H210	2.822
C213	H22A	2.569	C213	H22B	2.497

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C213	H22C	3.157	C213	H22D	3.403
C213	H197	3.155	C213	H211	2.656
C217	H23E	3.463	C217	H23F	3.354
C217	H208	2.720	C217	H209	2.458
C219	H20B	3.446	C219	H20C	3.093
C219	H210	2.386	C221	H21A	2.524
C221	H21B	2.549	C222	H23A	3.315
C222	H23B	2.681	C222	H24B	2.688
C222	H24F	3.566	C222	H24I	3.382
C222	H224	2.748	C222	H225	3.273
C222	H226	2.591	C222	H239	2.549
C222	H240	3.539	C223	H23A	2.544
C223	H23B	2.592	C223	H23C	3.191
C223	H23D	3.075	C223	H24F	3.354
C223	H225	2.764	C223	H226	3.240
C223	H239	3.468	C224	H23D	2.511
C224	H23E	2.686	C224	H23F	3.197
C224	H24F	3.113	C224	H208	3.459
C224	H222	3.352	C224	H226	2.792
C225	H22D	2.785	C225	H22E	2.698
C225	H208	2.436	C225	H223	2.702
C226	H24B	3.419	C226	H208	3.594
C226	H222	3.233	C226	H223	3.196
C226	H224	2.813	C227	H23G	2.504
C227	H23H	2.607	C227	H23I	3.184
C227	H212	3.427	C227	H225	2.664
C231	H222	2.692	C231	H223	2.488
C231	H239	3.260	C233	H21D	3.306
C233	H21E	3.501	C233	H24F	3.572
C233	H224	2.380	C235	H17K	3.474
C235	H22D	2.467	C235	H22E	2.669
C236	H15E	3.112	C236	H24E	3.123
C236	H154	2.428	C236	H238	2.806
C236	H239	3.269	C236	H240	2.576
C237	H24C	3.152	C237	H24D	2.672
C237	H24E	2.452	C237	H24H	3.539
C237	H239	2.764	C237	H240	3.154

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C238	H24D	3.508	C238	H24F	2.716
C238	H24G	3.225	C238	H24H	2.517
C238	H236	3.364	C238	H240	2.677
C239	H23B	3.269	C239	H24A	3.395
C239	H24B	2.847	C239	H24F	3.212
C239	H222	2.427	C239	H237	2.744
C240	H15E	2.842	C240	H222	3.062
C240	H236	3.240	C240	H237	3.247
C240	H238	2.750	C241	H15E	3.080
C241	H24I	2.556	C241	H24J	2.632
C241	H24K	3.216	C241	H222	2.737
C241	H239	2.751	C245	H16E	3.485
C245	H16F	3.231	C245	H236	3.203
C245	H237	2.332	C247	H224	3.228
C247	H238	2.407	C249	H24A	2.655
C249	H24B	2.552	C249	H222	2.936
H10A	H94	3.393	H10A	H95	2.439
H10B	H94	2.186	H10B	H95	2.558
H10B	H111	2.877	H10C	H94	3.527
H10C	H95	3.429	H10C	H111	3.515
H10D	H89B	2.808	H10D	H89C	2.767
H10D	H96	3.362	H10E	H11G	2.861
H10E	H95	3.534	H10E	H96	2.490
H10F	H11G	3.198	H10F	H89B	3.125
H10F	H89C	3.077	H10F	H96	2.331
H10G	H85A	2.565	H10G	H99A	2.863
H10G	H99B	2.216	H10H	H99A	2.472
H10H	H99B	2.808	H10I	H99A	3.505
H10I	H99B	3.355	H11A	H12A	2.942
H11A	H12B	2.375	H11A	H12C	3.458
H11A	H12E	2.513	H11A	H112	2.395
H11B	H12A	2.399	H11B	H12B	2.802
H11B	H12C	3.462	H11B	H94	2.465
H11B	H98	3.497	H11B	H99A	3.527
H11B	H111	3.081	H11B	H112	2.347
H11C	H108	3.359	H11C	H109	2.375
H11D	H13C	3.342	H11D	H108	2.207

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H11D	H109	2.545	H11D	H125	3.323
H11E	H13B	2.992	H11E	H13C	2.399
H11E	H108	3.595	H11E	H109	3.387
H11F	H96	3.430	H11F	H110	1.979
H11G	H96	2.487	H11G	H110	2.925
H11H	H110	3.160	H12A	H94	2.866
H12D	H13D	2.391	H12D	H13E	2.214
H12D	H13F	3.274	H12D	H14A	2.675
H12D	H15B	2.800	H12D	H125	3.588
H12D	H126	2.358	H12E	H13D	3.200
H12E	H13E	3.304	H12E	H15B	3.323
H12E	H108	3.472	H12E	H112	2.520
H12E	H125	3.039	H12E	H126	2.305
H13	H14	2.463	H13	H48	3.115
H13A	H123	3.550	H13A	H124	2.434
H13B	H124	2.331	H13C	H124	3.344
H14	H33	2.949	H14A	H15A	2.862
H14A	H15B	2.388	H14A	H15C	3.453
H14A	H122	3.529	H14A	H126	2.228
H14A	H140	2.632	H14A	H141	2.490
H14B	H15A	2.384	H14B	H15B	2.886
H14B	H15C	3.452	H14B	H140	2.704
H14B	H141	2.828	H14C	H137	2.878
H14C	H138	2.186	H14D	H55	2.952
H14D	H137	2.332	H14D	H138	2.947
H14E	H138	3.317	H14F	H63B	2.969
H14F	H138	3.567	H14F	H139	2.366
H14G	H63B	3.506	H14G	H139	2.355
H14H	H139	3.323	H15B	H126	3.257
H15D	H16G	2.142	H15D	H16H	2.786
H15D	H16I	3.303	H15D	H17A	2.707
H15D	H154	3.556	H15D	H155	2.394
H15E	H16G	3.224	H15E	H24A	2.475
H15E	H154	3.010	H15E	H155	2.318
H15E	H236	3.453	H15E	H240	2.537
H16A	H151	3.281	H16A	H152	2.251
H16B	H17G	2.923	H16B	H17H	2.924

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H16B	H151	2.235	H16B	H152	2.593
H16C	H17G	2.511	H16C	H17H	2.669
H16C	H152	3.343	H16D	H152	3.529
H16D	H153	2.544	H16E	H24C	3.037
H16E	H153	2.227	H16F	H24C	2.478
H16F	H24E	3.583	H16F	H153	3.335
H16H	H154	3.308	H17A	H17I	3.520
H17A	H17J	3.317	H17A	H151	3.241
H17A	H155	2.466	H17A	H168	2.355
H17A	H169	2.582	H17B	H17I	2.836
H17B	H17J	2.187	H17B	H17K	3.327
H17B	H168	2.745	H17B	H169	2.819
H17C	H165	2.803	H17C	H166	2.252
H17D	H165	2.341	H17D	H166	3.030
H17D	H182	2.427	H17E	H166	3.360
H17F	H19B	2.894	H17F	H19C	3.422
H17F	H166	3.555	H17F	H167	2.381
H17G	H19B	3.258	H17G	H167	2.361
H17H	H167	3.336	H17I	H18A	3.322
H17I	H18B	2.312	H17I	H169	2.613
H17I	H183	3.491	H17J	H18B	3.221
H17J	H169	3.543	H17K	H23H	3.090
H17K	H23I	2.982	H18	H19	2.473
H18	H36	2.951	H18A	H19D	2.698
H18A	H19E	2.316	H18A	H19F	3.398
H18A	H19G	3.045	H18A	H20E	3.168
H18A	H183	2.357	H18B	H19D	2.433
H18B	H19E	3.003	H18B	H19F	3.482
H18B	H165	2.578	H18B	H169	3.449
H18B	H182	3.061	H18B	H183	2.329
H18C	H179	2.843	H18C	H180	2.247
H18D	H179	2.331	H18D	H180	2.938
H18D	H196	2.480	H18E	H180	3.365
H19	H41	2.890	H19A	H181	2.229
H19B	H167	2.531	H19B	H181	2.540
H19C	H181	3.331	H19D	H165	3.379
H19E	H20E	3.449	H19G	H20D	2.785

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19G	H20E	2.369	H19G	H20F	3.432
H19G	H179	2.526	H19G	H183	3.294
H19G	H196	2.823	H19G	H197	2.441
H19H	H20D	2.297	H19H	H20E	2.873
H19H	H20F	3.396	H19H	H179	3.107
H19H	H196	2.621	H19H	H197	2.864
H20A	H193	3.577	H20A	H194	2.234
H20B	H21G	3.433	H20B	H21H	3.069
H20B	H193	2.511	H20B	H194	2.484
H20C	H21G	2.859	H20C	H21H	2.582
H20C	H194	3.309	H20F	H22A	2.816
H20F	H22B	3.574	H21A	H22A	2.882
H21A	H22B	2.299	H21A	H22C	3.396
H21A	H22D	2.861	H21A	H23H	3.222
H21A	H211	3.596	H21A	H212	2.325
H21B	H22A	2.406	H21B	H22B	2.808
H21B	H22C	3.452	H21B	H197	2.260
H21B	H211	2.837	H21B	H212	2.389
H21C	H208	2.840	H21C	H209	2.130
H21D	H23E	3.428	H21D	H23F	3.149
H21D	H208	2.307	H21D	H209	2.925
H21D	H225	3.267	H21E	H23E	3.440
H21E	H23F	3.040	H21E	H209	3.283
H21F	H23E	3.365	H21F	H210	2.486
H21G	H210	2.277	H21H	H210	3.339
H22D	H23G	2.625	H22D	H23H	2.352
H22D	H23I	3.403	H22D	H208	3.445
H22D	H212	2.527	H22D	H225	2.993
H22D	H226	2.375	H22E	H23G	2.458
H22E	H23H	3.094	H22E	H23I	3.498
H22E	H208	3.426	H22E	H225	2.446
H22E	H226	2.890	H23	H24	2.446
H23	H38	2.963	H23A	H222	2.979
H23A	H223	2.274	H23B	H222	2.125
H23B	H223	2.799	H23B	H239	2.507
H23C	H222	3.573	H23C	H223	3.381
H23D	H24F	2.952	H23D	H24G	3.538

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H23D	H223	3.577	H23D	H224	2.341
H23E	H24F	3.513	H23E	H224	2.422
H23F	H224	3.337	H24	H43	2.742
H24A	H24I	2.929	H24A	H24J	2.527
H24A	H24K	3.546	H24A	H240	2.417
H24B	H24I	2.331	H24B	H24J	2.888
H24B	H24K	3.433	H24B	H222	2.491
H24B	H226	3.429	H24B	H239	3.160
H24B	H240	2.316	H24C	H237	3.283
H24D	H237	2.454	H24E	H236	2.756
H24E	H237	2.207	H24F	H224	2.249
H24F	H238	2.665	H24F	H239	3.573
H24G	H238	3.326	H24H	H238	2.164
H24I	H222	2.677	H24K	H222	3.201
H28	H29	2.462	H28	H46	2.634
H29	H51	3.108	H33	H34	2.340
H35	H36	2.320	H38	H39	2.312
H40	H41	2.313	H43	H44	2.311
H45	H46	2.297	H48	H49	2.298
H50	H51	2.306	H52	H53	2.322
H52	H56	3.458	H52	H61B	3.519
H52	H69	2.034	H52	H71B	3.066
H52	H79A	3.420	H53	H54	2.883
H53	H55	2.561	H53	H61A	2.723
H53	H61B	2.242	H53	H61C	3.360
H54	H55	2.872	H54	H56	2.542
H54	H61A	3.474	H54	H63A	2.176
H54	H63B	2.579	H54	H63C	3.312
H54	H77B	2.539	H55	H56	2.875
H55	H57A	3.577	H55	H57B	3.201
H55	H65B	3.177	H55	H137	2.193
H56	H57A	2.411	H56	H57B	2.262
H56	H71B	2.886	H56	H141	3.192
H57A	H65A	2.250	H57A	H65B	2.583
H57A	H65C	3.341	H57A	H71B	2.728
H57A	H79A	3.284	H57B	H65A	3.271
H57B	H65B	3.527	H57B	H137	2.902

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H57B	H141	2.948	H61A	H63A	2.975
H61A	H63C	3.079	H61C	H77C	3.493
H63A	H77B	3.091	H63A	H77C	3.559
H63B	H139	2.531	H65A	H79A	3.172
H65B	H79A	2.913	H66	H67	2.338
H66	H70	3.464	H66	H75B	2.699
H66	H83	2.130	H67	H68	2.882
H67	H69	2.425	H67	H75A	2.381
H67	H75B	2.248	H67	H75C	3.285
H68	H69	2.882	H68	H70	2.464
H68	H77A	2.291	H68	H77B	2.465
H68	H77C	3.332	H69	H70	2.872
H69	H71B	3.198	H70	H71A	2.355
H70	H71B	2.304	H70	H84	3.386
H70	H85B	2.296	H71A	H79A	2.918
H71A	H79B	2.264	H71A	H79C	3.376
H71A	H85B	2.472	H71A	H93A	2.467
H71A	H93B	3.367	H71B	H79A	2.437
H71B	H79B	2.761	H71B	H79C	3.464
H71B	H85B	3.451	H75B	H91C	3.205
H75C	H91B	2.824	H75C	H91C	2.445
H79B	H93A	3.444	H80	H81	2.320
H80	H84	3.523	H80	H89A	3.083
H80	H89B	2.461	H80	H97	2.048
H80	H99B	3.455	H81	H82	2.863
H81	H83	2.763	H81	H89A	2.145
H81	H89B	2.824	H81	H89C	3.295
H81	H91A	3.350	H82	H83	2.867
H82	H84	2.756	H82	H91A	2.644
H82	H91B	2.219	H82	H91C	3.342
H83	H84	2.880	H83	H85A	3.566
H83	H85B	2.946	H84	H85A	2.374
H84	H85B	2.360	H84	H98	3.229
H84	H99B	2.475	H85A	H93A	3.077
H85A	H93B	2.309	H85A	H93C	3.384
H85A	H99B	2.467	H85B	H93A	2.534
H85B	H93B	2.679	H85B	H93C	3.491

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H89A	H91A	3.581	H89B	H97	3.401
H89C	H91A	3.382	H94	H95	2.371
H94	H98	3.504	H94	H111	2.168
H95	H96	2.880	H95	H97	2.655
H96	H97	2.888	H96	H98	2.784
H97	H98	2.877	H97	H99A	3.526
H97	H99B	3.015	H98	H99A	2.410
H98	H99B	2.296	H108	H109	2.315
H108	H112	3.471	H108	H125	2.022
H109	H110	2.868	H109	H111	2.636
H110	H111	2.874	H110	H112	2.600
H111	H112	2.889	H112	H126	3.410
H122	H123	2.329	H122	H126	3.540
H122	H140	2.121	H123	H124	2.871
H123	H125	2.555	H124	H125	2.885
H124	H126	2.646	H125	H126	2.891
H126	H141	3.544	H137	H138	2.388
H137	H141	3.477	H138	H139	2.860
H138	H140	2.647	H139	H140	2.886
H139	H141	2.725	H140	H141	2.878
H151	H152	2.349	H151	H155	3.529
H151	H168	2.147	H152	H153	2.881
H152	H154	2.618	H153	H154	2.877
H153	H155	2.729	H154	H155	2.883
H154	H236	2.038	H155	H169	3.172
H155	H240	3.368	H165	H166	2.401
H165	H169	3.545	H165	H182	2.136
H166	H167	2.882	H166	H168	2.663
H167	H168	2.877	H167	H169	2.829
H168	H169	2.870	H179	H180	2.304
H179	H183	3.474	H179	H196	2.073
H180	H181	2.870	H180	H182	2.678
H181	H182	2.896	H181	H183	2.607
H182	H183	2.875	H183	H197	3.529
H193	H194	2.417	H193	H195	3.570
H193	H197	3.540	H193	H211	2.133
H194	H195	2.879	H194	H196	2.429

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H195	H196	2.873	H195	H197	2.645
H196	H197	2.906	H197	H212	3.314
H208	H209	2.367	H208	H212	3.562
H208	H225	2.036	H209	H210	2.893
H209	H211	2.537	H210	H211	2.888
H210	H212	2.753	H211	H212	2.879
H212	H226	3.537	H222	H223	2.356
H222	H226	3.485	H222	H239	2.201
H223	H224	2.869	H223	H225	2.599
H224	H225	2.895	H224	H226	2.700
H225	H226	2.890	H226	H240	3.573
H236	H237	2.299	H236	H240	3.488
H237	H238	2.872	H237	H239	2.633
H238	H239	2.876	H238	H240	2.565
H239	H240	2.887			

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O10	O244	3.394(7)	O10	O250	2.809(10)
O11	O116	3.499(10)	O11	O251	3.00(6)
O11	O252	2.87(3)	O11	C134	3.398(17)
O11	C204	3.388(14)	O11	C205	3.19(3)
O58	C188[1]	3.599(10)	O62	C45[2]	3.388(9)
O64	O177[3]	3.337(7)	O64	C170[3]	3.526(8)
O64	C178[3]	3.526(10)	O74	O250	2.909(8)
O78	O203[1]	3.470(8)	O78	C194[1]	3.505(10)
O86	C131[4]	3.47(3)	O86	C132[4]	3.16(3)
O87	C23	3.423(8)	O87	C24	3.589(7)
O90	C34[4]	3.372(9)	O92	C131[4]	3.53(3)
O92	C132[4]	2.95(3)	O104	C65[5]	3.404(12)
O114	O242[6]	3.206(6)	O114	C236[6]	3.349(8)
O114	C237[6]	3.543(9)	O116	O11	3.499(10)
O116	O252	3.346(18)	O118	O252	3.215(14)
O129	C19	3.566(10)	O133	C164[6]	3.531(15)
O149	N7	3.209(11)	O149	C40	3.442(12)
O149	C178[3]	3.413(9)	O161	C136[7]	3.406(17)
O163	C117[7]	3.522(12)	O173	C91[8]	3.456(8)
O177	O64[9]	3.337(7)	O177	N9	3.495(10)
O177	C49	3.247(11)	O177	C57[9]	3.571(7)
O177	C65[9]	3.457(11)	O185	C61[10]	3.335(11)
O187	O251	3.20(5)	O187	C89[8]	3.505(12)
O189	C44[8]	3.485(10)	O189	C91[8]	3.590(11)
O191	C233[8]	3.423(11)	O199	C67[10]	3.571(9)
O201	O252	3.092(16)	O203	O78[10]	3.470(8)
O203	O251	3.51(6)	O203	O252	3.251(17)
O203	C79[10]	3.382(11)	O214	C107[9]	3.559(10)
O214	C160[5]	3.537(11)	O218	C35[5]	3.260(10)
O220	C160[5]	3.372(14)	O232	C192[4]	3.336(15)
O234	N9	3.354(10)	O234	C49	3.334(12)
O242	O114[7]	3.206(6)	O242	C108[7]	3.221(9)
O242	C109[7]	3.560(9)	O244	O10	3.394(7)
O248	C109[7]	3.387(9)	O250	O10	2.809(10)
O250	O74	2.909(8)	O250	N4	3.399(11)
O250	C24	3.579(12)	O250	C25	3.264(12)
O250	C75	3.559(15)	O250	C91	3.424(12)

Table 12. Intermolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
O250	C247	3.385(9)	O251	O11	3.00(6)
O251	O187	3.20(5)	O251	O203	3.51(6)
O251	N2	3.10(6)	O251	C12	3.21(6)
O251	C13	3.48(6)	O251	C14	3.50(6)
O251	C15	3.24(6)	O251	C134	3.19(5)
O251	C190	3.30(7)	O251	C204	2.04(7)
O251	C205	2.75(7)	O252	O11	2.87(3)
O252	O116	3.346(18)	O252	O118	3.215(14)
O252	O201	3.092(16)	O252	O203	3.251(17)
O252	C119	2.74(2)	O252	C204	3.10(3)
O252	C205	2.20(4)	N2	O251	3.10(6)
N4	O250	3.399(11)	N6	C148	3.561(9)
N7	O149	3.209(11)	N7	C150	3.266(12)
N7	C235[3]	3.457(9)	N8	C105	3.580(9)
N9	O177	3.495(10)	N9	O234	3.354(10)
N9	C178	3.221(12)	N9	C235	3.350(12)
C12	O251	3.21(6)	C13	O251	3.48(6)
C14	O251	3.50(6)	C15	O251	3.24(6)
C19	O129	3.566(10)	C23	O87	3.423(8)
C24	O87	3.589(7)	C24	O250	3.579(12)
C25	O250	3.264(12)	C25	C119	3.500(14)
C27	C247	3.417(10)	C28	C247	3.479(10)
C33	C190	3.441(9)	C34	O90[8]	3.372(9)
C34	C176	3.598(10)	C35	O218[2]	3.260(10)
C36	C63	3.538(9)	C40	O149	3.442(12)
C44	O189[4]	3.485(10)	C45	O62[5]	3.388(9)
C45	C105	3.401(9)	C46	C219	3.590(9)
C49	O177	3.247(11)	C49	O234	3.334(12)
C49	C178	3.528(12)	C57	O177[3]	3.571(7)
C57	C178[3]	3.381(10)	C61	O185[1]	3.335(11)
C63	C36	3.538(9)	C65	O104[2]	3.404(12)
C65	O177[3]	3.457(11)	C65	C105[2]	3.595(14)
C67	O199[1]	3.571(9)	C75	O250	3.559(15)
C79	O203[1]	3.382(11)	C79	C188[1]	3.571(14)
C81	C131[4]	3.586(18)	C89	O187[4]	3.505(12)
C89	C188[4]	3.506(15)	C91	O173[4]	3.456(8)
C91	O189[4]	3.590(11)	C91	O250	3.424(12)

Table 12. Intermolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C91	C174[4]	3.536(9)	C91	C190[4]	3.503(13)
C103	C231[6]	3.569(14)	C105	N8	3.580(9)
C105	C45	3.401(9)	C105	C65[5]	3.595(14)
C107	O214[3]	3.559(10)	C108	O242[6]	3.221(9)
C109	O242[6]	3.560(9)	C109	O248[6]	3.387(9)
C117	O163[6]	3.522(12)	C119	O252	2.74(2)
C119	C25	3.500(14)	C131	O86[8]	3.47(3)
C131	O92[8]	3.53(3)	C131	C81[8]	3.586(18)
C132	O86[8]	3.16(3)	C132	O92[8]	2.95(3)
C134	O11	3.398(17)	C134	O251	3.19(5)
C136	O161[6]	3.406(17)	C148	N6	3.561(9)
C150	N7	3.266(12)	C150	C178[3]	3.481(13)
C160	O214[2]	3.537(11)	C160	O220[2]	3.372(14)
C164	O133[7]	3.531(15)	C170	O64[9]	3.526(8)
C174	C91[8]	3.536(9)	C176	C34	3.598(10)
C178	O64[9]	3.526(10)	C178	O149[9]	3.413(9)
C178	N9	3.221(12)	C178	C49	3.528(12)
C178	C57[9]	3.381(10)	C178	C150[9]	3.481(13)
C188	O58[10]	3.599(10)	C188	C79[10]	3.571(14)
C188	C89[8]	3.506(15)	C190	O251	3.30(7)
C190	C33	3.441(9)	C190	C91[8]	3.503(13)
C192	O232[8]	3.336(15)	C192	C233[8]	3.590(17)
C194	O78[10]	3.505(10)	C204	O11	3.388(14)
C204	O251	2.04(7)	C204	O252	3.10(3)
C205	O11	3.19(3)	C205	O251	2.75(7)
C205	O252	2.20(4)	C219	C46	3.590(9)
C231	C103[7]	3.569(14)	C233	O191[4]	3.423(11)
C233	C192[4]	3.590(17)	C235	N7[9]	3.457(9)
C235	N9	3.350(12)	C236	O114[7]	3.349(8)
C237	O114[7]	3.543(9)	C247	O250	3.385(9)
C247	C27	3.417(10)	C247	C28	3.479(10)

Symmetry Operators:

(1) X+1,Y,Z+1
(2) X,Y,Z+1
(3) X+1,Y+1,Z+1
(4) X+1,Y,Z
(5) X,Y,Z-1
(6) X,Y+1,Z
(7) X,Y-1,Z
(8) X-1,Y,Z
(9) X-1,Y-1,Z-1
(10) X-1,Y,Z-1

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O10	H16E	3.074	O10	H24C	3.514
O10	H24H	2.950	O10	H77A	2.954
O11	H11F	3.111	O11	H11H	3.560
O11	H13B	2.578	O11	H13C	3.432
O58	H18C[1]	3.204	O58	H18D[1]	3.234
O59	H40	3.581	O59	H41	2.890
O60	H19H[1]	3.380	O60	H179[1]	3.002
O62	H21F[2]	3.345	O62	H21H[2]	3.545
O62	H45[2]	2.462	O64	H10A[2]	3.456
O64	H10D[2]	3.312	O64	H17B[3]	2.990
O64	H17J[3]	3.004	O72	H20A[1]	3.589
O72	H194[1]	2.991	O76	H19H[1]	2.668
O76	H20D[1]	2.923	O78	H18D[1]	3.023
O78	H20A[1]	3.127	O78	H194[1]	2.616
O78	H196[1]	3.079	O87	H23	2.770
O87	H24	3.135	O88	H19C[4]	3.225
O88	H24	3.043	O88	H44	3.480
O90	H19C[4]	2.781	O90	H34[4]	2.428
O92	H14H[4]	3.101	O100	H22B[3]	3.434
O100	H22C[3]	3.559	O101	H38	3.095
O102	H14C[5]	3.149	O102	H14D[5]	3.293
O102	H137[5]	3.594	O104	H65C[5]	2.526
O106	H16B[6]	3.369	O106	H151[6]	3.148
O114	H24E[7]	3.555	O114	H236[7]	2.886
O114	H237[7]	2.820	O115	H38	3.310
O118	H14C[5]	3.387	O118	H24K[7]	3.114
O120	H24D[7]	3.551	O120	H237[7]	2.667
O120	H239[7]	3.555	O129	H18	3.394
O129	H19	3.041	O130	H18	3.299
O133	H16I[7]	2.626	O135	H24E[7]	2.895
O135	H154[7]	3.414	O135	H236[7]	2.856
O143	H17J[3]	3.016	O145	H20C[2]	3.116
O145	H21H[2]	2.688	O147	H93C[8]	2.733
O149	H17J[3]	3.072	O149	H17K[3]	3.004
O149	H40	3.546	O158	H13	3.056
O158	H14	3.406	O159	H14	3.156
O161	H13D[9]	3.587	O161	H13F[9]	2.564

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O163	H11D[9]	2.592	O163	H108[9]	3.108
O163	H125[9]	3.310	O171	H10A[10]	3.479
O171	H23C[8]	3.313	O172	H13	3.466
O173	H12C[10]	3.145	O173	H75C[8]	3.513
O173	H91A[8]	3.495	O173	H91C[8]	2.649
O175	H12A[10]	3.035	O175	H22C[2]	2.992
O177	H49	2.901	O177	H57A[11]	3.265
O177	H57B[11]	3.459	O177	H65A[11]	2.834
O185	H61B[12]	2.720	O185	H61C[12]	3.131
O186	H50	3.501	O186	H51	2.842
O187	H89A[8]	3.288	O187	H89C[8]	2.843
O189	H44[8]	2.544	O189	H89A[8]	3.526
O189	H89C[8]	3.234	O189	H91A[8]	2.907
O189	H91C[8]	3.441	O191	H23D[8]	3.346
O191	H23F[8]	2.840	O199	H67[12]	2.582
O199	H69[12]	3.396	O199	H75B[12]	3.499
O203	H79C[12]	2.557	O206	H75A[12]	3.295
O214	H10H[11]	2.652	O214	H16A[5]	2.974
O214	H16C[5]	3.436	O215	H29	3.062
O216	H61A[5]	3.478	O216	H63C[5]	3.030
O218	H35[5]	2.338	O218	H63C[5]	3.062
O220	H10H[11]	3.343	O220	H16A[5]	3.551
O220	H16B[5]	2.992	O220	H16C[5]	3.050
O220	H17H[5]	3.183	O228	H93B[11]	3.140
O230	H17C[4]	3.080	O230	H17D[4]	3.409
O230	H19F[4]	3.117	O230	H165[4]	3.535
O232	H19F[4]	2.407	O234	H49	2.971
O234	H93B[11]	2.985	O242	H11D[9]	3.346
O242	H108[9]	2.627	O242	H109[9]	2.929
O243	H48	2.944	O246	H12C[9]	3.027
O246	H17C[4]	3.098	O246	H17E[4]	3.474
O248	H11C[9]	3.089	O248	H109[9]	2.392
O250	H17E[4]	3.295	O250	H24D	3.370
O250	H24G	2.763	O250	H24H	3.281
O250	H43	3.108	O250	H75C	3.256
O250	H77A	3.055	O250	H91B	2.477
O251	H13A	3.365	O251	H13B	3.212

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O251	H13C	2.538	O251	H19A	2.361
O251	H19B	3.553	O251	H33	3.551
O251	H181	2.947	O252	H11F	2.936
O252	H11G	3.518	O252	H11H	1.926
O252	H14E[5]	3.542	O252	H20C	3.390
O252	H21G	3.501	N2	H16E	3.218
N3	H13B	3.246	N4	H11F	2.973
N5	H24H	2.843	N6	H14F	3.468
N6	H14G	3.207	N6	H14H	3.425
N6	H17G	3.253	N6	H17H	3.484
N6	H66[8]	3.446	N6	H193[2]	3.449
N7	H15B	3.383	N7	H15C	2.742
N7	H23G[3]	3.016	N7	H23H[3]	3.476
N7	H23I[3]	3.323	N7	H99B	3.550
N8	H10D	3.177	N8	H10F	3.177
N8	H18C[4]	3.526	N8	H23E	3.411
N8	H23F	3.422	N8	H53[5]	3.052
N8	H61B[5]	3.046	N8	H89C	3.465
N8	H180[4]	2.773	N9	H17I	2.901
N9	H17K	2.892	N9	H22D	3.397
N9	H23H	2.682	C12	H16E	3.550
C12	H153	3.587	C13	H16E	3.584
C13	H19B	3.491	C13	H153	2.908
C13	H167	3.467	C13	H169	3.569
C14	H16D	3.294	C14	H16E	3.275
C14	H17G	3.503	C14	H19A	3.521
C14	H19B	3.022	C14	H153	2.989
C14	H167	3.302	C15	H16D	3.258
C15	H16E	3.032	C16	H13A	3.241
C16	H16D	3.304	C16	H16E	3.505
C17	H13A	3.125	C17	H13B	3.259
C18	H13A	3.253	C18	H13B	3.596
C18	H14G	3.565	C18	H63A	3.562
C18	H63B	3.403	C18	H124	3.146
C18	H139	3.314	C19	H124	2.961
C19	H141	3.476	C20	H13B	3.534
C20	H124	3.518	C22	H11F	3.130

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C23	H11F	3.240	C23	H82	2.944
C23	H84	3.579	C23	H96	3.354
C24	H10F	3.196	C24	H11F	3.117
C24	H11G	3.288	C24	H82	2.907
C24	H91B	3.567	C24	H96	3.142
C25	H11F	2.904	C25	H11G	3.454
C26	H11F	3.445	C26	H11H	3.526
C26	H24G	3.402	C26	H24H	3.376
C27	H24F	3.446	C27	H24G	3.447
C27	H24H	2.834	C28	H21G	3.276
C28	H23E	3.333	C28	H24F	3.109
C28	H24H	3.097	C28	H210	3.123
C28	H224	3.345	C29	H24F	3.379
C29	H24H	3.213	C29	H210	3.132
C29	H224	3.470	C30	H24H	3.024
C32	H13A	3.513	C32	H16D	3.414
C33	H13A	3.183	C33	H14G	3.489
C33	H17G	3.417	C33	H19A	3.406
C33	H19B	3.184	C33	H19C	3.163
C34	H14G	3.287	C34	H17F	3.366
C34	H17G	3.160	C34	H19C	3.361
C34	$H66^{8}$	3.586	C35	H14F	3.285
C35	H14G	3.264	C35	H16C	3.240
C35	H17G	3.521	C35	H63C	3.412
C35	$H209^{2}$	3.506	C35	$H211^{2}$	3.550
C36	H14G	3.481	C36	H16D	3.038
C36	H63A	3.360	C36	H63B	3.356
C36	H63C	3.310	C38	H98	3.017
C38	H110	3.394	C38	H112	3.112
C39	H15B	3.406	C39	H15C	3.338
C39	H98	2.854	C39	H99A	3.432
C39	H99B	3.540	C39	H112	3.284
C40	H15C	3.566	C40	$H23G^{3}$	3.539
C40	$H23I^{3}$	3.445	C40	H56	3.147
C40	H70	2.994	C40	H84	3.597
C40	H85B	3.591	C41	H56	3.247
C41	H68	3.286	C41	H70	3.126

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C42	H10F	3.199	C42	H23E	3.577
C42	H24G	3.593	C43	H10F	3.277
C43	H17D[4]	3.435	C43	H17E[4]	3.307
C43	H24G	3.193	C43	H91A	3.014
C43	H91B	3.384	C44	H10F	3.236
C44	H17D[4]	3.307	C44	H23D	3.476
C44	H89C	3.263	C44	H91A	3.077
C44	H180[4]	2.942	C44	H182[4]	3.511
C45	H10D	3.213	C45	H10E	3.359
C45	H10F	3.068	C45	H14D[5]	3.517
C45	H21F	3.163	C45	H23E	3.250
C45	H53[5]	3.340	C46	H10E	3.446
C46	H10F	3.078	C46	H14D[5]	3.487
C46	H14E[5]	3.510	C46	H21F	3.040
C46	H21G	3.375	C46	H23E	3.354
C48	H155	3.527	C48	H226	3.355
C48	H238	3.408	C48	H240	3.180
C49	H17I	3.402	C49	H17K	3.325
C49	H23H	3.400	C49	H226	3.175
C49	H240	3.335	C50	H17I	3.430
C50	H23H	3.598	C50	H183	3.002
C50	H197	3.183	C50	H212	3.214
C51	H183	3.194	C51	H195	3.141
C51	H197	3.485	C52	H18C[1]	3.372
C52	H18D[1]	3.131	C52	H179[1]	3.330
C52	H196[1]	3.590	C53	H18C[1]	3.513
C53	H45[2]	3.500	C53	H179[1]	3.318
C54	H45[2]	3.331	C56	H40	3.433
C57	H17J[3]	2.946	C57	H17K[3]	3.198
C61	H19G[1]	3.532	C61	H21E[2]	2.791
C61	H23F[2]	3.338	C61	H179[1]	3.092
C63	H18	3.534	C63	H21E[2]	3.523
C63	H21F[2]	3.294	C63	H21H[2]	3.250
C63	H35	3.571	C63	H36	2.905
C63	H45[2]	3.544	C65	H10D[2]	3.028
C65	H15D[3]	2.974	C65	H16G[3]	3.366
C65	H17A[3]	3.347	C65	H17B[3]	3.342

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C67	H19H[1]	3.397	C68	H19H[1]	3.272
C68	H41	3.372	C69	H19H[1]	3.318
C69	H41	3.423	C69	H196[1]	3.455
C70	H40	3.305	C70	H41	3.555
C71	H40	3.357	C71	H194[1]	3.560
C75	H12B[9]	3.258	C75	H17F[4]	3.401
C75	H17H[4]	3.190	C75	H22A[1]	3.429
C77	H20D[1]	3.550	C77	H24C	3.126
C79	H11C[1]	3.236	C79	H18D[1]	3.012
C79	H18E[1]	3.226	C79	H20A[1]	3.293
C79	H24A[3]	3.537	C79	H24J[3]	3.251
C79	H194[1]	3.429	C81	H19C[4]	3.526
C82	H23	3.528	C82	H24	3.476
C82	H34[4]	3.445	C83	H34[4]	3.580
C84	H23	3.560	C85	H23G[3]	3.142
C89	H16G[6]	3.399	C89	H18C[4]	3.240
C89	H18E[4]	3.255	C89	H19C[4]	3.287
C91	H17E[4]	2.860	C91	H17F[4]	3.377
C91	H19C[4]	2.776	C91	H34[4]	3.373
C91	H43	2.925	C91	H44	3.478
C93	H14H[4]	3.105	C93	H22E[3]	3.405
C93	H24I[3]	3.344	C96	H24	3.539
C97	H23	3.587	C98	H39	3.313
C99	H22B[3]	3.429	C99	H39	3.379
C103	H14C[5]	3.197	C103	H17B[6]	3.327
C103	H23A[7]	3.422	C103	H23B[7]	3.310
C103	H23C[7]	3.382	C103	H137[5]	3.329
C105	H14D[5]	3.292	C105	H24	3.300
C105	H55[5]	3.560	C105	H65B[5]	3.584
C105	H65C[5]	2.995	C107	H16A[6]	3.297
C107	H16B[6]	3.360	C107	H22E[3]	3.515
C107	H152[6]	3.580	C108	H236[7]	3.160
C110	H38	3.287	C111	H38	3.401
C112	H38	3.287	C112	H39	3.575
C113	H22B[3]	3.530	C113	H237[7]	3.336
C117	H24A[7]	3.296	C117	H24J[7]	3.285
C117	H79C[12]	3.316	C119	H14C[5]	3.500

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C119	H14E[5]	3.312	C119	H46	3.572
C121	H17C[6]	3.177	C121	H22A[3]	3.540
C121	H22C[3]	3.170	C121	H24D[7]	3.208
C121	H75A[7]	3.594	C121	H75C[7]	3.325
C121	H166[6]	3.292	C121	H237[7]	3.279
C124	H16I[7]	3.545	C131	H33	3.417
C131	H34	3.474	C131	H81[8]	2.714
C131	H83[8]	3.223	C132	H81[8]	3.053
C132	H83[8]	3.181	C132	H93C[8]	3.513
C134	H16I[7]	3.553	C134	H33	3.431
C136	H24E[7]	3.338	C137	H10C[2]	3.541
C138	H10C[2]	3.479	C139	H18	3.480
C141	H19	3.439	C142	H17J[3]	3.410
C142	H19D[3]	3.143	C146	H10C[2]	3.260
C146	H10E[2]	3.259	C146	H11G[2]	3.399
C146	H11H[2]	3.358	C146	H20C[2]	3.094
C146	H21H[2]	2.930	C146	H24K[13]	3.497
C146	H46[2]	3.313	C148	H18	3.434
C148	H20B[2]	3.155	C148	H20C[2]	3.567
C148	H93C[8]	3.173	C150	H17I[3]	3.409
C150	H17J[3]	3.482	C150	H17K[3]	2.997
C150	H18A[3]	3.371	C150	H23H[3]	3.529
C150	H39	3.581	C153	H13F[9]	3.569
C156	H11D[9]	3.427	C156	H65A[11]	3.207
C160	H10H[10]	3.444	C160	H10I[10]	3.421
C160	H209[2]	2.872	C162	H13F[9]	3.505
C162	H36	3.347	C164	H11D[9]	3.228
C164	H80[10]	3.249	C164	H89B[10]	3.276
C165	H23C[8]	3.109	C166	H12A[10]	3.585
C166	H12C[10]	3.436	C166	H23C[8]	3.205
C167	H14	3.537	C169	H13	3.488
C170	H10A[10]	3.353	C170	H65A[11]	3.209
C170	H65C[11]	3.520	C174	H12C[10]	2.868
C174	H23C[8]	3.216	C174	H23D[8]	3.588
C174	H24G[8]	2.922	C174	H43[8]	3.275
C174	H44[8]	3.490	C174	H91A[8]	3.466
C174	H91C[8]	2.991	C176	H14	3.381

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C176	H22C[2]	3.214	C176	H75B[8]	3.281
C176	H75C[8]	3.320	C176	H91C[8]	3.403
C178	H15A[11]	3.018	C178	H15C[11]	3.496
C178	H49	3.376	C178	H57A[11]	3.231
C178	H57B[11]	2.896	C179	H52[12]	3.497
C179	H61B[12]	3.022	C180	H44[8]	3.210
C180	H61B[12]	3.504	C180	H89C[8]	3.390
C181	H44[8]	3.234	C182	H44[8]	3.496
C183	H50	3.586	C184	H15A[11]	3.113
C188	H52[12]	3.053	C188	H53[12]	3.523
C188	H65B[12]	3.257	C188	H79A[12]	3.233
C188	H79C[12]	3.216	C188	H89A[8]	3.511
C188	H89C[8]	2.823	C190	H14	3.464
C190	H33	2.759	C190	H89A[8]	3.241
C190	H91A[8]	3.080	C190	H91C[8]	3.285
C192	H14B[11]	2.985	C192	H23A[8]	3.348
C192	H23F[8]	3.173	C192	H223[8]	3.535
C193	H67[12]	3.462	C195	H51	3.108
C195	H79C[12]	3.579	C196	H51	3.356
C196	H52[12]	3.584	C196	H69[12]	3.339
C197	H50	3.346	C197	H67[12]	3.506
C197	H69[12]	3.558	C198	H67[12]	3.369
C198	H69[12]	3.405	C202	H14E[5]	3.445
C202	H14F[5]	3.315	C202	H14H[5]	3.361
C202	H24J[7]	3.553	C204	H11E	3.409
C204	H51	3.209	C205	H11E	3.257
C205	H79C[12]	3.337	C207	H13D[11]	3.493
C207	H24E[12]	3.557	C207	H75A[12]	3.415
C208	H10H[11]	3.477	C208	H16A[5]	3.174
C209	H16A[5]	3.189	C209	H16C[5]	3.405
C209	H35[5]	3.372	C210	H35[5]	3.218
C211	H35[5]	3.541	C217	H61A[5]	2.986
C217	H63C[5]	3.302	C219	H14E[5]	3.000
C219	H28	3.368	C219	H35[5]	3.349
C219	H45	3.520	C219	H46	2.909
C219	H63C[5]	2.891	C221	H11B[11]	3.226
C221	H12A[11]	3.113	C221	H12B[11]	3.484

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C221	H16B[5]	3.471	C221	H17H[5]	3.169
C221	H75A[12]	3.578	C221	H99A[11]	3.295
C223	H19F[4]	3.198	C224	H19F[4]	3.318
C227	H93B[11]	3.076	C231	H10B[9]	3.082
C231	H10C[9]	3.294	C231	H17C[4]	3.145
C231	H19D[4]	3.529	C231	H19F[4]	3.554
C231	H165[4]	3.255	C231	H166[4]	3.568
C233	H19F[4]	2.888	C233	H28	3.358
C235	H15C[11]	3.267	C235	H40[11]	3.476
C235	H49	3.446	C235	H85A[11]	3.264
C235	H93B[11]	3.516	C236	H108[9]	3.054
C238	H48	3.489	C240	H48	3.434
C240	H109[9]	3.561	C241	H11C[9]	3.285
C241	H79B[11]	3.460	C241	H109[9]	3.194
C245	H12B[9]	3.278	C245	H20D[1]	3.344
C245	H77C	3.350	C247	H17C[4]	3.290
C247	H17E[4]	3.207	C247	H43	3.516
C249	H11C[9]	3.089	C249	H20A[9]	3.440
C249	H79B[11]	3.251	C249	H109[9]	3.053
H10A	O64[5]	3.456	H10A	O171[6]	3.479
H10A	C170[6]	3.353	H10A	H17B[6]	2.398
H10A	H17J[6]	3.566	H10A	H23A[7]	3.517
H10A	H23C[7]	3.508	H10A	H137[5]	2.999
H10B	C231[7]	3.082	H10B	H17B[6]	3.577
H10B	H23A[7]	3.197	H10B	H23B[7]	2.795
H10B	H23C[7]	2.752	H10B	H166[6]	3.313
H10C	C137[5]	3.541	H10C	C138[5]	3.479
H10C	C146[5]	3.260	H10C	C231[7]	3.294
H10C	H14C[5]	2.463	H10C	H14D[5]	3.287
H10C	H23A[7]	3.007	H10C	H23B[7]	2.958
H10C	H23C[7]	3.384	H10C	H24K[7]	3.501
H10C	H137[5]	3.002	H10C	H138[5]	2.760
H10D	O64[5]	3.312	H10D	N8	3.177
H10D	C45	3.213	H10D	C65[5]	3.028
H10D	H14D[5]	3.532	H10D	H18C[4]	3.230
H10D	H45	3.336	H10D	H55[5]	2.974
H10D	H65B[5]	2.810	H10D	H65C[5]	2.625

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H10E	C45	3.359	H10E	C46	3.446
H10E	C146[5]	3.259	H10E	H14C[5]	3.448
H10E	H14D[5]	2.375	H10E	H45	3.411
H10E	H46	3.545	H10E	H55[5]	3.233
H10E	H65C[5]	3.336	H10E	H137[5]	3.259
H10F	N8	3.177	H10F	C24	3.196
H10F	C42	3.199	H10F	C43	3.277
H10F	C44	3.236	H10F	C45	3.068
H10F	C46	3.078	H10F	H24	2.387
H10F	H45	3.535	H10F	H46	3.536
H10G	H22E[3]	3.001	H10H	O214[3]	2.652
H10H	O220[3]	3.343	H10H	C160[6]	3.444
H10H	C208[3]	3.477	H10H	H16A[6]	2.944
H10H	H16B[6]	3.050	H10H	H21A[3]	3.278
H10H	H22D[3]	3.417	H10H	H22E[3]	3.155
H10H	H208[3]	3.179	H10I	C160[6]	3.421
H10I	H16A[6]	2.831	H10I	H16B[6]	3.166
H10I	H151[6]	3.445	H10I	H152[6]	2.764
H10I	H208[3]	3.456	H11A	H20F[3]	2.681
H11A	H22A[3]	3.448	H11A	H22B[3]	3.435
H11A	H24D[7]	3.469	H11A	H24E[7]	2.960
H11A	H237[7]	3.219	H11B	C221[3]	3.226
H11B	H22A[3]	3.358	H11B	H22B[3]	2.756
H11B	H22C[3]	3.053	H11B	H39	3.231
H11C	O248[7]	3.089	H11C	C79[12]	3.236
H11C	C241[7]	3.285	H11C	C249[7]	3.089
H11C	H24A[7]	2.619	H11C	H24J[7]	2.356
H11C	H24K[7]	3.549	H11C	H79A[12]	3.497
H11C	H79B[12]	3.053	H11C	H79C[12]	2.685
H11D	O163[7]	2.592	H11D	O242[7]	3.346
H11D	C156[7]	3.427	H11D	C164[7]	3.228
H11D	H15E[7]	3.215	H11D	H16G[7]	3.487
H11D	H16I[7]	2.995	H11D	H24A[7]	3.103
H11E	C204	3.409	H11E	C205	3.257
H11E	H16I[7]	3.511	H11E	H18E	3.335
H11E	H79C[12]	3.075	H11F	O11	3.111
H11F	O252	2.936	H11F	N4	2.973

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H11F	C22	3.130	H11F	C23	3.240
H11F	C24	3.117	H11F	C25	2.904
H11F	C26	3.445	H11G	O252	3.518
H11G	C24	3.288	H11G	C25	3.454
H11G	C146[5]	3.399	H11G	H14C[5]	3.250
H11G	H14D[5]	3.206	H11G	H14E[5]	3.168
H11G	H24	3.355	H11G	H46	3.266
H11H	O11	3.560	H11H	O252	1.926
H11H	C26	3.526	H11H	C146[5]	3.358
H11H	H14C[5]	3.301	H11H	H14D[5]	3.548
H11H	H14E[5]	2.733	H11H	H46	3.023
H12A	O175[6]	3.035	H12A	C166[6]	3.585
H12A	C221[3]	3.113	H12A	H17C[6]	3.454
H12A	H17H[6]	3.515	H12A	H22A[3]	3.149
H12A	H22B[3]	3.368	H12A	H22C[3]	2.396
H12A	H75C[7]	3.391	H12A	H166[6]	2.931
H12B	C75[7]	3.258	H12B	C221[3]	3.484
H12B	C245[7]	3.278	H12B	H20F[3]	3.360
H12B	H22A[3]	3.048	H12B	H22C[3]	3.125
H12B	H24D[7]	2.501	H12B	H24E[7]	3.227
H12B	H75A[7]	2.782	H12B	H75C[7]	2.837
H12B	H237[7]	3.214	H12C	O173[6]	3.145
H12C	O246[7]	3.027	H12C	C166[6]	3.436
H12C	C174[6]	2.868	H12C	H17C[6]	2.225
H12C	H17E[6]	2.961	H12C	H23C[7]	3.561
H12C	H24D[7]	3.287	H12C	H75C[7]	3.217
H12C	H166[6]	2.798	H12C	H237[7]	3.301
H12D	H19E[3]	3.219	H12D	H20E[3]	3.110
H12D	H20F[3]	3.259	H12E	H20F[3]	3.236
H12E	H24E[7]	3.367	H13	O158	3.056
H13	O172	3.466	H13	C169	3.488
H13	H19B	3.544	H13	H153	2.974
H13	H167	3.032	H13	H169	2.635
H13	H181	3.423	H13A	O251	3.365
H13A	C16	3.241	H13A	C17	3.125
H13A	C18	3.253	H13A	C32	3.513
H13A	C33	3.183	H13A	H18	3.383

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H13A	H33	2.619	H13B	O11	2.578
H13B	O251	3.212	H13B	N3	3.246
H13B	C17	3.259	H13B	C18	3.596
H13B	C20	3.534	H13C	O11	3.432
H13C	O251	2.538	H13C	H16I[7]	3.393
H13C	H19A	3.358	H13C	H33	3.421
H13C	H89A[8]	3.436	H13D	O161[7]	3.587
H13D	C207[3]	3.493	H13D	H16F[7]	3.560
H13D	H19E[3]	3.499	H13D	H20D[3]	3.457
H13D	H20E[3]	2.955	H13D	H20F[3]	3.521
H13D	H21D[13]	3.575	H13D	H24C[7]	3.346
H13D	H24E[7]	3.012	H13E	H19E[3]	3.180
H13E	H21D[13]	3.388	H13F	O161[7]	2.564
H13F	C153[7]	3.569	H13F	C162[7]	3.505
H13F	H16F[7]	3.341	H13F	H21C[13]	3.457
H13F	H21D[13]	3.423	H13F	H24E[7]	3.524
H13F	H152[7]	3.294	H13F	H154[7]	3.066
H13F	H236[7]	3.477	H14	O158	3.406
H14	O159	3.156	H14	C167	3.537
H14	C176	3.381	H14	C190	3.464
H14	H16D	3.274	H14	H17F	3.536
H14	H17G	2.556	H14	H19A	3.505
H14	H19B	2.636	H14	H153	3.112
H14	H167	2.670	H14A	H19D[3]	3.315
H14A	H19E[3]	3.361	H14B	C192[3]	2.985
H14B	H17I[3]	3.595	H14B	H17J[3]	2.993
H14B	H18A[3]	3.496	H14B	H18B[3]	3.343
H14B	H19D[3]	2.217	H14B	H19E[3]	2.933
H14C	O102[2]	3.149	H14C	O118[2]	3.387
H14C	C103[2]	3.197	H14C	C119[2]	3.500
H14C	H10C[2]	2.463	H14C	H10E[2]	3.448
H14C	H11G[2]	3.250	H14C	H11H[2]	3.301
H14C	H20C[2]	3.289	H14C	H24K[13]	2.718
H14D	O102[2]	3.293	H14D	C45[2]	3.517
H14D	C46[2]	3.487	H14D	C105[2]	3.292
H14D	H10C[2]	3.287	H14D	H10D[2]	3.532
H14D	H10E[2]	2.375	H14D	H11G[2]	3.206

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H14D	H11H[2]	3.548	H14D	H21H[2]	3.335
H14D	H45[2]	3.080	H14D	H46[2]	3.033
H14E	O252[2]	3.542	H14E	C46[2]	3.510
H14E	C119[2]	3.312	H14E	C202[2]	3.445
H14E	C219[2]	3.000	H14E	H11G[2]	3.168
H14E	H11H[2]	2.733	H14E	H20C[2]	2.492
H14E	H21F[2]	3.344	H14E	H21G[2]	2.862
H14E	H21H[2]	2.386	H14E	H24K[13]	3.514
H14E	H46[2]	2.707	H14F	N6	3.468
H14F	C35	3.285	H14F	C202[2]	3.315
H14F	H18	3.538	H14F	H20B[2]	2.749
H14F	H20C[2]	2.998	H14F	H21H[2]	2.881
H14F	H35	3.265	H14G	N6	3.207
H14G	C18	3.565	H14G	C33	3.489
H14G	C34	3.287	H14G	C35	3.264
H14G	C36	3.481	H14G	H18	2.651
H14H	O92[8]	3.101	H14H	N6	3.425
H14H	C93[8]	3.105	H14H	C202[2]	3.361
H14H	H20A[2]	3.548	H14H	H20B[2]	2.678
H14H	H20C[2]	3.380	H14H	H83[8]	3.560
H14H	H93A[8]	3.114	H14H	H93C[8]	2.658
H15A	C178[3]	3.018	H15A	C184[3]	3.113
H15A	H17I[3]	2.714	H15A	H17J[3]	3.081
H15A	H17K[3]	2.757	H15A	H18A[3]	2.473
H15A	H18B[3]	2.862	H15A	H19D[3]	3.405
H15A	H19E[3]	3.437	H15B	N7	3.383
H15B	C39	3.406	H15B	H18A[3]	3.503
H15B	H39	3.156	H15C	N7	2.742
H15C	C39	3.338	H15C	C40	3.566
H15C	C178[3]	3.496	H15C	C235[3]	3.267
H15C	H17I[3]	3.507	H15C	H17K[3]	2.793
H15C	H23G[3]	3.503	H15C	H23H[3]	2.590
H15C	H23I[3]	3.250	H15C	H39	3.269
H15D	C65[11]	2.974	H15D	H65A[11]	2.255
H15D	H65B[11]	3.423	H15D	H65C[11]	2.903
H15E	H11D[9]	3.215	H15E	H65A[11]	3.433
H16A	O214[2]	2.974	H16A	O220[2]	3.551

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H16A	C107[10]	3.297	H16A	C208[2]	3.174
H16A	C209[2]	3.189	H16A	H10H[10]	2.944
H16A	H10I[10]	2.831	H16A	H21C[2]	2.991
H16A	H208[2]	2.867	H16A	H209[2]	2.421
H16B	O106[10]	3.369	H16B	O220[2]	2.992
H16B	C107[10]	3.360	H16B	C221[2]	3.471
H16B	H10H[10]	3.050	H16B	H10I[10]	3.166
H16B	H22C[2]	3.014	H16C	O214[2]	3.436
H16C	O220[2]	3.050	H16C	C35	3.240
H16C	C209[2]	3.405	H16C	H35	3.123
H16C	H209[2]	2.475	H16C	H211[2]	2.953
H16D	C14	3.294	H16D	C15	3.258
H16D	C16	3.304	H16D	C32	3.414
H16D	C36	3.038	H16D	H14	3.274
H16D	H21C[2]	3.282	H16D	H36	2.532
H16E	O10	3.074	H16E	N2	3.218
H16E	C12	3.550	H16E	C13	3.584
H16E	C14	3.275	H16E	C15	3.032
H16E	C16	3.505	H16F	H13D[9]	3.560
H16F	H13F[9]	3.341	H16F	H21C[2]	3.362
H16F	H36	3.393	H16F	H77C	2.806
H16G	C65[11]	3.366	H16G	C89[10]	3.399
H16G	H11D[9]	3.487	H16G	H65A[11]	3.210
H16G	H65B[11]	3.437	H16G	H65C[11]	2.912
H16G	H80[10]	3.202	H16G	H89A[10]	3.363
H16G	H89B[10]	2.605	H16H	H80[10]	2.814
H16H	H89B[10]	3.499	H16H	H97[10]	3.217
H16I	O133[9]	2.626	H16I	C124[9]	3.545
H16I	C134[9]	3.553	H16I	H11D[9]	2.995
H16I	H11E[9]	3.511	H16I	H13C[9]	3.393
H16I	H80[10]	3.197	H16I	H89A[10]	3.344
H16I	H89B[10]	3.260	H16I	H123[9]	2.981
H16I	H125[9]	3.252	H17A	C65[11]	3.347
H17A	H65A[11]	2.925	H17A	H65C[11]	3.094
H17A	H95[10]	3.404	H17B	O64[11]	2.990
H17B	C65[11]	3.342	H17B	C103[10]	3.327
H17B	H10A[10]	2.398	H17B	H10B[10]	3.577

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17B	H65A[11]	3.216	H17B	H65C[11]	3.215
H17B	H95[10]	3.181	H17C	O230[8]	3.080
H17C	O246[8]	3.098	H17C	C121[10]	3.177
H17C	C231[8]	3.145	H17C	C247[8]	3.290
H17C	H12A[10]	3.454	H17C	H12C[10]	2.225
H17C	H23B[8]	3.519	H17C	H23C[8]	2.478
H17C	H24F[8]	3.423	H17C	H24G[8]	2.837
H17D	O230[8]	3.409	H17D	C43[8]	3.435
H17D	C44[8]	3.307	H17D	H23C[8]	3.224
H17D	H23D[8]	2.812	H17D	H24G[8]	3.112
H17D	H43[8]	3.100	H17D	H44[8]	2.861
H17D	H91A[8]	3.548	H17D	H91C[8]	3.482
H17E	O246[8]	3.474	H17E	O250[8]	3.295
H17E	C43[8]	3.307	H17E	C91[8]	2.860
H17E	C247[8]	3.207	H17E	H12C[10]	2.961
H17E	H24F[8]	3.563	H17E	H24G[8]	2.369
H17E	H43[8]	2.580	H17E	H44[8]	3.348
H17E	H75C[8]	3.185	H17E	H91A[8]	2.896
H17E	H91B[8]	2.747	H17E	H91C[8]	2.464
H17F	C34	3.366	H17F	C75[8]	3.401
H17F	C91[8]	3.377	H17F	H14	3.536
H17F	H34	3.210	H17F	H75B[8]	3.054
H17F	H75C[8]	2.842	H17F	H91C[8]	2.448
H17G	N6	3.253	H17G	C14	3.503
H17G	C33	3.417	H17G	C34	3.160
H17G	C35	3.521	H17G	H14	2.556
H17G	H34	3.463	H17H	O220[2]	3.183
H17H	N6	3.484	H17H	C75[8]	3.190
H17H	C221[2]	3.169	H17H	H12A[10]	3.515
H17H	H22A[2]	3.361	H17H	H22C[2]	2.561
H17H	H75A[8]	3.536	H17H	H75B[8]	2.627
H17H	H75C[8]	2.969	H17I	N9	2.901
H17I	C49	3.402	H17I	C50	3.430
H17I	C150[11]	3.409	H17I	H14B[11]	3.595
H17I	H15A[11]	2.714	H17I	H15C[11]	3.507
H17I	H49	3.517	H17I	H50	3.580
H17J	O64[11]	3.004	H17J	O143[11]	3.016

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17J	O149[11]	3.072	H17J	C57[11]	2.946
H17J	C142[11]	3.410	H17J	C150[11]	3.482
H17J	H10A[10]	3.566	H17J	H14B[11]	2.993
H17J	H15A[11]	3.081	H17J	H57A[11]	3.089
H17J	H57B[11]	2.338	H17K	O149[11]	3.004
H17K	N9	2.892	H17K	C49	3.325
H17K	C57[11]	3.198	H17K	C150[11]	2.997
H17K	H15A[11]	2.757	H17K	H15C[11]	2.793
H17K	H49	3.095	H17K	H57A[11]	2.872
H17K	H57B[11]	2.709	H18	O129	3.394
H18	O130	3.299	H18	C63	3.534
H18	C139	3.480	H18	C148	3.434
H18	H13A	3.383	H18	H14F	3.538
H18	H14G	2.651	H18	H63A	3.364
H18	H63B	2.839	H18	H124	3.361
H18	H139	2.585	H18A	C150[11]	3.371
H18A	H14B[11]	3.496	H18A	H15A[11]	2.473
H18A	H15B[11]	3.503	H18A	H50	3.520
H18B	H14B[11]	3.343	H18B	H15A[11]	2.862
H18C	O58[12]	3.204	H18C	N8[8]	3.526
H18C	C52[12]	3.372	H18C	C53[12]	3.513
H18C	C89[8]	3.240	H18C	H10D[8]	3.230
H18C	H52[12]	2.933	H18C	H53[12]	2.782
H18C	H65B[12]	2.833	H18C	H89A[8]	3.516
H18C	H89B[8]	3.386	H18C	H89C[8]	2.425
H18D	O58[12]	3.234	H18D	O78[12]	3.023
H18D	C52[12]	3.131	H18D	C79[12]	3.012
H18D	H52[12]	2.331	H18D	H53[12]	3.406
H18D	H65B[12]	3.524	H18D	H79A[12]	2.853
H18D	H79C[12]	2.721	H18E	C79[12]	3.226
H18E	C89[8]	3.255	H18E	H11E	3.335
H18E	H65B[12]	2.930	H18E	H79A[12]	2.803
H18E	H79C[12]	2.827	H18E	H89A[8]	3.152
H18E	H89B[8]	3.267	H18E	H89C[8]	2.816
H19	O129	3.041	H19	C141	3.439
H19	H124	3.029	H19	H139	3.266
H19	H141	2.575	H19A	O251	2.361

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19A	C14	3.521	H19A	C33	3.406
H19A	H13C	3.358	H19A	H14	3.505
H19A	H33	2.571	H19A	H89A[8]	3.027
H19A	H89C[8]	3.588	H19B	O251	3.553
H19B	C13	3.491	H19B	C14	3.022
H19B	C33	3.184	H19B	H13	3.544
H19B	H14	2.636	H19B	H33	2.707
H19B	H34	3.523	H19B	H91A[8]	3.541
H19B	H91C[8]	3.295	H19C	O88[8]	3.225
H19C	O90[8]	2.781	H19C	C33	3.163
H19C	C34	3.361	H19C	C81[8]	3.526
H19C	C89[8]	3.287	H19C	C91[8]	2.776
H19C	H33	2.530	H19C	H34	2.894
H19C	H81[8]	3.092	H19C	H89A[8]	2.801
H19C	H89C[8]	3.357	H19C	H91A[8]	2.447
H19C	H91C[8]	2.715	H19D	C142[11]	3.143
H19D	C231[8]	3.529	H19D	H14A[11]	3.315
H19D	H14B[11]	2.217	H19D	H15A[11]	3.405
H19D	H23A[8]	2.815	H19D	H140[11]	3.585
H19D	H223[8]	3.481	H19E	H12D[11]	3.219
H19E	H13D[11]	3.499	H19E	H13E[11]	3.180
H19E	H14A[11]	3.361	H19E	H14B[11]	2.933
H19E	H15A[11]	3.437	H19E	H23F[8]	3.552
H19F	O230[8]	3.117	H19F	O232[8]	2.407
H19F	C223[8]	3.198	H19F	C224[8]	3.318
H19F	C231[8]	3.554	H19F	C233[8]	2.888
H19F	H21D[8]	3.591	H19F	H23A[8]	3.092
H19F	H23D[8]	3.059	H19F	H23F[8]	2.666
H19F	H223[8]	2.739	H19G	C61[12]	3.532
H19G	H61B[12]	3.509	H19G	H61C[12]	2.988
H19H	O60[12]	3.380	H19H	O76[12]	2.668
H19H	C67[12]	3.397	H19H	C68[12]	3.272
H19H	C69[12]	3.318	H19H	H52[12]	3.572
H19H	H61C[12]	3.405	H19H	H67[12]	2.680
H19H	H69[12]	2.593	H19H	H75A[12]	3.434
H20A	O72[12]	3.589	H20A	O78[12]	3.127
H20A	C79[12]	3.293	H20A	C249[7]	3.440

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H20A	H14H[5]	3.548	H20A	H24I[7]	3.353
H20A	H24J[7]	2.885	H20A	H24K[7]	3.555
H20A	H71A[12]	3.535	H20A	H79B[12]	3.059
H20A	H79C[12]	3.152	H20A	H93A[12]	3.133
H20B	C148[5]	3.155	H20B	H14F[5]	2.749
H20B	H14H[5]	2.678	H20C	O145[5]	3.116
H20C	O252	3.390	H20C	C146[5]	3.094
H20C	C148[5]	3.567	H20C	H14C[5]	3.289
H20C	H14E[5]	2.492	H20C	H14F[5]	2.998
H20C	H14H[5]	3.380	H20C	H24J[7]	3.364
H20C	H24K[7]	3.348	H20D	O76[12]	2.923
H20D	C77[12]	3.550	H20D	C245[12]	3.344
H20D	H13D[11]	3.457	H20D	H24C[12]	3.052
H20D	H24D[12]	3.242	H20D	H24E[12]	3.177
H20D	H61C[12]	3.451	H20D	H75A[12]	2.994
H20D	H77C[12]	3.131	H20E	H12D[11]	3.110
H20E	H13D[11]	2.955	H20E	H61C[12]	3.170
H20F	H11A[11]	2.681	H20F	H12B[11]	3.360
H20F	H12D[11]	3.259	H20F	H12E[11]	3.236
H20F	H13D[11]	3.521	H20F	H24D[12]	3.546
H20F	H24E[12]	3.138	H20F	H75A[12]	3.429
H21A	H10H[11]	3.278	H21A	H50	3.501
H21A	H99A[11]	3.365	H21B	H50	3.165
H21C	H13F[14]	3.457	H21C	H16A[5]	2.991
H21C	H16D[5]	3.282	H21C	H16F[5]	3.362
H21C	H36[5]	3.550	H21C	H61A[5]	3.524
H21C	H63C[5]	3.292	H21D	H13D[14]	3.575
H21D	H13E[14]	3.388	H21D	H13F[14]	3.423
H21D	H19F[4]	3.591	H21D	H61A[5]	3.505
H21E	C61[5]	2.791	H21E	C63[5]	3.523
H21E	H61A[5]	2.037	H21E	H61B[5]	3.347
H21E	H61C[5]	2.746	H21E	H63A[5]	3.386
H21E	H63C[5]	3.019	H21F	O62[5]	3.345
H21F	C45	3.163	H21F	C46	3.040
H21F	C63[5]	3.294	H21F	H14E[5]	3.344
H21F	H28	2.981	H21F	H45	2.779
H21F	H46	2.577	H21F	H63C[5]	2.554

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H21G	O252	3.501	H21G	C28	3.276
H21G	C46	3.375	H21G	H14E^{5}	2.862
H21G	H28	2.898	H21G	H46	2.584
H21H	O62^{5}	3.545	H21H	O145^{5}	2.688
H21H	C63^{5}	3.250	H21H	C146^{5}	2.930
H21H	H14D^{5}	3.335	H21H	H14E^{5}	2.386
H21H	H14F^{5}	2.881	H21H	H35^{5}	3.299
H21H	H45	3.500	H21H	H46	3.108
H21H	H63B^{5}	3.151	H21H	H63C^{5}	2.701
H22A	C75^{12}	3.429	H22A	C121^{11}	3.540
H22A	H11A^{11}	3.448	H22A	H11B^{11}	3.358
H22A	H12A^{11}	3.149	H22A	H12B^{11}	3.048
H22A	H17H^{5}	3.361	H22A	H75A^{12}	2.780
H22A	H75B^{12}	3.347	H22B	O100^{11}	3.434
H22B	C99^{11}	3.429	H22B	C113^{11}	3.530
H22B	H11A^{11}	3.435	H22B	H11B^{11}	2.756
H22B	H12A^{11}	3.368	H22B	H99A^{11}	2.514
H22C	O100^{11}	3.559	H22C	O175^{5}	2.992
H22C	C121^{11}	3.170	H22C	C176^{5}	3.214
H22C	H11B^{11}	3.053	H22C	H12A^{11}	2.396
H22C	H12B^{11}	3.125	H22C	H16B^{5}	3.014
H22C	H17H^{5}	2.561	H22C	H75A^{12}	3.584
H22C	H99A^{11}	3.448	H22D	N9	3.397
H22D	H10H^{11}	3.417	H22E	C93^{11}	3.405
H22E	C107^{11}	3.515	H22E	H10G^{11}	3.001
H22E	H10H^{11}	3.155	H22E	H85A^{11}	3.038
H22E	H93B^{11}	2.451	H23	O87	2.770
H23	C82	3.528	H23	C84	3.560
H23	C97	3.587	H23	H82	2.705
H23	H84	2.705	H23	H96	3.208
H23	H98	2.875	H23A	C103^{9}	3.422
H23A	C192^{4}	3.348	H23A	H10A^{9}	3.517
H23A	H10B^{9}	3.197	H23A	H10C^{9}	3.007
H23A	H19D^{4}	2.815	H23A	H19F^{4}	3.092
H23A	H165^{4}	3.395	H23B	C103^{9}	3.310
H23B	H10B^{9}	2.795	H23B	H10C^{9}	2.958
H23B	H17C^{4}	3.519	H23C	O171^{4}	3.313

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H23C	C103[9]	3.382	H23C	C165[4]	3.109
H23C	C166[4]	3.205	H23C	C174[4]	3.216
H23C	H10A[9]	3.508	H23C	H10B[9]	2.752
H23C	H10C[9]	3.384	H23C	H12C[9]	3.561
H23C	H17C[4]	2.478	H23C	H17D[4]	3.224
H23C	H165[4]	2.527	H23C	H166[4]	2.593
H23D	O191[4]	3.346	H23D	C44	3.476
H23D	C174[4]	3.588	H23D	H17D[4]	2.812
H23D	H19F[4]	3.059	H23D	H28	3.522
H23D	H182[4]	3.488	H23E	N8	3.411
H23E	C28	3.333	H23E	C42	3.577
H23E	C45	3.250	H23E	C46	3.354
H23E	H28	2.489	H23E	H45	3.590
H23F	O191[4]	2.840	H23F	N8	3.422
H23F	C61[5]	3.338	H23F	C192[4]	3.173
H23F	H19E[4]	3.552	H23F	H19F[4]	2.666
H23F	H61A[5]	3.102	H23F	H61B[5]	2.959
H23F	H61C[5]	3.412	H23F	H182[4]	3.517
H23G	N7[11]	3.016	H23G	C40[11]	3.539
H23G	C85[11]	3.142	H23G	H15C[11]	3.503
H23G	H40[11]	3.281	H23G	H85A[11]	2.386
H23G	H85B[11]	3.028	H23G	H93B[11]	3.145
H23G	H99B[11]	3.414	H23H	N7[11]	3.476
H23H	N9	2.682	H23H	C49	3.400
H23H	C50	3.598	H23H	C150[11]	3.529
H23H	H15C[11]	2.590	H23H	H49	3.312
H23I	N7[11]	3.323	H23I	C40[11]	3.445
H23I	H15C[11]	3.250	H23I	H40[11]	2.849
H23I	H49	3.405	H23I	H57A[11]	3.373
H23I	H71A[11]	3.351	H23I	H71B[11]	3.365
H23I	H85A[11]	3.588	H23I	H85B[11]	3.577
H24	O87	3.135	H24	O88	3.043
H24	C82	3.476	H24	C96	3.539
H24	C105	3.300	H24	H10F	2.387
H24	H11G	3.355	H24	H82	2.626
H24	H91A	3.479	H24	H91B	3.368
H24	H96	2.788	H24A	C79[11]	3.537

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H24A	C117[9]	3.296	H24A	H11C[9]	2.619
H24A	H11D[9]	3.103	H24A	H79A[11]	3.566
H24A	H79B[11]	2.832	H24A	H109[9]	3.160
H24B	H49	3.561	H24B	H79B[11]	3.363
H24C	O10	3.514	H24C	C77	3.126
H24C	H13D[9]	3.346	H24C	H20D[1]	3.052
H24C	H77A	3.093	H24C	H77C	2.431
H24D	O120[9]	3.551	H24D	O250	3.370
H24D	C121[9]	3.208	H24D	H11A[9]	3.469
H24D	H12B[9]	2.501	H24D	H12C[9]	3.287
H24D	H20D[1]	3.242	H24D	H20F[1]	3.546
H24D	H75A	3.363	H24D	H77C	3.529
H24E	O114[9]	3.555	H24E	O135[9]	2.895
H24E	C136[9]	3.338	H24E	C207[1]	3.557
H24E	H11A[9]	2.960	H24E	H12B[9]	3.227
H24E	H12E[9]	3.367	H24E	H13D[9]	3.012
H24E	H13F[9]	3.524	H24E	H20D[1]	3.177
H24E	H20F[1]	3.138	H24F	C27	3.446
H24F	C28	3.109	H24F	C29	3.379
H24F	H17C[4]	3.423	H24F	H17E[4]	3.563
H24F	H28	3.239	H24G	O250	2.763
H24G	C26	3.402	H24G	C27	3.447
H24G	C42	3.593	H24G	C43	3.193
H24G	C174[4]	2.922	H24G	H17C[4]	2.837
H24G	H17D[4]	3.112	H24G	H17E[4]	2.369
H24G	H43	2.635	H24H	O10	2.950
H24H	O250	3.281	H24H	N5	2.843
H24H	C26	3.376	H24H	C27	2.834
H24H	C28	3.097	H24H	C29	3.213
H24H	C30	3.024	H24I	C93[11]	3.344
H24I	H20A[9]	3.353	H24I	H79B[11]	3.191
H24I	H93A[11]	2.916	H24I	H93B[11]	3.389
H24I	H93C[11]	3.185	H24J	C79[11]	3.251
H24J	C117[9]	3.285	H24J	C202[9]	3.553
H24J	H11C[9]	2.356	H24J	H20A[9]	2.885
H24J	H20C[9]	3.364	H24J	H79B[11]	2.539
H24J	H79C[11]	3.101	H24J	H109[9]	3.016

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H24K	O118[9]	3.114	H24K	C146[14]	3.497
H24K	H10C[9]	3.501	H24K	H11C[9]	3.549
H24K	H14C[14]	2.718	H24K	H14E[14]	3.514
H24K	H20A[9]	3.555	H24K	H20C[9]	3.348
H24K	H109[9]	3.125	H28	C219	3.368
H28	C233	3.358	H28	H21F	2.981
H28	H21G	2.898	H28	H23D	3.522
H28	H23E	2.489	H28	H24F	3.239
H28	H210	2.702	H28	H224	3.019
H29	O215	3.062	H29	H210	2.718
H29	H212	3.131	H29	H224	3.276
H29	H226	3.072	H33	O251	3.551
H33	C131	3.417	H33	C134	3.431
H33	C190	2.759	H33	H13A	2.619
H33	H13C	3.421	H33	H19A	2.571
H33	H19B	2.707	H33	H19C	2.530
H34	O90[8]	2.428	H34	C82[8]	3.445
H34	C83[8]	3.580	H34	C91[8]	3.373
H34	C131	3.474	H34	H17F	3.210
H34	H17G	3.463	H34	H19B	3.523
H34	H19C	2.894	H34	H66[8]	3.010
H34	H81[8]	3.364	H34	H83[8]	2.903
H34	H91C[8]	3.216	H35	O218[2]	2.338
H35	C63	3.571	H35	C209[2]	3.372
H35	C210[2]	3.218	H35	C211[2]	3.541
H35	C219[2]	3.349	H35	H14F	3.265
H35	H16C	3.123	H35	H21H[2]	3.299
H35	H63B	3.485	H35	H63C	2.894
H35	H193[2]	3.436	H35	H209[2]	2.775
H35	H211[2]	2.926	H36	C63	2.905
H36	C162	3.347	H36	H16D	2.532
H36	H16F	3.393	H36	H21C[2]	3.550
H36	H63A	2.569	H36	H63B	2.936
H36	H63C	2.723	H38	O101	3.095
H38	O115	3.310	H38	C110	3.287
H38	C111	3.401	H38	C112	3.287
H38	H98	2.935	H38	H110	2.457

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H38	H112	2.444	H39	C98	3.313
H39	C99	3.379	H39	C112	3.575
H39	C150	3.581	H39	H11B	3.231
H39	H15B	3.156	H39	H15C	3.269
H39	H98	2.635	H39	H99A	2.900
H39	H99B	3.421	H39	H112	2.756
H40	O59	3.581	H40	O149	3.546
H40	C56	3.433	H40	C70	3.305
H40	C71	3.357	H40	C235[3]	3.476
H40	H23G[3]	3.281	H40	H23I[3]	2.849
H40	H56	2.603	H40	H57A	3.345
H40	H57B	3.458	H40	H70	2.555
H40	H71A	3.491	H40	H71B	2.797
H40	H85B	3.295	H41	O59	2.890
H41	C68	3.372	H41	C69	3.423
H41	C70	3.555	H41	H54	3.406
H41	H56	2.818	H41	H68	2.603
H41	H70	2.837	H41	H77A	3.592
H41	H77B	3.109	H43	O250	3.108
H43	C91	2.925	H43	C174[4]	3.275
H43	C247	3.516	H43	H17D[4]	3.100
H43	H17E[4]	2.580	H43	H24G	2.635
H43	H91A	2.485	H43	H91B	2.550
H43	H91C	3.376	H44	O88	3.480
H44	O189[4]	2.544	H44	C91	3.478
H44	C174[4]	3.490	H44	C180[4]	3.210
H44	C181[4]	3.234	H44	C182[4]	3.496
H44	H17D[4]	2.861	H44	H17E[4]	3.348
H44	H89C	2.958	H44	H91A	2.576
H44	H180[4]	2.427	H44	H182[4]	2.842
H45	O62[5]	2.462	H45	C53[5]	3.500
H45	C54[5]	3.331	H45	C63[5]	3.544
H45	C219	3.520	H45	H10D	3.336
H45	H10E	3.411	H45	H10F	3.535
H45	H14D[5]	3.080	H45	H21F	2.779
H45	H21H	3.500	H45	H23E	3.590
H45	H53[5]	2.865	H45	H55[5]	3.024

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H45	H61A[5]	3.238	H45	H61B[5]	3.429
H45	H63C[5]	3.492	H46	C119	3.572
H46	C146[5]	3.313	H46	C219	2.909
H46	H10E	3.545	H46	H10F	3.536
H46	H11G	3.266	H46	H11H	3.023
H46	H14D[5]	3.033	H46	H14E[5]	2.707
H46	H21F	2.577	H46	H21G	2.584
H46	H21H	3.108	H48	O243	2.944
H48	C238	3.489	H48	C240	3.434
H48	H153	3.580	H48	H155	3.072
H48	H226	3.556	H48	H238	2.637
H48	H240	2.518	H49	O177	2.901
H49	O234	2.971	H49	C178	3.376
H49	C235	3.446	H49	H17I	3.517
H49	H17K	3.095	H49	H23H	3.312
H49	H23I	3.405	H49	H24B	3.561
H49	H155	3.326	H49	H226	3.264
H49	H240	2.813	H50	O186	3.501
H50	C183	3.586	H50	C197	3.346
H50	H17I	3.580	H50	H18A	3.520
H50	H21A	3.501	H50	H21B	3.165
H50	H183	2.709	H50	H197	2.412
H50	H212	3.107	H51	O186	2.842
H51	C195	3.108	H51	C196	3.356
H51	C204	3.209	H51	H181	3.515
H51	H183	3.056	H51	H195	2.282
H51	H197	3.053	H52	C179[1]	3.497
H52	C188[1]	3.053	H52	C196[1]	3.584
H52	H18C[1]	2.933	H52	H18D[1]	2.331
H52	H19H[1]	3.572	H52	H179[1]	2.536
H52	H196[1]	2.619	H53	N8[2]	3.052
H53	C45[2]	3.340	H53	C188[1]	3.523
H53	H18C[1]	2.782	H53	H18D[1]	3.406
H53	H45[2]	2.865	H53	H179[1]	3.034
H53	H180[1]	3.326	H54	H41	3.406
H55	C105[2]	3.560	H55	H10D[2]	2.974
H55	H10E[2]	3.233	H55	H45[2]	3.024

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H56	C40	3.147	H56	C41	3.247
H56	H40	2.603	H56	H41	2.818
H57A	O177[3]	3.265	H57A	C178[3]	3.231
H57A	H17J[3]	3.089	H57A	H17K[3]	2.872
H57A	H23I[3]	3.373	H57A	H40	3.345
H57B	O177[3]	3.459	H57B	C178[3]	2.896
H57B	H17J[3]	2.338	H57B	H17K[3]	2.709
H57B	H40	3.458	H61A	O216[2]	3.478
H61A	C217[2]	2.986	H61A	H21C[2]	3.524
H61A	H21D[2]	3.505	H61A	H21E[2]	2.037
H61A	H23F[2]	3.102	H61A	H45[2]	3.238
H61B	O185[1]	2.720	H61B	N8[2]	3.046
H61B	C179[1]	3.022	H61B	C180[1]	3.504
H61B	H19G[1]	3.509	H61B	H21E[2]	3.347
H61B	H23F[2]	2.959	H61B	H45[2]	3.429
H61B	H179[1]	2.557	H61B	H180[1]	2.946
H61C	O185[1]	3.131	H61C	H19G[1]	2.988
H61C	H19H[1]	3.405	H61C	H20D[1]	3.451
H61C	H20E[1]	3.170	H61C	H21E[2]	2.746
H61C	H23F[2]	3.412	H61C	H179[1]	3.283
H63A	C18	3.562	H63A	C36	3.360
H63A	H18	3.364	H63A	H21E[2]	3.386
H63A	H36	2.569	H63B	C18	3.403
H63B	C36	3.356	H63B	H18	2.839
H63B	H21H[2]	3.151	H63B	H35	3.485
H63B	H36	2.936	H63C	O216[2]	3.030
H63C	O218[2]	3.062	H63C	C35	3.412
H63C	C36	3.310	H63C	C217[2]	3.302
H63C	C219[2]	2.891	H63C	H21C[2]	3.292
H63C	H21E[2]	3.019	H63C	H21F[2]	2.554
H63C	H21H[2]	2.701	H63C	H35	2.894
H63C	H36	2.723	H63C	H45[2]	3.492
H65A	O177[3]	2.834	H65A	C156[3]	3.207
H65A	C170[3]	3.209	H65A	H15D[3]	2.255
H65A	H15E[3]	3.433	H65A	H16G[3]	3.210
H65A	H17A[3]	2.925	H65A	H17B[3]	3.216
H65B	C105[2]	3.584	H65B	C188[1]	3.257

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H65B	H10D[2]	2.810	H65B	H15D[3]	3.423
H65B	H16G[3]	3.437	H65B	H18C[1]	2.833
H65B	H18D[1]	3.524	H65B	H18E[1]	2.930
H65B	H89B[2]	3.506	H65C	O104[2]	2.526
H65C	C105[2]	2.995	H65C	C170[3]	3.520
H65C	H10D[2]	2.625	H65C	H10E[2]	3.336
H65C	H15D[3]	2.903	H65C	H16G[3]	2.912
H65C	H17A[3]	3.094	H65C	H17B[3]	3.215
H65C	H89B[2]	3.168	H65C	H95[2]	3.435
H66	N6[4]	3.446	H66	C34[4]	3.586
H66	H34[4]	3.010	H66	H193[1]	3.526
H67	O199[1]	2.582	H67	C193[1]	3.462
H67	C197[1]	3.506	H67	C198[1]	3.369
H67	H19H[1]	2.680	H67	H193[1]	3.340
H67	H194[1]	3.492	H68	C41	3.286
H68	H41	2.603	H69	O199[1]	3.396
H69	C196[1]	3.339	H69	C197[1]	3.558
H69	C198[1]	3.405	H69	H19H[1]	2.593
H69	H179[1]	3.502	H69	H194[1]	3.094
H69	H196[1]	2.474	H70	C40	2.994
H70	C41	3.126	H70	H40	2.555
H70	H41	2.837	H71A	H20A[1]	3.535
H71A	H23I[3]	3.351	H71A	H40	3.491
H71B	H23I[3]	3.365	H71B	H40	2.797
H75A	O206[1]	3.295	H75A	C121[9]	3.594
H75A	C207[1]	3.415	H75A	C221[1]	3.578
H75A	H12B[9]	2.782	H75A	H17H[4]	3.536
H75A	H19H[1]	3.434	H75A	H20D[1]	2.994
H75A	H20F[1]	3.429	H75A	H22A[1]	2.780
H75A	H22C[1]	3.584	H75A	H24D	3.363
H75B	O199[1]	3.499	H75B	C176[4]	3.281
H75B	H17F[4]	3.054	H75B	H17H[4]	2.627
H75B	H22A[1]	3.347	H75C	O173[4]	3.513
H75C	O250	3.256	H75C	C121[9]	3.325
H75C	C176[4]	3.320	H75C	H12A[9]	3.391
H75C	H12B[9]	2.837	H75C	H12C[9]	3.217
H75C	H17E[4]	3.185	H75C	H17F[4]	2.842

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H75C	H17H[4]	2.969	H77A	O10	2.954
H77A	O250	3.055	H77A	H24C	3.093
H77A	H41	3.592	H77B	H41	3.109
H77C	C245	3.350	H77C	H16F	2.806
H77C	H20D[1]	3.131	H77C	H24C	2.431
H77C	H24D	3.529	H79A	C188[1]	3.233
H79A	H11C[1]	3.497	H79A	H18D[1]	2.853
H79A	H18E[1]	2.803	H79A	H24A[3]	3.566
H79B	C241[3]	3.460	H79B	C249[3]	3.251
H79B	H11C[1]	3.053	H79B	H20A[1]	3.059
H79B	H24A[3]	2.832	H79B	H24B[3]	3.363
H79B	H24I[3]	3.191	H79B	H24J[3]	2.539
H79C	O203[1]	2.557	H79C	C117[1]	3.316
H79C	C188[1]	3.216	H79C	C195[1]	3.579
H79C	C205[1]	3.337	H79C	H11C[1]	2.685
H79C	H11E[1]	3.075	H79C	H18D[1]	2.721
H79C	H18E[1]	2.827	H79C	H20A[1]	3.152
H79C	H24J[3]	3.101	H79C	H194[1]	3.230
H80	C164[6]	3.249	H80	H16G[6]	3.202
H80	H16H[6]	2.814	H80	H16I[6]	3.197
H81	C131[4]	2.714	H81	C132[4]	3.053
H81	H19C[4]	3.092	H81	H34[4]	3.364
H82	C23	2.944	H82	C24	2.907
H82	H23	2.705	H82	H24	2.626
H83	C131[4]	3.223	H83	C132[4]	3.181
H83	H14H[4]	3.560	H83	H34[4]	2.903
H84	C23	3.579	H84	C40	3.597
H84	H23	2.705	H85A	C235[3]	3.264
H85A	H22E[3]	3.038	H85A	H23G[3]	2.386
H85A	H23I[3]	3.588	H85B	C40	3.591
H85B	H23G[3]	3.028	H85B	H23I[3]	3.577
H85B	H40	3.295	H89A	O187[4]	3.288
H89A	O189[4]	3.526	H89A	C188[4]	3.511
H89A	C190[4]	3.241	H89A	H13C[4]	3.436
H89A	H16G[6]	3.363	H89A	H16I[6]	3.344
H89A	H18C[4]	3.516	H89A	H18E[4]	3.152
H89A	H19A[4]	3.027	H89A	H19C[4]	2.801

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H89B	C164[6]	3.276	H89B	H16G[6]	2.605
H89B	H16H[6]	3.499	H89B	H16I[6]	3.260
H89B	H18C[4]	3.386	H89B	H18E[4]	3.267
H89B	H65B[5]	3.506	H89B	H65C[5]	3.168
H89C	O187[4]	2.843	H89C	O189[4]	3.234
H89C	N8	3.465	H89C	C44	3.263
H89C	C180[4]	3.390	H89C	C188[4]	2.823
H89C	H18C[4]	2.425	H89C	H18E[4]	2.816
H89C	H19A[4]	3.588	H89C	H19C[4]	3.357
H89C	H44	2.958	H89C	H180[4]	2.973
H91A	O173[4]	3.495	H91A	O189[4]	2.907
H91A	C43	3.014	H91A	C44	3.077
H91A	C174[4]	3.466	H91A	C190[4]	3.080
H91A	H17D[4]	3.548	H91A	H17E[4]	2.896
H91A	H19B[4]	3.541	H91A	H19C[4]	2.447
H91A	H24	3.479	H91A	H43	2.485
H91A	H44	2.576	H91B	O250	2.477
H91B	C24	3.567	H91B	C43	3.384
H91B	H17E[4]	2.747	H91B	H24	3.368
H91B	H43	2.550	H91C	O173[4]	2.649
H91C	O189[4]	3.441	H91C	C174[4]	2.991
H91C	C176[4]	3.403	H91C	C190[4]	3.285
H91C	H17D[4]	3.482	H91C	H17E[4]	2.464
H91C	H17F[4]	2.448	H91C	H19B[4]	3.295
H91C	H19C[4]	2.715	H91C	H34[4]	3.216
H91C	H43	3.376	H93A	H14H[4]	3.114
H93A	H20A[1]	3.133	H93A	H24I[3]	2.916
H93B	O228[3]	3.140	H93B	O234[3]	2.985
H93B	C227[3]	3.076	H93B	C235[3]	3.516
H93B	H22E[3]	2.451	H93B	H23G[3]	3.145
H93B	H24I[3]	3.389	H93C	O147[4]	2.733
H93C	C132[4]	3.513	H93C	C148[4]	3.173
H93C	H14H[4]	2.658	H93C	H24I[3]	3.185
H93C	H122[4]	3.504	H95	H17A[6]	3.404
H95	H17B[6]	3.181	H95	H65C[5]	3.435
H95	H168[6]	2.938	H96	C23	3.354
H96	C24	3.142	H96	H23	3.208

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H96	H24	2.788	H97	H16H^{6}	3.217
H98	C38	3.017	H98	C39	2.854
H98	H23	2.875	H98	H38	2.935
H98	H39	2.635	H99A	C39	3.432
H99A	C221^{3}	3.295	H99A	H21A^{3}	3.365
H99A	H22B^{3}	2.514	H99A	H22C^{3}	3.448
H99A	H39	2.900	H99B	N7	3.550
H99B	C39	3.540	H99B	H23G^{3}	3.414
H99B	H39	3.421	H108	O163^{7}	3.108
H108	O242^{7}	2.627	H108	C236^{7}	3.054
H108	H154^{7}	3.549	H108	H236^{7}	2.523
H109	O242^{7}	2.929	H109	O248^{7}	2.392
H109	C240^{7}	3.561	H109	C241^{7}	3.194
H109	C249^{7}	3.053	H109	H24A^{7}	3.160
H109	H24J^{7}	3.016	H109	H24K^{7}	3.125
H110	C38	3.394	H110	H38	2.457
H112	C38	3.112	H112	C39	3.284
H112	H38	2.444	H112	H39	2.756
H122	H93C^{8}	3.504	H123	H16I^{7}	2.981
H124	C18	3.146	H124	C19	2.961
H124	C20	3.518	H124	H18	3.361
H124	H19	3.029	H125	O163^{7}	3.310
H125	H16I^{7}	3.252	H125	H154^{7}	3.496
H125	H236^{7}	3.295	H137	O102^{2}	3.594
H137	C103^{2}	3.329	H137	H10A^{2}	2.999
H137	H10C^{2}	3.002	H137	H10E^{2}	3.259
H138	H10C^{2}	2.760	H139	C18	3.314
H139	H18	2.585	H139	H19	3.266
H140	H19D^{3}	3.585	H141	C19	3.476
H141	H19	2.575	H151	O106^{10}	3.148
H151	H10I^{10}	3.445	H152	C107^{10}	3.580
H152	H10I^{10}	2.764	H152	H13F^{9}	3.294
H153	C12	3.587	H153	C13	2.908
H153	C14	2.989	H153	H13	2.974
H153	H14	3.112	H153	H48	3.580
H154	O135^{9}	3.414	H154	H13F^{9}	3.066
H154	H108^{9}	3.549	H154	H125^{9}	3.496

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H155	C48	3.527	H155	H48	3.072
H155	H49	3.326	H165	O230[8]	3.535
H165	C231[8]	3.255	H165	H23A[8]	3.395
H165	H23C[8]	2.527	H166	C121[10]	3.292
H166	C231[8]	3.568	H166	H10B[10]	3.313
H166	H12A[10]	2.931	H166	H12C[10]	2.798
H166	H23C[8]	2.593	H167	C13	3.467
H167	C14	3.302	H167	H13	3.032
H167	H14	2.670	H168	H95[10]	2.938
H169	C13	3.569	H169	H13	2.635
H179	O60[12]	3.002	H179	C52[12]	3.330
H179	C53[12]	3.318	H179	C61[12]	3.092
H179	H52[12]	2.536	H179	H53[12]	3.034
H179	H61B[12]	2.557	H179	H61C[12]	3.283
H179	H69[12]	3.502	H180	N8[8]	2.773
H180	C44[8]	2.942	H180	H44[8]	2.427
H180	H53[12]	3.326	H180	H61B[12]	2.946
H180	H89C[8]	2.973	H181	O251	2.947
H181	H13	3.423	H181	H51	3.515
H182	C44[8]	3.511	H182	H23D[8]	3.488
H182	H23F[8]	3.517	H182	H44[8]	2.842
H183	C50	3.002	H183	C51	3.194
H183	H50	2.709	H183	H51	3.056
H193	N6[5]	3.449	H193	H35[5]	3.436
H193	H66[12]	3.526	H193	H67[12]	3.340
H194	O72[12]	2.991	H194	O78[12]	2.616
H194	C71[12]	3.560	H194	C79[12]	3.429
H194	H67[12]	3.492	H194	H69[12]	3.094
H194	H79C[12]	3.230	H195	C51	3.141
H195	H51	2.282	H196	O78[12]	3.079
H196	C52[12]	3.590	H196	C69[12]	3.455
H196	H52[12]	2.619	H196	H69[12]	2.474
H197	C50	3.183	H197	C51	3.485
H197	H50	2.412	H197	H51	3.053
H208	H10H[11]	3.179	H208	H10I[11]	3.456
H208	H16A[5]	2.867	H209	C35[5]	3.506
H209	C160[5]	2.872	H209	H16A[5]	2.421

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H209	H16C[5]	2.475	H209	H35[5]	2.775
H210	C28	3.123	H210	C29	3.132
H210	H28	2.702	H210	H29	2.718
H211	C35[5]	3.550	H211	H16C[5]	2.953
H211	H35[5]	2.926	H212	C50	3.214
H212	H29	3.131	H212	H50	3.107
H223	C192[4]	3.535	H223	H19D[4]	3.481
H223	H19F[4]	2.739	H224	C28	3.345
H224	C29	3.470	H224	H28	3.019
H224	H29	3.276	H226	C48	3.355
H226	C49	3.175	H226	H29	3.072
H226	H48	3.556	H226	H49	3.264
H236	O114[9]	2.886	H236	O135[9]	2.856
H236	C108[9]	3.160	H236	H13F[9]	3.477
H236	H108[9]	2.523	H236	H125[9]	3.295
H237	O114[9]	2.820	H237	O120[9]	2.667
H237	C113[9]	3.336	H237	C121[9]	3.279
H237	H11A[9]	3.219	H237	H12B[9]	3.214
H237	H12C[9]	3.301	H238	C48	3.408
H238	H48	2.637	H239	O120[9]	3.555
H240	C48	3.180	H240	C49	3.335
H240	H48	2.518	H240	H49	2.813

Symmetry Operators:

(1) X+1,Y,Z+1
(2) X,Y,Z+1
(3) X+1,Y+1,Z+1
(4) X+1,Y,Z
(5) X,Y,Z-1
(6) X+1,Y+1,Z
(7) X,Y+1,Z
(8) X-1,Y,Z
(9) X,Y-1,Z
(10) X-1,Y-1,Z
(11) X-1,Y-1,Z-1
(12) X-1,Y,Z-1
(13) X,Y+1,Z+1
(14) X,Y-1,Z-1