Supporting Information

for

Synthesis of (Arylimido)niobium(V) Complexes Containing Ketimide, Phenoxide Ligands, and Some Reactions with Phenols, Alcohols

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Contents

1. Experimental procedure for some reactions with phenol, tables for crystal data and collection parameters of NbCl$_2$(N-2,6- Me$_2$C$_6$H$_3$)(O-2,6-Pr$_2$C$_6$H$_3$)(dme) (1a), NbCl$_2$(N-2,6- Me$_2$C$_6$H$_3$)(O-2,6-Ph$_2$C$_6$H$_3$)(dme) (1d), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(O-2,6-Pr$_2$C$_6$H$_3$) (4a), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(2,6- Me$_2$C$_6$H$_3$OH) (4b), Nb(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)$_3$(HN=C'Bu$_2$) (7), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)$_3$(HN=C'Bu$_2$)-[OCH(CF$_3$)$_2$]$_2$(HN=C'Bu$_2$) (9), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11), and NMR spectra for synthesized (arylimido)niobium complexes.

2. NMR spectra monitoring some reactions with phenols.

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4. Structure reports and cif, xyz files for 1a, 1d, 4a, 4b, 7, 8, 9, and 11.

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1. Experimental procedure for some reactions with phenol, tables for crystal data and collection parameters of NbCl$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-Pr$_2$C$_6$H$_3$)(dme) (1a), NbCl$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-Ph$_2$C$_6$H$_3$)(dme) (1d), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$O(2,6-Pr$_2$C$_6$H$_3$) (4a), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(2,6-Bu$_2$C$_6$H$_3$OH) (4b), Nb(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)$_3$(HN=C'Bu$_2$) (7), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$[OC(CF$_3$)$_2$]$_2$(HN=C'Bu$_2$) (8), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)-[OCH(CF$_3$)$_2$]$_2$(HN=C'Bu$_2$) (9), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11), and NMR spectra for synthesized (arylimido)niobium complexes.

Monitoring the reaction of Nb(NAr)(N=C'Bu$_2$)$_3$ (3a) with 2,6-'^Bu$_2$C$_6$H$_3$OH. The reaction was monitored by $^1$H NMR spectra (shown below, Figures S2-4-8)

(i) Reaction of 3a with 1.0 equiv of 2,6-'^Bu$_2$C$_6$H$_3$OH at 25 °C. Into a n-hexane solution (8 mL) containing Nb(NAr)(N=C'Bu$_2$)$_3$ (3a) (79 mg, 0.13 mmol), a n-hexane solution (4 mL) containing 2,6-'^Bu$_2$C$_6$H$_3$OH (27 mg, 0.13 mmol) was added slowly at -30 °C. The reaction mixture was stirred at room temperature overnight. The volatiles were then evaporated in vacuo, and the resultant mixture was measured by $^1$H NMR spectrum (36.3 % conversion of 3a).

(ii) Reaction of 3a with 2.0 equiv of 2,6-'^Bu$_2$C$_6$H$_3$OH at 70 °C. Into a C$_6$D$_6$ solution (0.5 mL) containing Nb(NAr)(N=C'Bu$_2$)$_3$ (3a) (35 mg, 0.06 mmol) in J Young NMR tubes, a C$_6$D$_6$ solution (0.3 mL) containing 2,6-'^Bu$_2$C$_6$H$_3$OH (24 mg, 0.12 mmol) was added slowly at -30 °C. The reaction mixture was heated at 70 °C. The solution was partly taken out were and evaporated in vacuo (1 day, 2 days and 1 week). The resultant mixture was measured by $^1$H NMR spectrum in C$_6$D$_6$ (>99 % conversion of 3a), and only mono phenoxide complex (4b) was observed as product.

(iii) Reaction of 3a with 2.0 equiv of 2,6-'^Bu$_2$C$_6$H$_3$OH at 100 °C. The reaction was conducted as the similar procedure to that conducted at 70 °C, except the reaction was conducted in toluene-$d_8$ at 100 °C for 1 day. The resultant mixture was measured by $^1$H NMR spectrum in C$_6$D$_6$ (>99 % conversion of 3a), and only mono phenoxide complex (4b) was observed as product.

Reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_3$(3a) with C$_6$F$_5$OH. See Figures S2-9-16.

Synthesis of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11). (i) Reaction of 3a with 0.5 equiv of C$_6$F$_5$OH. A n-hexane solution (6.0 mL) containing C$_6$F$_5$OH (15 mg, 0.08 mmol) was added to a n-hexane solution (15.0 mL) containing 3a (103 mg, 0.16 mmol) at -30 °C. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The orange-yellow mixture was dried in vacuo, and the crude product was measured by $^1$H and $^{19}$F NMR spectra (conversion of 3a 45 %). Microcrystals suitable for X-ray crystallographic analysis was collected (in small amount) from the chilled n-hexane solution. $^1$H NMR (C$_6$D$_6$): δ 9.70 (b, 1H, NH), 6.93 (d, 2H, $J = 6.8$ Hz, Ar), 6.74 (t, 1H, $J =$

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7.6 Hz, Ar), 2.57 (s, 6H, ArCH), 1.34 (s, 9H, C(CH₃)₃), 1.20 (s, 36H, C(CH₃)₃), 0.95 (s, 9H, C(CH₃)₃). ¹⁹F NMR (CDCl₃): δ -162.01 (d), -166.28 (t), -173.05 (t). ¹³C NMR (CDCl₃): 133.2, 126.9, 122.5, 44.9, 30.6, 19.2. These chemical shifts were assigned from the mixture of 3a and 13 (different ratios shown below).

(ii) Reaction of 3a with 0.5 equiv of C₆F₅OH (under diluted conditions). A n-hexane solution (6.0 mL) containing C₆F₅OH (8 mg, 0.04 mmol) was added to an n-hexane solution (15.0 mL) containing 3a (50 mg, 0.08 mmol) at -30 °C. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The orange-yellow mixture was dried in vacuo, and the crude product was measured by ¹H and ¹⁹F NMR spectra (conversion of 3a 35%).

(iii) Reaction of 3a with 0.8 equiv of C₆F₅OH (diluted conditions, 2 step C₆F₅OH addition). A n-hexane solution (12.0 mL) containing C₆F₅OH (13 mg, 0.07 mmol) was added to a n-hexane solution (30.0 mL) containing 3a (90 mg, 0.14 mmol) at -30 °C. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The solution was then cooled to -30 °C, and a n-hexane solution (8.0 mL) containing C₆F₅OH (8 mg, 0.04 mmol) was added was added to the chilled mixture. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The orange-yellow mixture was dried in vacuo, and the crude product was measured by ¹H and ¹⁹F NMR spectra (conversion of 3a 46%).

(iv) Reaction of 3a with 0.8 equiv of C₆F₅OH (diluted conditions, 3 step C₆F₅OH addition). A n-hexane solution (12.0 mL) containing C₆F₅OH (13 mg, 0.07 mmol) was added to an n-hexane solution (30.0 mL) containing 3a (90 mg, 0.14 mmol) at -30 °C. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The solution was then cooled to -30 °C, and a n-hexane solution (4.0 mL) containing C₆F₅OH (4 mg, 0.02 mmol) was added was added to the chilled mixture. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The solution was then cooled to -30 °C, and a n-hexane solution (4.0 mL) containing C₆F₅OH (4 mg, 0.02 mmol) was added was added to the chilled mixture. The reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The orange-yellow mixture was dried in vacuo, and the crude product was measured by ¹H and ¹⁹F NMR spectra (conversion of 3a 66%). Microcrystals suitable for X-ray crystallographic analysis was collected (in small amount) from the chilled n-hexane solution.

Reaction of 3a with 2.0 equiv of C₆F₅OH (after 3 step reactions with 1 equiv of C₆F₅OH under diluted conditions): Confirmation of formation of 7 from 11. A n-hexane solution (24.0 mL) containing C₆F₅OH (26 mg, 0.14 mmol) was added to an orange-yellow mixture obtained after the reaction [reaction of 3a with 1.0 equiv of C₆F₅OH with 3 step additions shown above in (iv)], and the reaction mixture was warmed slowly to room temperature and was stirred for 1 h. The orange-yellow mixture was dried in vacuo, and the
crude product was measured by $^1$H and $^{19}$F NMR spectra. The crude product was then dissolved in small amount of $n$-pentane to give an orange solid (22 mg, 15%). And the solid was characterized as 7 by $^1$H and $^{19}$F NMR spectra.

**Reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4a) with 2,4,6-Me$_3$C$_6$H$_2$OH.** Into a $n$-hexane solution (1 mL) containing Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$-(O-2,6-iPr$_2$C$_6$H$_3$) (4a) (43 mg, 0.06 mmol), a $n$-hexane solution (0.5 mL) containing 2,4,6-Me$_3$C$_6$H$_2$OH (9 mg, 0.06 mmol) was added slowly at -30 °C. The reaction mixture was warmed slowly to room temperature and solution was monitored by $^1$H-NMR spectra (after 2 h and 1 day). See also Figure S2-17-19.
Table S1. Crystal data and collection parameters of NbCl$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-\textsuperscript{2}Pr$_2$C$_6$H$_3$)(dme) (1a), NbCl$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-Ph$_2$C$_6$H$_3$)(dme) (1d), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C\textsuperscript{2}Bu$_2$)(O-2,6-\textsuperscript{2}Pr$_2$C$_6$H$_3$) (4a), Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C\textsuperscript{2}Bu$_2$)(2,6-\textsuperscript{2}Bu$_2$C$_6$H$_3$OH) (4b).\(^a\)

|     | 1a                              | 1d                              | 4a                                | 4b                                |
|-----|---------------------------------|---------------------------------|----------------------------------|----------------------------------|
| **Formula** | C$_{24}$H$_{36}$Cl$_2$NNbO$_3$ | C$_{30}$H$_{32}$Cl$_2$NNbO$_3$ | C$_{39}$H$_{64}$Cl$_2$NNbO       | C$_{80}$H$_{132}$N$_6$Nb$_2$O$_2$ |
| **Formula weight** | 550.37                          | 618.40                          | 754.77                           | 1395.77                          |
| **Crystal color, Habit** | yellow, block                   | colourless, prism               | yellow, prism                    | yellow, block                    |
| **Crystal size (mm)** | 0.260×0.230×0.220                | 0.200×0.160×0.080              | 0.200×0.180×0.180                | 0.231×0.146×0.064               |
| **Crystal system** | monoclinic                       | triclinic                       | monoclinic                       | triclinic                        |
| **Space group** | P2$_1$/c (#14)                  | P-1 (#2)                        | P2$_1$/c (#14)                   | P-1 (#2)                         |
| **a (Å)** | 13.572(4)                       | 9.9108(3)                       | 15.469(3)                        | 12.5502(4)                       |
| **b (Å)** | 9.116(2)                        | 12.5655(5)                      | 10.6814(19)                      | 14.0719(5)                       |
| **c (Å)** | 21.854(6)                       | 13.0149(5)                      | 24.897(4)                        | 23.5634(9)                       |
| **α (deg)** | 95.967(3)                       | 89.366(3)                       | 89.366(3)                        | 89.366(3)                        |
| **β (deg)** | 103.824(3)                      | 101.025(3)                      | 93.169(5)                        | 88.443(3)                        |
| **γ (deg)** | 106.341(3)                      | 93.169(5)                       | 88.443(3)                        | 75.219(3)                        |
| **V (Å$^3$)** | 2625.6(11)                      | 1505.05(10)                     | 4107.5(13)                       | 4022.2(3)                        |
| **Z value** | 4                               | 2                               | 4                                | 2                                |
| **D$_{calc}$ (g/cm$^3$)** | 1.392                           | 1.364                           | 1.220                            | 1.152                            |
| **F$_{000}$** | 1144.00                         | 636.00                          | 1608.00                          | 1504.00                          |
| **Temp (K)** | 273                             | 93                              | 93                               | 93                               |
| **μ (MoKα) (cm$^{-1}$)** | 6.855                           | 6.067                           | 4.542                            | 3.304                            |
| **No. of reflections** | Total: 26903                     | Total: 16099                     | Total: 60816                      | Total: 67935                      |
| **measured (R$_{int}$)** | Unique: 6010                     | Unique: 6894                     | Unique: 8829                      | Unique: 17259                     |
| (R$_{int}$ = 0.0223) | (R$_{int}$ = 0.0323)             | (R$_{int}$ = 0.0646)             | (R$_{int}$ = 0.0777)              |
| **2θ$_{max}$ (deg)** | 55.0                            | 55.0                            | 55.1                             | 55.0                             |
| **No. of observations** | 6010                            | 6894                            | 8829                             | 17259                            |
| **[1 > 2.00σ(I)]** |                                |                                 |                                  |                                  |
| **No. of variables** | 280                             | 334                             | 415                              | 811                              |
| **R1 [1 > 2.00σ(I)]** | 0.0246                          | 0.0275                          | 0.0495                           | 0.1366                           |
| **wR2 [1 > 2.00σ(I)]** | 0.0585                          | 0.0733                          | 0.1291                           | 0.3184                           |
| **Goodness of Fit** | 1.062                           | 1.013                           | 1.103                            | 1.251                            |

\(^a\)Structure reports and cif, xyz files are shown in the Supporting Information (shown below).
Table S2. Crystal data and collection parameters of Nb(N=C′Bu2)2(OC₆F₃)₃(HN=C′Bu2) (7), Nb(N-2,6-Me₂C₆H₃)(N=C′Bu2)₂[OC(CF₃)₃](HN=C′Bu2) (8), Nb(N-2,6-Me₂C₆H₃)(N=C′Bu2)-[OCH(CF₃)₂]₂(HN=C′Bu2)(9), Nb(N-2,6-Me₂C₆H₃)(N=C′Bu2)₂(OC₆F₅)(HN=C′Bu2) (11).."  

|       | 7                  | 8                  | 9                  | 11                 |
|-------|--------------------|--------------------|--------------------|--------------------|
| Formula | C₄₅H₅₅F₁₃N₃NbO₃ | C₃₉H₄₈F₁₃N₄NbO    | C₃₂H₃₈F₁₂N₃NbO₂  | C₄₁H₆₄F₁₃N₄NbO    |
| Formula weight | 1063.83 | 868.85            | 827.64            | 816.68            |
| Crystal color, Habit | orange, block | yellow, block | yellow, prism | yellow, block |
| Crystal size (mm) | 0.340x0.253x0.238 | 0.300x0.250x0.200 | 0.380x0.250x0.130 | 0.180x0.170x0.140 |
| Crystal system | triclinic | monoclinic | monoclinic | monoclinic |
| Space group | P-1 (#2) | P2₁/n (#14) | P2₁/n (#14) | P2₁/n (#14) |
| a (Å) | 11.3778(5) | 11.7181(3) | 17.905(3) | 11.903(3) |
| b (Å) | 12.9307(5) | 18.3197(5) | 12.035(4) | 18.130(5) |
| c (Å) | 18.9950(6) | 20.1982(5) | 19.691(3) | 20.798(6) |
| α (deg) | 86.879(3) | 81.525(3) | 91.823(2) | 115.352(2) |
| β (deg) | 81.525(3) | 91.823(2) | 115.352(2) | 104.299(5) |
| γ (deg) | 77.672(3) | 77.672(3) | 77.672(3) | 77.672(3) |
| V (Å³) | 2699.58(18) | 4333.79(19) | 3834.6(10) | 4349(2) |
| Z value | 2        | 4          | 4        | 4       |
| Dcalc (g/cm³) | 1.309 | 1.332 | 1.433 | 1.247 |
| F₀₀₀ | 1092.00 | 1824.00 | 1704.00 | 1728.00 |
| Temp (K) | 93 | 93 | 93 | 93 |
| μ (MoKα) (cm⁻¹) | 3.118 | 3.500 | 4.364 | 3.320 |
| No. of reflections measured (Rint) | Total: 22400 | Total: 34505 | Total: 32113 | Total: 41166 |
| Unique: 11596 | Unique: 9907 | Unique: 8561 | Unique: 9916 |
| R₁ [I > 2.00σ(I)] | 0.0643 | 0.0340 | 0.0313 | 0.0736 |
| wR₂ [I > 2.00σ(I)] | 0.2013 | 0.0890 | 0.0946 | 0.2163 |
| Goodness of Fit | 1.043 | 1.070 | 1.000 | 1.058 |

"Structure reports and cif, xyz files are shown in the Supporting Information (shown below)."
Figure S1-1. $^1$H NMR spectrum of Nb(N-2,6-iPr$_2$C$_6$H$_3$)Cl$_2$(O-2,6-iPr$_2$C$_6$H$_3$)(dme) (1b, in CDCl$_3$).

Figure S1-2. $^{13}$C NMR spectrum of Nb(N-2,6-iPr$_2$C$_6$H$_3$)Cl$_2$(O-2,6-iPr$_2$C$_6$H$_3$)(dme) (1b, in CDCl$_3$).
Figure S1-3. $^1$H NMR spectrum of Nb(NAd)Cl$_2$(O-2,6-$^t$Pr$_2$C$_6$H$_3$)(dme) (1c, in CDCl$_3$).

Figure S1-4. $^{13}$C NMR spectrum of Nb(NAd)Cl$_2$(O-2,6-$^t$Pr$_2$C$_6$H$_3$)(dme) (1c, in CDCl$_3$).
Figure S1-5. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(OTf)$_3$(dme) (2b, in CDCl$_3$). *impurity

Figure S1-6. $^{19}$F NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(OTf)$_3$(dme) (2b, in CDCl$_3$).
Figure S1-7. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_5$)(OTf)$_3$(dme) (2b, in CDCl$_3$).

Figure S1-8. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_5$)(N=C'Bu$_2$)$_3$ (3a, in C$_6$D$_6$).
Figure S1-9. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_3$ (3a, in C$_6$D$_6$).

Figure S1-10. $^1$H NMR spectrum of trans-NbCl$_2$(N=C'Bu$_2$)$_3$ (3b, in C$_6$D$_6$).
Figure S1-11. $^{13}$C NMR spectrum of trans-NbCl$_2$(N=C'Bu$_2$)$_3$ (3b, in C$_6$D$_6$).

* $n$-hexane

Figure S1-12. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_5$)(N=C'Bu$_2$)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4a, in CDCl$_3$).

* $n$-hexane and dichloromethane
Figure S1-13. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4a, in CDCl$_3$).

Figure S1-14. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4b, in C$_6$D$_6$).

*impurity
Figure S1-15. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=CNtBu)$_2$(O-2,6-tBu$_2$C$_6$H$_3$)$_2$ (4b, in C$_6$D$_6$).

Figure S1-16. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=CN'Bu$_2$)(O-2,6-iPr$_2$C$_6$H$_3$)$_2$ (5, in CDCl$_3$).

*n*-hexane and dichloromethane
Figure S1-17. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C‘Bu$_2$)(O-2,6-iPr$_2$C$_6$H$_3$)$_2$ (5, in C$_6$D$_6$).

Figure S1-18. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-iPr$_2$C$_6$H$_3$)$_3$ (6, in CDCl$_3$).
Figure S1-19. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6'-tBuC$_6$H$_3$)$_3$ (6, in CDCl$_3$).

Figure S1-20. $^1$H NMR spectrum of Nb(N=C'Bu$_2$)$_2$(OC$_6$F$_3$)$_3$(HN=C'Bu$_2$) (7, in C$_6$D$_6$).

$n$-hexane, toluene, dichloromethane
**Figure S1-21.** $^{19}$F NMR spectrum of Nb(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)$_3$(HN=C'Bu$_2$) (7, in C$_6$D$_6$).

**Figure S1-22.** $^{13}$C NMR spectrum of Nb(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)$_3$(HN=C'Bu$_2$) (7, in C$_6$D$_6$).
Figure S1-23. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$[OC(CF$_3$)$_3$]-(HN=C'Bu$_2$) (8, in C$_6$D$_6$). *impurity

Figure S1-24. $^{19}$F NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$[OC(CF$_3$)$_3$]-(HN=C'Bu$_2$) (8, in C$_6$D$_6$). *impurity
Figure S1-25. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)[OCH(CF$_3$)$_2$]$_2$-(HN=C'Bu$_2$) (9, in C$_6$D$_6$). *n-hexane and impurity.

Figure S1-26. $^{19}$F NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)[OCH(CF$_3$)$_2$]$_2$-(HN=C'Bu$_2$) (9, in C$_6$D$_6$).
Figure S1-27. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)[OCH(CF$_3$)$_2$]$_2$-(HN=C'Bu$_2$) (9, in C$_6$D$_6$).
Figure S1.1-28. $^1$H NMR spectra (in C$_6$D$_6$) of 9 and 10. Confirmation of removal of HN=C'Bu$_2$ from Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)[OCH(CF$_3$)$_2$]$_2$(HN=C'Bu$_2$) (9, in C$_6$D$_6$).
Disappearances of two resonances ascribed to 'Bu group in 9 (marked with #) suggested a formation of 10.

Figure S1.29. $^{19}$F NMR spectra (in C$_6$D$_6$) of 9 and 10. Confirmation of removal of HN=C'Bu$_2$ from Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)[OCH(CF$_3$)$_2$]$_2$(HN=C'Bu$_2$) (9, in C$_6$D$_6$). *impurity or side product derived from CF$_3$ in OCH(CF$_3$)$_2$ group.
Figure S1-30. $^1$H NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C' Bu$_2$)(2,4,6-Me$_3$C$_6$H$_2$OH)$_2$-(HN=C' Bu$_2$) (12, in C$_6$D$_6$). *n-hexane

Figure S1-31. $^{13}$C NMR spectrum of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C' Bu$_2$)(2,4,6-Me$_3$C$_6$H$_2$OH)$_2$-(HN=C' Bu$_2$) (12, in C$_6$D$_6$).
Figure S1-32. $^1$H NMR spectra of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)(2,4,6-Me$_3$C$_6$H$_2$OH)$_2$ (13, in C$_6$D$_6$). Confirmation of removal of HN=C'C'Bu$_2$ from 12. Disappearances of resonances ascribed to 'Bu group and N-H in 12 (marked with #) suggested a formation of 13.
2. NMR spectra monitoring some reactions with phenols or triflate compound.

Figure S2-1. VT-$^1$H NMR spectra of NbCl$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-'Pr$_2$C$_6$H$_3$)(dme) (1a in CDCl$_3$).
Figure S2-2. $^1$H NMR spectra of Nb(CF$_3$SO$_3$)$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-iPr$_2$C$_6$H$_3$)(dme) (2a): (a) reaction time = 3.5 h, (b) reaction time = 21 h (2a in CDCl$_3$).
Figure S2-3. $^{19}$F NMR spectra of Nb(CF$_3$SO$_3$)$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-$^t$Pr$_2$C$_6$H$_3$)(dme) (2a): (a) reaction time = 3.5 h, (b) reaction time = 21 h (2a in CDCl$_3$).
Figure S2-4. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with 2,6'-Bu$_2$C$_6$H$_3$OH (1 equiv at 25 °C, overnight). *impurity
Fig. S2-5. ¹H NMR spectra (in C₆D₆) monitoring reaction of Nb(N-2,6-Me₂C₆H₃)-(N=C'Bu₂)₃ (3a) with 2,6-tBu₂C₆H₅OH (2 equiv at 70°C, 7 days). *impurity or free HN=C'Bu₂
Figure S2-6. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu)$_3$ (3a) with 2,6'-Bu$_2$C$_6$H$_3$OH (2 equiv at 70 ºC, 1 day, 2 days, and 7 days).

Figure S2-7. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu)$_3$ (3a) with 2,6'-Bu$_2$C$_6$H$_3$OH (2 equiv at 70 ºC, 1 day).
**Figure S2-8.** $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with 2,6'-Bu$_2$C$_6$H$_3$OH in toluene-$d_8$ (2 equiv at 100ºC, 1 day). *n-hexane
Figure S2.9. $^1$H NMR spectrum (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with C$_6$F$_5$OH (0.5 equiv at -30 to 25 °C, 1 h). Formation of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11). $^*$n-hexane, toluene and dichloromethane
Figure S2-10. $^{19}$F NMR spectrum (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with C$_6$F$_5$OH (0.5 equiv at -30 to 25 ºC, 1 h). Formation of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11).

Figure S2-11. $^{13}$C NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with C$_6$F$_5$OH (0.5 equiv at -30 to 25 ºC, 1 h). Formation of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11).
Figure S2-12. $^{13}$C NMR spectrum (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with C$_6$F$_5$OH (0.5 equiv at -30 to 25 °C, 1 h). Formation of Nb(N-2,6-Me$_2$C$_6$H$_3$)(N=C'Bu$_2$)$_2$(OC$_6$F$_5$)(HN=C'Bu$_2$) (11). *impurity
Figure S2-13. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with C$_6$F$_5$OH. Reaction of 3a with (a) 0.50 equiv of C$_6$F$_5$OH [described as (i)], (b) 0.50 equiv of C$_6$F$_5$OH [described as (ii) under diluted conditions], (c) 0.50 + 0.30 equiv of C$_6$F$_5$OH [described as (iii), 2 step additions], and (d) 0.50 + 0.15 + 0.15 equiv of C$_6$F$_5$OH [described as (iv), 3 step additions].

*n-hexane, toluene and dichloromethane

Figure S2-14. $^{19}$F NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu$_2$)$_3$ (3a) with C$_6$F$_5$OH. Reaction of 3a with (a) 0.50 equiv of C$_6$F$_5$OH [described as (i)], (b) 0.50 equiv of C$_6$F$_5$OH [described as (ii) under diluted conditions], (c) 0.50 + 0.30 equiv of C$_6$F$_5$OH [described as (iii), 2 step additions], and (d) 0.50 + 0.15 + 0.15 equiv of C$_6$F$_5$OH [described as (iv), 3 step additions]. * impurity
Figure S2-15. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu)$_3$ (3a) with C$_6$F$_5$OH. Reaction of 3a with (a) 0.50 + 0.15 + 0.15 equiv of C$_6$F$_5$OH [described as (iv), 3 step additions], (b) 3a, (c) reaction mixture [(a) and 1 equiv of C$_6$F$_5$OH], (d) purified solid from the mixture (c), (e) Nb(N=C'Bu)$_2$(OC$_6$F$_5$)$_3$(HN=C'Bu)$_2$(7).

Note: The third step reaction conversion should be equal or less than 80% (conversion theory). And the unexpected higher conversion probably due to the tiny scale reaction (0.15 equiv of C$_6$F$_5$OH).
Figure S2-16. $^{19}$F NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C′Bu$_2$)$_3$ (3a) with (in C$_6$D$_6$) with C$_6$F$_5$OH. NMR spectra of (a) reaction mixture [described as (iv), 3 step addition and 1 equiv of C$_6$F$_5$OH], (b) purified solid from the mixture, (c) Nb(N=C′Bu$_2$)$_2$(OC$_6$F$_5$)$_3$(HN=C′Bu$_2$) (7). * impurity
Figure S2-17. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C'Bu)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4a) with 1 equiv of 2,4,6-Me$_3$C$_6$H$_2$OH (1 day).
Figure S2-18. $^1$H NMR spectrum (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C$'$Bu$_2$)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4a) with 1 equiv of 2,4,6-Me$_3$C$_6$H$_2$OH (1 day).

(a) 2 h

(b) 1 day

$5:12 = 49:51$

% conv = 80.0

$5:12 = 49:51$

% conv = 85.0

Figure S2-19. $^1$H NMR spectra (in C$_6$D$_6$) monitoring reaction of Nb(N-2,6-Me$_2$C$_6$H$_3$)-(N=C$'$Bu$_2$)$_2$(O-2,6-iPr$_2$C$_6$H$_3$) (4a) with 1 equiv of 2,4,6-Me$_3$C$_6$H$_2$OH (2 h and 1 day).
3. ORTEP Drawings for NbCl₂(N-2,6-Me₂C₆H₃)(O-2,6-Pr₂C₆H₃)(dme) (1a), NbCl₂(N-2,6-Me₂C₆H₃)(O-2,6-Ph₂C₆H₃)(dme) (1d) and selected bond distances and angles.

**Figure S3-1.** ORTEP drawing for Nb(N-2,6-Me₂C₆H₃)Cl₂(O-2,6-Pr₂C₆H₃)(dme) (1a). Selected bond distances (Å): Nb(1)-N(1) 1.7643(15), Nb(1)-O(1) 1.8878(12), Nb(1)-O(2) 2.3714(13), Nb(1)-O(3) 2.2434(12), Nb(1)-Cl(1) 2.4254(8), Nb(1)-Cl(2) 2.4473(8). Selected bond angles (°): Cl(1)-Nb(1)-Cl(2) 159.77(3), Cl(1)-Nb(1)-O(1) 93.20(4), Cl(1)-Nb(1)-O(2) 83.98(4), Cl(1)-Nb(1)-O(3) 80.60(4), Cl(1)-Nb(1)-N(1) 98.13(5), Cl(2)-Nb(1)-O(1) 96.97(4), Cl(2)-Nb(1)-O(2) 79.22(4), Cl(2)-Nb(1)-O(3) 83.59(4), Cl(2)-Nb(1)-N(1) 96.07(5), O(1)-Nb(1)-O(2) 86.68(5), O(1)-Nb(1)-O(3) 158.51(6), O(1)-Nb(1)-N(1) 104.97(6), O(3)-Nb(1)-O(2) 72.26(5), O(3)-Nb(1)-N(1) 96.30(6), O(2)-Nb(1)-N(1) 167.95(5), Nb(1)-O(1)-C(9) 158.00(10), Nb(1)-N(1)-C(1) 176.53(12).
Figure S3-2. ORTEP drawing for Nb(N-2,6-Me₂C₆H₃)Cl₂(O-2,6-Ph₂C₆H₃)(dme) (1d).
Selected bond distances (Å): Nb(1)-Cl(1) 2.4131(5), Nb(1)-Cl(2) 2.4407(4), Nb(1)-O(1) 1.9127(15), Nb(1)-O(2) 2.3802(14), Nb(1)-O(3) 2.2556(16), Nb(1)-N(1) 1.7569(16).
Selected bond angles (°): Cl(1)-Nb(1)-Cl(2) 156.28(2), Cl(1)-Nb(1)-O(1) 96.62(4), Cl(1)-Nb(1)-O(2) 80.56(3), Cl(1)-Nb(1)-O(3) 80.31(3), Cl(1)-Nb(1)-N(1) 96.53(5), Cl(2)-Nb(1)-O(1) 95.41(4), Cl(2)-Nb(1)-O(2) 78.67(3), Cl(2)-Nb(1)-O(3) 82.13(3), Cl(2)-Nb(1)-N(1) 100.02(5), O(1)-Nb(1)-O(2) 91.94(6), O(1)-Nb(1)-O(3) 162.67(5), O(1)-Nb(1)-N(1) 104.90(7), O(2)-Nb(1)-O(3) 70.74(5), O(2)-Nb(1)-N(1) 163.15(7), O(3)-Nb(1)-N(1) 92.42(7), Nb(1)-O(1)-C(9) 159.95(13), Nb(1)-N(1)-C(1) 175.74(14).
X-ray Structure Report

for

NbCl$_2$(N-2,6-Me$_2$C$_6$H$_3$)(O-2,6-Pr$_2$C$_6$H$_3$)(dme) (1a)

February 13, 2014
Experimental

Data Collection

A yellow block crystal of C_{24}H_{36}Cl_2NNbO_3 having approximate dimensions of 0.260 x 0.230 x 0.220 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer Mo-Kα radiation.

The crystal-to-detector distance was 0.00 mm.

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

\[
\begin{align*}
a &= 13.572(4) \text{ Å} \\
b &= 9.116(2) \text{ Å} \quad \beta &= 103.824(3)^\circ \\
c &= 21.854(6) \text{ Å} \\
V &= 2625.6(11) \text{ Å}^3
\end{align*}
\]

For Z = 4 and F.W. = 550.37, the calculated density is 1.392 g/cm\(^3\). The reflection conditions of:

\[
\begin{align*}
h0l &: l = 2n \\
0k0 &: k = 2n
\end{align*}
\]

uniquely determine the space group to be:

\[P2_1/c (#14)\]

The data were collected at a temperature of 0 ± 1°C to a maximum 2θ value of 55.0°. The crystal-to-detector distance was 0.00 mm. Readout was performed in the 0.000 mm pixel mode.

Data Reduction
Of the 26903 reflections that were collected, 6010 were unique ($R_{\text{int}} = 0.0223$); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, $\mu$, for Mo-K{$\alpha$} radiation is 6.855 cm{$^{-1}$}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.794 to 0.860. The data were corrected for Lorentz and polarization effects.

**Structure Solution and Refinement**

The structure was solved by direct methods$^2$ and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement$^3$ on $F^2$ was based on 6010 observed reflections and 280 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \frac{\sum ||Fo|| - |Fc||}{\sum |Fo|} = 0.0246$$

$$wR2 = \left[ \frac{\sum w(Fo^2 - Fc^2)^2}{\sum w(Fo^2)^2} \right]^{1/2} = 0.0585$$

The standard deviation of an observation of unit weight$^4$ was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.61 and -0.39 e/$\textrm{Å}^3$, respectively.

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$^{10}$. 

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References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User’s Guide, Molecular Structure Corporation, (c) 2000. J.W. Pflugrath (1999) Acta Cryst. D55, 1718-1725.

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

(3) Least Squares function minimized: (SHELXL97)

\[ \sum w(F_o^2 - F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.} \]

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

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

where: \( N_o = \text{number of observations} \)

\( N_v = \text{number of variables} \)

(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).

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(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

| Property                      | Value                                      |
|-------------------------------|--------------------------------------------|
| **Empirical Formula**         | \( \text{C}_24\text{H}_{36}\text{Cl}_2\text{NNbO}_3 \)               |
| **Formula Weight**            | 550.37                                     |
| **Crystal Color, Habit**      | yellow, block                              |
| **Crystal Dimensions**        | 0.260 X 0.230 X 0.220 mm                   |
| **Crystal System**            | monoclinic                                 |
| **Lattice Type**              | Primitive                                  |
| **Lattice Parameters**        | \( a = 13.572(4) \text{ Å} \)             |
|                               | \( b = 9.116(2) \text{ Å} \)              |
|                               | \( c = 21.854(6) \text{ Å} \)             |
|                               | \( \beta = 103.824(3) \text{ °} \)       |
|                               | \( V = 2625.6(11) \text{ Å}^3 \)          |
| **Space Group**               | \( \text{P2}_1/c \) (#14)                 |
| **Z value**                   | 4                                          |
| **D_{calc}**                  | 1.392 g/cm\(^3\)                          |
| **F_{000}**                   | 1144.00                                    |
| **\( \mu(\text{MoK}\alpha) \)** | 6.855 cm\(^{-1}\)                        |
B. Intensity Measurements

| Parameter                  | Value                                       |
|----------------------------|---------------------------------------------|
| Diffractometer             | XtaLAB mini                                 |
| Radiation                  | MoK\(\alpha\) (\lambda = 0.71075 \text{ Å}) |
| Voltage, Current           | 50kV, 12mA                                  |
| Temperature                | 0.0°C                                       |
| Detector Aperture          | 75 mm (diameter)                            |
| Detector Position          | 0.00 mm                                     |
| Pixel Size                 | 0.073 mm                                    |
| \(2\theta_{\text{max}}\)  | 55.0°                                       |
| No. of Reflections Measured| Total: 26903                                 |
|                            | Unique: 6010 (R\text{int} = 0.0223)         |
| Corrections                | Lorentz-polarization                        |
|                            | Absorption                                  |
|                            | (trans. factors: 0.794 - 0.860)             |
C. Structure Solution and Refinement

Structure Solution
Direct Methods (SHELX97)

Refinement
Full-matrix least-squares on $F^2$

Function Minimized
$\Sigma w (F_o^2 - F_c^2)^2$

Least Squares Weights
$w = 1 / [ \sigma^2 (F_o^2) + (0.0257 \cdot P)^2 + 1.7772 \cdot P ]$
where $P = (\text{Max}(F_o^2,0) + 2 F_c^2)/3$

$\theta_{\text{max}}$ cutoff
55.0°

Anomalous Dispersion
All non-hydrogen atoms

No. Observations (All reflections)
6010

No. Variables
280

Reflection/Parameter Ratio
21.46

Residuals: R1 ($I>2.00\sigma(I)$)
0.0246

Residuals: R (All reflections)
0.0272

Residuals: wR2 (All reflections)
0.0585

Goodness of Fit Indicator
1.062

Max Shift/Error in Final Cycle
0.002

Maximum peak in Final Diff. Map
0.61 e^-Å^3

Minimum peak in Final Diff. Map
-0.39 e^-Å^3
Table S3-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$

| atom | $x$           | $y$           | $z$           | $B_{\text{eq}}$ |
|------|--------------|--------------|--------------|----------------|
| Nb1  | 0.21600(2)   | 0.10799(2)   | 0.34521(2)   | 1.019(4)       |
| Cl2  | 0.38136(3)   | 0.02123(4)   | 0.33714(2)   | 1.663(7)       |
| Cl3  | 0.03439(3)   | 0.16352(5)   | 0.31525(2)   | 1.902(7)       |
| O1   | 0.26175(8)   | 0.30254(12)  | 0.36272(5)   | 1.25(2)        |
| O2   | 0.16882(9)   | -0.09699(12) | 0.28904(5)   | 1.51(2)        |
| O3   | 0.19508(9)   | 0.1675(2)    | 0.23723(5)   | 1.87(2)        |
| N1   | 0.21588(9)   | 0.0313(2)    | 0.41932(6)   |               |
| C1   | 0.04010(13)  | -0.1208(2)   | 0.43694(10)  | 2.40(4)        |
| C2   | 0.13226(13)  | -0.0980(2)   | 0.48990(9)   | 1.79(3)        |
| C3   | 0.21664(12)  | -0.0206(2)   | 0.47933(7)   | 1.30(3)        |
| C4   | 0.30253(13)  | 0.0080(2)    | 0.52881(7)   | 1.51(3)        |
| C5   | 0.38963(12)  | 0.0957(2)    | 0.51674(8)   | 1.70(3)        |
| C6   | 0.3032(2)    | -0.0450(2)   | 0.58864(8)   | 2.19(3)        |
| C7   | 0.2214(2)    | -0.1225(2)   | 0.59950(9)   | 2.67(4)        |
| C8   | 0.1373(2)    | -0.1483(2)   | 0.55089(10)  | 2.52(4)        |
| C9   | 0.30971(11)  | 0.4184(2)    | 0.39714(7)   | 1.13(3)        |
| C10  | 0.40288(13)  | 0.6601(2)    | 0.46340(8)   | 1.79(3)        |
| C11  | 0.32145(12)  | 0.5935(2)    | 0.48052(7)   | 1.46(3)        |
| C12  | 0.43778(13)  | 0.6043(2)    | 0.41340(8)   | 1.65(3)        |
| C13  | 0.39215(11)  | 0.4836(2)    | 0.37889(7)   | 1.26(3)        |
| C14  | 0.27397(11)  | 0.4704(2)    | 0.44853(7)   | 1.20(3)        |
| C15  | 0.1992(2)    | -0.2399(2)   | 0.31639(9)   | 2.25(3)        |
| C16  | 0.1783(2)    | -0.0898(2)   | 0.22429(8)   | 2.20(3)        |
| C17  | 0.1383(2)    | 0.0554(3)    | 0.19778(8)   | 2.38(4)        |
| C18  | 0.1649(2)    | 0.3124(3)    | 0.21360(9)   | 2.80(4)        |
| C20  | 0.54123(13)  | 0.3694(3)    | 0.34716(9)   | 2.22(3)        |
| C21  | 0.4264(2)    | 0.5416(3)    | 0.27275(8)   | 2.39(4)        |
| C22  | 0.43221(12)  | 0.4253(2)    | 0.32421(7)   | 1.47(3)        |
| C23  | 0.18382(12)  | 0.3986(2)    | 0.46647(8)   | 1.41(3)        |
| C24  | 0.1897(2)    | 0.4055(3)    | 0.53711(9)   | 2.59(4)        |
| C25  | 0.08504(13)  | 0.4681(3)    | 0.42895(10)  | 2.60(4)        |

$B_{\text{eq}} = 8/3 (U_{11}^{\text{aa*}})^2 + U_{22}^{\text{bb*}})^2 + U_{33}^{\text{cc*}})^2 + 2U_{12}^{\text{aa*bb*}}\cos \Theta + 2U_{13}^{\text{aa*cc*}}\cos \Theta + 2U_{23}^{\text{bb*cc*}}\cos \Theta$
Table S3-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogen atoms

| atom  | x     | y     | z     | $B_{\text{iso}}$ |
|-------|-------|-------|-------|------------------|
| H1A   | 0.0196| -0.0287| 0.4165| 2.89             |
| H1B   | -0.0141| -0.1596| 0.4534| 2.89             |
| H1C   | 0.0559| -0.1886| 0.4071| 2.89             |
| H5A   | 0.4465| 0.0884| 0.5525| 2.03             |
| H5B   | 0.3698| 0.1966| 0.5100| 2.03             |
| H5C   | 0.4083| 0.0582| 0.4800| 2.03             |
| H6    | 0.3594| -0.0281| 0.6218| 2.63             |
| H7    | 0.2231| -0.1573| 0.6397| 3.21             |
| H8    | 0.0828| -0.2004| 0.5590| 3.02             |
| H10   | 0.4339| 0.7418| 0.4854| 2.14             |
| H11   | 0.2981| 0.6316| 0.5139| 1.75             |
| H12   | 0.4930| 0.6486| 0.4026| 1.98             |
| H15A  | 0.2705| -0.2538| 0.3199| 2.70             |
| H15B  | 0.1616| -0.3149| 0.2899| 2.70             |
| H15C  | 0.1856| -0.2454| 0.3575| 2.70             |
| H16A  | 0.1399| -0.1685| 0.1998| 2.64             |
| H16B  | 0.2489| -0.1001| 0.2229| 2.64             |
| H17A  | 0.1461| 0.0655| 0.1550| 2.86             |
| H17B  | 0.0668| 0.0638| 0.1971| 2.86             |
| H18A  | 0.2014| 0.3843| 0.2423| 3.36             |
| H18B  | 0.0934| 0.3246| 0.2096| 3.36             |
| H18C  | 0.1797| 0.3247| 0.1731| 3.36             |
| H20A  | 0.5436| 0.2953| 0.3787| 2.66             |
| H20B  | 0.5848| 0.4494| 0.3649| 2.66             |
| H20C  | 0.5636| 0.3285| 0.3123| 2.66             |
| H21A  | 0.4546| 0.5027| 0.2399| 2.86             |
| H21B  | 0.4640| 0.6269| 0.2905| 2.86             |
| H21C  | 0.3568| 0.5681| 0.2556| 2.86             |
| H22   | 0.3895| 0.3423| 0.3056| 1.76             |
| H23   | 0.1831| 0.2949| 0.4545| 1.69             |
| H24A  | 0.2527| 0.3638| 0.5599| 3.11             |
| H24B  | 0.1343| 0.3512| 0.5462| 3.11             |
| H24C  | 0.1857| 0.5059| 0.5496| 3.11             |
| H25A  | 0.0795| 0.4546| 0.3847| 3.12             |
| H25B  | 0.0853| 0.5711| 0.4382| 3.12             |
| H25C  | 0.0284| 0.4223| 0.4404| 3.12             |
### Table S3-3. Anisotropic displacement parameters

| Atom | U$_{11}$   | U$_{22}$   | U$_{33}$   | U$_{12}$  | U$_{13}$  | U$_{23}$  |
|------|------------|------------|------------|-----------|-----------|-----------|
| Nb1  | 0.01233(7) | 0.01442(7) | 0.01157(7) | -0.00083(5) | 0.00209(5) | -0.00225(5) |
| Cl2  | 0.0146(2)  | 0.0248(2)  | 0.0248(2)  | 0.0008(2)  | 0.0065(2)  | -0.0033(2) |
| Cl3  | 0.0147(2)  | 0.0286(2)  | 0.0272(2)  | 0.0039(2)  | 0.0015(2)  | -0.0012(2) |
| O1   | 0.0169(5)  | 0.0158(6)  | 0.0152(5)  | -0.0020(5) | 0.0047(4)  | -0.0023(5) |
| O2   | 0.0203(6)  | 0.0188(6)  | 0.0186(6)  | -0.0024(5) | 0.0051(5)  | -0.0067(5) |
| O3   | 0.0263(7)  | 0.0287(7)  | 0.0138(6)  | -0.0067(5) | 0.0008(5)  | 0.0001(5)  |
| N1   | 0.0130(6)  | 0.0145(6)  | 0.0179(6)  | -0.0013(5) | 0.0036(5)  | -0.0028(5) |
| C1   | 0.0212(9)  | 0.0227(9)  | 0.0499(12) | -0.0063(7) | 0.0134(8)  | 0.0004(8)  |
| C2   | 0.0266(9)  | 0.0130(8)  | 0.0334(10)| -0.0007(7) | 0.0166(8)  | -0.0007(7) |
| C3   | 0.0212(8)  | 0.0120(7)  | 0.0181(8)  | 0.0009(6)  | 0.0084(6)  | 0.0000(6)  |
| C4   | 0.0267(9)  | 0.0143(8)  | 0.0171(8)  | 0.0021(7)  | 0.0063(7)  | -0.0003(6) |
| C5   | 0.0208(8)  | 0.0241(9)  | 0.0170(8)  | -0.0009(7) | -0.0004(6) | 0.0003(7)  |
| C6   | 0.0430(11) | 0.0226(9)  | 0.0180(8)  | 0.0023(8)  | 0.0078(8)  | 0.0018(7)  |
| C7   | 0.0583(13) | 0.0249(10)| 0.0247(9)  | 0.0027(9)  | 0.0224(9)  | 0.0077(8)  |
| C8   | 0.0430(11) | 0.0192(9)  | 0.0432(11)| -0.0014(8) | 0.0297(10) | 0.0046(8)  |
| C9   | 0.0152(7)  | 0.0134(7)  | 0.0138(7)  | -0.0001(6) | 0.0029(6)  | 0.0003(6)  |
| C10  | 0.0244(9)  | 0.0208(8)  | 0.0238(9)  | -0.0080(7) | 0.0080(7)  | -0.0072(7) |
| C11  | 0.0219(8)  | 0.0185(8)  | 0.0171(8)  | -0.0021(6) | 0.0088(6)  | -0.0037(6) |
| C12  | 0.0210(8)  | 0.0214(8)  | 0.0224(8)  | -0.0065(7) | 0.0094(7)  | -0.0019(7) |
| C13  | 0.0173(8)  | 0.0172(8)  | 0.0138(7)  | 0.0006(6)  | 0.0044(6)  | 0.0012(6)  |
| C14  | 0.0166(7)  | 0.0150(7)  | 0.0144(7)  | -0.0001(6) | 0.0047(6)  | 0.0013(6)  |
| C15  | 0.0271(9)  | 0.0173(8)  | 0.0393(11)| 0.0015(7)  | 0.0046(8)  | -0.0049(8) |
| C16  | 0.0292(9)  | 0.0361(10)| 0.0216(9)  | -0.0122(8) | 0.0127(7)  | -0.0168(8) |
| C17  | 0.0320(10)| 0.0451(12)| 0.0120(8)  | -0.0145(9) | 0.0026(7)  | -0.0073(8) |
| C18  | 0.0414(11)| 0.0378(11)| 0.0224(9)  | -0.0046(9) | -0.0019(8) | 0.0106(8)  |
| C20  | 0.0222(9)  | 0.0360(10)| 0.0268(9)  | 0.0037(8)  | 0.0073(7)  | -0.0064(8) |
| C21  | 0.0378(11)| 0.0346(10)| 0.0221(9)  | 0.0015(9)  | 0.0146(8)  | 0.0046(8)  |
| C22  | 0.0194(8)  | 0.0224(8)  | 0.0157(7)  | -0.0021(7) | 0.0075(6)  | -0.0020(6) |
| C23  | 0.0196(8)  | 0.0157(8)  | 0.0207(8)  | -0.0033(6) | 0.0098(6)  | -0.0029(6) |
| C24  | 0.0440(12)| 0.0340(11)| 0.0280(10)| -0.0167(9) | 0.0236(9)  | -0.0062(8) |
| C25  | 0.0197(9)  | 0.0269(10)| 0.0541(13)| 0.0004(8)  | 0.0126(9)  | -0.0006(9) |

The general temperature factor expression: \( \exp(-2\pi^2[a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2ab^*U_{12}hk + 2ac^*U_{13}hl + 2b^c*U_{23}kl]) \)
Table S3-4. Bond lengths (Å)

| atom | atom | distance   | atom | atom | distance   |
|------|------|------------|------|------|------------|
| Nb1  | Cl2  | 2.4254(8)  | Nb1  | Cl3  | 2.4473(8)  |
| Nb1  | O1   | 1.8878(12) | Nb1  | O2   | 2.2434(12) |
| Nb1  | O3   | 2.3714(13) | Nb1  | N1   | 1.7643(15) |
| O1   | C9   | 1.3682(18) | O2   | C15  | 1.451(2)   |
| O2   | C16  | 1.453(3)   | O3   | C17  | 1.437(3)   |
| O3   | C18  | 1.441(3)   | N1   | C3   | 1.392(2)   |
| C1   | C2   | 1.502(3)   | C2   | C3   | 1.410(3)   |
| C2   | C8   | 1.396(3)   | C3   | C4   | 1.412(2)   |
| C4   | C5   | 1.502(3)   | C4   | C6   | 1.392(3)   |
| C6   | C7   | 1.384(3)   | C7   | C8   | 1.382(3)   |
| C9   | C13  | 1.406(3)   | C9   | C14  | 1.408(3)   |
| C10  | C11  | 1.389(3)   | C10  | C12  | 1.387(3)   |
| C11  | C14  | 1.396(2)   | C12  | C13  | 1.393(3)   |
| C13  | C22  | 1.522(3)   | C14  | C23  | 1.519(3)   |
| C16  | C17  | 1.494(3)   | C20  | C22  | 1.532(3)   |
| C21  | C22  | 1.534(3)   | C23  | C24  | 1.528(3)   |
| C23  | C25  | 1.532(3)   |      |      |            |
Table S3-5. Bond lengths involving hydrogens (Å)

| atom  | atom | distance | atom  | atom | distance |
|-------|------|----------|-------|------|----------|
| C1    | H1A  | 0.960    | C1    | H1B  | 0.960    |
| C1    | H1C  | 0.960    | C5    | H5A  | 0.960    |
| C5    | H5B  | 0.960    | C5    | H5C  | 0.960    |
| C6    | H6   | 0.930    | C7    | H7   | 0.930    |
| C8    | H8   | 0.930    | C10   | H10  | 0.930    |
| C11   | H11  | 0.930    | C12   | H12  | 0.930    |
| C15   | H15A | 0.960    | C15   | H15B | 0.960    |
| C15   | H15C | 0.960    | C16   | H16A | 0.970    |
| C16   | H16B | 0.970    | C17   | H17A | 0.970    |
| C17   | H17B | 0.970    | C18   | H18A | 0.960    |
| C18   | H18B | 0.960    | C18   | H18C | 0.960    |
| C20   | H20A | 0.960    | C20   | H20B | 0.960    |
| C20   | H20C | 0.960    | C21   | H21A | 0.960    |
| C21   | H21B | 0.960    | C21   | H21C | 0.960    |
| C22   | H22  | 0.980    | C23   | H23  | 0.980    |
| C24   | H24A | 0.960    | C24   | H24B | 0.960    |
| C24   | H24C | 0.960    | C25   | H25A | 0.960    |
| C25   | H25B | 0.960    | C25   | H25C | 0.960    |
Table S3-6. Bond angles (°)

| atom | atom | atom | angle  | atom | atom | atom | angle  |
|------|------|------|--------|------|------|------|--------|
| Cl2  | Nb1  | Cl3  | 159.77(3) | Cl2  | Nb1  | O1   | 93.20(4) |
| Cl2  | Nb1  | O2   | 80.60(4)  | Cl2  | Nb1  | O3   | 83.98(4) |
| Cl2  | Nb1  | N1   | 98.13(5)  | Cl3  | Nb1  | O1   | 96.97(4) |
| Cl3  | Nb1  | O2   | 83.59(4)  | Cl3  | Nb1  | O3   | 79.22(4) |
| Cl3  | Nb1  | N1   | 96.07(5)  | O1   | Nb1  | O2   | 158.51(6) |
| O1   | Nb1  | O3   | 86.68(5)  | O1   | Nb1  | N1   | 104.97(6) |
| O2   | Nb1  | O3   | 72.26(5)  | O2   | Nb1  | N1   | 96.30(6)  |
| O3   | Nb1  | N1   | 167.95(5) | Nb1  | O1   | C9   | 158.00(10) |
| Nb1  | O2   | C15  | 120.42(10)| Nb1  | O2   | C16  | 114.54(10) |
| C15  | O2   | C16  | 111.05(14)| Nb1  | O3   | C17  | 110.73(11) |
| Nb1  | O3   | C18  | 121.49(11)| C17  | O3   | C18  | 111.76(13) |
| Nb1  | N1   | C3   | 176.53(12)| C1   | C2   | C3   | 120.16(17) |
| C1   | C2   | C8   | 122.13(18)| C3   | C2   | C8   | 117.69(16) |
| N1   | C3   | C2   | 120.06(14)| N1   | C3   | C4   | 118.52(15) |
| C2   | C3   | C4   | 121.41(15)| C3   | C4   | C5   | 120.29(15) |
| C3   | C4   | C6   | 118.31(17)| C5   | C4   | C6   | 121.39(14) |
| C4   | C6   | C7   | 120.85(16)| C6   | C7   | C8   | 120.34(19) |
| C2   | C8   | C7   | 121.4(2)  | O1   | C9   | C13  | 118.46(15) |
| O1   | C9   | C14  | 119.28(14)| C13  | C9   | C14  | 122.24(14) |
| C11  | C10  | C12  | 119.69(16)| C10  | C11  | C14  | 121.25(16) |
| C10  | C12  | C13  | 121.66(17)| C9   | C13  | C12  | 117.46(16) |
| C9   | C13  | C22  | 122.21(14)| C12  | C13  | C22  | 120.32(15) |
| C9   | C14  | C11  | 117.67(15)| C9   | C14  | C23  | 120.88(14) |
| C11  | C14  | C23  | 121.40(15)| O2   | C16  | C17  | 108.01(15) |
| O3   | C17  | C16  | 107.72(14)| C13  | C22  | C20  | 110.94(13) |
| C13  | C22  | C21  | 111.64(14)| C20  | C22  | C21  | 110.31(16) |
| C14  | C23  | C24  | 113.10(14)| C14  | C23  | C25  | 109.85(14) |
| C24  | C23  | C25  | 110.57(16)|      |      |      |        |
Table S3-7. Bond angles involving hydrogens (°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C2   | C1   | H1A  | 109.5 | C2   | C1   | H1B  | 109.5 |
| C2   | C1   | H1C  | 109.5 | H1A  | C1   | H1B  | 109.5 |
| H1A  | C1   | H1C  | 109.5 | H1B  | C1   | H1C  | 109.5 |
| C4   | C5   | H5A  | 109.5 | C4   | C5   | H5B  | 109.5 |
| C4   | C5   | H5C  | 109.5 | H5A  | C5   | H5B  | 109.5 |
| H5A  | C5   | H5C  | 109.5 | H5B  | C5   | H5C  | 109.5 |
| C4   | C6   | H6   | 119.6 | C7   | C6   | H6   | 119.6 |
| C6   | C7   | H7   | 119.8 | C8   | C7   | H7   | 119.8 |
| C2   | C8   | H8   | 119.3 | C7   | C8   | H8   | 119.3 |
| C11  | C10  | H10  | 120.2 | C12  | C10  | H10  | 120.2 |
| C10  | C11  | H11  | 119.4 | C14  | C11  | H11  | 119.4 |
| C10  | C12  | H12  | 119.2 | C13  | C12  | H12  | 119.2 |
| O2   | C15  | H15A | 109.5 | O2   | C15  | H15B | 109.5 |
| O2   | C15  | H15C | 109.5 | H15A | C15  | H15B | 109.5 |
| H15A | C15  | H15C | 109.5 | H15B | C15  | H15C | 109.5 |
| O2   | C16  | H16A | 110.1 | O2   | C16  | H16B | 110.1 |
| C17  | C16  | H16A | 110.1 | C14  | C16  | H16B | 110.1 |
| H16A | C16  | H16B | 108.4 | O3   | C17  | H17A | 108.2 |
| O3   | C17  | H17B | 110.2 | C16  | C17  | H17B | 108.2 |
| C16  | C17  | H17B | 110.2 | H17A | C17  | H17B | 108.5 |
| O3   | C18  | H18A | 109.5 | O3   | C18  | H18B | 109.5 |
| O3   | C18  | H18C | 109.5 | H18A | C18  | H18B | 109.5 |
| H18A | C18  | H18C | 109.5 | H18B | C18  | H18C | 109.5 |
| C22  | C20  | H20A | 109.5 | C22  | C20  | H20B | 109.5 |
| C22  | C20  | H20C | 109.5 | H20A | C20  | H20B | 109.5 |
| H20A | C20  | H20C | 109.5 | H20B | C20  | H20C | 109.5 |
| C22  | C21  | H21A | 109.5 | C22  | C21  | H21B | 109.5 |
| C22  | C21  | H21C | 109.5 | H21A | C21  | H21B | 109.5 |
| H21A | C21  | H21C | 109.5 | H21B | C21  | H21C | 109.5 |
| C13  | C22  | H22  | 107.9 | C20  | C22  | H22  | 107.9 |
| C21  | C22  | H22  | 107.9 | C14  | C23  | H23  | 107.7 |
| C24  | C23  | H23  | 107.7 | C25  | C23  | H23  | 107.7 |
| C23  | C24  | H24A | 109.5 | C23  | C24  | H24B | 109.5 |
| C23  | C24  | H24C | 109.5 | H24A | C24  | H24B | 109.5 |
| H24A | C24  | H24C | 109.5 | H24B | C24  | H24C | 109.5 |
| C23  | C25  | H25A | 109.5 | C23  | C25  | H25B | 109.5 |
| C23  | C25  | H25C | 109.5 | H25A | C25  | H25B | 109.5 |
Table S3-7. Bond angles involving hydrogens (°) (continued)

| atom  | atom | atom | angle | atom  | atom | atom | angle |
|-------|------|------|-------|-------|------|------|-------|
| H25A  | C25  | H25C | 109.5 | H25B  | C25  | H25C | 109.5 |
Table S3-8. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle   | atom1 | atom2 | atom3 | atom4 | angle   |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| Cl2   | Nb1   | O1    | C9    | -76.6(3)| Cl2   | Nb1   | O2    | C15   | 65.20(8)|
| Cl2   | Nb1   | O2    | C16   | -71.34(7)| Cl2   | Nb1   | O3    | C17   | 98.32(7)|
| Cl2   | Nb1   | O3    | C18   | -127.52(8)| Cl3   | Nb1   | O1    | C9    | 121.0(3)|
| Cl3   | Nb1   | O2    | C15   | -127.47(9)| Cl3   | Nb1   | O2    | C16   | 95.99(7)|
| Cl3   | Nb1   | O3    | C17   | -70.36(7)| Cl3   | Nb1   | O3    | C18   | 63.80(8)|
| O1    | Nb1   | O2    | C15   | 139.78(11)| O1    | Nb1   | O2    | C16   | 3.24(17)|
| O2    | Nb1   | O1    | C9    | -148.84(18)| O1    | Nb1   | O3    | C17   | -168.10(8)|
| O3    | Nb1   | O3    | C18   | -33.94(9)| O3    | Nb1   | O1    | C9    | -160.3(3)|
| N1    | Nb1   | O1    | C9    | 22.7(3)| O2    | Nb1   | O3    | C17   | 16.29(7)|
| O2    | Nb1   | O3    | C18   | 150.45(9)| O3    | Nb1   | O2    | C15   | 151.83(10)|
| O3    | Nb1   | O2    | C16   | 15.30(7)| N1    | Nb1   | O2    | C15   | -32.04(10)|
| N1    | Nb1   | O2    | C16   | -168.58(8)| Nb1   | O1    | C9    | C13   | 115.7(3)|
| Nb1   | O1    | C9    | C14   | -65.6(4)| Nb1   | O2    | C16   | C17   | -43.80(14)|
| C15   | O2    | C16   | C17   | 175.67(12)| Nb1   | O3    | C17   | C16   | -43.86(16)|
| C18   | O3    | C17   | C16   | 177.33(14)| C1    | C2    | C3    | N1    | -1.8(3)|
| C1    | C2    | C3    | C4    | 177.21(14)| C1    | C2    | C8    | C7    | -177.97(15)|
| C3    | C2    | C8    | C7    | 0.6(3)| C8    | C2    | C3    | N1    | 179.65(15)|
| C8    | C2    | C3    | C4    | -1.3(3)| N1    | C3    | C4    | C5    | 1.4(3)|
| N1    | C3    | C4    | C6    | -179.58(13)| C2    | C3    | C4    | C5    | -177.61(13)|
| C2    | C3    | C4    | C6    | 1.4(3)| C3    | C4    | C6    | C7    | -0.6(3)|
| C5    | C4    | C6    | C7    | 178.36(15)| C4    | C6    | C7    | C8    | -0.1(3)|
| C6    | C7    | C8    | C2    | 0.2(3)| O1    | C9    | C13   | C12   | 178.03(11)|
| O1    | C9    | C13   | C22   | -2.72(19)| O1    | C9    | C14   | C11   | -176.77(11)|
| O1    | C9    | C14   | C23   | 0.58(19)| C13   | C9    | C14   | C11   | 1.9(2)|
| C13   | C9    | C14   | C23   | 179.21(12)| C14   | C9    | C13   | C12   | -0.6(2)|
| C14   | C9    | C13   | C22   | 178.64(12)| C11   | C10   | C12   | C13   | 1.0(3)|
| C12   | C10   | C11   | C14   | 0.3(3)| C10   | C11   | C14   | C9    | -1.7(2)|
| C10   | C11   | C14   | C23   | -179.03(13)| C10   | C12   | C13   | C9    | -0.9(3)|
| C10   | C12   | C13   | C22   | 179.88(13)| C9    | C13   | C22   | C20   | -116.12(14)|
| C9    | C13   | C22   | C21   | 120.41(14)| C12   | C13   | C22   | C20   | 63.12(18)|
| C12   | C13   | C22   | C21   | -60.35(17)| C9    | C14   | C23   | C24   | 148.62(12)|
| C9    | C14   | C23   | C25   | -87.31(16)| C11   | C14   | C23   | C24   | -34.13(19)|
| C11   | C14   | C23   | C25   | 89.93(16)| O2    | C16   | C17   | O3    | 57.48(19)|
Table S3-9. Intramolecular contacts less than 3.60 Å

| atom | atom | distance   | atom | atom | distance   |
|------|------|------------|------|------|------------|
| Cl2  | C15  | 3.383(2)   | Cl2  | C16  | 3.3844(18) |
| Cl3  | C17  | 3.359(3)   | Cl3  | C18  | 3.434(3)   |
| O1   | C18  | 3.211(3)   | O1   | C22  | 2.871(3)   |
| O1   | C23  | 2.859(3)   | O1   | C25  | 3.433(3)   |
| N1   | C1   | 2.864(3)   | N1   | C5   | 2.8353(19) |
| N1   | C15  | 3.314(3)   | N1   | C23  | 3.560(3)   |
| C2   | C6   | 2.807(3)   | C3   | C7   | 2.772(3)   |
| C4   | C8   | 2.795(3)   | C9   | C10  | 2.770(3)   |
| C9   | C20  | 3.592(3)   | C9   | C25  | 3.317(3)   |
| C11  | C13  | 2.806(3)   | C11  | C24  | 2.953(3)   |
| C11  | C25  | 3.338(3)   | C12  | C14  | 2.800(3)   |
| C12  | C20  | 3.102(3)   | C12  | C21  | 3.094(3)   |
Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H5C  | 3.468    | Nb1  | H15A | 3.453    |
| Nb1  | H15C | 3.267    | Nb1  | H16B | 3.393    |
| Nb1  | H17B | 3.407    | Nb1  | H18A | 3.351    |
| Nb1  | H22  | 3.440    | Nb1  | H23  | 3.053    |
| Cl2  | H5C  | 3.075    | Cl2  | H15A | 2.902    |
| Cl2  | H16B | 2.923    | Cl2  | H20A | 3.310    |
| Cl2  | H22  | 3.015    | Cl3  | H1A  | 2.867    |
| Cl3  | H2B  | 2.440    | Cl3  | H25A | 3.045    |
| O1   | H5B  | 3.344    | O1   | H18A | 2.668    |
| O1   | H18B | 3.578    | O1   | H22  | 2.394    |
| O1   | H23  | 2.488    | O1   | H25A | 2.972    |
| O2   | H1A  | 3.404    | O2   | H17A | 3.231    |
| O2   | H17B | 2.602    | O3   | H16A | 3.213    |
| O3   | H16B | 2.587    | O3   | H22  | 3.139    |
| N1   | H1A  | 2.706    | N1   | H1C  | 2.920    |
| N1   | H5B  | 2.930    | N1   | H5C  | 2.643    |
| N1   | H15A | 3.577    | N1   | H15C | 2.845    |
| N1   | H23  | 2.594    | C1   | H8   | 2.690    |
| C1   | H15C | 3.138    | C2   | H7   | 3.256    |
| C2   | H15C | 3.422    | C3   | H1A  | 2.700    |
| C3   | H1B  | 3.299    | C3   | H1C  | 2.820    |
| C3   | H5A  | 3.300    | C3   | H5B  | 2.833    |
| C3   | H5C  | 2.695    | C3   | H6   | 3.250    |
| C3   | H8   | 3.244    | C3   | H15C | 3.307    |
| C3   | H23  | 2.943    | C4   | H7   | 3.249    |
| C4   | H23  | 3.294    | C4   | H24A | 3.414    |
| C5   | H6   | 2.676    | C5   | H23  | 3.345    |
| C5   | H24A | 3.340    | C6   | H5A  | 2.572    |
| C6   | H5B  | 3.060    | C6   | H5C  | 3.189    |
| C6   | H8   | 3.233    | C8   | H1A  | 3.182    |
| C8   | H1B  | 2.584    | C8   | H1C  | 3.095    |
| C8   | H6   | 3.234    | C9   | H5B  | 3.142    |
| C9   | H11  | 3.241    | C9   | H12  | 3.235    |
| C9   | H18A | 3.366    | C9   | H20A | 3.480    |
| C9   | H21C | 3.574    | C9   | H22  | 2.586    |
| C9   | H23  | 2.612    | C9   | H25A | 3.088    |
Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom | distance | atom   | atom | distance |
|--------|------|----------|--------|------|----------|
| C11    | H12  | 3.235    | C11    | H23  | 3.278    |
| C11    | H24A | 3.007    | C11    | H24C | 2.764    |
| C11    | H25B | 3.123    | C12    | H11  | 3.236    |
| C12    | H20A | 3.331    | C12    | H20B | 2.849    |
| C12    | H21B | 2.799    | C12    | H21C | 3.375    |
| C12    | H22  | 3.308    | C13    | H10  | 3.263    |
| C13    | H18A | 3.569    | C13    | H20A | 2.679    |
| C13    | H20B | 2.722    | C13    | H20C | 3.339    |
| C13    | H21A | 3.348    | C13    | H21B | 2.699    |
| C13    | H21C | 2.731    | C14    | H5B  | 2.981    |
| C14    | H10  | 3.262    | C14    | H24A | 2.700    |
| C14    | H24B | 3.356    | C14    | H24C | 2.771    |
| C14    | H25A | 2.678    | C14    | H25B | 2.679    |
| C14    | H25C | 3.325    | C15    | H1C  | 3.126    |
| C15    | H16A | 2.566    | C15    | H16B | 2.628    |
| C16    | H15A | 2.630    | C16    | H15B | 2.544    |
| C16    | H15C | 3.218    | C17    | H18A | 3.205    |
| C17    | H18B | 2.556    | C17    | H18C | 2.603    |
| C18    | H17A | 2.571    | C18    | H17B | 2.609    |
| C18    | H21C | 3.453    | C18    | H22  | 3.238    |
| C20    | H12  | 2.959    | C20    | H21A | 2.653    |
| C20    | H21B | 2.742    | C20    | H21C | 3.340    |
| C21    | H12  | 2.933    | C21    | H18A | 3.294    |
| C21    | H20A | 3.343    | C21    | H20B | 2.705    |
| C21    | H20C | 2.687    | C22    | H12  | 2.662    |
| C22    | H18A | 3.236    | C23    | H5B  | 3.085    |
| C23    | H11  | 2.688    | C24    | H5B  | 3.263    |
| C24    | H11  | 2.651    | C24    | H25A | 3.339    |
| C24    | H25B | 2.738    | C24    | H25C | 2.659    |
| C25    | H11  | 3.386    | C25    | H24A | 3.341    |
| C25    | H24B | 2.707    | C25    | H24C | 2.686    |
| H1A    | H8   | 3.406    | H1A    | H15C | 3.469    |
| H1B    | H8   | 2.396    | H1C    | H8   | 3.254    |
| H1C    | H15B | 3.420    | H1C    | H15C | 2.336    |
| H5A    | H6   | 2.381    | H5B    | H6   | 3.216    |
| H5B    | H23  | 2.688    | H5B    | H24A | 2.620    |
| H5C    | H6   | 3.411    | H6     | H7   | 2.305    |
Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H7   | H8   | 2.299    | H10  | H11  | 2.312    |
| H10  | H12  | 2.308    | H11  | H23  | 3.546    |
| H11  | H24A | 2.765    | H11  | H24B | 3.567    |
| H11  | H24C | 2.194    | H11  | H25B | 3.017    |
| H12  | H20A | 3.361    | H12  | H20B | 2.454    |
| H12  | H21B | 2.395    | H12  | H21C | 3.382    |
| H12  | H22  | 3.584    | H15A | H16A | 2.900    |
| H15A | H16B | 2.499    | H15B | H16B | 2.339    |
| H15B | H16B | 2.865    | H15B | H16A | 3.425    |
| H15C | H16B | 3.513    | H15A | H16A | 2.357    |
| H16A | H17B | 2.333    | H16B | H17B | 2.332    |
| H16B | H17B | 2.827    | H17A | H18A | 3.459    |
| H17A | H18B | 2.815    | H17A | H18C | 2.421    |
| H17B | H18A | 3.463    | H17B | H18B | 2.411    |
| H17B | H18C | 2.944    | H18A | H21C | 2.654    |
| H18A | H22  | 2.625    | H18C | H21C | 3.447    |
| H18C | H22  | 3.547    | H20A | H21A | 3.534    |
| H20A | H22  | 2.347    | H20B | H21A | 2.918    |
| H20B | H21B | 2.583    | H20B | H21C | 3.594    |
| H20B | H22  | 2.831    | H20C | H21A | 2.469    |
| H20C | H21B | 3.024    | H20C | H21C | 3.539    |
| H20C | H22  | 2.335    | H21A | H22  | 2.364    |
| H21B | H22  | 2.832    | H21C | H22  | 2.323    |
| H23  | H24A | 2.357    | H23  | H24B | 2.313    |
| H23  | H24C | 2.825    | H23  | H25A | 2.322    |
| H23  | H25B | 2.828    | H23  | H25C | 2.354    |
| H24A | H25B | 3.595    | H24A | H25C | 3.546    |
| H24B | H25A | 3.556    | H24B | H25B | 3.047    |
| H24B | H25C | 2.498    | H24C | H25A | 3.578    |
| H24C | H25B | 2.560    | H24C | H25C | 2.898    |
Table S3-11. Intermolecular contacts less than 3.60 Å

| atom | atom   | distance | atom  | atom   | distance |
|------|--------|----------|-------|--------|----------|
| Cl3  | C16\(^1\) | 3.598(2) | C1    | C8\(^2\) | 3.491(3) |
| C5   | C10\(^3\) | 3.534(3) | C8    | C1\(^2\)  | 3.491(3) |
| C10  | C5\(^3\)  | 3.534(3) | C16   | Cl3\(^4\) | 3.598(2) |

Symmetry Operators:

1. -X, Y+1/2, -Z+1/2
2. -X, -Y, -Z+1
3. -X+1, -Y+1, -Z+1
4. -X, Y+1/2-1, -Z+1/2
Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Cl2  | H5A  | 3.096    | Cl2  | H6   | 3.418    |
| Cl2  | H21A | 3.100    | Cl3  | H8   | 3.505    |
| Cl3  | H15B | 3.078    | Cl3  | H16A | 2.770    |
| Cl3  | H1B  | 3.521    | C1   | H1B  | 3.319    |
| Cl3  | H24B | 3.250    | Cl2  | H1A  | 3.432    |
| Cl2  | H25B | 2.874    | Cl2  | H11  | 3.295    |
| C2   | H1B  | 3.251    | C3   | H11  | 3.384    |
| C4   | H10  | 3.283    | C4   | H11  | 3.447    |
| C5   | H5A  | 3.415    | C5   | H10  | 2.826    |
| C5   | H12  | 3.119    | C6   | H11  | 3.363    |
| C6   | H18C | 3.425    | C6   | H20A | 3.054    |
| C6   | H20C | 3.573    | C6   | H21A | 3.471    |
| C6   | H21C | 3.553    | C7   | H1A  | 3.489    |
| C7   | H11  | 3.246    | C7   | H16A | 3.289    |
| C7   | H18C | 3.273    | C7   | H24C | 3.557    |
| C7   | H21C | 3.503    | C8   | H1B  | 3.257    |
| C8   | H11  | 3.207    | C8   | H24C | 3.222    |
| C8   | H25B | 3.504    | C8   | H25C | 3.396    |
| C9   | H15A | 3.411    | C9   | H15C | 3.504    |
| C10  | H5A  | 3.146    | C10  | H5B  | 3.272    |
| C10  | H15A | 3.315    | C10  | H15C | 3.396    |
| C10  | H20A | 3.377    | C11  | H15C | 3.228    |
| C11  | H20A | 3.340    | C11  | H20B | 3.337    |
| C12  | H5A  | 3.211    | C12  | H5B  | 3.290    |
| C12  | H15A | 2.965    | C13  | H15A | 3.017    |
| C14  | H15C | 3.312    | C15  | H21C | 3.279    |
| C16  | H7   | 3.104    | C17  | H24B | 3.408    |
| C17  | H24C | 3.494    | C17  | H25A | 3.208    |
| C17  | H25C | 3.528    | C18  | H1C  | 3.486    |
| C20  | H6   | 3.395    | C20  | H11  | 3.287    |
| C20  | H16B | 3.553    | C21  | H6   | 3.209    |
| C21  | H15A | 3.171    | C21  | H20C | 3.230    |
| C24  | H1B  | 3.314    | C24  | H17A | 2.790    |
Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C24  | H20B | 3.546    | C24  | H25C | 3.487    |
| C25  | H1C  | 3.176    | C25  | H8   | 3.392    |
| C25  | H15C | 3.485    | C25  | H17A | 3.353    |
| C25  | H17B | 3.144    | C25  | H24B | 3.555    |
| H1A  | C2   | 3.432    | H1A  | C7   | 3.489    |
| H1A  | C8   | 2.893    | H1A  | H1B  | 3.337    |
| H1A  | H8   | 2.634    | H1A  | H18B | 3.117    |
| H1A  | H18C | 3.225    | H1B  | Cl3  | 3.578    |
| H1B  | C2   | 3.251    | H1B  | C8   | 3.257    |
| H1B  | C24  | 3.314    | H1B  | H1A  | 3.337    |
| H1B  | H1B  | 3.519    | H1B  | H8   | 3.404    |
| H1B  | H18B | 3.471    | H1B  | H18C | 3.122    |
| H1B  | H24B | 2.392    | H1B  | H25B | 2.859    |
| H1B  | H25C | 3.372    | H1C  | C18  | 3.486    |
| H1C  | C25  | 3.176    | H1C  | H17A | 3.550    |
| H1C  | H17B | 3.353    | H1C  | H18B | 2.855    |
| H1C  | H18C | 3.260    | H1C  | H24B | 3.341    |
| H1C  | H25A | 3.317    | H1C  | H25B | 2.300    |
| H5A  | Cl2  | 3.096    | H5A  | C5   | 3.415    |
| H5A  | C10  | 3.146    | H5A  | C12  | 3.211    |
| H5A  | H5A  | 3.400    | H5A  | H5C  | 2.616    |
| H5A  | H10  | 3.470    | H5A  | H10  | 2.522    |
| H5A  | H12  | 2.646    | H5B  | C10  | 3.272    |
| H5B  | C12  | 3.290    | H5B  | H10  | 2.701    |
| H5B  | H12  | 2.721    | H5C  | C5   | 3.066    |
| H5C  | H5A  | 2.616    | H5C  | H5C  | 2.654    |
| H5C  | H10  | 2.904    | H5C  | H10  | 2.777    |
| H6   | Cl2  | 3.418    | H6   | C20  | 3.395    |
| H6   | C21  | 3.209    | H6   | H18C | 3.457    |
| H6   | H20A | 2.770    | H6   | H20C | 3.155    |
| H6   | H21A | 2.606    | H6   | H21C | 2.958    |
| H7   | C16  | 3.104    | H7   | H15B | 3.583    |
| H7   | H16A | 2.495    | H7   | H16B | 2.831    |
| H7   | H18A | 3.409    | H7   | H18C | 3.206    |
| H7   | H20A | 3.518    | H7   | H20C | 3.235    |
| H7   | H21C | 2.859    | H8   | Cl3  | 3.505    |
| H8   | Cl3  | 3.381    | H8   | C25  | 3.392    |
Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom     | distance | atom | atom     | distance |
|------|----------|----------|------|----------|----------|
| H8   | H1A³     | 2.634    | H8   | H1B³     | 3.404    |
| H8   | H16A⁹    | 3.218    | H8   | H24B³    | 3.552    |
| H8   | H24C⁶    | 3.050    | H8   | H25B⁶    | 3.369    |
| H8   | H25C³    | 2.526    | H10  | C⁴¹⁰     | 3.283    |
| H10  | C⁵¹⁰     | 3.382    | H10  | C⁵⁷      | 2.826    |
| H10  | H5A¹⁰    | 3.470    | H10  | H5C¹⁰    | 2.904    |
| H10  | H5B³     | 2.701    | H10  | H5A⁷     | 2.522    |
| H10  | H5C⁷     | 2.777    | H10  | H20A⁷    | 2.933    |
| H11  | C²¹⁰     | 3.295    | H11  | C³¹⁰     | 3.384    |
| H11  | C⁴¹⁰     | 3.447    | H11  | C⁶¹⁰     | 3.363    |
| H11  | C⁷¹⁰     | 3.246    | H11  | C⁸¹⁰     | 3.207    |
| H11  | C²⁰⁷     | 3.287    | H11  | H15C¹⁰   | 3.576    |
| H11  | H20A⁷    | 2.856    | H11  | H20B⁷    | 2.841    |
| H12  | C⁵⁷      | 3.119    | H12  | H5A⁷     | 2.646    |
| H12  | H5B³     | 2.721    | H12  | H15A¹⁰   | 3.252    |
| H12  | H24A⁷    | 3.353    | H15A | C⁹⁶      | 3.411    |
| H15A | C¹⁰⁶     | 3.315    | H15A | C¹²⁶     | 2.965    |
| H15A | C¹³⁶     | 3.017    | H15A | C²¹⁶     | 3.171    |
| H15A | H12⁶     | 3.252    | H15A | H21B⁶    | 3.050    |
| H15A | H21C⁶    | 2.601    | H15B | C¹³⁵     | 3.078    |
| H15B | H²¹¹²    | 3.583    | H15B | H15A     | 3.504    |
| H15B | H18A⁶    | 3.027    | H15B | H21C⁶    | 3.107    |
| H15B | H25A⁶    | 3.325    | H15C | C⁹⁶      | 3.504    |
| H15C | C¹⁰⁶     | 3.396    | H15C | C¹¹⁶     | 3.228    |
| H15C | C¹⁴⁶     | 3.312    | H15C | C²⁵⁶     | 3.485    |
| H15C | H¹¹⁶     | 3.576    | H15C | H25A⁶    | 3.212    |
| H15C | H25B⁶    | 2.985    | H16A | C¹³⁵     | 2.770    |
| H16A | C⁷¹¹²    | 3.289    | H16A | H7¹¹²    | 2.495    |
| H16A | H¹¹¹²    | 3.218    | H16A | H25A⁵    | 3.303    |
| H16A | H25C³    | 3.456    | H16A | H20²     | 3.553    |
| H16B | H¹¹¹²    | 2.831    | H16B | H20B²    | 3.324    |
| H16B | H20C²    | 2.904    | H16B | H21C⁶    | 3.362    |
| H17A | C²⁴¹²    | 2.790    | H17A | C²⁵⁵     | 3.353    |
| H17A | H¹¹⁴     | 3.550    | H17A | H24A¹²   | 2.875    |
| H17A | H²⁴B¹²    | 2.465    | H17A | H²⁴C¹²   | 2.572    |
| H17A | H²⁵A⁵    | 3.144    | H17A | H²⁵B⁵    | 3.310    |
| H17A | H²⁵C³    | 3.050    | H17B | C²⁵⁵     | 3.144    |
Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H17B   | H1C    | 3.353    | H17B   | H15B   | 3.367    |
| H17B   | H25A   | 2.537    | H17B   | H25B   | 3.177    |
| H17B   | H25C   | 3.242    | H18A   | H7     | 3.409    |
| H18A   | H15B   | 3.027    | H18B   | C1     | 3.521    |
| H18B   | C1     | 3.319    | H18B   | H1A    | 3.117    |
| H18B   | H1B    | 3.471    | H18B   | H1C    | 2.855    |
| H18C   | C1     | 3.391    | H18C   | C6     | 3.425    |
| H18C   | C7     | 3.273    | H18C   | H1A    | 3.225    |
| H18C   | H1B    | 3.122    | H18C   | H1C    | 3.260    |
| H18C   | H6     | 3.457    | H18C   | H7     | 3.206    |
| H18C   | H25A   | 2.537    | H18C   | H25B   | 3.177    |
| H20A   | C6     | 3.054    | H20A   | C7     | 3.486    |
| H20A   | C10    | 3.377    | H20A   | C11    | 3.340    |
| H20A   | H6     | 2.770    | H20A   | H7     | 3.518    |
| H20A   | H10    | 2.933    | H20A   | H11    | 2.856    |
| H20B   | C11    | 3.337    | H20B   | C24    | 3.546    |
| H20B   | H11    | 2.841    | H20B   | H16B   | 3.324    |
| H20B   | H24A   | 2.955    | H20B   | H24C   | 3.252    |
| H20C   | C6     | 3.573    | H20C   | C21    | 3.230    |
| H20C   | H6     | 3.155    | H20C   | H7     | 3.235    |
| H20C   | H16B   | 2.904    | H20C   | H21A   | 3.170    |
| H20C   | H21B   | 2.858    | H20C   | H21C   | 3.127    |
| H21A   | C12    | 3.100    | H21A   | C6     | 3.471    |
| H21A   | H6     | 2.606    | H21A   | H20C   | 3.170    |
| H21B   | H15A   | 3.050    | H21B   | H20C   | 2.858    |
| H21C   | C6     | 3.553    | H21C   | C7     | 3.503    |
| H21C   | C15    | 3.279    | H21C   | H6     | 2.958    |
| H21C   | H7     | 2.859    | H21C   | H15A   | 2.601    |
| H21C   | H15B   | 3.107    | H21C   | H16B   | 3.362    |
| H21C   | H20C   | 3.127    | H21C   | H7     | 3.353    |
| H24A   | H17A   | 2.875    | H24A   | H18C   | 3.350    |
| H24A   | H20B   | 2.955    | H24B   | C1     | 3.250    |
| H24B   | C17    | 3.408    | H24B   | C25    | 3.555    |
| H24B   | H1B    | 2.392    | H24B   | H1C    | 3.341    |
| H24B   | H8     | 3.552    | H24B   | H17A   | 2.465    |
| H24B   | H18C   | 3.135    | H24B   | H25B   | 3.160    |
| H24B   | H25C   | 3.087    | H24C   | C7     | 3.557    |
Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom    | distance | atom | atom    | distance |
|------|---------|----------|------|---------|----------|
| H24C | C8\textsuperscript{10} | 3.222    | H24C | C17\textsuperscript{8} | 3.494    |
| H24C | H8\textsuperscript{10} | 3.050    | H24C | H17A\textsuperscript{8} | 2.572    |
| H24C | H20B\textsuperscript{7} | 3.252    | H24C | H25C\textsuperscript{14} | 3.037    |
| H25A | C17\textsuperscript{4} | 3.208    | H25A | H1C\textsuperscript{10} | 3.317    |
| H25A | H15B\textsuperscript{10} | 3.325    | H25A | H15C\textsuperscript{10} | 3.212    |
| H25A | H16A\textsuperscript{4} | 3.303    | H25A | H17A\textsuperscript{4} | 3.144    |
| H25A | H17B\textsuperscript{4} | 2.537    | H25B | C1\textsuperscript{10} | 2.874    |
| H25B | C2\textsuperscript{10} | 3.231    | H25B | C8\textsuperscript{10} | 3.504    |
| H25B | H1B\textsuperscript{10} | 2.859    | H25B | H1C\textsuperscript{10} | 2.300    |
| H25B | H8\textsuperscript{10} | 3.369    | H25B | H15C\textsuperscript{10} | 2.985    |
| H25B | H17A\textsuperscript{4} | 3.310    | H25B | H17B\textsuperscript{4} | 3.177    |
| H25B | H24B\textsuperscript{14} | 3.160    | H25B | H25C\textsuperscript{14} | 3.373    |
| H25C | C8\textsuperscript{3} | 3.396    | H25C | C1\textsuperscript{7} | 3.528    |
| H25C | C24\textsuperscript{14} | 3.487    | H25C | H1B\textsuperscript{3} | 3.372    |
| H25C | H8\textsuperscript{3} | 2.526    | H25C | H16A\textsuperscript{4} | 3.456    |
| H25C | H17A\textsuperscript{4} | 3.050    | H25C | H17B\textsuperscript{4} | 3.242    |
| H25C | H24B\textsuperscript{14} | 3.087    | H25C | H24C\textsuperscript{14} | 3.037    |
| H25C | H25B\textsuperscript{14} | 3.373    | H25C | H25C\textsuperscript{14} | 3.215    |

Symmetry Operators:

1. $-X+1,-Y,-Z+1$
2. $-X+1,Y+1/2,-Z+1/2$
3. $-X,-Y,-Z+1$
4. $-X,Y+1/2,-Z+1/2$
5. $-X,Y+1/2-1,-Z+1/2$
6. $X,Y-1,Z$
7. $-X+1,Y+1,-Z+1/2$
8. $X,-Y+1/2,Z+1/2$
9. $X,-Y+1/2-1,Z+1/2$
10. $X,Y+1,Z$
11. $X,-Y+1/2-1,Z+1/2-1$
12. $X,-Y+1/2,Z+1/2-1$
13. $-X+1,Y+1/2,-Z+1/2$
14. $-X,-Y+1,-Z+1$
X-ray Structure Report

for

NbCl_2(N-2,6-MexC_6H_3)(O-2,6-PhC_6H_3)(dme) (1d)

February 7, 2018
Experimental

Data Collection

A colourless prism crystal of $\text{C}_3\text{H}_2\text{Cl}_2\text{NNbO}_3$ having approximate dimensions of 0.200 x 0.160 x 0.080 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 49.66 mm.

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

$$a = 9.9108(3) \text{ Å} \quad \alpha = 95.967(3)^{\circ}$$
$$b = 12.5655(5) \text{ Å} \quad \beta = 101.025(3)^{\circ}$$
$$c = 13.0149(5) \text{ Å} \quad \gamma = 106.341(3)^{\circ}$$
$$V = 1505.05(10) \text{ Å}^3$$

For $Z = 2$ and F.W. = 618.40, the calculated density is 1.364 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:

P-1 (#2)

The data were collected at a temperature of -180 ± 1°C to a maximum 2θ value of 65.2°. A total of 540 oscillation images were collected. A sweep of data was done using $\omega$ scans from -60.0 to 120.0° in 1.00° step, at $\chi$=54.0° and $\phi = 0.0°$. The exposure rate was 64.0 [sec./°]. The detector swing angle was 30.00°. A second sweep was performed using $\omega$ scans from -60.0 to 120.0° in 1.00° step, at $\chi$=54.0° and $\phi = 120.0°$. The exposure rate was 64.0 [sec./°]. The detector swing angle was 30.00°. Another sweep was performed using $\omega$ scans from -60.0 to 120.0° in 1.00° step, at $\chi$=54.0° and $\phi = 240.0°$. The exposure rate
was 64.0 [sec./°]. The detector swing angle was 30.00°. The crystal-to-detector distance was 49.66 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R_{int} = 0.0323); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).

The linear absorption coefficient, \( \mu \), for Mo-K\(\alpha \) radiation is 6.067 cm\(^{-1}\). An empirical absorption correction was applied which resulted in transmission factors ranging from 0.785 to 0.953. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods\(^2\) and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement\(^3\) on \( F^2 \) was based on 6894 observed reflections and 334 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

\[
R1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} = 0.0275
\]

\[
wR^2 = \frac{\sum w(Fo^2 - Fc^2)^2}{\sum w(Fo^2)^2}^{1/2} = 0.0733
\]

The goodness of fit\(^4\) was 1.01. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.67 and -0.74 e/Å\(^3\), respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4\(^5\). Anomalous dispersion effects were included in Fcalc\(^6\); the values for \( f' \) and \( \Delta f'' \) were those of Creagh and McAuley\(^7\). The values for the mass attenuation coefficients are those of Creagh and
Hubbell\textsuperscript{8}. All calculations were performed using the CrystalStructure\textsuperscript{9} crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7\textsuperscript{10}.

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

$$\sum w(F_o^2 - F_c^2)^2$$ where \(w = \text{Least Squares weights.}\)

(4) Goodness of fit is defined as:

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

where: \(N_o = \text{number of observations}\)

\(N_v = \text{number of variables}\)

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2.5: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
### EXPERIMENTAL DETAILS

#### A. Crystal Data

| Property                          | Value                        |
|----------------------------------|-----------------------------|
| Empirical Formula                | C$_{30}$H$_{32}$Cl$_2$NNbO$_3$ |
| Formula Weight                   | 618.40                       |
| Crystal Color, Habit             | colourless, prism            |
| Crystal Dimensions               | 0.200 X 0.160 X 0.080 mm     |
| Crystal System                   | triclinic                    |
| Lattice Type                     | Primitive                    |
| Lattice Parameters               | a = 9.9108(3) Å              |
|                                  | b = 12.5655(5) Å             |
|                                  | c = 13.0149(5) Å             |
|                                  | $\alpha$ = 95.967(3)°       |
|                                  | $\beta$ = 101.025(3)°       |
|                                  | $\gamma$ = 106.341(3)°      |
|                                  | V = 1505.05(10) Å$^3$       |
| Space Group                      | P-1 (#2)                     |
| Z value                          | 2                            |
| $D_{\text{calc}}$                | 1.364 g/cm$^3$               |
| F$_{000}$                        | 636.00                       |
| $\mu$(MoK$\alpha$)              | 6.067 cm$^{-1}$              |
### B. Intensity Measurements

| Parameter                        | Value                                      |
|----------------------------------|--------------------------------------------|
| Diffractometer                   | XtaLAB mini                                |
| Radiation                        | MoKα ($\lambda = 0.71075 \, \text{Å}$)   |
|                                  | graphite monochromated                     |
| Voltage, Current                 | 50kV, 12mA                                 |
| Temperature                      | -180.0°C                                   |
| Detector Aperture                | 75.0 mm (diameter)                         |
| Data Images                      | 540 exposures                              |
| $\omega$ oscillation Range ($\chi$=54.0, $\phi$=0.0) | -60.0 - 120.0°                             |
| Exposure Rate                    | 64.0 sec./°                                |
| Detector Swing Angle             | 30.00°                                     |
| $\omega$ oscillation Range ($\chi$=54.0, $\phi$=120.0) | -60.0 - 120.0°                             |
| Exposure Rate                    | 64.0 sec./°                                |
| Detector Swing Angle             | 30.00°                                     |
| $\omega$ oscillation Range ($\chi$=54.0, $\phi$=240.0) | -60.0 - 120.0°                             |
| Exposure Rate                    | 64.0 sec./°                                |
| Detector Swing Angle             | 30.00°                                     |
| Parameter                        | Value            |
|---------------------------------|------------------|
| Detector Position               | 49.66 mm         |
| Pixel Size                      | 0.073 mm         |
| $2\theta_{\text{max}}$          | 55.0°            |
| No. of Reflections Measured     | Total: 16099     |
|                                 | Unique: 6894 ($R_{\text{int}} = 0.0323$) |
| Corrections                     | Lorentz-polarization |
|                                 | Absorption       |
|                                 | (trans. factors: 0.785 - 0.953)   |
C. Structure Solution and Refinement

Structure Solution

Direct Methods (SHELXT)

Refinement

Full-matrix least-squares on $F^2$

Function Minimized

$$\sum w (Fo^2 - Fc^2)^2$$

Least Squares Weights

$$w = \frac{1}{\sigma^2(Fo^2) + (0.0331 \cdot P)^2 + 1.0758 \cdot P}$$

where $P = (\text{Max}(Fo^2,0) + 2Fc^2)/3$

$2\theta_{\text{max}}$ cutoff

55.0°

Anomalous Dispersion

All non-hydrogen atoms

No. Observations (All reflections)

6894

No. Variables

334

Reflection/Parameter Ratio

20.64

Residuals: $R_1$ ($I > 2.00\sigma(I)$)

0.0275

Residuals: $R$ (All reflections)

0.0330

Residuals: $wR^2$ (All reflections)

0.0733

Goodness of Fit Indicator

1.013

Max Shift/Error in Final Cycle

0.001

Maximum peak in Final Diff. Map

$0.67 \text{e}^-/\text{Å}^3$

Minimum peak in Final Diff. Map

$-0.74 \text{e}^-/\text{Å}^3$
Table S4-1. Atomic coordinates and B_{iso}/B_{eq}

| atom | x          | y          | z          | B_{eq}  |
|------|------------|------------|------------|---------|
| Nb1  | 0.44959(2) | 0.21682(2) | 0.71667(2) | 0.724(4) |
| Cl1  | 0.67026(5) | 0.28358(4) | 0.85343(4) | 1.225(8) |
| Cl2  | 0.30172(5) | 0.16346(4) | 0.53544(3) | 1.206(8) |
| O1   | 0.37021(13)| 0.33249(11)| 0.75762(10)| 0.93(2)  |
| O2   | 0.60009(14)| 0.35552(11)| 0.62515(10)| 1.14(2)  |
| O3   | 0.58242(14)| 0.12215(11)| 0.64685(10)| 1.16(2)  |
| N1   | 0.36491(17)| 0.10186(13)| 0.77244(12)| 0.96(2)  |
| C1   | 0.30772(19)| 0.01142(15)| 0.82145(15)| 0.94(3)  |
| C2   | 0.3217(2)  | 0.02994(16)| 0.93255(15)| 1.12(3)  |
| C3   | 0.2622(2)  | -0.06086(17)| 0.97954(16)| 1.38(3)  |
| C4   | 0.1908(2)  | -0.16710(18)| 0.92013(17)| 1.55(3)  |
| C5   | 0.1796(2)  | -0.18411(17)| 0.81164(16)| 1.40(3)  |
| C6   | 0.2371(2)  | -0.09580(16)| 0.76028(15)| 1.12(3)  |
| C7   | 0.3979(2)  | 0.14436(17)| 0.99784(16)| 1.56(3)  |
| C8   | 0.2203(2)  | -0.11550(17)| 0.64186(16)| 1.60(3)  |
| C9   | 0.29552(19)| 0.38839(15)| 0.80814(14)| 0.84(3)  |
| C10  | 0.3533(2)  | 0.50613(15)| 0.83673(14)| 0.92(3)  |
| C11  | 0.2769(2)  | 0.56483(16)| 0.88688(15)| 1.11(3)  |
| C12  | 0.1462(2)  | 0.50992(17)| 0.90891(16)| 1.28(3)  |
| C13  | 0.0893(2)  | 0.39417(16)| 0.87949(15)| 1.15(3)  |
| C14  | 0.1614(2)  | 0.33145(16)| 0.82871(14)| 0.94(3)  |
| C15  | 0.4931(2)  | 0.56929(15)| 0.81474(15)| 0.99(3)  |
| C16  | 0.4982(2)  | 0.65317(16)| 0.75140(16)| 1.29(3)  |
| C17  | 0.6290(2)  | 0.71417(17)| 0.73208(17)| 1.57(3)  |
| C18  | 0.7555(2)  | 0.69257(18)| 0.77579(17)| 1.76(3)  |
| C19  | 0.7515(2)  | 0.60984(18)| 0.83902(17)| 1.71(3)  |
| C20  | 0.6211(2)  | 0.54855(16)| 0.85840(15)| 1.27(3)  |
| C21  | 0.08901(19)| 0.20882(16)| 0.79393(15)| 1.00(3)  |
| C22  | 0.0559(2)  | 0.16202(16)| 0.68690(15)| 1.12(3)  |
| C23  | -0.0181(2) | 0.04886(17)| 0.65305(17)| 1.37(3)  |
| C24  | -0.0598(2) | -0.01965(17)| 0.72607(18)| 1.57(3)  |
| C25  | -0.0288(2) | 0.02599(17)| 0.83235(17)| 1.53(3)  |
| C26  | 0.0448(2)  | 0.13954(17)| 0.86680(16)| 1.29(3)  |
| C27  | 0.5537(2)  | 0.42132(17)| 0.57662(16)| 1.49(3)  |
| C28  | 0.6588(2)  | 0.27466(17)| 0.55530(16)| 1.42(3)  |
| C29  | 0.7059(2)  | 0.18953(18)| 0.61361(16)| 1.44(3)  |
| C30  | 0.6181(3)  | 0.03171(19)| 0.69486(17)| 1.84(4)  |
Table S4-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

| atom | x | y | z | $B_{\text{eq}}$ |
|------|---|---|---|----------------|

$$B_{\text{eq}} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$
Table S4-2. Atomic coordinates and $B_{iso}$ involving hydrogen atoms

| atom | x    | y    | z    | $B_{iso}$ |
|------|------|------|------|-----------|
| H3   | 0.27050 | -0.04999 | 1.05410 | 1.658     |
| H4   | 0.14980 | -0.22787 | 0.95375 | 1.859     |
| H5   | 0.13190 | -0.25722 | 0.77142 | 1.680     |
| H7A  | 0.43260 | 0.19754  | 0.95160 | 1.873     |
| H7B  | 0.33072 | 0.16947  | 1.03325 | 1.873     |
| H7C  | 0.48012 | 0.14085  | 1.05133 | 1.873     |
| H8A  | 0.26684 | -0.04497 | 0.61927 | 1.917     |
| H8B  | 0.26583 | -0.17215 | 0.62251 | 1.917     |
| H8C  | 0.11736 | -0.14220 | 0.60665 | 1.917     |
| H11  | 0.31541 | 0.64428  | 0.90635 | 1.334     |
| H12  | 0.09616 | 0.55111  | 0.94380 | 1.540     |
| H13  | -0.00077 | 0.35655  | 0.89414 | 1.375     |
| H16  | 0.41183 | 0.66855  | 0.72144 | 1.542     |
| H17  | 0.63158 | 0.77077  | 0.68880 | 1.889     |
| H18  | 0.84472 | 0.73425  | 0.76252 | 2.107     |
| H19  | 0.83816 | 0.59505  | 0.86916 | 2.047     |
| H20  | 0.61920 | 0.49206  | 0.90176 | 1.522     |
| H22  | 0.08454 | 0.20826  | 0.63667 | 1.341     |
| H23  | -0.04061 | 0.01789  | 0.57981 | 1.639     |
| H24  | -0.10936 | -0.09759 | 0.70296 | 1.882     |
| H25  | -0.05808 | -0.02066 | 0.88211 | 1.831     |
| H26  | 0.06536 | 0.17039  | 0.93993 | 1.549     |
| H27A | 0.51424 | 0.46143  | 0.62601 | 1.782     |
| H27B | 0.53640 | 0.47451  | 0.55949 | 1.782     |
| H27C | 0.47910 | 0.38629  | 0.51140 | 1.782     |
| H28A | 0.74213 | 0.32658  | 0.53609 | 1.698     |
| H28B | 0.58468 | 0.23662  | 0.48938 | 1.698     |
| H29A | 0.74040 | 0.14118  | 0.56658 | 1.729     |
| H29B | 0.78579 | 0.22789  | 0.67623 | 1.729     |
| H30A | 0.53405 | -0.01346 | 0.71712 | 2.207     |
| H30B | 0.64518 | -0.01596 | 0.64310 | 2.207     |
| H30C | 0.69919 | 0.06334  | 0.75685 | 2.207     |
| atom | U$_{11}$   | U$_{22}$   | U$_{33}$   | U$_{12}$   | U$_{13}$   | U$_{23}$   |
|------|-----------|-----------|-----------|-----------|-----------|-----------|
| Nb1  | 0.00974(9)| 0.00967(8)| 0.00843(8)| 0.00388(6)| 0.00198(6)| 0.00064(6)|
| Cl1  | 0.0131(2) | 0.0203(2) | 0.0114(2) | 0.00534(17)| -0.00027(16)| 0.00029(17)|
| Cl2  | 0.0137(2) | 0.0191(2) | 0.0104(2) | 0.00351(17)| 0.00010(16)| 0.00028(17)|
| O1   | 0.0110(6) | 0.0109(6) | 0.0133(6) | 0.0037(5)  | 0.0029(5)  | 0.0006(5)  |
| O2   | 0.0168(7) | 0.0157(7) | 0.0130(7) | 0.0066(5)  | 0.0057(5)  | 0.0035(5)  |
| O3   | 0.0171(7) | 0.0168(7) | 0.0143(7) | 0.0101(5)  | 0.0060(5)  | 0.0037(5)  |
| N1   | 0.0136(8) | 0.0127(8) | 0.0101(7) | 0.0051(6)  | 0.0026(6)  | -0.0007(6)|
| C1   | 0.0116(9) | 0.0129(9) | 0.0134(9) | 0.0062(7)  | 0.0036(7)  | 0.0036(7)  |
| C2   | 0.0136(9) | 0.0168(9) | 0.0134(9) | 0.0070(7)  | 0.0026(7)  | 0.0016(7)  |
| C3   | 0.0190(10)| 0.0233(11)| 0.0128(9) | 0.0086(8)  | 0.0048(8)  | 0.0063(8)  |
| C4   | 0.0203(10)| 0.0201(10)| 0.0229(11)| 0.0085(8)  | 0.0076(8)  | 0.0115(8)  |
| C5   | 0.0183(10)| 0.0118(9) | 0.0227(10)| 0.0048(8)  | 0.0036(8)  | 0.0030(8)  |
| C6   | 0.0159(9) | 0.0134(9) | 0.0148(9) | 0.0068(7)  | 0.0039(7)  | 0.0010(7)  |
| C7   | 0.0229(11)| 0.0221(11)| 0.0115(9) | 0.0043(8)  | 0.0039(8)  | -0.0019(8)|
| C8   | 0.0262(11)| 0.0158(10)| 0.0159(10)| 0.0049(8)  | 0.0034(8)  | -0.0023(8)|
| C9   | 0.0123(9) | 0.0127(9) | 0.0082(8) | 0.0063(7)  | 0.0018(7)  | 0.0012(7)  |
| C10  | 0.0130(9) | 0.0121(9) | 0.0094(8) | 0.0036(7)  | 0.0009(7)  | 0.0025(7)  |
| C11  | 0.0175(10)| 0.0108(9) | 0.0137(9) | 0.0060(7)  | 0.0015(7)  | 0.0001(7)  |
| C12  | 0.0173(10)| 0.0175(10)| 0.0165(9) | 0.0091(8)  | 0.0058(8)  | 0.0004(7)  |
| C13  | 0.0117(9) | 0.0171(9) | 0.0148(9) | 0.0046(7)  | 0.0039(7)  | 0.0012(7)  |
| C14  | 0.0124(9) | 0.0134(9) | 0.0096(8) | 0.0043(7)  | 0.0012(7)  | 0.0018(7)  |
| C15  | 0.0145(9) | 0.0095(9) | 0.0121(9) | 0.0024(7)  | 0.0035(7)  | -0.0016(7)|
| C16  | 0.0186(10)| 0.0141(9) | 0.0162(9) | 0.0058(8)  | 0.0030(8)  | 0.0026(7)  |
| C17  | 0.0256(11)| 0.0133(10)| 0.0215(11)| 0.0040(8)  | 0.0084(8)  | 0.0057(8)  |
| C18  | 0.0191(11)| 0.0188(11)| 0.0269(11)| -0.0005(8)| 0.0100(9)  | 0.0047(8)  |
| C19  | 0.0153(10)| 0.0227(11)| 0.0249(11)| 0.0047(8)  | 0.0012(8)  | 0.0049(9)  |
| C20  | 0.0155(10)| 0.0159(10)| 0.0163(9) | 0.0042(7)  | 0.0021(7)  | 0.0045(7)  |
| C21  | 0.0083(8) | 0.0123(9) | 0.0176(9) | 0.0034(7)  | 0.0037(7)  | 0.0020(7)  |
| C22  | 0.0105(9) | 0.0146(9) | 0.0171(9) | 0.0033(7)  | 0.0037(7)  | 0.0022(7)  |
| C23  | 0.0110(9) | 0.0176(10)| 0.0211(10)| 0.0042(7)  | 0.0022(7)  | -0.0027(8)|
| C24  | 0.0102(9) | 0.0129(9) | 0.0344(12)| 0.0019(7)  | 0.0039(8)  | 0.0019(8)  |
| C25  | 0.0143(10)| 0.0183(10)| 0.0293(11)| 0.0063(8)  | 0.0081(8)  | 0.0115(8)|
| C26  | 0.0128(9) | 0.0200(10)| 0.0182(10)| 0.0067(8)  | 0.0049(7)  | 0.0050(8)  |
| C27  | 0.0253(11)| 0.0165(10)| 0.0177(10)| 0.0083(8)  | 0.0072(8)  | 0.0066(8)  |
| C28  | 0.0192(10)| 0.0224(10)| 0.0167(10)| 0.0088(8)  | 0.0103(8)  | 0.0045(8)  |
| C29  | 0.0145(10)| 0.0272(11)| 0.0167(10)| 0.0104(8)  | 0.0067(8)  | 0.0028(8)  |
| C30  | 0.0320(12)| 0.0257(11)| 0.0240(11)| 0.0224(10)| 0.0114(9)  | 0.0093(9)  |
Table S4-3. Anisotropic displacement parameters (continued)

| atom | U₁₁ | U₂₂ | U₃₃ | U₁₂ | U₁₃ | U₂₃ |
|------|-----|-----|-----|-----|-----|-----|

The general temperature factor expression: $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$
Table S4-4. Bond lengths (Å)

| atom  | atom | distance   | atom  | atom | distance   |
|-------|------|------------|-------|------|------------|
| Nb1   | Cl1  | 2.4131(5)  | Nb1   | Cl2  | 2.4407(4)  |
| Nb1   | O1   | 1.9127(15) | Nb1   | O2   | 2.3802(14) |
| Nb1   | O3   | 2.2556(16) | Nb1   | N1   | 1.7569(16) |
| O1    | C9   | 1.362(3)   | O2    | C27  | 1.443(3)   |
| O2    | C28  | 1.434(3)   | O3    | C29  | 1.448(2)   |
| O3    | C30  | 1.448(3)   | N1    | C1   | 1.395(3)   |
| C1    | C2   | 1.414(3)   | C1    | C6   | 1.404(2)   |
| C2    | C3   | 1.389(3)   | C2    | C7   | 1.500(2)   |
| C3    | C4   | 1.388(3)   | C4    | C5   | 1.384(3)   |
| C5    | C6   | 1.395(3)   | C6    | C8   | 1.505(3)   |
| C9    | C10  | 1.408(2)   | C9    | C14  | 1.411(3)   |
| C10   | C11  | 1.395(3)   | C10   | C15  | 1.487(3)   |
| C11   | C12  | 1.384(3)   | C12   | C13  | 1.386(3)   |
| C13   | C14  | 1.399(3)   | C14   | C21  | 1.484(3)   |
| C15   | C16  | 1.400(3)   | C15   | C20  | 1.393(3)   |
| C16   | C17  | 1.392(3)   | C17   | C18  | 1.386(3)   |
| C18   | C19  | 1.388(3)   | C19   | C20  | 1.390(3)   |
| C21   | C22  | 1.393(3)   | C21   | C26  | 1.402(3)   |
| C22   | C23  | 1.383(3)   | C23   | C24  | 1.391(3)   |
| C24   | C25  | 1.382(3)   | C25   | C26  | 1.388(3)   |
| C28   | C29  | 1.501(3)   |
Table S4-5. Bond lengths involving hydrogens (Å)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C3   | H3   | 0.950    | C4   | H4   | 0.950    |
| C5   | H5   | 0.950    | C7   | H7A  | 0.980    |
| C7   | H7B  | 0.980    | C7   | H7C  | 0.980    |
| C8   | H8A  | 0.980    | C8   | H8B  | 0.980    |
| C8   | H8C  | 0.980    | C11  | H11  | 0.950    |
| C12  | H12  | 0.950    | C13  | H13  | 0.950    |
| C16  | H16  | 0.950    | C17  | H17  | 0.950    |
| C18  | H18  | 0.950    | C19  | H19  | 0.950    |
| C20  | H20  | 0.950    | C22  | H22  | 0.950    |
| C23  | H23  | 0.950    | C24  | H24  | 0.950    |
| C25  | H25  | 0.950    | C26  | H26  | 0.950    |
| C27  | H27A | 0.980    | C27  | H27B | 0.980    |
| C27  | H27C | 0.980    | C28  | H28A | 0.990    |
| C28  | H28B | 0.990    | C29  | H29A | 0.990    |
| C29  | H29B | 0.990    | C30  | H30A | 0.980    |
| C30  | H30B | 0.980    | C30  | H30C | 0.980    |
Table S4-6. Bond angles (°)

| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| Cl1  | Nb1  | Cl2  | 156.28(2) | Cl1  | Nb1  | O1   | 96.62(4) |
| Cl1  | Nb1  | O2   | 80.56(3)  | Cl1  | Nb1  | O3   | 80.31(3)  |
| Cl1  | Nb1  | N1   | 96.53(5)  | Cl2  | Nb1  | O1   | 95.41(4)  |
| Cl2  | Nb1  | O2   | 78.67(3)  | Cl2  | Nb1  | O3   | 82.13(3)  |
| Cl2  | Nb1  | N1   | 100.02(5) | O1   | Nb1  | O2   | 91.94(6)  |
| O1   | Nb1  | O3   | 162.67(5) | O1   | Nb1  | N1   | 104.90(7) |
| O2   | Nb1  | O3   | 70.74(5)  | O2   | Nb1  | N1   | 163.15(7) |
| O3   | Nb1  | N1   | 92.42(7)  | Nb1  | O1   | C9   | 159.95(13) |
| Nb1  | O2   | C27  | 120.11(12)| Nb1  | O2   | C28  | 112.83(11)|
| C27  | O2   | C28  | 111.27(16)| Nb1  | O3   | C29  | 116.18(12)|
| Nb1  | O3   | C30  | 120.61(13)| C29  | O3   | C30  | 109.96(17)|
| Nb1  | N1   | C1   | 175.74(14)| N1   | C1   | C2   | 118.99(15)|
| N1   | C1   | C6   | 119.87(17)| C2   | C1   | C6   | 121.15(18)|
| C1   | C2   | C3   | 118.06(16)| C1   | C2   | C7   | 121.08(18)|
| C3   | C2   | C7   | 120.86(18)| C2   | C3   | C4   | 121.53(19)|
| C3   | C4   | C5   | 119.7(2)  | C4   | C5   | C6   | 121.19(17)|
| C1   | C6   | C5   | 118.39(18)| C1   | C6   | C8   | 121.29(18)|
| C5   | C6   | C8   | 120.31(16)| O1   | C9   | C10  | 118.23(16)|
| O1   | C9   | C14  | 121.53(16)| C10  | C9   | C14  | 120.21(19)|
| C9   | C10  | C11  | 118.93(17)| C9   | C10  | C15  | 121.77(19)|
| C11  | C10  | C15  | 119.30(16)| C10  | C11  | C12  | 121.48(18)|
| C11  | C12  | C13  | 119.3(2)  | C12  | C13  | C14  | 121.48(18)|
| C9   | C14  | C13  | 118.62(17)| C9   | C14  | C21  | 123.14(19)|
| C13  | C14  | C21  | 118.15(17)| C10  | C15  | C16  | 119.98(18)|
| C10  | C15  | C20  | 121.11(18)| C16  | C15  | C20  | 118.89(18)|
| C15  | C16  | C17  | 120.4(2)  | C16  | C17  | C18  | 120.2(2)  |
| C17  | C18  | C19  | 119.8(2)  | C18  | C19  | C20  | 120.2(2)  |
| C15  | C20  | C19  | 120.5(2)  | C14  | C21  | C22  | 120.23(18)|
| C14  | C21  | C26  | 120.75(17)| C22  | C21  | C26  | 118.90(16)|
| C21  | C22  | C23  | 120.63(19)| C22  | C23  | C24  | 120.11(19)|
| C23  | C24  | C25  | 119.81(18)| C24  | C25  | C26  | 120.4(2)  |
| C21  | C26  | C25  | 120.14(18)| O2   | C28  | C29  | 107.05(17)|
| O3   | C29  | C28  | 107.65(17)|       |      |      |          |
Table S4-7. Bond angles involving hydrogens (°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C2   | C3   | H3   | 119.2 | C4   | C3   | H3   | 119.2 |
| C3   | C4   | H4   | 120.2 | C5   | C4   | H4   | 120.2 |
| C4   | C5   | H5   | 119.4 | C6   | C5   | H5   | 119.4 |
| C2   | C7   | H7A  | 109.5 | C2   | C7   | H7B  | 109.5 |
| C2   | C7   | H7C  | 109.5 | H7A  | C7   | H7C  | 109.5 |
| H7A  | C7   | H7C  | 109.5 | H7B  | C7   | H7C  | 109.5 |
| C6   | C8   | H8A  | 109.5 | C6   | C8   | H8B  | 109.5 |
| C6   | C8   | H8C  | 109.5 | H8A  | C8   | H8B  | 109.5 |
| H8A  | C8   | H8C  | 109.5 | H8B  | C8   | H8C  | 109.5 |
| C10  | C11  | H11  | 120.4 | C12  | C11  | H11  | 120.4 |
| C11  | C12  | H12  | 119.3 | C13  | C12  | H12  | 120.4 |
| C12  | C13  | H13  | 119.3 | C14  | C13  | H13  | 119.3 |
| C15  | C16  | H16  | 119.8 | C17  | C16  | H16  | 119.8 |
| C16  | C17  | H17  | 119.9 | C18  | C17  | H17  | 119.9 |
| C17  | C18  | H18  | 120.1 | C19  | C18  | H18  | 120.1 |
| C18  | C19  | H19  | 119.9 | C20  | C19  | H19  | 119.9 |
| C15  | C20  | H20  | 119.7 | C19  | C20  | H20  | 119.7 |
| C21  | C22  | H22  | 119.7 | C23  | C22  | H22  | 119.7 |
| C22  | C23  | H23  | 119.9 | C24  | C23  | H23  | 119.9 |
| C23  | C24  | H24  | 120.1 | C25  | C24  | H24  | 120.1 |
| C24  | C25  | H25  | 119.8 | C26  | C25  | H25  | 119.8 |
| C21  | C26  | H26  | 119.9 | C25  | C26  | H26  | 119.9 |
| O2   | C27  | H27A | 109.5 | O2   | C27  | H27B | 109.5 |
| O2   | C27  | H27C | 109.5 | H27A | C27  | H27B | 109.5 |
| H27A | C27  | H27C | 109.5 | H27B | C27  | H27C | 109.5 |
| O2   | C28  | H28A | 110.3 | O2   | C28  | H28B | 110.3 |
| C29  | C28  | H28A | 110.3 | C29  | C28  | H28B | 110.3 |
| H28A | C28  | H28B | 108.6 | O3   | C29  | H29A | 110.2 |
| O3   | C29  | H29B | 110.2 | C28  | C29  | H29B | 110.2 |
| C28  | C29  | H29B | 110.2 | H29A | C29  | H29B | 108.5 |
| O3   | C30  | H30A | 109.5 | O3   | C30  | H30B | 109.5 |
| O3   | C30  | H30C | 109.5 | H30A | C30  | H30B | 109.5 |
| H30A | C30  | H30C | 109.5 | H30B | C30  | H30C | 109.5 |
Table S4-8. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle  | atom1 | atom2 | atom3 | atom4 | angle  |
|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|
| C1    | Nb1   | O1    | C9    | -88.5(2) | C11   | Nb1   | O2    | C27   | -127.04(7) |
| C1    | Nb1   | O2    | C28   | 98.62(7)  | C11   | Nb1   | O3    | C29   | -67.30(7)  |
| C1    | Nb1   | O3    | C30   | 69.82(7)  | C12   | Nb1   | O1    | C9    | 112.0(2)   |
| C12   | Nb1   | O2    | C27   | 64.48(7)  | C12   | Nb1   | O2    | C28   | -69.87(6)  |
| C12   | Nb1   | O3    | C29   | 96.69(7)  | C12   | Nb1   | O3    | C30   | -126.19(7) |
| O1    | Nb1   | O2    | C27   | -30.65(8) | O1    | Nb1   | O2    | C28   | -165.00(7) |
| O2    | Nb1   | O1    | C9    | -169.3(2) | N1    | Nb1   | O1    | C9    | 10.1(2)    |
| O2    | Nb1   | O3    | C29   | 16.01(7)  | O2    | Nb1   | O3    | C30   | 153.13(8)  |
| O3    | Nb1   | O2    | C27   | 150.01(8) | O3    | Nb1   | O2    | C28   | 15.66(7)   |
| N1    | Nb1   | O3    | C29   | -163.52(8) | N1    | Nb1   | O3    | C30   | -26.40(8)  |
| Nb1   | O1    | C9    | C10   | 143.6(2)  | Nb1   | O1    | C9    | C14   | -38.5(4)   |
| Nb1   | O2    | C28   | C29   | -42.61(13) | C27   | O2    | C28   | C29   | 178.98(11) |
| Nb1   | O3    | C29   | C28   | -43.90(15) | C30   | O3    | C29   | C28   | 174.64(13) |
| N1    | C1    | C2    | C3    | 179.06(16) | N1    | C1    | C2    | C7    | -0.6(3)    |
| N1    | C1    | C6    | C5    | -179.21(17) | N1    | C1    | C6    | C8    | -0.6(3)    |
| C2    | C1    | C6    | C5    | 0.6(3)    | C2    | C1    | C6    | C8    | 179.19(17) |
| C6    | C1    | C2    | C3    | -0.7(3)   | C6    | C1    | C2    | C7    | 179.64(17) |
| C1    | C2    | C3    | C4    | 0.0(3)    | C7    | C2    | C3    | C4    | 179.69(18) |
| C2    | C3    | C4    | C5    | 0.8(3)    | C3    | C4    | C5    | C6    | -0.9(3)    |
| C4    | C5    | C6    | C1    | 0.3(3)    | C4    | C5    | C6    | C8    | -178.37(19) |
| O1    | C9    | C10   | C11   | 178.91(14) | O1    | C9    | C10   | C15   | -1.0(2)    |
| O1    | C9    | C14   | C13   | -179.04(14) | O1    | C9    | C14   | C21   | -2.4(3)    |
| C10   | C9    | C14   | C13   | -1.1(3)   | C10   | C9    | C14   | C21   | 175.47(15) |
| C14   | C9    | C10   | C11   | 0.9(3)    | C14   | C9    | C10   | C15   | -178.97(15) |
| C9    | C10   | C11   | C12   | -0.0(3)   | C9    | C10   | C15   | C16   | 120.87(19) |
| C9    | C10   | C15   | C20   | -60.8(2)  | C11   | C10   | C15   | C16   | -59.0(2)   |
| C11   | C10   | C15   | C20   | 119.33(19) | C15   | C10   | C11   | C12   | 179.90(15) |
| C10   | C11   | C12   | C13   | -0.7(3)   | C11   | C12   | C13   | C14   | 0.5(3)    |
| C12   | C13   | C14   | C9    | 0.4(3)    | C12   | C13   | C14   | C21   | -176.35(16) |
| C9    | C14   | C21   | C22   | -57.3(3)  | C9    | C14   | C21   | C26   | 126.68(19) |
| C13   | C14   | C21   | C22   | 119.31(19) | C13   | C14   | C21   | C26   | 56.7(2)    |
| C10   | C15   | C16   | C17   | 178.77(15) | C10   | C15   | C20   | C19   | -178.63(15) |
| C16   | C15   | C20   | C19   | -0.3(3)   | C20   | C15   | C16   | C17   | 0.4(3)    |
| C15   | C16   | C17   | C18   | -0.2(3)   | C16   | C17   | C18   | C19   | -0.0(3)   |
| C17   | C18   | C19   | C20   | 0.1(3)    | C18   | C19   | C20   | C15   | 0.0(3)    |
| C14   | C21   | C22   | C23   | -176.65(17) | C14   | C21   | C26   | C25   | 176.95(17) |
| C22   | C21   | C26   | C25   | 0.9(3)    | C26   | C21   | C22   | C23   | -0.6(3)   |
Table S4-8. Torsion angles (°) (continued)

| atom1 | atom2 | atom3 | atom4 | angle  | atom1 | atom2 | atom3 | atom4 | angle  |
|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|
| C21   | C22   | C23   | C24   | -0.4(3)| C22   | C23   | C24   | C25   | 1.0(3) |
| C23   | C24   | C25   | C26   | -0.6(3)| C24   | C25   | C26   | C21   | -0.3(3)|
| O2    | C28   | C29   | O3    | 55.44(16)|      |       |       |       |        |
Table S4-9. Intramolecular contacts less than 3.60 Å

| atom  | atom | distance  | atom  | atom | distance  |
|-------|------|----------|-------|------|----------|
| Cl1   | C20  | 3.494(2) | Cl1   | C29  | 3.340(2) |
| Cl1   | C30  | 3.443(2) | Cl2   | C22  | 3.412(2) |
| Cl2   | C27  | 3.4055(19)| Cl2   | C28  | 3.367(2) |
| O1    | C15  | 2.836(2) | O1    | C20  | 3.0800(19)|
| O1    | C21  | 2.937(2) | O1    | C22  | 3.143(2) |
| O1    | C27  | 3.339(3) | N1    | C7   | 2.865(3) |
| N1    | C8   | 2.881(2) | N1    | C21  | 3.412(3) |
| N1    | C22  | 3.371(3) | N1    | C30  | 3.181(3) |
| C1    | C4   | 2.780(3) | C1    | C24  | 3.511(3) |
| C1    | C25  | 3.420(3) | C1    | C26  | 3.533(3) |
| C2    | C5   | 2.799(2) | C2    | C25  | 3.454(3) |
| C2    | C6   | 3.411(3) | C3    | C6   | 2.794(3) |
| C6    | C4   | 3.308(3) | C7    | C26  | 3.568(3) |
| C8    | C23  | 3.562(3) | C9    | C12  | 2.800(3) |
| C9    | C20  | 3.186(2) | C9    | C22  | 3.170(2) |
| C10   | C13  | 2.790(3) | C11   | C14  | 2.793(3) |
| C11   | C16  | 3.109(3) | C11   | C20  | 3.560(3) |
| C13   | C22  | 3.539(3) | C13   | C26  | 3.087(3) |
| C15   | C18  | 2.797(3) | C16   | C19  | 2.775(3) |
| C17   | C20  | 2.776(3) | C21   | C24  | 2.791(3) |
| C22   | C25  | 2.772(3) | C23   | C26  | 2.776(3) |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H7A  | 3.125    | Nb1  | H8A  | 3.257    |
| Nb1  | H22  | 3.536    | Nb1  | H27A | 3.344    |
| Nb1  | H27C | 3.590    | Nb1  | H28B | 3.476    |
| Nb1  | H29B | 3.439    | Nb1  | H30A | 3.231    |
| Nb1  | H30C | 3.537    | Cl1  | H7A  | 2.890    |
| Cl1  | H20  | 2.835    | Cl1  | H29B | 2.871    |
| Cl1  | H30C | 3.030    | Cl2  | H8A  | 2.898    |
| Cl2  | H22  | 2.881    | Cl2  | H23  | 3.559    |
| Cl2  | H27C | 2.941    | Cl2  | H28B | 2.894    |
| O1   | H7A  | 3.243    | O1   | H20  | 2.880    |
| O1   | H22  | 2.868    | O1   | H27A | 2.794    |
| O2   | H29A | 3.226    | O2   | H29B | 2.603    |
| O3   | H8A  | 3.168    | O3   | H28A | 3.246    |
| O3   | H28B | 2.623    | N1   | H7A  | 2.387    |
| N1   | H7B  | 3.516    | N1   | H7C  | 3.528    |
| N1   | H8A  | 2.410    | N1   | H8B  | 3.549    |
| N1   | H8C  | 3.528    | N1   | H30A | 2.653    |
| N1   | H30C | 3.520    | C1   | H3   | 3.264    |
| C1   | H5   | 3.264    | C1   | H7A  | 2.572    |
| C1   | H7B  | 3.156    | C1   | H7C  | 3.160    |
| C1   | H8A  | 2.576    | C1   | H8B  | 3.163    |
| C1   | H8C  | 3.148    | C1   | H30A | 2.906    |
| C2   | H4   | 3.276    | C2   | H25  | 3.553    |
| C2   | H26  | 3.487    | C3   | H5   | 3.251    |
| C3   | H7A  | 3.305    | C3   | H7B  | 2.760    |
| C3   | H7C  | 2.760    | C3   | H25  | 3.381    |
| C4   | H25  | 3.463    | C5   | H3   | 3.250    |
| C5   | H8A  | 3.311    | C5   | H8B  | 2.761    |
| C5   | H8C  | 2.761    | C5   | H24  | 3.451    |
| C6   | H4   | 3.277    | C6   | H24  | 3.365    |
| C6   | H30A | 3.014    | C7   | H3   | 2.662    |
| C7   | H26  | 3.353    | C8   | H5   | 2.663    |
| C8   | H23  | 3.474    | C8   | H24  | 3.568    |
| C8   | H30A | 2.933    | C9   | H7A  | 3.588    |
| C9   | H11  | 3.272    | C9   | H13  | 3.275    |
| C9   | H20  | 3.049    | C9   | H22  | 2.996    |
| C9   | H27A | 3.530    | C10  | H12  | 3.280    |
Table S4-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C10  | H16  | 2.656    | C10  | H20  | 2.671    |
| C10  | H27A | 3.498    | C11  | H13  | 3.245    |
| C11  | H16  | 2.971    | C13  | H12  | 3.286    |
| C13  | H26  | 2.956    | C14  | H26  | 2.674    |
| C14  | H22  | 2.651    | C15  | H17  | 3.278    |
| C15  | H19  | 3.272    | C15  | H27A | 2.753    |
| C16  | H11  | 2.948    | C16  | H18  | 3.326    |
| C16  | H20  | 3.265    | C16  | H27A | 2.827    |
| C17  | H19  | 3.257    | C17  | H27A | 3.121    |
| C17  | H27B | 3.592    | C18  | H27A | 3.329    |
| C18  | H18  | 3.264    | C18  | H16  | 3.326    |
| C18  | H27B | 3.483    | C19  | H17  | 3.257    |
| C19  | H27A | 3.264    | C20  | H16  | 3.264    |
| C20  | H18  | 3.266    | C20  | H27A | 2.984    |
| C21  | H13  | 3.609    | C21  | H23  | 3.268    |
| C21  | H25  | 3.274    | C22  | H24  | 3.261    |
| C22  | H26  | 3.266    | C23  | H8A  | 3.435    |
| C23  | H8C  | 3.123    | C23  | H25  | 3.257    |
| C24  | H8C  | 3.152    | C24  | H22  | 3.260    |
| C24  | H26  | 3.259    | C25  | H23  | 3.256    |
| C25  | H7B  | 3.122    | C26  | H13  | 2.884    |
| C26  | H22  | 3.266    | C26  | H24  | 3.261    |
| C26  | H28A | 2.584    | C27  | H28B | 2.599    |
| C27  | H27A | 3.218    | C28  | H27B | 2.578    |
| C28  | H27C | 2.578    | C29  | H30A | 3.220    |
| C29  | H30B | 2.568    | C29  | H30C | 2.568    |
| C30  | H8A  | 3.259    | C30  | H8B  | 3.584    |
| C30  | H29A | 2.542    | C30  | H29B | 2.621    |
| H3   | H4   | 2.329    | H3   | H7A  | 3.592    |
| H3   | H7B  | 2.707    | H3   | H7C  | 2.704    |
| H4   | H5   | 2.328    | H5   | H8A  | 3.595    |
| H5   | H8B  | 2.698    | H5   | H8C  | 2.711    |
| H5   | H24  | 3.576    | H7A  | H26  | 3.531    |
| H7B  | H26  | 2.681    | H8A  | H23  | 3.318    |
| H8A  | H30A | 2.609    | H8B  | H30A | 2.795    |
| H8C  | H23  | 2.886    | H8C  | H24  | 2.928    |
Table S4-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom  | distance | atom  | atom  | distance |
|------|-------|----------|------|-------|----------|
| H11  | H12   | 2.329    | H11  | H16   | 2.769    |
| H12  | H13   | 2.330    | H13  | H26   | 2.694    |
| H16  | H17   | 2.338    | H16  | H27A  | 3.262    |
| H17  | H18   | 2.336    | H18  | H19   | 2.338    |
| H19  | H20   | 2.335    | H20  | H27A  | 3.489    |
| H22  | H23   | 2.328    | H23  | H24   | 2.342    |
| H24  | H25   | 2.330    | H25  | H26   | 2.334    |
| H27A | H28A  | 3.478    | H27A | H28B  | 3.488    |
| H27B | H28A  | 2.397    | H27B | H28B  | 2.902    |
| H27C | H28A  | 2.880    | H27C | H28B  | 2.413    |
| H28A | H29A  | 2.399    | H28A | H29B  | 2.350    |
| H28B | H29A  | 2.351    | H28B | H29B  | 2.868    |
| H29A | H30A  | 3.447    | H29A | H30B  | 2.345    |
| H29A | H30C  | 2.814    | H29B | H30A  | 3.506    |
| H29B | H30B  | 2.934    | H29B | H30C  | 2.431    |
Table S4-11. Intermolecular contacts less than 3.60 Å

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| Cl1    | Cl1\(^1\) | 3.571(2) | Cl2    | C23\(^2\) | 3.5802(17) |
| C11    | Cl1\(^1\) | 3.571(2) | C22    | C29\(^3\) | 3.541(3)   |
| C23    | Cl2\(^2\) | 3.5802(17)| C24    | C30\(^3\) | 3.390(3)   |
| C27    | C27\(^4\) | 3.196(3) | C29    | C22\(^5\) | 3.541(3)   |
| C30    | C24\(^5\) | 3.390(3) |

Symmetry Operators:

(1) \(-X+1,-Y+1,-Z+2\)  (2) \(-X,-Y,-Z+1\)
(3) \(X-1,Y,Z\)  (4) \(-X+1,-Y+1,-Z+1\)
(5) \(X+1,Y,Z\)
Table S4-12. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom | atom  | distance | atom | atom  | distance |
|------|-------|----------|------|-------|----------|
| Cl1  | H3$^1$| 3.441    | Cl1  | H4$^1$| 3.054    |
| Cl1  | H11$^2$| 3.128    | Cl1  | H12$^2$| 3.234    |
| Cl1  | H13$^3$| 3.051    | Cl2  | H17$^4$| 3.251    |
| Cl2  | H23$^5$| 2.937    | Cl2  | H24$^6$| 3.203    |
| Cl2  | H30B$^6$| 3.039    | C1   | H7C$^1$| 3.523    |
| C2   | H25$^7$| 3.249    | C3   | H26$^7$| 3.552    |
| C3   | H30C$^1$| 3.383    | C4   | H7C$^1$| 3.129    |
| C4   | H11$^8$| 2.970    | C4   | H12$^8$| 3.461    |
| C4   | H18$^9$| 3.449    | C4   | H26$^9$| 3.389    |
| C5   | H7C$^1$| 3.364    | C5   | H11$^8$| 3.087    |
| C5   | H18$^9$| 3.101    | C6   | H7C$^1$| 3.569    |
| C7   | H11$^{10}$| 3.224  | C8   | H28A$^6$| 3.485    |
| C8   | H28B$^6$| 3.368    | C8   | H29A$^6$| 2.812    |
| C10  | H20$^{10}$| 3.359   | C11  | H4$^{10}$| 3.305    |
| C11  | H5$^{10}$| 3.317    | C11  | H20$^{10}$| 2.980    |
| C12  | H4$^{10}$| 3.275    | C12  | H12$^{11}$| 3.326    |
| C12  | H19$^{12}$| 3.476   | C12  | H19$^{12}$| 3.293    |
| C12  | H20$^{12}$| 3.055   | C13  | H12$^{11}$| 3.337    |
| C13  | H19$^{12}$| 3.192    | C13  | H20$^{12}$| 3.490    |
| C13  | H29B$^{12}$| 3.561   | C15  | H7B$^{3}$| 3.441    |
| C16  | H7B$^{3}$| 3.233    | C16  | H7C$^{2}$| 3.381    |
| C16  | H27C$^4$| 3.464    | C17  | H7B$^{3}$| 3.147    |
| C17  | H24$^{13}$| 3.094   | C17  | H27C$^4$| 3.145    |
| C17  | H28B$^4$| 3.457    | C18  | H7B$^{3}$| 3.265    |
| C18  | H24$^{13}$| 2.943    | C18  | H25$^{13}$| 3.543    |
| C19  | H7B$^{3}$| 3.457    | C19  | H26$^{2}$| 3.568    |
| C20  | H7B$^{2}$| 3.539    | C21  | H29B$^{12}$| 3.187    |
| C22  | H29A$^{12}$| 3.143   | C22  | H29B$^{12}$| 3.000    |
| C23  | H23$^6$| 3.263    | C23  | H29A$^{12}$| 3.024    |
| C23  | H29B$^{12}$| 3.387   | C23  | H30B$^{12}$| 3.178    |
| C23  | H30C$^{12}$| 3.375   | C24  | H17$^{6}$| 3.341    |
| C24  | H18$^9$| 3.084    | C24  | H30B$^{12}$| 2.932    |
| C24  | H30C$^{12}$| 2.939   | C25  | H3$^7$| 3.112    |
| C25  | H18$^9$| 3.482    | C25  | H30B$^{12}$| 3.537    |
| C25  | H30C$^{12}$| 2.872   | C26  | H3$^7$| 3.404    |
| C26  | H4$^7$| 3.577    | C26  | H30C$^{12}$| 3.270    |
Table S4-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom     | atom     | distance | atom     | atom     | distance |
|----------|----------|----------|----------|----------|----------|
| C27      | H27A<sup>4</sup> | 3.204    | C27      | H27B<sup>4</sup> | 2.999    |
| C27      | H27C<sup>4</sup> | 2.853    | C28      | H8B<sup>6</sup>  | 2.856    |
| C29      | H8A<sup>6</sup>  | 3.465    | C29      | H8B<sup>6</sup>  | 3.130    |
| C30      | H3<sup>1</sup>   | 3.204    | C30      | H17<sup>8</sup>  | 3.312    |
| C30      | H24<sup>1</sup>  | 3.513    | H3       | C11<sup>1</sup>  | 3.441    |
| H3       | C25<sup>7</sup>  | 3.112    | H3       | C26<sup>7</sup>  | 3.404    |
| H3       | C30<sup>1</sup>  | 3.204    | H3       | H7C<sup>1</sup>  | 3.443    |
| H3       | H25<sup>7</sup>  | 2.734    | H3       | H26<sup>7</sup>  | 3.266    |
| H3       | H30A<sup>1</sup> | 3.112    | H3       | H30C<sup>1</sup> | 2.450    |
| H4       | C11<sup>1</sup>  | 3.054    | H4       | C11<sup>8</sup>  | 3.305    |
| H4       | C12<sup>8</sup>  | 3.275    | H4       | C26<sup>7</sup>  | 3.577    |
| H4       | H7C<sup>1</sup>  | 3.536    | H4       | H11<sup>8</sup>  | 2.706    |
| H4       | H12<sup>8</sup>  | 2.661    | H4       | H13<sup>7</sup>  | 3.026    |
| H4       | H18<sup>9</sup>  | 3.410    | H4       | H19<sup>9</sup>  | 3.166    |
| H4       | H26<sup>7</sup>  | 2.962    | H5       | C11<sup>8</sup>  | 3.317    |
| H5       | H11<sup>8</sup>  | 2.902    | H5       | H12<sup>8</sup>  | 3.451    |
| H5       | H16<sup>8</sup>  | 3.318    | H5       | H18<sup>8</sup>  | 2.797    |
| H5       | H19<sup>9</sup>  | 3.522    | H7A      | H11<sup>2</sup>  | 2.878    |
| H7B      | C15<sup>2</sup>  | 3.441    | H7B      | C16<sup>2</sup>  | 3.233    |
| H7B      | C17<sup>2</sup>  | 3.147    | H7B      | C18<sup>8</sup>  | 3.265    |
| H7B      | C19<sup>2</sup>  | 3.457    | H7B      | C20<sup>3</sup>  | 3.539    |
| H7B      | H11<sup>2</sup>  | 3.513    | H7B      | H17<sup>2</sup>  | 3.543    |
| H7B      | H25<sup>7</sup>  | 3.276    | H7C      | C1<sup>1</sup>   | 3.523    |
| H7C      | C2<sup>1</sup>   | 3.288    | H7C      | C3<sup>1</sup>   | 3.074    |
| H7C      | C4<sup>1</sup>   | 3.129    | H7C      | C5<sup>1</sup>   | 3.364    |
| H7C      | C6<sup>1</sup>   | 3.569    | H7C      | C6<sup>2</sup>   | 3.381    |
| H7C      | H3<sup>1</sup>   | 3.443    | H7C      | H4<sup>1</sup>   | 3.536    |
| H7C      | H11<sup>2</sup>  | 2.808    | H7C      | H16<sup>2</sup>  | 3.391    |
| H7C      | H30A<sup>1</sup>| 3.564    | H8A      | C29<sup>6</sup>  | 3.465    |
| H8A      | H23<sup>10</sup>| 3.201    | H8A      | H28B<sup>6</sup> | 3.471    |
| H8A      | H29A<sup>6</sup>| 2.568    | H8B      | C28<sup>8</sup>  | 2.856    |
| H8B      | C29<sup>6</sup>  | 3.130    | H8B      | H16<sup>8</sup>  | 3.035    |
| H8B      | H28A<sup>6</sup>| 2.655    | H8B      | H28B<sup>6</sup}| 2.495    |
| H8B      | H29A<sup>6</sup>| 2.523    | H8B      | H22<sup>5</sup>  | 3.289    |
| H8C      | H23<sup>8</sup>  | 3.108    | H8C      | H28A<sup>6</sup}| 3.559    |
| H8C      | H29A<sup>6</sup>| 2.878    | H11      | C11<sup>2</sup>  | 3.128    |
| H11      | C4<sup>10</sup>  | 2.970    | H11      | C5<sup>10</sup>  | 3.087    |
Table S4-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H11    | C7\(^2\) | 3.224    | H11    | H4\(^{10}\) | 2.706    |
| H11    | H5\(^{10}\) | 2.902    | H11    | H7A\(^2\)  | 2.878    |
| H11    | H7B\(^2\) | 3.513    | H11    | H7C\(^2\)  | 2.808    |
| H11    | H20\(^2\) | 3.238    | H12    | C11\(^2\)  | 3.234    |
| H12    | C4\(^{10}\) | 3.461    | H12    | C12\(^{11}\) | 3.326   |
| H12    | C13\(^{11}\) | 3.337    | H12    | H4\(^{10}\) | 2.661    |
| H12    | H5\(^{10}\) | 3.451    | H12    | H12\(^{11}\) | 2.739   |
| H12    | H13\(^{11}\) | 2.750    | H12    | H19\(^{12}\) | 2.783   |
| H12    | H19\(^2\) | 3.274    | H12    | H20\(^2\)  | 3.348    |
| H13    | C11\(^{12}\) | 3.051    | H13    | H4\(^{7}\)  | 3.026    |
| H13    | H12\(^{11}\) | 2.750    | H13    | H19\(^2\)  | 3.101    |
| H13    | H29B\(^{12}\) | 3.156    | H16    | H5\(^{10}\) | 3.318    |
| H16    | H7C\(^2\) | 3.391    | H16    | H8B\(^{40}\) | 3.035   |
| H16    | H27C\(^4\) | 3.473    | H16    | H28A\(^{4}\) | 3.421   |
| H16    | H28B\(^{4}\) | 3.105    | H17    | C12\(^{4}\) | 3.251    |
| H17    | C24\(^{13}\) | 3.341    | H17    | C30\(^{10}\) | 3.312   |
| H17    | H7B\(^2\) | 3.543    | H17    | H24\(^{13}\) | 2.594   |
| H17    | H27C\(^4\) | 2.917    | H17    | H28B\(^{4}\) | 2.815   |
| H17    | H30A\(^{10}\) | 3.134    | H17    | H30B\(^{10}\) | 2.777   |
| H17    | H30C\(^{10}\) | 3.530    | H18    | C4\(^{13}\)  | 3.449    |
| H18    | C5\(^{13}\) | 3.101    | H18    | C24\(^{13}\) | 3.084    |
| H18    | C25\(^{13}\) | 3.482    | H18    | H4\(^{13}\)  | 3.410    |
| H18    | H5\(^{13}\) | 2.797    | H18    | H24\(^{13}\) | 2.282    |
| H18    | H25\(^{13}\) | 3.098    | H19    | C12\(^3\)  | 3.476    |
| H19    | C12\(^{2}\) | 3.293    | H19    | C13\(^3\)  | 3.192    |
| H19    | H4\(^{13}\) | 3.166    | H19    | H5\(^{13}\)  | 3.522    |
| H19    | H12\(^3\) | 2.783    | H19    | H12\(^2\)  | 3.274    |
| H19    | H13\(^{2}\) | 3.101    | H19    | H26\(^2\)  | 3.429    |
| H20    | C10\(^{2}\) | 3.359    | H20    | C11\(^2\)  | 2.980    |
| H20    | C12\(^{2}\) | 3.055    | H20    | C13\(^3\)  | 3.490    |
| H20    | H11\(^{2}\) | 3.238    | H20    | H12\(^{2}\) | 3.348    |
| H22    | H8C\(^{5}\) | 3.289    | H22    | H29A\(^{12}\) | 3.195   |
| H22    | H29B\(^{12}\) | 3.172    | H23    | C12\(^{5}\) | 2.937    |
| H23    | C23\(^{5}\) | 3.263    | H23    | H8A\(^{5}\) | 3.201    |
| H23    | H8C\(^{5}\) | 3.108    | H23    | H23\(^{3}\) | 2.411    |
| H23    | H29A\(^{12}\) | 2.991    | H23    | H30B\(^{12}\) | 3.296   |
| H24    | C12\(^{5}\) | 3.203    | H24    | C17\(^{9}\) | 3.094    |
| atom  | atom       | distance | atom  | atom       | distance |
|-------|------------|----------|-------|------------|----------|
| H24   | C18\(^9\) | 2.943    | H24   | C30\(^{12}\) | 3.513    |
| H24   | H17\(^9\) | 2.594    | H24   | H18\(^8\)  | 2.282    |
| H24   | H30B\(^{12}\) | 2.902 | H24   | H30C\(^{12}\) | 3.249    |
| H25   | C3\(^7\)  | 3.249    | H25   | C18\(^9\)  | 3.543    |
| H25   | H3\(^7\)  | 2.734    | H25   | H7B\(^7\)  | 3.276    |
| H25   | H18\(^8\) | 3.098    | H25   | H25\(^7\)  | 2.999    |
| H25   | H26\(^7\) | 3.131    | H25   | H30C\(^{12}\) | 3.138    |
| H26   | C3\(^7\)  | 3.552    | H26   | C4\(^7\)   | 3.389    |
| H26   | C19\(^2\) | 3.568    | H26   | H3\(^7\)   | 3.266    |
| H26   | H4\(^7\)  | 2.962    | H26   | H19\(^2\)  | 3.429    |
| H26   | H25\(^7\) | 3.131    | H27A  | H27A\(^4\) | 3.498    |
| H27A  | H27A\(^4\) | 3.498   | H27A  | H27B\(^4\) | 2.900    |
| H27A  | H27C\(^4\) | 2.748   | H27B  | C27\(^4\)  | 2.999    |
| H27B  | H27A\(^4\) | 2.900   | H27B  | H27B\(^4\) | 3.114    |
| H27B  | H27C\(^4\) | 2.506   | H27C  | C16\(^4\)  | 3.464    |
| H27C  | C17\(^4\) | 3.145    | H27C  | C27\(^4\)  | 2.853    |
| H27C  | H16\(^4\) | 3.473    | H27C  | H17\(^4\)  | 2.917    |
| H27C  | H27C\(^4\) | 2.748   | H27C  | H27B\(^4\) | 2.506    |
| H27C  | H27C\(^4\) | 2.825   | H28A  | C8\(^6\)   | 3.485    |
| H28A  | H8B\(^6\) | 2.655    | H28A  | H8C\(^6\)  | 3.559    |
| H28A  | H16\(^4\) | 3.421    | H28B  | C8\(^6\)   | 3.368    |
| H28B  | C17\(^4\) | 3.457    | H28B  | H8A\(^6\)  | 3.471    |
| H28B  | H8B\(^6\) | 2.495    | H28B  | H16\(^4\)  | 3.105    |
| H28B  | H17\(^4\) | 2.815    | H28B  | H30A\(^6\) | 3.441    |
| H28B  | H30B\(^6\) | 3.130   | H29A  | C8\(^6\)   | 2.812    |
| H29A  | C22\(^3\) | 3.143    | H29A  | C23\(^3\)  | 3.024    |
| H29A  | H8A\(^6\) | 2.568    | H29A  | H8B\(^6\)  | 2.523    |
| H29A  | H8C\(^6\) | 2.878    | H29A  | H23\(^3\)  | 3.195    |
| H29A  | H23\(^3\) | 2.991    | H29B  | C13\(^3\)  | 3.561    |
| H29B  | C21\(^3\) | 3.187    | H29B  | C23\(^3\)  | 3.000    |
| H29B  | C23\(^3\) | 3.387    | H29B  | H13\(^3\)  | 3.156    |
| H29B  | H22\(^3\) | 3.172    | H30A  | H3\(^1\)   | 3.112    |
| H30A  | H7C\(^1\) | 3.564    | H30A  | H17\(^8\)  | 3.134    |
| H30A  | H28B\(^6\) | 3.441   | H30B  | Cl2\(^6\)  | 3.039    |
| H30B  | C23\(^3\) | 3.178    | H30B  | C24\(^4\)  | 2.932    |
| H30B  | C25\(^3\) | 3.537    | H30B  | H17\(^8\)  | 2.777    |
| H30B  | H23\(^3\) | 3.296    | H30B  | H24\(^3\)  | 2.902    |
Table S4-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom     | distance | atom   | atom     | distance |
|--------|----------|----------|--------|----------|----------|
| H30B   | H28B\textsuperscript{6} | 3.130    | H30C   | C3\textsuperscript{1} | 3.383    |
| H30C   | C23\textsuperscript{3}  | 3.375    | H30C   | C24\textsuperscript{3} | 2.939    |
| H30C   | C25\textsuperscript{3}  | 2.872    | H30C   | C26\textsuperscript{3}  | 3.270    |
| H30C   | H3\textsuperscript{1}   | 2.450    | H30C   | H17\textsuperscript{8} | 3.530    |
| H30C   | H24\textsuperscript{8}  | 3.249    | H30C   | H25\textsuperscript{3}  | 3.138    |

Symmetry Operators:

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

for

\[
\text{Nb}(\text{N-2,6- Me}_{2}\text{C}_{6}\text{H}_{3})(\text{N=C'Bu})_{2}(\text{O-2,6-Pr}_{2}\text{C}_{6}\text{H}_{3}) \quad (4a)
\]

July 14, 2016
**Experimental**

Data Collection

A yellow prism crystal of C$_{39}$H$_{64}$Cl$_2$N$_3$NbO having approximate dimensions of 0.200 x 0.180 x 0.180 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 44.95 mm.

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

\[
\begin{align*}
    a &= 15.469(3) \text{ Å} \\
    b &= 10.6814(19) \text{ Å} \\
    c &= 24.897(4) \text{ Å} \\
    \beta &= 93.169(5)^\circ \\
    V &= 4107.5(13) \text{ Å}^3
\end{align*}
\]

For $Z = 4$ and F.W. = 754.77, the calculated density is 1.220 g/cm$^3$. The reflection conditions of:

- $h0l$: $l = 2n$
- $0k0$: $k = 2n$

uniquely determine the space group to be:

P2$_1$/c (#14)

The data were collected at a temperature of -180 ± 1°C to a maximum 2θ value of 55.1°. A total of 2477 oscillation images were collected. A sweep of data was done using ω scans from -98.0 to 82.0° in 0.25° step, at $\chi$=0.0° and $\phi$ = -72.0°. The exposure rate was 64.0 [sec./°]. The detector swing angle was -7.95°. A second sweep was performed using ω scans from -98.0 to 82.0° in 0.25° step, at $\chi$=55.0° and $\phi$ = 36.0°. The exposure rate was 64.0 [sec./°]. The detector swing angle was -7.95°. Another sweep was
performed using $\omega$ scans from -98.0 to 82.0° in 0.25° step, at $\chi$=44.0° and $\phi$ = -108.0°. The exposure rate was 64.0 [sec./°]. The detector swing angle was -7.95°. Another sweep was performed using $\omega$ scans from -98.0 to -18.8° in 0.25° step, at $\chi$=0.0° and $\phi$ = 0.0°. The exposure rate was 64.0 [sec./°]. The detector swing angle was -7.95°. The crystal-to-detector distance was 44.95 mm. Readout was performed in the 0.172 mm pixel mode.

Data Reduction

Of the 60816 reflections were collected, where 8829 were unique ($R_{int} = 0.0646$); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku). \(^1\)

The linear absorption coefficient, $\mu$, for Mo-K\(\alpha\) radiation is 4.542 cm\(^{-1}\). An empirical absorption correction was applied which resulted in transmission factors ranging from 0.770 to 0.922. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods\(^2\) and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement\(^3\) on $F^2$ was based on 8829 observed reflections and 415 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma ||Fo| - |Fc|| / \Sigma |Fo| = 0.0495$$

$$wR2 = [ \Sigma (w(Fo^2 - Fe^2)^2) / \Sigma w(Fo^2)^2]^{1/2} = 0.1291$$

The goodness of fit\(^4\) was 1.10. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.85 and -0.68 e\(^{-}/Å^3\), respectively.
Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4. Anomalous dispersion effects were included in $F_{\text{calc}}$; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley. The values for the mass attenuation coefficients are those of Creagh and Hubbell. All calculations were performed using the CrystalStructure crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7.

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

$$\sum w(F_o^2 - F_c^2)^2$$

where $w =$ Least Squares weights.

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.
(10) **SHELXL Version 2014/7**: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula \( \text{C}_{39}\text{H}_{64}\text{Cl}_{2}\text{N}_{3}\text{NbO} \)

Formula Weight 754.77

Crystal Color, Habit yellow, prism

Crystal Dimensions 0.200 X 0.180 X 0.180 mm

Crystal System monoclinic

Lattice Type Primitive

Lattice Parameters
\[ a = 15.469(3) \, \text{Å} \]
\[ b = 10.6814(19) \, \text{Å} \]
\[ c = 24.897(4) \, \text{Å} \]
\[ \beta = 93.169(5) \, ^{\circ} \]
\[ V = 4107.5(13) \, \text{Å}^3 \]

Space Group \( P2_1/c (\#14) \)

Z value 4

\( D_{\text{calc}} \) 1.220 g/cm\(^3\)

\( F_{000} \) 1608.00

\( \mu(\text{MoK}\alpha) \) 4.542 cm\(^{-1}\)
### B. Intensity Measurements

| Parameter                                      | Value                                |
|------------------------------------------------|--------------------------------------|
| **Diffractometer**                             | XtaLAB P200                          |
| **Radiation**                                  | MoKα (λ = 0.71075 Å) multi-layer mirror monochromated |
| **Voltage, Current**                           | 50kV, 24mA                           |
| **Temperature**                                | -180.0°C                             |
| **Detector Aperture**                          | 83.8 x 70.0 mm                       |
| **Data Images**                                | 2477 exposures                        |
| ω oscillation Range (χ=0.0, φ=-72.0)           | -98.0 - 82.0°                         |
| **Exposure Rate**                              | 64.0 sec./°                          |
| **Detector Swing Angle**                       | -7.95°                               |
| ω oscillation Range (χ=55.0, φ=36.0)           | -98.0 - 82.0°                         |
| **Exposure Rate**                              | 64.0 sec./°                          |
| **Detector Swing Angle**                       | -7.95°                               |
| ω oscillation Range (χ=44.0, φ=-108.0)         | -98.0 - 82.0°                         |
| **Exposure Rate**                              | 64.0 sec./°                          |
| **Detector Swing Angle**                       | -7.95°                               |
$\omega$ oscillation Range ($\chi=0.0$, $\phi=0.0$) -98.0 - 18.8°

Exposure Rate 64.0 sec./°

Detector Swing Angle -7.95°

Detector Position 44.95 mm

Pixel Size 0.172 mm

$2\theta_{\text{max}}$ 55.1°

No. of Reflections Measured
Total: 60816
Unique: 8829 ($R_{\text{int}} = 0.0646$)

Corrections Lorentz-polarization Absorption
(trans. factors: 0.770 - 0.922)
C. Structure Solution and Refinement

Structure Solution
Direct Methods (SHELXT)

Refinement
Full-matrix least-squares on F^2

Function Minimized
Σ w (Fo^2 - Fc^2)^2

Least Squares Weights
w = 1/ [ σ^2(Fo^2) + (0.0505 · P)^2 + 6.9906 · P ]
where P = (Max(Fo^2,0) + 2Fc^2)/3

2θ_{max} cutoff
55.1°

Anomalous Dispersion
All non-hydrogen atoms

No. Observations (All reflections)
8829

No. Variables
415

Reflection/Parameter Ratio
21.27

Residuals: R1 (I>2.00σ(I))
0.0495

Residuals: R (All reflections)
0.0769

Residuals: wR2 (All reflections)
0.1291

Goodness of Fit Indicator
1.103

Max Shift/Error in Final Cycle
0.001

Maximum peak in Final Diff. Map
0.85 e^-/Å^3

Minimum peak in Final Diff. Map
-0.68 e^-/Å^3
Table S5-1. Atomic coordinates and $B_{iso}/B_{eq}$

| atom | x        | y        | z        | $B_{eq}$ |
|------|----------|----------|----------|----------|
| Nb1  | 0.30236(2) | 0.36674(3) | 0.58571(2) | 1.521(7) |
| Cl1  | -0.12921(8) | 0.41144(11) | 0.66153(6) | 4.52(3)  |
| Cl2  | -0.10053(7) | 0.16300(10) | 0.61900(5) | 3.59(2)  |
| O1   | 0.22582(15) | 0.3138(2)  | 0.64048(10) | 2.00(4)  |
| N1   | 0.30934(17) | 0.5320(3)  | 0.57674(11) | 1.83(5)  |
| N2   | 0.25560(18) | 0.2995(3)  | 0.51700(12) | 2.03(5)  |
| N3   | 0.41833(17) | 0.3157(3)  | 0.61113(11) | 1.80(5)  |
| C1   | 0.1764(2)   | 0.2992(3)  | 0.68311(13) | 1.72(6)  |
| C2   | 0.1530(2)   | 0.4054(3)  | 0.71295(14) | 1.82(6)  |
| C3   | 0.0999(2)   | 0.3871(4)  | 0.75548(14) | 2.32(6)  |
| C4   | 0.0699(3)   | 0.2690(4)  | 0.76843(15) | 2.59(7)  |
| C5   | 0.0953(3)   | 0.1659(4)  | 0.74008(15) | 2.54(7)  |
| C6   | 0.1493(2)   | 0.1783(3)  | 0.69689(14) | 1.84(6)  |
| C7   | 0.1831(2)   | 0.5339(3)  | 0.69688(15) | 2.30(6)  |
| C8   | 0.1926(3)   | 0.6267(4)  | 0.74397(19) | 4.01(9)  |
| C9   | 0.1228(3)   | 0.5853(4)  | 0.65216(18) | 3.17(8)  |
| C10  | 0.1802(2)   | 0.0629(3)  | 0.6698(16)  | 2.31(6)  |
| C11  | 0.2474(3)   | -0.0077(5) | 0.7029(2)   | 3.92(9)  |
| C12  | 0.1072(3)   | -0.0238(4) | 0.6482(2)   | 4.18(10) |
| C13  | 0.3142(2)   | 0.6623(3)  | 0.57505(14) | 2.15(6)  |
| C14  | 0.3818(3)   | 0.7245(4)  | 0.60440(15) | 2.72(7)  |
| C15  | 0.3869(4)   | 0.8541(4)  | 0.60053(19) | 4.00(10) |
| C16  | 0.3291(4)   | 0.9219(5)  | 0.5693(2)   | 4.96(13) |
| C17  | 0.2622(3)   | 0.8599(5)  | 0.5402(2)   | 4.48(12) |
| C18  | 0.2532(3)   | 0.7307(4)  | 0.54219(17) | 3.05(8)  |
| C19  | 0.4464(3)   | 0.6500(4)  | 0.6374(17)  | 3.49(9)  |
| C20  | 0.1842(3)   | 0.6620(5)  | 0.50925(19) | 4.06(10) |
| C21  | 0.2170(2)   | 0.2574(3)  | 0.47486(14) | 1.91(6)  |
| C22  | 0.2712(2)   | 0.2230(3)  | 0.42617(14) | 2.13(6)  |
| C23  | 0.2649(3)   | 0.3298(5)  | 0.3851(2)   | 4.09(10) |
| C24  | 0.2443(3)   | 0.0984(5)  | 0.3986(2)   | 3.97(9)  |
| C25  | 0.3664(3)   | 0.2089(5)  | 0.44480(17) | 3.29(8)  |
| C26  | 0.1160(2)   | 0.2454(4)  | 0.47437(15) | 2.32(6)  |
| C27  | 0.0933(3)   | 0.1107(5)  | 0.4872(3)   | 5.38(13) |
| C28  | 0.0690(3)   | 0.2845(7)  | 0.4223(2)   | 5.59(14) |
| C29  | 0.0808(3)   | 0.3255(6)  | 0.5195(2)   | 5.21(13) |
| C30  | 0.4940(2)   | 0.2848(3)  | 0.62768(14) | 1.73(6)  |
Table S5-1. Atomic coordinates and $B_{iso}/B_{eq}$ (continued)

| atom | x       | y       | z       | $B_{eq}$ |
|------|---------|---------|---------|----------|
| C31  | 0.5624(2) | 0.2643(3) | 0.58504(14) | 2.08(6) |
| C32  | 0.5521(3) | 0.3691(4) | 0.54280(15) | 2.86(7) |
| C33  | 0.5406(3) | 0.1373(4) | 0.55828(16) | 2.79(7) |
| C34  | 0.6581(2) | 0.2627(4) | 0.60535(18) | 3.02(8) |
| C35  | 0.5114(2) | 0.2626(4) | 0.68883(15) | 2.27(6) |
| C36  | 0.5346(3) | 0.1243(4) | 0.69913(16) | 3.15(8) |
| C37  | 0.5826(3) | 0.3491(4) | 0.71370(16) | 3.07(8) |
| C38  | 0.4285(3) | 0.2917(5) | 0.71848(16) | 3.28(8) |
| C39  | -0.0526(3) | 0.3054(4) | 0.64111(18) | 2.90(7) |

$B_{eq} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$
Table S5-2. Atomic coordinates and \( B_{\text{iso}} \) involving hydrogen atoms

| atom | x    | y    | z    | \( B_{\text{iso}} \) |
|------|------|------|------|----------------------|
| H3   | 0.08366 | 0.45719 | 0.77619 | 2.786 |
| H4   | 0.03181 | 0.25933 | 0.79680 | 3.109 |
| H5   | 0.07606 | 0.08509 | 0.74993 | 3.045 |
| H7   | 0.24152 | 0.52397 | 0.68207 | 2.762 |
| H8A  | 0.21223 | 0.70778 | 0.73081 | 4.815 |
| H8B  | 0.13654 | 0.63708 | 0.75994 | 4.815 |
| H8C  | 0.23506 | 0.59450 | 0.77120 | 4.815 |
| H9A  | 0.14251 | 0.66865 | 0.64184 | 3.807 |
| H9B  | 0.12278 | 0.52930 | 0.62098 | 3.807 |
| H9C  | 0.06398 | 0.59123 | 0.66474 | 3.807 |
| H10  | 0.20942 | 0.09249 | 0.63446 | 2.777 |
| H11A | 0.29420 | 0.04958 | 0.71468 | 4.707 |
| H11B | 0.21982 | -0.04086 | 0.73441 | 4.707 |
| H11C | 0.27130 | -0.07702 | 0.68260 | 4.707 |
| H12A | 0.13085 | -0.09558 | 0.62943 | 5.018 |
| H12B | 0.07691 | -0.05327 | 0.67937 | 5.018 |
| H12C | 0.06648 | 0.02154 | 0.62370 | 5.018 |
| H15  | 0.43222 | 0.89668 | 0.62030 | 4.794 |
| H16  | 0.33412 | 1.01039 | 0.56734 | 5.955 |
| H17  | 0.22175 | 0.90733 | 0.51854 | 5.376 |
| H19A | 0.43146 | 0.56097 | 0.63484 | 4.193 |
| H19B | 0.50418 | 0.66312 | 0.62408 | 4.193 |
| H19C | 0.44622 | 0.67687 | 0.67504 | 4.193 |
| H20A | 0.18910 | 0.57205 | 0.51648 | 4.876 |
| H20B | 0.12711 | 0.69165 | 0.51879 | 4.876 |
| H20C | 0.19140 | 0.67759 | 0.47096 | 4.876 |
| H23A | 0.20430 | 0.34122 | 0.37235 | 4.908 |
| H23B | 0.28655 | 0.40733 | 0.40208 | 4.908 |
| H23C | 0.29969 | 0.30935 | 0.35459 | 4.908 |
| H24A | 0.18321 | 0.10290 | 0.38585 | 4.768 |
| H24B | 0.28012 | 0.08364 | 0.36799 | 4.768 |
| H24C | 0.25220 | 0.02959 | 0.42443 | 4.768 |
| H25A | 0.37251 | 0.14097 | 0.47121 | 3.953 |
| H25B | 0.40041 | 0.18929 | 0.41384 | 3.953 |
| H25C | 0.38727 | 0.28727 | 0.46133 | 3.953 |
| H27A | 0.12392 | 0.08558 | 0.52097 | 6.462 |
| H27B | 0.03073 | 0.10360 | 0.49076 | 6.462 |
Table S5-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

| atom  | x      | y      | z      | B_{eq} |
|-------|--------|--------|--------|--------|
| H27C  | 0.11064| 0.05603| 0.45804| 6.462  |
| H28A  | 0.08373| 0.37138| 0.41416| 6.707  |
| H28B  | 0.08629| 0.22992| 0.39314| 6.707  |
| H28C  | 0.00637| 0.27749| 0.42586| 6.707  |
| H29A  | 0.11008| 0.30231| 0.55392| 6.253  |
| H29B  | 0.09131| 0.41418| 0.51214| 6.253  |
| H29C  | 0.01838| 0.31116| 0.52109| 6.253  |
| H32A  | 0.49167| 0.37296| 0.52887| 3.438  |
| H32B  | 0.56859| 0.44938| 0.55944| 3.438  |
| H32C  | 0.58954| 0.35170| 0.51318| 3.438  |
| H33A  | 0.54720| 0.07052| 0.58519| 3.353  |
| H33B  | 0.48082| 0.13858| 0.54313| 3.353  |
| H33C  | 0.58006| 0.12197| 0.52950| 3.353  |
| H34A  | 0.66724| 0.19680| 0.63246| 3.620  |
| H34B  | 0.69455| 0.24633| 0.57515| 3.620  |
| H34C  | 0.67360| 0.34401| 0.62140| 3.620  |
| H36A  | 0.48866| 0.07089| 0.68305| 3.780  |
| H36B  | 0.58940| 0.10495| 0.68295| 3.780  |
| H36C  | 0.54066| 0.10901| 0.73797| 3.780  |
| H37A  | 0.56669| 0.43660| 0.70673| 3.689  |
| H37B  | 0.58888| 0.33483| 0.75261| 3.689  |
| H37C  | 0.63762| 0.33077| 0.69759| 3.689  |
| H38A  | 0.41223| 0.37947| 0.71255| 3.936  |
| H38B  | 0.38134| 0.23737| 0.70458| 3.936  |
| H38C  | 0.43938| 0.27663| 0.75709| 3.936  |
| H39A  | -0.01020| 0.28842| 0.67148| 3.484  |
| H39B  | -0.02096| 0.34254| 0.61152| 3.484  |
| atom | U11  | U22  | U33  | U12  | U13  | U23  |
|------|------|------|------|------|------|------|
| Nb1  | 0.0151(14) | 0.01944(16) | 0.02311(15) | 0.00037(12) | -0.0008(10) | -0.00087(13) |
| C1   | 0.0415(6) | 0.0372(6) | 0.0918(9) | 0.0098(5) | -0.0083(6) | -0.0203(6) |
| C2   | 0.0479(6) | 0.0303(6) | 0.0564(6) | 0.0026(4) | -0.0123(5) | -0.0081(5) |
| O1   | 0.0226(12) | 0.0225(13) | 0.0315(13) | -0.0005(10) | 0.0079(10) | -0.0004(11) |
| N1   | 0.0204(14) | 0.0256(16) | 0.0236(15) | -0.0005(12) | 0.0031(11) | 0.0026(12) |
| N2   | 0.0193(14) | 0.0264(17) | 0.0310(16) | 0.0023(12) | -0.0021(12) | -0.0030(13) |
| N3   | 0.0189(14) | 0.0234(15) | 0.0259(15) | -0.0002(11) | 0.0005(11) | 0.0022(12) |
| C1   | 0.0165(15) | 0.0243(19) | 0.0244(17) | 0.0016(13) | -0.0019(13) | 0.0012(14) |
| C2   | 0.0191(16) | 0.0243(18) | 0.0252(17) | 0.0008(13) | -0.0030(13) | -0.0006(14) |
| C3   | 0.0300(19) | 0.029(2) | 0.0286(18) | 0.0015(15) | -0.0010(14) | -0.0030(16) |
| C4   | 0.037(2) | 0.036(2) | 0.0264(19) | -0.0001(17) | 0.0104(16) | 0.0041(17) |
| C5   | 0.035(2) | 0.027(2) | 0.035(2) | -0.0006(16) | 0.0299(16) | 0.0082(16) |
| C6   | 0.0225(17) | 0.0207(17) | 0.0265(17) | 0.0032(13) | -0.0007(14) | 0.0026(14) |
| C7   | 0.0273(19) | 0.0234(19) | 0.037(2) | -0.0007(15) | 0.0060(15) | -0.0026(16) |
| C8   | 0.061(3) | 0.037(3) | 0.054(3) | -0.010(2) | 0.004(2) | -0.06(2) |
| C9   | 0.043(2) | 0.030(2) | 0.048(2) | 0.0051(18) | 0.0087(19) | 0.0040(19) |
| C10  | 0.0286(19) | 0.0193(19) | 0.041(2) | 0.0039(14) | 0.0097(16) | 0.0027(16) |
| C11  | 0.044(3) | 0.046(3) | 0.059(3) | 0.022(2) | 0.006(2) | 0.004(2) |
| C12  | 0.038(2) | 0.037(3) | 0.084(4) | 0.0008(19) | 0.005(2) | -0.021(3) |
| C13  | 0.034(2) | 0.0190(19) | 0.0304(19) | 0.0024(14) | 0.0133(15) | 0.0016(14) |
| C14  | 0.045(2) | 0.029(2) | 0.030(2) | -0.0083(17) | 0.0160(17) | -0.0054(16) |
| C15  | 0.077(3) | 0.027(2) | 0.051(3) | -0.015(2) | 0.030(2) | -0.013(2) |
| C16  | 0.091(4) | 0.024(2) | 0.079(4) | 0.000(3) | 0.052(3) | -0.003(3) |
| C17  | 0.060(3) | 0.037(3) | 0.077(3) | 0.027(2) | 0.040(3) | 0.030(3) |
| C18  | 0.034(2) | 0.038(2) | 0.047(2) | 0.0134(18) | 0.0180(18) | 0.0116(19) |
| C19  | 0.053(3) | 0.045(3) | 0.034(2) | -0.026(2) | -0.0065(19) | -0.0034(19) |
| C20  | 0.028(2) | 0.068(3) | 0.058(3) | 0.011(2) | 0.0011(19) | 0.034(2) |
| C21  | 0.0215(17) | 0.0192(18) | 0.0313(18) | 0.0038(13) | -0.0039(14) | 0.0013(14) |
| C22  | 0.0263(18) | 0.0251(19) | 0.0287(18) | 0.0013(14) | -0.0043(14) | -0.0030(15) |
| C23  | 0.053(3) | 0.050(3) | 0.053(3) | 0.012(2) | 0.016(2) | 0.022(2) |
| C24  | 0.047(3) | 0.049(3) | 0.056(3) | -0.008(2) | 0.011(2) | -0.027(2) |
| C25  | 0.028(2) | 0.061(3) | 0.036(2) | 0.0109(19) | -0.0006(17) | -0.012(2) |
| C26  | 0.0212(18) | 0.030(2) | 0.036(2) | -0.0013(14) | -0.0047(15) | -0.0028(16) |
| C27  | 0.042(3) | 0.048(3) | 0.116(5) | -0.006(2) | 0.017(3) | 0.015(3) |
| C28  | 0.030(2) | 0.121(5) | 0.060(3) | 0.010(3) | -0.009(2) | 0.015(3) |
| C29  | 0.025(2) | 0.090(4) | 0.083(4) | 0.001(2) | -0.002(2) | -0.036(3) |
| C30  | 0.0199(16) | 0.0175(17) | 0.0279(17) | -0.0027(13) | -0.0009(13) | 0.0039(14) |
Table S5-3. Anisotropic displacement parameters (continued)

| atom | U\(_{11}\)  | U\(_{22}\)  | U\(_{33}\)  | U\(_{12}\)  | U\(_{13}\)  | U\(_{23}\)  |
|------|-------------|-------------|-------------|-------------|-------------|-------------|
| C31  | 0.0193(17)  | 0.029(2)    | 0.0311(19)  | 0.0022(14)  | 0.0002(14)  | 0.0012(15)  |
| C32  | 0.0291(19)  | 0.046(2)    | 0.035(2)    | 0.0035(18)  | 0.0080(15)  | 0.0070(19)  |
| C33  | 0.0305(19)  | 0.036(2)    | 0.040(2)    | 0.0035(17)  | 0.0023(16)  | -0.0060(19) |
| C34  | 0.0185(18)  | 0.049(3)    | 0.047(2)    | 0.0005(17)  | -0.0015(16) | -0.000(2)   |
| C35  | 0.0289(19)  | 0.029(2)    | 0.0277(18)  | 0.0018(15)  | -0.0054(15) | 0.0013(16)  |
| C36  | 0.049(2)    | 0.035(2)    | 0.034(2)    | 0.0002(19)  | -0.0077(18) | 0.0094(19)  |
| C37  | 0.040(2)    | 0.040(2)    | 0.036(2)    | 0.0003(18)  | -0.0120(17) | -0.0027(18) |
| C38  | 0.043(2)    | 0.056(3)    | 0.0254(19)  | 0.009(2)    | 0.0021(17)  | 0.0070(19)  |
| C39  | 0.0255(19)  | 0.037(2)    | 0.047(2)    | -0.0047(16) | -0.0001(17) | -0.0080(19) |

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 S5-4. Fragment Analysis

| fragment: 1 |  |  |  |  |  |
|-------------|---|---|---|---|---|
| Nb(1)       | O(1) | N(1) | N(2) | N(3) |
| C(1)        | C(2) | C(3) | C(4) | C(5) |
| C(6)        | C(7) | C(8) | C(9) | C(10) |
| C(11)       | 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) |  |  |

| fragment: 2 |  |  |  |
|-------------|---|---|---|
| Cl(1)       | Cl(2) | C(39) |  |  |
Table S5-5. Bond lengths (Å)

| atom | atom | distance  | atom | atom | distance  |
|------|------|-----------|------|------|-----------|
| Nb1  | O1   | 1.939(3)  | Nb1  | N1   | 1.783(3)  |
| Nb1  | N2   | 1.957(3)  | Nb1  | N3   | 1.947(3)  |
| Cl1  | C39  | 1.736(4)  | Cl2  | C39  | 1.766(4)  |
| O1   | C1   | 1.351(4)  | N1   | C13  | 1.395(5)  |
| N2   | C21  | 1.261(4)  | N3   | C30  | 1.264(4)  |
| C1   | C2   | 1.414(5)  | C1   | C6   | 1.406(5)  |
| C2   | C3   | 1.390(5)  | C2   | C7   | 1.511(5)  |
| C3   | C4   | 1.388(6)  | C4   | C5   | 1.377(6)  |
| C5   | C6   | 1.404(5)  | C6   | C10  | 1.531(5)  |
| C7   | C8   | 1.536(6)  | C7   | C9   | 1.516(6)  |
| C10  | C11  | 1.532(6)  | C10  | C12  | 1.514(6)  |
| C13  | C14  | 1.409(5)  | C13  | C18  | 1.416(5)  |
| C14  | C15  | 1.390(6)  | C14  | C19  | 1.489(6)  |
| C15  | C16  | 1.361(8)  | C16  | C17  | 1.397(8)  |
| C17  | C18  | 1.388(7)  | C18  | C20  | 1.501(6)  |
| C21  | C22  | 1.555(5)  | C21  | C26  | 1.567(5)  |
| C22  | C23  | 1.532(6)  | C22  | C24  | 1.545(6)  |
| C22  | C25  | 1.526(5)  | C26  | C27  | 1.518(7)  |
| C26  | C28  | 1.510(7)  | C26  | C29  | 1.536(7)  |
| C30  | C31  | 1.555(5)  | C30  | C35  | 1.550(5)  |
| C31  | C32  | 1.538(5)  | C31  | C33  | 1.540(5)  |
| C31  | C34  | 1.538(5)  | C35  | C36  | 1.538(6)  |
| C35  | C37  | 1.541(6)  | C35  | C38  | 1.546(6)  |
Table S5-6. Bond lengths involving hydrogens (Å)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C3   | H3   | 0.950    | C4   | H4   | 0.950    |
| C5   | H5   | 0.950    | C7   | H7   | 1.000    |
| C8   | H8A  | 0.980    | C8   | H8B  | 0.980    |
| C8   | H8C  | 0.980    | C9   | H9A  | 0.980    |
| C9   | H9B  | 0.980    | C9   | H9C  | 0.980    |
| C10  | H10  | 1.000    | C11  | H11A | 0.980    |
| C11  | H11B | 0.980    | C11  | H11C | 0.980    |
| C12  | H12A | 0.980    | C12  | H12B | 0.980    |
| C12  | H12C | 0.980    | C15  | H15  | 0.950    |
| C16  | H16  | 0.950    | C17  | H17  | 0.950    |
| C19  | H19A | 0.980    | C19  | H19B | 0.980    |
| C19  | H19C | 0.980    | C20  | H20A | 0.980    |
| C20  | H20B | 0.980    | C20  | H20C | 0.980    |
| C23  | H23A | 0.980    | C23  | H23B | 0.980    |
| C23  | H23C | 0.980    | C24  | H24A | 0.980    |
| C24  | H24B | 0.980    | C24  | H24C | 0.980    |
| C25  | H25A | 0.980    | C25  | H25B | 0.980    |
| C25  | H25C | 0.980    | C27  | H27A | 0.980    |
| C27  | H27B | 0.980    | C27  | H27C | 0.980    |
| C28  | H28A | 0.980    | C28  | H28B | 0.980    |
| C28  | H28C | 0.980    | C29  | H29A | 0.980    |
| C29  | H29B | 0.980    | C29  | H29C | 0.980    |
| C32  | H32A | 0.980    | C32  | H32B | 0.980    |
| C32  | H32C | 0.980    | C33  | H33A | 0.980    |
| C33  | H33B | 0.980    | C33  | H33C | 0.980    |
| C34  | H34A | 0.980    | C34  | H34B | 0.980    |
| C34  | H34C | 0.980    | C36  | H36A | 0.980    |
| C36  | H36B | 0.980    | C36  | H36C | 0.980    |
| C37  | H37A | 0.980    | C37  | H37B | 0.980    |
| C37  | H37C | 0.980    | C38  | H38A | 0.980    |
| C38  | H38B | 0.980    | C38  | H38C | 0.980    |
| C39  | H39A | 0.990    | C39  | H39B | 0.990    |
Table S5-7. Bond angles (°)

| atom | atom | atom | angle    | atom | atom | atom | angle    |
|------|------|------|----------|------|------|------|----------|
| O1   | Nb1  | N1   | 114.86(12) | O1   | Nb1  | N2   | 107.28(11) |
| O1   | Nb1  | N3   | 106.09(11) | N1   | Nb1  | N2   | 106.01(12) |
| N1   | Nb1  | N3   | 104.88(12) | N2   | Nb1  | N3   | 118.09(12) |
| Nb1  | O1   | C1   | 168.6(2)   | Nb1  | N1   | C13  | 174.5(2)  |
| Nb1  | N2   | C21  | 173.4(3)   | Nb1  | N3   | C30  | 178.9(3)  |
| O1   | C1   | C2   | 119.5(3)   | O1   | C1   | C6   | 119.1(3)  |
| C2   | C1   | C6   | 121.4(3)   | C1   | C2   | C3   | 117.9(3)  |
| C1   | C2   | C7   | 119.9(3)   | C3   | C2   | C7   | 122.2(3)  |
| C2   | C3   | C4   | 121.6(3)   | C3   | C4   | C5   | 119.9(4)  |
| C4   | C5   | C6   | 121.1(4)   | C1   | C6   | C5   | 118.1(3)  |
| C1   | C6   | C10  | 121.1(3)   | C5   | C6   | C10  | 120.8(3)  |
| C2   | C7   | C8   | 113.7(3)   | C2   | C7   | C9   | 109.7(3)  |
| C8   | C7   | C9   | 110.8(3)   | C6   | C10  | C11  | 109.4(3)  |
| C6   | C10  | C12  | 113.2(3)   | C11  | C10  | C12  | 110.5(3)  |
| N1   | C13  | C14  | 119.6(3)   | N1   | C13  | C18  | 119.8(3)  |
| C14  | C13  | C18  | 120.5(3)   | C13  | C14  | C15  | 118.5(4)  |
| C13  | C14  | C19  | 119.4(4)   | C15  | C14  | C19  | 122.1(4)  |
| C14  | C15  | C16  | 122.1(5)   | C15  | C16  | C17  | 119.2(5)  |
| C16  | C17  | C18  | 121.7(5)   | C13  | C18  | C17  | 117.9(4)  |
| C13  | C18  | C20  | 119.6(4)   | C17  | C18  | C20  | 122.4(4)  |
| N2   | C21  | C22  | 118.8(3)   | N2   | C21  | C26  | 117.5(3)  |
| C22  | C21  | C26  | 123.7(3)   | C21  | C22  | C23  | 109.1(3)  |
| C21  | C22  | C24  | 113.9(3)   | C21  | C22  | C25  | 109.8(3)  |
| C23  | C22  | C24  | 109.8(3)   | C23  | C22  | C25  | 107.6(3)  |
| C24  | C22  | C25  | 106.4(3)   | C21  | C26  | C27  | 108.5(3)  |
| C21  | C26  | C28  | 114.6(3)   | C21  | C26  | C29  | 110.0(3)  |
| C27  | C26  | C28  | 109.7(4)   | C27  | C26  | C29  | 106.2(4)  |
| C28  | C26  | C29  | 107.4(4)   | N3   | C30  | C31  | 117.9(3)  |
| N3   | C30  | C35  | 117.9(3)   | C31  | C30  | C35  | 124.2(3)  |
| C30  | C31  | C32  | 108.4(3)   | C30  | C31  | C33  | 106.2(3)  |
| C30  | C31  | C34  | 117.1(3)   | C32  | C31  | C33  | 109.5(3)  |
| C32  | C31  | C34  | 107.1(3)   | C33  | C31  | C34  | 108.4(3)  |
| C30  | C35  | C36  | 109.7(3)   | C30  | C35  | C37  | 112.6(3)  |
| C30  | C35  | C38  | 109.6(3)   | C36  | C35  | C37  | 110.7(3)  |
| C36  | C35  | C38  | 107.8(3)   | C37  | C35  | C38  | 106.3(3)  |
| Cl1  | C39  | C12  | 111.8(2)   |
Table S5-8. Bond angles involving hydrogens (°)

| atom | atom | atom | angle  | atom | atom | atom | angle  |
|------|------|------|--------|------|------|------|--------|
| C2   | C3   | H3   | 119.2  | C4   | C3   | H3   | 119.2  |
| C3   | C4   | H4   | 120.0  | C5   | C4   | H4   | 120.0  |
| C4   | C5   | H5   | 119.4  | C6   | C5   | H5   | 119.5  |
| C2   | C7   | H7   | 107.4  | C8   | C7   | H7   | 107.4  |
| C9   | C7   | H7   | 107.4  | C7   | C8   | H8A  | 109.5  |
| C7   | C8   | H8B  | 109.5  | C7   | C8   | H8C  | 109.5  |
| H8A  | C8   | H8B  | 109.5  | H8A  | C8   | H8C  | 109.5  |
| H8B  | C8   | H8C  | 109.5  | C7   | C9   | H9A  | 109.5  |
| C7   | C9   | H9B  | 109.5  | C7   | C9   | H9C  | 109.5  |
| H9A  | C9   | H9B  | 109.5  | H9A  | C9   | H9C  | 109.5  |
| H9B  | C9   | H9C  | 109.5  | C6   | C10  | H10  | 107.8  |
| C11  | C10  | H10  | 107.8  | C12  | C10  | H10  | 107.8  |
| C10  | C11  | H11A | 109.5  | C10  | C11  | H11B | 109.5  |
| C10  | C11  | H11C | 109.5  | H11A | C11  | H11B | 109.5  |
| H11A | C11  | H11C | 109.5  | H11B | C11  | H11C | 109.5  |
| C10  | C12  | H12A | 109.5  | C10  | C12  | H12B | 109.5  |
| C10  | C12  | H12C | 109.5  | H12A | C12  | H12B | 109.5  |
| H12A | C12  | H12C | 109.5  | H12B | C12  | H12C | 109.5  |
| C14  | C15  | H15  | 119.0  | C16  | C15  | H15  | 118.9  |
| C15  | C16  | H16  | 120.4  | C17  | C16  | H16  | 120.4  |
| C16  | C17  | H17  | 119.1  | C18  | C17  | H17  | 119.1  |
| C14  | C19  | H19A | 109.5  | C14  | C19  | H19B | 109.5  |
| C14  | C19  | H19C | 109.5  | H19A | C19  | H19B | 109.5  |
| H19A | C19  | H19C | 109.5  | H19B | C19  | H19C | 109.5  |
| C18  | C20  | H20A | 109.5  | C18  | C20  | H20B | 109.5  |
| C18  | C20  | H20C | 109.5  | H20A | C20  | H20B | 109.5  |
| H20A | C20  | H20C | 109.5  | H20B | C20  | H20C | 109.5  |
| C22  | C23  | H23A | 109.5  | C22  | C23  | H23B | 109.5  |
| C22  | C23  | H23C | 109.5  | H23A | C23  | H23B | 109.5  |
| H23A | C23  | H23C | 109.5  | H23B | C23  | H23C | 109.5  |
| C22  | C24  | H24A | 109.5  | C22  | C24  | H24B | 109.5  |
| C22  | C24  | H24C | 109.5  | H24A | C24  | H24B | 109.5  |
| H24A | C24  | H24C | 109.5  | H24B | C24  | H24C | 109.5  |
| C22  | C25  | H25A | 109.5  | C22  | C25  | H25B | 109.5  |
| C22  | C25  | H25C | 109.5  | H25A | C25  | H25B | 109.5  |
| H25A | C25  | H25C | 109.5  | H25B | C25  | H25C | 109.5  |
| C26  | C27  | H27A | 109.5  | C26  | C27  | H27B | 109.5  |
Table S5-8. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C26  | C27  | H27C | 109.5 | H27A | C27  | H27B | 109.5 |
| H27A | C27  | H27C | 109.5 | H27B | C27  | H27C | 109.5 |
| C26  | C28  | H28A | 109.5 | C26  | C28  | H28B | 109.5 |
| C26  | C28  | H28C | 109.5 | H28A | C28  | H28B | 109.5 |
| H28A | C28  | H28C | 109.5 | H28B | C28  | H28C | 109.5 |
| C26  | C29  | H29A | 109.5 | C26  | C29  | H29B | 109.5 |
| C26  | C29  | H29C | 109.5 | H29A | C29  | H29B | 109.5 |
| H29A | C29  | H29C | 109.5 | H29B | C29  | H29C | 109.5 |
| C31  | C32  | H32A | 109.5 | C31  | C32  | H32B | 109.5 |
| C31  | C32  | H32C | 109.5 | H32A | C32  | H32B | 109.5 |
| H32A | C32  | H32C | 109.5 | H32B | C32  | H32C | 109.5 |
| C31  | C33  | H33A | 109.5 | C31  | C33  | H33B | 109.5 |
| C31  | C33  | H33C | 109.5 | H33A | C33  | H33B | 109.5 |
| H33A | C33  | H33C | 109.5 | H33B | C33  | H33C | 109.5 |
| C31  | C34  | H34A | 109.5 | C31  | C34  | H34B | 109.5 |
| C31  | C34  | H34C | 109.5 | H34A | C34  | H34B | 109.5 |
| H34A | C34  | H34C | 109.5 | H34B | C34  | H34B | 109.5 |
| C35  | C36  | H36A | 109.5 | C35  | C36  | H36B | 109.5 |
| C35  | C36  | H36C | 109.5 | H36A | C36  | H36B | 109.5 |
| H36A | C36  | H36C | 109.5 | H36B | C36  | H36C | 109.5 |
| C35  | C37  | H37A | 109.5 | C35  | C37  | H37B | 109.5 |
| C35  | C37  | H37C | 109.5 | H37A | C37  | H37B | 109.5 |
| H37A | C37  | H37C | 109.5 | H37B | C37  | H37C | 109.5 |
| C35  | C38  | H38A | 109.5 | C35  | C38  | H38B | 109.5 |
| C35  | C38  | H38C | 109.5 | H38A | C38  | H38B | 109.5 |
| H38A | C38  | H38C | 109.5 | H38B | C38  | H38C | 109.5 |
| Cl1  | C39  | H39A | 109.3 | Cl1  | C39  | H39B | 109.2 |
| Cl2  | C39  | H39A | 109.3 | Cl2  | C39  | H39B | 109.3 |
| H39A | C39  | H39B | 107.9 |      |      |      |       |
Table S5-9. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle  | atom1 | atom2 | atom3 | atom4 | angle  |
|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|
| O1    | C1    | C2    | C3    | 178.0(2) | O1    | C1    | C2    | C7    | 0.2(4) |
| O1    | C1    | C6    | C5    | -177.7(2) | O1    | C1    | C6    | C10   | 4.4(4) |
| C2    | C1    | C6    | C5    | 2.4(5)   | C2    | C1    | C6    | C10   | -175.5(3) |
| C6    | C1    | C2    | C3    | -2.1(4)  | C6    | C1    | C2    | C7    | -179.9(3) |
| C1    | C2    | C3    | C4    | -0.4(5)  | C1    | C2    | C7    | C8    | -152.2(3) |
| C1    | C2    | C7    | C9    | 83.1(4)  | C3    | C2    | C7    | C8    | 30.1(4) |
| C3    | C2    | C7    | C9    | -94.6(4) | C7    | C2    | C3    | C4    | 177.4(3) |
| C2    | C3    | C4    | C5    | 2.4(5)   | C3    | C4    | C5    | C6    | -2.0(5) |
| C4    | C5    | C6    | C1    | -0.4(5)  | C4    | C5    | C6    | C10   | 177.6(3) |
| C1    | C6    | C10   | C11   | 105.9(3) | C1    | C6    | C10   | C12   | -130.3(3) |
| C5    | C6    | C10   | C11   | -72.0(4) | C5    | C6    | C10   | C12   | 51.8(4) |
| N1    | C13   | C14   | C15   | 177.8(3) | N1    | C13   | C14   | C19   | -0.8(5) |
| N1    | C13   | C18   | C17   | -177.8(3) | N1    | C13   | C18   | C20   | -0.3(5) |
| C14   | C13   | C18   | C17   | -0.4(5)  | C14   | C13   | C18   | C20   | 177.1(3) |
| C18   | C13   | C14   | C15   | 0.3(5)   | C18   | C13   | C14   | C19   | -178.3(3) |
| C13   | C14   | C15   | C16   | -0.2(7)  | C19   | C14   | C15   | C16   | 178.4(4) |
| C14   | C15   | C16   | C17   | 0.1(8)   | C15   | C16   | C17   | C18   | -0.2(8) |
| C16   | C17   | C18   | C13   | 0.3(7)   | C16   | C17   | C18   | C20   | -177.1(4) |
| N2    | C21   | C22   | C23   | -99.9(3) | N2    | C21   | C22   | C24   | 137.0(3) |
| N2    | C21   | C22   | C25   | 17.8(4)  | N2    | C21   | C26   | C27   | -98.3(3) |
| N2    | C21   | C26   | C28   | 138.8(3) | N2    | C21   | C26   | C29   | 17.6(4) |
| C22   | C21   | C26   | C27   | 83.1(4)  | C22   | C21   | C26   | C28   | -39.9(4) |
| C22   | C21   | C26   | C29   | -161.1(3) | C26   | C21   | C22   | C23   | 78.8(4) |
| C26   | C21   | C22   | C24   | -44.3(4) | C26   | C21   | C22   | C25   | -163.5(3) |
| N3    | C30   | C31   | C32   | 42.3(4)  | N3    | C30   | C31   | C33   | -75.2(4) |
| N3    | C30   | C31   | C34   | 163.6(3) | N3    | C30   | C35   | C36   | 115.0(3) |
| N3    | C30   | C35   | C37   | -121.2(3) | N3    | C30   | C35   | C38   | -3.1(4) |
| C31   | C30   | C35   | C36   | -61.5(4) | C31   | C30   | C35   | C37   | 62.2(4) |
| C31   | C30   | C35   | C38   | -179.6(3) | C35   | C30   | C31   | C32   | -141.1(3) |
| C35   | C30   | C31   | C33   | 101.3(3) | C35   | C30   | C31   | C34   | -19.9(5) |
Table S5-10. Intramolecular contacts less than 3.60 Å

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| O1   | C7   | 2.835(4) | O1   | C9   | 3.330(5) |
| O1   | C10  | 2.858(4) | N1   | C9   | 3.575(5) |
| N1   | C19  | 2.831(5) | N1   | C20  | 2.853(5) |
| N2   | C23  | 3.311(6) | N2   | C25  | 2.728(5) |
| N2   | C27  | 3.273(6) | N2   | C29  | 2.723(5) |
| N3   | C32  | 2.809(5) | N3   | C33  | 3.036(5) |
| N3   | C36  | 3.432(5) | N3   | C37  | 3.520(5) |
| N3   | C38  | 2.681(5) | C1   | C4   | 2.778(5) |
| C1   | C9   | 3.249(5) | C1   | C11  | 3.484(6) |
| C2   | C5   | 2.803(5) | C3   | C6   | 2.795(5) |
| C3   | C8   | 2.955(6) | C3   | C9   | 3.365(6) |
| C5   | C11  | 3.174(6) | C5   | C12  | 3.069(7) |
| C13  | C16  | 2.787(6) | C14  | C17  | 2.782(6) |
| C15  | C18  | 2.791(6) | C22  | C27  | 3.432(7) |
| C22  | C28  | 3.193(6) | C23  | C26  | 3.409(6) |
| C23  | C28  | 3.254(7) | C24  | C26  | 3.221(6) |
| C24  | C27  | 3.301(8) | C24  | C28  | 3.439(8) |
| C31  | C36  | 3.259(5) | C31  | C37  | 3.327(5) |
| C33  | C35  | 3.567(6) | C33  | C36  | 3.516(6) |
| C34  | C35  | 3.161(6) | C34  | C36  | 3.432(6) |
| C34  | C37  | 3.137(6) |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H7   | 3.116    | Nb1  | H9B  | 3.431    |
| Nb1  | H10  | 3.509    | Nb1  | H19A | 3.085    |
| Nb1  | H20A | 3.243    | Nb1  | H25C | 3.533    |
| Nb1  | H29A | 3.112    | Nb1  | H32A | 3.323    |
| Nb1  | H38A | 3.505    | Nb1  | H38B | 3.429    |
| O1   | H7   | 2.479    | O1   | H9B  | 2.827    |
| O1   | H10  | 2.381    | O1   | H11A | 3.504    |
| O1   | H29A | 2.727    | O1   | H38A | 3.385    |
| O1   | H38B | 2.928    | N1   | H7   | 2.879    |
| N1   | H9A  | 3.447    | N1   | H9B  | 3.145    |
| N1   | H19A | 2.336    | N1   | H19B | 3.470    |
| N1   | H19C | 3.507    | N1   | H20A | 2.363    |
| N1   | H20B | 3.534    | N1   | H20C | 3.486    |
| N1   | H32A | 3.554    | N2   | H20A | 3.088    |
| N2   | H23B | 3.145    | N2   | H25A | 2.769    |
| N2   | H25C | 2.530    | N2   | H27A | 3.066    |
| N2   | H29A | 2.478    | N2   | H29B | 2.818    |
| N3   | H19A | 2.691    | N3   | H32A | 2.472    |
| N3   | H32B | 3.071    | N3   | H33A | 3.375    |
| N3   | H33B | 2.750    | N3   | H36A | 3.319    |
| N3   | H37A | 3.463    | N3   | H38A | 2.622    |
| N3   | H38B | 2.567    | C1   | H3   | 3.263    |
| C1   | H5   | 3.269    | C1   | H7   | 2.605    |
| C1   | H9B  | 2.997    | C1   | H9C  | 3.588    |
| C1   | H10  | 2.583    | C1   | H11A | 3.300    |
| C1   | H29A | 3.322    | C1   | H38B | 3.254    |
| C2   | H4   | 3.277    | C2   | H8A  | 3.380    |
| C2   | H8B  | 2.755    | C2   | H8C  | 2.755    |
| C2   | H9A  | 3.322    | C2   | H9B  | 2.664    |
| C2   | H9C  | 2.664    | C3   | H5   | 3.249    |
| C3   | H7   | 3.274    | C3   | H8B  | 2.730    |
| C3   | H8C  | 3.056    | C3   | H9C  | 3.166    |
| C5   | H3   | 3.246    | C5   | H10  | 3.340    |
| C5   | H11A | 3.409    | C5   | H11B | 2.939    |
| C5   | H12B | 2.793    | C5   | H12C | 3.291    |
| C6   | H4   | 3.277    | C6   | H11A | 2.646    |
| C6   | H11B | 2.725    | C6   | H11C | 3.346    |
Table S5-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C6   | H12A | 3.377    | C6   | H12B | 2.740    |
| C6   | H12C | 2.740    | C7   | H3   | 2.697    |
| C8   | H3   | 2.629    | C8   | H9A  | 2.655    |
| C8   | H9B  | 3.356    | C8   | H9C  | 2.749    |
| C9   | H3   | 3.461    | C9   | H8A  | 2.676    |
| C9   | H8B  | 2.737    | C9   | H8C  | 3.353    |
| C9   | H20A | 3.587    | C9   | H20B | 3.514    |
| C10  | H5   | 2.699    | C11  | H5   | 3.119    |
| C11  | H12A | 2.667    | C11  | H12B | 2.714    |
| C11  | H12C | 3.348    | C11  | H3B  | 3.337    |
| C12  | H5   | 2.852    | C12  | H11A | 3.346    |
| C12  | H11B | 2.695    | C12  | H11C | 2.695    |
| C12  | H27A | 3.400    | C13  | H7   | 3.298    |
| C13  | H9A  | 3.211    | C13  | H9B  | 3.531    |
| C13  | H15  | 3.262    | C13  | H17  | 3.264    |
| C13  | H19A | 2.526    | C13  | H19B | 3.120    |
| C13  | H19C | 3.135    | C13  | H20A | 2.547    |
| C13  | H20B | 3.160    | C13  | H20C | 3.131    |
| C14  | H16  | 3.263    | C15  | H17  | 3.231    |
| C15  | H19A | 3.308    | C15  | H19B | 2.771    |
| C15  | H19C | 3.135    | C17  | H15  | 3.235    |
| C17  | H20A | 3.317    | C17  | H20B | 2.785    |
| C17  | H20C | 2.785    | C18  | H9A  | 3.162    |
| C18  | H16  | 3.286    | C19  | H15  | 2.676    |
| C19  | H32B | 3.512    | C19  | H37A | 3.358    |
| C19  | H38A | 3.498    | C20  | H9A  | 3.399    |
| C20  | H9B  | 3.308    | C20  | H17  | 2.691    |
| C20  | H29B | 3.015    | C21  | H20A | 3.551    |
| C21  | H23A | 2.702    | C21  | H23B | 2.687    |
| C21  | H23C | 3.367    | C21  | H24A | 2.789    |
| C21  | H24B | 3.430    | C21  | H24C | 2.805    |
| C21  | H25A | 2.714    | C21  | H25B | 3.371    |
| C21  | H25C | 2.693    | C21  | H27A | 2.635    |
| C21  | H27B | 3.359    | C21  | H27C | 2.726    |
| C21  | H28A | 2.770    | C21  | H28B | 2.803    |
| C21  | H28C | 3.422    | C21  | H29A | 2.683    |
| C21  | H29B | 2.765    | C21  | H29C | 3.389    |
Table S5-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C22  | H27C | 3.194    | C22  | H28A | 3.304    |
| C22  | H28B | 2.933    | C23  | H24A | 2.734    |
| C23  | H24B | 2.677    | C23  | H24C | 3.362    |
| C23  | H25A | 3.323    | C23  | H25B | 2.645    |
| C23  | H25C | 2.645    | C23  | H28A | 2.966    |
| C23  | H28B | 2.978    | C24  | H23C | 2.668    |
| C24  | H23B | 3.364    | C24  | H23C | 2.668    |
| C24  | H25A | 2.649    | C24  | H25B | 2.612    |
| C24  | H25C | 3.320    | C24  | H27C | 2.646    |
| C24  | H28B | 2.815    | C25  | H23A | 3.322    |
| C25  | H23B | 2.646    | C25  | H23C | 2.646    |
| C25  | H24A | 3.317    | C25  | H24B | 2.635    |
| C25  | H24C | 2.635    | C25  | H32A | 3.281    |
| C25  | H33B | 3.035    | C26  | H23A | 3.122    |
| C26  | H24A | 2.917    | C26  | H24C | 3.404    |
| C27  | H12C | 3.576    | C27  | H24A | 2.948    |
| C27  | H24C | 3.107    | C27  | H28A | 3.324    |
| C27  | H29A | 2.662    | C27  | H28C | 2.662    |
| C27  | H29C | 2.598    | C27  | H29B | 3.301    |
| C28  | H24A | 2.808    | C28  | H27A | 3.322    |
| C28  | H27B | 2.664    | C28  | H27C | 2.664    |
| C28  | H29A | 3.308    | C28  | H29B | 2.637    |
| C28  | H29C | 2.637    | C29  | H9B  | 3.372    |
| C29  | H20A | 3.125    | C29  | H27A | 2.648    |
| C29  | H27B | 2.582    | C29  | H27C | 3.304    |
| C29  | H28A | 2.670    | C29  | H28B | 3.312    |
| C29  | H28C | 2.592    | C30  | H19A | 3.113    |
| C30  | H32A | 2.633    | C30  | H32B | 2.743    |
| C30  | H32C | 3.360    | C30  | H33A | 2.670    |
| C30  | H33B | 2.620    | C30  | H33C | 3.336    |
| C30  | H34A | 2.836    | C30  | H34B | 3.457    |
| C30  | H34C | 2.862    | C30  | H36A | 2.672    |
| C30  | H36B | 2.745    | C30  | H36C | 3.371    |
| C30  | H37A | 2.743    | C30  | H37B | 3.407    |
| C30  | H37C | 2.789    | C30  | H38A | 2.717    |
| C30  | H38B | 2.707    | C30  | H38C | 3.377    |
Table S5-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C31  | H36A | 3.440    | C31  | H36B | 2.983    |
| C31  | H37A | 3.542    | C31  | H37C | 3.058    |
| C32  | H25C | 3.288    | C32  | H33A | 3.361    |
| C32  | H33B | 2.698    | C32  | H33C | 2.698    |
| C32  | H34A | 3.332    | C32  | H34B | 2.651    |
| C32  | H34C | 2.651    | C33  | H25A | 3.293    |
| C33  | H32A | 2.718    | C33  | H32B | 3.361    |
| C33  | H32C | 2.678    | C33  | H34A | 2.693    |
| C33  | H34B | 2.663    | C33  | H34C | 3.349    |
| C33  | H36A | 3.328    | C33  | H36B | 3.172    |
| C34  | H32A | 3.332    | C34  | H32B | 2.651    |
| C34  | H32C | 2.651    | C34  | H33A | 2.705    |
| C34  | H33B | 3.348    | C34  | H33C | 2.652    |
| C34  | H36B | 2.816    | C34  | H37A | 3.495    |
| C34  | H37C | 2.446    | C35  | H33A | 3.366    |
| C35  | H34A | 2.941    | C35  | H34C | 3.215    |
| C36  | H33A | 2.911    | C36  | H34A | 2.818    |
| C36  | H37A | 3.376    | C36  | H37B | 2.722    |
| C36  | H37C | 2.722    | C36  | H38A | 3.346    |
| C36  | H38B | 2.671    | C36  | H38C | 2.671    |
| C37  | H34A | 2.957    | C37  | H34C | 2.761    |
| C37  | H36A | 3.377    | C37  | H36B | 2.721    |
| C37  | H36C | 2.721    | C37  | H38A | 2.654    |
| C37  | H38B | 3.331    | C37  | H38C | 2.635    |
| C38  | H11A | 3.315    | C38  | H19A | 3.553    |
| C38  | H36A | 2.701    | C38  | H36B | 3.346    |
| C38  | H36C | 2.638    | C38  | H37A | 2.668    |
| C38  | H37B | 2.618    | C38  | H37C | 3.331    |
| H3   | H4   | 2.328    | H3   | H7   | 3.549    |
| H3   | H8A  | 3.556    | H3   | H8B  | 2.136    |
| H3   | H8C  | 2.772    | H3   | H9C  | 3.122    |
| H4   | H5   | 2.320    | H5   | H11A | 3.554    |
| H5   | H11B | 2.646    | H5   | H12B | 2.296    |
| H5   | H12C | 3.211    | H7   | H8A  | 2.365    |
| H7   | H8B  | 2.864    | H7   | H8C  | 2.351    |
| H7   | H9A  | 2.360    | H7   | H9B  | 2.320    |
| H7   | H9C  | 2.848    | H7   | H19A | 3.249    |
Table S5-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H7   | H19C | 3.576    | H7   | H38A | 3.116    |
| H8A  | H9A  | 2.445    | H8A  | H9B  | 3.551    |
| H8A  | H9C  | 3.016    | H8B  | H9A  | 2.966    |
| H8B  | H9C  | 2.612    | H8C  | H9A  | 3.541    |
| H9A  | H20A | 3.402    | H9A  | H20B | 3.070    |
| H9B  | H20A | 2.885    | H9B  | H20B | 3.083    |
| H9B  | H29A | 2.944    | H9B  | H29B | 2.991    |
| H10  | H11A | 2.373    | H10  | H11B | 2.864    |
| H10  | H11C | 2.346    | H10  | H12A | 2.348    |
| H10  | H12B | 2.851    | H10  | H12C | 2.339    |
| H10  | H27A | 3.054    | H10  | H29A | 3.326    |
| H10  | H38B | 3.464    | H11A | H12A | 3.564    |
| H11A | H12B | 3.599    | H11A | H36A | 3.160    |
| H11A | H38B | 2.437    | H11A | H38C | 3.432    |
| H11B | H12A | 2.944    | H11B | H12B | 2.539    |
| H11B | H12C | 3.598    | H11C | H12A | 2.489    |
| H11C | H12B | 3.014    | H11C | H12C | 3.575    |
| H12A | H27A | 3.319    | H12C | H27A | 2.837    |
| H12C | H27B | 3.439    | H12C | H29A | 3.549    |
| H15  | H16  | 2.301    | H15  | H19B | 2.731    |
| H15  | H19C | 2.717    | H16  | H17  | 2.340    |
| H17  | H20B | 2.730    | H17  | H20C | 2.754    |
| H19A | H32A | 3.483    | H19A | H32B | 3.144    |
| H19A | H37A | 2.988    | H19A | H38A | 2.767    |
| H19B | H32B | 2.995    | H19B | H37A | 3.287    |
| H19C | H37A | 3.243    | H19C | H38A | 3.361    |
| H20A | H29A | 3.285    | H20A | H29B | 2.264    |
| H20B | H29B | 3.018    | H20B | H29B | 3.397    |
| H23A | H24A | 2.591    | H23A | H24B | 2.995    |
| H23A | H25B | 3.544    | H23A | H25C | 3.544    |
| H23A | H28A | 2.209    | H23A | H28B | 2.262    |
| H23A | H28C | 3.473    | H23B | H24B | 3.560    |
| H23B | H25A | 3.546    | H23B | H25B | 2.925    |
| H23B | H25C | 2.448    | H23B | H28A | 3.191    |
| H23C | H24A | 2.978    | H23C | H24B | 2.455    |
| H23C | H24C | 3.554    | H23C | H25A | 3.546    |
| H23C | H25B | 2.448    | H23C | H25C | 2.925    |
Table S5-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H23C | H28B | 3.590    | H24A | H25A | 3.545    |
| H24A | H25B | 3.517    | H24A | H27A | 3.540    |
| H24A | H27C | 2.228    | H24A | H28A | 3.348    |
| H24A | H28B | 2.038    | H24A | H28C | 3.501    |
| H24B | H25A | 2.935    | H24B | H25B | 2.409    |
| H24B | H25C | 3.529    | H24B | H27C | 3.555    |
| H24B | H28B | 3.469    | H24C | H25A | 2.449    |
| H24C | H25B | 2.881    | H24C | H25C | 3.546    |
| H24C | H27A | 3.256    | H24C | H27C | 2.404    |
| H24C | H28B | 3.399    | H25A | H32A | 3.362    |
| H25A | H33B | 3.842    | H25A | H32C | 2.444    |
| H25B | H33B | 3.429    | H25C | H32A | 2.905    |
| H25C | H32C | 3.389    | H25C | H32C | 2.905    |
| H27A | H28B | 3.555    | H27A | H28C | 3.555    |
| H27A | H29A | 2.469    | H27A | H29B | 3.551    |
| H27A | H29C | 2.911    | H27B | H28A | 3.559    |
| H27B | H28B | 2.949    | H27B | H28B | 2.477    |
| H27B | H29A | 2.876    | H27B | H29B | 3.480    |
| H27B | H29C | 2.353    | H27C | H28A | 3.558    |
| H27C | H28B | 2.477    | H27C | H28C | 2.949    |
| H27C | H29A | 3.553    | H27C | H29C | 3.489    |
| H28A | H29A | 3.558    | H28A | H29B | 2.478    |
| H28A | H29C | 2.970    | H28B | H29B | 3.554    |
| H28B | H29C | 3.518    | H28C | H29A | 3.499    |
| H28C | H29B | 2.857    | H28C | H29C | 2.395    |
| H32A | H33B | 2.535    | H32A | H33C | 3.009    |
| H32A | H34B | 3.551    | H32A | H34C | 3.551    |
| H32B | H33C | 3.582    | H32B | H34A | 3.550    |
| H32B | H34B | 2.927    | H32B | H34C | 2.451    |
| H32C | H33A | 3.577    | H32C | H34B | 2.974    |
| H32C | H33C | 2.493    | H32C | H34A | 3.551    |
| H32C | H34B | 2.451    | H32C | H34C | 2.927    |
| H33A | H34A | 2.532    | H33A | H34B | 2.974    |
| H33A | H36A | 2.646    | H33A | H36B | 2.512    |
| H33B | H34A | 3.597    | H33B | H34B | 3.550    |
| H33B | H36A | 3.553    | H33C | H34A | 2.940    |
| H33C | H34B | 2.443    | H33C | H34A | 3.548    |
Table S5-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H34A  | H36A  | 3.378    | H34A  | H36B  | 2.040    |
| H34A  | H36C  | 3.490    | H34A  | H37A  | 3.566    |
| H34A  | H37C  | 2.229    | H34B  | H36B  | 3.551    |
| H34B  | H37C  | 3.343    | H34C  | H36B  | 3.284    |
| H34C  | H37A  | 2.935    | H34C  | H37B  | 3.588    |
| H34C  | H37C  | 2.011    | H36A  | H38A  | 3.591    |
| H36A  | H38B  | 2.511    | H36A  | H38C  | 2.994    |
| H36B  | H37B  | 3.006    | H36B  | H37C  | 2.545    |
| H36B  | H38B  | 3.583    | H36B  | H38C  | 3.554    |
| H36C  | H37B  | 2.545    | H36C  | H37C  | 3.006    |
| H36C  | H38A  | 3.543    | H36C  | H38B  | 2.901    |
| H36C  | H38C  | 2.443    | H37A  | H38A  | 2.478    |
| H37A  | H38B  | 3.569    | H37A  | H38C  | 2.940    |
| H37B  | H38A  | 2.896    | H37B  | H38B  | 3.521    |
| H37B  | H38C  | 2.403    | H37C  | H38A  | 3.565    |
| H37C  | H38C  | 3.526    |       |       |          |
Table S5-12. Intermolecular contacts less than 3.60 Å

| atom | atom  | distance |
|------|-------|----------|
| Cl2  | C24\(^1\) | 3.581(5) |
| C11  | C37\(^2\) | 3.600(6) |
| C37  | C11\(^3\) | 3.600(6) |

Symmetry Operators:

1. \(-X, -Y, -Z+1\)
2. \(-X+1, Y+1/2, -Z+1/2+1\)
3. \(-X+1, Y+1/2, -Z+1/2+1\)
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Cl1  | H5$^1$ | 2.962    | Cl1  | H8B$^2$ | 3.528    |
| Cl1  | H9C   | 3.549    | Cl1  | H11B$^1$ | 3.056    |
| Cl1  | H20C$^3$ | 3.516   | Cl1  | H23A$^3$ | 2.989    |
| Cl1  | H23B$^3$ | 3.428   | Cl1  | H28A$^3$ | 3.094    |
| Cl1  | H34C$^4$ | 3.238   | Cl2  | H3$^2$  | 3.411    |
| Cl2  | H8B$^2$ | 3.108    | Cl2  | H12C   | 2.990    |
| Cl2  | H20C$^3$ | 3.089    | Cl2  | H24A$^5$ | 3.114    |
| Cl2  | H24C$^5$ | 3.260    | Cl2  | H27C$^5$ | 3.024    |
| Cl2  | H29C   | 3.511    | Cl2  | H34B$^4$ | 3.413    |
| N1   | H32C$^6$ | 3.064    | N2   | H16$^6$ | 3.523    |
| C1   | H39A   | 2.887    | C1   | H39B   | 3.480    |
| C2   | H39A   | 2.951    | C3   | H5$^1$  | 3.443    |
| C3   | H12B$^1$ | 3.317    | C3   | H24A$^8$ | 3.427    |
| C3   | H39A   | 2.827    | C4   | H8B$^2$  | 3.526    |
| C4   | H9C$^2$ | 3.323    | C4   | H12B$^1$ | 3.282    |
| C4   | H23A$^8$ | 3.437    | C4   | H24A$^8$ | 3.595    |
| C4   | H28B$^8$ | 3.101    | C4   | H39A   | 2.659    |
| C5   | H3$^2$  | 3.561    | C5   | H39A   | 2.643    |
| C6   | H39A   | 2.775    | C8   | H11B$^9$ | 3.585    |
| C9   | H4$^1$  | 3.335    | C9   | H12A$^9$ | 3.459    |
| C9   | H28A$^3$ | 3.544    | C9   | H28C$^3$ | 3.079    |
| C9   | H39B   | 3.527    | C10  | H16$^6$ | 3.576    |
| C11  | H8A$^7$ | 3.171    | C11  | H37B$^{10}$ | 3.187 |
| C11  | H37C$^{10}$ | 3.433  | C12  | H3$^2$  | 3.593    |
| C12  | H4$^2$  | 3.491    | C12  | H9A$^7$  | 3.336    |
| C13  | H32C$^6$ | 2.725    | C14  | H11C$^9$ | 3.402    |
| C14  | H25B$^6$ | 3.546    | C14  | H32C$^6$ | 3.094    |
| C15  | H11C$^9$ | 2.884    | C15  | H25B$^6$ | 3.361    |
| C15  | H33A$^9$ | 3.427    | C15  | H33C$^6$ | 3.315    |
| C15  | H36A$^9$ | 3.421    | C16  | H10$^9$  | 3.116    |
| C16  | H11C$^9$ | 3.005    | C16  | H12A$^9$ | 3.491    |
| C16  | H25A$^9$ | 3.475    | C16  | H33B$^9$ | 3.385    |
| C16  | H33C$^6$ | 2.938    | C17  | H10$^9$  | 3.543    |
| C17  | H12A$^9$ | 3.128    | C17  | H24C$^9$ | 3.402    |
| C17  | H27A$^9$ | 3.241    | C17  | H32C$^6$ | 3.532    |
| C17  | H33C$^6$ | 3.078    | C17  | H34B$^6$ | 3.194    |
| C18  | H12A$^9$ | 3.493    | C18  | H32C$^6$ | 2.993    |
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C18  | H3C6 | 3.581    | C18  | H3B6 | 3.083    |
| C19  | H25B6| 3.244    | C19  | H3C11| 3.129    |
| C19  | H37B11| 3.444   | C19  | H3C11| 3.367    |
| C20  | H28C3| 3.499    | C20  | H29C3| 3.196    |
| C20  | H28C6| 3.577    | C20  | H3B6 | 3.054    |
| C23  | H19B6| 3.593    | C24  | H3A12| 3.540    |
| C25  | H19B6| 3.033    | C25  | H3A12| 3.371    |
| C27  | H177 | 3.017    | C27  | H27B5| 3.056    |
| C28  | H413 | 3.181    | C28  | H9A3 | 3.595    |
| C28  | H9C3 | 3.193    | C28  | H20B3| 3.451    |
| C29  | H20B3| 3.308    | C29  | H3B8 | 2.857    |
| C32  | H32A6| 3.332    | C33  | H157 | 3.477    |
| C33  | H167 | 3.489    | C33  | H25A12| 3.360   |
| C34  | H20C6| 3.150    | C34  | H24C12| 3.512   |
| C35  | H19C10| 3.537  | C36  | H157 | 3.454    |
| C36  | H19C10| 3.180   | C36  | H37A10| 3.518   |
| C36  | H38A10| 3.486   | C37  | H11A11| 3.320   |
| C37  | H11B11| 3.457   | C37  | H11C11| 3.428   |
| C37  | H19C10| 3.375   | C38  | H19C10| 3.423   |
| C38  | H36C11| 3.583   | C39  | H8B2 | 3.367    |
| C39  | H9C  | 3.579    | C39  | H12C | 3.586    |
| C39  | H20C3| 3.430    | C39  | H29A | 3.413    |
| C39  | H29C | 3.241    | C39  | CI21 | 3.411    |
| H3   | C51  | 3.561    | H3   | C121 | 3.593    |
| H3   | H51  | 2.866    | H3   | H12B1| 2.777    |
| H3   | H12C1| 3.566    | H3   | H24A8| 3.126    |
| H3   | H28B8| 3.530    | H3   | H39A | 3.426    |
| H4   | C92  | 3.335    | H4   | CI21 | 3.491    |
| H4   | C288 | 3.181    | H4   | H8B2 | 3.174    |
| H4   | H9A2 | 3.316    | H4   | H9C2 | 2.548    |
| H4   | H12A1| 3.552    | H4   | H12B1| 2.701    |
| H4   | H2A8 | 3.355    | H4   | H2A8 | 3.463    |
| H4   | H28A8| 3.297    | H4   | H28B8| 2.501    |
| H4   | H28C8| 3.282    | H4   | H39A | 3.167    |
| H5   | CI12 | 2.962    | H5   | C32  | 3.443    |
| H5   | H32  | 2.866    | H5   | H8B2 | 3.331    |
| H5   | H9C2 | 3.118    | H5   | H39A | 3.166    |
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom     | distance | atom  | atom     | distance |
|-------|----------|----------|-------|----------|----------|
| H8A   | C11\(^9\) | 3.171    | H8A   | H11B\(^9\) | 2.689    |
| H8A   | H11C\(^9\) | 2.771    | H8A   | H12A\(^9\) | 3.466    |
| H8A   | H12B\(^9\) | 3.499    | H8A   | H37B\(^{11}\) | 3.367    |
| H8A   | H37C\(^{11}\) | 3.137   | H8B   | C1\(^1\)    | 3.528    |
| H8B   | C12\(^1\) | 3.108    | H8B   | C4\(^1\)    | 3.526    |
| H8B   | C39\(^1\) | 3.367    | H8B   | H4\(^1\)    | 3.174    |
| H8B   | H5\(^1\)  | 3.331    | H8B   | H39A\(^1\)  | 3.117    |
| H8C   | H24B\(^8\) | 3.119   | H8C   | H34A\(^{11}\) | 2.972    |
| H8C   | H36B\(^{11}\) | 2.889  | H8C   | H36C\(^{11}\) | 3.493    |
| H8C   | H37C\(^{11}\) | 3.268  | H9A   | C12\(^9\)   | 3.336    |
| H9A   | C28\(^3\) | 3.595    | H9A   | H4\(^1\)    | 3.316    |
| H9A   | H11C\(^9\) | 3.486    | H9A   | H12A\(^9\)  | 2.542    |
| H9A   | H12B\(^9\) | 3.291    | H9A   | H28C\(^3\)  | 2.837    |
| H9B   | H28A\(^3\) | 3.433    | H9B   | H28C\(^3\)  | 3.058    |
| H9B   | H39A      | 3.566    | H9B   | H39B      | 2.987    |
| H9C   | C1\(^1\)  | 3.549    | H9C   | C4\(^1\)    | 3.323    |
| H9C   | C28\(^3\) | 3.193    | H9C   | C39        | 3.579    |
| H9C   | H4\(^1\)  | 2.548    | H9C   | H5\(^1\)   | 3.118    |
| H9C   | H28A\(^3\) | 2.957    | H9C   | H28B\(^3\) | 3.280    |
| H9C   | H28C\(^3\) | 2.823    | H9C   | H39A      | 3.439    |
| H9C   | H39B      | 3.216    | H10   | C16\(^7\)  | 3.116    |
| H10   | C17\(^7\) | 3.543    | H10   | H16\(^7\)  | 2.764    |
| H10   | H17\(^7\) | 3.513    | H11A  | C37\(^{10}\) | 3.320    |
| H11A  | H37A\(^{10}\) | 3.074  | H11A  | H37B\(^{10}\) | 3.006    |
| H11A  | H37C\(^{10}\) | 3.330  | H11B  | C1\(^2\)   | 3.056    |
| H11B  | C8\(^7\)  | 3.585    | H11B  | C1\(^2\)   | 3.056    |
| H11B  | H8A\(^7\) | 2.689    | H11B  | H37A\(^{10}\) | 3.546    |
| H11B  | H37B\(^{10}\) | 3.243  | H11B  | H37C\(^{10}\) | 3.033    |
| H11C  | C14\(^7\) | 3.402    | H11C  | C15\(^7\)  | 2.884    |
| H11C  | C16\(^7\) | 3.005    | H11C  | C37\(^{10}\) | 3.428    |
| H11C  | H8A\(^7\) | 2.771    | H11C  | H9A\(^7\)  | 3.486    |
| H11C  | H15\(^7\) | 3.018    | H11C  | H16\(^7\)  | 3.219    |
| H11C  | H37B\(^{10}\) | 2.789  | H11C  | H37C\(^{10}\) | 3.375    |
| H12A  | C9\(^7\)  | 3.459    | H12A  | C16\(^7\)  | 3.491    |
| H12A  | C17\(^7\) | 3.128    | H12A  | C18\(^7\)  | 3.493    |
| H12A  | H4\(^2\)  | 3.552    | H12A  | H8A\(^7\)  | 3.466    |
| H12A  | H9A\(^7\) | 2.542    | H12A  | H17\(^7\)  | 3.167    |
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H12A   | H20B^7 | 3.569    | H12A   | H28C^5 | 3.139    |
| H12B   | C3^2   | 3.317    | H12B   | C4^2   | 3.282    |
| H12B   | H3^2   | 2.777    | H12B   | H4^2   | 2.701    |
| H12B   | H8A^7  | 3.499    | H12B   | H9A^3  | 3.291    |
| H12B   | H28B^5 | 3.562    | H12C   | CI2^2  | 2.990    |
| H12C   | C39    | 3.586    | H12C   | H3^2   | 3.566    |
| H12C   | H27B^5 | 3.420    | H12C   | H27C^5 | 3.423    |
| H12C   | H28B^5 | 3.587    | H12C   | H28C^5 | 3.583    |
| H12C   | H39A   | 3.332    | H15    | C33^9  | 3.477    |
| H15    | C36^9  | 3.454    | H15    | H11C^9 | 3.018    |
| H15    | H25B^6 | 2.918    | H15    | H33A^9 | 2.747    |
| H15    | H33B^9 | 3.331    | H15    | H36A^9 | 2.552    |
| H15    | H36B^9 | 3.588    | H15    | H37B^11| 3.266    |
| H16    | N2^9   | 3.523    | H16    | CI0^9  | 3.576    |
| H16    | C33^9  | 3.489    | H16    | H10^9  | 2.764    |
| H16    | H11C^9 | 3.219    | H16    | H25A^9 | 2.861    |
| H16    | H27A^9 | 3.484    | H16    | H33A^9 | 3.363    |
| H16    | H33B^9 | 2.746    | H16    | H33C^6 | 3.151    |
| H17    | C27^9  | 3.017    | H17    | H10^9  | 3.513    |
| H17    | H12A^9 | 3.167    | H17    | H24C^9 | 2.746    |
| H17    | H27A^9 | 2.435    | H17    | H27C^9 | 2.731    |
| H17    | H33C^6 | 3.366    | H17    | H34B^6 | 3.185    |
| H19A   | H36C^11| 3.213    | H19B   | C23^6  | 3.593    |
| H19B   | C25^6  | 3.033    | H19B   | H23B^6 | 3.421    |
| H19B   | H23C^6 | 3.065    | H19B   | H25B^6 | 2.389    |
| H19B   | H25C^6 | 2.831    | H19B   | H36C^11| 3.588    |
| H19B   | H38C^11| 3.271    | H19C   | C35^11 | 3.537    |
| H19C   | C36^11 | 3.180    | H19C   | C37^11 | 3.375    |
| H19C   | C38^11 | 3.423    | H19C   | H36C^11| 2.282    |
| H19C   | H37B^11| 2.548    | H19C   | H38C^11| 2.606    |
| H20A   | H29C^3 | 3.521    | H20A   | H34B^6 | 3.558    |
| H20B   | C28^3  | 3.451    | H20B   | C29^3  | 3.308    |
| H20B   | H12A^9 | 3.569    | H20B   | H27B^3 | 3.277    |
| H20B   | H28C^3 | 2.566    | H20B   | H29C^3 | 2.409    |
| H20B   | H39B^3 | 3.573    | H20C   | CI1^3  | 3.516    |
| H20C   | CI2^3  | 3.089    | H20C   | C34^8  | 3.150    |
| H20C   | C39^3  | 3.430    | H20C   | H29C^3 | 3.264    |
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H20C  | H32C  | 3.404    | H20C  | H34B  | 2.305    |
| H20C  | H34C  | 3.199    | H20C  | H39B  | 3.258    |
| H23A  | Cl1   | 2.989    | H23A  | C4    | 3.437    |
| H23A  | H4    | 3.355    | H23B  | Cl1   | 3.428    |
| H23B  | H19B  | 3.421    | H23B  | H32B  | 2.836    |
| H23B  | H34C  | 2.796    | H23C  | H19B  | 3.065    |
| H23C  | H38C  | 3.462    | H24A  | Cl2   | 3.114    |
| H24A  | C3    | 3.427    | H24A  | C4    | 3.595    |
| H24A  | H3    | 3.126    | H24A  | H4    | 3.463    |
| H24B  | H8C   | 3.119    | H24B  | H33A  | 3.296    |
| H24B  | H34A  | 3.104    | H24B  | H36B  | 3.166    |
| H24C  | Cl2   | 3.260    | H24C  | C17   | 3.402    |
| H24C  | C34   | 3.512    | H24C  | H17   | 2.746    |
| H24C  | H33A  | 3.303    | H24C  | H33C  | 3.216    |
| H24C  | H34A  | 3.099    | H24C  | H34B  | 3.060    |
| H25A  | C16   | 3.475    | H25A  | C33   | 3.360    |
| H25A  | H16   | 2.861    | H25A  | H33A  | 2.968    |
| H25A  | H33C  | 2.903    | H25B  | C14   | 3.546    |
| H25B  | C15   | 3.361    | H25B  | C19   | 3.244    |
| H25B  | H15   | 2.918    | H25B  | H19B  | 2.389    |
| H25B  | H33A  | 2.891    | H25C  | H19B  | 2.831    |
| H25C  | H32B  | 2.947    | H25C  | C17   | 3.241    |
| H25C  | H32B  | 2.947    | H27A  | H17   | 2.435    |
| H27A  | H16   | 3.484    | H27A  | H17   | 2.435    |
| H27A  | H27B  | 3.133    | H27B  | C27   | 3.056    |
| H27B  | H12C  | 3.420    | H27B  | H20B  | 3.277    |
| H27B  | H27A  | 3.133    | H27B  | H27B  | 2.462    |
| H27B  | H27C  | 3.102    | H27B  | Cl2   | 3.024    |
| H27C  | H12C  | 3.423    | H27C  | H17   | 2.731    |
| H27C  | H27B  | 3.102    | H27C  | H17   | 2.731    |
| H27C  | H27B  | 3.102    | H28A  | Cl1   | 3.094    |
| H28A  | C9    | 3.544    | H28A  | H4    | 3.297    |
| H28A  | H9B   | 3.433    | H28A  | H9C   | 2.957    |
| H28A  | H39B  | 3.259    | H28B  | C4    | 3.101    |
| H28B  | H3    | 3.530    | H28B  | H4    | 2.501    |
| H28B  | H9C   | 3.280    | H28B  | H12B  | 3.562    |
| H28B  | H12C  | 3.587    | H28C  | C9    | 3.079    |
| H28C  | C20   | 3.499    | H28C  | H4    | 3.282    |
| H28C  | H9A   | 2.837    | H28C  | H9B   | 3.058    |
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H28C | H9C^3 | 2.823 | H28C | H12C^5 | 3.583 |
| H28C | H12C^5 | 3.583 | H28C | H20B^3 | 2.566 |
| H29A | C39 | 3.413 | H29A | H39A | 3.557 |
| H29A | H39B | 2.583 | H29B | H29B^3 | 3.394 |
| H29B | H29C^3 | 3.466 | H29B | H39B | 3.194 |
| H29C | Cl2 | 3.511 | H29C | C20^3 | 3.196 |
| H29C | C39 | 3.241 | H29C | H20A^3 | 3.521 |
| H29C | H20B^3 | 2.409 | H29C | H20C^3 | 3.264 |
| H29C | H29B^3 | 3.466 | H29C | H39B | 2.388 |
| H32A | C32^6 | 3.332 | H32A | H32A^6 | 3.089 |
| H32A | H32B^6 | 3.013 | H32A | H32C^6 | 3.343 |
| H32B | H23B^6 | 2.836 | H32B | H25C^6 | 2.947 |
| H32B | H32A^6 | 3.013 | H32B | H32C | N1^6 | 3.064 |
| H32C | C13^6 | 2.725 | H32C | C14^6 | 3.094 |
| H32C | C17^6 | 3.532 | H32C | C18^6 | 2.993 |
| H32C | C20^6 | 3.577 | H32C | H20C^6 | 3.404 |
| H32C | H32A^6 | 3.343 | H32C | C15^7 | 3.427 |
| H33A | C25^12 | 3.371 | H33A | C15^7 | 2.747 |
| H33A | H16^7 | 3.363 | H33A | H24B^12 | 3.296 |
| H33A | H24C^12 | 3.303 | H33A | H25A^12 | 2.968 |
| H33A | H25B^12 | 2.891 | H33B | C16^7 | 3.385 |
| H33B | H15^7 | 3.331 | H33B | H16^7 | 2.746 |
| H33B | H33C^12 | 3.423 | H33B | C17^6 | 3.078 |
| H33C | C16^6 | 2.938 | H33C | C17^6 | 3.078 |
| H33C | C18^6 | 3.581 | H33C | H16^6 | 3.151 |
| H33C | H17^6 | 3.366 | H33C | H24C^12 | 3.216 |
| H33C | H25A^12 | 2.903 | H33C | H33B^12 | 3.423 |
| H34A | C24^12 | 3.540 | H34A | H8C^10 | 2.972 |
| H34A | H24B^12 | 3.104 | H34A | H24C^12 | 3.099 |
| H34B | C12^14 | 3.413 | H34B | C17^6 | 3.194 |
| H34B | C18^6 | 3.083 | H34B | C20^6 | 3.054 |
| H34B | H17^6 | 3.185 | H34B | H20A^6 | 3.558 |
| H34B | H20C^6 | 2.305 | H34B | H24C^12 | 3.060 |
| H34C | Cl1^14 | 3.238 | H34C | H20C^6 | 3.199 |
| H34C | H23B^6 | 2.796 | H36A | C15^7 | 3.421 |
| H36A | H15^7 | 2.552 | H36A | H37A^10 | 3.253 |
| H36A | H37B^10 | 3.252 | H36A | H38A^10 | 3.584 |
Table S5-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H36B   | H8C\textsuperscript{10} | 2.889    | H36B   | H15\textsuperscript{7} | 3.588    |
| H36B   | H24B\textsuperscript{12} | 3.166    | H36B   | H38A\textsuperscript{10} | 3.546    |
| H36C   | C19\textsuperscript{10} | 3.129    | H36C   | C38\textsuperscript{10} | 3.583    |
| H36C   | H8C\textsuperscript{10} | 3.493    | H36C   | H19A\textsuperscript{10} | 3.213    |
| H36C   | H19B\textsuperscript{10} | 3.588    | H36C   | H19C\textsuperscript{10} | 2.282    |
| H36C   | H37A\textsuperscript{10} | 2.881    | H36C   | H37B\textsuperscript{10} | 3.564    |
| H36C   | H38A\textsuperscript{10} | 2.821    | H36C   | H38C\textsuperscript{10} | 3.565    |
| H37A   | C36\textsuperscript{11} | 3.518    | H37A   | H11A\textsuperscript{11} | 3.074    |
| H37A   | H11B\textsuperscript{11} | 3.546    | H37A   | H36A\textsuperscript{11} | 3.253    |
| H37A   | H36C\textsuperscript{11} | 2.881    | H37B   | C11\textsuperscript{11} | 3.187    |
| H37B   | C19\textsuperscript{10} | 3.444    | H37B   | H8A\textsuperscript{10} | 3.367    |
| H37B   | H11A\textsuperscript{11} | 3.006    | H37B   | H11B\textsuperscript{11} | 3.243    |
| H37B   | H11C\textsuperscript{11} | 2.789    | H37B   | H15\textsuperscript{10} | 3.266    |
| H37B   | H19C\textsuperscript{10} | 2.548    | H37B   | H36A\textsuperscript{11} | 3.252    |
| H37B   | H36C\textsuperscript{11} | 3.564    | H37C   | C11\textsuperscript{11} | 3.433    |
| H37C   | H8A\textsuperscript{10} | 3.137    | H37C   | H8C\textsuperscript{10} | 3.268    |
| H37C   | H11A\textsuperscript{11} | 3.330    | H37C   | H11B\textsuperscript{11} | 3.033    |
| H37C   | H11C\textsuperscript{11} | 3.375    | H38A   | C36\textsuperscript{11} | 3.486    |
| H38A   | H36A\textsuperscript{11} | 3.584    | H38A   | H36B\textsuperscript{11} | 3.546    |
| H38A   | H36C\textsuperscript{11} | 2.821    | H38C   | C19\textsuperscript{10} | 3.367    |
| H38C   | H19B\textsuperscript{10} | 3.271    | H38C   | H19C\textsuperscript{10} | 2.606    |
| H38C   | H23C\textsuperscript{8} | 3.462    | H38C   | H36C\textsuperscript{11} | 3.565    |
| H39A   | C1     | 2.887    | H39A   | C2     | 2.951    |
| H39A   | C3     | 2.827    | H39A   | C4     | 2.659    |
| H39A   | C5     | 2.643    | H39A   | C6     | 2.775    |
| H39A   | H3     | 3.426    | H39A   | H4     | 3.167    |
| H39A   | H5     | 3.166    | H39A   | H8B\textsuperscript{2} | 3.117    |
| H39A   | H9B    | 3.566    | H39A   | H9C    | 3.439    |
| H39A   | H12C   | 3.332    | H39A   | H29A   | 3.557    |
| H39B   | C1     | 3.480    | H39B   | C9     | 3.527    |
| H39B   | C29    | 2.857    | H39B   | H9B    | 2.987    |
| H39B   | H9C    | 3.216    | H39B   | H20B\textsuperscript{3} | 3.573    |
| H39B   | H20C\textsuperscript{3} | 3.258    | H39B   | H28A\textsuperscript{3} | 3.259    |
| H39B   | H29A   | 2.583    | H39B   | H29B   | 3.194    |
| H39B   | H29C   | 2.388    |        |        |          |

Symmetry Operators:

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

for

\[ \text{Nb}({\text{N-2,6-Me}_{2}C_{6}H_{3}})(\text{N=C'Bu}_2)(2,6-{\text{Bu}_{2}C_{6}H_{3}}\text{OH}) \] (4b)

June 6, 2017
Experimental

Data Collection

A yellow block crystal of C₈₀H₁₃₂N₆Nb₂O₂ having approximate dimensions of 0.231 x 0.146 x 0.064 mm was mounted in a loop. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 45.00 mm.

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

\[
a = 12.5502(4) \text{ Å} \quad \alpha = 89.366(3)^{\circ} \\
b = 14.0719(5) \text{ Å} \quad \beta = 88.443(3)^{\circ} \\
c = 23.5634(9) \text{ Å} \quad \gamma = 75.219(3)^{\circ} \\
V = 4022.2(3) \text{ Å}^3
\]

For \( Z = 2 \) and F.W. = 1395.77, the calculated density is 1.152 g/cm³. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -180 ± 1°C to a maximum 2θ value of 61.4°. A total of 1440 oscillation images were collected. A sweep of data was done using ω scans from -105.0 to 75.0° in 0.50° step, at \( \chi = 45.0^\circ \) and \( \phi = 0.0^\circ \). The exposure rate was 10.0 [sec./°]. The detector swing angle was -15.00°. A second sweep was performed using ω scans from -105.0 to 75.0° in 0.50° step, at \( \chi = 45.0^\circ \) and \( \phi \)
= 90.0°. The exposure rate was 10.0 [sec./°]. The detector swing angle was -15.00°. Another sweep was performed using ω scans from -105.0 to 75.0° in 0.50° step, at χ=45.0° and ϕ = 90.0°. The exposure rate was 10.0 [sec./°]. The detector swing angle was -15.00°. Another sweep was performed using ω scans from -105.0 to 75.0° in 0.50° step, at χ=45.0° and ϕ = 90.0°. The exposure rate was 10.0 [sec./°]. The detector swing angle was -15.00°. The crystal-to-detector distance was 45.00 mm. Readout was performed in the 0.172 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R\text{int} = 0.0777); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). 1

The linear absorption coefficient, μ, for Mo-Kα radiation is 3.304 cm⁻¹. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.510 to 0.979. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods 2 and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement 3 on \( F^2 \) was based on 17259 observed reflections and 811 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

\[
R1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} = 0.1366
\]

\[
wR2 = \left[ \frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum w(F_o^2)^2} \right]^{1/2} = 0.3184
\]
The goodness of fit\(^4\) was 1.25. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 4.07 and -2.36 e\(^-\)/Å\(^3\), respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4\(^5\). Anomalous dispersion effects were included in Fcalc\(^6\); the values for f' and Δf\(^\prime\) 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 Version 2014/7\(^{10}\).

References

(1) CrystAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

\[ \Sigma w(F_0^2-F_c^2)^2 \] where w = Least Squares weights.

(4) Goodness of fit is defined as:

\[ \left[ \Sigma w(F_0^2-F_c^2)^2/(N_o-N_v) \right]^{1/2} \]

where \( N_o \) = number of observations

\( N_v \) = number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.
(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula \( \text{C}_80\text{H}_{132}\text{N}_6\text{Nb}_2\text{O}_2 \)

Formula Weight 1395.77

Crystal Color, Habit yellow, block

Crystal Dimensions 0.231 X 0.146 X 0.064 mm

Crystal System triclinic

Lattice Type Primitive

Lattice Parameters
\[ a = 12.5502(4) \text{ Å} \]
\[ b = 14.0719(5) \text{ Å} \]
\[ c = 23.5634(9) \text{ Å} \]
\[ \alpha = 89.366(3) ^\circ \]
\[ \beta = 88.443(3) ^\circ \]
\[ \gamma = 75.219(3) ^\circ \]
\[ V = 4022.2(3) \text{ Å}^3 \]

Space Group P-1 (#2)

Z value 2

D\text{calc} 1.152 g/cm\text{3}

F\text{000} 1504.00

\( \mu(\text{MoK}\alpha) \) 3.304 cm\text{-1}
B. Intensity Measurements

Diffractometer  
XtaLAB P200

Radiation  
MoKα (λ = 0.71073 Å)  
multi-layer mirror monochromated

Voltage, Current  
50kV, 24mA

Temperature  
-180.0°C

Detector Aperture  
83.8 x 70.0 mm

Data Images  
1440 exposures

ω oscillation Range (χ=45.0, φ=0.0)  
-105.0 - 75.0°

Exposure Rate  
10.0 sec./°

Detector Swing Angle  
-15.00°

ω oscillation Range (χ=45.0, φ=90.0)  
-105.0 - 75.0°

Exposure Rate  
10.0 sec./°

Detector Swing Angle  
-15.00°

ω oscillation Range (χ=45.0, φ=90.0)  
-105.0 - 75.0°

Exposure Rate  
10.0 sec./°

Detector Swing Angle  
-15.00°
| Parameter                              | Value                  |
|----------------------------------------|------------------------|
| $\omega$ oscillation Range ($\chi=45.0$, $\phi=90.0$) | $-105.0 - 75.0^\circ$ |
| Exposure Rate                          | 10.0 sec./$^\circ$     |
| Detector Swing Angle                   | $-15.00^\circ$         |
| Detector Position                      | 45.00 mm               |
| Pixel Size                             | 0.172 mm               |
| $2\theta_{\text{max}}$                | 55.0$^\circ$           |
| No. of Reflections Measured            | Total: 67935           |
|                                        | Unique: 17259 ($R_{\text{int}} = 0.0777$) |
| Corrections                            | Lorentz-polarization   |
|                                        | Absorption             |
|                                        | (trans. factors: 0.510 - 0.979) |
C. Structure Solution and Refinement

| Structure Solution | Direct Methods (SHELXT) |
|--------------------|-------------------------|
| Refinement         | Full-matrix least-squares on $F^2$ |
| Function Minimized | $\sum w (Fo^2 - Fc^2)^2$ |
| Least Squares Weights | $w = 1/ \left[ \sigma^2(Fo^2) + (0.0000 \cdot P)^2 + 93.3720 \cdot P \right]$ where $P = (\text{Max}(Fo^2,0) + 2Fc^2)/3$ |
| $2\theta_{\text{max}}$ cutoff | 55.0° |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. Observations (All reflections) | 17259 |
| No. Variables | 811 |
| Reflection/Parameter Ratio | 21.28 |
| Residuals: R1 ($I > 2.00\sigma(I)$) | 0.1366 |
| Residuals: R (All reflections) | 0.1584 |
| Residuals: wR2 (All reflections) | 0.3184 |
| Goodness of Fit Indicator | 1.251 |
| Max Shift/Error in Final Cycle | 0.001 |
| Maximum peak in Final Diff. Map | $4.07 \text{ e}^-/\text{Å}^3$ |
| Minimum peak in Final Diff. Map | $-2.36 \text{ e}^-/\text{Å}^3$ |
Table S6-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$

| atom | x         | y         | z          | $B_{\text{eq}}$ |
|------|-----------|-----------|------------|----------------|
| Nb1  | 0.26438(7)| 0.73789(6)| 0.61332(4) | 1.454(17)      |
| Nb2  | 0.27171(7)| 1.23869(6)| 0.88233(4) | 1.357(17)      |
| O1   | 0.2794(5) | 0.6684(5) | 0.5405(3)  | 1.58(11)       |
| O2   | 0.2728(5) | 1.1677(4) | 0.9543(3)  | 1.26(10)       |
| N1   | 0.2891(7) | 0.8572(6) | 0.6061(4)  | 1.65(13)       |
| N2   | 0.3831(7) | 0.6688(6) | 0.6615(4)  | 1.69(13)       |
| N3   | 0.1117(7) | 0.7671(6) | 0.6409(4)  | 1.68(14)       |
| N4   | 0.2997(7) | 1.3568(6) | 0.8878(4)  | 1.74(14)       |
| N5   | 0.3922(6) | 1.1616(6) | 0.8345(4)  | 1.73(14)       |
| N6   | 0.1207(6) | 1.2723(5) | 0.8560(4)  | 1.50(13)       |
| C1   | 0.2298(7) | 0.6355(6) | 0.4971(4)  | 1.42(15)       |
| C2   | 0.1964(8) | 0.5463(7) | 0.5042(4)  | 1.64(15)       |
| C3   | 0.1339(8) | 0.5198(8) | 0.4615(4)  | 2.04(17)       |
| C4   | 0.1089(9) | 0.5753(8) | 0.4130(5)  | 2.18(18)       |
| C5   | 0.1489(8) | 0.6590(8) | 0.4054(4)  | 2.04(17)       |
| C6   | 0.2110(8) | 0.6903(7) | 0.4460(4)  | 1.63(15)       |
| C7   | 0.2348(8) | 0.4763(7) | 0.5553(4)  | 1.81(16)       |
| C8   | 0.3593(8) | 0.4426(8) | 0.5540(5)  | 2.7(2)         |
| C9   | 0.1924(9) | 0.3835(7) | 0.5510(5)  | 2.5(2)         |
| C10  | 0.1950(12)| 0.5226(8) | 0.6123(5)  | 3.1(2)         |
| C11  | 0.2585(8) | 0.7794(7) | 0.4344(4)  | 1.76(16)       |
| C12  | 0.3806(8) | 0.7550(8) | 0.4447(5)  | 2.25(18)       |
| C13  | 0.1962(9) | 0.8678(7) | 0.4720(5)  | 2.22(18)       |
| C14  | 0.2400(9) | 0.8142(8) | 0.3715(4)  | 2.16(18)       |
| C15  | 0.3079(8) | 0.9465(7) | 0.5907(4)  | 1.46(15)       |
| C16  | 0.2190(8) | 1.0313(7) | 0.5892(4)  | 1.66(16)       |
| C17  | 0.2420(9) | 1.1194(7) | 0.5718(5)  | 2.17(18)       |
| C18  | 0.3470(9) | 1.1259(7) | 0.5585(5)  | 2.17(18)       |
| C19  | 0.4343(9) | 1.0426(8) | 0.5608(5)  | 2.20(18)       |
| C20  | 0.4147(8) | 0.9525(7) | 0.5786(4)  | 1.90(17)       |
| C21  | 0.1055(9) | 1.0242(7) | 0.6037(5)  | 2.5(2)         |
| C22  | 0.5096(8) | 0.8616(7) | 0.5817(5)  | 2.12(18)       |
| C23  | 0.4572(8) | 0.6313(8) | 0.6974(4)  | 1.94(17)       |
| C24  | 0.4258(10)| 0.6567(13)| 0.7616(5)  | 3.9(3)         |
| C25  | 0.3341(12)| 0.6070(13)| 0.7754(5)  | 4.5(3)         |
| C26  | 0.5142(13)| 0.6267(17)| 0.8050(7)  | 6.6(5)         |
| C27  | 0.3838(13)| 0.7690(14)| 0.7663(7)  | 5.8(4)         |
Table S6-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

| atom | x         | y         | z         | $B_{\text{eq}}$ |
|------|-----------|-----------|-----------|-----------------|
| C28  | 0.5685(8) | 0.5671(7) | 0.6762(5) | 2.23(18)        |
| C29  | 0.5744(12)| 0.4577(9) | 0.6919(7) | 4.4(3)          |
| C30  | 0.6682(9) | 0.5965(9) | 0.6991(5) | 2.8(2)          |
| C31  | 0.5777(9) | 0.5726(9) | 0.6107(5) | 2.9(2)          |
| C32  | 0.0087(7) | 0.7852(7) | 0.6568(4) | 1.59(15)        |
| C33  | -0.0169(10)| 0.7961(9)| 0.7213(5) | 2.8(2)          |
| C34  | 0.0683(12)| 0.8364(12)| 0.7489(6)| 4.5(3)          |
| C35  | -0.1295(11)| 0.8608(12)| 0.7386(5)| 4.5(3)          |
| C36  | -0.0047(13)| 0.6915(12)| 0.7456(7)| 5.0(4)          |
| C37  | -0.0786(8)| 0.7934(7) | 0.6116(5) | 2.08(17)        |
| C38  | -0.1515(9)| 0.7216(8) | 0.6258(6) | 3.1(2)          |
| C39  | -0.1558(10)| 0.8994(8) | 0.6085(5)| 2.9(2)          |
| C40  | -0.0279(9)| 0.7687(9) | 0.5532(5) | 2.6(2)          |
| C41  | 0.2220(7) | 1.1367(6) | 0.9995(4) | 1.35(14)        |
| C42  | 0.2031(8) | 1.1928(7) | 1.0505(4) | 1.60(15)        |
| C43  | 0.1394(8) | 1.1631(7) | 1.0923(4) | 1.88(17)        |
| C44  | 0.1011(8) | 1.0790(8) | 1.0874(4) | 1.96(17)        |
| C45  | 0.1287(8) | 1.0210(7) | 1.0395(4) | 1.78(16)        |
| C46  | 0.1898(7) | 1.0458(6) | 0.9952(4) | 1.53(15)        |
| C47  | 0.2495(8) | 1.2820(7) | 1.0589(4) | 1.58(15)        |
| C48  | 0.3711(8) | 1.2583(8) | 1.0456(5) | 2.11(17)        |
| C49  | 0.2343(9) | 1.3191(7) | 1.1212(4) | 2.05(17)        |
| C50  | 0.1853(8) | 1.3690(7) | 1.0223(4) | 1.94(17)        |
| C51  | 0.2263(8) | 0.9747(7) | 0.9443(4) | 1.54(15)        |
| C52  | 0.1919(9) | 0.8794(7) | 0.9536(5) | 2.16(18)        |
| C53  | 0.1749(9) | 1.0174(7) | 0.8887(4) | 2.18(18)        |
| C54  | 0.3523(9) | 0.9475(8) | 0.9376(6) | 3.0(2)          |
| C55  | 0.3163(8) | 1.4459(6) | 0.9063(4) | 1.60(16)        |
| C56  | 0.2237(8) | 1.5282(7) | 0.9106(4) | 1.73(16)        |
| C57  | 0.2411(8) | 1.6157(7) | 0.9323(4) | 1.82(16)        |
| C58  | 0.3456(9) | 1.6235(7) | 0.9457(5) | 2.28(19)        |
| C59  | 0.4370(9) | 1.5418(8) | 0.9395(5) | 2.51(19)        |
| C60  | 0.4230(9) | 1.4536(7) | 0.9192(5) | 2.03(17)        |
| C61  | 0.1120(8) | 1.5227(8) | 0.8943(5) | 2.41(19)        |
| C62  | 0.5203(9) | 1.3647(8) | 0.9117(6) | 2.8(2)          |
| C63  | 0.4691(8) | 1.1112(7) | 0.8036(4) | 1.77(16)        |
| C64  | 0.5815(8) | 1.0611(7) | 0.8304(5) | 2.03(17)        |
Table S6-1. Atomic coordinates and $B_{iso}/B_{eq}$ (continued)

| atom | x     | y     | z     | $B_{eq}$ |
|------|-------|-------|-------|----------|
| C65  | 0.5777(8) | 1.0836(8) | 0.8942(5) | 2.34(19) |
| C66  | 0.6065(9)  | 0.9471(8)  | 0.8260(6)  | 2.7(2)   |
| C67  | 0.6761(9)  | 1.0972(8)  | 0.8047(5)  | 2.44(19) |
| C68  | 0.4488(9)  | 1.1070(10) | 0.7389(5)  | 2.7(2)   |
| C69  | 0.5314(10) | 1.0255(12) | 0.7043(6)  | 4.2(3)   |
| C70  | 0.3364(9)  | 1.0897(10) | 0.7315(5)  | 3.2(2)   |
| C71  | 0.4532(13) | 1.2068(12) | 0.7146(6)  | 4.7(3)   |
| C72  | 0.0231(7)  | 1.2917(7)  | 0.8375(4)  | 1.66(16) |
| C73  | -0.0748(8) | 1.2976(7)  | 0.8809(5)  | 2.02(18) |
| C74  | -0.0302(8) | 1.2668(8)  | 0.9388(5)  | 2.23(18) |
| C75  | -0.1431(10) | 1.2293(8)  | 0.8630(6)  | 3.3(3)   |
| C76  | -0.1475(9) | 1.4047(8)  | 0.8863(5)  | 2.6(2)   |
| C77  | 0.0090(8)  | 1.3103(8)  | 0.7717(5)  | 2.4(2)   |
| C78  | -0.0999(10) | 1.3824(10) | 0.7554(5)  | 3.3(2)   |
| C79  | 0.0159(10) | 1.2089(9)  | 0.7445(5)  | 3.3(2)   |
| C80  | 0.1028(11) | 1.3505(10) | 0.7472(5)  | 3.3(2)   |

$B_{eq} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$
Table S6-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogen atoms

| atom | x     | y     | z     | $B_{\text{iso}}$ |
|------|-------|-------|-------|-----------------|
| H3   | 0.10824 | 0.46217 | 0.46622 | 2.446 |
| H4   | 0.06497 | 0.55709 | 0.38491 | 2.621 |
| H5   | 0.13296 | 0.69579 | 0.37128 | 2.449 |
| H8A  | 0.38517 | 0.41264 | 0.51718 | 3.236 |
| H8B  | 0.38985 | 0.49920 | 0.55977 | 3.236 |
| H8C  | 0.38345 | 0.39424 | 0.58430 | 3.236 |
| H9A  | 0.11160 | 0.40202 | 0.55171 | 2.972 |
| H9B  | 0.21985 | 0.34938 | 0.51547 | 2.972 |
| H9C  | 0.21865 | 0.33987 | 0.58321 | 2.972 |
| H10A | 0.11428 | 0.54449 | 0.61318 | 3.750 |
| H10B | 0.21922 | 0.47420 | 0.64253 | 3.750 |
| H10C | 0.22562 | 0.57915 | 0.61800 | 3.750 |
| H12A | 0.40817 | 0.81315 | 0.43696 | 2.696 |
| H12B | 0.39396 | 0.73463 | 0.48434 | 2.696 |
| H12C | 0.41883 | 0.70144 | 0.41956 | 2.696 |
| H13A | 0.11709 | 0.88269 | 0.46477 | 2.665 |
| H13B | 0.20861 | 0.85071 | 0.51211 | 2.665 |
| H13C | 0.22373 | 0.92540 | 0.46266 | 2.665 |
| H14A | 0.16103 | 0.83052 | 0.36378 | 2.592 |
| H14B | 0.26805 | 0.87249 | 0.36511 | 2.592 |
| H14C | 0.27929 | 0.76150 | 0.34602 | 2.592 |
| H17  | 0.18288 | 1.17678 | 0.56914 | 2.602 |
| H18  | 0.35996 | 1.18734 | 0.54784 | 2.599 |
| H19  | 0.50683 | 1.04624 | 0.55033 | 2.640 |
| H21A | 0.10731 | 0.95646 | 0.61471 | 3.040 |
| H21B | 0.07527 | 1.06842 | 0.63525 | 3.040 |
| H21C | 0.05901 | 1.04293 | 0.57054 | 3.040 |
| H22A | 0.57873 | 0.87887 | 0.57194 | 2.545 |
| H22B | 0.51317 | 0.83441 | 0.62027 | 2.545 |
| H22C | 0.49843 | 0.81248 | 0.55485 | 2.545 |
| H25A | 0.27641 | 0.62631 | 0.74719 | 5.432 |
| H25B | 0.36390 | 0.53547 | 0.77460 | 5.432 |
| H25C | 0.30271 | 0.62700 | 0.81324 | 5.432 |
| H26A | 0.57360 | 0.65866 | 0.79623 | 7.933 |
| H26B | 0.48273 | 0.64673 | 0.84285 | 7.933 |
| H26C | 0.54392 | 0.55519 | 0.80422 | 7.933 |
| H27A | 0.32569 | 0.79300 | 0.73887 | 6.930 |
Table S6-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogens/\(B_{eq}\) (continued)

| atom | x    | y    | z    | \(B_{eq}\) |
|------|------|------|------|------------|
| H27B | 0.35414 | 0.78629 | 0.80482 | 6.930      |
| H27C | 0.44484 | 0.79929 | 0.75838 | 6.930      |
| H29A | 0.51012 | 0.43955 | 0.67704 | 5.285      |
| H29B | 0.64190 | 0.41496 | 0.67527 | 5.285      |
| H29C | 0.57482 | 0.44995 | 0.73329 | 5.285      |
| H30A | 0.73602 | 0.55229 | 0.68372 | 3.394      |
| H30B | 0.66535 | 0.66420 | 0.68758 | 3.394      |
| H30C | 0.66712 | 0.59179 | 0.74060 | 3.394      |
| H31A | 0.51513 | 0.55421 | 0.58372 | 3.420      |
| H31B | 0.57734 | 0.63977 | 0.59913 | 3.420      |
| H31C | 0.64663 | 0.52727 | 0.59745 | 3.420      |
| H34A | 0.14193 | 0.79608 | 0.73850 | 5.454      |
| H34B | 0.06106 | 0.90419 | 0.73607 | 5.454      |
| H34C | 0.05749 | 0.83535 | 0.79024 | 5.454      |
| H35A | -0.18706 | 0.83612 | 0.72112 | 5.368      |
| H35B | -0.13873 | 0.85955 | 0.78002 | 5.368      |
| H35C | -0.13516 | 0.92838 | 0.72585 | 5.368      |
| H36A | -0.05917 | 0.66222 | 0.72862 | 6.043      |
| H36B | 0.06964 | 0.65093 | 0.73679 | 6.043      |
| H36C | -0.01686 | 0.69511 | 0.78689 | 6.043      |
| H38A | -0.18552 | 0.73626 | 0.66371 | 3.705      |
| H38B | -0.20923 | 0.72933 | 0.59769 | 3.705      |
| H38C | -0.10564 | 0.65380 | 0.62506 | 3.705      |
| H39A | -0.19034 | 0.91804 | 0.64593 | 3.460      |
| H39B | -0.11239 | 0.94559 | 0.59696 | 3.460      |
| H39C | -0.21301 | 0.90134 | 0.58075 | 3.460      |
| H40A | -0.08635 | 0.77476 | 0.52564 | 3.099      |
| H40B | 0.01725 | 0.81401 | 0.54290 | 3.099      |
| H40C | 0.01853 | 0.70110 | 0.55310 | 3.099      |
| H43  | 0.12081 | 1.20150 | 1.12573 | 2.253      |
| H44  | 0.05634 | 1.06153 | 1.11684 | 2.347      |
| H45  | 0.10464 | 0.96241 | 1.03724 | 2.131      |
| H48A | 0.39813 | 1.31684 | 1.05135 | 2.532      |
| H48B | 0.40968 | 1.20539 | 1.07072 | 2.532      |
| H48C | 0.38501 | 1.23704 | 1.00599 | 2.532      |
| H49A | 0.15578 | 1.33573 | 1.13201 | 2.465      |
| H49B | 0.27493 | 1.26748 | 1.14641 | 2.465      |
Table S6-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogens/$B_{\text{eq}}$ (continued)

| atom | x       | y       | z       | $B_{\text{eq}}$ |
|------|---------|---------|---------|-----------------|
| H49C | 0.26247 | 1.37766 | 1.12435 | 2.465           |
| H50A | 0.10638 | 1.38252 | 1.03199 | 2.326           |
| H50B | 0.21144 | 1.42743 | 1.02978 | 2.326           |
| H50C | 0.19727 | 1.35194 | 0.98201 | 2.326           |
| H52A | 0.22277 | 0.84829 | 0.98900 | 2.596           |
| H52B | 0.11133 | 0.89361 | 0.95599 | 2.596           |
| H52C | 0.21957 | 0.83489 | 0.92177 | 2.596           |
| H53A | 0.19427 | 1.07941 | 0.88042 | 2.615           |
| H53B | 0.20277 | 0.97080 | 0.85788 | 2.615           |
| H53C | 0.09452 | 1.02953 | 0.89210 | 2.615           |
| H54A | 0.37743 | 1.00735 | 0.93151 | 3.547           |
| H54B | 0.38497 | 0.91395 | 0.97202 | 3.547           |
| H54C | 0.37489 | 0.90383 | 0.90492 | 3.547           |
| H57  | 0.17981 | 1.67074 | 0.93803 | 2.178           |
| H58  | 0.35537 | 1.68408 | 0.95900 | 2.732           |
| H59  | 0.50826 | 1.54704 | 0.94925 | 3.015           |
| H61A | 0.11553 | 1.45676 | 0.88014 | 2.890           |
| H61B | 0.06191 | 1.53646 | 0.92756 | 2.890           |
| H61C | 0.08477 | 1.57134 | 0.86453 | 2.890           |
| H62A | 0.49470 | 1.30969 | 0.89707 | 3.386           |
| H62B | 0.57410 | 1.38068 | 0.88474 | 3.386           |
| H62C | 0.55493 | 1.34641 | 0.94835 | 3.386           |
| H65A | 0.51739 | 1.06136 | 0.91275 | 2.804           |
| H65B | 0.64776 | 1.04911 | 0.91090 | 2.804           |
| H65C | 0.56545 | 1.15450 | 0.89966 | 2.804           |
| H66A | 0.54465 | 0.92487 | 0.84271 | 3.249           |
| H66B | 0.61683 | 0.92774 | 0.78598 | 3.249           |
| H66C | 0.67374 | 0.91702 | 0.84648 | 3.249           |
| H67A | 0.68184 | 1.08446 | 0.76379 | 2.929           |
| H67B | 0.66267 | 1.16802 | 0.81124 | 2.929           |
| H67C | 0.74498 | 1.06263 | 0.82248 | 2.929           |
| H69A | 0.60617 | 1.03367 | 0.70788 | 5.003           |
| H69B | 0.52853 | 0.96078 | 0.71904 | 5.003           |
| H69C | 0.51149 | 1.03079 | 0.66428 | 5.003           |
| H70A | 0.33507 | 1.02532 | 0.74732 | 3.859           |
| H70B | 0.28078 | 1.14111 | 0.75122 | 3.859           |
| H70C | 0.32032 | 1.09133 | 0.69093 | 3.859           |
Table S6-2. Atomic coordinates and $B_{iso}$ involving hydrogens/$B_{eq}$ (continued)

| atom | x      | y      | z      | $B_{eq}$ |
|------|--------|--------|--------|----------|
| H71A | 0.52675| 1.21682| 0.71979| 5.651    |
| H71B | 0.43760| 1.20896| 0.67397| 5.651    |
| H71C | 0.39806| 1.25874| 0.73426| 5.651    |
| H74A | -0.09162| 1.27073| 0.96598| 2.676    |
| H74B | 0.01568| 1.19913| 0.93723| 2.676    |
| H74C | -0.17259| 1.24871| 0.82535| 3.901    |
| H75A | -0.09690| 1.16176| 0.86170| 3.901    |
| H75B | -0.20421| 1.23335| 0.89046| 3.901    |
| H76A | -0.17819| 1.42757| 0.84935| 3.133    |
| H76B | -0.20768| 1.40658| 0.91401| 3.133    |
| H76C | -0.10238| 1.44752| 0.89908| 3.133    |
| H78A | -0.16190| 1.35864| 0.77049| 3.960    |
| H78B | -0.10351| 1.44729| 0.77123| 3.960    |
| H78C | -0.10370| 1.38741| 0.71391| 3.960    |
| H79B | 0.04404| 1.18256| 0.75998| 4.019    |
| H79A | 0.00905| 1.21670| 0.70327| 4.019    |
| H79C | 0.08691| 1.16349| 0.75306| 4.019    |
| H80A | 0.17372| 1.30596| 0.75695| 3.922    |
| H80B | 0.09736| 1.35574| 0.70584| 3.922    |
| H80C | 0.09755| 1.41562| 0.76316| 3.922    |
Table S6-3. Anisotropic displacement parameters

| atom | U_{11}  | U_{22}  | U_{33}  | U_{12}   | U_{13}   | U_{23}  |
|------|---------|---------|---------|----------|----------|---------|
| Nb1  | 0.0215(5) | 0.0132(4) | 0.0192(4) | -0.0017(3) | -0.0025(3) | 0.0005(3) |
| Nb2  | 0.0169(4) | 0.0138(4) | 0.0196(4) | -0.0014(3) | -0.0013(3) | -0.0019(3) |
| O1   | 0.023(3)  | 0.015(3)  | 0.023(3)  | -0.006(3)  | -0.006(3)  | 0.002(3)  |
| O2   | 0.017(3)  | 0.013(3)  | 0.018(3)  | -0.003(2)  | 0.002(2)   | 0.003(2)  |
| N1   | 0.021(4)  | 0.015(4)  | 0.027(4)  | -0.006(3)  | 0.003(3)   | -0.000(3) |
| N2   | 0.019(4)  | 0.019(4)  | 0.026(4)  | -0.005(3)  | 0.000(3)   | -0.006(3) |
| N3   | 0.022(4)  | 0.019(4)  | 0.026(4)  | -0.010(3)  | -0.018(3)  | 0.013(3)  |
| N4   | 0.024(4)  | 0.016(4)  | 0.028(4)  | -0.009(3)  | 0.001(3)   | -0.006(3) |
| N5   | 0.017(4)  | 0.022(4)  | 0.028(5)  | -0.007(3)  | -0.001(3)  | 0.007(3)  |
| N6   | 0.016(4)  | 0.013(4)  | 0.028(4)  | -0.004(3)  | 0.008(3)   | -0.003(3) |
| C1   | 0.007(4)  | 0.012(4)  | 0.031(5)  | 0.003(3)   | 0.001(4)   | -0.007(4) |
| C2   | 0.023(5)  | 0.012(4)  | 0.027(5)  | -0.003(4)  | 0.001(4)   | -0.002(4) |
| C3   | 0.023(5)  | 0.023(5)  | 0.031(6)  | -0.005(4)  | -0.005(4)  | -0.003(4) |
| C4   | 0.026(5)  | 0.032(6)  | 0.027(5)  | -0.009(4)  | -0.003(4)  | -0.004(4) |
| C5   | 0.025(5)  | 0.029(5)  | 0.020(5)  | -0.001(4)  | 0.001(4)   | 0.002(4)  |
| C6   | 0.019(5)  | 0.016(4)  | 0.023(5)  | 0.002(4)   | 0.003(4)   | -0.003(4) |
| C7   | 0.023(5)  | 0.019(5)  | 0.028(5)  | -0.006(4)  | -0.002(4)  | -0.001(4) |
| C8   | 0.018(5)  | 0.031(6)  | 0.054(7)  | -0.006(4)  | -0.006(5)  | 0.017(5)  |
| C9   | 0.036(6)  | 0.012(4)  | 0.052(7)  | -0.016(4)  | -0.006(5)  | 0.005(4)  |
| C10  | 0.069(9)  | 0.014(5)  | 0.029(6)  | -0.001(5)  | 0.022(6)   | 0.006(4)  |
| C11  | 0.020(5)  | 0.016(4)  | 0.031(5)  | -0.004(4)  | 0.003(4)   | -0.001(4) |
| C12  | 0.014(5)  | 0.032(6)  | 0.040(6)  | -0.008(4)  | -0.004(4)  | 0.011(5)  |
| C13  | 0.035(6)  | 0.015(4)  | 0.030(6)  | 0.003(4)   | -0.008(4)  | 0.004(4)  |
| C14  | 0.030(6)  | 0.025(5)  | 0.029(6)  | -0.012(4)  | -0.006(4)  | 0.005(4)  |
| C15  | 0.023(5)  | 0.018(4)  | 0.015(4)  | -0.007(4)  | -0.004(4)  | 0.004(3)  |
| C16  | 0.027(5)  | 0.018(4)  | 0.021(5)  | -0.009(4)  | -0.010(4)  | -0.005(4) |
| C17  | 0.032(6)  | 0.014(4)  | 0.036(6)  | -0.002(4)  | -0.012(5)  | 0.003(4)  |
| C18  | 0.039(6)  | 0.015(4)  | 0.031(6)  | -0.010(4)  | -0.008(5)  | 0.003(4)  |
| C19  | 0.030(6)  | 0.030(5)  | 0.028(6)  | -0.015(5)  | -0.002(4)  | -0.003(4) |
| C20  | 0.022(5)  | 0.017(4)  | 0.032(6)  | -0.002(4)  | -0.009(4)  | 0.001(4)  |
| C21  | 0.024(5)  | 0.016(5)  | 0.053(7)  | 0.001(4)   | -0.004(5)  | -0.005(5) |
| C22  | 0.022(5)  | 0.024(5)  | 0.039(6)  | -0.013(4)  | 0.000(4)   | -0.002(4) |
| C23  | 0.026(5)  | 0.030(5)  | 0.025(5)  | -0.018(4)  | -0.004(4)  | 0.005(4)  |
| C24  | 0.032(7)  | 0.097(12) | 0.021(6)  | -0.022(7)  | -0.002(5)  | 0.005(7)  |
| C25  | 0.063(9)  | 0.095(12) | 0.025(7)  | -0.041(9)  | -0.006(6)  | 0.023(7)  |
| C26  | 0.045(9)  | 0.17(2)   | 0.043(9)  | -0.037(11) | -0.015(7)  | 0.009(11) |
| C27  | 0.052(9)  | 0.097(14) | 0.073(11) | -0.026(9)  | 0.023(8)   | -0.055(10) |
Table S6-3. Anisotropic displacement parameters (continued)

| atom | U11   | U22   | U33   | U12   | U13   | U23   |
|------|-------|-------|-------|-------|-------|-------|
| C28  | 0.016(5) | 0.022(5) | 0.043(6) | 0.003(4) | -0.010(4) | 0.007(4) |
| C29  | 0.048(8) | 0.028(6) | 0.091(12) | -0.008(6) | -0.023(8) | 0.020(7) |
| C30  | 0.019(5) | 0.037(6) | 0.050(7) | -0.004(5) | -0.006(5) | 0.004(5) |
| C31  | 0.025(6) | 0.040(7) | 0.036(6) | 0.003(5) | 0.002(5) | -0.011(5) |
| C32  | 0.013(4) | 0.016(4) | 0.025(5) | 0.006(3) | 0.002(4) | 0.004(4) |
| C33  | 0.032(6) | 0.043(7) | 0.024(6) | 0.007(5) | 0.002(5) | 0.008(5) |
| C34  | 0.051(9) | 0.077(11) | 0.034(7) | 0.005(8) | 0.000(6) | -0.012(7) |
| C35  | 0.042(8) | 0.082(11) | 0.032(7) | 0.009(7) | 0.001(6) | -0.007(7) |
| C36  | 0.058(10) | 0.066(10) | 0.052(9) | 0.010(8) | 0.013(7) | 0.026(8) |
| C37  | 0.019(5) | 0.020(5) | 0.038(6) | -0.001(4) | 0.003(4) | 0.002(4) |
| C38  | 0.017(5) | 0.026(6) | 0.075(9) | -0.005(4) | -0.019(5) | 0.001(6) |
| C39  | 0.032(6) | 0.023(5) | 0.048(7) | 0.006(5) | -0.014(5) | 0.004(5) |
| C40  | 0.018(5) | 0.040(6) | 0.037(6) | -0.003(4) | -0.006(4) | -0.001(5) |
| C41  | 0.011(4) | 0.015(4) | 0.024(5) | -0.001(3) | -0.002(4) | 0.002(4) |
| C42  | 0.019(5) | 0.018(4) | 0.020(5) | 0.003(4) | -0.005(4) | -0.001(4) |
| C43  | 0.018(5) | 0.026(5) | 0.025(5) | -0.002(4) | -0.004(4) | -0.005(4) |
| C44  | 0.018(5) | 0.032(5) | 0.024(5) | -0.007(4) | 0.001(4) | 0.006(4) |
| C45  | 0.018(5) | 0.018(4) | 0.032(6) | -0.005(4) | -0.001(4) | 0.002(4) |
| C46  | 0.016(4) | 0.013(4) | 0.028(5) | -0.001(3) | -0.007(4) | -0.002(4) |
| C47  | 0.022(5) | 0.022(5) | 0.016(5) | -0.006(4) | 0.001(4) | 0.000(4) |
| C48  | 0.021(5) | 0.024(5) | 0.036(6) | -0.006(4) | 0.002(4) | -0.001(4) |
| C49  | 0.029(5) | 0.020(5) | 0.028(5) | -0.002(4) | -0.012(4) | -0.005(4) |
| C50  | 0.022(5) | 0.016(4) | 0.031(6) | 0.002(4) | 0.010(4) | -0.004(4) |
| C51  | 0.022(5) | 0.016(4) | 0.020(5) | -0.004(4) | -0.001(4) | 0.001(4) |
| C52  | 0.033(6) | 0.016(5) | 0.036(6) | -0.012(4) | 0.010(5) | -0.008(4) |
| C53  | 0.039(6) | 0.016(5) | 0.028(6) | -0.008(4) | 0.001(5) | -0.004(4) |
| C54  | 0.027(6) | 0.027(6) | 0.059(8) | -0.006(5) | -0.003(5) | -0.017(5) |
| C55  | 0.027(5) | 0.010(4) | 0.027(5) | -0.012(4) | 0.011(4) | -0.001(4) |
| C56  | 0.020(5) | 0.016(4) | 0.029(5) | -0.003(4) | 0.005(4) | -0.004(4) |
| C57  | 0.028(5) | 0.009(4) | 0.033(6) | -0.008(4) | 0.006(4) | -0.005(4) |
| C58  | 0.036(6) | 0.011(4) | 0.043(6) | -0.012(4) | 0.001(5) | -0.010(4) |
| C59  | 0.031(6) | 0.026(5) | 0.040(6) | -0.010(5) | -0.006(5) | -0.000(5) |
| C60  | 0.027(5) | 0.015(4) | 0.039(6) | -0.014(4) | 0.005(4) | -0.003(4) |
| C61  | 0.022(5) | 0.023(5) | 0.042(6) | 0.003(4) | 0.004(5) | -0.006(5) |
| C62  | 0.023(5) | 0.029(6) | 0.058(8) | -0.012(5) | -0.003(5) | -0.009(5) |
| C63  | 0.020(5) | 0.028(5) | 0.021(5) | -0.008(4) | -0.002(4) | -0.007(4) |
| C64  | 0.022(5) | 0.017(5) | 0.040(6) | -0.010(4) | -0.002(4) | -0.006(4) |
| atom | U_{11}  | U_{22}  | U_{33}  | U_{12}  | U_{13}  | U_{23}  |
|------|---------|---------|---------|---------|---------|---------|
| C65  | 0.017(5)| 0.036(6)| 0.034(6)| -0.002(4)| -0.006(4)| -0.003(5)|
| C66  | 0.021(5)| 0.028(6)| 0.055(8)| -0.008(4)| 0.000(5) | -0.003(5)|
| C67  | 0.022(5)| 0.030(6)| 0.041(7)| -0.007(4)| -0.000(5)| -0.006(5)|
| C68  | 0.023(5)| 0.055(7)| 0.026(6)| -0.014(5)| -0.005(4)| -0.000(5)|
| C69  | 0.029(7)| 0.084(11)| 0.039(7)| -0.002(7)| -0.009(5)| -0.018(7)|
| C70  | 0.026(6)| 0.065(9)| 0.033(6)| -0.014(6)| -0.010(5)| -0.014(6)|
| C71  | 0.063(10)| 0.082(11)| 0.037(8)| -0.022(9)| 0.013(7) | 0.009(7) |
| C72  | 0.008(4)| 0.019(4)| 0.031(5)| 0.007(3) | -0.008(3)| -0.011(4)|
| C73  | 0.014(4)| 0.017(5)| 0.044(6)| 0.002(4) | -0.006(4)| -0.007(4)|
| C74  | 0.017(5)| 0.029(6)| 0.041(6)| -0.011(4)| 0.005(4) | -0.001(5)|
| C75  | 0.036(6)| 0.029(6)| 0.058(8)| -0.003(5)| -0.036(6)| -0.005(5)|
| C76  | 0.029(6)| 0.019(5)| 0.050(7)| -0.005(4)| 0.006(5) | -0.008(5)|
| C77  | 0.016(5)| 0.037(6)| 0.034(6)| 0.004(4) | -0.008(4)| -0.012(5)|
| C78  | 0.033(6)| 0.047(7)| 0.036(7)| 0.008(5) | -0.017(5)| -0.004(5)|
| C79  | 0.029(6)| 0.048(7)| 0.040(7)| 0.011(5) | -0.013(5)| -0.014(6)|
| C80  | 0.048(8)| 0.052(8)| 0.025(6)| -0.013(6)| 0.000(5) | 0.003(5) |

The general temperature factor expression: \( \exp(-2\pi^2 (a^2 U_{11} h^2 + b^2 U_{22} k^2 + c^2 U_{33} l^2 + 2a'b'U_{12}hl + 2a'c'U_{13}hl + 2b'c'U_{23}kl)) \)
Table S6-4. Fragment Analysis

fragment: 1

|   | Nb(1) | O(1) | N(1) | N(2) | N(3) |
|---|-------|------|------|------|------|
| C(1) | C(2) | C(3) | C(4) | C(5) |
| C(6) | C(7) | C(8) | C(9) | C(10) |
| C(11) | 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) |

fragment: 2

|   | Nb(2) | O(2) | N(4) | N(5) | N(6) |
|---|-------|------|------|------|------|
| C(41) | C(42) | C(43) | C(44) | C(45) |
| C(46) | C(47) | C(48) | C(49) | C(50) |
| C(51) | C(52) | C(53) | C(54) | C(55) |
| C(56) | C(57) | C(58) | C(59) | C(60) |
| C(61) | C(62) | C(63) | C(64) | C(65) |
| C(66) | C(67) | C(68) | C(69) | C(70) |
| C(71) | C(72) | C(73) | C(74) | C(75) |
Table S6-4. Fragment Analysis (continued)

| C(76) | C(77) | C(78) | C(79) |
|-------|-------|-------|-------|
| C(80) |       |       |       |
Table S6-5. Bond lengths (Å)

| atom  | atom | distance  | atom  | atom | distance |
|-------|------|-----------|-------|------|----------|
| Nb1   | O1   | 1.965(7)  | Nb1   | N1   | 1.790(9) |
| Nb1   | N2   | 1.946(8)  | Nb1   | N3   | 1.949(8) |
| Nb2   | O2   | 1.957(6)  | Nb2   | N4   | 1.791(9) |
| Nb2   | N5   | 1.957(8)  | Nb2   | N6   | 1.949(8) |
| O1    | C1   | 1.358(12) | O2    | C41  | 1.351(11) |
| N1    | C15  | 1.380(13) | N2    | C23  | 1.280(13) |
| N3    | C32  | 1.298(12) | N4    | C55  | 1.397(13) |
| N5    | C63  | 1.260(12) | N6    | C72  | 1.273(12) |
| C1    | C2   | 1.427(14) | C1    | C6   | 1.415(13) |
| C2    | C3   | 1.403(15) | C2    | C7   | 1.554(13) |
| C3    | C4   | 1.375(15) | C4    | C5   | 1.400(17) |
| C5    | C6   | 1.394(15) | C6    | C11  | 1.538(15) |
| C7    | C8   | 1.512(14) | C7    | C9   | 1.536(16) |
| C7    | C10  | 1.515(15) | C11   | C12  | 1.508(14) |
| C11   | C13  | 1.559(13) | C11   | C14  | 1.561(15) |
| C15   | C16  | 1.411(12) | C15   | C20  | 1.385(15) |
| C16   | C17  | 1.397(15) | C16   | C21  | 1.484(15) |
| C17   | C18  | 1.372(16) | C18   | C19  | 1.387(13) |
| C19   | C20  | 1.410(16) | C20   | C22  | 1.512(12) |
| C23   | C24  | 1.575(16) | C23   | C26  | 1.531(13) |
| C24   | C25  | 1.52(2)   | C24   | C26  | 1.51(2)   |
| C24   | C27  | 1.54(2)   | C28   | C29  | 1.563(17) |
| C28   | C30  | 1.528(17) | C28   | C31  | 1.546(16) |
| C32   | C33  | 1.547(15) | C32   | C37  | 1.532(14) |
| C33   | C34  | 1.50(2)   | C33   | C35  | 1.520(17) |
| C33   | C36  | 1.55(2)   | C37   | C38  | 1.555(17) |
| C37   | C39  | 1.560(13) | C37   | C40  | 1.506(15) |
| C41   | C42  | 1.427(13) | C41   | C46  | 1.442(14) |
| C42   | C43  | 1.379(14) | C42   | C47  | 1.530(15) |
| C43   | C44  | 1.392(16) | C44   | C45  | 1.384(14) |
| C45   | C46  | 1.372(14) | C46   | C51  | 1.554(13) |
| C47   | C48  | 1.502(14) | C47   | C49  | 1.554(14) |
| C47   | C50  | 1.550(13) | C51   | C52  | 1.521(15) |
| C51   | C53  | 1.525(14) | C51   | C54  | 1.533(14) |
| C55   | C56  | 1.418(12) | C55   | C60  | 1.413(15) |
| C56   | C57  | 1.408(14) | C56   | C61  | 1.485(15) |
| C57   | C58  | 1.388(16) | C58   | C59  | 1.407(13) |
Table S6-5. Bond lengths (Å) (continued)

| atom  | atom  | distance   | atom  | atom  | distance   |
|-------|-------|------------|-------|-------|------------|
| C59   | C60   | 1.389(16)  | C60   | C62   | 1.516(13)  |
| C63   | C64   | 1.554(13)  | C63   | C68   | 1.556(15)  |
| C64   | C65   | 1.538(16)  | C64   | C66   | 1.558(15)  |
| C64   | C67   | 1.516(16)  | C68   | C69   | 1.557(17)  |
| C68   | C70   | 1.506(18)  | C68   | C71   | 1.53(2)    |
| C72   | C73   | 1.562(14)  | C72   | C77   | 1.577(15)  |
| C73   | C74   | 1.505(15)  | C73   | C75   | 1.511(17)  |
| C73   | C76   | 1.555(13)  | C77   | C78   | 1.536(15)  |
| C77   | C79   | 1.551(18)  | C77   | C80   | 1.528(19)  |
Table S6-6. Bond lengths involving hydrogens (Å)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C3   | H3   | 0.950    | C4   | H4   | 0.950    |
| C5   | H5   | 0.950    | C8   | H8A  | 0.980    |
| C8   | H8B  | 0.980    | C8   | H8C  | 0.980    |
| C9   | H9A  | 0.980    | C9   | H9B  | 0.980    |
| C9   | H9C  | 0.980    | C10  | H10A | 0.980    |
| C10  | H10B | 0.980    | C10  | H10C | 0.980    |
| C12  | H12A | 0.980    | C12  | H12B | 0.980    |
| C12  | H12C | 0.980    | C13  | H13A | 0.980    |
| C13  | H13B | 0.980    | C13  | H13C | 0.980    |
| C14  | H14A | 0.980    | C14  | H14B | 0.980    |
| C14  | H14C | 0.980    | C17  | H17  | 0.950    |
| C18  | H18  | 0.950    | C19  | H19  | 0.950    |
| C21  | H21A | 0.980    | C21  | H21B | 0.980    |
| C21  | H21C | 0.980    | C22  | H22A | 0.980    |
| C22  | H22B | 0.980    | C22  | H22C | 0.980    |
| C25  | H25A | 0.980    | C25  | H25B | 0.980    |
| C25  | H25C | 0.980    | C26  | H26A | 0.980    |
| C26  | H26B | 0.980    | C26  | H26C | 0.980    |
| C27  | H27A | 0.980    | C27  | H27B | 0.980    |
| C27  | H27C | 0.980    | C29  | H29A | 0.980    |
| C29  | H29B | 0.980    | C29  | H29C | 0.980    |
| C30  | H30A | 0.980    | C30  | H30B | 0.980    |
| C30  | H30C | 0.980    | C31  | H31A | 0.980    |
| C31  | H31B | 0.980    | C31  | H31C | 0.980    |
| C34  | H34A | 0.980    | C34  | H34B | 0.980    |
| C34  | H34C | 0.980    | C35  | H35A | 0.980    |
| C35  | H35B | 0.980    | C35  | H35C | 0.980    |
| C36  | H36A | 0.980    | C36  | H36B | 0.980    |
| C36  | H36C | 0.980    | C38  | H38A | 0.980    |
| C38  | H38B | 0.980    | C38  | H38C | 0.980    |
| C39  | H39A | 0.980    | C39  | H39B | 0.980    |
| C39  | H39C | 0.980    | C40  | H40A | 0.980    |
| C40  | H40B | 0.980    | C40  | H40C | 0.980    |
| C43  | H43  | 0.950    | C44  | H44  | 0.950    |
| C45  | H45  | 0.950    | C48  | H48A | 0.980    |
| C48  | H48B | 0.980    | C48  | H48C | 0.980    |
| C49  | H49A | 0.980    | C49  | H49B | 0.980    |
Table S6-6. Bond lengths involving hydrogens (Å) (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C49  | H49C | 0.980    | C50  | H50A | 0.980    |
| C50  | H50B | 0.980    | C50  | H50C | 0.980    |
| C52  | H52A | 0.980    | C52  | H52B | 0.980    |
| C52  | H52C | 0.980    | C53  | H53A | 0.980    |
| C53  | H53B | 0.980    | C53  | H53C | 0.980    |
| C54  | H54A | 0.980    | C54  | H54B | 0.980    |
| C54  | H54C | 0.980    | C57  | H57  | 0.950    |
| C58  | H58  | 0.950    | C59  | H59  | 0.950    |
| C61  | H61A | 0.980    | C61  | H61B | 0.980    |
| C61  | H61C | 0.980    | C62  | H62A | 0.980    |
| C62  | H62B | 0.980    | C62  | H62C | 0.980    |
| C65  | H65A | 0.980    | C65  | H65B | 0.980    |
| C65  | H65C | 0.980    | C66  | H66A | 0.980    |
| C66  | H66B | 0.980    | C66  | H66C | 0.980    |
| C67  | H67A | 0.980    | C67  | H67B | 0.980    |
| C67  | H67C | 0.980    | C69  | H69A | 0.980    |
| C69  | H69B | 0.980    | C69  | H69C | 0.980    |
| C70  | H70A | 0.980    | C70  | H70B | 0.980    |
| C70  | H70C | 0.980    | C71  | H71A | 0.980    |
| C71  | H71B | 0.980    | C71  | H71C | 0.980    |
| C74  | H74A | 0.980    | C74  | H74B | 0.980    |
| C74  | H74C | 0.980    | C75  | H75A | 0.980    |
| C75  | H75B | 0.980    | C75  | H75C | 0.980    |
| C76  | H76A | 0.980    | C76  | H76B | 0.980    |
| C76  | H76C | 0.980    | C78  | H78A | 0.980    |
| C78  | H78B | 0.980    | C78  | H78C | 0.980    |
| C79  | H79A | 0.980    | C79  | H79B | 0.980    |
| C79  | H79C | 0.980    | C80  | H80A | 0.980    |
| C80  | H80B | 0.980    | C80  | H80C | 0.980    |
Table S6-7. Bond angles (°)

| atom | atom | atom | angle  | atom | atom | atom | angle  |
|------|------|------|--------|------|------|------|--------|
| O1   | Nb1  | N1   | 112.3(3)| O1   | Nb1  | N2   | 108.2(3) |
| O1   | Nb1  | N3   | 109.9(3)| N1   | Nb1  | N2   | 102.9(4) |
| N1   | Nb1  | N3   | 102.9(3)| N2   | Nb1  | N3   | 120.4(3) |
| O2   | Nb2  | N4   | 114.8(3)| O2   | Nb2  | N5   | 107.2(3) |
| O2   | Nb2  | N6   | 107.4(3)| N4   | Nb2  | N5   | 104.9(4) |
| N4   | Nb2  | N6   | 102.3(3)| N5   | Nb2  | N6   | 120.5(3) |
| Nb1  | O1   | C1   | 148.2(6)| Nb2  | O2   | C41  | 152.4(5) |
| Nb1  | N1   | C15  | 170.1(7)| Nb1  | N2   | C23  | 173.4(7) |
| Nb1  | N3   | C32  | 177.0(8)| Nb2  | N4   | C55  | 165.9(7) |
| Nb2  | N5   | C63  | 179.3(9)| Nb2  | N6   | C72  | 178.0(7) |
| O1   | C1   | C2   | 119.1(8)| O1   | C1   | C6   | 119.6(9) |
| C2   | C1   | C6   | 121.3(9)| C1   | C2   | C3   | 118.0(9) |
| C1   | C2   | C7   | 121.5(9)| C3   | C2   | C7   | 120.4(9) |
| C2   | C3   | C4   | 121.5(10)| C3   | C4   | C5   | 119.3(10) |
| C4   | C5   | C6   | 122.6(9)| C1   | C6   | C5   | 117.0(9) |
| C1   | C6   | C11  | 122.3(9)| C5   | C6   | C11  | 120.7(9) |
| C2   | C7   | C8   | 109.3(9)| C2   | C7   | C9   | 110.8(9) |
| C2   | C7   | C10  | 113.4(7)| C8   | C7   | C9   | 106.7(8) |
| C8   | C7   | C10  | 109.4(10)| C9   | C7   | C10  | 107.0(9) |
| C6   | C11  | C12  | 111.5(8)| C6   | C11  | C13  | 109.9(8) |
| C6   | C11  | C14  | 110.4(9)| C12  | C11  | C13  | 110.5(9) |
| C12  | C11  | C14  | 108.0(9)| C13  | C11  | C14  | 106.3(7) |
| N1   | C15  | C16  | 119.8(9)| N1   | C15  | C20  | 119.5(8) |
| C16  | C15  | C20  | 120.7(9)| C15  | C16  | C17  | 117.6(9) |
| C15  | C16  | C21  | 120.0(9)| C17  | C16  | C21  | 122.4(8) |
| C16  | C17  | C18  | 122.3(8)| C17  | C18  | C19  | 119.9(10) |
| C18  | C19  | C20  | 119.5(10)| C15  | C20  | C19  | 119.9(8) |
| C15  | C20  | C22  | 120.2(9)| C19  | C20  | C22  | 119.8(9) |
| N2   | C23  | C24  | 116.0(9)| N2   | C23  | C28  | 119.5(9) |
| C24  | C23  | C28  | 124.5(9)| C23  | C24  | C25  | 104.5(11) |
| C23  | C24  | C26  | 118.6(10)| C23  | C24  | C27  | 107.8(11) |
| C25  | C24  | C26  | 109.3(13)| C25  | C24  | C27  | 111.0(12) |
| C26  | C24  | C27  | 105.7(15)| C23  | C28  | C29  | 108.6(10) |
| C23  | C28  | C30  | 114.2(9)| C23  | C28  | C31  | 110.2(8) |
| C29  | C28  | C30  | 110.1(9)| C29  | C28  | C31  | 106.9(10) |
| C30  | C28  | C31  | 106.6(9)| N3   | C32  | C33  | 116.6(9) |
| N3   | C32  | C37  | 119.0(9)| C33  | C32  | C37  | 124.4(8) |
Table S6-7. Bond angles (°) (continued)

| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| C32  | C33  | C34  | 109.6(10) | C32  | C33  | C35  | 116.2(9) |
| C32  | C33  | C36  | 107.1(10) | C34  | C33  | C35  | 107.6(11) |
| C34  | C33  | C36  | 106.7(11) | C35  | C33  | C36  | 109.3(12) |
| C32  | C37  | C38  | 109.9(9)  | C32  | C37  | C39  | 111.5(9)  |
| C32  | C37  | C40  | 112.1(9)  | C34  | C33  | C35  | 107.9(8)  |
| C34  | C33  | C36  | 107.1(10) | C34  | C33  | C35  | 107.3(9)  |
| O2   | C41  | C42  | 120.0(9)  | C42  | C43  | C44  | 119.7(9)  |
| C42  | C41  | C46  | 121.2(9)  | C41  | C42  | C43  | 121.2(9)  |
| C42  | C41  | C47  | 122.3(9)  | C43  | C42  | C44  | 119.7(10) |
| C42  | C43  | C44  | 122.6(9)  | C43  | C42  | C45  | 119.7(10) |
| C44  | C45  | C46  | 121.8(10) | C46  | C51  | C52  | 111.6(8)  |
| C46  | C51  | C52  | 111.5(8)  | C46  | C51  | C53  | 112.9(7)  |
| C52  | C51  | C54  | 107.2(8)  | C53  | C51  | C54  | 109.6(9)  |
| N4   | C55  | C56  | 118.3(9)  | C56  | C51  | C54  | 120.5(8)  |
| C56  | C55  | C60  | 121.2(9)  | C56  | C51  | C54  | 117.3(9)  |
| C55  | C56  | C61  | 121.9(9)  | C57  | C56  | C61  | 120.8(8)  |
| C56  | C57  | C58  | 121.6(8)  | C57  | C58  | C59  | 120.2(10) |
| C58  | C59  | C60  | 120.0(11) | C55  | C60  | C59  | 119.5(8)  |
| C55  | C60  | C62  | 119.4(9)  | C59  | C60  | C62  | 121.1(10) |
| N5   | C63  | C64  | 119.4(9)  | N5   | C63  | C68  | 117.9(8)  |
| C64  | C63  | C68  | 122.7(8)  | C63  | C68  | C65  | 110.3(8)  |
| C63  | C64  | C66  | 111.0(9)  | C63  | C66  | C67  | 112.7(9)  |
| C65  | C64  | C66  | 105.7(9)  | C65  | C64  | C67  | 106.4(9)  |
| C66  | C64  | C67  | 110.4(8)  | C63  | C68  | C69  | 116.7(9)  |
| C63  | C68  | C70  | 108.5(9)  | C63  | C68  | C71  | 106.2(11) |
| C69  | C68  | C70  | 106.4(11) | C69  | C68  | C71  | 108.5(11) |
| C70  | C68  | C71  | 110.6(10) | N6   | C72  | C73  | 118.7(9)  |
| N6   | C72  | C77  | 117.1(8)  | C73  | C72  | C77  | 124.1(8)  |
| C72  | C73  | C74  | 109.5(8)  | C72  | C73  | C75  | 109.9(9)  |
| C72  | C73  | C76  | 111.1(8)  | C74  | C73  | C75  | 108.8(9)  |
| C74  | C73  | C76  | 106.9(9)  | C75  | C73  | C76  | 110.6(8)  |
| C72  | C77  | C78  | 114.6(8)  | C72  | C77  | C79  | 106.6(9)  |
Table S6-7. Bond angles (°) (continued)

| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| C72  | C77  | C80  | 110.1(9)| C78  | C77  | C79  | 109.0(10)|
| C78  | C77  | C80  | 107.4(10)| C79  | C77  | C80  | 108.9(9) |
Table S6-8. Bond angles involving hydrogens (°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C2   | C3   | H3   | 119.3 | C4   | C3   | H3   | 119.2 |
| C3   | C4   | H4   | 120.4 | C5   | C4   | H4   | 120.4 |
| C4   | C5   | H5   | 118.7 | C6   | C5   | H5   | 118.7 |
| C7   | C8   | H8A  | 109.5 | C7   | C8   | H8B  | 109.5 |
| C7   | C8   | H8C  | 109.5 | H8B  | C8   | H8C  | 109.5 |
| C7   | C9   | H9A  | 109.5 | C7   | C9   | H9B  | 109.5 |
| C7   | C9   | H9C  | 109.5 | H9A  | C9   | H9B  | 109.5 |
| H9A  | C9   | H9C  | 109.5 | H9B  | C9   | H9C  | 109.5 |
| C7   | C10  | H10A | 109.5 | H10A | C10  | H10B | 109.5 |
| H10A | C10  | H10C | 109.5 | H10B | C10  | H10C | 109.5 |
| C11  | C12  | H12A | 109.5 | C11  | C12  | H12B | 109.5 |
| C11  | C12  | H12C | 109.5 | H12A | C12  | H12B | 109.5 |
| H12A | C12  | H12C | 109.5 | H12B | C12  | H12C | 109.5 |
| C11  | C13  | H13A | 109.5 | C11  | C13  | H13B | 109.5 |
| C11  | C13  | H13C | 109.5 | H13A | C13  | H13B | 109.5 |
| H13A | C13  | H13C | 109.5 | H13B | C13  | H13C | 109.5 |
| C11  | C14  | H14A | 109.5 | C11  | C14  | H14B | 109.5 |
| C11  | C14  | H14C | 109.5 | H14A | C14  | H14B | 109.5 |
| H14A | C14  | H14C | 109.5 | H14B | C14  | H14C | 109.5 |
| C16  | C17  | H17  | 118.9 | C18  | C17  | H17  | 118.9 |
| C17  | C18  | H18  | 120.0 | C19  | C18  | H18  | 120.0 |
| C18  | C19  | H19  | 120.2 | C20  | C19  | H19  | 120.2 |
| C16  | C21  | H21A | 109.5 | C16  | C21  | H21B | 109.5 |
| C16  | C21  | H21C | 109.5 | H21A | C21  | H21B | 109.5 |
| H21A | C21  | H21C | 109.5 | H21B | C21  | H21C | 109.5 |
| C20  | C22  | H22A | 109.5 | C20  | C22  | H22B | 109.5 |
| C20  | C22  | H22C | 109.5 | H22A | C22  | H22B | 109.5 |
| H22A | C22  | H22C | 109.5 | H22B | C22  | H22C | 109.5 |
| C24  | C25  | H25A | 109.5 | C24  | C25  | H25B | 109.5 |
| C24  | C25  | H25C | 109.5 | H25A | C25  | H25B | 109.5 |
| H25A | C25  | H25C | 109.5 | H25B | C25  | H25C | 109.5 |
| C24  | C26  | H26A | 109.5 | C24  | C26  | H26B | 109.5 |
| C24  | C26  | H26C | 109.5 | H26A | C26  | H26B | 109.5 |
| H26A | C26  | H26C | 109.5 | H26B | C26  | H26C | 109.5 |
| C24  | C27  | H27A | 109.5 | C24  | C27  | H27B | 109.5 |
Table S6-8. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C24  | C27  | H27C | 109.5 | H27A | C27  | H27B | 109.5 |
| H27A | C27  | H27C | 109.5 | H27B | C27  | H27C | 109.5 |
| C28  | C29  | H29A | 109.5 | C28  | C29  | H29B | 109.5 |
| C28  | C29  | H29C | 109.5 | H29A | C29  | H29B | 109.5 |
| H29A | C29  | H29C | 109.5 | H29B | C29  | H29C | 109.5 |
| C28  | C30  | H30A | 109.5 | C28  | C30  | H30B | 109.5 |
| C28  | C30  | H30C | 109.5 | H30A | C30  | H30B | 109.5 |
| H30A | C30  | H30C | 109.5 | H30B | C30  | H30C | 109.5 |
| C28  | C31  | H31A | 109.5 | C28  | C31  | H31B | 109.5 |
| C28  | C31  | H31C | 109.5 | H31A | C31  | H31B | 109.5 |
| H31A | C31  | H31C | 109.5 | H31B | C31  | H31C | 109.5 |
| C33  | C34  | H34A | 109.5 | C33  | C34  | H34B | 109.5 |
| C33  | C34  | H34C | 109.5 | H34A | C34  | H34B | 109.5 |
| H34A | C34  | H34C | 109.5 | H34B | C34  | H34C | 109.5 |
| C33  | C35  | H35A | 109.5 | C33  | C35  | H35B | 109.5 |
| C33  | C35  | H35C | 109.5 | H35A | C35  | H35B | 109.5 |
| H35A | C35  | H35C | 109.5 | H35B | C35  | H35C | 109.5 |
| C33  | C36  | H36A | 109.5 | C33  | C36  | H36B | 109.5 |
| C33  | C36  | H36C | 109.5 | H36A | C36  | H36B | 109.5 |
| H36A | C36  | H36C | 109.5 | H36B | C36  | H36C | 109.5 |
| C37  | C38  | H38A | 109.5 | C37  | C38  | H38B | 109.5 |
| C37  | C38  | H38C | 109.5 | H38A | C38  | H38B | 109.5 |
| H38A | C38  | H38C | 109.5 | H38B | C38  | H38C | 109.5 |
| C37  | C39  | H39A | 109.5 | C37  | C39  | H39B | 109.5 |
| C37  | C39  | H39C | 109.5 | H39A | C39  | H39B | 109.5 |
| H39A | C39  | H39C | 109.5 | H39B | C39  | H39C | 109.5 |
| C37  | C40  | H40A | 109.5 | C37  | C40  | H40B | 109.5 |
| C37  | C40  | H40C | 109.5 | H40A | C40  | H40B | 109.5 |
| H40A | C40  | H40C | 109.5 | H40B | C40  | H40C | 109.5 |
| C42  | C43  | H43  | 118.7 | C44  | C43  | H43  | 118.7 |
| C43  | C44  | H44  | 120.2 | C45  | C44  | H44  | 120.1 |
| C44  | C45  | H45  | 119.1 | C46  | C45  | H45  | 119.1 |
| C47  | C48  | H48A | 109.5 | C47  | C48  | H48B | 109.5 |
| C47  | C48  | H48C | 109.5 | H48A | C48  | H48B | 109.5 |
| H48A | C48  | H48C | 109.5 | H48B | C48  | H48C | 109.5 |
| C47  | C49  | H49A | 109.5 | C47  | C49  | H49B | 109.5 |
| C47  | C49  | H49C | 109.5 | H49A | C49  | H49B | 109.5 |
| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| H49A | C49  | H49C | 109.5 | H49B| C49  | H49C | 109.5 |
| C47  | C50  | H50A | 109.5 | C47 | C50  | H50B | 109.5 |
| C47  | C50  | H50C | 109.5 | H50A| C50  | H50B | 109.5 |
| H50A | C50  | H50C | 109.5 | H50B| C50  | H50C | 109.5 |
| C51  | C52  | H52A | 109.5 | C51 | C52  | H52B | 109.5 |
| C51  | C52  | H52C | 109.5 | H52A| C52  | H52B | 109.5 |
| H52A | C52  | H52C | 109.5 | H52B| C52  | H52C | 109.5 |
| C51  | C53  | H53A | 109.5 | C51 | C53  | H53B | 109.5 |
| C51  | C53  | H53C | 109.5 | H53A| C53  | H53B | 109.5 |
| H53A | C53  | H53C | 109.5 | H53B| C53  | H53B | 109.5 |
| C51  | C54  | H54A | 109.5 | C51 | C54  | H54B | 109.5 |
| C51  | C54  | H54C | 109.5 | H54A| C54  | H54B | 109.5 |
| H54A | C54  | H54C | 109.5 | H54B| C54  | H54C | 109.5 |
| C56  | C57  | H57  | 119.2 | C56 | C57  | H57  | 119.9 |
| C57  | C58  | H58  | 119.9 | C57 | C58  | H58  | 119.9 |
| C58  | C59  | H59  | 120.0 | C60 | C59  | H59  | 120.0 |
| C60  | C61  | H61A | 109.5 | C56 | C61  | H61B | 109.5 |
| C61  | H61C | 109.5 | C61  | H61B| C61  | H61C | 109.5 |
| H61A | C61  | H61C | 109.5 | H61B| C61  | H61C | 109.5 |
| C60  | C62  | H62A | 109.5 | C60 | C62  | H62B | 109.5 |
| C60  | C62  | H62C | 109.5 | C62 | H62B | 109.5 |
| H62A | C62  | H62C | 109.5 | H62B| C62  | H62C | 109.5 |
| C64  | C65  | H65A | 109.5 | C64 | C65  | H65B | 109.5 |
| C64  | C65  | H65C | 109.5 | H65A| C65  | H65B | 109.5 |
| H65A | C65  | H65C | 109.5 | H65B| C65  | H65C | 109.5 |
| C64  | C66  | H66A | 109.5 | C64 | C66  | H66B | 109.5 |
| C64  | C66  | H66C | 109.5 | H66A| C66  | H66B | 109.5 |
| H66A | C66  | H66C | 109.5 | H66B| C66  | H66C | 109.5 |
| C64  | C67  | H67A | 109.5 | C64 | C67  | H67B | 109.5 |
| C64  | C67  | H67C | 109.5 | H67A| C67  | H67B | 109.5 |
| H67A | C67  | H67C | 109.5 | H67B| C67  | H67C | 109.5 |
| C68  | C69  | H69A | 109.5 | C68 | C69  | H69B | 109.5 |
| C68  | C69  | H69C | 109.5 | H69A| C69  | H69B | 109.5 |
| H69A | C69  | H69C | 109.5 | H69B| C69  | H69C | 109.5 |
| C68  | C70  | H70A | 109.5 | C68 | C70  | H70B | 109.5 |
| C68  | C70  | H70C | 109.5 | H70A| C70  | H70B | 109.5 |
| H70A | C70  | H70C | 109.5 | H70B| C70  | H70C | 109.5 |
Table S6-8. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C68  | C71  | H71A | 109.5 | C68  | C71  | H71B | 109.5 |
| C68  | C71  | H71C | 109.5 | H71A | C71  | H71B | 109.5 |
| H71A | C71  | H71C | 109.5 | H71B | C71  | H71C | 109.5 |
| C73  | C74  | H74A | 109.5 | C73  | C74  | H74B | 109.5 |
| C73  | C74  | H74C | 109.5 | H74A | C74  | H74B | 109.5 |
| H74A | C74  | H74C | 109.5 | H74B | C74  | H74C | 109.5 |
| C73  | C75  | H75A | 109.5 | C73  | C75  | H75B | 109.5 |
| C73  | C75  | H75C | 109.5 | H75A | C75  | H75B | 109.5 |
| H75A | C75  | H75C | 109.5 | H75B | C75  | H75C | 109.5 |
| C73  | C76  | H76A | 109.5 | C73  | C76  | H76B | 109.5 |
| C73  | C76  | H76C | 109.5 | H76A | C76  | H76B | 109.5 |
| H76A | C76  | H76C | 109.5 | H76B | C76  | H76C | 109.5 |
| C77  | C78  | H78A | 109.5 | C77  | C78  | H78B | 109.5 |
| C77  | C78  | H78C | 109.5 | H78A | C78  | H78B | 109.5 |
| H78A | C78  | H78C | 109.5 | H78B | C78  | H78C | 109.5 |
| C77  | C79  | H79A | 109.5 | C77  | C79  | H79B | 109.5 |
| C77  | C79  | H79C | 109.5 | H79A | C79  | H79B | 109.5 |
| H79A | C79  | H79C | 109.5 | H79B | C79  | H79C | 109.5 |
| C77  | C80  | H80A | 109.5 | C77  | C80  | H80B | 109.5 |
| C77  | C80  | H80C | 109.5 | H80A | C80  | H80B | 109.5 |
| H80A | C80  | H80C | 109.5 | H80B | C80  | H80C | 109.5 |
Table S6-9. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle   | atom1 | atom2 | atom3 | atom4 | angle   |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| N1    | Nb1   | O1    | C1    | -106.8(9) | N2    | Nb1   | O1    | C1    | 140.3(8) |
| N3    | Nb1   | O1    | C1    | 7.0(9)    | N4    | Nb2   | O2    | C41   | 100.9(10) |
| N5    | Nb2   | O2    | C41   | -143.0(9) | N6    | Nb2   | O2    | C41   | -12.2(10) |
| Nb1   | O1    | C1    | C2    | -80.4(11) | Nb1   | O1    | C1    | C6    | 98.9(12)  |
| Nb2   | O2    | C41   | C42   | -93.4(14) | Nb2   | O2    | C41   | C46   | 87.8(13)  |
| O1    | C1    | C2    | C3    | 172.6(6)  | O1    | C1    | C2    | C7    | -11.8(11) |
| O1    | C1    | C6    | C5    | -173.0(6) | O1    | C1    | C6    | C11   | 8.3(11)   |
| C2    | C1    | C6    | C5    | 6.4(11)   | C2    | C1    | C6    | C11   | -172.3(7) |
| C6    | C1    | C2    | C3    | -6.7(12)  | C6    | C1    | C2    | C7    | 168.9(7)  |
| C1    | C2    | C3    | C4    | 2.6(13)   | C1    | C2    | C7    | C8    | -59.6(10) |
| C1    | C2    | C7    | C9    | -176.9(7) | C1    | C2    | C7    | C10   | 62.7(11)  |
| C3    | C2    | C7    | C8    | 115.9(9)  | C3    | C2    | C7    | C9    | 1.4(11)   |
| C3    | C2    | C7    | C10   | -121.8(9) | C7    | C2    | C3    | C4    | -173.0(7) |
| C2    | C3    | C4    | C5    | 1.5(13)   | C3    | C4    | C5    | C6    | -1.8(14)  |
| C4    | C5    | C6    | C1    | -2.1(13)  | C4    | C5    | C6    | C11   | 176.6(8)  |
| C1    | C6    | C11   | C12   | 50.9(11)  | C1    | C6    | C11   | C13   | -72.0(10) |
| C1    | C6    | C11   | C14   | 171.0(7)  | C5    | C6    | C11   | C12   | -127.8(8) |
| C5    | C6    | C11   | C13   | 109.4(9)  | C5    | C6    | C11   | C14   | -7.7(11)  |
| N1    | C15   | C16   | C17   | -178.4(7) | N1    | C15   | C16   | C21   | -0.6(13)  |
| N1    | C15   | C20   | C19   | 177.7(8)  | N1    | C15   | C20   | C22   | 0.7(14)   |
| C16   | C15   | C20   | C19   | -4.5(14)  | C16   | C15   | C20   | C22   | 178.5(8)  |
| C20   | C15   | C16   | C17   | 3.8(13)   | C20   | C15   | C16   | C21   | -178.4(8) |
| C15   | C16   | C17   | C18   | -2.4(15)  | C21   | C16   | C17   | C18   | 179.9(9)  |
| C16   | C17   | C18   | C19   | 1.6(16)   | C17   | C18   | C19   | C20   | -2.2(15)  |
| C18   | C19   | C20   | C15   | 3.6(15)   | C18   | C19   | C20   | C22   | -179.4(9) |
| N2    | C23   | C24   | C25   | 66.4(13)  | N2    | C23   | C24   | C26   | -171.7(11) |
| N2    | C23   | C24   | C27   | -51.7(14) | N2    | C23   | C28   | C29   | -107.7(11) |
| N2    | C23   | C28   | C30   | 129.1(10) | N2    | C23   | C28   | C31   | 9.1(14)   |
| C24   | C23   | C28   | C29   | 73.0(14)  | C24   | C23   | C28   | C30   | -50.2(15) |
| C24   | C23   | C28   | C31   | -170.2(11)| C28   | C23   | C24   | C25   | -114.3(11) |
| C28   | C23   | C24   | C26   | 8.2(2)    | C28   | C23   | C24   | C27   | 127.6(10) |
| N3    | C32   | C33   | C34   | 30.4(12)  | N3    | C32   | C33   | C35   | 152.6(9)  |
| N3    | C32   | C33   | C36   | -85.0(11) | N3    | C32   | C37   | C38   | 125.6(9)  |
| N3    | C32   | C37   | C39   | -114.7(9) | N3    | C32   | C37   | C40   | 5.5(12)   |
| C33   | C32   | C37   | C38   | -53.7(11) | C33   | C32   | C37   | C39   | 65.9(12)  |
| C33   | C32   | C37   | C40   | -173.8(8) | C37   | C32   | C33   | C34   | -150.3(8) |
| C37   | C32   | C33   | C35   | -28.0(15) | C37   | C32   | C33   | C36   | 94.4(10)  |

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| atom1 | atom2 | atom3 | atom4 | angle  | atom1 | atom2 | atom3 | atom4 | angle  |
|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|
| O2    | C41   | C42   | C43   | 172.5(6) | O2    | C41   | C42   | C47   | -6.9(12) |
| O2    | C41   | C46   | C45   | -173.7(6) | O2    | C41   | C46   | C51   | 9.2(11)  |
| C42   | C41   | C46   | C45   | 7.6(12)  | C42   | C41   | C46   | C51   | -169.6(7) |
| C46   | C41   | C42   | C43   | -8.8(11) | C46   | C41   | C42   | C47   | 171.8(7) |
| C41   | C42   | C43   | C44   | 4.4(12)  | C41   | C42   | C47   | C48   | -51.4(10) |
| C41   | C42   | C47   | C49   | -170.3(7) | C41   | C42   | C47   | C50   | 72.7(9)  |
| C43   | C42   | C47   | C48   | 129.3(8) | C43   | C42   | C47   | C49   | 10.3(11) |
| C43   | C42   | C47   | C50   | -106.6(9) | C47   | C42   | C43   | C44   | -176.2(7) |
| C42   | C43   | C44   | C45   | 1.1(13)  | C43   | C44   | C45   | C46   | -2.5(13) |
| C44   | C45   | C46   | C41   | -1.8(13) | C44   | C45   | C46   | C51   | 175.4(7) |
| C41   | C46   | C51   | C52   | 173.6(7) | C41   | C46   | C51   | C53   | -67.6(11) |
| C41   | C46   | C51   | C54   | 55.0(10) | C45   | C46   | C51   | C52   | -3.5(11) |
| C45   | C46   | C51   | C53   | 115.3(9) | C45   | C46   | C51   | C54   | -122.1(9) |
| N4    | C55   | C56   | C57   | 176.4(8) | N4    | C55   | C56   | C61   | -2.0(14) |
| N4    | C55   | C60   | C59   | -177.6(8) | N4    | C55   | C60   | C62   | 1.4(14)  |
| C56   | C55   | C60   | C59   | 3.6(15)  | C56   | C55   | C60   | C62   | -177.4(8) |
| C60   | C55   | C56   | C57   | -4.7(14) | C60   | C55   | C56   | C61   | 176.8(8) |
| C55   | C56   | C57   | C58   | 4.1(14)  | C61   | C56   | C57   | C58   | -177.5(8) |
| C56   | C57   | C58   | C59   | -2.3(15) | C57   | C58   | C59   | C60   | 1.0(16)  |
| C58   | C59   | C60   | C55   | -1.6(16) | C58   | C59   | C60   | C62   | 179.4(9) |
| N5    | C63   | C64   | C65   | 0.2(14)  | N5    | C63   | C64   | C66   | 116.9(10) |
| N5    | C63   | C64   | C67   | -118.6(10) | N5    | C63   | C68   | C69   | -165.4(9) |
| N5    | C63   | C68   | C70   | -45.3(13) | N5    | C63   | C68   | C71   | 73.6(12) |
| C64   | C63   | C68   | C69   | 18.1(16) | C64   | C63   | C68   | C70   | 138.2(9) |
| C64   | C63   | C68   | C71   | -102.9(10) | C68   | C63   | C64   | C65   | 176.6(9) |
| C68   | C63   | C64   | C66   | -66.6(13) | C68   | C63   | C64   | C67   | 57.8(13) |
| N6    | C72   | C73   | C74   | -6.2(12) | N6    | C72   | C73   | C75   | -125.7(9) |
| N6    | C72   | C73   | C76   | 111.6(9) | N6    | C72   | C77   | C78   | -149.1(8) |
| N6    | C72   | C77   | C79   | 90.1(10) | N6    | C72   | C77   | C80   | -27.9(11) |
| C73   | C72   | C77   | C78   | 29.7(14) | C73   | C72   | C77   | C79   | -91.0(9) |
| C73   | C72   | C77   | C80   | 150.9(8) | C77   | C72   | C73   | C74   | 175.0(8) |
| C77   | C72   | C73   | C75   | 55.5(11) | C77   | C72   | C73   | C76   | -67.2(12) |
Table S6-10. Intramolecular contacts less than 3.60 Å

| atom | atom | distance     | atom | atom | distance     |
|------|------|--------------|------|------|--------------|
| Nb1  | C10  | 3.359(13)    | O1   | C7   | 2.913(13)    |
| O1   | C8   | 3.094(13)    | O1   | C10  | 3.022(14)    |
| O1   | C11  | 2.916(12)    | O1   | C12  | 2.960(13)    |
| O1   | C13  | 3.172(11)    | O2   | C47  | 2.925(11)    |
| O2   | C48  | 2.963(13)    | O2   | C50  | 3.196(11)    |
| O2   | C51  | 2.934(12)    | O2   | C53  | 3.142(13)    |
| O2   | C54  | 3.030(13)    | N1   | C13  | 3.387(14)    |
| N1   | C21  | 2.841(11)    | N1   | C22  | 2.827(14)    |
| N2   | C25  | 2.909(16)    | N2   | C27  | 2.86(2)      |
| N2   | C29  | 3.392(14)    | N2   | C30  | 3.593(13)    |
| N2   | C31  | 2.724(13)    | N3   | C10  | 3.401(13)    |
| N3   | C34  | 2.726(16)    | N3   | C36  | 3.145(19)    |
| N3   | C38  | 3.550(15)    | N3   | C39  | 3.498(13)    |
| N3   | C40  | 2.742(14)    | N4   | C50  | 3.431(13)    |
| N4   | C61  | 2.865(12)    | N4   | C62  | 2.869(15)    |
| N5   | C65  | 2.728(13)    | N5   | C66  | 3.496(12)    |
| N5   | C67  | 3.499(13)    | N5   | C70  | 2.814(15)    |
| N5   | C71  | 3.012(17)    | N6   | C53  | 3.556(12)    |
| N6   | C74  | 2.697(13)    | N6   | C75  | 3.514(15)    |
| N6   | C76  | 3.466(12)    | N6   | C79  | 3.204(16)    |
| N6   | C80  | 2.770(15)    | C1   | C4   | 2.793(15)    |
| C1   | C8   | 3.097(13)    | C1   | C10  | 3.205(15)    |
| C1   | C12  | 3.064(15)    | C1   | C13  | 3.237(13)    |
| C1   | C40  | 3.528(13)    | C2   | C5   | 2.793(14)    |
| C3   | C6   | 2.824(16)    | C3   | C8   | 3.556(15)    |
| C3   | C9   | 2.818(15)    | C5   | C13  | 3.534(16)    |
| C5   | C14  | 2.812(17)    | C13  | C15  | 3.477(15)    |
| C15  | C18  | 2.784(15)    | C16  | C19  | 2.809(16)    |
| C17  | C20  | 2.766(12)    | C24  | C29  | 3.359(19)    |
| C24  | C30  | 3.257(16)    | C26  | C28  | 3.17(2)      |
| C26  | C29  | 3.53(2)      | C26  | C30  | 3.080(19)    |
| C33  | C38  | 3.191(18)    | C33  | C39  | 3.330(16)    |
| C35  | C37  | 3.150(17)    | C35  | C38  | 3.38(2)      |
| C35  | C39  | 3.119(18)    | C36  | C37  | 3.504(19)    |
| C36  | C38  | 3.38(2)      | C41  | C44  | 2.771(14)    |
| C41  | C48  | 3.065(15)    | C41  | C50  | 3.231(13)    |
| C41  | C53  | 3.266(15)    | C41  | C54  | 3.102(14)    |
Table S6-10. Intramolecular contacts less than 3.60 Å (continued)

| atom | atom | distance   | atom | atom | distance   |
|------|------|-----------|------|------|-----------|
| C41  | C74  | 3.556(13) | C42  | C45  | 2.821(15) |
| C43  | C46  | 2.798(14) | C43  | C49  | 2.849(16) |
| C43  | C50  | 3.484(15) | C45  | C52  | 2.810(14) |
| C45  | C53  | 3.584(14) | C45  | C54  | 3.595(15) |
| C50  | C55  | 3.457(15) | C50  | C56  | 3.541(14) |
| C55  | C58  | 2.790(15) | C56  | C59  | 2.834(16) |
| C57  | C60  | 2.799(12) | C64  | C69  | 3.124(18) |
| C64  | C71  | 3.560(18) | C66  | C68  | 3.321(16) |
| C66  | C69  | 3.141(18) | C67  | C68  | 3.255(16) |
| C67  | C69  | 3.337(19) | C67  | C71  | 3.573(18) |
| C73  | C78  | 3.171(16) | C73  | C79  | 3.514(16) |
| C75  | C77  | 3.226(17) | C75  | C78  | 3.431(18) |
| C75  | C79  | 3.360(18) | C76  | C77  | 3.373(15) |
| C76  | C78  | 3.131(17) |       |      |           |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H8B  | 3.555    | Nb1  | H10C | 2.405    |
| Nb1  | H12B | 3.403    | Nb1  | H13B | 2.853    |
| Nb1  | H21A | 3.202    | Nb1  | H22C | 3.599    |
| Nb1  | H25A | 3.498    | Nb1  | H27A | 3.229    |
| Nb1  | H31A | 3.548    | Nb1  | H34A | 3.301    |
| Nb1  | H40B | 3.474    | Nb1  | H40C | 3.588    |
| Nb2  | H48C | 3.274    | Nb2  | H50C | 2.852    |
| Nb2  | H53A | 2.662    | Nb2  | H54A | 3.391    |
| Nb2  | H61A | 3.193    | Nb2  | H62A | 3.231    |
| Nb2  | H65A | 3.522    | Nb2  | H70B | 3.382    |
| Nb2  | H74A | 3.485    | Nb2  | H80A | 3.268    |
| O1   | H8A  | 3.548    | O1   | H8B  | 2.475    |
| O1   | H10A | 3.443    | O1   | H10C | 2.384    |
| O1   | H12B | 2.288    | O1   | H12C | 3.393    |
| O1   | H13B | 2.578    | O1   | H31A | 3.265    |
| O1   | H40B | 3.403    | O1   | H40C | 3.194    |
| O2   | H48B | 3.393    | O2   | H48C | 2.289    |
| O2   | H50C | 2.607    | O2   | H53A | 2.512    |
| O2   | H54A | 2.362    | O2   | H54B | 3.513    |
| O2   | H65A | 3.185    | O2   | H74A | 3.356    |
| O2   | H74C | 3.180    | N1   | H12B | 3.419    |
| N1   | H13B | 2.472    | N1   | H13C | 3.563    |
| N1   | H21A | 2.356    | N1   | H21B | 3.518    |
| N1   | H21C | 3.479    | N1   | H22B | 2.777    |
| N1   | H22C | 2.786    | N1   | H27A | 3.258    |
| N2   | H8B  | 3.386    | N2   | H10C | 2.822    |
| N2   | H22B | 3.293    | N2   | H25A | 2.542    |
| N2   | H25B | 3.281    | N2   | H27A | 2.500    |
| N2   | H27C | 3.177    | N2   | H29A | 3.234    |
| N2   | H30B | 3.595    | N2   | H31A | 2.534    |
| N2   | H31B | 2.753    | N2   | H34A | 3.559    |
| N3   | H10A | 3.199    | N3   | H10C | 2.719    |
| N3   | H13B | 3.539    | N3   | H21A | 2.715    |
| N3   | H25A | 3.543    | N3   | H34A | 2.397    |
| N3   | H34B | 2.923    | N3   | H36A | 3.515    |
| N3   | H36B | 2.890    | N3   | H38C | 3.523    |
| N3   | H39B | 3.433    | N3   | H40B | 2.625    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| N3   | H40C | 2.691    | N4   | H48C | 3.298    |
| N4   | H50B | 3.565    | N4   | H50C | 2.543    |
| N4   | H61A | 2.390    | N4   | H61B | 3.497    |
| N4   | H61C | 3.547    | N4   | H62A | 2.382    |
| N4   | H62B | 3.543    | N4   | H62C | 3.509    |
| N5   | H53A | 3.158    | N5   | H54A | 3.169    |
| N5   | H62A | 3.116    | N5   | H65A | 2.613    |
| N5   | H62B | 2.676    | N5   | H66A | 3.398    |
| N5   | H70B | 2.501    | N5   | H71A | 3.337    |
| N5   | H71C | 2.725    | N5   | H80A | 3.512    |
| N6   | H50C | 3.432    | N6   | H53A | 2.696    |
| N6   | H61A | 2.648    | N6   | H70B | 3.387    |
| N6   | H74A | 2.562    | N6   | H76C | 3.366    |
| N6   | H75B | 3.470    | N6   | H79C | 2.979    |
| N6   | H79A | 3.555    | N6   | H80C | 2.928    |
| C1   | H3   | 3.287    | C1   | H5   | 3.256    |
| C1   | H8A  | 3.280    | C1   | H8B  | 2.833    |
| C1   | H10A | 3.446    | C1   | H10C | 2.951    |
| C1   | H12B | 2.776    | C1   | H12C | 3.268    |
| C1   | H13A | 3.489    | C1   | H13B | 2.996    |
| C1   | H40B | 3.328    | C1   | H40C | 2.866    |
| C2   | H4   | 3.281    | C2   | H8A  | 2.645    |
| C2   | H8B  | 2.716    | C2   | H8C  | 3.352    |
| C2   | H9A  | 2.738    | C2   | H9B  | 2.722    |
| C2   | H9C  | 3.388    | C2   | H10A | 2.743    |
| C2   | H10B | 3.400    | C2   | H10C | 2.775    |
| C2   | H40C | 2.914    | C3   | H5   | 3.244    |
| C3   | H8A  | 3.420    | C3   | H9A  | 2.733    |
| C3   | H9B  | 2.687    | C3   | H10A | 3.590    |
| C3   | H40C | 3.366    | C5   | H3   | 3.252    |
| C5   | H13A | 3.384    | C5   | H14A | 2.635    |
| C5   | H14C | 2.785    | C6   | H4   | 3.302    |
| C6   | H12A | 3.361    | C6   | H12B | 2.708    |
| C6   | H12C | 2.708    | C6   | H13A | 2.699    |
| C6   | H13B | 2.750    | C6   | H13C | 3.380    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C6   | H14A | 2.718    | C6   | H14B | 3.387    |
| C6   | H14C | 2.750    | C6   | H40B | 3.433    |
| C6   | H40C | 3.423    | C7   | H3   | 2.705    |
| C8   | H9A  | 3.303    | C8   | H9B  | 2.625    |
| C8   | H9C  | 2.625    | C8   | H10A | 3.319    |
| C8   | H10B | 2.657    | C8   | H10C | 2.657    |
| C8   | H29A | 3.499    | C9   | H3   | 2.409    |
| C9   | H3   | 2.409    | C9   | H8A  | 2.656    |
| C9   | H8B  | 3.306    | C9   | H8C  | 2.584    |
| C9   | H10A | 2.664    | C9   | H10B | 2.590    |
| C9   | H10C | 3.311    | C10  | H8B  | 2.656    |
| C10  | H9A  | 2.656    | C10  | H9B  | 3.308    |
| C10  | H9C  | 2.609    | C10  | H36B | 3.572    |
| C10  | H40C | 3.226    | C11  | H5   | 2.681    |
| C12  | H13A | 3.360    | C12  | H13B | 2.715    |
| C12  | H13C | 2.715    | C12  | H14A | 3.332    |
| C12  | H14B | 2.670    | C12  | H14C | 2.670    |
| C12  | H22C | 3.232    | C13  | H12A | 2.683    |
| C13  | H12B | 2.722    | C13  | H12C | 3.369    |
| C13  | H14A | 2.679    | C13  | H14B | 2.657    |
| C13  | H14C | 3.356    | C13  | H21C | 3.490    |
| C13  | H40B | 3.007    | C14  | H5   | 2.393    |
| C14  | H12A | 2.645    | C14  | H12B | 3.342    |
| C14  | H12C | 2.669    | C14  | H13A | 2.692    |
| C14  | H13B | 3.356    | C14  | H13C | 2.645    |
| C15  | H13B | 2.799    | C15  | H13C | 3.264    |
| C15  | H17  | 3.260    | C15  | H19  | 3.276    |
| C15  | H21A | 2.535    | C15  | H21B | 3.145    |
| C15  | H21C | 3.119    | C15  | H22A | 3.306    |
| C15  | H22B | 2.759    | C15  | H22C | 2.759    |
| C16  | H13B | 3.172    | C16  | H13C | 3.340    |
| C16  | H18  | 3.277    | C17  | H19  | 3.246    |
| C17  | H21A | 3.312    | C17  | H21B | 2.775    |
| C17  | H21C | 2.775    | C19  | H17  | 3.240    |
| C19  | H22A | 2.558    | C19  | H22B | 3.168    |
| C19  | H22C | 3.135    | C20  | H18  | 3.276    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom  | distance | atom  | atom  | distance |
|------|-------|----------|------|-------|----------|
| C21  | H13B  | 3.262    | C21  | H17   | 2.683    |
| C21  | H39B  | 3.209    | C22  | H12B  | 3.486    |
| C22  | H19   | 2.686    | C22  | H31B  | 3.045    |
| C23  | H22B  | 3.578    | C23  | H25A  | 2.543    |
| C23  | H25B  | 2.672    | C23  | H25C  | 3.315    |
| C23  | H26A  | 2.864    | C23  | H26B  | 3.466    |
| C23  | H26C  | 2.858    | C23  | H27A  | 2.628    |
| C23  | H27B  | 3.369    | C23  | H27C  | 2.749    |
| C23  | H29A  | 2.654    | C23  | H29B  | 3.358    |
| C23  | H29C  | 2.740    | C23  | H30A  | 3.398    |
| C23  | H30B  | 2.770    | C23  | H30C  | 2.770    |
| C23  | H31A  | 2.680    | C23  | H31B  | 2.746    |
| C23  | H31C  | 3.366    | C24  | H29A  | 3.577    |
| C24  | H29C  | 3.099    | C24  | H30B  | 3.458    |
| C24  | H30C  | 2.961    | C25  | H26A  | 3.318    |
| C25  | H26B  | 2.653    | C25  | H26C  | 2.653    |
| C25  | H27A  | 2.724    | C25  | H27B  | 2.699    |
| C25  | H27C  | 3.359    | C25  | H29C  | 3.387    |
| C25  | H34A  | 3.231    | C25  | H36B  | 3.365    |
| C26  | H25A  | 3.316    | C26  | H25B  | 2.656    |
| C26  | H25C  | 2.656    | C26  | H27A  | 3.286    |
| C26  | H27B  | 2.604    | C26  | H27C  | 2.603    |
| C26  | H29C  | 2.946    | C26  | H30B  | 3.424    |
| C26  | H30C  | 2.367    | C27  | H25A  | 2.736    |
| C27  | H25B  | 3.362    | C27  | H25C  | 2.679    |
| C27  | H26A  | 2.600    | C27  | H26B  | 2.591    |
| C27  | H26C  | 3.292    | C27  | H34A  | 3.050    |
| C28  | H25B  | 3.522    | C28  | H26A  | 3.131    |
| C28  | H26C  | 3.032    | C29  | H25B  | 3.204    |
| C29  | H26C  | 2.965    | C29  | H30A  | 2.697    |
| C29  | H30B  | 3.382    | C29  | H30C  | 2.734    |
| C29  | H31A  | 2.687    | C29  | H31B  | 3.357    |
| C29  | H31C  | 2.652    | C30  | H26A  | 2.604    |
| C30  | H26C  | 3.021    | C30  | H29A  | 3.376    |
| C30  | H29B  | 2.724    | C30  | H29C  | 2.724    |
| C30  | H31A  | 3.322    | C30  | H31B  | 2.641    |
| C30  | H31C  | 2.641    | C31  | H8B   | 3.081    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C31  | H22B | 3.573    | C31  | H22C | 3.518    |
| C31  | H29A | 2.709    | C31  | H29B | 2.639    |
| C31  | H29C | 3.352    | C31  | H30A | 2.621    |
| C31  | H30B | 2.652    | C31  | H30C | 3.325    |
| C32  | H10A | 4.464    | C32  | H10C | 3.543    |
| C32  | H21A | 3.118    | C32  | H34A | 2.616    |
| C32  | H34B | 2.725    | C32  | H34C | 3.338    |
| C32  | H35A | 2.788    | C32  | H35B | 3.426    |
| C32  | H35C | 2.833    | C32  | H36A | 2.683    |
| C32  | H36B | 2.641    | C32  | H36C | 3.344    |
| C32  | H38A | 2.697    | C32  | H38B | 3.371    |
| C32  | H38C | 2.735    | C32  | H39A | 2.727    |
| C32  | H39B | 2.772    | C32  | H39C | 3.392    |
| C32  | H40A | 3.360    | C32  | H40B | 2.712    |
| C32  | H40C | 2.712    | C33  | H38A | 2.850    |
| C33  | H38C | 3.431    | C33  | H39A | 3.012    |
| C33  | H25A | 3.409    | C34  | H27A | 3.134    |
| C33  | H35A | 3.289    | C34  | H35B | 2.619    |
| C34  | H35C | 2.619    | C34  | H36A | 3.296    |
| C34  | H36B | 2.624    | C34  | H36C | 2.624    |
| C35  | H34A | 3.293    | C35  | H34B | 2.613    |
| C35  | H34C | 2.613    | C35  | H36A | 2.718    |
| C35  | H36B | 3.346    | C35  | H36C | 2.660    |
| C35  | H38A | 2.729    | C35  | H39A | 2.396    |
| C35  | H39B | 3.552    | C36  | H25A | 3.412    |
| C36  | H34A | 2.634    | C36  | H34B | 3.305    |
| C36  | H34C | 2.590    | C36  | H35A | 2.717    |
| C36  | H35B | 2.649    | C36  | H35C | 2.351    |
| C36  | H38A | 2.959    | C36  | H38C | 3.245    |
| C37  | H35A | 2.882    | C37  | H35C | 3.269    |
| C37  | H36A | 3.282    | C38  | H35A | 2.739    |
| C38  | H36A | 2.742    | C38  | H39A | 2.727    |
| C38  | H39B | 3.371    | C38  | H39C | 2.667    |
| C38  | H40A | 2.640    | C38  | H40B | 3.335    |
| C38  | H40C | 2.659    | C39  | H21A | 3.598    |
| C39  | H35A | 2.839    | C39  | H35C | 2.827    |
| C39  | H38A | 2.729    | C39  | H38B | 2.662    |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C39  | H38C | 3.372    | C39  | H40A | 2.618    |
| C39  | H40B | 2.660    | C39  | H40C | 3.330    |
| C40  | H10A | 3.507    | C40  | H13A | 3.382    |
| C40  | H13B | 3.556    | C40  | H38A | 3.325    |
| C40  | H38B | 2.662    | C40  | H38C | 2.662    |
| C40  | H39A | 3.320    | C40  | H39B | 2.653    |
| C40  | H39C | 2.653    | C41  | H43  | 3.250    |
| C41  | H45  | 3.272    | C41  | H48B | 3.273    |
| C41  | H48C | 2.774    | C41  | H50A | 3.477    |
| C41  | H50C | 2.989    | C41  | H53A | 2.981    |
| C41  | H53C | 3.574    | C41  | H54A | 2.787    |
| C41  | H54B | 3.336    | C41  | H74A | 3.308    |
| C41  | H74C | 2.940    | C42  | H44  | 3.280    |
| C42  | H48A | 3.351    | C42  | H48B | 2.699    |
| C42  | H48C | 2.699    | C42  | H49A | 2.739    |
| C42  | H49B | 2.770    | C42  | H49C | 3.393    |
| C42  | H50A | 2.673    | C42  | H50B | 3.361    |
| C42  | H50C | 2.734    | C42  | H74A | 3.478    |
| C42  | H74C | 3.591    | C43  | H45  | 3.254    |
| C43  | H49A | 2.672    | C43  | H49B | 2.849    |
| C43  | H50A | 3.318    | C45  | H43  | 3.250    |
| C45  | H52A | 2.691    | C45  | H52B | 2.727    |
| C45  | H53C | 3.509    | C45  | H54B | 3.528    |
| C45  | H74C | 3.513    | C46  | H44  | 3.260    |
| C46  | H52A | 2.708    | C46  | H52B | 2.753    |
| C46  | H52C | 3.385    | C46  | H53A | 2.743    |
| C46  | H53B | 3.402    | C46  | H53C | 2.775    |
| C46  | H54A | 2.697    | C46  | H54B | 2.715    |
| C46  | H54C | 3.373    | C46  | H74C | 2.998    |
| C47  | H43  | 2.670    | C48  | H49A | 3.300    |
| C48  | H49B | 2.625    | C48  | H49C | 2.625    |
| C48  | H50A | 3.359    | C48  | H50B | 2.722    |
| C48  | H50C | 2.722    | C49  | H43  | 2.443    |
| C49  | H48A | 2.592    | C49  | H48B | 2.631    |
| C49  | H48C | 3.310    | C49  | H50A | 2.683    |
| C49  | H50B | 2.604    | C49  | H50C | 3.335    |
| C50  | H43  | 3.590    | C50  | H48A | 2.689    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C50  | H48B | 3.368    | C50  | H48C | 2.733    |
| C50  | H49A | 2.655    | C50  | H49B | 3.335    |
| C50  | H49C | 2.633    | C50  | H61B | 3.338    |
| C50  | H74A | 3.040    | C51  | H45  | 2.664    |
| C51  | H74C | 3.570    | C52  | H45  | 2.394    |
| C52  | H53A | 3.291    | C52  | H53B | 2.601    |
| C52  | H53C | 2.602    | C52  | H54A | 3.314    |
| C52  | H54B | 2.638    | C52  | H54C | 2.638    |
| C53  | H52A | 3.291    | C53  | H52B | 2.601    |
| C53  | H52C | 2.601    | C53  | H54A | 2.730    |
| C53  | H54B | 3.345    | C53  | H54C | 2.645    |
| C53  | H74C | 3.028    | C53  | H75B | 3.566    |
| C54  | H52A | 2.659    | C54  | H52B | 3.316    |
| C54  | H52C | 2.611    | C54  | H53A | 2.721    |
| C54  | H53B | 2.649    | C54  | H53C | 3.347    |
| C54  | H65A | 2.969    | C54  | H66A | 3.203    |
| C55  | H50B | 3.196    | C55  | H50C | 2.824    |
| C55  | H57  | 3.275    | C55  | H59  | 3.282    |
| C55  | H61A | 2.576    | C55  | H61B | 3.149    |
| C55  | H61C | 3.166    | C55  | H62A | 2.555    |
| C55  | H62B | 3.158    | C55  | H62C | 3.147    |
| C56  | H50B | 3.151    | C56  | H50C | 3.065    |
| C56  | H58  | 3.294    | C57  | H50B | 3.571    |
| C57  | H59  | 3.278    | C57  | H61A | 3.311    |
| C57  | H61B | 2.759    | C57  | H61C | 2.758    |
| C59  | H57  | 3.275    | C59  | H62A | 3.320    |
| C59  | H62B | 2.779    | C59  | H62C | 2.779    |
| C60  | H58  | 3.277    | C61  | H50B | 3.579    |
| C61  | H50C | 3.145    | C61  | H57  | 2.669    |
| C61  | H76C | 3.131    | C61  | H80C | 3.483    |
| C62  | H48C | 3.509    | C62  | H59  | 2.689    |
| C62  | H65C | 2.882    | C63  | H65A | 2.703    |
| C63  | H65B | 3.383    | C63  | H65C | 2.741    |
| C63  | H66A | 2.711    | C63  | H66B | 2.796    |
| C63  | H66C | 3.404    | C63  | H67A | 2.741    |
| C63  | H67B | 2.756    | C63  | H67C | 3.395    |
| C63  | H69A | 2.850    | C63  | H69B | 2.866    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C63  | H69C | 3.467    | C63  | H70A | 2.691    |
| C63  | H70B | 2.631    | C63  | H70C | 3.341    |
| C63  | H71A | 2.653    | C63  | H71B | 3.327    |
| C63  | H71C | 2.614    | C64  | H69A | 2.914    |
| C64  | H69B | 3.157    | C64  | H71A | 3.356    |
| C65  | H54A | 3.078    | C65  | H62A | 3.086    |
| C65  | H66A | 2.681    | C65  | H66B | 3.325    |
| C65  | H66C | 2.599    | C65  | H67A | 3.308    |
| C65  | H67B | 2.618    | C65  | H67C | 2.618    |
| C66  | H54C | 3.587    | C66  | H65A | 2.655    |
| C66  | H65B | 2.614    | C66  | H65C | 3.331    |
| C66  | H67A | 2.752    | C66  | H67B | 3.371    |
| C66  | H67C | 2.665    | C66  | H69A | 3.025    |
| C67  | H69B | 2.715    | C67  | H65A | 3.304    |
| C67  | H65B | 2.624    | C67  | H65C | 2.624    |
| C67  | H66A | 3.365    | C67  | H66B | 2.717    |
| C67  | H66C | 2.717    | C67  | H69A | 2.707    |
| C67  | H71A | 2.978    | C68  | H66A | 3.527    |
| C68  | H66B | 3.064    | C68  | H67A | 2.935    |
| C68  | H67B | 3.508    | C69  | H66A | 3.532    |
| C69  | H66B | 2.459    | C69  | H67A | 2.680    |
| C69  | H70A | 2.639    | C69  | H70B | 3.317    |
| C69  | H70C | 2.600    | C69  | H71A | 2.706    |
| C69  | H71B | 2.649    | C69  | H71C | 3.355    |
| C70  | H69A | 3.307    | C70  | H69B | 2.633    |
| C70  | H69C | 2.633    | C70  | H71A | 3.334    |
| C70  | H71B | 2.685    | C70  | H71C | 2.685    |
| C70  | H79C | 3.067    | C70  | H80A | 3.255    |
| C71  | H67A | 3.187    | C71  | H67B | 3.459    |
| C71  | H69A | 2.693    | C71  | H69B | 3.349    |
| C71  | H69C | 2.677    | C71  | H70A | 3.338    |
| C71  | H70B | 2.680    | C71  | H70C | 2.680    |
| C71  | H80A | 3.548    | C72  | H53A | 3.367    |
| C72  | H61A | 3.040    | C72  | H74A | 2.682    |
| C72  | H74B | 3.359    | C72  | H74C | 2.684    |
| C72  | H75A | 2.698    | C72  | H75B | 2.696    |
| C72  | H75C | 3.368    | C72  | H76A | 2.761    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance |
|-------|-------|----------|
| C72   | C72   | 3.412    |
| C72   | H76B  | 2.797    |
| C72   | H78A  | 3.450    |
| C72   | H79B  | 3.369    |
| C72   | H80A  | 2.685    |
| C72   | H80C  | 2.768    |
| C73   | H78B  | 2.385    |
| C74   | H50A  | 3.481    |
| C74   | H53A  | 3.586    |
| C74   | H75A  | 3.303    |
| C74   | H75C  | 2.638    |
| C74   | H76B  | 2.642    |
| C75   | H74A  | 3.304    |
| C75   | H74C  | 2.636    |
| C75   | H76B  | 2.702    |
| C75   | H78A  | 2.800    |
| C76   | H61A  | 3.558    |
| C76   | H74B  | 2.624    |
| C76   | H75A  | 2.726    |
| C76   | H75C  | 2.683    |
| C76   | H78B  | 2.841    |
| C77   | H75B  | 3.435    |
| C78   | H75A  | 2.796    |
| C78   | H76C  | 3.515    |
| C78   | H79B  | 2.676    |
| C78   | H80A  | 3.327    |
| C78   | H80C  | 2.647    |
| C79   | H75A  | 2.939    |
| C79   | H78A  | 2.711    |
| C79   | H78C  | 2.679    |
| C79   | H80B  | 2.670    |
| C80   | H61A  | 3.510    |
| C80   | H78A  | 3.326    |
| C80   | H78C  | 2.649    |
| C80   | H79B  | 2.691    |
| H3    | H4    | 2.319    |
| H3    | H9B   | 2.177    |

| atom  | atom  | distance |
|-------|-------|----------|
| C72   | H76C  | 2.753    |
| C72   | H78B  | 2.836    |
| C72   | H79A  | 2.686    |
| C72   | H79C  | 2.667    |
| C72   | H80B  | 3.394    |
| C73   | C73   | 2.886    |
| C73   | H79A  | 3.257    |
| C74   | C74   | 3.543    |
| C74   | H53C  | 3.483    |
| C74   | H75B  | 2.638    |
| C74   | H76A  | 3.312    |
| C74   | H76C  | 2.642    |
| C75   | C75   | 2.636    |
| C75   | H76A  | 2.728    |
| C75   | H76C  | 3.360    |
| C75   | H79A  | 2.707    |
| C76   | C76   | 2.633    |
| C76   | H74A  | 3.322    |
| C76   | H75B  | 3.368    |
| C76   | H78A  | 2.834    |
| C76   | C77   | 2.893    |
| C77   | C77   | 3.074    |
| C78   | C78   | 2.423    |
| C78   | C78   | 2.721    |
| C78   | C78   | 3.362    |
| C78   | C78   | 2.647    |
| C78   | C79   | 3.224    |
| C79   | C79   | 3.209    |
| C79   | C79   | 3.365    |
| C79   | C79   | 2.701    |
| C79   | C79   | 3.358    |
| C80   | C80   | 3.213    |
| C80   | C80   | 2.649    |
| C80   | C80   | 2.691    |
| H3    | H3    | 2.174    |
| H3    | H3    | 3.371    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H4   | H5   | 2.337    | H5   | H13A | 3.413    |
| H5   | H14A | 2.020    | H5   | H14B | 3.348    |
| H5   | H14C | 2.319    | H8A  | H9A  | 3.547    |
| H8A  | H9B  | 2.459    | H8A  | H9C  | 2.952    |
| H8A  | H10B | 3.552    | H8A  | H10C | 3.552    |
| H8A  | H31A | 3.437    | H8B  | H9B  | 3.543    |
| H8B  | H9C  | 3.509    | H8B  | H10A | 3.551    |
| H8B  | H10B | 2.942    | H8B  | H10C | 2.469    |
| H8B  | H29A | 3.186    | H8B  | H31A | 2.105    |
| H8B  | H31B | 3.584    | H8B  | H31C | 3.485    |
| H8C  | H9A  | 3.492    | H8C  | H9B  | 2.848    |
| H8C  | H9C  | 2.382    | H8C  | H10A | 3.551    |
| H8C  | H10B | 2.469    | H8C  | H10C | 2.942    |
| H8C  | H29A | 2.906    | H8C  | H31A | 3.128    |
| H9A  | H10A | 2.494    | H9A  | H10B | 2.888    |
| H9A  | H10C | 3.568    | H9B  | H10A | 3.565    |
| H9B  | H10B | 3.487    | H9C  | H10A | 2.928    |
| H9C  | H10B | 2.365    | H9C  | H10C | 3.497    |
| H10A | H36A | 3.581    | H10A | H36B | 3.259    |
| H10A | H38C | 2.804    | H10A | H40C | 2.641    |
| H10B | H25A | 3.489    | H10B | H36B | 3.486    |
| H10C | H25A | 3.237    | H10C | H31A | 3.590    |
| H10C | H36B | 3.383    | H10C | H40C | 3.150    |
| H12A | H13A | 3.577    | H12A | H13B | 2.965    |
| H12A | H13C | 2.510    | H12A | H14A | 3.542    |
| H12A | H14B | 2.457    | H12A | H14C | 2.926    |
| H12A | H22C | 3.027    | H12B | H13B | 2.551    |
| H12B | H13C | 3.022    | H12B | H14B | 3.565    |
| H12B | H14C | 3.576    | H12B | H22C | 2.563    |
| H12C | H13C | 3.600    | H12C | H14A | 3.560    |
| H12C | H14B | 2.960    | H12C | H14C | 2.482    |
| H13A | H14A | 2.503    | H13A | H14B | 2.958    |
| H13A | H14C | 3.593    | H13A | H21C | 3.319    |
| H13A | H40A | 3.552    | H13A | H40B | 2.519    |
| H13B | H14A | 3.588    | H13B | H14B | 3.550    |
| H13B | H21A | 2.936    | H13B | H21C | 3.176    |
| H13B | H40B | 2.663    | H13C | H14A | 2.921    |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H13C | H14B | 2.430 | H13C | H14C | 3.546 |
| H13C | H21C | 3.396 | H17  | H18  | 2.306 |
| H17  | H21B | 2.731 | H17  | H21C | 2.730 |
| H18  | H19  | 2.341 | H19  | H22A | 2.353 |
| H19  | H22B | 3.374 | H19  | H22C | 3.318 |
| H21A | H34B | 3.023 | H21A | H39B | 2.843 |
| H21B | H40B | 3.081 | H21B | H34B | 3.329 |
| H21B | H39B | 3.402 | H21B | H39B | 2.881 |
| H21C | H40B | 3.464 | H22A | H31B | 3.422 |
| H22B | H27C | 3.406 | H22B | H30B | 3.106 |
| H22B | H31B | 2.698 | H22C | H31B | 2.598 |
| H25A | H26B | 3.547 | H25A | H26C | 3.547 |
| H25A | H27A | 2.578 | H25A | H27B | 3.021 |
| H25A | H34A | 2.559 | H25A | H36B | 2.547 |
| H25B | H26A | 3.551 | H25B | H26B | 2.939 |
| H25B | H26C | 2.465 | H25B | H27B | 3.579 |
| H25B | H29A | 3.008 | H25B | H29C | 2.768 |
| H25C | H26A | 3.551 | H25C | H26B | 2.465 |
| H25C | H26C | 2.939 | H25C | H27A | 2.973 |
| H25C | H27B | 2.490 | H25C | H27C | 3.570 |
| H25C | H34A | 3.238 | H25C | H26B | 3.418 |
| H26A | H27A | 3.500 | H26A | H27B | 2.882 |
| H26A | H27C | 2.394 | H26A | H29C | 3.301 |
| H26A | H30A | 3.415 | H26A | H30B | 2.787 |
| H26A | H30C | 1.833 | H26B | H27A | 3.494 |
| H26B | H27B | 2.385 | H26B | H27C | 2.869 |
| H26B | H30C | 3.253 | H26C | H27B | 3.507 |
| H26C | H27C | 3.510 | H26C | H29A | 3.513 |
| H26C | H29C | 2.205 | H26C | H30C | 2.273 |
| H27A | H34A | 2.296 | H27A | H34B | 3.293 |
| H27A | H34C | 3.453 | H27B | H34A | 3.097 |
| H27C | H30B | 3.345 | H27C | H30C | 3.506 |
| H29A | H30A | 3.592 | H29A | H31A | 2.530 |
| H29A | H31C | 2.971 | H29B | H30A | 2.521 |
| H29B | H30C | 3.029 | H29B | H31A | 2.919 |
| H29B | H31B | 3.540 | H29B | H31C | 2.417 |
| H29C | H30A | 2.975 | H29C | H30C | 2.560 |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H29C  | H31A  | 3.597    | H29C  | H31C  | 3.537    |
| H30A  | H31A  | 3.525    | H30A  | H31B  | 2.892    |
| H30A  | H31C  | 2.420    | H30B  | H31A  | 3.549    |
| H30B  | H31B  | 2.453    | H30B  | H31C  | 2.937    |
| H30C  | H31B  | 3.550    | H30C  | H31C  | 3.536    |
| H34A  | H35B  | 3.520    | H34A  | H35C  | 3.520    |
| H34A  | H36A  | 3.527    | H34A  | H36B  | 2.438    |
| H34A  | H36C  | 2.928    | H34B  | H35A  | 3.511    |
| H34B  | H35B  | 2.899    | H34B  | H35C  | 2.417    |
| H34B  | H36B  | 3.538    | H34B  | H36C  | 3.518    |
| H34C  | H35A  | 3.511    | H34C  | H35B  | 2.417    |
| H34C  | H35C  | 2.899    | H34C  | H36A  | 3.493    |
| H34C  | H36B  | 2.864    | H34C  | H36C  | 2.391    |
| H35A  | H36A  | 2.569    | H35A  | H36B  | 2.975    |
| H35A  | H38A  | 1.958    | H35A  | H38B  | 3.339    |
| H35A  | H38C  | 3.379    | H35A  | H39A  | 2.099    |
| H35A  | H39B  | 3.507    | H35A  | H39C  | 3.425    |
| H35B  | H36A  | 2.961    | H35B  | H36B  | 3.535    |
| H35B  | H36C  | 2.433    | H35B  | H38A  | 3.403    |
| H35B  | H39A  | 3.296    | H35C  | H36C  | 3.546    |
| H35C  | H38A  | 3.296    | H35C  | H39A  | 2.043    |
| H35C  | H39B  | 3.055    | H36A  | H38A  | 2.279    |
| H36A  | H38C  | 2.535    | H36B  | H38A  | 3.599    |
| H36B  | H38C  | 3.470    | H36C  | H38A  | 3.593    |
| H38A  | H39A  | 2.573    | H38A  | H39C  | 2.977    |
| H38A  | H40A  | 3.537    | H38A  | H40C  | 3.552    |
| H38B  | H39A  | 2.967    | H38B  | H39B  | 3.553    |
| H38B  | H39C  | 2.438    | H38B  | H40A  | 2.451    |
| H38B  | H40B  | 3.558    | H38B  | H40C  | 2.949    |
| H38C  | H39C  | 3.555    | H38C  | H40A  | 2.922    |
| H38C  | H40B  | 3.567    | H38C  | H40C  | 2.471    |
| H39A  | H40A  | 3.519    | H39A  | H40B  | 3.552    |
| H39B  | H40A  | 2.893    | H39B  | H40B  | 2.470    |
| H39B  | H40C  | 3.565    | H39C  | H40A  | 2.425    |
| H39C  | H40B  | 2.954    | H39C  | H40C  | 3.545    |
| H43   | H44   | 2.326    | H43   | H49A  | 2.053    |
| H43   | H49B  | 2.412    | H43   | H49C  | 3.399    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H43   | H50A  | 3.326    | H44   | H45   | 2.323    |
| H45   | H52A  | 2.192    | H45   | H52B  | 2.145    |
| H45   | H52C  | 3.358    | H45   | H53C  | 3.535    |
| H48A  | H49A  | 3.495    | H48A  | H49B  | 2.866    |
| H48A  | H49C  | 2.392    | H48A  | H50A  | 3.581    |
| H48A  | H50B  | 2.521    | H48A  | H50C  | 2.973    |
| H48A  | H62C  | 3.174    | H48B  | H49A  | 3.526    |
| H48B  | H49B  | 2.433    | H48B  | H49C  | 2.923    |
| H48C  | H49B  | 3.539    | H48C  | H49C  | 3.521    |
| H48C  | H50B  | 3.037    | H48C  | H50C  | 2.568    |
| H48C  | H62A  | 3.162    | H48C  | H62C  | 3.199    |
| H48C  | H65A  | 3.395    | H48C  | H65C  | 3.342    |
| H49A  | H50A  | 2.492    | H49A  | H50B  | 2.873    |
| H49A  | H50C  | 3.572    | H49B  | H50A  | 3.582    |
| H49B  | H50B  | 3.510    | H49C  | H50A  | 2.956    |
| H49C  | H50B  | 2.383    | H49C  | H50C  | 3.518    |
| H50A  | H61B  | 3.225    | H50A  | H74A  | 2.603    |
| H50B  | H61B  | 3.221    | H50C  | H61A  | 2.876    |
| H50C  | H61B  | 3.011    | H50C  | H74A  | 2.633    |
| H52A  | H53B  | 3.505    | H52A  | H53C  | 3.505    |
| H52A  | H54A  | 3.552    | H52A  | H54B  | 2.463    |
| H52A  | H54C  | 2.950    | H52B  | H53A  | 3.504    |
| H52B  | H53B  | 2.877    | H52B  | H53C  | 2.391    |
| H52B  | H54B  | 3.549    | H52B  | H54C  | 3.526    |
| H52C  | H53A  | 3.504    | H52C  | H53B  | 2.391    |
| H52C  | H53C  | 2.877    | H52C  | H54A  | 3.515    |
| H52C  | H54B  | 2.879    | H52C  | H54C  | 2.411    |
| H53A  | H54A  | 2.588    | H53A  | H54C  | 2.959    |
| H53A  | H70A  | 3.550    | H53A  | H70B  | 3.383    |
| H53A  | H74C  | 2.759    | H53A  | H75B  | 3.579    |
| H53A  | H79C  | 3.398    | H53B  | H54A  | 2.980    |
| H53B  | H54B  | 3.529    | H53B  | H54C  | 2.419    |
| H53B  | H70A  | 3.241    | H53C  | H54C  | 3.531    |
| H53C  | H74C  | 2.569    | H53C  | H75B  | 2.744    |
| H54A  | H65A  | 2.119    | H54A  | H65C  | 3.575    |
| H54A  | H66A  | 2.950    | H54B  | H65A  | 3.253    |
| H54C  | H65A  | 3.193    | H54C  | H66A  | 2.630    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H57  | H58  | 2.325    | H57  | H61B | 2.698    |
| H57  | H61C | 2.720    | H58  | H59  | 2.356    |
| H59  | H62B | 2.738    | H59  | H62C | 2.733    |
| H61A | H74A | 3.124    | H61A | H76C | 2.794    |
| H61A | H80A | 3.563    | H61A | H80C | 2.850    |
| H61B | H74A | 3.416    | H61B | H76C | 2.771    |
| H61C | H76C | 3.342    | H61C | H80C | 3.232    |
| H62A | H65A | 3.449    | H62A | H65C | 2.138    |
| H62A | H67B | 3.197    | H62B | H65C | 2.916    |
| H62B | H67B | 3.392    | H62C | H65C | 2.916    |
| H65A | H66A | 2.497    | H65A | H66B | 3.518    |
| H65A | H66C | 2.878    | H65A | H66B | 3.518    |
| H65B | H67B | 3.518    | H65B | H66A | 2.940    |
| H65B | H67C | 3.527    | H65B | H66C | 2.365    |
| H65B | H67C | 2.416    | H65B | H66B | 2.898    |
| H65B | H67C | 3.510    | H65B | H66C | 2.365    |
| H65C | H66C | 3.503    | H65C | H66A | 2.956    |
| H65C | H66C | 3.565    | H65C | H66B | 2.956    |
| H65C | H66C | 3.510    | H65C | H66B | 2.956    |
| H66A | H67B | 2.932    | H66A | H66B | 2.340    |
| H66B | H67B | 1.936    | H66B | H66B | 3.348    |
| H66B | H70A | 3.590    | H66C | H66C | 3.061    |
| H66C | H67B | 3.588    | H66C | H67C | 2.490    |
| H66C | H67B | 3.522    | H67A | H69A | 1.893    |
| H67A | H69B | 3.115    | H67A | H69A | 3.431    |
| H67A | H71A | 2.559    | H67B | H69A | 3.300    |
| H67B | H71A | 2.756    | H67C | H69A | 3.337    |
| H69A | H70A | 3.533    | H69A | H70C | 3.503    |
| H69A | H71A | 2.531    | H69A | H71B | 2.930    |
| H69B | H70A | 2.442    | H69B | H70B | 3.546    |
| H69B | H70B | 2.874    | H69B | H71A | 3.598    |
| H69B | H71B | 3.546    | H69C | H70A | 2.930    |
| H69C | H70B | 3.528    | H69C | H70C | 2.401    |
| H69C | H71A | 2.991    | H69C | H71B | 2.452    |
| H69C | H71C | 3.563    | H70A | H71B | 3.577    |
| H70A | H71C | 3.577    | H70A | H79C | 3.224    |
Table S6-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H70B | H71A | 3.571    | H70B | H71B | 2.971    |
| H70B | H71C | 2.503    | H70B | H79B | 3.517    |
| H70B | H79C | 2.372    | H70B | H80A | 2.369    |
| H70B | H80B | 3.476    | H70C | H71A | 3.571    |
| H70C | H71B | 2.503    | H70C | H71C | 2.971    |
| H70C | H79C | 3.168    | H70C | H80A | 3.470    |
| H71C | H80A | 2.762    | H74A | H75B | 3.535    |
| H74A | H75C | 3.535    | H74A | H76A | 3.530    |
| H74A | H76B | 2.919    | H74A | H76C | 2.439    |
| H74B | H75A | 3.532    | H74B | H75B | 2.922    |
| H74B | H75C | 2.445    | H74B | H76A | 3.523    |
| H74B | H76B | 2.429    | H74B | H76C | 2.906    |
| H74C | H75A | 3.532    | H74C | H75B | 2.445    |
| H74C | H75C | 2.922    | H74C | H76B | 3.543    |
| H74C | H76C | 3.547    | H75A | H76A | 2.569    |
| H75A | H76B | 3.008    | H75A | H78A | 2.033    |
| H75A | H78B | 3.359    | H75A | H78C | 3.475    |
| H75A | H79A | 2.230    | H75A | H79B | 3.581    |
| H75A | H79C | 3.563    | H75B | H76B | 3.589    |
| H75B | H78A | 3.431    | H75B | H79A | 2.504    |
| H75B | H79C | 3.403    | H75C | H76A | 2.982    |
| H75C | H76B | 2.495    | H75C | H76C | 3.571    |
| H75C | H78A | 3.416    | H76A | H78A | 2.087    |
| H76A | H78B | 2.091    | H76A | H78C | 3.315    |
| H76B | H78A | 3.460    | H76C | H78A | 3.462    |
| H76C | H78B | 3.013    | H78A | H79A | 2.552    |
| H78A | H79B | 2.966    | H78A | H80B | 3.546    |
| H78A | H80C | 3.546    | H78B | H79B | 3.570    |
| H78B | H80A | 3.549    | H78B | H80B | 2.927    |
| H78B | H80C | 2.450    | H78C | H79A | 2.987    |
| H78C | H79B | 2.469    | H78C | H79C | 3.565    |
| H78C | H80A | 3.549    | H78C | H80B | 2.450    |
| H78C | H80C | 2.927    | H79A | H80A | 3.591    |
| H79A | H80B | 3.568    | H79B | H80A | 2.992    |
| H79B | H80B | 2.485    | H79B | H80C | 3.580    |
| H79C | H80A | 2.518    | H79C | H80B | 2.946    |
| H79C | H80C | 3.595    |
Table S6-12. Intermolecular contacts less than 3.60 Å

| atom | atom   | distance     | atom   | atom   | distance     |
|------|--------|--------------|--------|--------|--------------|
| C19  | C19\(^1\) | 3.341(15)    | C26    | C59\(^2\) | 3.57(2)      |
| C30  | C38\(^3\) | 3.599(18)    | C38    | C30\(^4\) | 3.599(18)    |
| C59  | C26\(^3\) | 3.57(2)      | C59    | C59\(^6\) | 3.351(16)    |
| C67  | C75\(^3\) | 3.588(18)    | C75    | C67\(^4\) | 3.588(18)    |

Symmetry Operators:

1. \(-X+1,-Y+2,-Z+1\)
2. \(X,Y-1,Z\)
3. \(X+1,Y,Z\)
4. \(X-1,Y,Z\)
5. \(X,Y+1,Z\)
6. \(-X+1,-Y+3,-Z+2\)
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens

| Atom | Atom | Distance | Atom | Atom | Distance |
|------|------|----------|------|------|----------|
| C1   | H31C¹ | 3.275    | C2   | H31C¹ | 3.074    |
| C3   | H3²   | 3.396    | C3   | H9A²  | 3.019    |
| C3   | H31C¹ | 2.973    | C3   | H38C² | 3.293    |
| C4   | H9A²  | 2.807    | C4   | H30A¹ | 3.205    |
| C4   | H31C¹ | 3.044    | C4   | H38C² | 3.366    |
| C4   | H78C³ | 3.030    | C5   | H29B¹ | 3.158    |
| C5   | H31C¹ | 3.166    | C5   | H78C³ | 2.995    |
| C5   | H79B³ | 3.458    | C6   | H29B¹ | 3.490    |
| C6   | H31C¹ | 3.285    | C8   | H12B¹ | 3.548    |
| C8   | H12C¹ | 3.072    | C8   | H18⁴  | 3.595    |
| C8   | H31C¹ | 3.590    | C9   | H4²   | 3.434    |
| C9   | H17⁴  | 2.967    | C9   | H18⁴  | 3.014    |
| C9   | H40A² | 3.424    | C12  | H8A¹  | 3.402    |
| C12  | H8C¹  | 3.225    | C12  | H18⁴  | 3.560    |
| C12  | H19⁵  | 3.445    | C13  | H21C³ | 3.307    |
| C13  | H39B³ | 3.038    | C13  | H39C³ | 3.520    |
| C14  | H29B¹ | 3.371    | C14  | H39B³ | 3.431    |
| C14  | H71A⁵ | 3.523    | C15  | H69C  | 3.574    |
| C15  | H70C  | 3.170    | C16  | H70C  | 2.973    |
| C17  | H9B⁶  | 3.432    | C17  | H9C⁶  | 3.055    |
| C17  | H40A³ | 3.161    | C17  | H70C  | 2.987    |
| C18  | H9B⁶  | 3.305    | C18  | H9C⁶  | 3.084    |
| C18  | H12A⁵ | 3.399    | C18  | H22A⁵ | 3.185    |
| C18  | H22C⁵ | 3.490    | C18  | H69C  | 3.325    |
| C18  | H70C  | 3.174    | C18  | H71B  | 3.312    |
| C19  | H12A⁵ | 3.176    | C19  | H19⁵  | 2.908    |
| C19  | H22A⁵ | 3.299    | C19  | H22C⁵ | 3.595    |
| C19  | H69C  | 2.637    | C19  | H70C  | 3.352    |
| C19  | H71B  | 3.577    | C20  | H19⁵  | 3.169    |
| C20  | H69C  | 2.763    | C20  | H70C  | 3.315    |
| C21  | H13A³ | 3.233    | C21  | H14A³ | 3.516    |
| C21  | H79B  | 3.554    | C22  | H18⁴  | 3.416    |
| C22  | H19⁵  | 3.348    | C22  | H38B⁷ | 3.573    |
| C22  | H69B  | 3.577    | C22  | H69C  | 3.097    |
| C26  | H49B⁸ | 3.569    | C26  | H49C⁸ | 3.285    |
| C26  | H59⁴  | 3.572    | C27  | H70A  | 3.527    |
| C29  | H12C¹ | 3.456    | C29  | H14C¹ | 3.281    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C30  | H38A | 3.108    | C30  | H38B | 3.569    |
| C30  | H38C | 3.552    | C30  | H78B | 3.553    |
| C30  | H78C | 3.565    | C31  | H8A  | 3.050    |
| C35  | H43  | 3.303    | C35  | H66B | 3.251    |
| C35  | H66C | 3.449    | C35  | H67A | 3.468    |
| C35  | H67C | 3.482    | C36  | H43  | 3.510    |
| C36  | H49A | 3.479    | C36  | H61C | 3.327    |
| C38  | H3   | 3.321    | C38  | H30A | 3.327    |
| C38  | H30B | 2.965    | C39  | H13C | 2.920    |
| C39  | H14B | 3.219    | C39  | H22A | 3.547    |
| C40  | H17  | 3.490    | C41  | H65B | 3.443    |
| C42  | H65B | 3.562    | C42  | H66C | 3.093    |
| C43  | H35B | 3.022    | C43  | H36C | 3.574    |
| C43  | H65B | 3.462    | C44  | H66C | 2.766    |
| C44  | H34C | 3.502    | C44  | H35B | 3.328    |
| C44  | H52B | 2.814    | C44  | H53C | 3.229    |
| C44  | H65B | 3.208    | C44  | H66C | 3.276    |
| C44  | H67C | 3.221    | C44  | H75B | 3.594    |
| C45  | H45  | 3.440    | C45  | H52B | 2.944    |
| C45  | H53C | 3.420    | C45  | H65B | 2.992    |
| C45  | H75B | 3.540    | C46  | H65B | 3.102    |
| C47  | H66C | 3.514    | C48  | H54B | 3.403    |
| C48  | H59  | 3.456    | C49  | H26A | 3.218    |
| C49  | H36C | 3.482    | C49  | H66C | 3.315    |
| C49  | H76A | 3.526    | C49  | H76C | 3.314    |
| C50  | H61B | 3.243    | C50  | H76B | 3.590    |
| C50  | H76C | 3.133    | C52  | H44  | 3.476    |
| C52  | H57  | 3.005    | C52  | H58  | 2.984    |
| C52  | H74B | 3.283    | C53  | H44  | 3.367    |
| C54  | H48B | 3.208    | C54  | H65B | 3.571    |
| C55  | H25B | 3.431    | C55  | H25C | 3.318    |
| C56  | H25C | 2.947    | C57  | H25C | 2.904    |
| C57  | H52A | 3.499    | C57  | H52C | 3.035    |
| C57  | H74B | 3.182    | C58  | H25C | 3.179    |
| C58  | H26B | 2.997    | C58  | H48A | 3.528    |
| C58  | H52A | 3.305    | C58  | H52C | 3.046    |
| C58  | H62C | 2.905    | C59  | H25C | 3.507    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom     | distance | atom   | atom     | distance |
|--------|----------|----------|--------|----------|----------|
| C59    | H26B^6   | 2.826    | C59    | H26C^6   | 3.447    |
| C59    | H48A^12  | 3.228    | C59    | H59^12   | 2.914    |
| C59    | H62C^12  | 3.107    | C60    | H25C^6   | 3.559    |
| C60    | H26B^6   | 3.471    | C60    | H26C^6   | 3.534    |
| C60    | H59^12   | 3.238    | C61    | H49A^13  | 3.509    |
| C61    | H50A^13  | 3.199    |        |          |          |
|        |          |          | C62    | H59      | 3.238    |
| C65    | H54B^8   | 3.201    | C66    | H26B^6   | 3.471    |
| C66    | H35B^7   | 3.278    | C66    | H26C^6   | 3.534    |
| C66    | H49B^8   | 3.078    | C67    | H35C^7   | 3.420    |
| C67    | H35C^7   | 3.405    |        |          |          |
| C67    | H35B^7   | 3.507    | C67    | H75C^7   | 3.424    |
| C69    | H14B^5   | 3.555    | C69    | H22B     | 3.415    |
| C74    | H57^13   | 3.412    | C75    | H45^10   | 3.506    |
| C75    | H67B^11  | 3.071    | C75    | H67C^11  | 3.193    |
| C76    | H49C^13  | 3.045    | C76    | H50B^13  | 3.030    |
| C76    | H62B^11  | 3.597    | C78    | H4^3     | 3.448    |
| C78    | H5^3     | 3.265    | C78    | H30A^14  | 3.224    |
| C79    | H5^3     | 3.413    | C79    | H14A^3   | 3.566    |
| C79    | H21B     | 3.217    | C80    | H10B^6   | 3.501    |
| H3     | C3^2     | 3.396    | H3     | C3^2     | 3.321    |
| H3     | H3^2     | 3.062    | H3     | H9A^2    | 2.966    |
| H3     | H10A^2   | 3.425    | H3     | H31C^1   | 3.423    |
| H3     | H38B^2   | 3.063    | H3     | H38C^2   | 2.720    |
| H3     | H40A^2   | 3.417    | H3     | H40C^2   | 3.154    |
| H4     | C9^2     | 3.434    | H4     | C78^3    | 3.448    |
| H4     | H9A^2    | 2.581    | H4     | H9C^2    | 3.547    |
| H4     | H10A^2   | 2.956    | H4     | H30A^1   | 3.016    |
| H4     | H31C^1   | 3.544    | H4     | H38C^2   | 2.891    |
| H4     | H78C^3   | 2.522    | H4     | H80B^3   | 3.022    |
| H5     | C78^3    | 3.265    | H5     | C79^3    | 3.413    |
| H5     | H29B^1   | 3.039    | H5     | H78A^3   | 3.424    |
| H5     | H78C^3   | 2.418    | H5     | H79A^3   | 3.583    |
| H5     | H79B^3   | 2.604    | H8A    | C12^1    | 3.402    |
| H8A    | C31^1    | 3.050    | H8A    | H12B^1   | 3.007    |
| H8A    | H12C^1   | 2.997    | H8A    | H18^4    | 3.335    |
| H8A    | H22C^1   | 3.560    | H8A    | H31A^1   | 2.958    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom       | distance | atom   | atom       | distance |
|--------|------------|----------|--------|------------|----------|
| H8A    | H31B\(^1\) | 2.841    | H8A    | H31C\(^1\) | 2.829    |
| H8B    | H12C\(^1\) | 3.248    | H8C    | C12\(^1\)  | 3.225    |
| H8C    | H12A\(^1\) | 3.417    | H8C    | H12B\(^1\) | 3.308    |
| H8C    | H12C\(^1\) | 2.503    | H8C    | H18\(^4\)  | 3.132    |
| H8C    | H71B\(^4\) | 3.283    | H9A    | C3\(^2\)   | 3.019    |
| H9A    | C4\(^2\)   | 2.807    | H9A    | H3\(^2\)   | 2.966    |
| H9A    | H4\(^2\)   | 2.581    | H9A    | H17\(^4\)  | 3.092    |
| H9A    | H40A\(^2\) | 3.185    | H9A    | H40C\(^2\) | 3.519    |
| H9B    | C17\(^4\)  | 3.432    | H9B    | C18\(^4\)  | 3.305    |
| H9B    | H17\(^4\)  | 2.862    | H9B    | H18\(^4\)  | 2.619    |
| H9B    | H38B\(^2\) | 2.918    | H9B    | H40A\(^2\) | 2.901    |
| H9C    | C17\(^4\)  | 3.055    | H9C    | C18\(^4\)  | 3.084    |
| H9C    | H4\(^2\)   | 3.547    | H9C    | H17\(^4\)  | 2.476    |
| H9C    | H18\(^4\)  | 2.542    | H9C    | H80B\(^4\) | 3.212    |
| H10A   | H3\(^2\)   | 3.425    | H10A   | H4\(^2\)   | 2.956    |
| H10A   | H80B\(^4\) | 3.464    | H10A   | C80\(^4\)  | 3.501    |
| H10B   | H80B\(^4\) | 2.909    | H10B   | H80C\(^4\) | 3.383    |
| H12A   | C18\(^5\)  | 3.399    | H12A   | C19\(^5\)  | 3.176    |
| H12A   | H8C\(^1\)  | 3.417    | H12A   | H18\(^5\)  | 2.940    |
| H12A   | H19\(^5\)  | 2.500    | H12A   | H69C\(^5\) | 3.523    |
| H12A   | H71B\(^5\) | 3.180    | H12B   | C8\(^1\)   | 3.548    |
| H12B   | H8A\(^1\)  | 3.007    | H12B   | H8C\(^1\)  | 3.308    |
| H12B   | H18\(^5\)  | 3.592    | H12C   | C8\(^1\)   | 3.072    |
| H12C   | C29\(^1\)  | 3.456    | H12C   | H8A\(^1\)  | 2.997    |
| H12C   | H8B\(^1\)  | 3.248    | H12C   | H8C\(^1\)  | 2.503    |
| H12C   | H29A\(^1\) | 3.000    | H12C   | H29B\(^1\) | 3.011    |
| H12C   | H31A\(^1\) | 3.496    | H12C   | H31C\(^1\) | 3.548    |
| H12C   | H71A\(^5\) | 3.573    | H12C   | H71B\(^5\) | 3.252    |
| H13A   | C21\(^3\)  | 3.233    | H13A   | H21B\(^3\) | 3.359    |
| H13A   | H21C\(^3\) | 2.361    | H13A   | H39B\(^3\) | 2.795    |
| H13C   | C39\(^3\)  | 2.920    | H13C   | H19\(^5\)  | 3.510    |
| H13C   | H21C\(^3\) | 3.569    | H13C   | H39A\(^3\) | 3.322    |
| H13C   | H39B\(^3\) | 2.445    | H13C   | H39C\(^3\) | 2.606    |
| H14A   | C21\(^3\)  | 3.516    | H14A   | C79\(^3\)  | 3.566    |
| H14A   | H21B\(^3\) | 2.943    | H14A   | H21C\(^3\) | 3.242    |
| H14A   | H39B\(^3\) | 3.195    | H14A   | H79A\(^3\) | 3.328    |
| H14A   | H79B\(^3\) | 2.902    | H14B   | C39\(^3\)  | 3.219    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H14B  | C69^5 | 3.555    | H14B  | H35C^3| 3.592    |
| H14B  | H39A^3| 2.870    | H14B  | H39B^3| 2.928    |
| H14B  | H39C^3| 3.340    | H14B  | H67A^5| 3.168    |
| H14B  | H69A^5| 2.839    | H14B  | H69C^5| 3.433    |
| H14B  | H71A^5| 3.215    | H14C  | C29^1 | 3.281    |
| H14C  | H29A^1| 3.380    | H14C  | H29B^1| 2.479    |
| H14C  | H29C^1| 3.585    | H14C  | H67A^5| 3.461    |
| H14C  | H71A^5| 2.930    | H17   | C9^6  | 2.967    |
| H17   | C40^3 | 3.490    | H17   | H9A^6 | 3.092    |
| H17   | H9B^6 | 2.862    | H17   | H9C^6 | 2.476    |
| H17   | H40A^3| 2.571    | H17   | H70C  | 3.434    |
| H18   | C8^6  | 3.595    | H18   | C9^6  | 3.014    |
| H18   | C12^3 | 3.560    | H18   | C22^3 | 3.416    |
| H18   | H8A^6 | 3.335    | H18   | H8C^6 | 3.132    |
| H18   | H9B^6 | 2.619    | H18   | H9C^6 | 2.542    |
| H18   | H12A^5| 2.940    | H18   | H12B^5| 3.592    |
| H18   | H22A^5| 3.000    | H18   | H22C^5| 2.963    |
| H18   | H71B  | 3.194    | H19   | C12^3 | 3.445    |
| H19   | C19^3 | 2.908    | H19   | C20^3 | 3.169    |
| H19   | C22^3 | 3.348    | H19   | H12A^5| 2.500    |
| H19   | H13C^5| 3.510    | H19   | H19^5 | 2.748    |
| H19   | H22A^5| 3.176    | H19   | H22C^5| 3.152    |
| H19   | H69C  | 2.692    | H21B  | C79   | 3.217    |
| H21B  | H13A^3| 3.359    | H21B  | H14A^3| 2.943    |
| H21B  | H70C  | 3.467    | H21B  | H79A  | 3.478    |
| H21B  | H79B  | 2.594    | H21B  | H79C  | 3.118    |
| H21C  | C13^3 | 3.307    | H21C  | H13A^3| 2.361    |
| H21C  | H13C^3| 3.569    | H21C  | H14A^3| 3.242    |
| H21C  | H40A^3| 3.480    | H21C  | H40B^3| 3.339    |
| H22A  | C18^3 | 3.185    | H22A  | C19^3 | 3.299    |
| H22A  | C39^7 | 3.547    | H22A  | H18^5 | 3.000    |
| H22A  | H19^5 | 3.176    | H22A  | H38B^7| 3.013    |
| H22A  | H39A^7| 3.585    | H22A  | H39C^7| 2.725    |
| H22A  | H69C  | 3.017    | H22B  | C69   | 3.415    |
| H22B  | H38B^7| 3.449    | H22B  | H69B  | 2.984    |
| H22B  | H69C  | 2.957    | H22C  | C18^3 | 3.490    |
| H22C  | C19^5 | 3.595    | H22C  | H8A^1 | 3.560    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom     | atom     | distance | atom     | atom     | distance |
|----------|----------|----------|----------|----------|----------|
| H22C     | H18      | 2.963    | H22C     | H19      | 3.152    |
| H25C     | C55      | 3.431    | H25C     | C55      | 3.318    |
| H25C     | C56      | 2.947    | H25C     | C57      | 2.904    |
| H25C     | C58      | 3.179    | H25C     | C59      | 3.507    |
| H25C     | C60      | 3.559    | H25C     | H57      | 3.273    |
| H25C     | H61      | 3.232    | H26A     | C49      | 3.218    |
| H26A     | H49B     | 2.775    | H26A     | H49C     | 2.765    |
| H26B     | C58      | 2.997    | H26B     | C59      | 2.826    |
| H26B     | C60      | 3.471    | H26B     | H48A     | 3.055    |
| H26B     | H48B     | 3.461    | H26B     | H49B     | 3.563    |
| H26B     | H49C     | 3.242    | H26B     | H58      | 3.112    |
| H26B     | H59      | 2.845    | H26B     | C59      | 3.447    |
| H26C     | C60      | 3.534    | H26C     | H49C     | 3.326    |
| H26C     | H59      | 3.439    | H26C     | H62B     | 3.039    |
| H27A     | H70      | 3.310    | H27B     | H52      | 3.180    |
| H27B     | H53B     | 3.056    | H27B     | H54      | 2.951    |
| H27C     | H66A     | 3.585    | H27B     | H70A     | 3.566    |
| H27C     | H66A     | 3.160    | H27C     | H66B     | 3.231    |
| H27C     | H69B     | 2.871    | H27C     | H70A     | 3.138    |
| H29A     | H12C     | 3.000    | H29A     | H14C     | 3.380    |
| H29A     | H71A     | 3.239    | H29A     | H71B     | 3.589    |
| H29A     | H71C     | 3.452    | H29B     | C5       | 3.158    |
| H29B     | C6       | 3.490    | H29B     | C14      | 3.371    |
| H29B     | H5       | 3.039    | H29B     | H12C     | 3.011    |
| H29B     | H14C     | 2.479    | H29B     | H71A     | 3.588    |
| H29B     | H78A     | 3.315    | H29B     | H78C     | 3.270    |
| H29C     | H14C     | 3.585    | H29C     | H71A     | 3.503    |
| H29C     | H78A     | 3.362    | H30A     | C4       | 3.205    |
| H30A     | C38      | 3.327    | H30A     | C7       | 3.224    |
| H30A     | H4       | 3.016    | H30A     | H36A     | 3.512    |
| H30A     | H38A     | 3.024    | H30A     | H38B     | 3.387    |
| H30A     | H38C     | 3.026    | H30A     | H78A     | 3.389    |
| H30A     | H78B     | 3.022    | H30A     | H78C     | 2.756    |
| H30B     | C38      | 2.965    | H30B     | H35A     | 3.510    |
| H30B     | H38A     | 2.397    | H30B     | H38B     | 2.884    |
| H30B     | H38C     | 3.164    | H30C     | H38A     | 3.534    |
| H30C     | H49B     | 3.535    | H30C     | H49C     | 3.387    |
Table S6-13: Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom        | distance | atom   | atom        | distance |
|--------|-------------|----------|--------|-------------|----------|
| H30C   | H78A\textsuperscript{9} | 3.508    | H30C   | H78B\textsuperscript{9} | 3.168    |
| H30C   | H78C\textsuperscript{9} | 3.558    | H31A   | H8A\textsuperscript{1}  | 2.958    |
| H31A   | H12C\textsuperscript{1} | 3.496    | H31B   | H8A\textsuperscript{1}  | 2.841    |
| H31B   | H38B\textsuperscript{7} | 3.237    | H31C   | C1\textsuperscript{1}  | 3.275    |
| H31C   | C2\textsuperscript{1}  | 3.074    | H31C   | C3\textsuperscript{1}  | 2.973    |
| H31C   | C4\textsuperscript{1}  | 3.044    | H31C   | C5\textsuperscript{1}  | 3.166    |
| H31C   | C6\textsuperscript{1}  | 3.285    | H31C   | C8\textsuperscript{1}  | 3.590    |
| H31C   | H3\textsuperscript{1}  | 3.423    | H31C   | H4\textsuperscript{1}  | 3.544    |
| H31C   | H8A\textsuperscript{1} | 2.829    | H31C   | H12C\textsuperscript{1} | 3.548    |
| H34C   | C44\textsuperscript{10} | 3.502    | H34C   | H43\textsuperscript{10} | 3.086    |
| H34C   | H44\textsuperscript{10} | 2.790    | H34C   | H53B         | 3.391    |
| H35A   | C66\textsuperscript{11} | 3.596    | H35A   | H30B\textsuperscript{11} | 3.510    |
| H35A   | H66B\textsuperscript{11} | 2.877    | H35A   | H66C\textsuperscript{11} | 3.443    |
| H35A   | H69A\textsuperscript{11} | 3.302    | H35A   | H69B\textsuperscript{11} | 3.554    |
| H35B   | C43\textsuperscript{10} | 3.022    | H35B   | C44\textsuperscript{10} | 3.328    |
| H35B   | C66\textsuperscript{11} | 3.278    | H35B   | C67\textsuperscript{11} | 3.596    |
| H35B   | H43\textsuperscript{10} | 2.368    | H35B   | H44\textsuperscript{10} | 2.999    |
| H35B   | H49A\textsuperscript{10} | 3.470    | H35B   | H49B\textsuperscript{10} | 3.233    |
| H35B   | H66B\textsuperscript{11} | 2.971    | H35B   | H66C\textsuperscript{11} | 2.739    |
| H35B   | H67A\textsuperscript{11} | 3.408    | H35B   | H67C\textsuperscript{11} | 3.025    |
| H35C   | C67\textsuperscript{11} | 3.420    | H35C   | H14B\textsuperscript{3} | 3.592    |
| H35C   | H66B\textsuperscript{11} | 3.387    | H35C   | H67A\textsuperscript{11} | 2.873    |
| H35C   | H67C\textsuperscript{11} | 3.078    | H35C   | H67A\textsuperscript{11} | 3.243    |
| H36A   | H30A\textsuperscript{11} | 3.512    | H36A   | H49A\textsuperscript{10} | 3.468    |
| H36A   | H78B\textsuperscript{4} | 3.351    | H36B   | H61C\textsuperscript{4} | 3.193    |
| H36B   | H80C\textsuperscript{4} | 3.294    | H36C   | C43\textsuperscript{10} | 3.574    |
| H36C   | C49\textsuperscript{10} | 3.482    | H36C   | H43\textsuperscript{10} | 2.648    |
| H36C   | H49A\textsuperscript{10} | 2.658    | H36C   | H49B\textsuperscript{10} | 3.480    |
| H36C   | H61C\textsuperscript{4} | 2.632    | H38A   | C30\textsuperscript{11} | 3.108    |
| H38A   | H30A\textsuperscript{11} | 3.024    | H38A   | H30B\textsuperscript{11} | 2.397    |
| H38A   | H30C\textsuperscript{11} | 3.534    | H38B   | C2\textsuperscript{21}  | 3.573    |
| H38B   | C30\textsuperscript{11} | 3.569    | H38B   | H3\textsuperscript{2}  | 3.063    |
| H38B   | H9B\textsuperscript{3}  | 2.918    | H38B   | H22A\textsuperscript{11} | 3.013    |
| H38B   | H22B\textsuperscript{11} | 3.449    | H38B   | H30A\textsuperscript{11} | 3.387    |
| H38B   | H30B\textsuperscript{11} | 2.884    | H38B   | H31B\textsuperscript{11} | 3.237    |
| H38C   | C3\textsuperscript{2}   | 3.293    | H38C   | C4\textsuperscript{2}   | 3.366    |
| H38C   | C30\textsuperscript{11} | 3.552    | H38C   | H3\textsuperscript{2}  | 2.720    |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H38C | H4   | 2.891    | H38C | H30A | 3.026    |
| H38C | H30B | 3.164    | H39A | H13C | 3.322    |
| H39A | H14B | 2.870    | H39A | H22A | 3.585    |
| H39A | H69A | 3.005    | H39B | C13  | 3.038    |
| H39B | C14  | 3.431    | H39B | H13A | 2.795    |
| H39B | H13C | 2.445    | H39B | H14A | 3.195    |
| H39B | H14B | 2.928    | H39C | C13  | 3.520    |
| H39C | H13C | 2.606    | H39C | H14B | 3.340    |
| H39C | H22A | 2.725    | H40A | C9   | 3.424    |
| H40A | C17  | 3.161    | H40A | H3   | 3.417    |
| H40A | H9A  | 3.185    | H40A | H9B  | 2.901    |
| H40A | H17  | 2.571    | H40A | H21C | 3.480    |
| H40B | H21C | 3.339    | H40C | H3   | 3.154    |
| H40C | H9A  | 3.519    | H43  | C35  | 3.303    |
| H43  | C36  | 3.510    | H43  | H34C | 3.086    |
| H43  | H35B | 2.368    | H43  | H36C | 2.648    |
| H43  | H61C | 3.564    | H43  | H66C | 2.781    |
| H44  | C52  | 3.476    | H44  | C53  | 3.367    |
| H44  | H34C | 2.790    | H44  | H35B | 2.999    |
| H44  | H52B | 2.696    | H44  | H52C | 3.537    |
| H44  | H53B | 3.432    | H44  | H53C | 2.557    |
| H44  | H67C | 3.038    | H44  | H75B | 3.090    |
| H45  | C45  | 3.440    | H45  | C75  | 3.506    |
| H45  | H45  | 3.145    | H45  | H52B | 2.943    |
| H45  | H53C | 2.944    | H45  | H65B | 3.335    |
| H45  | H74B | 3.328    | H45  | H74C | 3.079    |
| H45  | H75B | 2.952    | H45  | H75C | 3.211    |
| H48A | C58  | 3.528    | H48A | C59  | 3.228    |
| H48A | H26B | 3.055    | H48A | H58  | 3.093    |
| H48A | H59  | 2.489    | H48B | C48  | 3.208    |
| H48B | C66  | 3.264    | H48B | H26B | 3.461    |
| H48B | H54A | 3.467    | H48B | H54B | 2.857    |
| H48B | H54C | 2.819    | H48B | H66A | 2.701    |
| H48B | H66C | 2.933    | H48C | H54B | 3.169    |
| H49A | C36  | 3.479    | H49A | C61  | 3.509    |
| H49A | H35B | 3.470    | H49A | H36A | 3.468    |
| H49A | H36C | 2.658    | H49A | H61B | 3.212    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H49A | H61C\textsuperscript{13} | 2.967 | H49A | H76A\textsuperscript{13} | 3.447 |
| H49A | H76C\textsuperscript{13} | 3.037 | H49B | C26\textsuperscript{8} | 3.569 |
| H49B | C66\textsuperscript{8} | 3.078 | H49B | H26A\textsuperscript{8} | 2.775 |
| H49B | H26B\textsuperscript{8} | 3.563 | H49B | H30C\textsuperscript{8} | 3.535 |
| H49B | H35B\textsuperscript{10} | 3.233 | H49B | H36C\textsuperscript{10} | 3.480 |
| H49B | H66A\textsuperscript{8} | 3.067 | H49B | H66B\textsuperscript{8} | 3.170 |
| H49B | H66C\textsuperscript{8} | 2.515 | H49C | C26\textsuperscript{8} | 3.285 |
| H49C | C76\textsuperscript{13} | 3.045 | H49C | H26A\textsuperscript{8} | 2.765 |
| H49C | H26B\textsuperscript{8} | 3.242 | H49C | H26C\textsuperscript{8} | 3.326 |
| H49C | H30C\textsuperscript{8} | 3.387 | H49C | H76A\textsuperscript{13} | 2.745 |
| H49C | H76C\textsuperscript{13} | 3.069 | H49C | H76C\textsuperscript{13} | 2.811 |
| H50A | C61\textsuperscript{13} | 3.199 | H50A | H61B\textsuperscript{13} | 2.314 |
| H50A | H61C\textsuperscript{13} | 3.323 | H50A | H76C\textsuperscript{13} | 2.895 |
| H50B | C76\textsuperscript{13} | 3.030 | H50B | H61B\textsuperscript{13} | 3.460 |
| H50B | H76A\textsuperscript{13} | 3.475 | H50B | H76B\textsuperscript{13} | 2.687 |
| H50B | H76C\textsuperscript{13} | 2.548 | H52A | C57\textsuperscript{4} | 3.499 |
| H52A | C58\textsuperscript{8} | 3.305 | H52A | H57\textsuperscript{4} | 2.960 |
| H52A | H58\textsuperscript{4} | 2.573 | H52A | H65B\textsuperscript{8} | 3.431 |
| H52A | H74B\textsuperscript{10} | 2.813 | H52A | H75C\textsuperscript{10} | 3.077 |
| H52B | C44\textsuperscript{10} | 2.814 | H52B | C45\textsuperscript{10} | 2.944 |
| H52B | H44\textsuperscript{10} | 2.696 | H52B | H45\textsuperscript{10} | 2.943 |
| H52B | H57\textsuperscript{4} | 3.064 | H52B | H74B\textsuperscript{10} | 2.994 |
| H52B | H74C\textsuperscript{10} | 3.368 | H52C | C57\textsuperscript{4} | 3.035 |
| H52C | C58\textsuperscript{8} | 3.046 | H52C | H27B | 3.180 |
| H52C | H44\textsuperscript{10} | 3.537 | H52C | H57\textsuperscript{4} | 2.508 |
| H52C | H58\textsuperscript{4} | 2.524 | H52C | H74B\textsuperscript{10} | 3.561 |
| H53B | H27B | 3.056 | H53B | H34C | 3.391 |
| H53B | H44\textsuperscript{10} | 3.432 | H53C | C44\textsuperscript{10} | 3.229 |
| H53C | C45\textsuperscript{10} | 3.420 | H53C | H44\textsuperscript{10} | 2.557 |
| H53C | H45\textsuperscript{10} | 2.944 | H54A | H48B\textsuperscript{8} | 3.467 |
| H54B | C48\textsuperscript{8} | 3.403 | H54B | C65\textsuperscript{8} | 3.201 |
| H54B | H48B\textsuperscript{8} | 2.857 | H54B | H48C\textsuperscript{8} | 3.169 |
| H54B | H58\textsuperscript{4} | 3.367 | H54B | H65A\textsuperscript{8} | 3.068 |
| H54B | H65B\textsuperscript{8} | 2.813 | H54B | H65C\textsuperscript{8} | 3.192 |
| H54C | H27B | 2.951 | H54C | H48B\textsuperscript{8} | 2.819 |
| H54C | H58\textsuperscript{4} | 3.395 | H57 | C52\textsuperscript{6} | 3.005 |
| H57 | C74\textsuperscript{15} | 3.412 | H57 | H25C\textsuperscript{6} | 3.273 |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom       | distance | atom   | atom       | distance |
|--------|------------|----------|--------|------------|----------|
| H57    | H52A       | 2.960    | H57    | H52B       | 3.064    |
| H57    | H52C       | 2.508    | H57    | H74A       | 3.494    |
| H57    | H74B       | 2.542    | H58    | C52        | 2.984    |
| H58    | C62        | 3.443    | H58    | H26B       | 3.112    |
| H58    | H48A       | 3.093    | H58    | H52A       | 2.573    |
| H58    | H52C       | 2.524    | H58    | H54B       | 3.367    |
| H58    | H54C       | 3.395    | H58    | H62C       | 2.467    |
| H59    | C26        | 3.572    | H59    | C48        | 3.456    |
| H59    | C59        | 2.914    | H59    | C60        | 3.238    |
| H59    | C62        | 3.494    | H59    | H26B       | 2.845    |
| H59    | H26C       | 3.439    | H59    | H48A       | 2.489    |
| H59    | H59        | 2.749    | H59    | H62C       | 2.840    |
| H61B   | C50        | 3.243    | H61B   | H49A       | 3.212    |
| H61B   | H50A       | 2.314    | H61B   | H50B       | 3.460    |
| H61B   | H74A       | 3.563    | H61C   | C36        | 3.327    |
| H61C   | H25C       | 3.232    | H61C   | H36B       | 3.193    |
| H61C   | H36C       | 2.632    | H61C   | H43        | 3.564    |
| H61C   | H49A       | 2.967    | H61C   | H50A       | 3.323    |
| H62B   | C76        | 3.597    | H62B   | H26C       | 3.039    |
| H62B   | H75A       | 3.510    | H62B   | H75C       | 3.021    |
| H62B   | H76A       | 3.419    | H62B   | H76B       | 2.954    |
| H62B   | H76C       | 3.290    | H62C   | C59        | 3.107    |
| H62C   | H58        | 2.467    | H62C   | H59        | 2.840    |
| H62C   | H75C       | 3.301    | H62C   | H76B       | 3.375    |
| H65A   | H54B       | 3.068    | H65B   | C41        | 3.443    |
| H65B   | C42        | 3.562    | H65B   | C43        | 3.462    |
| H65B   | C44        | 3.208    | H65B   | C45        | 2.992    |
| H65B   | C46        | 3.102    | H65B   | C48        | 3.571    |
| H65B   | H45        | 3.335    | H65B   | H52A       | 3.431    |
| H65B   | H54B       | 2.813    | H65B   | H75C       | 3.576    |
| H65C   | H54B       | 3.192    | H65C   | H75C       | 3.351    |
| H66A   | H27B       | 3.585    | H66A   | H27C       | 3.160    |
| H66A   | H48B       | 2.701    | H66A   | H49B       | 3.067    |
| H66B   | C35        | 3.251    | H66B   | H27C       | 3.231    |
| H66B   | H35A       | 2.877    | H66B   | H35B       | 2.971    |
| H66B   | H35C       | 3.387    | H66B   | H49B       | 3.170    |
| H66C   | C35        | 3.449    | H66C   | C42        | 3.093    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H66C | C43^8 | 2.766 | H66C | C44^8 | 3.276 |
| H66C | C47^8 | 3.514 | H66C | C49^8 | 3.315 |
| H66C | H35A^7 | 3.443 | H66C | H35B^7 | 2.739 |
| H66C | H43^8 | 2.781 | H66C | H48B^8 | 2.933 |
| H66C | H49B^8 | 2.515 | H67A | C35^2 | 3.468 |
| H67A | H14B^5 | 3.168 | H67A | H14C^5 | 3.461 |
| H67A | H35B^7 | 3.408 | H67A | H35C^7 | 2.873 |
| H67B | C75^7 | 3.071 | H67B | H75A^7 | 2.630 |
| H67B | H75B^7 | 3.253 | H67B | H75C^7 | 2.848 |
| H67C | C35^2 | 3.482 | H67C | C44^8 | 3.221 |
| H67C | C75^7 | 3.193 | H67C | H35B^7 | 3.025 |
| H67C | H35C^7 | 3.078 | H67C | H44^8 | 3.038 |
| H67C | H75A^7 | 3.053 | H67C | H75B^7 | 2.877 |
| H67C | H75C^7 | 3.109 | H69A | H14B^5 | 2.839 |
| H69A | H35A^7 | 3.302 | H69A | H35C^7 | 3.243 |
| H69A | H39A^7 | 3.005 | H69B | C22 | 3.577 |
| H69B | H22B | 2.984 | H69B | H27C | 2.871 |
| H69B | H35A^7 | 3.554 | H69C | C15 | 3.574 |
| H69C | C18 | 3.325 | H69C | C19 | 2.637 |
| H69C | C20 | 2.763 | H69C | C22 | 3.097 |
| H69C | H12A^5 | 3.523 | H69C | H14B^5 | 3.433 |
| H69C | H19 | 2.692 | H69C | H22A | 3.017 |
| H69C | H22B | 2.957 | H70A | C27 | 3.527 |
| H70A | H27A | 3.310 | H70A | H27B | 3.566 |
| H70A | H27C | 3.138 | H70C | C15 | 3.170 |
| H70C | C16 | 2.973 | H70C | C17 | 2.987 |
| H70C | C18 | 3.174 | H70C | C19 | 3.352 |
| H70C | C20 | 3.315 | H70C | H17 | 3.434 |
| H70C | H21B | 3.467 | H71A | C14^4 | 3.523 |
| H71A | H12C^3 | 3.573 | H71A | H14B^5 | 3.215 |
| H71A | H14C^5 | 2.930 | H71A | H29A^6 | 3.239 |
| H71A | H29B^6 | 3.588 | H71A | H29C^6 | 3.503 |
| H71B | C18 | 3.312 | H71B | C19 | 3.577 |
| H71B | H8C^6 | 3.283 | H71B | H12A^5 | 3.180 |
| H71B | H12C^3 | 3.252 | H71B | H18 | 3.194 |
| H71B | H29A^6 | 3.589 | H71C | H29A^6 | 3.452 |
| H74A | H57^13 | 3.494 | H74A | H61B^13 | 3.563 |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom    | distance | atom  | atom    | distance |
|-------|---------|----------|-------|---------|----------|
| H74B  | C52     | 3.283    | H74B  | C57     | 3.182    |
| H74B  | H45     | 3.328    | H74B  | H52A    | 2.813    |
| H74B  | H52B    | 2.994    | H74B  | H52C    | 3.561    |
| H74B  | H57     | 2.542    | H74C  | H45     | 3.079    |
| H74C  | H52B    | 3.368    | H75A  | C67     | 3.244    |
| H75A  | H62B    | 3.510    | H75A  | H67B    | 2.630    |
| H75A  | H67C    | 3.053    | H75B  | C44     | 3.594    |
| H75B  | C45     | 3.540    | H75B  | C67     | 3.507    |
| H75B  | H44     | 3.090    | H75B  | H45     | 2.952    |
| H75B  | H67B    | 3.253    | H75B  | H67C    | 2.877    |
| H75C  | C62     | 3.505    | H75C  | C67     | 3.424    |
| H75C  | H45     | 3.211    | H75C  | H52A    | 3.077    |
| H75C  | H62B    | 3.021    | H75C  | H62C    | 3.301    |
| H75C  | H65B    | 3.576    | H75C  | H65C    | 3.351    |
| H75C  | H67B    | 2.848    | H75C  | H67C    | 3.109    |
| H76A  | C49     | 3.526    | H76A  | H49A    | 3.447    |
| H76A  | H49C    | 2.745    | H76A  | H50B    | 3.475    |
| H76A  | H62B    | 3.419    | H76B  | C50     | 3.590    |
| H76B  | H49C    | 3.069    | H76B  | H50B    | 2.687    |
| H76B  | H62B    | 2.954    | H76B  | H62C    | 3.375    |
| H76C  | C49     | 3.314    | H76C  | C50     | 3.133    |
| H76C  | H49A    | 3.037    | H76C  | H49C    | 2.811    |
| H76C  | H50A    | 2.895    | H76C  | H50B    | 2.548    |
| H78A  | H5      | 3.424    | H78A  | H29B    | 3.315    |
| H78A  | H29C    | 3.362    | H78A  | H30A    | 3.389    |
| H78A  | H30C    | 3.508    | H78B  | C30     | 3.553    |
| H78B  | H30A    | 3.022    | H78B  | H30C    | 3.168    |
| H78B  | H36A    | 3.351    | H78C  | C4      | 3.030    |
| H78C  | C5      | 2.995    | H78C  | C30     | 3.565    |
| H78C  | H4      | 2.522    | H78C  | H5      | 2.418    |
| H78C  | H29B    | 3.270    | H78C  | H30A    | 2.756    |
| H78C  | H30C    | 3.558    | H79A  | H5      | 3.583    |
| H79A  | H14A    | 3.328    | H79A  | H21B    | 3.478    |
| H79B  | C5      | 3.458    | H79B  | C21     | 3.554    |
| H79B  | H5      | 2.604    | H79B  | H14A    | 2.902    |
| H79B  | H21B    | 2.594    | H79C  | H21B    | 3.118    |
| H80B  | H4      | 3.022    | H80B  | H9C     | 3.212    |
Table S6-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom    | distance | atom   | atom    | distance |
|--------|---------|----------|--------|---------|----------|
| H80B   | H10A^6  | 3.464    | H80B   | H10B^6  | 2.909    |
| H80C   | H10B^6  | 3.383    | H80C   | H36B^6  | 3.294    |

Symmetry Operators:

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

\[ \text{Nb}(\text{N}=\text{C} \cdot \text{Bu}_2)_2(\text{OC}_6\text{F}_5)_3(\text{HN}=\text{C} \cdot \text{Bu}_2) \] (7)

November 21, 2017
Experimental

Data Collection

An orange block crystal of C$_{45}$H$_{55}$F$_{15}$N$_3$NbO$_3$ having approximate dimensions of 0.340 x 0.253 x 0.238 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-K$\alpha$ radiation.

The crystal-to-detector distance was 45.00 mm.

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

\begin{align*}
    a &= 11.3778(5) \text{ Å} & \alpha &= 86.879(3)^\circ \\
    b &= 12.9307(5) \text{ Å} & \beta &= 81.525(3)^\circ \\
    c &= 18.9950(6) \text{ Å} & \gamma &= 77.672(3)^\circ \\
    V &= 2699.58(18) \text{ Å}^3 \\
\end{align*}

For Z = 2 and F.W. = 1063.83, the calculated density is 1.309 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:

P-1 (#2)

The data were collected at a temperature of -180 ± 1°C to a maximum 2$\theta$ value of 61.3$^\circ$. A total of 720 oscillation images were collected. A sweep of data was done using $\omega$ scans from -105.0 to 75.0$^\circ$ in 0.50$^\circ$ step, at $\chi$=45.0$^\circ$ and $\phi$ = 0.0$^\circ$. The exposure rate was 32.0 [sec./$^\circ$]. The detector swing angle was -15.00$^\circ$. A second sweep was performed using $\omega$ scans from -105.0 to 75.0$^\circ$ in 0.50$^\circ$ step, at $\chi$=45.0$^\circ$ and $\phi$ = 90.0$^\circ$. The exposure rate was 32.0 [sec./$^\circ$]. The detector swing angle was -15.00$^\circ$. The crystal-to-detector distance was 45.00 mm. Readout was performed in the 0.172 mm pixel mode.
**Data Reduction**

Of the 0 reflections were collected, where 0 were unique ($R_{int} = 0.0339$). Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).  \(^1\)

The linear absorption coefficient, $\mu$, for Mo-K$\alpha$ radiation is 3.118 cm$^{-1}$. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.760 to 0.928. The data were corrected for Lorentz and polarization effects.

**Structure Solution and Refinement**

The structure was solved by direct methods\(^2\) and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model. The final cycle of full-matrix least-squares refinement\(^3\) on $F^2$ was based on 11596 observed reflections and 652 variable parameters and converged (largest parameter shift was 0.03 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum ||Fo| - |Fc|| / \sum |Fo| = 0.0643$$

$$wR2 = [\sum (w(Fo^2 - Fc^2)^2)/\sum w(Fo^2)^2]^{1/2} = 0.2013$$

The goodness of fit\(^4\) was 1.04. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.28 and -1.27 e$^\cdot/\text{Å}^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 \(^5\). 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 Version 2014/7\textsuperscript{10}.

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT Version 2014/5: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

\[
\sum w(F_0^2-F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.}
\]

(4) Goodness of fit is defined as:

\[
[w(F_0^2-F_c^2)^2/(N_O-N_V)]^{1/2}
\]

where: \(N_O = \) number of observations

\(N_V = \) number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2.5: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
### EXPERIMENTAL DETAILS

#### A. Crystal Data

| Property                              | Value                        |
|---------------------------------------|------------------------------|
| **Empirical Formula**                 | $\text{C}_{45}\text{H}_{55}\text{F}_{15}\text{N}_{3}\text{NbO}_{3}$ |
| **Formula Weight**                    | 1063.83                      |
| **Crystal Color, Habit**              | orange, block                |
| **Crystal Dimensions**                | $0.340 \times 0.253 \times 0.238 \text{ mm}$ |
| **Crystal System**                    | triclinic                    |
| **Lattice Type**                      | Primitive                    |
| **Lattice Parameters**                |                              |
| a                                      | $11.3778(5) \text{ Å}$       |
| b                                      | $12.9307(5) \text{ Å}$       |
| c                                      | $18.9950(6) \text{ Å}$       |
| $\alpha$                               | $86.879(3)^\circ$            |
| $\beta$                                | $81.525(3)^\circ$            |
| $\gamma$                               | $77.672(3)^\circ$            |
| V                                      | $2699.58(18) \text{ Å}^3$    |
| **Space Group**                       | P-1 (#2)                     |
| **Z value**                            | 2                            |
| **$D_{calc}$**                         | $1.309 \text{ g/cm}^3$       |
| **$F_{000}$**                          | 1092.00                      |
| **$\mu(\text{MoK}\alpha)$**          | $3.118 \text{ cm}^{-1}$     |
B. Intensity Measurements

Diffractometer  XtaLAB P200
Radiation  MoKα ($\lambda = 0.71075$ Å)
             multi-layer mirror monochromated
Voltage, Current  50kV, 24mA
Temperature  -180.0°C
Detector Aperture  83.8 x 70.0 mm
Data Images  720 exposures
$\omega$ oscillation Range ($\chi=45.0$, $\phi=0.0$)  -105.0 - 75.0°
Exposure Rate  32.0 sec./°
Detector Swing Angle  -15.00°
$\omega$ oscillation Range ($\chi=45.0$, $\phi=90.0$)  -105.0 - 75.0°
Exposure Rate  32.0 sec./°
Detector Swing Angle  -15.00°
Detector Position  45.00 mm
Pixel Size  0.172 mm
$2\theta_{\text{max}}$  55.0°
No. of Reflections Measured  Total: 22400
Unique: 11596 ($R_{\text{int}} = 0.0339$)

Corrections

Lorentz-polarization Absorption
(trans. factors: 0.760 - 0.928)
### C. Structure Solution and Refinement

| Structure Solution | Direct Methods (SHELXT Version 2014/5) |
|--------------------|----------------------------------------|
| Refinement         | Full-matrix least-squares on $F^2$      |
| Function Minimized | $\sum w (Fo^2 - Fc^2)^2$                |
| Least Squares Weights | $w = 1/ \left[ \sigma^2(Fo^2) + (0.0883 \cdot P)^2 + 11.0188 \cdot P \right]$ |
|                     | where $P = (\text{Max}(Fo^2,0) + 2Fc^2)/3$ |
| $2\theta_{\text{max}}$ cutoff | 55.0° |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. Observations (All reflections) | 11596 |
| No. Variables | 652 |
| Reflection/Parameter Ratio | 17.79 |
| Residuals: R1 ($I > 2.00\sigma(I)$) | 0.0643 |
| Residuals: R (All reflections) | 0.0723 |
| Residuals: wR2 (All reflections) | 0.2013 |
| Goodness of Fit Indicator | 1.043 |
| Max Shift/Error in Final Cycle | 0.032 |
| Maximum peak in Final Diff. Map | $1.28 \text{ e}^{-/\AA^3}$ |
| Minimum peak in Final Diff. Map | $-1.27 \text{ e}^{-/\AA^3}$ |
Table S7-1. Atomic coordinates and $B_{iso}/B_{eq}$ and occupancy

| atom  | x           | y           | z           | $B_{eq}$   | occ  |
|-------|-------------|-------------|-------------|------------|------|
| Nb1   | 0.60505(3)  | 0.28604(3)  | 0.71893(2)  | 2.140(10)  | 1    |
| F1    | 0.8874(3)   | 0.1173(2)   | 0.58205(15) | 3.13(5)    | 1    |
| F2    | 1.0662(3)   | 0.1384(2)   | 0.47469(16) | 3.86(6)    | 1    |
| F3    | 1.0742(2)   | 0.3317(2)   | 0.41165(14) | 3.31(5)    | 1    |
| F4    | 0.8978(3)   | 0.5029(2)   | 0.45545(14) | 3.08(5)    | 1    |
| F5    | 0.7183(3)   | 0.4826(2)   | 0.56250(14) | 3.10(5)    | 1    |
| F6    | 0.2630(2)   | 0.4506(2)   | 0.68884(14) | 2.63(4)    | 1    |
| F7    | 0.1209(2)   | 0.6433(2)   | 0.67403(15) | 3.31(5)    | 1    |
| F8    | 0.2162(3)   | 0.8203(2)   | 0.66778(17) | 3.88(6)    | 1    |
| F9    | 0.4550(3)   | 0.8017(2)   | 0.68216(15) | 3.19(5)    | 1    |
| F10   | 0.5985(2)   | 0.6100(2)   | 0.69836(14) | 2.49(4)    | 1    |
| F11   | 0.2773(2)   | 0.4059(3)   | 0.83333(14) | 3.52(6)    | 1    |
| F12   | 0.1284(2)   | 0.3943(3)   | 0.95731(15) | 3.71(6)    | 1    |
| F13   | 0.1951(3)   | 0.2450(3)   | 1.05854(17) | 4.96(8)    | 1    |
| F14   | 0.4124(4)   | 0.1054(3)   | 1.03393(18) | 5.88(9)    | 1    |
| F15   | 0.5619(3)   | 0.1143(2)   | 0.90982(16) | 4.00(6)    | 1    |
| O1    | 0.7108(3)   | 0.2905(3)   | 0.62867(16) | 2.57(5)    | 1    |
| O2    | 0.5053(3)   | 0.4300(2)   | 0.70281(16) | 2.24(5)    | 1    |
| O3    | 0.4945(3)   | 0.2627(2)   | 0.80607(16) | 2.65(5)    | 1    |
| N1    | 0.6990(3)   | 0.1427(3)   | 0.73511(18) | 2.11(6)    | 1    |
| N2    | 0.7092(3)   | 0.3664(3)   | 0.77004(19) | 2.41(6)    | 1    |
| N3    | 0.4688(3)   | 0.2327(3)   | 0.66375(18) | 2.22(6)    | 1    |
| C1    | 0.7570(4)   | 0.0503(3)   | 0.7462(2)   | 2.10(6)    | 1    |
| C2    | 0.8722(4)   | 0.0342(4)   | 0.7833(3)   | 2.91(8)    | 1    |
| C3    | 0.8530(5)   | -0.0210(6)  | 0.8549(3)   | 4.57(12)   | 1    |
| C4    | 0.9006(5)   | 0.1414(4)   | 0.7932(4)   | 4.89(14)   | 1    |
| C5    | 0.9845(5)   | -0.0306(6)  | 0.7354(4)   | 5.10(14)   | 1    |
| C6    | 0.7029(5)   | -0.0426(3)  | 0.7243(3)   | 2.86(8)    | 1    |
| C7    | 0.7861(8)   | -0.1523(5)  | 0.7167(4)   | 6.07(18)   | 1    |
| C8    | 0.6601(5)   | -0.0169(4)  | 0.6508(3)   | 3.63(9)    | 1    |
| C9    | 0.5921(7)   | -0.0464(6)  | 0.7796(3)   | 5.13(15)   | 1    |
| C10   | 0.7494(4)   | 0.4242(4)   | 0.8090(2)   | 2.26(7)    | 1    |
| C11   | 0.6779(5)   | 0.4464(4)   | 0.8844(3)   | 3.53(10)   | 1    |
| C12   | 0.6740(9)   | 0.3394(8)   | 0.9225(4)   | 3.23(15)   | 0.735(14) |
| C12A  | 0.626(3)    | 0.367(3)    | 0.9193(18)  | 4.7(7)     | 0.265(14) |
| C13   | 0.5393(6)   | 0.4975(6)   | 0.8713(4)   | 3.32(16)   | 0.735(14) |
| C13A  | 0.607(2)    | 0.557(2)    | 0.8819(12)  | 5.7(8)     | 0.265(14) |
Table S7-1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

| atom | x        | y        | z        | B_{eq}  | occ    |
|------|----------|----------|----------|---------|--------|
| C14  | 0.7088(12)| 0.5211(10)| 0.9320(4)| 5.9(3)  | 0.735(14) |
| C14A | 0.7839(16)| 0.4581(19)| 0.9386(7)| 3.6(4)  | 0.265(14) |
| C15  | 0.8655(4) | 0.4642(4) | 0.7791(3)| 3.09(9) | 1      |
| C16  | 0.9745(5) | 0.4042(5) | 0.8162(5)| 5.79(18)| 1      |
| C17  | 0.8489(5) | 0.5853(5) | 0.7871(4)| 4.30(11)| 1      |
| C18  | 0.8972(6) | 0.4407(5) | 0.6989(3)| 5.10(15)| 1      |
| C19  | 0.4021(4) | 0.2208(3) | 0.6181(2)| 1.89(6) | 1      |
| C20  | 0.2892(4) | 0.1718(4) | 0.6431(3)| 3.04(8) | 1      |
| C21  | 0.3097(5) | 0.0617(4) | 0.6092(4)| 4.97(15)| 1      |
| C22  | 0.1715(4) | 0.2419(4) | 0.6241(3)| 3.31(9) | 1      |
| C23  | 0.2713(6) | 0.1563(7) | 0.7243(4)| 6.9(2)  | 1      |
| C24  | 0.4435(4) | 0.2498(4) | 0.5392(2)| 2.33(7) | 1      |
| C25  | 0.3536(5) | 0.2532(4) | 0.4856(3)| 3.34(9) | 1      |
| C26  | 0.5605(4) | 0.1686(4) | 0.5142(3)| 3.01(8) | 1      |
| C27  | 0.4724(4) | 0.3614(4) | 0.5363(3)| 2.83(8) | 1      |
| C28  | 0.7975(3) | 0.2993(3) | 0.5756(2)| 1.91(6) | 1      |
| C29  | 0.8874(4) | 0.2135(3) | 0.5506(2)| 2.14(6) | 1      |
| C30  | 0.9796(4) | 0.2234(4) | 0.4959(2)| 2.53(7) | 1      |
| C31  | 0.9838(4) | 0.3209(4) | 0.4637(2)| 2.43(7) | 1      |
| C32  | 0.8948(4) | 0.4073(3) | 0.4864(2)| 2.21(7) | 1      |
| C33  | 0.8037(4) | 0.3967(3) | 0.5407(2)| 2.12(6) | 1      |
| C34  | 0.4358(3) | 0.5229(3) | 0.69419(19)| 1.66(6) | 1      |
| C35  | 0.3125(3) | 0.5365(3) | 0.6873(2)| 1.90(6) | 1      |
| C36  | 0.2397(4) | 0.6350(4) | 0.6789(2)| 2.21(7) | 1      |
| C37  | 0.2871(4) | 0.7244(3) | 0.6764(2)| 2.47(7) | 1      |
| C38  | 0.4081(5) | 0.7146(3) | 0.6832(2)| 2.13(6) | 1      |
| C39  | 0.4805(3) | 0.6163(3) | 0.6918(2)| 1.87(6) | 1      |
| C40  | 0.4234(4) | 0.2575(3) | 0.8666(2)| 1.94(6) | 1      |
| C41  | 0.3108(4) | 0.3287(3) | 0.8818(2)| 2.14(6) | 1      |
| C42  | 0.2347(4) | 0.3246(4) | 0.9449(2)| 2.73(8) | 1      |
| C43  | 0.2685(5) | 0.2485(4) | 0.9963(3)| 3.30(9) | 1      |
| C44  | 0.3796(6) | 0.1777(4) | 0.9839(3)| 3.63(10)| 1      |
| C45  | 0.4538(6) | 0.1825(3) | 0.9202(2)| 2.64(7) | 1      |

B_{eq} = \frac{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 S7-2. Atomic coordinates and B\textsubscript{iso} and occupancy involving hydrogen atoms

| atom  | x          | y          | z          | B\textsubscript{iso} | occ |
|-------|------------|------------|------------|-----------------------|-----|
| H1    | 0.4177(12) | 0.228(2)   | 0.7016(3)  | 15(4)                 | 1   |
| H3A   | 0.81992    | -0.08375   | 0.84967    | 5.480                 | 1   |
| H3B   | 0.79586    | 0.02745    | 0.88805    | 5.480                 | 1   |
| H3C   | 0.93081    | -0.04247   | 0.87339    | 5.480                 | 1   |
| H4A   | 0.91309    | 0.17722    | 0.74674    | 5.873                 | 1   |
| H4B   | 0.83267    | 0.18446    | 0.82358    | 5.873                 | 1   |
| H4C   | 0.97450    | 0.13180    | 0.81573    | 5.873                 | 1   |
| H5A   | 0.99609    | 0.00592    | 0.68916    | 6.115                 | 1   |
| H5B   | 1.05721    | -0.03694   | 0.75868    | 6.115                 | 1   |
| H5C   | 0.97064    | -0.10135   | 0.72850    | 6.115                 | 1   |
| H7A   | 0.85682    | -0.14875   | 0.68102    | 7.278                 | 1   |
| H7B   | 0.81326    | -0.17627   | 0.76257    | 7.278                 | 1   |
| H7C   | 0.74152    | -0.20233   | 0.70157    | 7.278                 | 1   |
| H8A   | 0.73041    | -0.01415   | 0.61466    | 4.359                 | 1   |
| H8B   | 0.61937    | -0.07189   | 0.63903    | 4.359                 | 1   |
| H8C   | 0.60331    | 0.05188    | 0.65207    | 4.359                 | 1   |
| H9A   | 0.53967    | 0.02435    | 0.78390    | 6.152                 | 1   |
| H9B   | 0.54687    | -0.09602   | 0.76470    | 6.152                 | 1   |
| H9C   | 0.61861    | -0.06995   | 0.82570    | 6.152                 | 1   |
| H12A  | 0.63943    | 0.27980    | 0.89558    | 2.393                 | 0.735(14) |
| H12B  | 0.75489    | 0.30745    | 0.93760    | 2.319                 | 0.735(14) |
| H12C  | 0.61956    | 0.33791    | 0.97051    | 3.778                 | 0.735(14) |
| H12D  | 0.68621    | 0.29948    | 0.91540    | 5.694                 | 0.265(14) |
| H12E  | 0.60113    | 0.38369    | 0.96961    | 5.694                 | 0.265(14) |
| H12F  | 0.55551    | 0.35994    | 0.89754    | 5.694                 | 0.265(14) |
| H13A  | 0.51256    | 0.45198    | 0.83996    | 3.990                 | 0.735(14) |
| H13B  | 0.48594    | 0.50332    | 0.91697    | 3.990                 | 0.735(14) |
| H13C  | 0.53583    | 0.56802    | 0.84893    | 3.990                 | 0.735(14) |
| H13D  | 0.65821    | 0.60175    | 0.85511    | 6.817                 | 0.265(14) |
| H13E  | 0.53575    | 0.55851    | 0.85837    | 6.817                 | 0.265(14) |
| H13F  | 0.58138    | 0.58227    | 0.93043    | 6.817                 | 0.265(14) |
| H14A  | 0.71076    | 0.58886    | 0.90665    | 7.070                 | 0.735(14) |
| H14B  | 0.64735    | 0.53218    | 0.97435    | 7.070                 | 0.735(14) |
| H14C  | 0.78863    | 0.49135    | 0.94639    | 7.070                 | 0.735(14) |
| H14D  | 0.82724    | 0.51339    | 0.91903    | 4.292                 | 0.265(14) |
| H14E  | 0.74252    | 0.47691    | 0.98656    | 4.292                 | 0.265(14) |
| H14F  | 0.84204    | 0.39047    | 0.94085    | 4.292                 | 0.265(14) |
Table S7-2. Atomic coordinates and $B_{iso}$ involving hydrogens/$B_{eq}$ and occupancy (continued)

| atom  | x       | y       | z       | $B_{eq}$ | occ |
|-------|---------|---------|---------|----------|-----|
| H16A  | 1.04769 | 0.43039 | 0.79671 | 6.954    | 1   |
| H16B  | 0.95647 | 0.41636 | 0.86751 | 6.954    | 1   |
| H16C  | 0.98797 | 0.32825 | 0.80776 | 6.954    | 1   |
| H17A  | 0.91608 | 0.61025 | 0.75765 | 5.154    | 1   |
| H17B  | 0.84841 | 0.60083 | 0.83706 | 5.154    | 1   |
| H17C  | 0.77180 | 0.62135 | 0.77160 | 5.154    | 1   |
| H18A  | 0.83309 | 0.48190 | 0.67337 | 6.118    | 1   |
| H18B  | 0.90372 | 0.36503 | 0.69195 | 6.118    | 1   |
| H18C  | 0.97473 | 0.46029 | 0.68047 | 6.118    | 1   |
| H21A  | 0.38529 | 0.01712 | 0.62163 | 5.964    | 1   |
| H21B  | 0.24146 | 0.02795 | 0.62736 | 5.964    | 1   |
| H21C  | 0.31521 | 0.07040 | 0.55737 | 5.964    | 1   |
| H22A  | 0.17852 | 0.25414 | 0.57246 | 3.968    | 1   |
| H22B  | 0.10368 | 0.20662 | 0.63992 | 3.968    | 1   |
| H22C  | 0.15680 | 0.30981 | 0.64783 | 3.968    | 1   |
| H23A  | 0.34386 | 0.10973 | 0.73909 | 8.334    | 1   |
| H23B  | 0.20064 | 0.12416 | 0.73901 | 8.334    | 1   |
| H23C  | 0.25789 | 0.22507 | 0.74679 | 8.334    | 1   |
| H25A  | 0.27861 | 0.30460 | 0.50087 | 4.008    | 1   |
| H25B  | 0.38992 | 0.27417 | 0.43842 | 4.008    | 1   |
| H25C  | 0.33507 | 0.18289 | 0.48345 | 4.008    | 1   |
| H26A  | 0.61866 | 0.16563 | 0.54794 | 3.608    | 1   |
| H26B  | 0.54120 | 0.09866 | 0.51198 | 3.608    | 1   |
| H26C  | 0.59604 | 0.18993 | 0.46695 | 3.608    | 1   |
| H27A  | 0.52969 | 0.36397 | 0.56962 | 3.392    | 1   |
| H27B  | 0.50845 | 0.37743 | 0.48791 | 3.392    | 1   |
| H27C  | 0.39723 | 0.41382 | 0.54951 | 3.392    | 1   |
| atom | U11    | U22    | U33    | U12    | U13    | U23    |
|------|--------|--------|--------|--------|--------|--------|
| Nb1  | 0.0337(2) | 0.0175(2) | 0.02332(19) | 0.00190(13) | 0.00531(14) | 0.00539(13) |
| F1   | 0.0454(16) | 0.0245(13) | 0.0427(15) | -0.0035(11) | 0.0054(12) | 0.0086(11) |
| F2   | 0.0461(17) | 0.0397(16) | 0.0480(17) | 0.0060(13) | 0.0141(13) | -0.0010(13) |
| F3   | 0.0286(13) | 0.0552(18) | 0.0365(14) | -0.0096(12) | 0.0104(11) | 0.0091(12) |
| F4   | 0.0435(15) | 0.0337(14) | 0.0382(14) | -0.0127(12) | 0.0005(11) | 0.0153(11) |
| F5   | 0.0405(14) | 0.0301(14) | 0.0364(14) | 0.0069(11) | 0.0051(11) | 0.0101(11) |
| F6   | 0.0334(13) | 0.0293(13) | 0.0422(14) | -0.0169(11) | -0.0066(11) | 0.0015(11) |
| F7   | 0.0201(12) | 0.0557(18) | 0.0474(16) | -0.0018(12) | -0.0081(11) | 0.0054(13) |
| F8   | 0.0430(16) | 0.0267(14) | 0.066(2) | 0.0138(12) | -0.0044(14) | 0.0074(13) |
| F9   | 0.0515(16) | 0.0201(13) | 0.0524(16) | -0.0146(11) | -0.0059(13) | 0.0014(11) |
| F10  | 0.0223(11) | 0.0319(13) | 0.0426(14) | -0.0093(10) | -0.0085(10) | 0.0038(11) |
| F11  | 0.0321(14) | 0.0605(19) | 0.0308(13) | 0.0088(13) | -0.0026(11) | 0.0116(12) |
| F12  | 0.0283(13) | 0.071(2) | 0.0374(15) | -0.0056(13) | 0.0048(11) | -0.0073(14) |
| F13  | 0.072(2) | 0.069(2) | 0.0386(16) | -0.0173(18) | 0.0256(15) | 0.0069(15) |
| F14  | 0.106(3) | 0.054(2) | 0.0444(18) | 0.002(2) | 0.0135(19) | 0.0269(16) |
| F15  | 0.0580(19) | 0.0335(15) | 0.0473(17) | 0.0086(13) | 0.0037(14) | 0.0128(13) |
| O1   | 0.0247(14) | 0.0370(17) | 0.0293(14) | -0.0017(12) | 0.0050(11) | 0.0135(12) |
| O2   | 0.0290(14) | 0.0181(14) | 0.0358(15) | -0.0006(11) | -0.0056(12) | 0.0038(11) |
| O3   | 0.0272(14) | 0.0303(16) | 0.0353(16) | -0.0002(12) | 0.0087(12) | 0.0097(12) |
| N1   | 0.0256(16) | 0.0203(17) | 0.0326(18) | -0.0060(13) | 0.0003(13) | 0.0061(13) |
| N2   | 0.0267(17) | 0.0266(18) | 0.0357(19) | 0.0046(14) | -0.0086(14) | -0.0061(14) |
| N3   | 0.0336(18) | 0.0224(17) | 0.0262(17) | 0.0015(14) | -0.0087(14) | 0.0006(13) |
| C1   | 0.0215(18) | 0.0170(19) | 0.037(2) | -0.0099(14) | 0.0023(15) | 0.0068(15) |
| C2   | 0.027(2) | 0.028(2) | 0.054(3) | -0.0020(17) | -0.0067(19) | 0.010(2) |
| C3   | 0.043(3) | 0.081(4) | 0.053(3) | -0.020(3) | -0.017(2) | 0.019(3) |
| C4   | 0.044(3) | 0.035(3) | 0.114(6) | -0.009(2) | -0.036(3) | 0.004(3) |
| C5   | 0.033(3) | 0.073(4) | 0.077(4) | 0.008(3) | -0.002(3) | -0.004(3) |
| C6   | 0.049(3) | 0.018(2) | 0.042(2) | -0.0079(18) | -0.008(2) | 0.0049(17) |
| C7   | 0.097(6) | 0.038(3) | 0.098(6) | 0.007(3) | -0.051(5) | -0.008(3) |
| C8   | 0.056(3) | 0.037(3) | 0.044(3) | -0.011(2) | -0.004(2) | 0.000(2) |
| C9   | 0.089(5) | 0.076(5) | 0.044(3) | -0.056(4) | 0.001(3) | -0.004(3) |
| C10  | 0.0243(19) | 0.035(2) | 0.0274(19) | -0.0088(17) | -0.0034(15) | 0.0034(16) |
| C11  | 0.059(3) | 0.050(3) | 0.028(2) | -0.025(3) | 0.006(2) | -0.008(2) |
| C12  | 0.046(5) | 0.057(5) | 0.024(3) | -0.021(4) | -0.009(3) | 0.007(3) |
| C12A | 0.060(9) | 0.060(9) | 0.060(9) | -0.013(3) | -0.008(2) | -0.002(2) |
| C13  | 0.039(4) | 0.038(4) | 0.046(4) | -0.010(3) | 0.013(3) | -0.014(3) |
| C13A | 0.048(13) | 0.10(2) | 0.045(12) | 0.037(14) | -0.006(10) | -0.029(13) |
### Table S7-3. Anisotropic displacement parameters (continued)

| atom | U_{11}  | U_{22}  | U_{33}  | U_{12}  | U_{13}  | U_{23}  |
|------|---------|---------|---------|---------|---------|---------|
| C14  | 0.105(9)| 0.102(9)| 0.038(4)| -0.076(8)| 0.009(5)| -0.022(5)|
| C14A | 0.054(13)| 0.056(13)| 0.026(9)| -0.006(10)| -0.007(8)| -0.012(8)|
| C15  | 0.0198(19)| 0.039(3)| 0.056(3)| -0.0066(18)| -0.0047(19)| 0.020(2) |
| C16  | 0.042(3)| 0.057(4)| 0.132(7)| -0.022(3)| -0.046(4)| 0.039(4) |
| C17  | 0.043(3)| 0.047(3)| 0.076(4)| -0.021(2)| -0.009(3)| 0.018(3) |
| C18  | 0.055(3)| 0.059(4)| 0.056(3)| 0.012(3)| 0.028(3)| 0.022(3) |
| C19  | 0.0256(19)| 0.0147(18)| 0.0297(19)| -0.0003(14)| -0.0040(15)| 0.0016(14) |
| C20  | 0.028(2)| 0.038(3)| 0.047(3)| -0.0074(19)| -0.0016(19)| 0.013(2) |
| C21  | 0.039(3)| 0.023(3)| 0.125(6)| -0.010(2)| -0.009(3)| 0.014(3) |
| C22  | 0.030(2)| 0.036(3)| 0.059(3)| -0.0060(19)| -0.004(2)| -0.000(2) |
| C23  | 0.050(4)| 0.141(7)| 0.058(4)| -0.010(4)| 0.007(3)| 0.051(4) |
| C24  | 0.034(2)| 0.031(2)| 0.0238(19)| -0.0070(17)| -0.0051(16)| 0.0029(16) |
| C25  | 0.049(3)| 0.053(3)| 0.029(2)| -0.015(2)| -0.014(2)| 0.001(2) |
| C26  | 0.037(2)| 0.040(3)| 0.033(2)| -0.003(2)| 0.0014(18)| -0.0004(19) |
| C27  | 0.042(2)| 0.031(2)| 0.036(2)| -0.0120(19)| -0.0116(19)| 0.0120(18) |
| C28  | 0.0198(17)| 0.032(2)| 0.0207(17)| -0.0076(15)| -0.0025(14)| 0.0057(15) |
| C29  | 0.031(2)| 0.023(2)| 0.0278(19)| -0.0091(16)| -0.0015(16)| 0.0041(15) |
| C30  | 0.026(2)| 0.036(2)| 0.031(2)| -0.0023(17)| 0.0015(16)| -0.0017(17) |
| C31  | 0.0239(19)| 0.044(3)| 0.0245(19)| -0.0124(18)| 0.0025(15)| 0.0047(17) |
| C32  | 0.031(2)| 0.029(2)| 0.0262(19)| -0.0136(17)| -0.0064(16)| 0.0098(16) |
| C33  | 0.0251(19)| 0.029(2)| 0.0251(19)| -0.0038(16)| -0.0034(15)| 0.0049(16) |
| C34  | 0.0209(17)| 0.0186(18)| 0.0223(17)| -0.0033(14)| -0.0017(13)| 0.0019(14) |
| C35  | 0.0227(18)| 0.024(2)| 0.0270(19)| -0.0097(15)| -0.0024(14)| 0.0003(15) |
| C36  | 0.0184(17)| 0.035(2)| 0.029(2)| -0.0020(16)| -0.0039(14)| 0.0021(16) |
| C37  | 0.031(2)| 0.022(2)| 0.035(2)| 0.0053(16)| -0.0033(17)| 0.0043(16) |
| C38  | 0.033(2)| 0.0165(19)| 0.031(2)| -0.0072(15)| -0.0015(16)| 0.0018(15) |
| C39  | 0.0183(17)| 0.026(2)| 0.0270(18)| -0.0054(14)| -0.0024(14)| 0.0009(15) |
| C40  | 0.0248(18)| 0.0221(19)| 0.0270(19)| -0.0094(15)| 0.0014(14)| 0.0016(15) |
| C41  | 0.0248(19)| 0.032(2)| 0.0246(19)| -0.0063(16)| -0.0037(15)| 0.0010(16) |
| C42  | 0.029(2)| 0.047(3)| 0.030(2)| -0.0159(19)| 0.0001(17)| -0.0051(19) |
| C43  | 0.051(3)| 0.044(3)| 0.030(2)| -0.021(2)| 0.013(2)| -0.001(2) |
| C44  | 0.072(4)| 0.032(3)| 0.032(2)| -0.016(2)| 0.003(2)| 0.013(2) |
| C45  | 0.039(2)| 0.021(2)| 0.036(2)| -0.0032(17)| 0.0021(18)| 0.0029(17)|

The general temperature factor expression: \( \exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2ab'U_{12}hl + 2ac'U_{13}kh + 2bc'U_{23}lj)) \)
Table S7-4. Bond lengths (Å)

| atom    | atom    | distance    | atom    | atom    | distance    |
|---------|---------|-------------|---------|---------|-------------|
| Nb1     | O1      | 1.950(3)    | Nb1     | O2      | 1.996(3)    |
| Nb1     | O3      | 1.976(3)    | Nb1     | N1      | 1.965(3)    |
| Nb1     | N2      | 2.098(4)    | Nb1     | N3      | 2.234(4)    |
| F1      | C29     | 1.342(5)    | F2      | C30     | 1.345(5)    |
| F3      | C31     | 1.349(4)    | F4      | C32     | 1.345(5)    |
| F5      | C33     | 1.346(5)    | F6      | C35     | 1.345(5)    |
| F7      | C36     | 1.350(5)    | F8      | C37     | 1.344(5)    |
| F9      | C38     | 1.342(5)    | F10     | C39     | 1.351(5)    |
| F11     | C41     | 1.353(5)    | F12     | C42     | 1.343(5)    |
| F13     | C43     | 1.347(6)    | F14     | C44     | 1.333(6)    |
| F15     | C45     | 1.346(5)    | O1      | C28     | 1.321(5)    |
| O2      | C34     | 1.307(4)    | O3      | C40     | 1.312(5)    |
| N1      | C1      | 1.260(5)    | N2      | C10     | 1.273(6)    |
| N3      | C19     | 1.268(6)    | C1      | C2      | 1.548(7)    |
| C1      | C6      | 1.563(7)    | C2      | C3      | 1.510(8)    |
| C2      | C4      | 1.517(8)    | C2      | C5      | 1.563(7)    |
| C6      | C7      | 1.529(7)    | C6      | C8      | 1.541(8)    |
| C6      | C9      | 1.525(8)    | C10     | C11     | 1.548(6)    |
| C10     | C15     | 1.541(6)    | C11     | C12     | 1.532(11)   |
| C11     | C12A    | 1.39(4)     | C11     | C13     | 1.624(9)    |
| C11     | C13A    | 1.48(3)     | C11     | C14     | 1.485(14)   |
| C11     | C14A    | 1.73(2)     | C15     | C16     | 1.557(8)    |
| C15     | C17     | 1.550(8)    | C15     | C18     | 1.544(8)    |
| C19     | C20     | 1.553(7)    | C19     | C24     | 1.554(5)    |
| C20     | C21     | 1.553(8)    | C20     | C22     | 1.528(7)    |
| C20     | C23     | 1.534(9)    | C24     | C25     | 1.539(7)    |
| C24     | C26     | 1.539(6)    | C24     | C27     | 1.544(7)    |
| C28     | C29     | 1.390(5)    | C28     | C33     | 1.402(6)    |
| C29     | C30     | 1.386(6)    | C30     | C31     | 1.378(7)    |
| C31     | C32     | 1.379(6)    | C32     | C33     | 1.373(6)    |
| C34     | C35     | 1.401(5)    | C34     | C39     | 1.402(6)    |
| C35     | C36     | 1.378(5)    | C36     | C37     | 1.372(7)    |
| C37     | C38     | 1.380(6)    | C38     | C39     | 1.375(5)    |
| C40     | C41     | 1.410(5)    | C40     | C45     | 1.397(6)    |
| C41     | C42     | 1.377(6)    | C42     | C43     | 1.385(7)    |
| C43     | C44     | 1.390(7)    | C44     | C45     | 1.376(7)    |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| N3   | H1   | 0.864(10)| C3   | H3A  | 0.980    |
| C3   | H3B  | 0.980    | C3   | H3C  | 0.980    |
| C4   | H4A  | 0.980    | C4   | H4B  | 0.980    |
| C4   | H4C  | 0.980    | C5   | H5A  | 0.980    |
| C5   | H5B  | 0.980    | C5   | H5C  | 0.980    |
| C7   | H7A  | 0.980    | C7   | H7B  | 0.980    |
| C7   | H7C  | 0.980    | C8   | H8A  | 0.980    |
| C8   | H8B  | 0.980    | C8   | H8C  | 0.980    |
| C9   | H9A  | 0.980    | C9   | H9B  | 0.980    |
| C9   | H9C  | 0.980    | C12  | H12A | 1.115    |
| C12  | H12B | 1.001    | C12  | H12C | 1.026    |
| C12A | H12D | 0.980    | C12A | H12E | 0.980    |
| C12A | H12F | 0.980    | C13  | H13A | 0.980    |
| C13  | H13B | 0.980    | C13  | H13C | 0.980    |
| C13A | H13D | 0.980    | C13A | H13E | 0.980    |
| C13A | H13F | 0.980    | C14  | H14A | 0.980    |
| C14  | H14B | 0.980    | C14  | H14C | 0.980    |
| C14A | H14D | 0.980    | C14A | H14E | 0.980    |
| C14A | H14F | 0.980    | C16  | H16A | 0.980    |
| C16  | H16B | 0.980    | C16  | H16C | 0.980    |
| C17  | H17A | 0.980    | C17  | H17B | 0.980    |
| C17  | H17C | 0.980    | C18  | H18A | 0.980    |
| C18  | H18B | 0.980    | C18  | H18C | 0.980    |
| C21  | H21A | 0.980    | C21  | H21B | 0.980    |
| C21  | H21C | 0.980    | C22  | H22A | 0.980    |
| C22  | H22B | 0.980    | C22  | H22C | 0.980    |
| C23  | H23A | 0.980    | C23  | H23B | 0.980    |
| C23  | H23C | 0.980    | C25  | H25A | 0.980    |
| C25  | H25B | 0.980    | C25  | H25C | 0.980    |
| C26  | H26A | 0.980    | C26  | H26B | 0.980    |
| C26  | H26C | 0.980    | C27  | H27A | 0.980    |
| C27  | H27B | 0.980    | C27  | H27C | 0.980    |
Table S7-6. Bond angles (°)

| atom | atom | atom | angle     | atom | atom | atom | angle     |
|------|------|------|-----------|------|------|------|-----------|
| O1   | Nb1  | O2   | 93.10(12) | O1   | Nb1  | O3   | 172.10(14)|
| O1   | Nb1  | N1   | 87.80(13) | O1   | Nb1  | N2   | 91.66(14) |
| O1   | Nb1  | N3   | 90.48(13) | O2   | Nb1  | O3   | 91.66(13) |
| O2   | Nb1  | N1   | 178.35(14)| O2   | Nb1  | N2   | 84.84(13) |
| O2   | Nb1  | N3   | 83.58(13) | O3   | Nb1  | N1   | 87.29(13) |
| O3   | Nb1  | N2   | 95.04(14) | O3   | Nb1  | N3   | 83.79(13) |
| N1   | Nb1  | N2   | 96.51(15) | N1   | Nb1  | N3   | 95.04(14) |
| N2   | Nb1  | N3   | 168.32(12)| Nb1  | O1   | C28  | 168.3(3)  |
| Nb1  | O2   | C34  | 177.3(3)  | Nb1  | O3   | C40  | 173.3(3)  |
| Nb1  | N1   | C1   | 178.7(3)  | Nb1  | N2   | C10  | 167.1(3)  |
| Nb1  | N3   | C19  | 163.0(3)  | N1   | C1   | C2   | 119.5(4)  |
| N1   | C1   | C6   | 116.6(4)  | C2   | C1   | C6   | 123.8(3)  |
| C1   | C2   | C3   | 110.7(4)  | C1   | C2   | C4   | 109.0(4)  |
| C1   | C2   | C5   | 110.7(4)  | C3   | C2   | C4   | 109.5(5)  |
| C3   | C2   | C5   | 110.2(4)  | C4   | C2   | C5   | 106.8(5)  |
| C1   | C6   | C7   | 118.0(5)  | C1   | C6   | C8   | 109.5(4)  |
| C1   | C6   | C9   | 105.6(4)  | C7   | C6   | C8   | 104.7(5)  |
| C7   | C6   | C9   | 110.3(5)  | C8   | C6   | C9   | 108.5(5)  |
| N2   | C10  | C11  | 116.4(4)  | N2   | C10  | C15  | 118.5(4)  |
| C11  | C10  | C15  | 125.1(4)  | C10  | C11  | C12  | 107.7(5)  |
| C10  | C11  | C12A | 117.8(14)| C10  | C11  | C13  | 104.9(4)  |
| C10  | C11  | C13A | 106.3(9)  | C10  | C11  | C14  | 121.3(6)  |
| C10  | C11  | C14A | 106.1(6)  | C12  | C11  | C13  | 106.0(6)  |
| C12  | C11  | C14  | 110.8(6)  | C12A | C11  | C13A | 120.9(17) |
| C12A | C11  | C14A | 101.7(17)| C13  | C11  | C14  | 104.9(6)  |
| C13A | C11  | C14A | 101.6(14)| C10  | C15  | C16  | 110.3(4)  |
| C10  | C15  | C17  | 112.0(4)  | C10  | C15  | C18  | 109.1(5)  |
| C16  | C15  | C17  | 110.2(5)  | C16  | C15  | C18  | 107.5(4)  |
| C17  | C15  | C18  | 107.6(5)  | N3   | C19  | C20  | 118.6(4)  |
| N3   | C19  | C24  | 117.5(4)  | C20  | C19  | C24  | 123.8(4)  |
| C19  | C20  | C21  | 108.9(4)  | C19  | C20  | C22  | 112.8(4)  |
| C19  | C20  | C23  | 110.6(5)  | C21  | C20  | C22  | 109.9(5)  |
| C21  | C20  | C23  | 108.2(5)  | C22  | C20  | C23  | 106.4(4)  |
| C19  | C24  | C25  | 117.8(4)  | C19  | C24  | C26  | 106.9(3)  |
| C19  | C24  | C27  | 108.3(3)  | C25  | C24  | C26  | 108.6(4)  |
| C25  | C24  | C27  | 105.9(4)  | C26  | C24  | C27  | 109.3(4)  |
| O1   | C28  | C29  | 122.6(4)  | O1   | C28  | C33  | 121.5(3)  |
Table S7-6. Bond angles (°) (continued)

| atom | atom | atom | angle  | atom | atom | atom | angle  |
|------|------|------|--------|------|------|------|--------|
| C29  | C28  | C33  | 115.9(3)| F1   | C29  | C28  | 119.1(3)|
| F1   | C29  | C30  | 118.5(3)| C28  | C29  | C30  | 122.4(4)|
| F2   | C30  | C29  | 120.2(4)| F2   | C30  | C31  | 119.8(4)|
| C29  | C30  | C31  | 119.9(4)| F3   | C31  | C30  | 120.4(4)|
| F3   | C31  | C32  | 120.6(4)| C30  | C31  | C32  | 119.1(4)|
| F4   | C32  | C31  | 119.6(4)| F4   | C32  | C33  | 119.8(3)|
| C31  | C32  | C33  | 120.6(4)| F5   | C33  | C32  | 118.4(3)|
| F5   | C33  | C32  | 119.5(4)| C28  | C33  | C32  | 122.1(3)|
| O2   | C34  | C35  | 122.8(4)| O2   | C34  | C39  | 121.7(4)|
| C35  | C34  | C39  | 115.5(3)| F6   | C35  | C34  | 119.1(3)|
| F6   | C35  | C36  | 118.6(4)| C34  | C35  | C36  | 122.3(4)|
| F7   | C36  | C35  | 119.6(4)| F7   | C36  | C37  | 120.0(4)|
| C35  | C36  | C37  | 120.4(4)| F8   | C37  | C36  | 120.3(4)|
| F8   | C37  | C38  | 120.5(4)| C36  | C37  | C38  | 119.2(4)|
| F9   | C38  | C37  | 119.8(3)| F9   | C38  | C39  | 119.9(4)|
| C37  | C38  | C39  | 120.3(4)| F10  | C39  | C34  | 119.2(3)|
| F10  | C39  | C38  | 118.6(4)| C34  | C39  | C38  | 122.3(4)|
| O3   | C40  | C41  | 121.6(3)| O3   | C40  | C45  | 122.7(3)|
| C41  | C40  | C45  | 115.6(3)| F11  | C41  | C40  | 118.9(3)|
| F11  | C41  | C42  | 118.5(3)| C40  | C41  | C42  | 122.6(4)|
| F12  | C42  | C41  | 120.7(4)| F12  | C42  | C43  | 119.6(4)|
| C41  | C42  | C43  | 119.7(4)| F13  | C43  | C42  | 119.9(4)|
| F13  | C43  | C44  | 120.6(4)| C42  | C43  | C44  | 119.5(4)|
| F14  | C44  | C43  | 119.2(4)| F14  | C44  | C45  | 120.8(5)|
| C43  | C44  | C45  | 119.9(4)| F15  | C45  | C40  | 118.5(4)|
| F15  | C45  | C44  | 118.8(4)| C40  | C45  | C44  | 122.6(4)|
Table S7-7. Bond angles involving hydrogens (°)

| atom | atom | atom | angle  | atom | atom | atom | angle  |
|------|------|------|--------|------|------|------|--------|
| Nb1  | N3   | H1   | 95.9(12) | C19  | N3   | H1   | 98.0(10) |
| C2   | C3   | H3A  | 109.5   | C2   | C3   | H3B  | 109.5  |
| C2   | C3   | H3C  | 109.5   | H3A  | C3   | H3B  | 109.5  |
| H3A  | C3   | H3C  | 109.5   | H3B  | C3   | H3C  | 109.5  |
| C2   | C4   | H4A  | 109.5   | C2   | C4   | H4B  | 109.5  |
| C2   | C4   | H4C  | 109.5   | H4A  | C4   | H4B  | 109.5  |
| C2   | C5   | H5A  | 109.5   | C2   | C5   | H5B  | 109.5  |
| C2   | C5   | H5C  | 109.5   | H5A  | C5   | H5B  | 109.5  |
| H5A  | C5   | H5C  | 109.5   | H5B  | C5   | H5C  | 109.5  |
| C6   | C7   | H7A  | 109.5   | C6   | C7   | H7B  | 109.5  |
| C6   | C7   | H7C  | 109.5   | H7A  | C7   | H7B  | 109.5  |
| H7A  | C7   | H7C  | 109.5   | H7B  | C7   | H7C  | 109.5  |
| C6   | C8   | H8A  | 109.5   | C6   | C8   | H8B  | 109.5  |
| C6   | C8   | H8C  | 109.5   | H8A  | C8   | H8B  | 109.5  |
| H8A  | C8   | H8C  | 109.5   | H8B  | C8   | H8C  | 109.5  |
| C6   | C9   | H9A  | 109.5   | C6   | C9   | H9B  | 109.5  |
| C6   | C9   | H9C  | 109.5   | H9A  | C9   | H9B  | 109.5  |
| H9A  | C9   | H9C  | 109.5   | H9B  | C9   | H9C  | 109.5  |
| C11  | C12  | H12A | 118.2   | C11  | C12  | H12B | 110.2  |
| C11  | C12  | H12C | 118.7   | H12A | C12  | H12B | 110.6  |
| H12A | C12  | H12C | 97.4    | H12B | C12  | H12C | 99.7   |
| C11  | C12A | H12D | 109.5   | C11  | C12A | H12E | 109.5  |
| C11  | C12A | H12F | 109.5   | H12D | C12A | H12E | 109.5  |
| H12D | C12A | H12F | 109.5   | H12E | C12A | H12F | 109.5  |
| C11  | C13  | H13A | 109.5   | C11  | C13  | H13B | 109.5  |
| C11  | C13  | H13C | 109.5   | H13B | C13  | H13C | 109.5  |
| H13A | C13  | H13C | 109.5   | H13B | C13  | H13C | 109.5  |
| C11  | C13A | H13D | 109.5   | C11  | C13A | H13B | 109.5  |
| C11  | C13A | H13F | 109.5   | H13D | C13A | H13E | 109.5  |
| H13D | C13A | H13F | 109.5   | H13E | C13A | H13E | 109.5  |
| C11  | C14  | H14A | 109.5   | C11  | C14  | H14B | 109.5  |
| C11  | C14  | H14C | 109.5   | H14A | C14  | H14B | 109.5  |
| H14A | C14  | H14C | 109.5   | H14B | C14  | H14C | 109.5  |
| C11  | C14A | H14D | 109.5   | C11  | C14A | H14E | 109.5  |
| C11  | C14A | H14F | 109.5   | H14D | C14A | H14E | 109.5  |
| H14D | C14A | H14F | 109.5   | H14E | C14A | H14F | 109.5  |
Table S7-7. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C15  | C16  | H16A | 109.5 | C15  | C16  | H16B | 109.5 |
| C15  | C16  | H16C | 109.5 | H16A | C16  | H16C | 109.5 |
| H16A | C16  | H16C | 109.5 | C15  | C17  | H17B | 109.5 |
| C15  | C17  | H17A | 109.5 | C15  | C17  | H17A | 109.5 |
| C15  | C17  | H17C | 109.5 | H17A | C17  | H17B | 109.5 |
| H17A | C17  | H17C | 109.5 | H17B | C17  | H17C | 109.5 |
| C15  | C18  | H18A | 109.5 | C15  | C18  | H18B | 109.5 |
| C15  | C18  | H18C | 109.5 | H18A | C18  | H18B | 109.5 |
| H18A | C18  | H18C | 109.5 | H18B | C18  | H18C | 109.5 |
| C20  | C21  | H21A | 109.5 | C20  | C21  | H21B | 109.5 |
| C20  | C21  | H21C | 109.5 | H21A | C21  | H21B | 109.5 |
| H21A | C21  | H21C | 109.5 | H21B | C21  | H21C | 109.5 |
| C20  | C22  | H22A | 109.5 | C20  | C22  | H22B | 109.5 |
| C20  | C22  | H22C | 109.5 | H22A | C22  | H22B | 109.5 |
| H22A | C22  | H22C | 109.5 | H22B | C22  | H22C | 109.5 |
| C20  | C23  | H23A | 109.5 | C20  | C23  | H23B | 109.5 |
| C20  | C23  | H23C | 109.5 | H23A | C23  | H23B | 109.5 |
| H23A | C23  | H23C | 109.5 | H23B | C23  | H23C | 109.5 |
| C24  | C25  | H25A | 109.5 | C24  | C25  | H25B | 109.5 |
| C24  | C25  | H25C | 109.5 | H25A | C25  | H25B | 109.5 |
| H25A | C25  | H25C | 109.5 | H25B | C25  | H25C | 109.5 |
| C24  | C26  | H26A | 109.5 | C24  | C26  | H26B | 109.5 |
| C24  | C26  | H26C | 109.5 | H26A | C26  | H26B | 109.5 |
| H26A | C26  | H26C | 109.5 | H26B | C26  | H26C | 109.5 |
| C24  | C27  | H27A | 109.5 | C24  | C27  | H27B | 109.5 |
| C24  | C27  | H27C | 109.5 | H27A | C27  | H27B | 109.5 |
| H27A | C27  | H27C | 109.5 | H27B | C27  | H27C | 109.5 |
Table S7-8. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle   | atom1 | atom2 | atom3 | atom4 | angle   |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| N1    | C1    | C2    | C3    | 114.8(4)| N1    | C1    | C2    | C4    | -5.6(5) |
| N1    | C1    | C2    | C5    | -122.7(4)| N1    | C1    | C6    | C7    | 162.8(3) |
| N1    | C1    | C6    | C8    | 43.3(5)  | N1    | C1    | C6    | C9    | -73.3(4) |
| C2    | C1    | C6    | C7    | -20.1(6) | C2    | C1    | C6    | C8    | -139.6(4) |
| C2    | C1    | C6    | C9    | 103.8(4) | C6    | C1    | C2    | C3    | -62.2(5) |
| C6    | C1    | C2    | C4    | 177.3(3) | C6    | C1    | C2    | C5    | 60.2(5)  |
| N2    | C10   | C11   | C12   | 57.0(5)  | N2    | C10   | C11   | C12A  | 35.1(6) |
| N2    | C10   | C11   | C13   | -55.7(5) | N2    | C10   | C11   | C13A  | -104.4(5) |
| N2    | C10   | C11   | C14   | -174.0(4)| N2    | C10   | C11   | C14A  | 148.1(3) |
| N2    | C10   | C15   | C16   | -107.2(4)| N2    | C10   | C15   | C17   | 129.6(4) |
| N2    | C10   | C15   | C18   | 10.6(5)  | C11   | C10   | C15   | C16   | 71.1(5)  |
| C11   | C10   | C15   | C17   | -52.0(6) | C11   | C10   | C15   | C18   | -171.1(4) |
| C15   | C10   | C11   | C12   | -121.4(4)| C15   | C10   | C11   | C12A  | -143.3(4) |
| C15   | C10   | C11   | C13   | 125.9(4) | C15   | C10   | C11   | C13A  | 77.2(5)  |
| C15   | C10   | C11   | C14   | 7.6(7)   | C15   | C10   | C11   | C14A  | -30.3(5) |
| N3    | C19   | C20   | C21   | -112.8(4)| N3    | C19   | C20   | C22   | 125.0(4) |
| N3    | C19   | C20   | C23   | 6.0(5)   | N3    | C19   | C24   | C25   | -170.2(3) |
| N3    | C19   | C24   | C26   | 67.4(4)  | N3    | C19   | C24   | C27   | -50.2(4) |
| C20   | C19   | C24   | C25   | 13.9(5)  | C20   | C19   | C24   | C26   | -108.5(4) |
| C20   | C19   | C24   | C27   | 133.9(3) | C24   | C19   | C20   | C21   | 63.1(4)  |
| C24   | C19   | C20   | C22   | -59.1(5) | C24   | C19   | C20   | C23   | -178.1(3) |
| O1    | C28   | C29   | F1    | -0.7(6)  | O1    | C28   | C29   | C30   | -178.7(4) |
| O1    | C28   | C33   | F5    | -0.1(6)  | O1    | C28   | C33   | C32   | 178.7(4) |
| C29   | C28   | C33   | F5    | 179.6(4) | C29   | C28   | C33   | C32   | -1.6(6)  |
| C33   | C28   | C29   | F1    | 179.6(4) | C33   | C28   | C30   | C30   | 1.5(6)   |
| F1    | C29   | C30   | F2    | 0.3(7)   | F1    | C29   | C30   | C31   | -178.6(4) |
| C28   | C29   | C30   | F2    | 178.4(4) | C28   | C29   | C30   | C31   | -0.5(7)  |
| F2    | C30   | C31   | F3    | -0.4(7)  | F2    | C30   | C31   | C32   | -179.5(4) |
| C29   | C30   | C31   | F3    | 178.5(4) | C29   | C30   | C31   | C32   | -0.5(7)  |
| F3    | C31   | C32   | F4    | 1.0(7)   | F3    | C31   | C32   | C33   | -178.6(4) |
| C30   | C31   | C32   | F4    | -180.0(4)| C30   | C31   | C32   | C33   | 0.5(7)   |
| F4    | C32   | C33   | F5    | -0.2(6)  | F4    | C32   | C33   | C28   | -178.9(3) |
| C31   | C32   | C33   | F5    | 179.4(4) | C31   | C32   | C33   | C28   | 0.6(7)   |
| O2    | C34   | C35   | F6    | -0.7(5)  | O2    | C34   | C35   | C36   | 179.4(3) |
| O2    | C34   | C39   | F10   | 0.2(5)   | O2    | C34   | C39   | C38   | -179.6(3) |
| C35   | C34   | C39   | F10   | 179.7(3) | C35   | C34   | C39   | C38   | -0.1(5)  |
| C39   | C34   | C35   | F6    | 179.8(3) | C39   | C34   | C35   | C36   | -0.1(5)  |
Table S7-8. Torsion angles (°) (continued)

| atom1 | atom2 | atom3 | atom4 | angle   | atom1 | atom2 | atom3 | atom4 | angle   |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| F6    | C35   | C36   | F7    | 1.5(5)  | F6    | C35   | C36   | C37   | -179.3(3) |
| C34   | C35   | C36   | F7    | -178.7(3) | C34   | C35   | C36   | C37   | 0.6(6)  |
| F7    | C36   | C37   | F8    | -1.2(6) | F7    | C36   | C37   | C38   | 178.4(3) |
| C35   | C36   | C37   | F8    | 179.6(3) | C35   | C36   | C37   | C38   | -0.8(6) |
| F8    | C37   | C38   | F9    | 0.9(6)  | F8    | C37   | C38   | C39   | -179.8(3) |
| C36   | C37   | C38   | F9    | -178.7(3) | C36   | C37   | C38   | C39   | 0.6(6)  |
| F9    | C38   | C39   | F10   | -0.7(5) | F9    | C38   | C39   | C40   | 179.2(3) |
| C37   | C38   | C39   | F10   | -179.9(3) | C37   | C38   | C39   | C40   | -0.1(6) |
| O3    | C40   | C41   | F11   | -1.8(7) | O3    | C40   | C41   | C42   | 179.9(4) |
| O3    | C40   | C45   | F15   | 1.6(7)  | O3    | C40   | C45   | C44   | 179.4(4) |
| C41   | C40   | C45   | F15   | -178.0(4) | C41   | C40   | C45   | C44   | -0.1(7) |
| C45   | C40   | C41   | F11   | 177.8(4) | C45   | C40   | C41   | C42   | -0.6(7) |
| F11   | C41   | C42   | F12   | 1.4(7)  | F11   | C41   | C42   | C43   | -178.1(4) |
| C40   | C41   | C42   | F12   | 179.7(4) | C40   | C41   | C42   | C43   | 0.3(7)  |
| F12   | C42   | C43   | F13   | -0.4(8) | F12   | C42   | C43   | C44   | -178.8(4) |
| C41   | C42   | C43   | F13   | 179.1(5) | C41   | C42   | C43   | C44   | 0.7(8)  |
| F13   | C43   | C44   | F14   | 0.7(9)  | F13   | C43   | C44   | C45   | -179.7(5) |
| C42   | C43   | C44   | F14   | 179.1(5) | C42   | C43   | C44   | C45   | -1.3(9) |
| F14   | C44   | C45   | F15   | -1.6(8) | F14   | C44   | C45   | C40   | -179.4(5) |
| C43   | C44   | C45   | F15   | 178.9(5) | C43   | C44   | C45   | C40   | 1.1(9)  |
Table S7-9. Intramolecular contacts less than 3.60 Å

| atom | atom | distance   | atom | atom | distance   |
|------|------|------------|------|------|------------|
| F1   | F2   | 2.706(4)   | F1   | O1   | 2.759(4)   |
| F1   | N1   | 3.335(4)   | F1   | C1   | 3.402(5)   |
| F1   | C5   | 3.578(8)   | F1   | C8   | 3.475(7)   |
| F2   | F3   | 2.726(4)   | F3   | F4   | 2.727(4)   |
| F4   | F5   | 2.706(4)   | F5   | F10  | 3.114(4)   |
| F5   | O1   | 2.734(4)   | F5   | O2   | 3.470(4)   |
| F5   | C18  | 3.475(7)   | F5   | C27  | 3.592(6)   |
| F5   | C39  | 3.585(4)   | F6   | F7   | 2.690(4)   |
| F6   | F11  | 2.795(4)   | F6   | O2   | 2.763(4)   |
| F6   | N3   | 3.264(4)   | F6   | C19  | 3.307(4)   |
| F6   | C22  | 3.438(6)   | F6   | C27  | 3.543(5)   |
| F7   | F8   | 2.724(5)   | F8   | F9   | 2.728(4)   |
| F9   | F10  | 2.691(3)   | F9   | C36  | 3.600(6)   |
| F10  | O2   | 2.748(4)   | F10  | N2   | 3.421(4)   |
| F10  | C10  | 3.448(5)   | F10  | C13  | 3.550(7)   |
| F10  | C13A | 3.53(2)    | F10  | C17  | 3.469(7)   |
| F11  | F12  | 2.708(4)   | F11  | O2   | 3.367(4)   |
| F11  | O3   | 2.752(4)   | F11  | C34  | 3.443(5)   |
| F11  | C35  | 3.187(5)   | F12  | F13  | 2.720(5)   |
| F13  | F14  | 2.727(5)   | F14  | F15  | 2.708(5)   |
| F15  | O3   | 2.750(4)   | F15  | N1   | 3.488(4)   |
| F15  | C1   | 3.568(5)   | F15  | C3   | 3.439(6)   |
| F15  | C9   | 3.249(8)   | F15  | C12  | 3.452(12)  |
| F15  | C12A | 3.51(4)    | O1   | C18  | 3.595(8)   |
| O1   | C26  | 3.571(7)   | O1   | C27  | 3.383(6)   |
| O2   | C13  | 3.459(8)   | O2   | C27  | 3.424(6)   |
| O3   | C12  | 3.533(11)  | O3   | C12A | 3.29(4)    |
| O3   | C13  | 3.502(8)   | N1   | C3   | 3.435(7)   |
| N1   | C4   | 2.685(8)   | N1   | C5   | 3.532(6)   |
| N1   | C8   | 2.824(7)   | N1   | C9   | 2.986(9)   |
| N2   | C4   | 3.293(6)   | N2   | C12  | 2.877(8)   |
| N2   | C12A | 2.85(3)    | N2   | C13  | 2.858(7)   |
| N2   | C13A | 3.24(3)    | N2   | C16  | 3.403(8)   |
| N2   | C17  | 3.580(8)   | N2   | C18  | 2.684(8)   |
| N3   | C8   | 3.484(6)   | N3   | C21  | 3.429(8)   |
| N3   | C22  | 3.549(6)   | N3   | C23  | 2.723(9)   |
| N3   | C26  | 2.975(6)   | N3   | C27  | 2.863(6)   |
Table S7-9. Intramolecular contacts less than 3.60 Å (continued)

| atom | atom | distance  | atom | atom | distance  |
|------|------|-----------|------|------|-----------|
| C2   | C7   | 3.176(10) | C2   | C9   | 3.569(10) |
| C3   | C6   | 3.268(9)  | C3   | C7   | 3.462(11) |
| C3   | C9   | 3.561(10) | C5   | C6   | 3.279(8)  |
| C5   | C7   | 3.085(11) | C8   | C26  | 3.577(7)  |
| C11  | C16  | 3.372(8)  | C11  | C17  | 3.240(8)  |
| C12  | C40  | 3.562(12) | C12  | C45  | 3.551(13) |
| C12A | C40  | 3.25(4)   | C12A | C45  | 3.39(4)   |
| C13A | C15  | 3.31(2)   | C13A | C17  | 3.14(3)   |
| C14  | C15  | 3.210(10) | C14  | C16  | 3.565(12) |
| C14  | C17  | 3.136(12) | C14A | C15  | 3.037(14) |
| C14A | C16  | 2.939(16) | C14A | C17  | 3.303(18) |
| C18  | C28  | 3.500(8)  | C18  | C33  | 3.445(8)  |
| C20  | C25  | 3.152(7)  | C21  | C24  | 3.262(8)  |
| C21  | C25  | 3.383(8)  | C22  | C24  | 3.292(6)  |
| C22  | C25  | 3.117(7)  | C28  | C31  | 2.819(5)  |
| C29  | C32  | 2.740(6)  | C30  | C33  | 2.747(5)  |
| C34  | C37  | 2.820(5)  | C35  | C38  | 2.742(6)  |
| C36  | C39  | 2.744(6)  | C40  | C43  | 2.823(6)  |
| C41  | C44  | 2.751(6)  | C42  | C45  | 2.758(6)  |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H4A  | 3.592    | Nb1  | H4B  | 3.488    |
| Nb1  | H8C  | 3.352    | Nb1  | H12A | 3.430    |
| Nb1  | H12F | 3.507    | Nb1  | H13A | 3.140    |
| Nb1  | H27A | 3.135    | F1   | H4A  | 3.332    |
| F1   | H5A  | 2.721    | F1   | H8A  | 2.705    |
| F1   | H8C  | 3.565    | F1   | H26A | 3.144    |
| F5   | H18A | 2.635    | F5   | H18B | 3.544    |
| F5   | H27A | 2.877    | F5   | H27B | 3.486    |
| F6   | H1   | 3.06(2)  | F6   | H22C | 2.599    |
| F6   | H23C | 3.070    | F6   | H27A | 3.520    |
| F6   | H27C | 2.863    | F10  | H13A | 3.441    |
| F10  | H13C | 2.894    | F10  | H13D | 3.142    |
| F10  | H13E | 3.088    | F10  | H17C | 2.608    |
| F10  | H18A | 2.814    | F11  | H1   | 3.462(17) |
| F11  | H12F | 3.481    | F11  | H13A | 2.885    |
| F11  | H13B | 3.515    | F11  | H23C | 2.994    |
| F15  | H3A  | 3.550    | F15  | H3B  | 2.640    |
| F15  | H4B  | 3.542    | F15  | H9A  | 2.783    |
| F15  | H9C  | 2.846    | F15  | H12A | 2.471    |
| F15  | H12C | 3.394    | F15  | H12D | 3.044    |
| F15  | H12F | 3.158    | O1   | H4A  | 3.493    |
| O1   | H8C  | 3.538    | O1   | H18A | 3.291    |
| O1   | H18B | 3.000    | O1   | H26A | 2.743    |
| O1   | H27A | 2.477    | O2   | H1   | 2.99(3)  |
| O2   | H13A | 2.651    | O2   | H13C | 3.478    |
| O2   | H13E | 3.563    | O2   | H27A | 2.671    |
| O2   | H27C | 3.357    | O3   | H1   | 2.384(13) |
| O3   | H9A  | 3.057    | O3   | H12A | 2.585    |
| O3   | H12D | 3.344    | O3   | H12F | 2.459    |
| O3   | H13A | 2.621    | O3   | H23A | 3.292    |
| O3   | H23C | 3.204    | N1   | H1   | 3.298(14) |
| N1   | H3B  | 3.413    | N1   | H4A  | 2.611    |
| N1   | H4B  | 2.575    | N1   | H5A  | 3.473    |
| N1   | H8A  | 3.071    | N1   | H8C  | 2.511    |
| N1   | H9A  | 2.650    | N1   | H9C  | 3.384    |
| N1   | H12A | 3.516    | N2   | H4A  | 2.992    |
| N2   | H4B  | 2.701    | N2   | H12A | 2.665    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| N2   | H12B | 3.322    | N2   | H12D | 2.840    |
| N2   | H12F | 2.779    | N2   | H13A | 2.494    |
| N2   | H13C | 3.208    | N2   | H13D | 3.422    |
| N2   | H13E | 3.204    | N2   | H16C | 3.283    |
| N2   | H17C | 3.520    | N2   | H18A | 2.725    |
| N2   | H18B | 2.473    | N3   | H8C  | 2.507    |
| N3   | H9A  | 3.473    | N3   | H21A | 3.304    |
| N3   | H22C | 3.530    | N3   | H23A | 2.592    |
| N3   | H23C | 2.688    | N3   | H26A | 2.640    |
| N3   | H26B | 3.351    | N3   | H27A | 2.523    |
| N3   | H27C | 3.164    | C1   | H3A  | 2.625    |
| C1   | H3B  | 2.783    | C1   | H3C  | 3.356    |
| C1   | H4A  | 2.665    | C1   | H4B  | 2.683    |
| C1   | H4C  | 3.347    | C1   | H5A  | 2.727    |
| C1   | H5B  | 3.400    | C1   | H5C  | 2.768    |
| C1   | H7A  | 2.852    | C1   | H7B  | 2.872    |
| C1   | H7C  | 3.466    | C1   | H8A  | 2.755    |
| C1   | H8B  | 3.383    | C1   | H8C  | 2.676    |
| C1   | H9A  | 2.558    | C1   | H9B  | 3.321    |
| C1   | H9C  | 2.695    | C2   | H7A  | 3.190    |
| C2   | H7B  | 2.997    | C2   | H9C  | 3.412    |
| C3   | H4A  | 3.319    | C3   | H4B  | 2.659    |
| C3   | H4C  | 2.659    | C3   | H5A  | 3.360    |
| C3   | H5B  | 2.714    | C3   | H5C  | 2.714    |
| C3   | H7B  | 2.884    | C3   | H9C  | 3.003    |
| C4   | H3A  | 3.314    | C4   | H3B  | 2.582    |
| C4   | H3C  | 2.739    | C4   | H5A  | 2.662    |
| C4   | H5B  | 2.643    | C4   | H5C  | 3.326    |
| C4   | H12A | 3.496    | C4   | H12B | 3.558    |
| C4   | H12D | 3.498    | C4   | H16C | 2.843    |
| C4   | H18B | 3.388    | C5   | H3A  | 2.807    |
| C5   | H3B  | 3.360    | C5   | H3C  | 2.605    |
| C5   | H4A  | 2.647    | C5   | H4B  | 3.335    |
| C5   | H4C  | 2.635    | C5   | H7A  | 2.660    |
| C5   | H7B  | 2.962    | C6   | H3A  | 2.867    |
| C6   | H5A  | 3.487    | C6   | H5C  | 2.990    |
| C7   | H3A  | 2.827    | C7   | H5A  | 3.431    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C7   | H5C  | 2.375    | C7   | H8A  | 2.617    |
| C7   | H8B  | 2.583    | C7   | H8C  | 3.295    |
| C7   | H9A  | 3.352    | C7   | H9B  | 2.695    |
| C7   | H9C  | 2.695    | C8   | H7A  | 2.625    |
| C8   | H7B  | 3.297    | C8   | H7C  | 2.570    |
| C8   | H9A  | 2.714    | C8   | H9B  | 2.624    |
| C8   | H9C  | 3.340    | C8   | H21A | 3.190    |
| C8   | H26A | 2.984    | C8   | H26B | 3.283    |
| C9   | H3A  | 3.022    | C9   | H7A  | 3.352    |
| C9   | H7B  | 2.696    | C9   | H7C  | 2.696    |
| C9   | H8A  | 3.339    | C9   | H8B  | 2.672    |
| C9   | H8C  | 2.672    | C9   | H23A | 3.268    |
| C10  | H4A  | 3.506    | C10  | H4B  | 3.052    |
| C10  | H12A | 2.796    | C10  | H12B | 2.803    |
| C10  | H12C | 3.440    | C10  | H12D | 2.630    |
| C10  | H12E | 3.334    | C10  | H12F | 2.815    |
| C10  | H13A | 2.623    | C10  | H13B | 3.368    |
| C10  | H13C | 2.760    | C10  | H13D | 2.459    |
| C10  | H13E | 2.740    | C10  | H13F | 3.271    |
| C10  | H14A | 2.821    | C10  | H14B | 3.446    |
| C10  | H14C | 2.919    | C10  | H14D | 2.780    |
| C10  | H14E | 3.464    | C10  | H14F | 2.835    |
| C10  | H16A | 3.385    | C10  | H16B | 2.730    |
| C10  | H16C | 2.730    | C10  | H17A | 3.388    |
| C10  | H17B | 2.860    | C10  | H17C | 2.663    |
| C10  | H18A | 2.733    | C10  | H18B | 2.659    |
| C10  | H18C | 3.360    | C10  | H18D | 3.080    |
| C11  | H17B | 3.083    | C11  | H17C | 3.268    |
| C12  | H4B  | 2.944    | C12  | H13A | 2.722    |
| C12  | H13B | 2.681    | C12  | H13C | 3.373    |
| C12  | H14A | 3.332    | C12  | H14B | 2.670    |
| C12  | H14C | 2.670    | C12  | H16B | 3.559    |
| C12A | H4B  | 3.347    | C12A | H3D  | 3.287    |
| C12A | H13E | 2.740    | C12A | H13F | 2.741    |
| C12A | H14D | 3.267    | C12A | H14E | 2.630    |
| C12A | H14F | 2.630    | C13  | H12A | 2.842    |
| C13  | H12B | 3.412    | C13  | H12C | 2.815    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| C13    | H14A   | 2.666    | C13    | H14B   | 2.567    |
| C13    | H14C   | 3.343    | C13A   | H12D   | 3.305    |
| C13A   | H12E   | 2.721    | C13A   | H12F   | 2.721    |
| C13A   | H14D   | 2.636    | C13A   | H14E   | 2.717    |
| C13A   | H14F   | 3.342    | C13A   | H17B   | 2.916    |
| C13A   | H17C   | 2.813    | C14    | H12A   | 3.504    |
| C14    | H12B   | 2.698    | C14    | H12C   | 2.792    |
| C14    | H13A   | 3.318    | C14    | H13B   | 2.652    |
| C14    | H13C   | 2.652    | C14    | H16B   | 2.968    |
| C14    | H17B   | 2.548    | C14    | H17C   | 3.286    |
| C14A   | H12D   | 2.617    | C14A   | H12E   | 2.455    |
| C14A   | H12F   | 3.329    | C14A   | H13D   | 2.688    |
| C14A   | H13E   | 3.387    | C14A   | H13F   | 2.532    |
| C14A   | H16B   | 2.194    | C14A   | H16C   | 3.387    |
| C14A   | H17B   | 2.728    | C15    | H13D   | 2.881    |
| C15    | H14A   | 3.087    | C15    | H14C   | 3.188    |
| C15    | H14D   | 2.718    | C15    | H14F   | 3.158    |
| C16    | H4A    | 3.524    | C16    | H4B    | 3.542    |
| C16    | H4C    | 3.523    | C16    | H12B   | 3.529    |
| C16    | H14C   | 3.099    | C16    | H14D   | 2.634    |
| C16    | H14F   | 2.632    | C16    | H17A   | 2.813    |
| C16    | H17B   | 2.657    | C16    | H17C   | 3.387    |
| C16    | H18A   | 3.355    | C16    | H18B   | 2.709    |
| C16    | H18C   | 2.640    | C17    | H13D   | 2.330    |
| C17    | H14A   | 2.561    | C17    | H14C   | 3.232    |
| C17    | H14D   | 2.621    | C17    | H16A   | 2.703    |
| C17    | H16B   | 2.766    | C17    | H16C   | 3.391    |
| C17    | H18A   | 2.649    | C17    | H18B   | 3.352    |
| C17    | H18C   | 2.697    | C18    | H4A    | 3.452    |
| C18    | H16A   | 2.686    | C18    | H16B   | 3.354    |
| C18    | H16C   | 2.668    | C18    | H17A   | 2.576    |
| C18    | H17B   | 3.340    | C18    | H17C   | 2.783    |
| C19    | H8C    | 2.928    | C19    | H21A   | 2.678    |
| C19    | H21B   | 3.376    | C19    | H21C   | 2.738    |
| C19    | H22A   | 2.748    | C19    | H22B   | 3.403    |
| C19    | H22C   | 2.769    | C19    | H23A   | 2.717    |
| C19    | H23B   | 3.384    | C19    | H23C   | 2.732    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| C19   | H25A  | 2.850    | C19   | H25B  | 3.463    |
| C19   | H25C  | 2.871    | C19   | H26A  | 2.596    |
| C19   | H26B  | 2.721    | C19   | H26C  | 3.340    |
| C19   | H27A  | 2.636    | C19   | H27B  | 3.362    |
| C19   | H27C  | 2.746    | C20   | H1    | 2.217(19)|
| C20   | H25A  | 3.125    | C20   | H25C  | 3.002    |
| C20   | H26B  | 3.509    | C21   | H1    | 3.37(2)  |
| C21   | H8C   | 3.528    | C21   | H22A  | 2.728    |
| C21   | H22B  | 2.681    | C21   | H22C  | 3.370    |
| C21   | H23A  | 2.678    | C21   | H23B  | 2.675    |
| C21   | H23C  | 3.355    | C21   | H25C  | 2.799    |
| C21   | H26B  | 3.097    | C22   | H1    | 3.319(14)|
| C22   | H21A  | 3.366    | C22   | H21B  | 2.710    |
| C22   | H21C  | 2.710    | C22   | H23A  | 3.310    |
| C22   | H23B  | 2.612    | C22   | H23C  | 2.640    |
| C22   | H25A  | 2.646    | C22   | H25C  | 3.055    |
| C23   | H1    | 2.05(2)  | C22   | H9A   | 3.478    |
| C23   | H21A  | 2.714    | C23   | H21B  | 2.649    |
| C23   | H21C  | 3.350    | C23   | H22A  | 3.312    |
| C23   | H22B  | 2.625    | C23   | H22C  | 2.625    |
| C24   | H1    | 3.059(7) | C24   | H21A  | 3.460    |
| C24   | H21C  | 2.973    | C24   | H22A  | 2.977    |
| C24   | H22C  | 3.551    | C25   | H21C  | 2.747    |
| C25   | H22A  | 2.390    | C25   | H22C  | 3.544    |
| C25   | H26A  | 3.350    | C25   | H26B  | 2.680    |
| C25   | H26C  | 2.680    | C25   | H27A  | 3.321    |
| C25   | H27B  | 2.632    | C25   | H27C  | 2.632    |
| C26   | H8A   | 3.407    | C26   | H8C   | 3.000    |
| C26   | H21A  | 3.465    | C26   | H21C  | 3.286    |
| C26   | H25A  | 3.350    | C26   | H25B  | 2.680    |
| C26   | H25C  | 2.680    | C26   | H27A  | 2.722    |
| C26   | H27B  | 2.674    | C26   | H27C  | 3.362    |
| C27   | H1    | 3.539(15)| C27   | H25A  | 2.652    |
| C27   | H25B  | 2.608    | C27   | H25C  | 3.322    |
| C27   | H26A  | 2.735    | C27   | H26B  | 3.362    |
| C27   | H26C  | 2.660    | C28   | H18A  | 3.209    |
| C28   | H18B  | 2.915    | C28   | H26A  | 3.053    |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C28  | H27A | 3.000    | C29  | H18B | 3.457    |
| C29  | H26A | 3.255    | C33  | H18A | 2.895    |
| C33  | H18B | 3.217    | C33  | H27A | 3.200    |
| C34  | H13A | 3.060    | C34  | H13C | 3.425    |
| C34  | H13E | 3.558    | C34  | H27A | 3.132    |
| C34  | H27C | 3.283    | C35  | H27A | 3.556    |
| C35  | H27C | 3.059    | C39  | H13A | 3.448    |
| C39  | H13C | 3.143    | C39  | H13E | 3.330    |
| C40  | H1   | 3.190(9) | C40  | H9A  | 3.392    |
| C40  | H12A | 2.673    | C40  | H12C | 3.531    |
| C40  | H12D | 3.414    | C40  | H12F | 2.356    |
| C40  | H13A | 2.899    | C40  | H23A | 3.497    |
| C40  | H23C | 3.257    | C41  | H12F | 2.956    |
| C41  | H13A | 3.054    | C41  | H13B | 3.463    |
| C41  | H23C | 3.148    | C44  | H12F | 3.588    |
| C45  | H9A  | 3.288    | C45  | H12A | 2.653    |
| C45  | H12C | 3.297    | C45  | H12D | 3.303    |
| C45  | H12F | 2.769    | H1   | H8C  | 2.850    |
| H1   | H9A  | 3.151    | H1   | H21A | 3.304    |
| H1   | H22C | 3.227    | H1   | H23A | 1.950    |
| H1   | H23B | 3.033    | H1   | H23C | 1.900    |
| H1   | H26A | 3.449    | H1   | H27A | 3.246    |
| H3A  | H4B  | 3.507    | H3A  | H4C  | 3.583    |
| H3A  | H5B  | 3.139    | H3A  | H5C  | 2.649    |
| H3A  | H7A  | 3.300    | H3A  | H7B  | 2.113    |
| H3A  | H7C  | 3.585    | H3A  | H9A  | 3.572    |
| H3A  | H9C  | 2.368    | H3B  | H4A  | 3.495    |
| H3B  | H4B  | 2.395    | H3B  | H4C  | 2.826    |
| H3B  | H5B  | 3.548    | H3B  | H9C  | 3.001    |
| H3B  | H12A | 3.366    | H3B  | H12D | 3.512    |
| H3C  | H4B  | 3.060    | H3C  | H4C  | 2.564    |
| H3C  | H5A  | 3.519    | H3C  | H5B  | 2.434    |
| H3C  | H5C  | 2.841    | H3C  | H7B  | 3.381    |
| H4A  | H5A  | 2.462    | H4A  | H5B  | 2.917    |
| H4A  | H5C  | 3.548    | H4A  | H16C | 2.670    |
| H4A  | H18B | 2.577    | H4B  | H5A  | 3.566    |
| H4B  | H5B  | 3.546    | H4B  | H12A | 2.523    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H4B  | H12B | 2.686    | H4B  | H12D | 2.529    |
| H4B  | H14F | 3.593    | H4B  | H16C | 2.803    |
| H4B  | H18B | 3.454    | H4C  | H5A  | 2.928    |
| H4C  | H5B  | 2.429    | H4C  | H5C  | 3.530    |
| H4C  | H16C | 2.572    | H5A  | H7A  | 2.827    |
| H5A  | H7B  | 3.564    | H5A  | H8A  | 3.584    |
| H5B  | H7A  | 3.478    | H5C  | H7A  | 1.900    |
| H5C  | H7B  | 2.212    | H5C  | H7C  | 3.268    |
| H7A  | H8A  | 2.432    | H7A  | H8B  | 2.885    |
| H7A  | H8C  | 3.531    | H7A  | H9B  | 3.587    |
| H7A  | H9C  | 3.587    | H7B  | H8A  | 3.532    |
| H7B  | H8B  | 3.479    | H7B  | H9A  | 3.589    |
| H7B  | H9B  | 2.982    | H7B  | H9C  | 2.516    |
| H7C  | H8A  | 2.856    | H7C  | H8B  | 2.336    |
| H7C  | H8C  | 3.472    | H7C  | H9A  | 3.589    |
| H7C  | H9B  | 2.516    | H7C  | H9C  | 2.982    |
| H8A  | H9A  | 3.598    | H8A  | H9B  | 3.531    |
| H8A  | H26A | 2.742    | H8A  | H26B | 3.186    |
| H8B  | H9A  | 3.016    | H8B  | H9B  | 2.434    |
| H8B  | H9C  | 3.546    | H8B  | H21A | 2.727    |
| H8B  | H26A | 3.441    | H8B  | H26B | 3.270    |
| H8C  | H9A  | 2.530    | H8C  | H9B  | 2.885    |
| H8C  | H9C  | 3.588    | H8C  | H21A | 2.760    |
| H8C  | H23A | 3.124    | H8C  | H26A | 2.408    |
| H8C  | H26B | 2.854    | H9A  | H23A | 2.513    |
| H9B  | H21A | 3.577    | H9B  | H23A | 3.196    |
| H12A | H13A | 2.642    | H12A | H13B | 3.055    |
| H12B | H13B | 3.587    | H12B | H14A | 3.593    |
| H12B | H14B | 2.980    | H12B | H14C | 2.506    |
| H12B | H16B | 3.048    | H12B | H16C | 3.390    |
| H12C | H13A | 3.087    | H12C | H13B | 2.598    |
| H12C | H14B | 2.604    | H12C | H14C | 3.020    |
| H12D | H14D | 3.490    | H12D | H14E | 2.953    |
| H12D | H14F | 2.443    | H12E | H13D | 3.578    |
| H12E | H13E | 3.058    | H12E | H13F | 2.606    |
| H12E | H14D | 3.360    | H12E | H14E | 2.273    |
| H12E | H14F | 2.734    | H12F | H13D | 3.578    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance |
|-------|-------|----------|
| H12F  | H13E  | 2.606    |
| H12F  | H14E  | 3.520    |
| H13A  | H14A  | 3.552    |
| H13B  | H14A  | 2.974    |
| H13B  | H14C  | 3.539    |
| H13C  | H14B  | 2.832    |
| H13C  | H17C  | 3.059    |
| H13D  | H14E  | 3.060    |
| H13D  | H17A  | 3.250    |
| H13D  | H17C  | 1.935    |
| H13E  | H14E  | 3.595    |
| H13F  | H14D  | 2.728    |
| H13F  | H14F  | 3.459    |
| H13F  | H17C  | 3.525    |
| H14A  | H17A  | 3.433    |
| H14A  | H17C  | 2.593    |
| H14C  | H16B  | 2.314    |
| H14D  | H16A  | 3.201    |
| H14D  | H16C  | 3.329    |
| H14D  | H17B  | 1.891    |
| H14E  | H16B  | 3.067    |
| H14F  | H16A  | 3.422    |
| H14F  | H16C  | 2.865    |
| H16A  | H17A  | 2.618    |
| H16A  | H18A  | 3.566    |
| H16A  | H18C  | 2.454    |
| H16B  | H17B  | 2.519    |
| H16B  | H18C  | 3.550    |
| H16C  | H18A  | 3.584    |
| H16C  | H18C  | 2.887    |
| H17A  | H18B  | 3.508    |
| H17B  | H18A  | 3.586    |
| H17C  | H18A  | 2.582    |
| H21A  | H22B  | 3.578    |
| H21A  | H23B  | 3.002    |
| H21A  | H26B  | 2.840    |
| H21B  | H22B  | 2.501    |
Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom     | atom     | distance | atom     | atom     | distance |
|----------|----------|----------|----------|----------|----------|
| H21B     | H23A     | 2.912    | H21B     | H23B     | 2.452    |
| H21B     | H23C     | 3.555    | H21B     | H25C     | 3.475    |
| H21C     | H22A     | 2.552    | H21C     | H22B     | 2.955    |
| H21C     | H23A     | 3.588    | H21C     | H23B     | 3.555    |
| H21C     | H25A     | 3.120    | H21C     | H25B     | 3.537    |
| H21C     | H25C     | 1.991    | H21C     | H26B     | 2.684    |
| H22A     | H23B     | 3.517    | H22A     | H23C     | 3.539    |
| H22A     | H25A     | 1.826    | H22A     | H25B     | 3.275    |
| H22A     | H25C     | 2.337    | H22A     | H27C     | 3.524    |
| H22B     | H23A     | 3.519    | H22B     | H23B     | 2.406    |
| H22B     | H23C     | 2.922    | H22B     | H25A     | 3.421    |
| H22C     | H23A     | 3.532    | H22C     | H23B     | 2.881    |
| H22C     | H23C     | 2.436    | H22C     | H25A     | 2.925    |
| H22C     | H27C     | 3.546    | H25A     | H26B     | 3.576    |
| H25A     | H26C     | 3.576    | H25A     | H27A     | 3.550    |
| H25A     | H27B     | 2.936    | H25A     | H27C     | 2.448    |
| H25B     | H26A     | 3.576    | H25B     | H26B     | 2.960    |
| H25B     | H26C     | 2.490    | H25B     | H27A     | 3.516    |
| H25B     | H27B     | 2.401    | H25B     | H27C     | 2.873    |
| H25C     | H26A     | 3.576    | H25C     | H26B     | 2.490    |
| H25C     | H26C     | 2.960    | H25C     | H27B     | 3.524    |
| H25C     | H27C     | 3.544    | H26A     | H27A     | 2.580    |
| H26A     | H27B     | 2.998    | H26B     | H27B     | 3.555    |
| H26C     | H27A     | 2.959    | H26C     | H27B     | 2.447    |
| H26C     | H27C     | 3.551    |
Table S7-11. Intermolecular contacts less than 3.60 Å

| atom | atom | distance  | atom | atom | distance  |
|------|------|-----------|------|------|-----------|
| F1   | F2   | 3.442(4)  | F2   | F1   | 3.442(4)  |
| F3   | F4   | 3.487(4)  | F3   | F7   | 2.896(4)  |
| F3   | C7   | 3.427(8)  | F3   | C18  | 3.565(7)  |
| F3   | C25  | 3.591(6)  | F4   | F3   | 3.487(4)  |
| F4   | F4   | 3.058(4)  | F4   | F6   | 3.471(4)  |
| F4   | F7   | 3.241(4)  | F4   | C22  | 3.535(6)  |
| F5   | C31  | 3.415(6)  | F4   | C18  | 3.195(6)  |
| F5   | C25  | 3.444(6)  | F5   | C27  | 3.349(5)  |
| F6   | F4   | 3.471(4)  | F7   | F3   | 2.896(4)  |
| F7   | F4   | 3.241(4)  | F7   | C31  | 3.004(5)  |
| F7   | C32  | 3.191(5)  | F8   | C5   | 3.069(6)  |
| F8   | C21  | 3.577(7)  | F9   | C9   | 3.504(9)  |
| F9   | C25  | 3.598(5)  | F11  | C16  | 3.512(7)  |
| F12  | C14  | 3.364(13) | F12  | C14A | 3.22(2)   |
| F12  | C16  | 3.394(9)  | F13  | C3   | 3.360(8)  |
| F13  | C14  | 3.451(15) | F14  | C9   | 3.578(7)  |
| F14  | F15  | 2.950(5)  | F14  | C9   | 3.578(7)  |
| F15  | F14  | 2.950(5)  | C7   | F3   | 3.427(8)  |
| C5   | F8   | 3.069(6)  | C7   | F3   | 3.427(8)  |
| C7   | C17  | 3.544(9)  | C9   | F9   | 3.504(9)  |
| C9   | F14  | 3.578(7)  | C14  | F12  | 3.364(13) |
| C14  | F13  | 3.451(15) | C14  | C42  | 3.371(13) |
| C14  | C43  | 3.417(14) | C14A | F12  | 3.22(2)   |
| C16  | F11  | 3.512(7)  | C16  | F12  | 3.394(9)  |
| C17  | C7   | 3.544(9)  | C18  | F3   | 3.565(7)  |
| C21  | F8   | 3.577(7)  | C22  | F4   | 3.535(6)  |
| C22  | C30  | 3.552(8)  | C25  | F3   | 3.591(6)  |
| C25  | F5   | 3.444(6)  | C25  | F9   | 3.598(5)  |
| C27  | F5   | 3.349(5)  | C30  | C22  | 3.552(8)  |
| C31  | F4   | 3.415(6)  | C31  | F7   | 3.004(5)  |
| C32  | F4   | 3.195(6)  | C32  | F7   | 3.191(5)  |
| C42  | C14  | 3.371(13) | C43  | C14A | 3.417(14) |

Symmetry Operators:

(1) -X+2,-Y,-Z+1  (2) -X+2,-Y+1,-Z+1
(3) -X+1,-Y+1,-Z+1  (4) X+1,Y,Z
(5) X-1,Y+1,Z  (6) X,Y+1,Z
(7) X-1,Y,Z  (8) -X+1,-Y+1,-Z+2
(9) $-X+1, Y, -Z+2$
(10) $X+1, Y-1, Z$
(11) $X, Y-1, Z$
Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| F1    | H22B  | 3.278    | F2    | H7A   | 2.963    |
| F2    | H8A   | 2.893    | F2    | H21C  | 3.371    |
| F2    | H22A  | 3.024    | F2    | H22B  | 3.416    |
| F2    | H25C  | 3.261    | F3    | H7A   | 2.927    |
| F3    | H7C   | 3.063    | F3    | H17A  | 3.253    |
| F3    | H18A  | 3.113    | F3    | H18C  | 3.121    |
| F3    | H22A  | 3.460    | F3    | H25A  | 3.025    |
| F3    | H25C  | 3.583    | F4    | H22A  | 3.049    |
| F4    | H22A  | 3.113    | F4    | H27C  | 3.313    |
| F4    | H25A  | 2.918    | F5    | H25A  | 3.123    |
| F5    | H25A  | 2.947    | F5    | H27C  | 2.795    |
| F5    | H27B  | 3.065    | F6    | H16A  | 3.283    |
| F6    | H16A  | 3.001    | F7    | H7A   | 3.570    |
| F7    | H5A   | 3.512    | F7    | H17A  | 3.158    |
| F8    | H5A   | 3.072    | F8    | H16A  | 3.283    |
| F8    | H5C   | 2.851    | F8    | H16B  | 3.072    |
| F9    | H7C   | 3.324    | F9    | H16B  | 2.748    |
| F9    | H26C  | 2.966    | F10   | H7C   | 3.206    |
| F10   | H5C   | 3.583    | F11   | H16A  | 2.751    |
| F11   | H21A  | 3.113    | F12   | H14A  | 3.420    |
| F12   | H14B  | 3.353    | F12   | H14C  | 2.797    |
| F12   | H14D  | 2.848    | F12   | H14C  | 2.787    |
| F12   | H14F  | 3.330    | F12   | H14D  | 3.575    |
| F12   | H16A  | 3.295    | F12   | H16B  | 2.741    |
| F13   | H3A   | 2.662    | F13   | H3B   | 3.597    |
| F13   | H3C   | 3.357    | F13   | H7B   | 3.458    |
| F13   | H13D  | 3.461    | F13   | H14A  | 2.747    |
| F13   | H14C  | 3.449    | F13   | H14D  | 3.127    |
| F13   | H17B  | 2.806    | F14   | H3A   | 3.237    |
| F14   | H3B   | 3.345    | F14   | H9C   | 2.665    |
| C4    | H23B  | 3.380    | C5    | H21B  | 3.513    |
| C5    | H23B  | 3.496    | C7    | H17A  | 3.218    |
| C7    | H17C  | 3.082    | C8    | H25C  | 3.409    |
Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| C12A   | H13F8  | 3.424    | C13    | H14B8  | 3.413    |
| C13A   | H12E8  | 3.416    | C14    | H13B8  | 3.401    |
| C17    | H7B7   | 3.042    | C17    | H7C7   | 3.216    |
| C18    | H22B1  | 3.535    | C18    | H22C1  | 3.120    |
| C21    | H26B11 | 3.216    | C21    | H26C11 | 3.521    |
| C22    | H18B5  | 3.236    | C22    | H18C5  | 3.325    |
| C25    | H8B11  | 3.358    | C26    | H21A11 | 3.519    |
| C26    | H21C11 | 3.381    | C27    | H27B4  | 3.432    |
| C29    | H22A1  | 3.548    | C29    | H22B1  | 3.171    |
| C30    | H22A1  | 2.969    | C30    | H22B1  | 3.236    |
| C31    | H22A1  | 3.204    | C31    | H25A1  | 3.490    |
| C33    | H27C4  | 3.532    | C37    | H26C4  | 3.105    |
| C38    | H25B4  | 3.030    | C38    | H26C4  | 3.048    |
| C39    | H27B4  | 3.451    | C39    | H25B4  | 3.120    |
| C41    | H14E8  | 3.539    | C41    | H14B8  | 3.495    |
| C42    | H14A8  | 3.278    | C42    | H14B8  | 3.092    |
| C42    | H14C8  | 3.178    | C42    | H14D8  | 3.315    |
| C42    | H14E8  | 3.016    | C43    | H13F8  | 3.503    |
| C43    | H14A8  | 2.939    | C43    | H14B8  | 3.281    |
| C43    | H14C8  | 3.490    | C43    | H14D8  | 3.442    |
| C43    | H14E8  | 3.558    | C43    | H14D8  | 3.442    |
| H3A    | F14g   | 3.237    | H3A    | F13g   | 2.662    |
| H3B    | F14g   | 3.345    | H3B    | F13g   | 3.597    |
| H4A    | H22B1  | 2.817    | H4A    | H23B1  | 3.179    |
| H4C    | H23B1  | 2.749    | H5A    | F812   | 3.072    |
| H5A    | H21B1  | 2.931    | H5A    | H22B1  | 3.141    |
| H5A    | H23B1  | 3.313    | H5B    | F812   | 2.768    |
| H5B    | H21B1  | 3.210    | H5B    | H23B1  | 2.886    |
| H5C    | F712   | 3.512    | H5C    | F812   | 2.851    |
| H7A    | F2     | 2.963    | H7A    | F3     | 2.927    |
| H7A    | F712   | 3.570    | H7A    | H17A10 | 3.344    |
| H7A    | H17C10 | 3.594    | H7B    | F13g   | 3.458    |
| H7B    | C1710  | 3.042    | H7B    | H17A10 | 2.759    |
| H7B    | H17B10 | 3.114    | H7B    | H17C10 | 2.749    |
| H7C    | F3q    | 3.063    | H7C    | F910   | 3.324    |
| H7C    | F1010  | 3.206    | H7C    | C1710  | 3.216    |
Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H7C   | H17A  | 3.040    | H7C   | H17C  | 2.560    |
| H7C   | H25B  | 3.494    | H8A   | F2    | 2.893    |
| H8A   | H21C  | 3.521    | H8A   | H25C  | 3.215    |
| H8B   | F9    | 2.748    | H8B   | C25   | 3.358    |
| H8B   | H25B  | 3.098    | H8B   | H25C  | 2.726    |
| H9B   | F9    | 2.569    | H9C   | F14   | 2.665    |
| H12C  | H13B  | 2.982    | H12C  | H14B  | 3.196    |
| H12E  | C13A  | 3.416    | H12E  | H12E  | 3.509    |
| H12E  | H13E  | 3.454    | H12E  | H13F  | 2.579    |
| H12F  | H13F  | 3.454    | H13B  | C14   | 3.401    |
| H13B  | H12C  | 2.982    | H13B  | H13B  | 3.212    |
| H13B  | H14B  | 2.458    | H13D  | F13   | 3.461    |
| H13E  | H12E  | 3.454    | H13F  | C12A  | 3.424    |
| H13F  | C43   | 3.503    | H12E  | H12E  | 2.579    |
| H13F  | H12F  | 3.454    | H14A  | F12   | 3.420    |
| H14A  | F13   | 2.747    | H14A  | C42   | 3.278    |
| H14A  | C43   | 2.939    | H14B  | F12   | 3.353    |
| H14B  | C13   | 3.413    | H14B  | C41   | 3.495    |
| H14B  | C42   | 3.092    | H14B  | C34   | 3.281    |
| H14B  | H12C  | 3.196    | H14B  | H13B  | 2.458    |
| H14C  | F12   | 2.797    | H14C  | F13   | 3.449    |
| H14C  | C42   | 3.178    | H14C  | C43   | 3.490    |
| H14D  | F12   | 2.848    | H14D  | F13   | 3.127    |
| H14D  | C42   | 3.315    | H14D  | C43   | 3.442    |
| H14E  | F12   | 2.787    | H14E  | C41   | 3.539    |
| H14E  | C42   | 3.016    | H14E  | C43   | 3.558    |
| H14F  | F12   | 3.330    | H14F  | F12   | 3.575    |
| H16A  | F6    | 3.001    | H16A  | F11   | 2.751    |
| H16A  | F12   | 3.295    | H16A  | C41   | 3.580    |
| H16A  | H22C  | 3.254    | H16A  | H23C  | 3.250    |
| H16B  | F11   | 3.587    | H16B  | F12   | 2.741    |
| H16C  | H22B  | 3.577    | H16C  | H22C  | 3.337    |
| H16C  | H23B  | 3.353    | H16C  | H23C  | 3.150    |
| H17A  | F3    | 3.253    | H17A  | F7    | 2.720    |
| H17A  | C7    | 3.218    | H17A  | H7A   | 3.344    |
| H17A  | H7B   | 2.759    | H17A  | H7C   | 3.040    |
| H17B  | F13   | 2.806    | H17B  | H7B   | 3.114    |
Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom | distance | atom   | atom | distance |
|--------|------|----------|--------|------|----------|
| H17C   | C7   | 3.082    | H17C   | H7A  | 3.594    |
| H17C   | H7B  | 2.749    | H17C   | H7C  | 2.560    |
| H18A   | F3   | 3.113    | H18B   | C22  | 3.236    |
| H18B   | H22B | 2.814    | H18B   | H22C | 2.825    |
| H18C   | F3   | 3.121    | H18C   | F4   | 2.838    |
| H18C   | F6   | 3.283    | H18C   | F7   | 3.158    |
| H18C   | C22  | 3.325    | H18C   | H22B | 3.375    |
| H18C   | H22C | 2.548    | H21A   | F8   | 3.507    |
| H21A   | F9   | 2.948    | H21A   | C26  | 3.519    |
| H21A   | H26B | 2.939    | H21A   | H26C | 3.192    |
| H21B   | F8   | 2.814    | H21B   | F9   | 3.595    |
| H21B   | C5   | 3.513    | H21B   | H5A  | 2.931    |
| H21B   | H5B  | 3.210    | H21B   | H26B | 3.552    |
| H21B   | H26C | 3.452    | H21C   | F2   | 3.371    |
| H21C   | C26  | 3.381    | H21C   | H8A  | 3.521    |
| H21C   | H26B | 2.709    | H21C   | H26C | 3.338    |
| H22A   | F2   | 3.024    | H22A   | F3   | 3.460    |
| H22A   | F4   | 3.113    | H22A   | C29  | 3.548    |
| H22A   | C30  | 2.969    | H22A   | C31  | 3.204    |
| H22B   | F1   | 3.278    | H22B   | F2   | 3.416    |
| H22B   | C18  | 3.535    | H22B   | C29  | 3.171    |
| H22B   | C30  | 3.236    | H22B   | H4A  | 2.817    |
| H22B   | H5A  | 3.141    | H22B   | H16C | 3.577    |
| H22B   | H18B | 2.814    | H22B   | H18C | 3.375    |
| H22C   | F4   | 3.049    | H22C   | C18  | 3.120    |
| H22C   | H16A | 3.254    | H22C   | H16C | 3.337    |
| H22C   | H18B | 2.825    | H22C   | H18C | 2.548    |
| H23B   | C4   | 3.380    | H23B   | C5   | 3.496    |
| H23B   | H4A  | 3.179    | H23B   | H4C  | 2.749    |
| H23B   | H5A  | 3.313    | H23B   | H5B  | 2.886    |
| H23B   | H16C | 3.353    | H23C   | H16A | 3.250    |
| H23C   | H16C | 3.150    | H25A   | F3   | 3.025    |
| H25A   | F4   | 2.918    | H25A   | F5   | 2.947    |
| H25A   | C31  | 3.490    | H25B   | F5   | 3.123    |
| H25B   | F9   | 2.763    | H25B   | F10  | 2.928    |
| H25B   | C38  | 3.030    | H25B   | C39  | 3.120    |
| H25B   | H7C  | 3.494    | H25B   | H8B  | 3.098    |
Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom     | distance | atom  | atom     | distance |
|-------|----------|----------|-------|----------|----------|
| H25C  | F2<sup>5</sup> | 3.261    | H25C  | F3<sup>3</sup> | 3.583    |
| H25C  | C8<sup>11</sup> | 3.409    | H25C  | H8A<sup>11</sup> | 3.215    |
| H25C  | H8B<sup>11</sup> | 2.726    | H26B  | C21<sup>11</sup> | 3.216    |
| H26B  | H21A<sup>11</sup> | 2.939    | H26B  | H21B<sup>11</sup> | 3.552    |
| H26B  | H21C<sup>11</sup> | 2.709    | H26B  | H26B<sup>11</sup> | 2.978    |
| H26C  | F8<sup>4</sup> | 3.072    | H26C  | C37<sup>4</sup> | 3.105    |
| H26C  | C21<sup>11</sup> | 3.521    | H26C  | H21A<sup>11</sup> | 3.338    |
| H26C  | C38<sup>4</sup> | 3.048    | H26C  | H21C<sup>11</sup> | 3.192    |
| H27A  | H27B<sup>4</sup> | 3.419    | H27B  | F5<sup>4</sup> | 3.065    |
| H27B  | C27<sup>4</sup> | 3.432    | H27B  | C38<sup>4</sup> | 3.451    |
| H27B  | C39<sup>4</sup> | 3.395    | H27B  | H27A<sup>4</sup> | 3.419    |
| H27B  | H27B<sup>4</sup> | 3.189    | H27B  | H27C<sup>4</sup> | 3.122    |
| H27C  | F4<sup>4</sup> | 3.313    | H27C  | F5<sup>4</sup> | 2.795    |
| H27C  | C33<sup>4</sup> | 3.532    | H27C  | H27B<sup>4</sup> | 3.122    |

Symmetry Operators:

1. X+1,Y,Z
2. -X+2,-Y,-Z+1
3. -X+2,-Y+1,-Z+1
4. -X+1,-Y+1,-Z+1
5. X-1,Y,Z
6. X-1,Y+1,Z
7. X,Y+1,Z
8. -X+1,-Y+1,-Z+2
9. -X+1,-Y,-Z+2
10. X,Y-1,Z
11. -X+1,-Y,-Z+1
12. X+1,Y-1,Z
X-ray Structure Report

for

\[ \text{Nb(N-2,6-MeC}_6\text{H}_3(\text{N=C}^\text{tBu}_2)\text{2[OC(CF}_3)_3]HN=C}^\text{tBu}_2) \ (8) \]

October 30, 2016
**Experimental**

**Data Collection**

A yellow block crystal of C_{39}H_{64}F_{9}N_{4}NbO having approximate dimensions of 0.300 x 0.250 x 0.200 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-K\(\alpha\) radiation.

The crystal-to-detector distance was 45.00 mm.

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

\[
\begin{align*}
    a &= 11.7181(3) \text{ Å} \\
    b &= 18.3197(5) \text{ Å} \\
    c &= 20.1982(5) \text{ Å} \\
    V &= 4333.79(19) \text{ Å}^3
\end{align*}
\]

For \(Z = 4\) and F.W. = 868.85, the calculated density is 1.332 g/cm\(^3\). The reflection conditions of:

\[
\begin{align*}
    h0l: & \quad h+l = 2n \\
    0k0: & \quad k = 2n
\end{align*}
\]

uniquely determine the space group to be:

\[P2_1/n \ (\#14)\]

The data were collected at a temperature of -180 ± 1\(^\circ\)C to a maximum 2\(\theta\) value of 61.3\(^\circ\). A total of 720 oscillation images were collected. A sweep of data was done using \(\omega\) scans from -105.0 to 75.0\(^\circ\) in 0.50\(^\circ\) step, at \(\chi=45.0^\circ\) and \(\phi = 0.0^\circ\). The exposure rate was 60.0 [sec./\(^\circ\)]. The detector swing angle was -15.00\(^\circ\).

A second sweep was performed using \(\omega\) scans from -105.0 to 75.0\(^\circ\) in 0.50\(^\circ\) step, at \(\chi=45.0^\circ\) and \(\phi = 90.0^\circ\). The exposure rate was 60.0 [sec./\(^\circ\)]. The detector swing angle was -15.00\(^\circ\). The crystal-to-detector distance was 45.00 mm. Readout was performed in the 0.172 mm pixel mode.
Data Reduction

Of the 0 reflections were collected, where 0 were unique ($R_{\text{int}} = 0.0218$); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). ¹

The linear absorption coefficient, $\mu$, for Mo-Kα radiation is 3.500 cm⁻¹. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.826 to 0.932. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods² and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement³ on $F^2$ was based on 9907 observed reflections and 804 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$R1 = \sum |F_o| - |F_c| / \sum |F_o| = 0.0340$

$wR2 = [ \sum (w(F_o^2 - F_c^2)^2) / \sum w(F_o^2)^2 ]^{1/2} = 0.0890$

The goodness of fit⁴ was 1.07. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.81 and -1.04 e⁻/Å³, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4.⁵ Anomalous dispersion effects were included in Fcalc⁶; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁷. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁸. All calculations were performed using the CrystalStructure⁹ crystallographic software package.
except for refinement, which was performed using SHELXL Version 2014/7\textsuperscript{10}.

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

\[ \sum w(F_o^2-F_c^2)^2 \] where \( w \) = Least Squares weights.

(4) Goodness of fit is defined as:

\[ \left[ \sum w(F_o^2-F_c^2)^2/(N_o-N_v) \right]^{1/2} \]

where:\n\( N_o \) = number of observations\n\( N_v \) = number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2.3: Crystal Structure Analysis Package, Rigaku Corporation (2000-2016). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
**EXPERIMENTAL DETAILS**

A. Crystal Data

| Property                  | Value                          |
|---------------------------|--------------------------------|
| Empirical Formula         | C$_{39}$H$_{64}$F$_9$N$_4$NbO   |
| Formula Weight            | 868.85                         |
| Crystal Color, Habit      | yellow, block                  |
| Crystal Dimensions        | 0.300 X 0.250 X 0.200 mm       |
| Crystal System            | monoclinic                     |
| Lattice Type              | Primitive                      |
| Lattice Parameters        | a = 11.7181(3) Å               |
|                           | b = 18.3197(5) Å               |
|                           | c = 20.1982(5) Å               |
|                           | β = 91.823(2)°                 |
|                           | V = 4333.79(19) Å$^3$          |
| Space Group               | P2$_1$/n (#14)                 |
| Z value                   | 4                              |
| D$_{calc}$                | 1.332 g/cm$^3$                 |
| F$_{000}$                 | 1824.00                        |
| μ(MoKα)                   | 3.500 cm$^{-1}$                |
B. Intensity Measurements

| Parameter                                      | Value                        |
|------------------------------------------------|------------------------------|
| Diffractometer                                 | XtaLAB P200                  |
| Radiation                                      | MoKα (λ = 0.71073 Å)         |
| multi-layer mirror monochromated               |                              |
| Voltage, Current                               | 50kV, 24mA                   |
| Temperature                                    | -180.0°C                     |
| Detector Aperture                              | 83.8 x 70.0 mm               |
| Data Images                                    | 720 exposures                |
| ω oscillation Range (χ=45.0, φ=0.0)            | -105.0 - 75.0°               |
| Exposure Rate                                  | 60.0 sec./°                  |
| Detector Swing Angle                           | -15.00°                      |
| ω oscillation Range (χ=45.0, φ=90.0)           | -105.0 - 75.0°               |
| Exposure Rate                                  | 60.0 sec./°                  |
| Detector Swing Angle                           | -15.00°                      |
| Detector Position                              | 45.00 mm                     |
| Pixel Size                                     | 0.172 mm                     |
| 2θ_{max}                                       | 55.0°                        |
| No. of Reflections Measured                    | Total: 34505                 |
Unique: 9907 ($R_{int} = 0.0218$)

| Corrections | Lorentz-polarization Absorption |
|-------------|--------------------------------|
|             | (trans. factors: 0.826 - 0.932) |
C. Structure Solution and Refinement

Structure Solution  Direct Methods (SHELXT)

Refinement  Full-matrix least-squares on $F^2$

Function Minimized  $\sum w (F_o^2 - F_c^2)^2$

Least Squares Weights  
$$w = 1/ \left[ \sigma^2 (F_o^2) + (0.0375 \cdot P)^2 + 4.0783 \cdot P \right]$$

where $P = (\text{Max}(F_o^2, 0) + 2F_c^2)/3$

$2\theta_{\text{max}}$ cutoff  55.0°

Anomalous Dispersion  All non-hydrogen atoms

No. Observations (All reflections)  9907

No. Variables  804

Reflection/Parameter Ratio  12.32

Residuals: $R_1$ (I>2.00$\sigma$(I))  0.0340

Residuals: $R$ (All reflections)  0.0387

Residuals: $wR^2$ (All reflections)  0.0890

Goodness of Fit Indicator  1.070

Max Shift/Error in Final Cycle  0.004

Maximum peak in Final Diff. Map  0.81 $e^{-}/\text{Å}^3$

Minimum peak in Final Diff. Map  -1.04 $e^{-}/\text{Å}^3$
Table S8-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ and occupancy

| atom | x         | y         | z         | $B_{\text{eq}}$ | occ |
|------|-----------|-----------|-----------|----------------|-----|
| Nb1  | 0.61143(2)| 0.27405(2)| 0.40167(2)| 1.810(5)       | 1   |
| F36A | 0.3729(3) | 0.08203(19)| 0.34643(13)| 3.65(7)        | 0.564(5) |
| F36B | 0.4573(10)| 0.0372(7) | 0.2511(7) | 4.3(2)         | 0.564(5) |
| F36C | 0.5415(12)| 0.0369(8) | 0.3501(7) | 3.7(2)         | 0.564(5) |
| F36D | 0.3232(3) | 0.1235(2) | 0.33269(16)| 3.21(8)        | 0.436(5) |
| F37A | 0.5567(8) | 0.1255(3) | 0.1814(4) | 4.93(15)       | 0.564(5) |
| F37B | 0.6620(11)| 0.2036(10)| 0.2337(8) | 5.1(2)         | 0.564(5) |
| F37C | 0.6787(3) | 0.0859(2) | 0.2558(2) | 4.59(8)        | 0.564(5) |
| F37D | 0.5141(16)| 0.0415(9) | 0.3528(7) | 3.5(2)         | 0.436(5) |
| F38A | 0.3575(13)| 0.2339(8) | 0.3100(9) | 3.56(13)       | 0.564(5) |
| F38B | 0.3286(10)| 0.1573(9) | 0.2314(7) | 3.40(13)       | 0.564(5) |
| F38C | 0.4585(6) | 0.2556(2) | 0.2341(2) | 5.60(12)       | 0.564(5) |
| F38D | 0.6763(14)| 0.1970(12)| 0.2402(10)| 3.07(15)       | 0.436(5) |
| O1   | 0.56409(11)| 0.18047(7)| 0.35093(6)| 1.84(2)        | 1   |
| N1   | 0.55287(13)| 0.34318(8)| 0.34816(7)| 1.95(2)        | 1   |
| N2   | 0.51839(17)| 0.28936(9)| 0.47969(8)| 2.67(3)        | 1   |
| N3   | 0.77439(14)| 0.29798(8)| 0.39555(7)| 2.09(3)        | 1   |
| N4   | 0.69393(16)| 0.16715(9)| 0.46788(8)| 2.48(3)        | 1   |
| C1   | 0.50814(16)| 0.39920(10)| 0.30861(9)| 2.06(3)        | 1   |
| C2   | 0.39929(18)| 0.42774(10)| 0.32129(12)| 2.76(4)        | 1   |
| C3   | 0.3558(2) | 0.48393(11)| 0.28173(12)| 3.21(4)        | 1   |
| C4   | 0.4184(2) | 0.51240(12)| 0.23063(11)| 3.30(4)        | 1   |
| C5   | 0.5250(2) | 0.48468(12)| 0.21879(10)| 3.03(4)        | 1   |
| C6   | 0.57209(17)| 0.42787(11)| 0.25647(9)| 2.41(3)        | 1   |
| C7   | 0.68784(18)| 0.39791(14)| 0.24272(11)| 3.15(4)        | 1   |
| C8   | 0.3340(2) | 0.39873(12)| 0.37881(16)| 4.20(6)        | 1   |
| C9   | 0.4556(2) | 0.29805(11)| 0.52896(10)| 3.02(4)        | 1   |
| C10  | 0.4730(3) | 0.36562(13)| 0.57510(13)| 5.35(8)        | 1   |
| C11  | 0.3910(9) | 0.4140(3) | 0.5824(4) | 3.28(14)       | 0.509(17) |
| C12  | 0.5290(10)| 0.3353(4) | 0.6496(3) | 3.33(15)       | 0.509(17) |
| C13  | 0.5939(9) | 0.4070(5) | 0.5543(4) | 2.72(13)       | 0.509(17) |
| C14  | 0.3672(2) | 0.23607(10)| 0.54298(10)| 2.65(3)        | 1   |
| C15  | 0.449(3) | 0.1742(17)| 0.5839(16)| 2.7(3)         | 0.29(3) |
| C16  | 0.326(3) | 0.2086(18)| 0.4830(14)| 2.6(3)         | 0.29(3) |
| C17  | 0.2845(15)| 0.2605(8) | 0.5908(8) | 2.32(19)       | 0.29(3) |
| C18  | 0.75232(19)| 0.13192(11)| 0.51239(9)| 2.74(4)        | 1   |
| C19  | 0.8080(2) | 0.17479(14)| 0.57054(10)| 3.59(5)        | 1   |
Table S8-1. Atomic coordinates and $B_{iso}/B_{eq}$ and occupancy (continued)

| atom | x      | y      | z      | $B_{eq}$     | occ   |
|------|--------|--------|--------|--------------|-------|
| C20  | 0.9466(6) | 0.1537(7) | 0.5768(5) | 4.27(19)     | 0.500(19) |
| C21  | 0.7826(16) | 0.1489(12) | 0.6384(11) | 3.6(3)       | 0.500(19) |
| C22  | 0.7992(10) | 0.2485(4)   | 0.5625(3)   | 2.41(12)     | 0.500(19) |
| C23  | 0.87783(18) | 0.31613(11) | 0.38988(9)  | 2.47(3)      | 1     |
| C24  | 0.7595(2)   | 0.04712(12) | 0.50596(10) | 2.91(4)      | 1     |
| C25  | 0.8003(3)   | 0.0265(2)   | 0.4356(2)   | 2.90(6)      | 0.793(7) |
| C26  | 0.8360(5)   | 0.0019(2)   | 0.5536(2)   | 5.48(12)     | 0.793(7) |
| C27  | 0.6355(3)   | 0.01800(15) | 0.51169(16) | 3.18(7)      | 0.793(7) |
| C28  | 0.95539(18) | 0.26587(13) | 0.34928(11) | 3.02(4)      | 1     |
| C29  | 0.9527(3)   | 0.2975(2)   | 0.27652(16) | 3.42(6)      | 0.710(4) |
| C30  | 1.0783(3)   | 0.2656(2)   | 0.3763(3)   | 4.95(10)     | 0.710(4) |
| C31  | 0.9094(3)   | 0.19134(17) | 0.34761(17) | 3.01(6)      | 0.710(4) |
| C32  | 0.9216(3)   | 0.38884(13) | 0.42244(11) | 3.85(5)      | 1     |
| C33  | 0.8426(9)   | 0.4217(5)   | 0.4575(5)   | 3.35(14)     | 0.524(18) |
| C34  | 0.9662(18)  | 0.4436(12)  | 0.3700(9)   | 3.9(3)       | 0.524(18) |
| C35  | 1.0359(8)   | 0.3674(4)   | 0.4701(4)   | 3.36(14)     | 0.524(18) |
| C36  | 0.4687(4)   | 0.0744(2)   | 0.3127(2)   | 2.30(7)      | 0.564(5) |
| C36A | 0.3752(4)   | 0.1681(3)   | 0.2912(3)   | 2.35(9)      | 0.436(5) |
| C37  | 0.6075(4)   | 0.1403(3)   | 0.24051(18) | 3.50(10)     | 0.564(5) |
| C37A | 0.5301(6)   | 0.0718(3)   | 0.2929(3)   | 2.66(10)     | 0.436(5) |
| C38  | 0.4195(5)   | 0.1994(3)   | 0.2683(2)   | 3.47(9)      | 0.564(5) |
| C38A | 0.5582(4)   | 0.1907(3)   | 0.2315(2)   | 2.43(9)      | 0.436(5) |
| C39  | 0.51278(16) | 0.15279(10)| 0.29508(8)  | 1.86(3)      | 1     |
| F0AA | 0.3501(14)  | 0.2245(10)  | 0.3183(11)  | 4.7(3)       | 0.436(5) |
| F1AA | 0.3511(14)  | 0.1620(11)  | 0.2263(8)   | 4.2(3)       | 0.436(5) |
| F2AA | 0.6375(4)   | 0.0584(3)   | 0.2778(2)   | 3.76(9)      | 0.436(5) |
| F3AA | 0.4456(10)  | 0.0318(9)   | 0.2588(8)   | 2.46(12)     | 0.436(5) |
| F4AA | 0.5121(4)   | 0.2561(3)   | 0.2197(3)   | 3.21(8)      | 0.436(5) |
| F5AA | 0.5404(9)   | 0.1509(4)   | 0.1764(5)   | 3.35(11)     | 0.436(5) |
| C30A | 1.0117(6)   | 0.2013(4)   | 0.4020(4)   | 2.75(13)     | 0.290(4) |
| C29A | 1.0543(7)   | 0.2870(5)   | 0.3084(4)   | 3.15(15)     | 0.290(4) |
| C31A | 0.8818(6)   | 0.2088(4)   | 0.3035(4)   | 2.56(13)     | 0.290(4) |
| C26A | 0.6761(10)  | 0.0191(5)   | 0.5583(8)   | 3.3(3)       | 0.207(7) |
| C25A | 0.8840(12)  | 0.0250(8)   | 0.5345(7)   | 3.2(3)       | 0.207(7) |
| C27A | 0.7433(19)  | 0.0255(8)   | 0.4410(8)   | 3.8(3)       | 0.207(7) |
| C20A | 0.9271(8)   | 0.1854(6)   | 0.5611(4)   | 4.00(16)     | 0.500(19) |
| C21A | 0.7513(13)  | 0.1469(13)  | 0.6368(10)  | 2.9(2)       | 0.500(19) |
Table S8-1. Atomic coordinates and \( B_{\text{iso}} \)/\( B_{\text{eq}} \) and occupancy (continued)

| atom | x         | y         | z         | \( B_{\text{eq}} \) | occ    |
|------|-----------|-----------|-----------|---------------------|--------|
| C22A | 0.7498(10)| 0.2609(4) | 0.5682(3) | 2.45(13)            | 0.500(19) |
| C35A | 0.9825(10)| 0.3822(4) | 0.4875(4) | 3.25(18)            | 0.476(18) |
| C33A | 0.7996(10)| 0.4373(4) | 0.4449(4) | 2.99(13)            | 0.476(18) |
| C34A | 0.981(2)  | 0.4367(12)| 0.3724(9) | 3.5(3)              | 0.476(18) |
| C13A | 0.5477(10)| 0.4167(5) | 0.5476(4) | 2.94(14)            | 0.491(17) |
| C11A | 0.3387(10)| 0.4162(3) | 0.5624(4) | 3.34(14)            | 0.491(17) |
| C12A | 0.4697(10)| 0.3502(4) | 0.6438(3) | 3.08(15)            | 0.491(17) |
| C17A | 0.2499(11)| 0.2572(3) | 0.5743(6) | 3.25(15)            | 0.71(3) |
| C15A | 0.4254(10)| 0.1789(7) | 0.5845(6) | 2.41(12)            | 0.71(3) |
| C16A | 0.3299(11)| 0.1985(8) | 0.4751(5) | 2.31(12)            | 0.71(3) |

\[ B_{eq} = \frac{8}{3} \pi^2 \left[ U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha \right] \]
| atom  | x       | y       | z       | $B_{iso}$ | occ  |
|-------|---------|---------|---------|-----------|------|
| H3    | 0.28224 | 0.50310 | 0.28980 | 3.858     | 1    |
| H4    | 0.66541 | 0.13480 | 0.43746 | 3.092     | 1    |
| H5    | 0.56763 | 0.50483 | 0.18398 | 3.634     | 1    |
| H7A   | 0.70636 | 0.35851 | 0.27408 | 3.776     | 1    |
| H7B   | 0.68804 | 0.37879 | 0.19741 | 3.776     | 1    |
| H7C   | 0.74488 | 0.43681 | 0.24767 | 3.776     | 1    |
| H8A   | 0.37787 | 0.35954 | 0.400   | 67        | 5.040|
| H8B   | 0.32150 | 0.43821 | 0.41051 | 5.040     | 1    |
| H8C   | 0.26014 | 0.37960 | 0.36262 | 5.040     | 1    |
| H11A  | 0.35852 | 0.42752 | 0.53881 | 4.923     | 0.509|
| H11B  | 0.42234 | 0.45748 | 0.60456 | 4.923     | 0.509|
| H11C  | 0.33115 | 0.39281 | 0.60926 | 4.923     | 0.509|
| H12A  | 0.47298 | 0.30426 | 0.67110 | 4.991     | 0.509|
| H12B  | 0.54746 | 0.37723 | 0.67816 | 4.991     | 0.509|
| H12C  | 0.59852 | 0.30713 | 0.64225 | 4.991     | 0.509|
| H13A  | 0.65750 | 0.37246 | 0.55846 | 4.086     | 0.509|
| H13B  | 0.60846 | 0.44869 | 0.58378 | 4.086     | 0.509|
| H13C  | 0.58645 | 0.42421 | 0.50839 | 4.086     | 0.509|
| H15A  | 0.51422 | 0.16120 | 0.55703 | 4.080     | 0.293|
| H15B  | 0.40376 | 0.13040 | 0.59233 | 4.080     | 0.293|
| H15C  | 0.47680 | 0.19498 | 0.62612 | 4.080     | 0.293|
| H16A  | 0.28967 | 0.24791 | 0.45716 | 3.942     | 0.293|
| H16B  | 0.27040 | 0.17006 | 0.49097 | 3.942     | 0.293|
| H16C  | 0.38977 | 0.18845 | 0.45841 | 3.942     | 0.293|
| H17A  | 0.32501 | 0.27741 | 0.63115 | 3.479     | 0.293|
| H17B  | 0.23412 | 0.21982 | 0.60170 | 3.479     | 0.293|
| H17C  | 0.23899 | 0.30057 | 0.57170 | 3.479     | 0.293|
| H20A  | 0.95552 | 0.10466 | 0.59561 | 6.407     | 0.500|
| H20B  | 0.98615 | 0.18913 | 0.60579 | 6.407     | 0.500|
| H20C  | 0.97933 | 0.15505 | 0.53282 | 6.407     | 0.500|
| H21A  | 0.70084 | 0.13839 | 0.64092 | 5.435     | 0.500|
| H21B  | 0.80384 | 0.18682 | 0.67076 | 5.435     | 0.500|
| H21C  | 0.82643 | 0.10444 | 0.64832 | 5.435     | 0.500|
| H22A  | 0.83672 | 0.26301 | 0.52189 | 3.610     | 0.500|
| H22B  | 0.83620 | 0.27315 | 0.60058 | 3.610     | 0.500|
| H22C  | 0.71846 | 0.26241 | 0.55940 | 3.610     | 0.500|
| H25A  | 0.74948 | 0.04889 | 0.40192 | 4.356     | 0.793|
Table S8-2. Atomic coordinates and B\textsubscript{iso} involving hydrogens/B\textsubscript{eq} and occupancy (continued)

| atom | x     | y     | z     | B\textsubscript{eq} | occ  |
|------|-------|-------|-------|------------------|------|
| H25B | 0.79872 | -0.02672 | 0.43038 | 4.356           | 0.793(7) |
| H25C | 0.87838 | 0.04424 | 0.43025 | 4.356           | 0.793(7) |
| H26A | 0.91597 | 0.01584 | 0.54846 | 8.219           | 0.793(7) |
| H26B | 0.82651 | -0.05009 | 0.54354 | 8.219           | 0.793(7) |
| H26C | 0.81429 | 0.01119 | 0.59934 | 8.219           | 0.793(7) |
| H27A | 0.60663 | 0.03095 | 0.55516 | 4.763           | 0.793(7) |
| H27B | 0.63520 | -0.03521 | 0.50668 | 4.763           | 0.793(7) |
| H27C | 0.58650 | 0.03992 | 0.47684 | 4.763           | 0.793(7) |
| H29A | 0.87400 | 0.29741 | 0.25859 | 5.128           | 0.793(7) |
| H29B | 1.00048 | 0.26721 | 0.24856 | 5.128           | 0.793(7) |
| H29C | 0.98208 | 0.34763 | 0.27726 | 5.128           | 0.793(7) |
| H30A | 1.10885 | 0.31538 | 0.37552 | 7.427           | 0.793(7) |
| H30B | 1.12462 | 0.23390 | 0.34875 | 7.427           | 0.793(7) |
| H30C | 1.08042 | 0.24737 | 0.42191 | 7.427           | 0.793(7) |
| H31A | 0.90787 | 0.17196 | 0.39280 | 4.508           | 0.793(7) |
| H31B | 0.95797 | 0.16030 | 0.32077 | 4.508           | 0.793(7) |
| H31C | 0.83175 | 0.19200 | 0.32816 | 4.508           | 0.793(7) |
| H33B | 0.87149 | 0.46915 | 0.47298 | 5.027           | 0.524(18) |
| H33C | 0.82457 | 0.39132 | 0.49566 | 5.027           | 0.524(18) |
| H34A | 1.02738 | 0.42058 | 0.34546 | 5.874           | 0.524(18) |
| H34B | 0.99574 | 0.48741 | 0.39249 | 5.874           | 0.524(18) |
| H34C | 0.90347 | 0.45713 | 0.33920 | 5.874           | 0.524(18) |
| H35A | 1.01430 | 0.33159 | 0.50350 | 5.047           | 0.524(18) |
| H35B | 1.06541 | 0.41148 | 0.49223 | 5.047           | 0.524(18) |
| H35C | 1.09516 | 0.34661 | 0.44260 | 5.047           | 0.524(18) |
| H4A  | 0.38789 | 0.55085 | 0.20393 | 3.959           | 1     |
| H30D | 1.06638 | 0.22432 | 0.43322 | 4.130           | 0.290(4) |
| H30E | 1.05079 | 0.16385 | 0.37648 | 4.130           | 0.290(4) |
| H30F | 0.95024 | 0.17857 | 0.42658 | 4.130           | 0.290(4) |
| H29D | 1.02807 | 0.31972 | 0.27271 | 4.730           | 0.290(4) |
| H29E | 1.08793 | 0.24306 | 0.28929 | 4.730           | 0.290(4) |
| H29F | 1.11190 | 0.31195 | 0.33643 | 4.730           | 0.290(4) |
| H31D | 0.83117 | 0.18043 | 0.33136 | 3.835           | 0.290(4) |
| H31E | 0.93383 | 0.17566 | 0.28115 | 3.835           | 0.290(4) |
| H31F | 0.83600 | 0.23582 | 0.27025 | 3.835           | 0.290(4) |
| H26D | 0.70716 | 0.03001 | 0.60277 | 5.011           | 0.207(7) |

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Table S8-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogens/Beq and occupancy (continued)

| atom   | x      | y      | z      | Beq   | occ   |
|--------|--------|--------|--------|-------|-------|
| H26E   | 0.66628| -0.03379| 0.55336| 5.011 | 0.207(7) |
| H26F   | 0.60201| 0.04329 | 0.55169| 5.011 | 0.207(7) |
| H25D   | 0.94174| 0.05442 | 0.51266| 4.790 | 0.207(7) |
| H25E   | 0.89771| -0.02682| 0.52586| 4.790 | 0.207(7) |
| H25F   | 0.88665| 0.03402 | 0.58231| 4.790 | 0.207(7) |
| H27D   | 0.66227| 0.02978 | 0.42805| 5.639 | 0.207(7) |
| H27E   | 0.76763| -0.02541| 0.43629| 5.639 | 0.207(7) |
| H27F   | 0.78851| 0.05664 | 0.41233| 5.639 | 0.207(7) |
| H20D   | 0.96598| 0.13799 | 0.56185| 6.005 | 0.500(19) |
| H20E   | 0.95914| 0.21627 | 0.59667| 6.005 | 0.500(19) |
| H20F   | 0.93802| 0.20910 | 0.51827| 6.005 | 0.500(19) |
| H21D   | 0.66829| 0.15272 | 0.63273| 4.377 | 0.500(19) |
| H21E   | 0.78099| 0.17562 | 0.67450| 4.377 | 0.500(19) |
| H21F   | 0.77002| 0.09529 | 0.56185| 4.377 | 0.500(19) |
| H22D   | 0.76335| 0.28324 | 0.52507| 3.681 | 0.500(19) |
| H22E   | 0.78543| 0.29075 | 0.60337| 3.681 | 0.500(19) |
| H22F   | 0.66746| 0.25769 | 0.57477| 3.681 | 0.500(19) |
| H35D   | 0.94121| 0.34829 | 0.51560| 4.874 | 0.476(18) |
| H35E   | 0.98664| 0.43025 | 0.50886| 4.874 | 0.476(18) |
| H35F   | 1.05988| 0.36384 | 0.48113| 4.874 | 0.476(18) |
| H33D   | 0.74897| 0.44406 | 0.40579| 4.888 | 0.476(18) |
| H33E   | 0.82229| 0.48510 | 0.46268| 4.888 | 0.476(18) |
| H33F   | 0.75945| 0.40987 | 0.47865| 4.888 | 0.476(18) |
| H34D   | 1.05408| 0.41445 | 0.36130| 5.259 | 0.476(18) |
| H34E   | 0.99496| 0.48519 | 0.39161| 5.259 | 0.476(18) |
| H34F   | 0.93259| 0.44136 | 0.33224| 5.259 | 0.476(18) |
| H13D   | 0.62578| 0.39746 | 0.54993| 4.411 | 0.491(17) |
| H13E   | 0.54456| 0.46254 | 0.57243| 4.411 | 0.491(17) |
| H13F   | 0.52478| 0.42558 | 0.50119| 4.411 | 0.491(17) |
| H11D   | 0.32140| 0.42125 | 0.51481| 5.015 | 0.491(17) |
| H11E   | 0.34630| 0.46478 | 0.58243| 5.015 | 0.491(17) |
| H11F   | 0.27662| 0.38967 | 0.58314| 5.015 | 0.491(17) |
| H12D   | 0.39961| 0.32330 | 0.65286| 4.617 | 0.491(17) |
| H12E   | 0.47105| 0.39600 | 0.66878| 4.617 | 0.491(17) |
| H12F   | 0.53614| 0.32053 | 0.65708| 4.617 | 0.491(17) |
| H17D   | 0.26441| 0.28037 | 0.61748| 4.883 | 0.71(3) |
| H17E   | 0.20384| 0.21315 | 0.57993| 4.883 | 0.71(3) |
Table S8-2. Atomic coordinates and $B_{iso}$ involving hydrogens/$B_{eq}$ and occupancy (continued)

| atom  | x     | y     | z     | $B_{eq}$ | occ   |
|-------|-------|-------|-------|----------|-------|
| H17F  | 0.20853 | 0.29136 | 0.54483 | 4.883    | 0.71(3) |
| H15D  | 0.49590 | 0.16375 | 0.56361 | 3.608    | 0.71(3) |
| H15E  | 0.37472 | 0.13672 | 0.58856 | 3.608    | 0.71(3) |
| H15F  | 0.44374 | 0.19882 | 0.62861 | 3.608    | 0.71(3) |
| H16D  | 0.29816 | 0.23538 | 0.44458 | 3.473    | 0.71(3) |
| H16E  | 0.27195 | 0.16122 | 0.48312 | 3.473    | 0.71(3) |
| H16F  | 0.39651 | 0.17558 | 0.45556 | 3.473    | 0.71(3) |
Table S8-3. Anisotropic displacement parameters

| atom | U_{11}     | U_{22}     | U_{33}     | U_{12}     | U_{13}     | U_{23}     |
|------|------------|------------|------------|------------|------------|------------|
| Nb1  | 0.0372(10) | 0.0181(8)  | 0.0135(8)  | -0.00988(6)| 0.00290(6) | -0.00039(5)|
| F36A | 0.0452(16) | 0.055(2)   | 0.0389(13) | -0.0242(15)| 0.0097(11) | -0.0041(12)|
| F36B | 0.090(6)   | 0.029(3)   | 0.044(4)   | -0.004(3)  | -0.025(4)  | -0.018(3)  |
| F36C | 0.063(4)   | 0.026(2)   | 0.049(4)   | -0.005(2)  | -0.026(3)  | 0.002(2)   |
| F36D | 0.0351(18) | 0.044(2)   | 0.0429(17) | -0.0175(16)| 0.0044(13) | -0.0012(14)|
| F37A | 0.106(5)   | 0.067(4)   | 0.0150(17) | -0.030(3)  | 0.008(2)   | -0.011(3)  |
| F37B | 0.076(8)   | 0.085(7)   | 0.034(4)   | -0.041(5)  | 0.021(5)   | -0.001(3)  |
| F37C | 0.0403(16) | 0.065(2)   | 0.070(2)   | -0.0013(16)| 0.0155(15) | -0.0365(18)|
| F37D | 0.092(10)  | 0.019(3)   | 0.021(3)   | -0.011(5)  | -0.007(4)  | 0.005(2)   |
| F38A | 0.040(3)   | 0.037(2)   | 0.059(3)   | -0.0032(18)| 0.003(2)   | -0.009(2)  |
| F38B | 0.032(2)   | 0.048(3)   | 0.048(2)   | -0.000219  | -0.0164(17)| -0.011(2)  |
| F38C | 0.134(5)   | 0.0280(15) | 0.048(3)   | -0.006(3)  | -0.053(3)  | 0.0120(16) |
| F38D | 0.032(3)   | 0.057(4)   | 0.027(4)   | -0.010(2)  | 0.002(2)   | 0.001(3)   |
| O1   | 0.0344(7)  | 0.0209(6)  | 0.0142(5)  | -0.0070(5) | -0.0026(5) | -0.0014(5) |
| N1   | 0.0308(8)  | 0.0208(7)  | 0.0227(7)  | -0.0068(6) | 0.0054(6)  | 0.0006(6)  |
| N2   | 0.0593(11) | 0.0209(8)  | 0.0219(8)  | -0.0143(7) | 0.0111(7)  | -0.0029(6) |
| N3   | 0.0414(9)  | 0.0214(7)  | 0.0162(7)  | -0.0105(6) | -0.0067(6) | 0.0042(6)  |
| N4   | 0.0526(11) | 0.0251(8)  | 0.0162(7)  | -0.0177(7) | -0.0065(7) | 0.0025(6)  |
| C1   | 0.0305(9)  | 0.0188(8)  | 0.0288(9)  | -0.0085(7) | -0.0023(7) | -0.0001(7) |
| C2   | 0.0367(11) | 0.0176(9)  | 0.0505(12) | -0.0069(8) | 0.0024(9)  | -0.0052(8) |
| C3   | 0.0392(11) | 0.0222(10) | 0.0600(14) | -0.0028(8) | -0.0112(10)| -0.0109(9) |
| C4   | 0.0589(14) | 0.0252(10) | 0.0397(12) | -0.0038(10)| -0.0235(10)| 0.0001(9)  |
| C5   | 0.0527(13) | 0.0339(11) | 0.0277(10) | -0.0092(10)| -0.0105(9) | 0.0076(8)  |
| C6   | 0.0373(10) | 0.0297(10) | 0.0240(9)  | -0.0098(8) | -0.0066(7) | 0.0053(7)  |
| C7   | 0.0352(11) | 0.0537(14) | 0.0308(10) | -0.0077(10)| 0.0039(8)  | 0.0197(10) |
| C8   | 0.0471(14) | 0.0232(10) | 0.091(2)   | -0.0020(9) | 0.0338(13) | 0.0003(11) |
| C9   | 0.0727(16) | 0.0176(9)  | 0.0257(9)  | -0.0114(9) | 0.0200(10) | -0.0034(7) |
| C10  | 0.143(3)   | 0.0248(11) | 0.0382(13) | -0.0332(15)| 0.0445(16) | -0.0157(10)|
| C11  | 0.056(5)   | 0.026(2)   | 0.044(3)   | -0.003(3)  | 0.019(3)   | -0.012(2)  |
| C12  | 0.067(5)   | 0.035(3)   | 0.024(2)   | -0.018(3)  | 0.005(3)   | -0.0051(19)|
| C13  | 0.051(5)   | 0.021(3)   | 0.032(3)   | -0.015(3)  | 0.009(3)   | -0.004(2)  |
| C14  | 0.0514(12) | 0.0202(9)  | 0.0302(10) | -0.0049(8) | 0.0178(9)  | 0.0006(7)  |
| C15  | 0.046(9)   | 0.024(5)   | 0.034(6)   | -0.011(5)  | 0.008(5)   | 0.011(4)   |
| C16  | 0.045(7)   | 0.019(7)   | 0.037(6)   | -0.005(5)  | 0.013(4)   | 0.001(4)   |
| C17  | 0.025(5)   | 0.034(4)   | 0.028(5)   | -0.012(4)  | -0.004(4)  | 0.000(3)   |
| C18  | 0.0521(12) | 0.0333(10) | 0.0180(8)  | -0.0225(9) | -0.0085(8) | 0.0077(7)  |
| C19  | 0.0653(15) | 0.0525(14) | 0.0175(9)  | -0.0309(12)| -0.0135(9) | 0.0043(9)  |
| atom  | U_{11}  | U_{22}  | U_{33}  | U_{12}  | U_{13}  | U_{23}  |
|-------|---------|---------|---------|---------|---------|---------|
| C20   | 0.045(3) | 0.058(5) | 0.058(5) | -0.005(3) | -0.027(3) | -0.017(4) |
| C21   | 0.074(10) | 0.037(4) | 0.027(3) | -0.016(7) | -0.008(6) | 0.011(3)  |
| C22   | 0.046(4)  | 0.024(3) | 0.020(2) | -0.007(3) | -0.011(2) | -0.0008(18) |
| C23   | 0.0438(11) | 0.0291(10) | 0.0202(8) | -0.0178(8) | -0.0104(8) | 0.0092(7)  |
| C24   | 0.0480(12) | 0.0311(11) | 0.0307(10) | -0.0120(9) | -0.0111(9) | 0.0120(8)  |
| C25   | 0.0352(17) | 0.0323(16) | 0.0424(17) | -0.0003(16) | -0.0059(16) | 0.0105(12) |
| C26   | 0.103(4)  | 0.043(2)  | 0.059(2)  | -0.028(2)  | -0.050(2)  | 0.0259(18) |
| C27   | 0.0589(19) | 0.0261(13) | 0.0360(17) | -0.0191(12) | 0.0076(14) | 0.0005(11) |
| C28   | 0.0319(10) | 0.0517(14) | 0.0307(10) | -0.0134(9) | -0.0064(8) | 0.0049(9)  |
| C29   | 0.0448(18) | 0.0503(19) | 0.0353(16) | 0.0006(15) | 0.0103(13) | 0.0088(14) |
| C30   | 0.0403(19) | 0.043(2)  | 0.103(3)  | -0.0140(16) | -0.031(2)  | 0.0182(2)  |
| C31   | 0.0391(16) | 0.0350(16) | 0.0400(19) | -0.0092(13) | -0.0001(13) | -0.0024(13) |
| C32   | 0.0765(17) | 0.0379(12) | 0.0308(11) | -0.0379(12) | -0.0148(11) | 0.0098(9)  |
| C33   | 0.042(4)  | 0.0273(2) | 0.058(4)  | -0.014(3)  | 0.008(3)  | -0.018(3)  |
| C34   | 0.049(5)  | 0.039(7)  | 0.062(8)  | -0.016(4)  | 0.013(6)  | 0.021(4)  |
| C35   | 0.044(4)  | 0.036(3)  | 0.047(3)  | -0.016(3)  | -0.017(3) | -0.005(2) |
| C36   | 0.037(2)  | 0.0278(19) | 0.0226(18) | -0.0085(16) | -0.0050(17) | -0.0024(15) |
| C36A  | 0.025(2)  | 0.031(3)  | 0.033(2)  | -0.0052(19) | -0.0036(18) | -0.006(2)  |
| C37   | 0.061(3)  | 0.050(3)  | 0.0220(17) | -0.022(2)  | 0.0087(17) | -0.0105(17) |
| C37A  | 0.052(4)  | 0.026(2)  | 0.023(2)  | 0.003(2)  | -0.012(2) | -0.0089(18) |
| C38   | 0.057(3)  | 0.034(2)  | 0.039(2)  | 0.003(2)  | -0.025(2) | -0.0028(19) |
| C38A  | 0.032(3)  | 0.045(3)  | 0.0147(19) | -0.004(2)  | -0.0044(16) | -0.0021(18) |
| C39   | 0.0301(9) | 0.0244(9) | 0.0162(7) | -0.0051(7) | -0.0014(6) | -0.0026(6) |
| F0AA  | 0.032(4)  | 0.064(8)  | 0.084(9)  | 0.018(5)  | -0.013(5) | -0.038(6) |
| F1AA  | 0.063(8)  | 0.045(3)  | 0.047(5)  | 0.004(5)  | -0.041(5) | 0.001(3) |
| F2AA  | 0.046(2)  | 0.048(2)  | 0.049(2)  | 0.0254(19) | -0.0129(17) | -0.0198(18) |
| F3AA  | 0.035(2)  | 0.027(3)  | 0.030(3)  | -0.009(2)  | -0.0144(19) | -0.0038(19) |
| F4AA  | 0.054(3)  | 0.039(2)  | 0.0278(19) | -0.0072(2) | -0.0114(17) | 0.0107(14) |
| F5AA  | 0.058(2)  | 0.052(4)  | 0.0165(19) | -0.0043(3) | -0.0028(15) | -0.0053(3) |
| C30A  | 0.034(4)  | 0.040(4)  | 0.031(3)  | 0.0063(3)  | -0.0023(3) | 0.0013(3) |
| C29A  | 0.0354(4) | 0.0515(4) | 0.0344(4) | -0.0103(3) | 0.0073(3)  | 0.0023(3) |
| C31A  | 0.0364(4) | 0.0374(4) | 0.0244(4) | -0.0033(3) | 0.0023(3)  | -0.0063(3) |
| C26A  | 0.0386(4) | 0.0175(4) | 0.07310(4) | -0.0034(4) | 0.0186(4)  | 0.0045(4) |
| C25A  | 0.0437(7) | 0.0266(7) | 0.0517(4) | 0.0205(4)  | -0.0196(4) | -0.0145(4) |
| C27A  | 0.07612(7) | 0.0195(4) | 0.0478(4) | 0.0118(4)  | -0.0249(4) | -0.0035(4) |
| C20A  | 0.0634(4) | 0.0474(4) | 0.0413(4) | -0.0113(4) | -0.0253(4) | 0.0043(4) |
| C21A  | 0.0486(4) | 0.0455(4) | 0.0183(4) | -0.0055(4) | -0.0044(4) | 0.0073(4) |

Table S8-3. Anisotropic displacement parameters (continued)
| atom  | $U_{11}$  | $U_{22}$  | $U_{33}$  | $U_{12}$  | $U_{13}$  | $U_{23}$  |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| C22A  | 0.051(5)  | 0.020(2)  | 0.021(2)  | -0.006(3) | -0.010(3) | -0.0002(16) |
| C35A  | 0.054(5)  | 0.032(3)  | 0.036(3)  | -0.016(3) | -0.017(3) | 0.004(2)   |
| C33A  | 0.044(5)  | 0.023(3)  | 0.046(3)  | -0.008(3) | 0.000(3)  | -0.006(2)  |
| C34A  | 0.068(8)  | 0.021(4)  | 0.043(6)  | -0.013(4) | -0.020(5) | 0.012(3)   |
| C13A  | 0.055(5)  | 0.022(3)  | 0.036(3)  | -0.011(3) | 0.004(3)  | -0.008(2)  |
| C11A  | 0.057(5)  | 0.021(2)  | 0.050(4)  | 0.004(3)  | 0.015(3)  | -0.008(2)  |
| C12A  | 0.060(5)  | 0.030(3)  | 0.027(2)  | -0.013(3) | 0.009(3)  | -0.0119(19)|
| C17A  | 0.046(4)  | 0.035(2)  | 0.043(3)  | -0.000(2) | 0.020(3)  | -0.001(2)  |
| C15A  | 0.038(3)  | 0.028(3)  | 0.026(2)  | -0.011(2) | 0.003(2)  | 0.0025(17) |
| C16A  | 0.035(2)  | 0.026(4)  | 0.028(2)  | -0.004(2) | 0.002(2)  | -0.0015(19)|

The general temperature factor expression: $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2abU_{12}hk + 2acU_{13}hl + 2bcU_{23}kl))$
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | O1   | 2.0642(13)| Nb1  | N1   | 1.7877(15)|
| Nb1  | N2   | 1.9647(18)| Nb1  | N3   | 1.9670(17)|
| Nb1  | N4   | 2.5448(17)| F36A | C36  | 1.339(5) |
| F36B | C36  | 1.422(14) | F36C | C36  | 1.314(14)|
| F36D | C36A | 1.333(6)  | F37A | C37  | 1.345(9) |
| F37B | C37  | 1.333(18) | F37C | C37  | 1.330(6) |
| F37D | C37A | 1.349(16) | F38A | C38  | 1.293(17)|
| F38B | C38  | 1.495(14) | F38C | C38  | 1.328(7) |
| F38D | C38A | 1.394(17) | O1   | C39  | 1.359(2) |
| N1   | C1   | 1.393(2)  | N2   | C9   | 1.266(3) |
| N3   | C23  | 1.266(3)  | N4   | C18  | 1.286(3) |
| C1   | C2   | 1.409(3)  | C1   | C6   | 1.413(3) |
| C2   | C3   | 1.390(3)  | C2   | C8   | 1.508(4) |
| C3   | C4   | 1.387(3)  | C4   | C5   | 1.376(4) |
| C5   | C6   | 1.393(3)  | C6   | C7   | 1.497(3) |
| C9   | C10  | 1.559(3)  | C9   | C14  | 1.569(3) |
| C10  | C11  | 1.319(10) | C10  | C12  | 1.715(7) |
| C10  | C13  | 1.672(11) | C10  | C13A | 1.408(11)|
| C10  | C11A | 1.838(11) | C10  | C12A | 1.417(6) |
| C14  | C15  | 1.68(3)   | C14  | C16  | 1.38(3)  |
| C14  | C17  | 1.460(17) | C14  | C17A | 1.580(13)|
| C14  | C15A | 1.492(12) | C14  | C16A | 1.584(11)|
| C18  | C19  | 1.540(3)  | C18  | C24  | 1.561(3) |
| C19  | C20  | 1.670(8)  | C19  | C21  | 1.49(2)  |
| C19  | C22  | 1.364(8)  | C19  | C20A | 1.429(10)|
| C19  | C21A | 1.60(2)   | C19  | C22A | 1.718(8) |
| C23  | C28  | 1.547(3)  | C23  | C32  | 1.565(3) |
| C24  | C25  | 1.561(5)  | C24  | C26  | 1.536(5) |
| C24  | C27  | 1.556(4)  | C24  | C26A | 1.550(14)|
| C24  | C25A | 1.603(14) | C24  | C27A | 1.379(16)|
| C28  | C29  | 1.579(4)  | C28  | C30  | 1.523(4) |
| C28  | C31  | 1.468(4)  | C28  | C30A | 1.711(8) |
| C28  | C29A | 1.495(8)  | C28  | C31A | 1.626(8) |
| C32  | C33  | 1.327(10) | C32  | C34  | 1.56(2)  |
| C32  | C35  | 1.672(9)  | C32  | C35A | 1.480(9) |
| C32  | C33A | 1.755(11) | C32  | C34A | 1.52(2)  |
| C36  | C39  | 1.572(4)  | C36A | C39  | 1.635(5) |
Table S8-4. Bond lengths (Å) (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C36A | F0AA | 1.21(2)  | C36A | F1AA | 1.337(17) |
| C37  | C39  | 1.605(5) | C37A | C39  | 1.498(5)  |
| C37A | F2AA | 1.327(9) | C37A | F3AA | 1.396(15) |
| C38  | C39  | 1.477(5) | C38A | C39  | 1.568(5)  |
| C38A | F4AA | 1.333(8) | C38A | F5AA | 1.342(10) |
Table S8-5. Bond lengths involving hydrogens (Å)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| N4   | H4   | 0.910    | C3   | H3   | 0.950    |
| C4   | H4A  | 0.950    | C5   | H5   | 0.950    |
| C7   | H7A  | 0.980    | C7   | H7B  | 0.980    |
| C7   | H7C  | 0.980    | C8   | H8A  | 0.980    |
| C8   | H8B  | 0.980    | C8   | H8C  | 0.980    |
| C11  | H11A | 0.980    | C11  | H11B | 0.980    |
| C11  | H11C | 0.980    | C12  | H12A | 0.980    |
| C12  | H12B | 0.980    | C12  | H12C | 0.980    |
| C13  | H13A | 0.980    | C13  | H13B | 0.980    |
| C13  | H13C | 0.980    | C15  | H15A | 0.980    |
| C15  | H15B | 0.980    | C15  | H15C | 0.980    |
| C16  | H16A | 0.980    | C16  | H16B | 0.980    |
| C16  | H16C | 0.980    | C17  | H17A | 0.980    |
| C17  | H17B | 0.980    | C17  | H17C | 0.980    |
| C20  | H20A | 0.980    | C20  | H20B | 0.980    |
| C20  | H20C | 0.980    | C21  | H21A | 0.980    |
| C21  | H21B | 0.980    | C21  | H21C | 0.980    |
| C22  | H22A | 0.980    | C22  | H22B | 0.980    |
| C22  | H22C | 0.980    | C25  | H25A | 0.980    |
| C25  | H25B | 0.980    | C25  | H25C | 0.980    |
| C26  | H26A | 0.980    | C26  | H26B | 0.980    |
| C26  | H26C | 0.980    | C27  | H27A | 0.980    |
| C27  | H27B | 0.980    | C27  | H27C | 0.980    |
| C29  | H29A | 0.980    | C29  | H29B | 0.980    |
| C29  | H29C | 0.980    | C30  | H30A | 0.980    |
| C30  | H30B | 0.980    | C30  | H30C | 0.980    |
| C31  | H31A | 0.980    | C31  | H31B | 0.980    |
| C31  | H31C | 0.980    | C33  | H33A | 0.980    |
| C33  | H33B | 0.980    | C33  | H33C | 0.980    |
| C34  | H34A | 0.980    | C34  | H34B | 0.980    |
| C34  | H34C | 0.980    | C35  | H35A | 0.980    |
| C35  | H35B | 0.980    | C35  | H35C | 0.980    |
| C30A | H30D | 0.980    | C30A | H30E | 0.980    |
| C30A | H30F | 0.980    | C29A | H29D | 0.980    |
| C29A | H29E | 0.980    | C29A | H29F | 0.980    |
| C31A | H31D | 0.980    | C31A | H31E | 0.980    |
| C31A | H31F | 0.980    | C26A | H26D | 0.980    |
Table S8-5. Bond lengths involving hydrogens (Å) (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| C26A  | H26E  | 0.980    | C26A  | H26F  | 0.980    |
| C25A  | H25D  | 0.980    | C25A  | H25E  | 0.980    |
| C25A  | H25F  | 0.980    | C27A  | H27D  | 0.980    |
| C27A  | H27E  | 0.980    | C27A  | H27F  | 0.980    |
| C20A  | H20D  | 0.980    | C20A  | H20E  | 0.980    |
| C20A  | H20F  | 0.980    | C21A  | H21D  | 0.980    |
| C21A  | H21E  | 0.980    | C21A  | H21F  | 0.980    |
| C22A  | H22D  | 0.980    | C22A  | H22E  | 0.980    |
| C22A  | H22F  | 0.980    | C35A  | H35D  | 0.980    |
| C35A  | H35E  | 0.980    | C35A  | H35F  | 0.980    |
| C33A  | H33D  | 0.980    | C33A  | H33E  | 0.980    |
| C33A  | H33F  | 0.980    | C34A  | H34D  | 0.980    |
| C34A  | H34E  | 0.980    | C34A  | H34F  | 0.980    |
| C13A  | H13D  | 0.980    | C13A  | H13E  | 0.980    |
| C13A  | H13F  | 0.980    | C11A  | H11D  | 0.980    |
| C11A  | H11E  | 0.980    | C11A  | H11F  | 0.980    |
| C12A  | H12D  | 0.980    | C12A  | H12E  | 0.980    |
| C12A  | H12F  | 0.980    | C17A  | H17D  | 0.980    |
| C17A  | H17E  | 0.980    | C17A  | H17F  | 0.980    |
| C15A  | H15D  | 0.980    | C15A  | H15E  | 0.980    |
| C15A  | H15F  | 0.980    | C16A  | H16D  | 0.980    |
| C16A  | H16E  | 0.980    | C16A  | H16F  | 0.980    |
| atom  | atom | atom | angle   | atom  | atom | atom | angle   |
|-------|------|------|---------|-------|------|------|---------|
| O1    | Nb1  | N1   | 101.32(6)| O1    | Nb1  | N2   | 111.69(6) |
| O1    | Nb1  | N3   | 113.58(6)| O1    | Nb1  | N4   | 73.34(5)   |
| N1    | Nb1  | N2   | 99.88(7) | N1    | Nb1  | N3   | 99.14(7)   |
| N1    | Nb1  | N4   | 174.27(6)| N2    | Nb1  | N3   | 125.68(7)  |
| N2    | Nb1  | N4   | 84.24(6) | N3    | Nb1  | N4   | 81.44(6)   |
| Nb1   | O1   | C39  | 145.75(11)| Nb1   | N1   | C1   | 177.56(13) |
| Nb1   | N2   | C9   | 178.00(17)| Nb1   | N3   | C23  | 177.13(14) |
| Nb1   | N4   | C18  | 159.78(14)| N1    | C1   | C6   | 120.13(18) |
| N1    | C1   | C6   | 120.17(17)| C2    | C1   | C6   | 120.13(18) |
| C1    | C2   | C3   | 119.2(2)  | C1    | C2   | C8   | 119.58(18) |
| C3    | C2   | C8   | 121.2(2)  | C2    | C3   | C4   | 120.9(2)   |
| C3    | C4   | C5   | 119.7(2)  | C4    | C5   | C6   | 121.8(2)   |
| C1    | C6   | C5   | 118.35(19)| C1    | C6   | C7   | 120.46(18) |
| C5    | C6   | C7   | 121.19(19)| C2    | C1   | C6   | 120.1(2)   |
| N2    | C9   | C14  | 117.02(18)| C10   | C9   | C14  | 122.8(2)   |
| C9    | C10  | C11  | 121.2(5)  | C9    | C10  | C12  | 107.9(3)   |
| C9    | C10  | C13  | 107.8(4)  | C9    | C10  | C13A | 111.3(4)   |
| C9    | C10  | C11A | 102.8(3)  | C9    | C10  | C12A | 114.8(3)   |
| C9    | C10  | C12  | 112.3(5)  | C11   | C10  | C13  | 110.5(5)   |
| C11   | C10  | C13  | 93.7(5)   | C13A  | C10  | C11A | 98.6(5)    |
| C12   | C10  | C13  | 118.69(18)| C11A  | C10  | C12A | 100.8(6)   |
| C13A  | C10  | C12A | 123.8(6)  | C11A  | C10  | C12A | 100.8(6)   |
| C9    | C14  | C15  | 101.9(10) | C9    | C14  | C16  | 108.5(14)  |
| C9    | C14  | C17  | 110.7(6)  | C9    | C14  | C17A | 118.8(3)   |
| C9    | C14  | C15A | 108.5(5)  | C9    | C14  | C16A | 108.9(5)   |
| C15   | C14  | C18  | 111.2(18) | C15   | C14  | C17  | 105.1(13)  |
| C16   | C14  | C17  | 118.2(16) | C17A  | C14  | C15A | 109.6(6)   |
| C17A  | C14  | C16A | 103.5(6)  | C15A  | C14  | C16A | 106.9(7)   |
| N4    | C18  | C19  | 118.69(18)| N4    | C18  | C24  | 118.05(17) |
| C19   | C18  | C24  | 123.22(17)| C18   | C19  | C20  | 109.1(4)   |
| C18   | C19  | C21  | 116.6(8)  | C18   | C19  | C22  | 112.7(4)   |
| C18   | C19  | C20A | 111.04(4) | C18   | C19  | C21A | 107.4(7)   |
| C18   | C19  | C22A | 106.8(3)  | C20   | C19  | C21  | 94.5(8)    |
| C20   | C19  | C22  | 107.9(7)  | C21   | C19  | C22  | 114.1(9)   |
| C20A  | C19  | C21A | 126.1(7)  | C20A  | C19  | C22A | 105.1(6)   |
| C21A  | C19  | C22A | 98.2(9)   | N3    | C23  | C28  | 118.17(18) |
| N3    | C23  | C32  | 119.20(19)| C28   | C23  | C32  | 122.62(19) |
| C18   | C24  | C25  | 109.6(2)  | C18   | C24  | C26  | 121.1(2)   |
Table S8-6. Bond angles (°) (continued)

| atom | atom | atom | angle    | atom | atom | atom | angle |
|------|------|------|----------|------|------|------|-------|
| C18  | C24  | C27  | 106.35(19) | C18  | C24  | C26A | 103.7(4) |
| C18  | C24  | C25A | 105.8(5)   | C18  | C24  | C27A | 111.0(6) |
| C25  | C24  | C26  | 104.5(3)   | C25  | C24  | C27  | 107.4(2) |
| C26  | C24  | C27  | 107.2(3)   | C26A | C24  | C25A | 105.0(7) |
| C26A | C24  | C27A | 118.9(10)  | C25A | C24  | C27A | 111.5(10) |
| C23  | C28  | C29  | 106.3(2)   | C23  | C28  | C30  | 112.1(2) |
| C23  | C28  | C31  | 110.2(2)   | C23  | C28  | C30A | 107.7(3) |
| C23  | C28  | C29A | 128.1(4)   | C23  | C28  | C31A | 112.0(3) |
| C29  | C28  | C30  | 108.9(3)   | C29  | C28  | C31  | 108.9(2) |
| C30  | C28  | C31  | 110.3(2)   | C30A | C28  | C29A | 103.4(4) |
| C30A | C28  | C31A | 95.5(4)    | C29A | C28  | C31A | 105.0(4) |
| C33  | C32  | C34  | 108.9(9)   | C33  | C32  | C35  | 111.0(5) |
| C34  | C32  | C34A | 110.3(3)   | C34  | C32  | C35A | 111.3(8) |
| C35A | C32  | C34A | 114.7(9)   | C34A | C32  | C35A | 105.9(5) |
| F36A | C36  | F36B | 116.1(6)   | F36A | C36  | F36C | 107.6(7) |
| F36A | C36  | C39  | 107.8(3)   | F36B | C36  | F36C | 107.1(8) |
| F36B | C36  | C39  | 105.2(6)   | F36C | C36  | C39  | 113.2(7) |
| F36D | C36A | C39  | 109.5(4)   | F36D | C36A | F0AA | 96.7(10) |
| F36D | C36A | F1AA | 118.6(9)   | C39  | C36A | F0AA | 112.2(9) |
| C39  | C36A | F1AA | 102.1(8)   | F0AA | C36A | F1AA | 118.0(14) |
| F37A | C37  | F37B | 106.4(8)   | F37A | C37  | F37C | 108.2(5) |
| F37A | C37  | C39  | 110.0(5)   | F37B | C37  | F37C | 112.1(7) |
| F37B | C37  | C39  | 106.9(7)   | F37C | C37  | C39  | 113.0(3) |
| F37D | C37A | C39  | 111.0(8)   | F37D | C37A | F2AA | 106.9(9) |
| F37D | C37A | F3AA | 96.3(10)   | C39  | C37A | F2AA | 108.7(5) |
| C39  | C37A | F3AA | 116.1(7)   | F2AA | C37A | F3AA | 116.9(7) |
| F38A | C38  | F38B | 99.8(9)    | F38A | C38  | F38C | 99.8(8) |
| F38A | C38  | C39  | 117.9(8)   | F38B | C38  | F38C | 113.1(7) |
| F38B | C38  | C39  | 113.0(6)   | F38C | C38  | C39  | 112.0(5) |
| F38D | C38A | C39  | 107.1(9)   | F38D | C38A | F4AA | 110.0(10) |
| F38D | C38A | F5AA | 106.1(10)  | C39  | C38A | F4AA | 113.5(4) |
| C39  | C38A | F5AA | 113.0(5)   | F4AA | C38A | F5AA | 106.8(5) |
| O1   | C39  | C36  | 107.05(19) | O1   | C39  | C36A | 112.7(2) |
| O1   | C39  | C37  | 109.0(2)   | O1   | C39  | C37A | 109.7(3) |
Table S8-6. Bond angles (°) (continued)

| atom | atom | atom | angle  | atom | atom | atom | angle |
|------|------|------|--------|------|------|------|-------|
| O1   | C39  | C38  | 113.0(2)| O1   | C39  | C38A | 111.2(2) |
| C36  | C39  | C37  | 105.3(3)| C36  | C39  | C38  | 111.5(3) |
| C36A | C39  | C37A | 107.6(4)| C36A | C39  | C38A | 104.1(3) |
| C37  | C39  | C38  | 110.6(3)| C37A | C39  | C38A | 111.4(3) |
| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| Nb1  | N4   | H4   | 91.2  | C18  | N4   | H4   | 108.7 |
| C2   | C3   | H3   | 119.6 | C4   | C3   | H3   | 119.5 |
| C3   | C4   | H4A  | 120.2 | C5   | C4   | H4A  | 120.2 |
| C4   | C5   | H5   | 119.1 | C6   | C5   | H5   | 119.1 |
| C6   | C7   | H7A  | 109.5 | C6   | C7   | H7B  | 109.5 |
| C6   | C7   | H7C  | 109.5 | H7A  | C7   | H7B  | 109.5 |
| C2   | C8   | H8A  | 109.5 | C2   | C8   | H8B  | 109.5 |
| C2   | C8   | H8C  | 109.5 | H8A  | C8   | H8B  | 109.5 |
| H8A  | C8   | H8C  | 109.5 | H8B  | C8   | H8C  | 109.5 |
| C10  | C11  | H11A | 109.5 | C10  | C11  | H11B | 109.5 |
| C10  | C11  | H11C | 109.5 | H11A | C11  | H11B | 109.5 |
| H11A | C11  | H11C | 109.5 | H11B | C11  | H11C | 109.5 |
| C10  | C12  | H12A | 109.5 | C10  | C12  | H12B | 109.5 |
| C10  | C12  | H12C | 109.5 | H12A | C12  | H12B | 109.5 |
| C10  | C12  | H12C | 109.5 | H12B | C12  | H12C | 109.5 |
| C10  | C13  | H13A | 109.5 | C10  | C13  | H13B | 109.5 |
| C10  | C13  | H13C | 109.5 | H13A | C13  | H13B | 109.5 |
| H13A | C13  | H13C | 109.5 | H13B | C13  | H13C | 109.5 |
| C14  | C15  | H15A | 109.5 | C14  | C15  | H15B | 109.5 |
| C14  | C15  | H15C | 109.5 | H15A | C15  | H15B | 109.5 |
| H15A | C15  | H15C | 109.5 | H15B | C15  | H15C | 109.5 |
| C14  | C16  | H16A | 109.5 | C14  | C16  | H16B | 109.5 |
| C14  | C16  | H16C | 109.5 | H16A | C16  | H16B | 109.5 |
| H16A | C16  | H16C | 109.5 | H16B | C16  | H16C | 109.5 |
| C14  | C17  | H17A | 109.5 | C14  | C17  | H17B | 109.5 |
| C14  | C17  | H17C | 109.5 | H17A | C17  | H17B | 109.5 |
| H17A | C17  | H17C | 109.5 | H17B | C17  | H17C | 109.5 |
| C19  | C20  | H20A | 109.5 | C19  | C20  | H20B | 109.5 |
| C19  | C20  | H20C | 109.5 | H20A | C20  | H20B | 109.5 |
| H20A | C20  | H20C | 109.5 | H20B | C20  | H20C | 109.5 |
| C19  | C21  | H21A | 109.5 | C19  | C21  | H21B | 109.5 |
| C19  | C21  | H21C | 109.5 | H21A | C21  | H21B | 109.5 |
| H21A | C21  | H21C | 109.5 | H21B | C21  | H21C | 109.5 |
| C19  | C22  | H22A | 109.5 | C19  | C22  | H22B | 109.5 |
| C19  | C22  | H22C | 109.5 | H22A | C22  | H22B | 109.5 |
| H22A | C22  | H22C | 109.5 | H22B | C22  | H22C | 109.5 |
Table S8-7. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C24  | C25  | H25A | 109.5 | C24  | C25  | H25B | 109.5 |
| C24  | C25  | H25C | 109.5 | H25A | C25  | H25B | 109.5 |
| H25A | C25  | H25C | 109.5 | H25B | C25  | H25C | 109.5 |
| C24  | C26  | H26A | 109.5 | C24  | C26  | H26B | 109.5 |
| C24  | C26  | H26C | 109.5 | H26A | C26  | H26B | 109.5 |
| H26A | C26  | H26C | 109.5 | H26B | C26  | H26C | 109.5 |
| C24  | C27  | H27A | 109.5 | C24  | C27  | H27B | 109.5 |
| C24  | C27  | H27C | 109.5 | H27A | C27  | H27B | 109.5 |
| H27A | C27  | H27C | 109.5 | H27B | C27  | H27C | 109.5 |
| C28  | C29  | H29A | 109.5 | C28  | C29  | H29B | 109.5 |
| C28  | C29  | H29C | 109.5 | H29A | C29  | H29B | 109.5 |
| H29A | C29  | H29C | 109.5 | H29B | C29  | H29C | 109.5 |
| C28  | C30  | H30A | 109.5 | C28  | C30  | H30B | 109.5 |
| C28  | C30  | H30C | 109.5 | H30A | C30  | H30B | 109.5 |
| H30A | C30  | H30C | 109.5 | H30B | C30  | H30C | 109.5 |
| C28  | C31  | H31A | 109.5 | C28  | C31  | H31B | 109.5 |
| C28  | C31  | H31C | 109.5 | H31A | C31  | H31B | 109.5 |
| H31A | C31  | H31C | 109.5 | H31B | C31  | H31C | 109.5 |
| C32  | C33  | H33A | 109.5 | C32  | C33  | H33B | 109.5 |
| C32  | C33  | H33C | 109.5 | H33A | C33  | H33B | 109.5 |
| H33A | C33  | H33C | 109.5 | H33B | C33  | H33C | 109.5 |
| C32  | C34  | H34A | 109.5 | C32  | C34  | H34B | 109.5 |
| C32  | C34  | H34C | 109.5 | H34A | C34  | H34B | 109.5 |
| H34A | C34  | H34C | 109.5 | H34B | C34  | H34C | 109.5 |
| C32  | C35  | H35A | 109.5 | C32  | C35  | H35B | 109.5 |
| C32  | C35  | H35C | 109.5 | H35A | C35  | H35B | 109.5 |
| H35A | C35  | H35C | 109.5 | H35B | C35  | H35C | 109.5 |
| C28  | C30A | H30D | 109.5 | C28  | C30A | H30E | 109.5 |
| C28  | C30A | H30F | 109.5 | H30D | C30A | H30E | 109.5 |
| H30D | C30A | H30F | 109.5 | H30E | C30A | H30F | 109.5 |
| C28  | C29A | H29D | 109.5 | C28  | C29A | H29E | 109.5 |
| C28  | C29A | H29F | 109.5 | H29D | C29A | H29E | 109.5 |
| H29D | C29A | H29F | 109.5 | H29E | C29A | H29F | 109.5 |
| C28  | C31A | H31D | 109.5 | C28  | C31A | H31E | 109.5 |
| C28  | C31A | H31F | 109.5 | H31D | C31A | H31E | 109.5 |
| H31D | C31A | H31F | 109.5 | H31E | C31A | H31F | 109.5 |
| C24  | C26A | H26D | 109.5 | C24  | C26A | H26E | 109.5 |
Table S8-7. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C24  | C26A | H26F | 109.5 | H26D | C26A | H26E | 109.5 |
| H26D | C26A | H26F | 109.5 | H26E | C26A | H26F | 109.5 |
| C24  | C25A | H25D | 109.5 | C24  | C25A | H25E | 109.5 |
| C24  | C25A | H25F | 109.5 | H25D | C25A | H25E | 109.5 |
| H25D | C25A | H25F | 109.5 | C24  | C27A | H27D | 109.5 |
| C24  | C27A | H27E | 109.5 | C25A | H27F | 109.5 |
| C24  | C27A | H27F | 109.5 | H27D | C27A | H27E | 109.5 |
| H27D | C27A | H27F | 109.5 | H27D | C27A | H27E | 109.5 |
| C19  | C20A | H20D | 109.5 | C19  | C20A | H20E | 109.5 |
| C19  | C20A | H20E | 109.5 | H20D | C20A | H20F | 109.5 |
| H20D | C20A | H20F | 109.5 | H20E | C20A | H20F | 109.5 |
| C19  | C21A | H21D | 109.5 | C19  | C21A | H21E | 109.5 |
| C19  | C21A | H21E | 109.5 | H21D | C21A | H21F | 109.5 |
| H21D | C21A | H21F | 109.5 | H21D | C21A | H21F | 109.5 |
| C19  | C22A | H22D | 109.5 | C19  | C22A | H22E | 109.5 |
| C19  | C22A | H22E | 109.5 | H22D | C22A | H22F | 109.5 |
| H22D | C22A | H22F | 109.5 | H22D | C22A | H22F | 109.5 |
| C32  | C35A | H35D | 109.5 | C32  | C35A | H35E | 109.5 |
| C32  | C35A | H35F | 109.5 | H35D | C35A | H35E | 109.5 |
| H35D | C35A | H35F | 109.5 | H35D | C35A | H35E | 109.5 |
| C32  | C33A | H33D | 109.5 | C32  | C33A | H33E | 109.5 |
| C32  | C33A | H33F | 109.5 | H33D | C33A | H33E | 109.5 |
| H33D | C33A | H33F | 109.5 | H33D | C33A | H33E | 109.5 |
| C32  | C34A | H34D | 109.5 | C32  | C34A | H34E | 109.5 |
| C32  | C34A | H34F | 109.5 | H34D | C34A | H34E | 109.5 |
| H34D | C34A | H34F | 109.5 | H34D | C34A | H34E | 109.5 |
| C10  | C13A | H13D | 109.5 | C10  | C13A | H13E | 109.5 |
| C10  | C13A | H13F | 109.5 | H13D | C13A | H13E | 109.5 |
| H13D | C13A | H13F | 109.5 | H13D | C13A | H13E | 109.5 |
| C10  | C11A | H11D | 109.5 | C10  | C11A | H11E | 109.5 |
| C10  | C11A | H11F | 109.5 | H11D | C11A | H11E | 109.5 |
| H11D | C11A | H11F | 109.5 | H11D | C11A | H11E | 109.5 |
| C10  | C12A | H12D | 109.5 | C10  | C12A | H12E | 109.5 |
| C10  | C12A | H12F | 109.5 | H12D | C12A | H12E | 109.5 |
| H12D | C12A | H12F | 109.5 | H12D | C12A | H12E | 109.5 |
| C14  | C17A | H17D | 109.5 | C14  | C17A | H17E | 109.5 |
| C14  | C17A | H17F | 109.5 | H17D | C17A | H17E | 109.5 |
Table S8-7. Bond angles involving hydrogens (°) (continued)

| atom  | atom  | atom  | angle | atom  | atom  | atom  | angle |
|-------|-------|-------|-------|-------|-------|-------|-------|
| H17D  | C17A  | H17F  | 109.5 | H17E  | C17A  | H17F  | 109.5 |
| C14   | C15A  | H15D  | 109.5 | C14   | C15A  | H15E  | 109.5 |
| C14   | C15A  | H15F  | 109.5 | H15D  | C15A  | H15E  | 109.5 |
| H15D  | C15A  | H15F  | 109.5 | H15E  | C15A  | H15F  | 109.5 |
| C14   | C16A  | H16D  | 109.5 | C14   | C16A  | H16E  | 109.5 |
| C14   | C16A  | H16F  | 109.5 | H16D  | C16A  | H16E  | 109.5 |
| H16D  | C16A  | H16F  | 109.5 | H16E  | C16A  | H16F  | 109.5 |
Table S8-8. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1   | atom2   | atom3 | atom4 | angle  | atom1   | atom2   | atom3 | atom4 | angle  |
|---------|---------|-------|-------|--------|---------|---------|-------|-------|--------|
| N1      | Nb1     | O1    | C39   | 3.57(17) | N2      | Nb1     | O1    | C39   | 109.12(16) |
| N3      | Nb1     | O1    | C39   | -101.74(15) | O1      | Nb1     | N4    | C18   | 171.9(4)    |
| N4      | Nb1     | O1    | C39   | -174.28(17) | N2      | Nb1     | N4    | C18   | -73.4(3)    |
| N3      | Nb1     | N4    | C18   | 54.1(3)   | Nb1     | O1    | C39   | C36   | -155.51(14) |
| Nb1     | O1      | C39   | C36A  | -68.8(2)  | Nb1     | O1    | C39   | C37   | 91.0(2)     |
| Nb1     | O1      | C39   | C37A  | 171.38(13) | Nb1     | O1    | C39   | C38   | -32.4(3)    |
| Nb1     | O1      | C39   | C38A  | 47.7(3)   | Nb1     | N4    | C18   | C19   | 11.0(5)     |
| Nb1     | N4      | C18   | C24   | -171.1(3) | N1      | C1    | C2    | C3    | 179.63(15)  |
| N1      | C1      | C2    | C8    | 1.8(3)    | N1      | C1    | C6    | C5    | -178.96(14) |
| N1      | C1      | C6    | C7    | 0.6(3)    | C2      | C1    | C2    | C3    | 0.3(3)      |
| C2      | C1      | C6    | C7    | 179.94(16) | C6      | C1    | C2    | C3    | 0.3(3)      |
| C6      | C1      | C2    | C8    | -177.53(15) | C1      | C2    | C3    | C4    | -0.5(3)     |
| C8      | C2      | C3    | C4    | 177.29(18) | C2      | C3    | C4    | C5    | 0.1(3)      |
| C3      | C4      | C5    | C6    | 0.6(3)    | C4      | C5    | C6    | C1    | -0.8(3)     |
| C4      | C5      | C6    | C7    | 179.57(18) | N2      | C9    | C10   | C11   | 118.8(3)    |
| N2      | C9      | C10   | C12   | -109.9(2) | N2      | C9    | C10   | C13   | -9.8(3)     |
| N2      | C9      | C10   | C13A  | 10.5(3)   | N2      | C9    | C10   | C11A  | 115.2(2)    |
| N2      | C9      | C10   | C12A  | -136.4(2) | N2      | C9    | C14   | C15   | 81.5(2)     |
| N2      | C9      | C14   | C16   | -35.9(3)  | N2      | C9    | C14   | C17   | -167.11(17) |
| N2      | C9      | C14   | C17A  | -147.89(18) | N2     | C9    | C14   | C15A  | 86.1(2)     |
| N2      | C9      | C14   | C16A  | -29.8(3)  | C10     | C9    | C14   | C15   | -94.7(2)    |
| C10     | C9      | C14   | C16   | 147.9(2)  | C10     | C9    | C14   | C17   | 16.7(3)     |
| C10     | C9      | C14   | C17A  | 35.9(3)   | C10     | C9    | C14   | C15A  | -90.0(2)    |
| C10     | C9      | C14   | C16A  | 154.0(2)  | C14     | C9    | C10   | C11   | -65.1(3)    |
| C14     | C9      | C10   | C12   | 66.2(3)   | C14     | C9    | C10   | C13   | 166.27(17)  |
| C14     | C9      | C10   | C13A  | -173.45(19) | C14    | C9    | C10   | C11A  | -68.8(2)    |
| C14     | C9      | C10   | C12A  | 39.7(4)   | N4      | C18   | C19   | C20   | -127.67(19) |
| N4      | C18     | C19   | C21   | 126.9(2)  | N4      | C18   | C19   | C22   | -7.8(3)     |
| N4      | C18     | C19   | C20A  | -101.7(2) | N4      | C18   | C19   | C21A  | 116.8(2)    |
| N4      | C18     | C19   | C22A  | 12.3(3)   | N4      | C18   | C24   | C25   | 52.9(2)     |
| N4      | C18     | C24   | C26   | 174.62(17) | N4      | C18   | C24   | C27   | -62.9(2)    |
| N4      | C18     | C24   | C26A  | -103.4(2) | N4      | C18   | C24   | C25A  | 146.44(18)  |
| N4      | C18     | C24   | C27A  | 25.3(3)   | C19     | C18   | C24   | C25   | -129.36(19) |
| C19     | C18     | C24   | C26   | -7.6(3)   | C19     | C18   | C24   | C27   | 114.9(2)    |
| C19     | C18     | C24   | C26A  | 74.4(2)   | C19     | C18   | C24   | C25A  | -35.8(2)    |
| C19     | C18     | C24   | C27A  | -156.90(19) | C24     | C18   | C19   | C20   | 54.6(2)     |
| C24     | C18     | C19   | C21   | -50.8(3)  | C24     | C18   | C19   | C22   | 174.41(18)  |
Table S8-8. Torsion angles (°) (continued)

| atom1 | atom2 | atom3 | atom4 | angle   | atom1 | atom2 | atom3 | atom4 | angle   |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| C24   | C18   | C19   | C20A  | 80.5(2) | C24   | C18   | C19   | C21A  | -61.0(3) |
| C24   | C18   | C19   | C22A  | -165.44(17) | N3    | C23   | C28   | C29   | 93.93(19) |
| N3    | C23   | C28   | C30   | -147.16(16) | N3    | C23   | C28   | C31   | -23.9(2)  |
| N3    | C23   | C28   | C30A  | -87.97(19)  | N3    | C23   | C28   | C29A  | 148.00(18) |
| N3    | C23   | C28   | C31A  | 15.8(2)    | N3    | C23   | C32   | C33   | 4.4(3)    |
| N3    | C23   | C32   | C34   | -118.8(2)  | N3    | C23   | C32   | C35   | 126.55(18)|
| N3    | C23   | C32   | C35A  | 98.6(2)    | N3    | C23   | C32   | C33A  | -12.6(2)  |
| N3    | C23   | C32   | C34A  | -127.42(19) | C28   | C23   | C32   | C33   | -177.10(17)|
| C28   | C23   | C32   | C34   | 59.7(3)    | C28   | C23   | C32   | C35   | -54.9(2)  |
| C28   | C23   | C32   | C35A  | -82.9(2)   | C28   | C23   | C32   | C33A  | 165.89(15)|
| C28   | C23   | C32   | C34A  | 51.1(3)    | C32   | C23   | C28   | C29   | -84.6(2)  |
| C32   | C23   | C28   | C30   | 34.3(3)    | C32   | C23   | C28   | C31   | 157.59(16)|
| C32   | C23   | C28   | C30A  | 93.5(2)    | C32   | C23   | C28   | C29A  | -30.5(3)  |
| C32   | C23   | C28   | C31A  | -162.75(16)| F36B  | C36   | C39   | O1    | 77.6(3)   |
| F36A  | C36   | C39   | C36A  | -33.4(3)   | F36A  | C36   | C39   | C38   | -46.5(3)  |
| F36A  | C36   | C39   | C37A  | 177.6(5)   | F36A  | C36   | C39   | C38   | -157.9(5)|
| F36A  | C36   | C39   | C38A  | -134.1(3)  | F36B  | C36   | C39   | O1    | 127.42(19)|
| F36B  | C36   | C39   | C36A  | 91.1(5)    | F36B  | C36   | C39   | C37   | -42.0(6)  |
| F36B  | C36   | C39   | C37A  | -57.9(5)   | F36B  | C36   | C39   | C38   | 78.0(5)   |
| F36B  | C36   | C39   | C38A  | -9.6(6)    | F36C  | C36   | C39   | O1    | -41.3(7)  |
| F36C  | C36   | C39   | C36A  | -152.3(7)  | F36C  | C36   | C39   | C37   | 74.6(7)   |
| F36C  | C36   | C39   | C37A  | 58.7(7)    | F36C  | C36   | C39   | C38   | -165.47(17)|
| F36C  | C36   | C39   | C38A  | 107.0(7)   | F36D  | C36A  | C39   | O1    | -75.2(4)  |
| F36D  | C36A  | C39   | C36   | 29.5(3)    | F36D  | C36A  | C39   | C37   | 131.8(3)  |
| F36D  | C36A  | C39   | C37A  | 45.9(4)    | F36D  | C36A  | C39   | C38   | -173.0(6)|
| F36D  | C36A  | C39   | C38A  | 164.2(3)   | F0AA  | C36A  | C39   | O1    | 31.0(12)  |
| F0AA  | C36A  | C39   | C36   | 135.6(12)  | F0AA  | C36A  | C39   | C37   | -122.0(11)|
| F0AA  | C36A  | C39   | C37A  | 152.0(11)  | F0AA  | C36A  | C39   | C38   | -66.8(12) |
| F0AA  | C36A  | C39   | C38A  | -89.6(11)  | F1AA  | C36A  | C39   | O1    | 158.3(9)  |
| F1AA  | C36A  | C39   | C36   | -97.0(9)   | F1AA  | C36A  | C39   | C37   | 5.3(10)   |
| F1AA  | C36A  | C39   | C37A  | -80.7(9)   | F1AA  | C36A  | C39   | C38   | 60.5(9)   |
| F1AA  | C36A  | C39   | C38A  | 37.7(9)    | F37A  | C37   | C39   | O1    | -169.0(4) |
| F37A  | C37   | C39   | C36   | 76.4(4)    | F37A  | C37   | C39   | C36A  | -15.3(5)  |
| F37A  | C37   | C39   | C37A  | 84.9(4)    | F37A  | C37   | C39   | C38   | -44.2(4)  |
| F37A  | C37   | C39   | C38A  | -68.3(4)   | F37B  | C37   | C39   | O1    | -53.8(7)  |
| F37B  | C37   | C39   | C36   | -168.4(7)  | F37B  | C37   | C39   | C36A  | 99.9(7)   |
| F37B  | C37   | C39   | C37A  | -159.9(7)  | F37B  | C37   | C39   | C38   | 71.0(7)   |

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Table S8-8. Torsion angles (°) (continued)

| atom1 | atom2 | atom3 | atom4 | angle  | atom1 | atom2 | atom3 | atom4 | angle  |
|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|
| F37B  | C37   | C39   | C38A  | 46.9(7)| F37C  | C37   | C39   | O1    | 70.0(4)|
| F37C  | C37   | C39   | C36   | -44.6(4)| F37C  | C37   | C39   | C36A  | -136.3(3)|
| F37C  | C37   | C39   | C37A  | -36.1(3)| F37C  | C37   | C39   | C37A  | -165.2(3)|
| F37C  | C37   | C39   | C38A  | 170.7(5)| F37D  | C37A  | C39   | O1    | 43.2(10)|
| F37D  | C37A  | C39   | C36   | -47.5(9)| F37D  | C37A  | C39   | C36A  | -79.7(9)|
| F37D  | C37A  | C39   | C37   | 148.4(9)| F37D  | C37A  | C39   | C38   | -107.2(9)|
| F2AA  | C37A  | C39   | C36   | -164.7(7)| F2AA  | C37A  | C39   | C36A  | 163.1(3)|
| F2AA  | C37A  | C39   | C37   | 31.2(3)| F2AA  | C37A  | C39   | C38   | 135.6(4)|
| F2AA  | C37A  | C39   | C38A  | 135.6(4)| F37B  | C37   | C39   | O1    | -74.0(4)|
| F37B  | C37   | C39   | C37A  | 170.4(9)| F37B  | C37   | C39   | C38   | 1.4(9)|
| F37B  | C37   | C39   | C38A  | -47.5(9)| F37B  | C37   | C39   | C38A  | -84.6(9)|
| F38B  | C37   | C39   | C37A  | 132.5(9)| F38B  | C37   | C39   | C38   | 151.8(9)|
| F38B  | C37   | C39   | C38A  | -94.6(9)| F38B  | C37   | C39   | C38A  | -157.9(9)|
| F38B  | C37   | C39   | C38B  | 151.8(9)| F38B  | C37   | C39   | C38B  | 101.8(9)|
| F38B  | C37   | C39   | C38C  | 101.8(9)| F38B  | C37   | C39   | C38C  | -10.4(10)|
| F38B  | C37   | C39   | C38D  | -10.4(10)| F38B  | C37   | C39   | C38D  | 164.4(9)|
| F38B  | C37   | C39   | C38A  | -52.0(9)| F38B  | C37   | C39   | C38A  | -79.9(10)|
| F4AA  | C38A  | C39   | C37   | 151.5(10)| F4AA  | C38A  | C39   | O1    | 42.8(10)|
| F4AA  | C38A  | C39   | C37   | 133.7(4)| F4AA  | C38A  | C39   | C37A  | 42.7(4)|
| F4AA  | C38A  | C39   | C37   | -173.7(6)| F4AA  | C38A  | C39   | C37A  | 158.4(3)|
| F4AA  | C38A  | C39   | C37   | 29.8(4)| F5AA  | C38A  | C39   | O1    | 159.3(5)|
| F5AA  | C38A  | C39   | C37   | 11.9(7)| F5AA  | C38A  | C39   | C36A  | -79.1(6)|
| F5AA  | C38A  | C39   | C37   | 64.5(5)| F5AA  | C38A  | C39   | C37A  | 36.7(6)|
| atom  | atom  | distance   | atom  | atom  | distance   |
|-------|-------|------------|-------|-------|------------|
| Nb1   | F38A  | 3.532(15)  | Nb1   | F0AA  | 3.565(18)  |
| F36A  | F38A  | 2.882(15)  | F36A  | F38B  | 2.737(15)  |
| F36A  | O1    | 2.875(3)   | F36A  | C38   | 2.733(6)   |
| F36B  | F37A  | 2.462(15)  | F36B  | F37C  | 2.743(12)  |
| F36B  | F38B  | 2.690(19)  | F36B  | O1    | 3.517(13)  |
| F36B  | C37   | 2.595(13)  | F36B  | C38   | 3.028(14)  |
| F36C  | F37C  | 2.685(15)  | F36C  | O1    | 2.643(15)  |
| F36C  | C25   | 3.447(14)  | F36C  | C27   | 3.429(14)  |
| F36C  | C37   | 3.031(15)  | F36D  | F37D  | 2.713(18)  |
| F36D  | O1    | 3.021(4)   | F36D  | C37A  | 2.746(8)   |
| F36D  | F3AA  | 2.692(15)  | F36D  | C16A  | 3.186(12)  |
| F37A  | F38B  | 2.946(16)  | F37A  | F38C  | 2.865(9)   |
| F37A  | O1    | 3.568(7)   | F37A  | C36   | 3.025(9)   |
| F37A  | C38   | 2.772(9)   | F37B  | F38C  | 2.568(16)  |
| F37B  | O1    | 2.698(16)  | F37B  | C7    | 3.578(18)  |
| F37B  | C38   | 2.949(15)  | F37C  | O1    | 2.943(4)   |
| F37C  | C36   | 2.758(6)   | F37D  | O1    | 2.612(17)  |
| F37D  | C36A  | 3.073(17)  | F37D  | C27A  | 3.19(3)    |
| F38A  | O1    | 2.715(15)  | F38A  | N1    | 3.119(15)  |
| F38A  | C1    | 3.506(15)  | F38A  | C2    | 3.591(15)  |
| F38A  | C8    | 3.339(15)  | F38A  | C16   | 3.56(3)    |
| F38A  | C36   | 3.199(15)  | F38B  | C36   | 2.743(14)  |
| F38B  | C37   | 3.283(13)  | F38B  | O1    | 2.968(5)   |
| F38C  | N1    | 2.991(5)   | F38C  | C1    | 3.078(5)   |
| F38C  | C6    | 3.450(5)   | F38C  | C37   | 2.741(7)   |
| F38D  | O1    | 2.647(19)  | F38D  | C37A  | 3.07(2)    |
| F38D  | F2AA  | 2.69(2)    | F38D  | C31A  | 2.698(18)  |
| O1    | F0AA  | 2.695(17)  | O1    | F1AA  | 3.504(16)  |
| O1    | F2AA  | 2.828(5)   | O1    | F3AA  | 3.556(15)  |
| O1    | F4AA  | 3.036(6)   | O1    | F5AA  | 3.569(9)   |
| N1    | C7    | 2.873(3)   | N1    | C8    | 2.846(3)   |
| N1    | C38   | 3.438(5)   | N1    | F0AA  | 3.263(18)  |
| N1    | F4AA  | 3.071(6)   | N2    | C8    | 3.543(3)   |
| N2    | C11   | 3.455(8)   | N2    | C12   | 3.533(6)   |
| N2    | C13   | 2.759(9)   | N2    | C15   | 3.11(3)    |
| N2    | C16   | 2.70(4)    | N2    | C22A  | 3.242(11)  |
| N2    | C13A  | 2.722(9)   | N2    | C11A  | 3.585(9)   |
Table S8-9. Intramolecular contacts less than 3.60 Å (continued)

| atom | atom | distance  | atom | atom | distance |
|------|------|-----------|------|------|----------|
| N2   | C12A | 3.559(7)  | N2   | C15A | 3.148(12) |
| N2   | C16A | 2.765(14) | N3   | C22  | 3.496(7)  |
| N3   | C29  | 3.235(4)  | N3   | C31  | 2.712(4)  |
| N3   | C33  | 2.698(9)  | N3   | C34  | 3.54(2)   |
| N3   | C30A | 3.297(8)  | N3   | C31A | 2.804(8)  |
| N3   | C22A | 3.573(7)  | N3   | C35A | 3.390(10) |
| N3   | C33A | 2.753(8)  | N3   | C34A | 3.55(2)   |
| N4   | C21  | 3.58(2)   | N4   | C22  | 2.693(8)  |
| N4   | C25  | 2.945(4)  | N4   | C27  | 2.959(3)  |
| N4   | C31  | 3.587(4)  | N4   | C26A | 3.280(12) |
| N4   | C27A | 2.718(14) | N4   | C20A | 3.286(9)  |
| N4   | C21A | 3.48(2)   | N4   | C22A | 2.720(7)  |
| C1   | C4   | 2.789(3)  | C1   | F4AA | 3.179(6)  |
| C2   | C5   | 2.782(3)  | C3   | C6   | 2.796(3)  |
| C6   | F4AA | 3.304(6)  | C7   | F4AA | 3.338(6)  |
| C8   | F0AA | 3.426(19) | C9   | C22A | 3.578(12) |
| C10  | C15  | 3.52(3)   | C10  | C17  | 2.955(17) |
| C10  | C17A | 3.283(11) | C10  | C15A | 3.471(13) |
| C11  | C14  | 3.364(6)  | C11  | C17  | 3.083(16) |
| C12  | C14  | 3.359(9)  | C12  | C15  | 3.36(3)   |
| C12  | C17  | 3.36(2)   | C13  | C33  | 3.572(14) |
| C14  | C11A | 3.342(6)  | C14  | C12A | 3.130(8)  |
| C19  | C26  | 3.203(5)  | C19  | C26A | 3.250(10) |
| C19  | C25A | 2.982(14) | C20  | C24  | 3.235(10) |
| C20  | C26  | 3.097(13) | C21  | C24  | 3.27(2)   |
| C21  | C26  | 3.26(2)   | C24  | C20A | 3.372(10) |
| C24  | C21A | 3.22(2)   | C28  | C34  | 3.28(2)   |
| C28  | C35  | 3.188(8)  | C28  | C35A | 3.519(8)  |
| C28  | C34A | 3.18(2)   | C29  | C32  | 3.419(4)  |
| C29  | C34  | 3.28(2)   | C30  | C32  | 3.073(5)  |
| C30  | C34  | 3.52(2)   | C30  | C35  | 2.716(9)  |
| C32  | C29A | 3.382(8)  | C36A | F3AA | 2.717(16) |
| C36A | F4AA | 2.721(8)  | C36A | F5AA | 3.083(11) |
| C37A | F0AA | 3.549(19) | C37A | F1AA | 2.959(18) |
| C37A | F5AA | 2.769(10) | C38A | F0AA | 3.11(2)   |
| C38A | F1AA | 2.482(17) | C38A | F2AA | 2.748(7)  |
| C38A | F3AA | 3.251(16) | F0AA | F4AA | 2.85(2)   |
Table S8-9. Intramolecular contacts less than 3.60 Å (continued)

| atom | atom | distance  | atom | atom | distance |
|------|------|-----------|------|------|----------|
| F0AA | C16A | 3.22(2)   | F1AA | F3AA | 2.70(2)  |
| F1AA | F4AA | 2.563(19) | F1AA | F5AA | 2.474(19) |
| F2AA | F5AA | 2.865(10) | F2AA | C27A | 3.536(17) |
| F3AA | F5AA | 2.980(17) | C30A | C20A | 3.405(10) |
| C29A | C34A | 3.16(2)   | C26A | C21A | 2.95(3)  |
| C25A | C20A | 3.026(18) | C25A | C21A | 3.45(3)  |
| C11A | C17A | 3.105(10) | C12A | C17A | 3.358(15) |
**Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens**

| atom | atom | distance |
|------|------|----------|
| Nb1  | H7A  | 3.233    |
| Nb1  | H13C | 3.513    |
| Nb1  | H22A | 3.535    |
| Nb1  | H31C | 3.372    |
| Nb1  | H31D | 3.438    |
| Nb1  | H22F | 3.550    |
| Nb1  | H33F | 3.383    |
| Nb1  | H16F | 3.310    |
| F36A | H16C | 2.988    |
| F36C | H25A | 2.631    |
| F36C | H27B | 3.569    |
| F36D | H16D | 3.072    |
| F36D | H16F | 2.770    |
| F37B | H7B  | 3.309    |
| F37B | H31C | 2.721    |
| F37C | H31C | 2.994    |
| F37D | H27D | 2.281    |
| F37D | H27F | 3.408    |
| F38A | H8A  | 2.946    |
| F38A | H16A | 3.112    |
| F38C | H7A  | 3.535    |
| F38D | H7B  | 3.445    |
| O1   | H4   | 2.243    |
| O1   | H25A | 3.384    |
| O1   | H31D | 3.167    |
| O1   | H16F | 2.932    |
| N1   | H7B  | 3.537    |
| N1   | H8A  | 2.358    |
| N1   | H8C  | 3.516    |
| N1   | H33A | 3.405    |
| N1   | H13F | 3.465    |
| N2   | H8A  | 2.597    |
| N2   | H12C | 3.402    |
| N2   | H13C | 2.654    |
| N2   | H15C | 3.474    |
| N2   | H16C | 2.415    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| N2   | H22D | 2.987    | N2   | H22F | 2.620    |
| N2   | H33F | 3.586    | N2   | H13D | 2.721    |
| N2   | H13F | 2.534    | N2   | H11D | 3.431    |
| N2   | H15D | 2.875    | N2   | H15F | 3.568    |
| N2   | H16D | 2.833    | N2   | H16F | 2.565    |
| N3   | H4   | 3.369    | N3   | H7A  | 2.786    |
| N3   | H22A | 2.709    | N3   | H22C | 3.456    |
| N3   | H29A | 3.037    | N3   | H29C | 3.582    |
| N3   | H31A | 2.790    | N3   | H31C | 2.476    |
| N3   | H33A | 2.497    | N3   | H33C | 2.699    |
| N3   | H34C | 3.492    | N3   | H35A | 3.556    |
| N3   | H30F | 3.057    | N3   | H31D | 2.611    |
| N3   | H31F | 2.888    | N3   | H20F | 3.488    |
| N3   | H22D | 2.637    | N3   | H35D | 3.201    |
| N3   | H33D | 2.701    | N3   | H33F | 2.659    |
| N3   | H34F | 3.482    | N4   | H15A | 2.816    |
| N4   | H16C | 3.585    | N4   | H20C | 3.560    |
| N4   | H21A | 3.533    | N4   | H22A | 2.638    |
| N4   | H22C | 2.552    | N4   | H25A | 2.636    |
| N4   | H25C | 3.229    | N4   | H27A | 3.240    |
| N4   | H27C | 2.658    | N4   | H31A | 2.972    |
| N4   | H31C | 3.327    | N4   | H30F | 3.150    |
| N4   | H31D | 3.245    | N4   | H26F | 3.048    |
| N4   | H27D | 2.664    | N4   | H27F | 2.582    |
| N4   | H20F | 3.102    | N4   | H21D | 3.363    |
| N4   | H22D | 2.542    | N4   | H22F | 2.748    |
| N4   | H15D | 3.068    | N4   | H16F | 3.490    |
| C1   | H3   | 3.273    | C1   | H5   | 3.268    |
| C1   | H7A  | 2.557    | C1   | H7B  | 3.151    |
| C1   | H7C  | 3.147    | C1   | H8A  | 2.549    |
| C1   | H8B  | 3.133    | C1   | H8C  | 3.157    |
| C1   | H33D | 3.484    | C2   | H4A  | 3.272    |
| C3   | H5   | 3.243    | C3   | H8A  | 3.315    |
| C3   | H8B  | 2.774    | C3   | H8C  | 2.774    |
| C5   | H3   | 3.244    | C5   | H7A  | 3.310    |
| C5   | H7B  | 2.766    | C5   | H7C  | 2.766    |
| C6   | H4A  | 3.273    | C7   | H5   | 2.669    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C7   | H29A | 2.865    | C7   | H34C | 3.324    |
| C7   | H31F | 3.476    | C7   | H33D | 3.453    |
| C7   | H34F | 3.435    | C8   | H3   | 2.681    |
| C8   | H11A | 3.278    | C8   | H16A | 3.234    |
| C8   | H13F | 3.317    | C8   | H11D | 2.786    |
| C8   | H16D | 3.306    | C9   | H8A  | 2.943    |
| C9   | H11A | 2.641    | C9   | H11B | 3.324    |
| C9   | H11C | 2.814    | C9   | H12A | 2.874    |
| C9   | H12B | 3.484    | C9   | H12C | 2.797    |
| C9   | H13A | 2.779    | C9   | H13B | 3.453    |
| C9   | H13C | 2.812    | C9   | H15A | 2.656    |
| C9   | H15B | 3.390    | C9   | H15C | 2.729    |
| C9   | H16A | 2.559    | C9   | H16B | 3.270    |
| C9   | H16C | 2.567    | C9   | H17A | 2.635    |
| C9   | H17B | 3.345    | C9   | H17C | 2.707    |
| C9   | H22C | 3.189    | C9   | H22F | 2.724    |
| C9   | H13D | 2.724    | C9   | H13E | 3.299    |
| C9   | H13F | 2.542    | C9   | H11D | 2.760    |
| C9   | H11E | 3.496    | C9   | H11F | 2.926    |
| C9   | H12D | 2.648    | C9   | H12E | 3.346    |
| C9   | H12F | 2.757    | C9   | H17D | 2.928    |
| C9   | H17E | 3.518    | C9   | H17F | 2.925    |
| C9   | H15D | 2.597    | C9   | H15E | 3.340    |
| C9   | H15F | 2.719    | C9   | H16D | 2.725    |
| C9   | H16E | 3.412    | C9   | H16F | 2.765    |
| C10  | H15C | 3.291    | C10  | H17A | 2.651    |
| C10  | H17C | 2.989    | C10  | H22C | 3.465    |
| C10  | H22F | 3.017    | C10  | H17D | 3.046    |
| C10  | H17F | 3.422    | C10  | H15F | 3.263    |
| C11  | H8B  | 3.569    | C11  | H12A | 2.839    |
| C11  | H12B | 2.707    | C11  | H12C | 3.319    |
| C11  | H13A | 3.265    | C11  | H13B | 2.626    |
| C11  | H13C | 2.781    | C11  | H17A | 2.806    |
| C11  | H17C | 2.740    | C12  | H11A | 3.402    |
| C12  | H11B | 2.707    | C12  | H11C | 2.651    |
| C12  | H13A | 2.510    | C12  | H13B | 2.651    |
| C12  | H13C | 3.372    | C12  | H15C | 2.681    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C12  | H17A | 2.631    | C12  | H22C | 3.208    |
| C13  | H11A | 2.791    | C13  | H11B | 2.461    |
| C13  | H11C | 3.316    | C13  | H12A | 3.366    |
| C13  | H12B | 2.635    | C13  | H12C | 2.550    |
| C13  | H22C | 3.025    | C13  | H33A | 3.357    |
| C13  | H33C | 3.000    | C14  | H11A | 3.510    |
| C14  | H11C | 3.202    | C14  | H12A | 3.097    |
| C14  | H12C | 3.566    | C14  | H22F | 3.578    |
| C14  | H11D | 3.479    | C14  | H11F | 3.124    |
| C14  | H12D | 2.751    | C14  | H12F | 3.366    |
| C15  | H12A | 2.971    | C15  | H12C | 3.203    |
| C15  | H16A | 3.400    | C15  | H16B | 2.768    |
| C15  | H16C | 2.620    | C15  | H17A | 2.586    |
| C15  | H17B | 2.689    | C15  | H17C | 3.382    |
| C15  | H21A | 3.201    | C15  | H22C | 3.595    |
| C15  | H27A | 3.271    | C16  | H8A  | 3.292    |
| C16  | H15A | 2.762    | C16  | H15B | 2.761    |
| C16  | H15C | 3.347    | C16  | H17A | 3.247    |
| C16  | H17B | 2.668    | C16  | H17C | 2.685    |
| C17  | H11A | 3.358    | C17  | H11C | 2.510    |
| C17  | H12A | 2.815    | C17  | H15A | 3.337    |
| C17  | H15B | 2.762    | C17  | H15C | 2.631    |
| C17  | H16A | 2.712    | C17  | H16B | 2.611    |
| C17  | H16C | 3.259    | C18  | H15A | 3.008    |
| C18  | H20A | 2.914    | C18  | H20B | 3.440    |
| C18  | H20C | 2.712    | C18  | H21A | 2.686    |
| C18  | H21B | 3.389    | C18  | H21C | 2.897    |
| C18  | H22A | 2.602    | C18  | H22B | 3.274    |
| C18  | H22C | 2.607    | C18  | H25A | 2.700    |
| C18  | H25B | 3.397    | C18  | H25C | 2.770    |
| C18  | H26A | 2.940    | C18  | H26B | 3.498    |
| C18  | H26C | 2.902    | C18  | H27A | 2.679    |
| C18  | H27B | 3.356    | C18  | H27C | 2.654    |
| C18  | H31A | 3.158    | C18  | H30F | 3.061    |
| C18  | H26D | 2.676    | C18  | H26E | 3.312    |
| C18  | H26F | 2.541    | C18  | H25D | 2.635    |
| C18  | H25E | 3.377    | C18  | H25F | 2.760    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom   | distance | atom | atom   | distance |
|------|--------|----------|------|--------|----------|
| C18  | H27D   | 2.721    | C18  | H27E   | 3.274    |
| C18  | H27F   | 2.494    | C18  | H20D   | 2.668    |
| C18  | H20E   | 3.301    | C18  | H20F   | 2.595    |
| C18  | H21D   | 2.679    | C18  | H21E   | 3.377    |
| C18  | H21F   | 2.739    | C18  | H22D   | 2.787    |
| C18  | H22E   | 3.457    | C18  | H22F   | 2.822    |
| C18  | H15D   | 3.261    | C19  | H4     | 3.204    |
| C19  | H15A   | 3.453    | C19  | H26A   | 3.212    |
| C19  | H26C   | 3.053    | C19  | H27A   | 3.544    |
| C19  | H30F   | 3.398    | C19  | H26D   | 2.984    |
| C19  | H26F   | 3.423    | C19  | H25D   | 2.967    |
| C19  | H25F   | 2.754    | C20  | H21A   | 3.207    |
| C20  | H21B   | 2.639    | C20  | H21C   | 2.238    |
| C20  | H22A   | 2.609    | C20  | H22B   | 2.594    |
| C20  | H22C   | 3.343    | C20  | H26A   | 2.613    |
| C20  | H26C   | 3.078    | C21  | H15A   | 3.510    |
| C21  | H20A   | 2.371    | C21  | H20B   | 2.602    |
| C21  | H20C   | 3.192    | C21  | H22A   | 3.227    |
| C21  | H22B   | 2.488    | C21  | H22C   | 2.713    |
| C21  | H26A   | 3.445    | C21  | H26C   | 2.673    |
| C21  | H27A   | 3.396    | C22  | H4     | 3.596    |
| C22  | H12C   | 3.085    | C22  | H13A   | 2.813    |
| C22  | H20A   | 3.266    | C22  | H20B   | 2.574    |
| C22  | H20C   | 2.798    | C22  | H21A   | 2.832    |
| C22  | H21B   | 2.460    | C22  | H21C   | 3.168    |
| C22  | H33C   | 2.963    | C22  | H35A   | 3.206    |
| C23  | H7A    | 3.132    | C23  | H22A   | 2.893    |
| C23  | H29A   | 2.673    | C23  | H29B   | 3.358    |
| C23  | H29C   | 2.679    | C23  | H30A   | 2.732    |
| C23  | H30B   | 3.388    | C23  | H30C   | 2.747    |
| C23  | H31A   | 2.665    | C23  | H31B   | 3.326    |
| C23  | H31C   | 2.641    | C23  | H33A   | 2.545    |
| C23  | H33B   | 3.269    | C23  | H33C   | 2.634    |
| C23  | H34A   | 2.764    | C23  | H34B   | 3.428    |
| C23  | H34C   | 2.798    | C23  | H35A   | 2.770    |
| C23  | H35B   | 3.445    | C23  | H35C   | 2.785    |
| C23  | H30D   | 2.890    | C23  | H30E   | 3.464    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom  | distance | atom | atom  | distance |
|------|-------|----------|------|-------|----------|
| C23  | H30F  | 2.753    | C23  | H29D  | 2.995    |
| C23  | H29E  | 3.507    | C23  | H29F  | 2.980    |
| C23  | H31D  | 2.799    | C23  | H31E  | 3.459    |
| C23  | H31F  | 2.858    | C23  | H20F  | 3.309    |
| C23  | H22D  | 3.139    | C23  | H35D  | 2.688    |
| C23  | H35E  | 3.402    | C23  | H35F  | 2.909    |
| C23  | H33D  | 2.812    | C23  | H33E  | 3.497    |
| C23  | H33F  | 2.872    | C23  | H34D  | 2.814    |
| C23  | H34E  | 3.387    | C23  | H34F  | 2.660    |
| C24  | H4    | 2.369    | C24  | H20A  | 3.066    |
| C24  | H20C  | 3.278    | C24  | H21A  | 3.289    |
| C24  | H21C  | 3.137    | C24  | H20D  | 3.118    |
| C24  | H21D  | 3.408    | C24  | H21F  | 2.920    |
| C25  | H4    | 2.538    | C25  | H26A  | 2.622    |
| C25  | H26B  | 2.603    | C25  | H26C  | 3.318    |
| C25  | H27A  | 3.368    | C25  | H27B  | 2.694    |
| C25  | H27C  | 2.677    | C25  | H31A  | 3.084    |
| C26  | H20A  | 2.479    | C26  | H20C  | 3.303    |
| C26  | H21A  | 3.471    | C26  | H21C  | 2.685    |
| C26  | H25A  | 3.311    | C26  | H25B  | 2.568    |
| C26  | H25C  | 2.672    | C26  | H27A  | 2.741    |
| C26  | H27B  | 2.599    | C26  | H27C  | 3.339    |
| C27  | H4    | 2.643    | C27  | H15A  | 3.134    |
| C27  | H21A  | 3.484    | C27  | H25A  | 2.685    |
| C27  | H25B  | 2.688    | C27  | H25C  | 3.367    |
| C27  | H26A  | 3.347    | C27  | H26B  | 2.625    |
| C27  | H26C  | 2.703    | C27  | H34A  | 2.959    |
| C28  | H34C  | 3.561    | C28  | H35A  | 3.390    |
| C28  | H35C  | 2.868    | C28  | H20F  | 3.580    |
| C28  | H35F  | 3.407    | C28  | H34D  | 2.964    |
| C28  | H34F  | 3.243    | C29  | H7A   | 3.095    |
| C29  | H7C   | 3.563    | C29  | H30A  | 2.687    |
| C29  | H30B  | 2.712    | C29  | H30C  | 3.380    |
| C29  | H31A  | 3.341    | C29  | H31B  | 2.668    |
| C29  | H31C  | 2.632    | C29  | H34A  | 2.776    |
| C29  | H34C  | 3.245    | C30  | H29A  | 3.370    |
| C30  | H29B  | 2.709    | C30  | H29C  | 2.717    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C30  | H31A | 2.662    | C30  | H31B | 2.620    |
| C30  | H31C | 3.306    | C30  | H34A | 2.963    |
| C30  | H35A | 2.958    | C30  | H35B | 3.560    |
| C30  | H35C | 2.005    | C31  | H4   | 3.588    |
| C31  | H25A | 3.414    | C31  | H25C | 3.197    |
| C31  | H29A | 2.671    | C31  | H29B | 2.685    |
| C31  | H29C | 3.319    | C31  | H30A | 3.295    |
| C31  | H30B | 2.639    | C31  | H30C | 2.670    |
| C32  | H22A | 3.235    | C32  | H29C | 3.131    |
| C32  | H30A | 2.767    | C32  | H30C | 3.191    |
| C32  | H30D | 3.462    | C32  | H29D | 3.542    |
| C32  | H29F | 3.197    | C32  | H22D | 3.424    |
| C33  | H13A | 3.156    | C33  | H13C | 3.204    |
| C33  | H22A | 3.187    | C33  | H34A | 3.181    |
| C33  | H34B | 2.557    | C33  | H34C | 2.597    |
| C33  | H35A | 2.742    | C33  | H35B | 2.688    |
| C33  | H35C | 3.286    | C34  | H7C  | 3.527    |
| C34  | H29C | 2.580    | C34  | H30A | 2.883    |
| C34  | H33A | 2.606    | C34  | H33B | 2.434    |
| C34  | H33C | 3.222    | C34  | H35A | 3.420    |
| C34  | H35B | 2.758    | C34  | H35C | 2.729    |
| C35  | H22A | 3.218    | C35  | H30A | 2.322    |
| C35  | H30C | 2.467    | C35  | H33A | 3.352    |
| C35  | H33B | 2.683    | C35  | H33C | 2.583    |
| C35  | H34A | 2.699    | C35  | H34B | 2.733    |
| C35  | H34C | 3.442    | C36  | H4   | 3.539    |
| C36A | H16D | 3.480    | C36A | H16F | 3.325    |
| C37  | H31C | 3.262    | C37A | H4   | 3.475    |
| C37A | H27D | 3.190    | C38A | H31F | 3.425    |
| C39  | H4   | 3.354    | C39  | H16F | 3.580    |
| H3   | H8B  | 2.738    | H3   | H8C  | 2.715    |
| H3   | H4A  | 2.333    | H4   | H15A | 3.079    |
| H4   | H16C | 3.415    | H4   | H22A | 3.498    |
| H4   | H22C | 3.438    | H4   | H25A | 2.002    |
| H4   | H25B | 3.351    | H4   | H25C | 3.004    |
| H4   | H27A | 3.138    | H4   | H27B | 3.437    |
| H4   | H27C | 2.134    | H4   | H31A | 3.084    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H4   | H31C | 3.169    | H4   | F2AA | 3.521    |
| H4   | H30F | 3.446    | H4   | H31D | 3.054    |
| H4   | C26A | 3.232    | H4   | H26F | 2.966    |
| H4   | C27A | 2.201    | H4   | H27D | 1.934    |
| H4   | H27E | 3.170    | H4   | H27F | 2.106    |
| H4   | H22D | 3.423    | H4   | H22F | 3.572    |
| H4   | H15D | 3.323    | H4   | H16F | 3.270    |
| H5   | H7A  | 3.599    | H5   | H7B  | 2.715    |
| H5   | H7C  | 2.711    | H5   | H4A  | 2.316    |
| H7A  | H29A | 2.292    | H7A  | H29C | 3.236    |
| H7A  | H31C | 3.543    | H7A  | H33A | 3.465    |
| H7A  | H34C | 3.184    | H7A  | F4AA | 3.122    |
| H7A  | C31A | 3.468    | H7A  | H31F | 2.715    |
| H7A  | H33D | 3.114    | H7A  | H34F | 3.242    |
| H7B  | H29A | 2.886    | H7B  | F4AA | 3.092    |
| H7B  | H31F | 3.445    | H7C  | H29A | 2.973    |
| H7C  | H29C | 3.263    | H7C  | H34C | 2.606    |
| H7C  | H33D | 3.195    | H7C  | H34F | 2.743    |
| H8A  | H11A | 3.070    | H8A  | H13C | 3.431    |
| H8A  | H16A | 2.574    | H8A  | H16C | 3.346    |
| H8A  | F0AA | 2.994    | H8A  | H13F | 2.886    |
| H8A  | C11A | 3.472    | H8A  | H11D | 2.670    |
| H8A  | C16A | 3.367    | H8A  | H16D | 2.624    |
| H8A  | H16F | 3.552    | H8B  | H11A | 2.621    |
| H8B  | H13F | 2.967    | H8B  | C11A | 3.094    |
| H8B  | H11D | 2.129    | H8B  | H11E | 3.509    |
| H8C  | H16A | 3.089    | H8C  | F0AA | 3.170    |
| H8C  | H11D | 3.226    | H8C  | H16D | 3.142    |
| H11A | H13B | 3.063    | H11A | H13C | 2.760    |
| H11A | H17A | 3.353    | H11A | H17C | 2.806    |
| H11B | H12A | 3.160    | H11B | H12B | 2.526    |
| H11B | H12C | 3.511    | H11B | H13A | 3.324    |
| H11B | H13B | 2.240    | H11B | H13C | 2.843    |
| H11B | H17A | 3.537    | H11C | H12A | 2.612    |
| H11C | H12B | 2.867    | H11C | H12C | 3.548    |
| H11C | H13B | 3.461    | H11C | H17A | 2.161    |
| H11C | H17B | 3.369    | H11C | H17C | 2.132    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H12A  | H13A  | 3.424    | H12A  | H13B  | 3.579    |
| H12A  | H15A  | 3.533    | H12A  | H15C  | 2.200    |
| H12A  | H17A  | 1.952    | H12A  | H17B  | 3.456    |
| H12A  | H17C  | 3.347    | H12B  | H13A  | 2.777    |
| H12B  | H13B  | 2.438    | H12B  | H13C  | 3.579    |
| H12B  | H15C  | 3.589    | H12B  | H17A  | 3.299    |
| H12B  | H17A  | 1.952    | H12B  | H17C  | 3.347    |
| H12C  | H13A  | 2.202    | H12C  | H13B  | 2.853    |
| H12C  | H13C  | 3.451    | H12C  | H15A  | 3.313    |
| H12C  | H15C  | 2.516    | H12C  | H17A  | 3.252    |
| H12C  | H21A  | 3.316    | H12C  | H21B  | 3.300    |
| H12C  | H22B  | 3.000    | H12C  | H22C  | 2.366    |
| H13A  | H22A  | 3.013    | H13A  | H22B  | 2.882    |
| H13A  | H22C  | 2.139    | H13A  | H33A  | 3.149    |
| H13A  | H33B  | 3.561    | H13A  | H33C  | 2.391    |
| H13B  | H33C  | 3.312    | H13C  | H22C  | 3.484    |
| H13C  | H33A  | 2.750    | H13C  | H33B  | 3.535    |
| H13C  | H33C  | 2.874    | H15A  | H16B  | 3.119    |
| H15A  | H16C  | 2.482    | H15A  | H17A  | 3.450    |
| H15A  | H17B  | 3.596    | H15A  | H21A  | 2.755    |
| H15A  | H22C  | 3.027    | H15A  | H27A  | 2.621    |
| H15A  | H27C  | 2.892    | H15B  | H16B  | 2.638    |
| H15B  | H16C  | 2.906    | H15B  | H17A  | 2.961    |
| H15B  | H17B  | 2.587    | H15B  | H21A  | 3.590    |
| H15B  | H27A  | 3.106    | H15C  | H16C  | 3.508    |
| H15C  | H17A  | 2.338    | H15C  | H17B  | 2.907    |
| H15C  | H17C  | 3.538    | H15C  | H21A  | 2.830    |
| H15C  | H22C  | 3.406    | H16A  | H17A  | 3.567    |
| H16A  | H17B  | 3.055    | H16A  | H17C  | 2.593    |
| H16B  | H17A  | 3.490    | H16B  | H17B  | 2.465    |
| H16B  | H17C  | 2.924    | H16C  | H17B  | 3.517    |
| H16C  | H17C  | 3.582    | H16C  | H27C  | 3.578    |
| H20A  | H21A  | 3.209    | H20A  | H21B  | 2.811    |
| H20A  | H21C  | 1.877    | H20A  | H22A  | 3.527    |
| H20A  | H22B  | 3.391    | H20A  | H26A  | 1.934    |
| H20A  | H26B  | 3.366    | H20A  | H26C  | 2.384    |
| H20B  | H21A  | 3.563    | H20B  | H21B  | 2.543    |
| H20B  | H21C  | 2.598    | H20B  | H22A  | 2.753    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H20B | H22B | 2.336    | H20B | H22C | 3.512    |
| H20B | H26A | 3.469    | H20B | H35A | 3.351    |
| H20C | H21B | 3.563    | H20C | H21C | 3.127    |
| H20C | H22A | 2.594    | H20C | H22B | 3.084    |
| H20C | H25C | 3.107    | H20C | H26A | 2.678    |
| H20C | H26C | 3.558    | H20C | H30C | 3.074    |
| H20C | H31A | 2.940    | H20C | H35A | 3.316    |
| H21A | H22B | 3.059    | H21A | H22C | 2.817    |
| H21A | H26C | 2.824    | H21A | H27A | 2.823    |
| H21B | H22A | 3.348    | H21B | H22B | 2.165    |
| H21B | H22C | 2.799    | H21B | H26C | 3.530    |
| H21C | H22B | 3.241    | H21C | H26A | 2.818    |
| H21C | H26B | 3.535    | H21C | H26C | 1.977    |
| H21C | H27A | 3.417    | H22A | H30C | 3.561    |
| H22A | H31A | 3.227    | H22A | H33C | 2.413    |
| H22A | H35A | 2.469    | H22B | H33C | 3.029    |
| H22B | H35A | 3.100    | H22C | H33C | 2.980    |
| H25A | H26A | 3.545    | H25A | H26B | 3.481    |
| H25A | H27A | 3.580    | H25A | H27B | 2.971    |
| H25A | H27C | 2.480    | H25A | H31A | 2.930    |
| H25A | H31C | 3.180    | H25B | H26A | 2.824    |
| H25B | H26B | 2.338    | H25B | H26C | 3.482    |
| H25B | H27A | 3.591    | H25B | H27B | 2.502    |
| H25B | H27C | 2.950    | H25B | H26A | 2.470    |
| H25C | H26B | 2.946    | H25C | H26C | 3.572    |
| H25C | H27B | 3.592    | H25C | H27C | 3.577    |
| H25C | H31A | 2.487    | H25C | H31B | 3.227    |
| H25C | H31C | 3.436    | H26A | H27B | 3.498    |
| H26B | H27A | 2.989    | H26B | H27B | 2.355    |
| H26B | H27C | 3.493    | H26C | H27A | 2.590    |
| H26C | H27B | 2.895    | H29A | H30A | 3.584    |
| H29A | H30B | 3.599    | H29A | H31A | 3.566    |
| H29A | H31B | 2.962    | H29A | H31C | 2.448    |
| H29A | H34A | 3.346    | H29A | H34C | 3.361    |
| H29B | H30A | 2.960    | H29B | H30B | 2.529    |
| H29B | H31A | 3.593    | H29B | H31B | 2.502    |
| H29B | H31C | 2.932    | H29B | H34A | 3.433    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H29C   | H30A   | 2.511    | H29C   | H30B   | 3.010    |
| H29C   | H31B   | 3.556    | H29C   | H31C   | 3.522    |
| H29C   | H34A   | 1.980    | H29C   | H34B   | 3.461    |
| H29C   | H34C   | 2.552    | H29C   | H35C   | 3.554    |
| H30A   | H31A   | 3.553    | H30A   | H31B   | 3.507    |
| H30A   | H34A   | 2.227    | H30A   | H34B   | 3.440    |
| H30A   | H35A   | 2.860    | H30A   | H35B   | 2.999    |
| H30A   | H35C   | 1.484    | H30A   | H31A   | 2.945    |
| H30B   | H31B   | 2.425    | H30B   | H31C   | 3.528    |
| H30B   | H35C   | 2.832    | H30B   | H31A   | 2.503    |
| H30C   | H31B   | 2.931    | H30C   | H31C   | 3.571    |
| H30C   | H34A   | 3.575    | H30C   | H35A   | 2.404    |
| H30C   | H35B   | 3.332    | H30C   | H35C   | 1.872    |
| H33A   | H34A   | 3.476    | H33A   | H34B   | 2.935    |
| H33A   | H34C   | 2.470    | H33B   | H34A   | 3.326    |
| H33B   | H34B   | 2.242    | H33B   | H34C   | 2.749    |
| H33B   | H35A   | 3.077    | H33B   | H35B   | 2.525    |
| H33B   | H35C   | 3.520    | H33C   | H34B   | 3.425    |
| H33C   | H34C   | 3.533    | H33C   | H35A   | 2.479    |
| H33C   | H35B   | 2.849    | H33C   | H35C   | 3.477    |
| H34A   | H35A   | 3.592    | H34A   | H35B   | 2.988    |
| H34A   | H35C   | 2.494    | H34B   | H35B   | 2.560    |
| H34B   | H35C   | 2.993    | F0AA   | H16D   | 2.649    |
| F0AA   | H16F   | 2.948    | F2AA   | H31D   | 3.341    |
| F2AA   | H27D   | 3.084    | F2AA   | H27F   | 3.195    |
| C30A   | H29D   | 3.406    | C30A   | H29E   | 2.588    |
| C30A   | H29F   | 2.710    | C30A   | H31D   | 2.543    |
| C30A   | H31E   | 2.621    | C30A   | H31F   | 3.373    |
| C30A   | H20E   | 3.487    | C30A   | H20F   | 2.532    |
| C30A   | H35F   | 3.419    | H30D   | H29F   | 2.598    |
| H30D   | H29E   | 2.946    | H30D   | H31D   | 3.481    |
| H30D   | C31A   | 3.357    | H30D   | C20A   | 3.180    |
| H30D   | H31E   | 3.513    | H30D   | H20E   | 3.573    |
| H30D   | H20D   | 3.291    | H30D   | C35A   | 3.257    |
| H30D   | H20F   | 2.336    | H30D   | H35F   | 2.735    |
| H30E   | C29A   | 2.643    | H30E   | H29D   | 3.547    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H30E   | H29E   | 2.334    | H30E   | H29F   | 2.927    |
| H30E   | C31A   | 2.567    | H30E   | H31D   | 2.720    |
| H30E   | H31E   | 2.338    | H30E   | H31F   | 3.512    |
| H30E   | H20F   | 3.298    | H30F   | C29A   | 3.364    |
| H30F   | H29E   | 3.460    | H30F   | C31A   | 2.647    |
| H30F   | H31D   | 2.340    | H30F   | H31E   | 2.938    |
| H30F   | H31F   | 3.549    | H30F   | H25D   | 2.866    |
| H30F   | H27F   | 2.938    | H30F   | C20A   | 2.742    |
| H30F   | H20D   | 2.832    | H30F   | H20E   | 3.503    |
| H30F   | H20F   | 1.944    | H30F   | H22D   | 3.565    |
| H30F   | H35D   | 3.595    | C29A   | H31D   | 3.308    |
| C29A   | H31E   | 2.531    | C29A   | H31F   | 2.810    |
| C29A   | H34D   | 2.568    | C29A   | H34F   | 3.211    |
| H29D   | C31A   | 2.743    | H29D   | H31E   | 2.868    |
| H29D   | H31F   | 2.725    | H29D   | C34A   | 3.004    |
| H29D   | H34D   | 2.504    | H29D   | H34F   | 2.784    |
| H29E   | C31A   | 2.521    | H29E   | H31D   | 3.355    |
| H29E   | H31E   | 2.189    | H29E   | H31F   | 2.968    |
| H29E   | H34D   | 3.488    | H29F   | C31A   | 3.343    |
| H29F   | H31E   | 3.419    | H29F   | H35F   | 3.151    |
| H29F   | C34A   | 2.859    | H29F   | H34D   | 2.064    |
| H29F   | H34F   | 3.167    | H31D   | H27F   | 2.849    |
| C26A   | H25D   | 3.338    | C26A   | H25E   | 2.826    |
| C26A   | H25F   | 2.537    | C26A   | H27D   | 2.637    |
| C26A   | H27E   | 2.838    | C26A   | H27F   | 3.338    |
| C26A   | H21D   | 2.876    | C26A   | H21F   | 2.455    |
| C26A   | H15D   | 3.392    | H26D   | C25A   | 2.527    |
| H26D   | H25D   | 3.374    | H26D   | H25E   | 2.950    |
| H26D   | H25F   | 2.181    | H26D   | C27A   | 3.310    |
| H26D   | H27D   | 3.551    | H26D   | C21A   | 2.303    |
| H26D   | H21D   | 2.376    | H26D   | H21E   | 3.144    |
| H26D   | H21F   | 1.619    | H26D   | H15D   | 3.554    |
| H26E   | C25A   | 2.807    | H26E   | H25E   | 2.788    |
| H26E   | H25F   | 2.929    | H26E   | C27A   | 2.698    |
| H26E   | H27D   | 2.785    | H26E   | H27E   | 2.684    |
| H26E   | H21F   | 3.204    | H26F   | C25A   | 3.350    |
| H26F   | H25F   | 3.400    | H26F   | C27A   | 2.844    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H26F   | H27D   | 2.628    | H26F   | H27E   | 3.327    |
| H26F   | C21A   | 3.071    | H26F   | H21D   | 2.687    |
| H26F   | H21F   | 2.831    | H26F   | C15A   | 3.314    |
| H26F   | H15D   | 2.548    | H26F   | H15E   | 3.272    |
| C25A   | H27D   | 3.320    | C25A   | H27E   | 2.544    |
| C25A   | H27F   | 2.738    | C25A   | H20D   | 2.340    |
| C25A   | H20F   | 3.448    | C25A   | H21F   | 2.916    |
| H25D   | C27A   | 2.752    | H25D   | H27D   | 3.499    |
| H25D   | H27F   | 2.665    | H25D   | C20A   | 2.598    |
| H25D   | H20D   | 1.842    | H25D   | H20E   | 3.419    |
| H25D   | H20F   | 2.836    | H25D   | H21F   | 3.459    |
| H25E   | C27A   | 2.633    | H25E   | H27D   | 3.499    |
| H25E   | H27E   | 2.328    | H25E   | H27F   | 3.008    |
| H25E   | H20D   | 3.201    | H25F   | C27A   | 3.281    |
| H25F   | H27E   | 3.410    | H25F   | C20A   | 2.844    |
| H25F   | H20D   | 2.155    | H25F   | H20E   | 3.449    |
| H25F   | H20F   | 3.513    | H25F   | C21A   | 2.862    |
| H25F   | H21D   | 3.550    | H25F   | H21E   | 3.455    |
| H25F   | H21F   | 2.201    | C20A   | H21D   | 3.454    |
| C20A   | H21E   | 2.909    | C20A   | H21F   | 3.017    |
| C20A   | H22D   | 2.709    | C20A   | H22E   | 2.703    |
| C20A   | H22F   | 3.338    | C20A   | H35D   | 3.129    |
| H20D   | C21A   | 2.981    | H20D   | H21E   | 3.266    |
| H20D   | H21F   | 2.978    | H20D   | C22A   | 3.394    |
| H20E   | C21A   | 2.885    | H20E   | H21E   | 2.755    |
| H20E   | H21F   | 3.296    | H20E   | C22A   | 2.632    |
| H20E   | H22D   | 2.941    | H20E   | H22E   | 2.458    |
| H20E   | H22F   | 3.515    | H20E   | H35D   | 2.925    |
| H20F   | C21A   | 3.485    | H20F   | C22A   | 2.631    |
| H20F   | H22D   | 2.464    | H20F   | H22E   | 2.930    |
| H20F   | H22F   | 3.518    | H20F   | C35A   | 3.277    |
| H20F   | H35D   | 2.551    | H20F   | H35F   | 3.272    |
| C21A   | H22D   | 3.372    | C21A   | H22E   | 2.752    |
| C21A   | H22F   | 2.564    | C21A   | H15D   | 3.310    |
| H21D   | C22A   | 2.572    | H21D   | H22D   | 3.441    |
| H21D   | H22E   | 2.946    | H21D   | H22F   | 2.251    |
| H21D   | H12F   | 3.484    | H21D   | C15A   | 3.017    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H21D | H15D | 2.427    | H21D | H15E | 3.538    |
| H21D | H15F | 2.762    | H21E | C22A | 2.671    |
| H21E | H22E | 2.553    | H21E | H22F | 2.814    |
| H21F | C22A | 3.401    | H21F | H22F | 3.483    |
| C22A | H35D | 2.979    | C22A | H33F | 3.278    |
| C22A | H13D | 2.911    | C22A | H12F | 3.313    |
| C22A | H15D | 3.465    | H22D | C35A | 3.253    |
| H22D | H35D | 2.414    | H22D | C33A | 3.289    |
| H22D | H33F | 2.502    | H22D | C13A | 3.555    |
| H22D | H13D | 2.698    | H22E | H35D | 2.791    |
| H22E | H33F | 3.339    | H22E | H13D | 2.891    |
| H22E | H12F | 3.195    | H22F | H33F | 3.583    |
| H22F | C13A | 3.272    | H22F | H13D | 2.652    |
| H22F | C12A | 3.223    | H22F | H12F | 2.573    |
| H22F | C15A | 3.194    | H22F | H15D | 2.651    |
| H22F | H15F | 3.066    | C35A | H33D | 3.348    |
| C35A | H33E | 2.695    | C35A | H33F | 2.662    |
| C35A | H34D | 2.772    | C35A | H34E | 2.711    |
| C35A | H34F | 3.351    | H35D | C33A | 2.702    |
| H35D | H33D | 3.571    | H35D | H33E | 3.045    |
| H35D | H33F | 2.503    | H35D | C34A | 3.360    |
| H35E | C33A | 2.512    | H35E | H33D | 3.433    |
| H35E | H33E | 2.340    | H35E | H33F | 2.738    |
| H35E | C34A | 2.757    | H35E | H34D | 3.121    |
| H35E | H34E | 2.578    | H35F | C33A | 3.392    |
| H35F | H33E | 3.572    | H35F | C34A | 2.707    |
| H35F | H34D | 2.591    | H35F | H34E | 2.950    |
| C33A | H34D | 3.498    | C33A | H34E | 2.706    |
| C33A | H34F | 2.799    | C33A | H13D | 3.076    |
| C33A | H13F | 3.456    | H33D | C34A | 2.826    |
| H33D | H34E | 3.002    | H33D | H34F | 2.654    |
| H33D | H13D | 3.399    | H33D | H13F | 3.324    |
| H33E | C34A | 2.791    | H33E | H34E | 2.518    |
| H33E | H34F | 3.077    | H33E | H13D | 3.353    |
| H33F | C34A | 3.456    | H33F | H34E | 3.594    |
| H33F | C13A | 2.886    | H33F | H13D | 2.173    |
| H33F | H13E | 3.341    | H33F | H13F | 2.816    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom     | atom     | distance | atom     | atom     | distance |
|----------|----------|----------|----------|----------|----------|
| C13A     | H11D     | 2.714    | C13A     | H11E     | 2.636    |
| C13A     | H11F     | 3.316    | C13A     | H12D     | 3.270    |
| C13A     | H12E     | 2.662    | C13A     | H12F     | 2.834    |
| H13D     | C11A     | 3.399    | H13D     | H11E     | 3.580    |
| H13D     | C12A     | 2.812    | H13D     | H12E     | 3.054    |
| H13D     | H12F     | 2.814    | H13E     | C11A     | 2.560    |
| H13E     | H11D     | 2.928    | H13E     | H11E     | 2.339    |
| H13E     | H11F     | 3.425    | H13E     | C12A     | 2.676    |
| H13E     | H12D     | 3.494    | H13E     | H12E     | 2.474    |
| H13E     | H12F     | 3.116    | H13F     | C11A     | 2.547    |
| H13F     | H11D     | 2.409    | H13F     | H11E     | 2.793    |
| H13F     | H11F     | 3.455    | H13F     | C12A     | 3.276    |
| H13F     | H12E     | 3.505    | C11A     | H12D     | 2.582    |
| C11A     | H12E     | 2.636    | C11A     | H12F     | 3.436    |
| C11A     | H17D     | 2.873    | C11A     | H17F     | 2.766    |
| H11D     | C12A     | 3.348    | H11D     | H12D     | 3.416    |
| H11D     | H12E     | 3.552    | H11D     | C17A     | 3.352    |
| H11D     | H17D     | 3.390    | H11D     | H17F     | 2.798    |
| H11E     | C12A     | 2.814    | H11E     | H12D     | 3.013    |
| H11E     | H12E     | 2.570    | H11E     | H17D     | 3.589    |
| H11F     | C12A     | 2.639    | H11F     | H12D     | 2.326    |
| H11F     | H12E     | 2.819    | H11F     | H12F     | 3.577    |
| H11F     | C17A     | 2.452    | H11F     | H17D     | 2.125    |
| H11F     | H17E     | 3.344    | H11F     | H17F     | 2.107    |
| C12A     | H17D     | 2.761    | C12A     | H15F     | 2.805    |
| H12D     | C17A     | 2.624    | H12D     | H17D     | 1.889    |
| H12D     | H17E     | 3.360    | H12D     | H17F     | 3.131    |
| H12D     | C15A     | 3.003    | H12D     | H15F     | 2.392    |
| H12E     | H17D     | 3.356    | H12F     | H17D     | 3.340    |
| H12F     | C15A     | 3.231    | H12F     | H15D     | 3.461    |
| H12F     | H15F     | 2.537    | C17A     | H15D     | 3.366    |
| C17A     | H15E     | 2.659    | C17A     | H15F     | 2.712    |
| C17A     | H16D     | 2.727    | C17A     | H16E     | 2.566    |
| C17A     | H16F     | 3.347    | H17D     | C15A     | 2.745    |
| H17D     | H15E     | 2.998    | H17D     | H15F     | 2.582    |
| H17D     | C16A     | 3.354    | H17D     | H16E     | 3.486    |
| H17E     | C15A     | 2.669    | H17E     | H15D     | 3.565    |
Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H17E  | H15E  | 2.445    | H17E  | H15F  | 2.960    |
| H17E  | C16A  | 2.634    | H17E  | H16D  | 3.009    |
| H17E  | H16E  | 2.338    | H17E  | H16F  | 3.499    |
| H17F  | C15A  | 3.348    | H17F  | H15E  | 3.534    |
| H17F  | C16A  | 2.651    | H17F  | H16D  | 2.528    |
| H17F  | H16E  | 2.802    | H17F  | H16F  | 3.585    |
| C15A  | H16D  | 3.318    | C15A  | H16E  | 2.701    |
| C15A  | H16F  | 2.616    | H15D  | C16A  | 2.677    |
| H15D  | H16D  | 3.538    | H15D  | H16E  | 3.043    |
| H15D  | H16F  | 2.450    | H15E  | C16A  | 2.595    |
| H15E  | H16D  | 3.516    | H15E  | H16E  | 2.454    |
| H15E  | H16F  | 2.799    | H15F  | C16A  | 3.336    |
| H15F  | H16E  | 3.576    | H15F  | H16F  | 3.547    |
Table S8-11. Intermolecular contacts less than 3.60 Å

| atom    | atom       | distance | atom    | atom       | distance |
|---------|------------|----------|---------|------------|----------|
| F36A    | C26        | 3.570(6) | F36A    | C27        | 3.406(4) |
| F36B    | C34        | 3.14(2)  | F36D    | C26A       | 3.416(13) |
| F37A    | C34        | 3.50(2)  | F37B    | C17        | 3.33(2)  |
| F37D    | C26A       | 3.11(2)  | F38C    | C20        | 3.583(12) |
| F38C    | C21        | 3.28(2)  | F38D    | C17A       | 3.59(2)  |
| C17     | F37B⁵      | 3.33(2)  | C20     | F38C⁶      | 3.583(12) |
| C21     | F38C⁶      | 3.28(2)  | C26     | F36A¹      | 3.570(6)  |
| C27     | F36A¹      | 3.406(4) | C27     | C27¹       | 3.263(5)  |
| C34     | F36B⁷      | 3.14(2)  | C34     | F37A⁷      | 3.50(2)  |
| F3AA    | C34A²      | 3.31(3)  | F4AA    | C20A⁴      | 3.492(9)  |
| C31A    | C12A³      | 3.584(10)| C26A    | F36D¹      | 3.416(13) |
| C26A    | F37D¹      | 3.11(2)  | C25A    | C25A⁸      | 3.23(2)  |
| C20A    | F4AA⁶      | 3.492(9) | C33A    | C11A⁹      | 3.135(12) |
| C34A    | F3AA⁷      | 3.31(3)  | C11A    | C33A⁹      | 3.135(12) |
| C12A    | C31A⁵      | 3.584(10)| C17A    | F38D⁵      | 3.59(2)  |

Symmetry Operators:

(1)  -X+1,-Y,-Z+1  (2)  -X+1/2+1,Y+1/2-1,-Z+1/2
(3)  X+1,-Y+1,Z   (4)  X,-Y+1,Z
(5)  X,-Y+1,Z+1   (6)  X+1,-Y+1,Z+1
(7)  -X+1/2+1,Y+1/2,-Z+1/2 (8)  -X+2,-Y,-Z+1
(9)  -X+1,-Y+1,-Z+1
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| F36A | H3$^1$ | 3.556 | F36A | H26B$^2$ | 3.327 |
| F36A | H26C$^2$ | 3.013 | F36A | H27A$^2$ | 2.874 |
| F36A | H27B$^2$ | 3.093 | F36A | H4A$^1$ | 3.241 |
| F36B | H3$^1$ | 2.967 | F36B | H29C$^3$ | 3.594 |
| F36B | H34A$^3$ | 2.901 | F36B | H34B$^3$ | 3.105 |
| F36B | H34C$^3$ | 2.885 | F36C | H15B$^2$ | 3.334 |
| F36C | H27A$^2$ | 2.904 | F36D | H3$^1$ | 3.509 |
| F36D | H4A$^1$ | 2.885 | F36D | H30E$^4$ | 3.421 |
| F36D | H26D$^2$ | 3.124 | F36D | H26E$^2$ | 2.827 |
| F37A | H11C$^3$ | 3.589 | F37A | H17C$^5$ | 3.407 |
| F37A | H22B$^6$ | 3.537 | F37A | H34B$^3$ | 2.991 |
| F37A | H34C$^3$ | 3.150 | F37B | H17A$^5$ | 2.883 |
| F37B | H17B$^5$ | 3.151 | F37B | H17C$^5$ | 3.422 |
| F37C | H5$^3$ | 3.505 | F37C | H7C$^3$ | 2.876 |
| F37C | H11C$^5$ | 3.527 | F37C | H34C$^3$ | 3.171 |
| F37D | H26D$^2$ | 3.065 | F37D | H26E$^2$ | 2.887 |
| F37D | H26F$^2$ | 2.856 | F38A | H21B$^6$ | 3.210 |
| F38A | H30A$^4$ | 3.566 | F38A | H30B$^4$ | 2.863 |
| F38B | H3$^1$ | 3.133 | F38B | H12B$^6$ | 3.490 |
| F38B | H12C$^6$ | 3.260 | F38B | H21B$^6$ | 3.118 |
| F38B | H22B$^6$ | 2.938 | F38B | H4A$^1$ | 3.486 |
| F38C | H20B$^6$ | 2.811 | F38C | H21B$^6$ | 2.426 |
| F38C | H21C$^6$ | 3.436 | F38C | H22B$^6$ | 3.059 |
| F38D | H12D$^5$ | 3.224 | F38D | H17D$^5$ | 2.748 |
| C1   | H11B$^7$ | 3.247 | C1   | H13E$^7$ | 3.559 |
| C2   | H11B$^7$ | 3.292 | C2   | H13B$^7$ | 2.970 |
| C2   | H13E$^7$ | 2.999 | C2   | H12E$^7$ | 3.572 |
| C3   | H11B$^7$ | 3.578 | C3   | H12B$^7$ | 2.890 |
| C3   | H13B$^7$ | 3.001 | C3   | H21C$^6$ | 3.153 |
| C3   | H21F$^6$ | 3.271 | C3   | H13E$^7$ | 3.284 |
| C3   | H12E$^7$ | 3.134 | C4   | H12B$^7$ | 2.756 |
| C4   | H20A$^6$ | 3.507 | C4   | H21C$^6$ | 2.897 |
| C4   | H26C$^6$ | 2.916 | C4   | H31B$^8$ | 3.258 |
| C4   | H30E$^8$ | 3.544 | C4   | H31E$^8$ | 3.468 |
| C4   | H25F$^6$ | 3.123 | C4   | H21F$^6$ | 3.130 |
| C4   | H12E$^7$ | 2.908 | C5   | H12B$^7$ | 3.401 |
| C5   | H20A$^6$ | 3.066 | C5   | H21C$^6$ | 3.146 |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom     | distance | atom | atom     | distance |
|------|----------|----------|------|----------|----------|
| C5   | H25C     | 3.428    | C5   | H26C     | 3.398    |
| C5   | H31B     | 3.323    | C5   | H31E     | 3.532    |
| C5   | H25F     | 3.161    | C5   | H12E     | 3.151    |
| C6   | H11B     | 3.505    | C6   | H20A     | 3.535    |
| C8   | H13B     | 2.968    | C8   | H30A     | 3.047    |
| C8   | H35C     | 3.261    | C8   | H29F     | 3.145    |
| C8   | H34D     | 3.300    | C8   | H13E     | 3.060    |
| C11  | H13C     | 3.500    | C11  | H33A     | 3.468    |
| C12  | H29B     | 2.770    | C12  | H31B     | 3.582    |
| C13  | H8B      | 3.079    | C15  | H27B     | 3.270    |
| C15  | H29B     | 3.528    | C16  | H26B     | 3.445    |
| C16  | H27B     | 3.215    | C16  | H30B     | 3.570    |
| C16  | H30C     | 3.178    | C17  | H7B      | 3.547    |
| C25  | H5       | 2.936    | C25  | H26A     | 3.419    |
| C26  | H16B     | 3.496    | C26  | H25C     | 3.457    |
| C26  | H4A      | 3.225    | C27  | H27B     | 3.197    |
| C27  | H27A     | 3.230    | C27  | H27B     | 3.197    |
| C27  | H27C     | 2.826    | C29  | H12A     | 2.846    |
| C29  | H15C     | 3.063    | C29  | H17A     | 3.531    |
| C30  | H8C      | 3.003    | C30  | H16A     | 2.942    |
| C31  | H5       | 3.488    | C33  | H35B     | 3.385    |
| C35  | H8C      | 3.468    | C35  | H17C     | 3.325    |
| C35  | H33B     | 3.374    | C36  | H27A     | 3.431    |
| C37A | H34F     | 3.516    | C38  | H21B     | 3.145    |
| C38  | H22B     | 3.532    | C38A | H20E     | 3.387    |
| C38A | H17D     | 3.432    | H3   | F36A     | 3.556    |
| H3   | F36B     | 2.967    | H3   | F36D     | 3.509    |
| H3   | F38B     | 3.133    | H3   | H12B     | 3.021    |
| H3   | H13B     | 2.955    | H3   | H21C     | 3.523    |
| H3   | H34A     | 3.561    | H3   | F1AA     | 3.314    |
| H3   | F3AA      | 2.864    | H3   | H21F     | 3.455    |
| H3   | H34D     | 3.481    | H3   | H13E     | 3.450    |
| H3   | H12E     | 3.510    | H5   | F37C     | 3.505    |
| H5   | C25      | 2.936    | H5   | C31      | 3.488    |
| H5   | H20A     | 2.964    | H5   | H21C     | 3.519    |
| H5   | H25A     | 2.914    | H5   | H25B     | 2.890    |
| H5   | H25C     | 2.517    | H5   | H26A     | 3.238    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H5    | H26C  | 3.391    | H5    | H31A  | 3.448    |
| H5    | H31B  | 2.865    | H5    | H30E  | 3.434    |
| H5    | H31D  | 3.446    | H5    | H31E  | 3.208    |
| H5    | H25F  | 2.975    | H5    | C27A  | 3.431    |
| H5    | H27E  | 3.199    | H5    | H27F  | 2.781    |
| H5    | H12E  | 3.527    | H7B   | H17A  | 3.563    |
| H7B   | H15B  | 3.356    | H7B   | H20A  | 3.375    |
| H7B   | H20B  | 3.208    | H7B   | H25B  | 3.116    |
| H7B   | H27E  | 3.276    | H7B   | H17D  | 3.464    |
| H7B   | H17E  | 2.921    | H7B   | H15E  | 3.163    |
| H7C   | F37C  | 2.876    | H7C   | F2AA  | 2.679    |
| H8A   | H13B  | 3.530    | H8A   | H30A  | 3.278    |
| H8A   | H35C  | 3.454    | H8A   | H29F  | 3.450    |
| H8A   | H13E  | 3.423    | H8B   | C13^  | 3.079    |
| H8B   | H11B  | 3.579    | H8B   | H13A  | 3.532    |
| H8B   | H13B  | 2.230    | H8B   | H13C  | 3.176    |
| H8B   | H30A  | 3.415    | H8B   | H35B  | 3.505    |
| H8B   | H35C  | 3.222    | H8B   | H33E  | 3.413    |
| H8B   | H34D  | 3.286    | H8B   | C13A  | 3.170    |
| H8B   | H13D  | 3.170    | H8B   | H13E  | 2.419    |
| H8B   | H13F  | 3.528    | H8C   | C30^  | 3.003    |
| H8C   | C35^  | 3.468    | H8C   | H30A  | 2.150    |
| H8C   | H30B  | 3.114    | H8C   | H30C  | 3.449    |
| H8C   | H34A  | 2.840    | H8C   | H35B  | 3.575    |
| H8C   | H35C  | 2.629    | H8C   | C29A  | 3.119    |
| H8C   | H29D  | 3.403    | H8C   | H29E  | 3.512    |
| H8C   | H29F  | 2.185    | H8C   | H35F  | 3.417    |
| H8C   | C34A  | 3.445    | H8C   | H34D  | 2.497    |
| H11A  | H13B  | 3.389    | H11A  | H13C  | 2.957    |
| H11A  | H33A  | 3.126    | H11A  | H33B  | 3.296    |
| H11A  | H35B  | 3.544    | H11B  | Cl^   | 3.247    |
| H11B  | C2^   | 3.292    | H11B  | C3^   | 3.578    |
| H11B  | C6^   | 3.505    | H11B  | H8B   | 3.579    |
| H11B  | H13C  | 3.146    | H11B  | H33A  | 3.158    |
| H11C  | F37A  | 3.589    | H11C  | F37C  | 3.527    |
| H11C  | H33A  | 3.566    | H12A  | C29^  | 2.846    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H12A | H9A  | 2.840    | H12A | H9B  | 2.058    |
| H12A | H9C  | 3.512    | H12A | H31B | 3.102    |
| H12B | F38B | 3.490    | H12B | C3   | 2.890    |
| H12B | C4   | 2.756    | H12B | C5   | 3.401    |
| H12B | H3   | 3.021    | H12B | H29B | 3.062    |
| H12B | H31B | 3.172    | H12B | H4   | 2.805    |
| H12C | F38B | 3.260    | H12C | H29B | 2.818    |
| H13A | H8B  | 3.532    | H13B | C2   | 2.970    |
| H13B | C3   | 3.001    | H13B | C8   | 2.968    |
| H13B | H3   | 2.955    | H13B | H8A  | 3.530    |
| H13B | H8B  | 2.230    | H13B | H11A | 3.389    |
| H13C | C11  | 3.500    | H13C | H8B  | 3.176    |
| H13C | H11A | 2.957    | H13C | H11B | 3.146    |
| H13C | H13C | 3.448    | H15A | H27B | 3.147    |
| H15B | F36C | 3.334    | H15B | C27  | 3.458    |
| H15B | H7B  | 3.356    | H15B | H25B | 3.062    |
| H15B | H27B | 2.682    | H15B | H27C | 3.422    |
| H15C | C29  | 3.063    | H15C | H29A | 2.972    |
| H15C | H29B | 2.575    | H15C | H29C | 3.150    |
| H16A | C30  | 2.942    | H16A | H30A | 2.918    |
| H16A | H30B | 2.886    | H16A | H30C | 2.531    |
| H16A | H35C | 2.917    | H16B | C26  | 3.496    |
| H16B | H20C | 3.551    | H16B | H25B | 3.187    |
| H16B | H26B | 2.560    | H16B | H27B | 2.707    |
| H16B | H30B | 3.497    | H16B | H30C | 2.951    |
| H16C | H26B | 3.584    | H16C | H27B | 2.912    |
| H17A | F37B | 2.883    | H17A | C29  | 3.531    |
| H17A | H7B  | 3.563    | H17A | H29A | 2.956    |
| H17A | H29B | 3.195    | H17B | F37B | 3.151    |
| H17B | H7B  | 2.713    | H17B | H20B | 2.963    |
| H17B | H20C | 3.463    | H17B | H29A | 3.535    |
| H17C | F37A | 3.407    | H17C | F37B | 3.422    |
| H17C | C35  | 3.325    | H17C | H35A | 2.987    |
| H17C | H35B | 3.261    | H17C | H35C | 3.174    |
| H20A | C4   | 3.507    | H20A | C5   | 3.066    |
| H20A | C6   | 3.535    | H20A | H5   | 2.964    |
| H20A | H7   | 3.375    | H20A | H25B | 3.272    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom   | distance | atom  | atom   | distance |
|-------|--------|----------|-------|--------|----------|
| H20A  | H25C\(^10\) | 3.401    | H20B  | F38C\(^{11}\) | 2.811    |
| H20B  | H7B\(^{11}\) | 3.208    | H20B  | H17B\(^{12}\) | 2.963    |
| H20C  | H16B\(^{12}\) | 3.551    | H20C  | H17B\(^{12}\) | 3.463    |
| H20C  | H25B\(^{10}\) | 3.567    | H20C  | H26B\(^{10}\) | 3.388    |
| H21B  | F38A\(^{11}\) | 3.210    | H21B  | F38B\(^{11}\) | 3.118    |
| H21B  | F38C\(^{11}\) | 2.426    | H21B  | C3\(^{11}\) | 3.145    |
| H21C  | F38C\(^{11}\) | 3.436    | H21C  | C3\(^{11}\) | 3.153    |
| H21C  | C4\(^{11}\) | 2.897    | H21C  | C5\(^{11}\) | 3.146    |
| H21C  | H3\(^{11}\) | 3.523    | H21C  | H5\(^{11}\) | 3.519    |
| H21C  | H4A\(^{11}\) | 3.134    | H22B  | F37A\(^{11}\) | 3.537    |
| H22B  | F38B\(^{11}\) | 2.938    | H22B  | F38C\(^{11}\) | 3.059    |
| H22B  | C3\(^{11}\) | 3.532    | H25A  | H5\(^3\) | 2.914    |
| H25B  | H5\(^3\) | 2.890    | H25B  | H7B\(^{3}\) | 3.116    |
| H25B  | H15B\(^2\) | 3.062    | H25B  | H16B\(^2\) | 3.187    |
| H25B  | H20A\(^{10}\) | 3.272    | H25B  | H20C\(^{10}\) | 3.567    |
| H25B  | H26A\(^{10}\) | 3.363    | H25C  | C5\(^3\) | 3.428    |
| H25C  | C26\(^{10}\) | 3.457    | H25C  | H5\(^3\) | 2.517    |
| H25C  | H20A\(^{10}\) | 3.401    | H25C  | H26A\(^{10}\) | 2.672    |
| H25C  | H26B\(^{10}\) | 3.483    | H26A  | H26A\(^{10}\) | 3.363    |
| H26A  | H5\(^{11}\) | 3.238    | H26A  | H26A\(^{10}\) | 2.880    |
| H26A  | H25C\(^{10}\) | 2.672    | H26A  | H26A\(^{10}\) | 2.880    |
| H26A  | H4A\(^{11}\) | 3.395    | H26B  | F36A\(^2\) | 3.327    |
| H26B  | C16\(^2\) | 3.445    | H26B  | H16B\(^2\) | 2.560    |
| H26B  | H16C\(^2\) | 3.584    | H26B  | H20C\(^{10}\) | 3.388    |
| H26B  | H25C\(^{10}\) | 3.483    | H26B  | H4A\(^{11}\) | 3.296    |
| H26C  | F36A\(^{2}\) | 3.013    | H26C  | C4\(^{11}\) | 2.916    |
| H26C  | C5\(^{11}\) | 3.398    | H26C  | H5\(^{11}\) | 3.391    |
| H26C  | H4A\(^{11}\) | 2.526    | H27A  | F36A\(^{2}\) | 2.874    |
| H27A  | F36C\(^2\) | 2.904    | H27A  | C27\(^2\) | 3.230    |
| H27A  | C36\(^2\) | 3.431    | H27A  | H27A\(^2\) | 3.485    |
| H27A  | H27B\(^2\) | 3.061    | H27A  | H27C\(^2\) | 2.671    |
| H27B  | F36A\(^{2}\) | 3.093    | H27B  | C15\(^2\) | 3.270    |
| H27B  | C16\(^2\) | 3.215    | H27B  | C27\(^2\) | 3.197    |
| H27B  | H15A\(^2\) | 3.147    | H27B  | H15B\(^2\) | 2.682    |
| H27B  | H16B\(^2\) | 2.707    | H27B  | H16C\(^2\) | 2.912    |
| H27B  | H27A\(^2\) | 3.061    | H27B  | H27B\(^2\) | 3.424    |
| H27B  | H27C\(^2\) | 2.631    | H27C  | C27\(^2\) | 2.826    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H27C   | H15B²  | 3.422    | H27C   | H27A²  | 2.671    |
| H27C   | H27B²  | 2.631    | H27C   | H27C²  | 2.692    |
| H29A   | H12A⁵  | 2.840    | H29A   | H15C⁵  | 2.972    |
| H29A   | H17A⁵  | 2.956    | H29A   | H17B⁵  | 3.535    |
| H29B   | C12⁵   | 2.770    | H29B   | C15⁵   | 3.528    |
| H29B   | H12A⁵  | 2.058    | H29B   | H12B⁵  | 3.062    |
| H29B   | H12C⁵  | 2.818    | H29B   | H15C⁵  | 2.575    |
| H29B   | H17A⁵  | 3.195    | H29C   | F36B⁸  | 3.594    |
| H29C   | H12A⁵  | 3.512    | H29C   | H15C⁵  | 3.150    |
| H30A   | F38A¹² | 3.566    | H30A   | C8¹²   | 3.047    |
| H30A   | H8A¹²  | 3.278    | H30A   | H8B¹²  | 3.415    |
| H30A   | H8C¹²  | 2.150    | H30A   | H16A¹² | 2.918    |
| H30B   | F38A¹² | 2.863    | H30B   | C16¹²  | 3.570    |
| H30B   | H8C¹²  | 3.114    | H30B   | H16A¹² | 2.886    |
| H30B   | H16B¹² | 3.497    | H30B   | H4A³   | 3.520    |
| H30C   | C16¹²  | 3.178    | H30C   | H8C¹²  | 3.449    |
| H30C   | H16A¹² | 2.531    | H30C   | H16B¹² | 2.951    |
| H31A   | H5³    | 3.448    | H31B   | C4³    | 3.258    |
| H31B   | C5³    | 3.323    | H31B   | C12³   | 3.582    |
| H31B   | H5³    | 2.865    | H31B   | H12A³  | 3.102    |
| H31B   | H12B⁵  | 3.172    | H31B   | H4A³   | 2.755    |
| H33A   | C11¹⁷  | 3.468    | H33A   | H11A⁷  | 3.126    |
| H33A   | H11B⁷  | 3.158    | H33A   | H11C⁷  | 3.566    |
| H33B   | C35¹³  | 3.374    | H33B   | H11A⁷  | 3.296    |
| H33B   | H33B¹³ | 3.366    | H33B   | H34B¹³ | 3.189    |
| H33B   | H35B¹³ | 2.406    | H34A   | F36B⁸  | 2.901    |
| H34A   | H3¹²   | 3.561    | H34A   | H8C¹²  | 2.840    |
| H34B   | F36B³  | 3.105    | H34B   | F37A⁸  | 2.991    |
| H34B   | H33B¹³ | 3.189    | H34B   | H35B¹³ | 3.078    |
| H34C   | F36B³  | 2.885    | H34C   | F37A⁸  | 3.150    |
| H34C   | F37C⁸  | 3.171    | H35A   | H17C¹² | 2.987    |
| H35B   | C33¹³  | 3.385    | H35B   | H8B¹²  | 3.505    |
| H35B   | H8C¹²  | 3.575    | H35B   | H11A¹² | 3.544    |
| H35B   | H17C¹² | 3.261    | H35B   | H33B¹³ | 2.406    |
| H35B   | H34B¹³ | 3.078    | H35C   | C8¹²   | 3.261    |
| H35C   | H8A¹²  | 3.454    | H35C   | H8B¹²  | 3.222    |
| H35C   | H8C¹²  | 2.629    | H35C   | H16A¹² | 2.917    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H35C   | H17C\(^1\) | 3.174    | H4A    | F36A\(^{14}\) | 3.241    |
| H4A    | F36D\(^{14}\) | 2.885    | H4A    | F38B\(^{14}\) | 3.486    |
| H4A    | C26\(^6\) | 3.225    | H4A    | H12B\(^7\) | 2.805    |
| H4A    | H21C\(^6\) | 3.134    | H4A    | H26A\(^6\) | 3.395    |
| H4A    | H26B\(^6\) | 3.296    | H4A    | H26C\(^6\) | 2.526    |
| H4A    | H30B\(^8\) | 3.520    | H4A    | H31B\(^8\) | 2.755    |
| H4A    | H30E\(^8\) | 2.741    | H4A    | H29E\(^8\) | 3.535    |
| H4A    | H31E\(^8\) | 3.105    | H4A    | H26D\(^6\) | 3.253    |
| H4A    | H25F\(^6\) | 2.907    | H4A    | H21F\(^6\) | 3.232    |
| H4A    | H12E\(^7\) | 3.165    | F0AA   | H29E\(^4\) | 3.128    |
| F0AA   | H29F\(^4\) | 3.250    | F0AA   | H21E\(^6\) | 3.506    |
| F1AA   | H3\(^1\) | 3.314    | F1AA   | H21E\(^6\) | 3.251    |
| F1AA   | H22E\(^6\) | 2.718    | F2AA   | H7C\(^3\) | 2.679    |
| F2AA   | H34F\(^3\) | 3.178    | F3AA   | H3\(^1\) | 2.864    |
| F3AA   | H26D\(^2\) | 3.553    | F3AA   | H34D\(^3\) | 3.241    |
| F3AA   | H34E\(^3\) | 3.252    | F3AA   | H34F\(^3\) | 2.885    |
| F4AA   | H20E\(^6\) | 2.591    | F4AA   | H21E\(^6\) | 3.094    |
| F4A    | H22E\(^6\) | 3.594    | F5AA   | H20E\(^6\) | 3.054    |
| F5AA   | H22E\(^6\) | 3.459    | F5AA   | H35D\(^6\) | 3.414    |
| F5AA   | H34E\(^3\) | 3.352    | F5AA   | H11F\(^5\) | 3.477    |
| F5AA   | H17D\(^5\) | 3.176    | F5AA   | H17F\(^5\) | 3.520    |
| C30A   | H16D\(^{12}\) | 3.495    | C30A   | H16E\(^{12}\) | 3.493    |
| H30D   | C17A\(^{12}\) | 3.566    | H30D   | H17E\(^{12}\) | 3.334    |
| H30D   | H17F\(^{12}\) | 3.021    | H30D   | C16A\(^{12}\) | 3.211    |
| H30D   | H16D\(^{12}\) | 2.726    | H30D   | H16E\(^{12}\) | 2.828    |
| H30E   | F36D\(^{12}\) | 3.421    | H30E   | C4\(^4\) | 3.544    |
| H30E   | H5\(^3\) | 3.434    | H30E   | H4A\(^3\) | 2.741    |
| H30E   | H25E\(^{10}\) | 3.237    | H30E   | H16D\(^{12}\) | 3.429    |
| H30E   | H16E\(^{12}\) | 3.317    | H30F   | H25E\(^{10}\) | 3.423    |
| C29A   | H8C\(^{12}\) | 3.119    | H29D   | H8C\(^{12}\) | 3.403    |
| H29D   | H21D\(^{5}\) | 3.353    | H29D   | H12F\(^5\) | 3.476    |
| H29D   | H15F\(^{5}\) | 3.063    | H29E   | H8C\(^{12}\) | 3.512    |
| H29E   | H4A\(^3\) | 3.535    | H29E   | F0A\(^{12}\) | 3.128    |
| H29E   | H12F\(^{5}\) | 2.959    | H29F   | C8\(^{12}\) | 3.145    |
| H29F   | H8A\(^{12}\) | 3.450    | H29F   | H8C\(^{12}\) | 2.185    |
| H29F   | F0AA\(^{12}\) | 3.250    | H29F   | H16D\(^{12}\) | 3.347    |
| C31A   | H12D\(^{5}\) | 3.112    | C31A   | H12E\(^{5}\) | 3.516    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| C31A  | H12F  | 3.555    | H31D  | H53   | 3.446    |
| H31E  | C43   | 3.468    | H31E  | C53   | 3.532    |
| H31E  | H53   | 3.208    | H31E  | H4A3  | 3.105    |
| H31E  | C12A5 | 2.859    | H31E  | H12D5 | 2.610    |
| H31E  | H12E5 | 2.670    | H31E  | H12F5 | 2.813    |
| H31F  | C12A5 | 3.423    | H31F  | H12D5 | 2.732    |
| H31F  | H12E5 | 3.570    | H31F  | H12F5 | 3.483    |
| H31F  | H17D5 | 3.186    | H31F  | H15F5 | 3.383    |
| C26A  | H16E2 | 3.466    | H26D  | F36D2 | 3.124    |
| H26D  | F37D2 | 3.065    | H26D  | H4A11 | 3.253    |
| H26D  | F3AA2 | 3.553    | H26E  | F36D2 | 2.827    |
| H26E  | F37D2 | 2.887    | H26E  | H15E2 | 3.452    |
| H26E  | C16A2 | 3.072    | H26E  | H16E2 | 2.559    |
| H26E  | H16F2 | 2.704    | H26F  | H37D2 | 2.856    |
| H26F  | H26F2 | 3.503    | H26F  | H27D2 | 3.410    |
| C25A  | H25D10| 2.705    | C25A  | H25E10| 2.868    |
| H25D  | C25A10| 2.705    | H25D  | H25D10| 2.479    |
| H25D  | H25E10| 2.120    | H25D  | H25F10| 3.240    |
| H25D  | H27E10| 3.567    | H25E  | H30E10| 3.237    |
| H25E  | H30F10| 3.423    | H25E  | C25A10| 2.868    |
| H25E  | H25D10| 2.120    | H25E  | H25E10| 2.822    |
| H25E  | H25F10| 3.377    | H25E  | H20D10| 3.165    |
| H25E  | H16E2 | 3.166    | H25F  | C411  | 3.123    |
| H25F  | C511  | 3.161    | H25F  | H511  | 2.975    |
| H25F  | H4A11 | 2.907    | H25F  | H25D10| 3.240    |
| H25F  | H25E10| 3.377    | C27A  | H53   | 3.431    |
| C27A  | H15E2 | 3.323    | H27D  | H26F2 | 3.410    |
| H27D  | H15E2 | 3.098    | H27E  | H53   | 3.199    |
| H27E  | H7B3  | 3.276    | H27E  | H25D10| 3.567    |
| H27E  | H17E2 | 3.472    | H27E  | H15E2 | 2.672    |
| H27E  | H16E2 | 3.017    | H27F  | H53   | 2.781    |
| C20A  | H17E12| 3.292    | H20D  | H25E10| 3.165    |
| H20D  | H17E12| 3.120    | H20E  | C38A11| 3.387    |
| H20E  | F4AA11| 2.591    | H20E  | F5AA11| 3.054    |
| H20E  | C17A12| 3.532    | H20E  | H17E12| 2.899    |
| H20E  | H17F12| 3.424    | H20F  | H17E12| 3.318    |
| H20F  | H17F12| 3.535    | H21D  | H29D9 | 3.353    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom          | distance | atom  | atom          | distance |
|-------|---------------|----------|-------|---------------|----------|
| H21E  | F0AA          | 3.506    | H21E  | F1AA          | 3.251    |
| H21E  | F4AA          | 3.094    | H21F  | C3            | 3.271    |
| H21F  | C4            | 3.130    | H21F  | H3            | 3.455    |
| H21F  | H4A           | 3.232    | H22E  | F1AA          | 2.718    |
| H22E  | F4AA          | 3.594    | H22E  | F5AA          | 3.459    |
| C35A  | H35E          | 3.454    | C35A  | H33E          | 3.465    |
| C35A  | H34E          | 3.448    | C35A  | H17F          | 3.307    |
| H35D  | F5AA          | 3.414    | H35D  | H17F          | 3.336    |
| H35E  | C35A          | 3.454    | H35E  | H35E          | 2.601    |
| H35E  | C33A          | 3.589    | H35E  | H35E          | 2.769    |
| H35E  | C34A          | 3.431    | H35E  | H34E          | 2.542    |
| H35F  | H8C           | 3.417    | H35F  | H33E          | 3.279    |
| H35F  | H11D          | 3.291    | H35F  | H17F          | 2.512    |
| H35F  | C17A          | 3.470    | H35F  | H17F          | 2.512    |
| C33A  | H35E          | 3.589    | C33A  | H11D          | 3.076    |
| C33A  | H11E          | 2.527    | C33A  | H11F          | 3.336    |
| H33D  | C11A          | 2.839    | H33D  | H11D          | 3.070    |
| H33D  | H11E          | 2.027    | H33D  | H11F          | 3.070    |
| H33E  | H8B           | 3.413    | H33E  | C35A          | 3.465    |
| H33E  | H35E          | 2.769    | H33E  | H35F          | 3.279    |
| H33E  | C11A          | 2.649    | H33E  | H11D          | 2.456    |
| H33E  | H11E          | 2.337    | H33E  | H11F          | 2.719    |
| H33F  | C11A          | 3.478    | H33F  | H11D          | 3.240    |
| H33F  | H11E          | 2.869    | C34A  | H8C           | 3.445    |
| C34A  | H35E          | 3.431    | H34D  | C8            | 3.300    |
| H34D  | H3            | 3.481    | H34D  | H8B           | 3.286    |
| H34D  | H8C           | 2.497    | H34D  | F3AA          | 3.241    |
| H34E  | F3AA          | 3.252    | H34E  | F5AA          | 3.352    |
| H34E  | C35A          | 3.448    | H34E  | H35E          | 2.542    |
| H34F  | C37A          | 3.516    | H34F  | F2AA          | 3.178    |
| H34F  | F3AA          | 2.885    | C13A  | H8B           | 3.170    |
| C13A  | H13E          | 3.431    | C13A  | H13F          | 3.161    |
| C13A  | H11D          | 3.589    | H13D  | H8B           | 3.170    |
| H13E  | C1            | 3.559    | H13E  | C2            | 2.999    |
| H13E  | C3            | 3.284    | H13E  | C8            | 3.060    |
| H13E  | H3            | 3.450    | H13E  | H8A           | 3.423    |
| H13E  | H8B           | 2.419    | H13E  | C13A          | 3.431    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom   | distance | atom  | atom   | distance |
|-------|--------|----------|-------|--------|----------|
| H13E  | H13E\(^7\) | 3.368    | H13E  | H13F\(^7\) | 2.645    |
| H13E  | H11D\(^7\) | 3.206    | H13F  | H8B\(^7\) | 3.528    |
| H13F  | C13A\(^7\) | 3.161    | H13F  | H13E\(^7\) | 2.645    |
| H13F  | H13F\(^7\) | 2.788    | H13F  | C11A\(^7\) | 3.569    |
| H13F  | H11D\(^7\) | 3.356    | H13F  | H11E\(^7\) | 3.055    |
| C11A  | H33D\(^7\) | 2.839    | C11A  | H13F\(^7\) | 3.569    |
| C11A  | H33F\(^7\) | 3.478    | C11A  | H13F\(^7\) | 3.569    |
| H11D  | H35F\(^4\) | 3.291    | H11D  | C33A\(^7\) | 3.076    |
| H11D  | H33D\(^7\) | 3.070    | H11D  | H33E\(^7\) | 2.456    |
| H11D  | H33F\(^7\) | 3.240    | H11D  | C13A\(^7\) | 3.589    |
| H11D  | H33E\(^7\) | 3.206    | H11D  | H13F\(^7\) | 3.356    |
| H11E  | C33A\(^7\) | 2.527    | H11E  | H33D\(^7\) | 2.027    |
| H11E  | H33E\(^7\) | 2.337    | H11E  | H33F\(^7\) | 2.869    |
| H11E  | H13F\(^7\) | 3.055    | H11F  | F5AA\(^9\) | 3.477    |
| H11F  | H35F\(^4\) | 3.254    | H11F  | C33A\(^7\) | 3.336    |
| H11F  | H33D\(^7\) | 3.070    | H11F  | H33E\(^7\) | 2.719    |
| C12A  | H31E\(^9\) | 2.859    | C12A  | H31F\(^9\) | 3.423    |
| H12D  | F38D\(^9\) | 3.224    | H12D  | C31A\(^9\) | 3.112    |
| H12D  | H31E\(^9\) | 2.610    | H12D  | H31F\(^9\) | 2.732    |
| H12E  | C2\(^7\) | 3.572    | H12E  | C3\(^7\) | 3.134    |
| H12E  | C4\(^7\) | 2.908    | H12E  | C5\(^7\) | 3.151    |
| H12E  | H3\(^7\) | 3.510    | H12E  | H5\(^7\) | 3.527    |
| H12E  | H4A\(^7\) | 3.165    | H12E  | C31A\(^9\) | 3.516    |
| H12E  | H31E\(^9\) | 2.670    | H12E  | H31F\(^9\) | 3.570    |
| H12F  | H29D\(^9\) | 3.476    | H12F  | H29E\(^9\) | 2.959    |
| H12F  | C31A\(^9\) | 3.555    | H12F  | H31E\(^9\) | 2.813    |
| H12F  | H31F\(^9\) | 3.483    | C17A  | H30D\(^4\) | 3.566    |
| C17A  | H20E\(^4\) | 3.532    | C17A  | H35F\(^4\) | 3.470    |
| H17D  | F38D\(^9\) | 2.748    | H17D  | C38A\(^9\) | 3.432    |
| H17D  | H7B\(^9\) | 3.464    | H17D  | F5AA\(^9\) | 3.176    |
| H17D  | H31F\(^9\) | 3.186    | H17E  | H7B\(^9\) | 2.921    |
| H17E  | H30D\(^4\) | 3.334    | H17E  | H27E\(^2\) | 3.472    |
| H17E  | C20A\(^4\) | 3.292    | H17E  | H20D\(^4\) | 3.120    |
| H17E  | H20E\(^4\) | 2.899    | H17E  | H20F\(^4\) | 3.318    |
| H17F  | F5AA\(^9\) | 3.520    | H17F  | H30D\(^4\) | 3.021    |
| H17F  | H20E\(^4\) | 3.424    | H17F  | H20F\(^4\) | 3.535    |
| H17F  | C35A\(^4\) | 3.307    | H17F  | H35D\(^4\) | 3.336    |
Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom       | distance | atom | atom       | distance |
|------|------------|----------|------|------------|----------|
| H17F | H35F$^4$   | 2.512    | H15E | H7B$^9$    | 3.163    |
| H15E | H26E$^2$   | 3.452    | H15E | C27A$^2$   | 3.323    |
| H15E | H27D$^2$   | 3.098    | H15E | H27E$^2$   | 2.672    |
| H15F | H29D$^9$   | 3.063    | H15F | H31F$^9$   | 3.383    |
| C16A | H30D$^4$   | 3.211    | C16A | H26E$^2$   | 3.072    |
| H16D | C30A$^4$   | 3.495    | H16D | H30F$^4$   | 3.347    |
| H16D | H30E$^4$   | 3.429    | H16D | H30D$^4$   | 2.726    |
| H16E | C30A$^4$   | 3.493    | H16E | C26A$^2$   | 3.466    |
| H16E | H30E$^4$   | 3.317    | H16E | H25E$^2$   | 3.166    |
| H16E | H26E$^2$   | 2.559    | H16F | H26E$^2$   | 2.704    |

Symmetry Operators:

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

for

\[
\text{Nb(N-2,6-\text{Me}_2\text{C}_6\text{H}_3)(N=\text{C}^{\text{Bu}}_2)(\text{OCH(CF}_3)_2)\text{[HN=\text{C}^{\text{Bu}}_2)}} (9)
\]

November 21, 2017
Experimental

Data Collection

A yellow prism crystal of C_{32}H_{48}F_{12}N_{3}NbO_{2} having approximate dimensions of 0.380 x 0.250 x 0.130 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 45.02 mm.

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

\[ a = 17.905(3) \text{ Å} \]
\[ b = 12.0354(15) \text{ Å} \quad \beta = 115.352(2)^\circ \]
\[ c = 19.691(3) \text{ Å} \]
\[ V = 3834.6(10) \text{ Å}^3 \]

For \( Z = 4 \) and \( F.W. = 827.64 \), the calculated density is 1.433 g/cm\(^3\). The reflection conditions of:

\[ h0l: \ h+l = 2n \]
\[ 0k0: \ k = 2n \]

uniquely determine the space group to be:

\[ P2_1/n \ (\#14) \]

The data were collected at a temperature of -180 ± 1°C to a maximum \( 2\theta \) value of 55.0°. A total of 720 oscillation images were collected. A sweep of data was done using \( \omega \) scans from -105.0 to 75.0° in 0.50° step, at \( \omega = 45.0^\circ \) and \( \phi = 0^\circ \). The exposure rate was 12.0 [sec./°]. The detector swing angle was -14.95°. A second sweep was performed using \( \omega \) scans from -105.0 to 75.0° in 0.50° step, at \( \chi = 45.0^\circ \) and \( \phi \)
The exposure rate was 12.0 [sec./°]. The detector swing angle was -14.95°. The crystal-to-detector distance was 45.02 mm. Readout was performed in the 0.172 mm pixel mode.

Data Reduction

Of the 32113 reflections were collected, where 8561 were unique (R_{int} = 0.0590); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).  

The linear absorption coefficient, μ, for Mo-Kα radiation is 4.036 cm\(^{-1}\). The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods\(^2\) and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement\(^3\) on F\(^2\) was based on 8561 observed reflections and 456 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

\[
R1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} = 0.0313
\]

\[
wR2 = \left[ \frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum w(F_o^2)^2} \right]^{1/2} = 0.0946
\]

The goodness of fit\(^4\) was 1.00. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.71 and -0.68 e\(^-\)/Å\(^3\), respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4\(^5\). Anomalous dispersion effects were included in Fcalc\(^6\); the values for Δf and Δf\(^*\) were those of Creagh and McAuley\(^7\). The values for the mass attenuation coefficients are those of Creagh and
Hubbell\textsuperscript{8}. All calculations were performed using the CrystalStructure\textsuperscript{9} crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7\textsuperscript{10}.

References

(1) **CrystalClear**: Data Collection and Processing Software, Rigaku Corporation (1998-2015). Tokyo 196-8666, Japan.

(2) **SHELXT**: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

\[ \sum w(F_o^2-F_c^2)^2 \quad \text{where } w = \text{Least Squares weights}. \]

(4) Goodness of fit is defined as:

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

where: \( N_o \) = number of observations

\( N_v \) = number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2.5**: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.

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(10) *SHELXL Version 2014/7*: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula \[ \text{C}_{32}\text{H}_{48}\text{F}_{12}\text{N}_{3}\text{NbO}_{2} \]

Formula Weight \[ 827.64 \]

Crystal Color, Habit yellow, prism

Crystal Dimensions \[ 0.380 \times 0.250 \times 0.130 \text{ mm} \]

Crystal System monoclinic

Lattice Type Primitive

Lattice Parameters \[ a = 17.905(3) \text{ Å} \]
\[ b = 12.0354(15) \text{ Å} \]
\[ c = 19.691(3) \text{ Å} \]
\[ \beta = 115.352(2) \degree \]
\[ V = 3834.6(10) \text{ Å}^3 \]

Space Group \[ \text{P2}_1/n \ (#14) \]

Z value \[ 4 \]

\( \text{D}_{\text{calc}} \) \[ 1.433 \text{ g/cm}^3 \]

\( F_{000} \) \[ 1704.00 \]

\( \beta(\text{MoK\alpha}) \) \[ 4.036 \text{ cm}^{-1} \]
B. Intensity Measurements

| Parameter                              | Specification                          |
|----------------------------------------|----------------------------------------|
| Diffractometer                         | XtaLAB P200                            |
| Radiation                              | MoKα ($\lambda = 0.71075$ Å)           |
|                                        | multi-layer mirror monochromated       |
| Voltage, Current                       | 50kV, 24mA                             |
| Temperature                            | -180.0°C                               |
| Detector Aperture                      | 83.8 x 70.0 mm                         |
| Data Images                            | 720 exposures                          |
| $\omega$ oscillation Range ($\chi=45.0, \phi=0.0$) | -105.0 - 75.0°                         |
| Exposure Rate                          | 12.0 sec./°                            |
| Detector Swing Angle                   | -14.95°                                |
| $\omega$ oscillation Range ($\chi=45.0, \phi=90.0$) | -105.0 - 75.0°                         |
| Exposure Rate                          | 12.0 sec./°                            |
| Detector Swing Angle                   | -14.95°                                |
| Detector Position                      | 45.02 mm                               |
| Pixel Size                             | 0.172 mm                               |
| $2\theta_{\text{max}}$                | 55.0°                                  |
| No. of Reflections Measured            | Total: 32113                            |
Unique: 8561 ($R_{\text{int}} = 0.0590$)

Corrections

Lorentz-polarization
C. Structure Solution and Refinement

| Structure Solution        | Direct Methods (SHELXT) |
|---------------------------|-------------------------|
| Refinement                | Full-matrix least-squares on $F^2$ |
| Function Minimized        | $\Sigma w (F_o^2 - F_c^2)^2$ |
| Least Squares Weights     | $w = 1/ [ \sigma^2(F_o^2) + (0.0589 \cdot P)^2 + 0.0000 \cdot P ]$ |
|                           | where $P = (\text{Max}(F_o^2,0) + 2F_c^2)/3$ |
| $2\theta_{\text{max}}$ cutoff | 55.0$^\circ$ |
| Anomalous Dispersion      | All non-hydrogen atoms |
| No. Observations (All reflections) | 8561 |
| No. Variables             | 456 |
| Reflection/Parameter Ratio| 18.77 |
| Residuals: $R_1$ ($I>2.00\theta(I)$) | 0.0313 |
| Residuals: $R$ (All reflections) | 0.0374 |
| Residuals: $wR^2$ (All reflections) | 0.0946 |
| Goodness of Fit Indicator | 1.000 |
| Max Shift/Error in Final Cycle | 0.002 |
| Maximum peak in Final Diff. Map | 0.71 e$^-$/Å$^3$ |
| Minimum peak in Final Diff. Map | -0.68 e$^-$/Å$^3$ |
Table S9-1. Atomic coordinates and $B_{iso}/B_{eq}$

| atom | x      | y      | z      | $B_{eq}$ |
|------|--------|--------|--------|----------|
| Nb1  | 0.46346(2) | 0.30661(2) | 0.72732(2) | 1.040(5) |
| F1   | 0.21491(9)  | 0.26490(12) | 0.64477(9)  | 3.42(3)  |
| F2   | 0.20702(9)  | 0.31068(12) | 0.53642(8)  | 2.99(3)  |
| F3   | 0.14415(8)  | 0.40870(13) | 0.58786(8)  | 3.40(3)  |
| F4   | 0.36000(8)  | 0.58427(10) | 0.63440(8)  | 2.74(2)  |
| F5   | 0.23196(10) | 0.60177(12) | 0.61092(10) | 3.92(3)  |
| F6   | 0.26666(10) | 0.52272(12) | 0.53009(8)  | 3.57(3)  |
| F7   | 0.68165(9)  | 0.31080(13) | 0.88927(9)  | 3.20(3)  |
| F8   | 0.73583(8)  | 0.39373(13) | 0.82444(8)  | 3.18(3)  |
| F9   | 0.73816(8)  | 0.47056(11) | 0.92421(7)  | 2.59(2)  |
| F10  | 0.66142(8)  | 0.59020(11) | 0.75649(7)  | 2.57(2)  |
| F11  | 0.64431(9)  | 0.64952(10) | 0.85265(7)  | 2.67(2)  |
| F12  | 0.53872(7)  | 0.61833(10) | 0.74748(7)  | 2.22(2)  |
| O1   | 0.35872(8)  | 0.36271(11) | 0.64508(7)  | 1.44(2)  |
| O2   | 0.56532(8)  | 0.39661(11) | 0.75433(7)  | 1.43(2)  |
| N1   | 0.44270(10) | 0.34188(13) | 0.80591(9)  | 1.33(3)  |
| N2   | 0.47293(10) | 0.14660(13) | 0.73995(9)  | 1.40(3)  |
| N3   | 0.47344(11) | 0.28140(13) | 0.60851(9)  | 1.41(3)  |
| C1   | 0.42589(11) | 0.37356(16) | 0.86653(10) | 1.33(3)  |
| C2   | 0.40708(12) | 0.48485(16) | 0.87551(11) | 1.60(3)  |
| C3   | 0.38848(13) | 0.51130(18) | 0.93578(11) | 1.98(3)  |
| C4   | 0.38816(14) | 0.4309(2)   | 0.98542(11) | 2.31(4)  |
| C5   | 0.40820(14) | 0.32212(19) | 0.97749(11) | 2.10(4)  |
| C6   | 0.42849(13) | 0.29128(16) | 0.91894(11) | 1.64(3)  |
| C7   | 0.45413(16) | 0.17439(17) | 0.91214(12) | 2.27(4)  |
| C8   | 0.40686(14) | 0.57580(17) | 0.82255(12) | 2.00(3)  |
| C9   | 0.47232(12) | 0.04143(16) | 0.74184(10) | 1.41(3)  |
| C10  | 0.38853(13) | -0.01688(16) | 0.69073(11) | 1.81(3)  |
| C11  | 0.55101(13) | -0.02177(16) | 0.79676(11) | 1.72(3)  |
| C12  | 0.35908(15) | 0.0422(2)   | 0.61397(12) | 2.56(4)  |
| C13  | 0.33021(14) | -0.0019(2)  | 0.72896(13) | 2.71(4)  |
| C14  | 0.39232(17) | -0.14156(19) | 0.67343(15) | 3.03(5)  |
| C15  | 0.61927(13) | 0.06140(18) | 0.84213(12) | 2.07(4)  |
| C16  | 0.58554(14) | -0.09707(17) | 0.75334(13) | 2.23(4)  |
| C17  | 0.53280(15) | -0.09112(18) | 0.85365(12) | 2.42(4)  |
| C18  | 0.50913(12) | 0.26997(15) | 0.56397(10) | 1.44(3)  |
| C19  | 0.45542(13) | 0.27702(19) | 0.47784(11) | 1.96(3)  |
Table S9-1. Atomic coordinates and $B_{iso}/B_{eq}$ (continued)

| atom | x           | y           | z           | $B_{eq}$ |
|------|-------------|-------------|-------------|----------|
| C20  | 0.60268(13) | 0.25112(17) | 0.59948(11) | 1.75(3)  |
| C21  | 0.36899(15) | 0.3241(2)   | 0.45972(12) | 2.68(4)  |
| C22  | 0.49367(15) | 0.3527(2)   | 0.43796(13) | 2.78(4)  |
| C23  | 0.44277(17) | 0.1576(2)   | 0.44502(14) | 3.16(5)  |
| C24  | 0.63527(16) | 0.1777(2)   | 0.55391(14) | 2.79(4)  |
| C25  | 0.64511(14) | 0.36625(19) | 0.61271(13) | 2.31(4)  |
| C26  | 0.62978(14) | 0.19462(18) | 0.67639(13) | 2.28(4)  |
| C27  | 0.29162(12) | 0.42127(16) | 0.64259(10) | 1.48(3)  |
| C28  | 0.21358(14) | 0.35202(19) | 0.60186(12) | 2.15(4)  |
| C29  | 0.28646(14) | 0.53331(18) | 0.60349(12) | 2.21(4)  |
| C30  | 0.60738(12) | 0.46126(15) | 0.81736(10) | 1.43(3)  |
| C31  | 0.69205(13) | 0.40903(17) | 0.86382(11) | 1.99(3)  |
| C32  | 0.61356(12) | 0.58039(17) | 0.79336(11) | 1.73(3)  |

$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$
Table S9-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogen atoms

| atom  | x       | y       | z       | $B_{\text{iso}}$ |
|-------|---------|---------|---------|------------------|
| H3    | 0.37586 | 0.58598 | 0.94256 | 2.370            |
| H4    | 0.37412 | 0.45015 | 1.02529 | 2.768            |
| H5    | 0.40818 | 0.26754 | 1.01233 | 2.520            |
| H7A   | 0.46582 | 0.16874 | 0.86798 | 2.722            |
| H7B   | 0.50388 | 0.15517 | 0.95735 | 2.722            |
| H7C   | 0.40941 | 0.12307 | 0.90665 | 2.722            |
| H8A   | 0.42097 | 0.54424 | 0.78365 | 2.397            |
| H8B   | 0.35183 | 0.60961 | 0.79893 | 2.397            |
| H8C   | 0.44764 | 0.63255 | 0.85070 | 2.397            |
| H12A  | 0.38779 | 0.03306 | 0.58918 | 3.077            |
| H12B  | 0.29694 | 0.00958 | 0.58253 | 3.077            |
| H12C  | 0.34432 | 0.12144 | 0.62136 | 3.077            |
| H13A  | 0.35364 | -0.03930| 0.77789 | 3.248            |
| H13B  | 0.32359 | 0.07742 | 0.73609 | 3.248            |
| H13C  | 0.27621 | -0.03443| 0.69726 | 3.248            |
| H14A  | 0.42941 | -0.15183| 0.64903 | 3.632            |
| H14B  | 0.41311 | -0.18406| 0.72039 | 3.632            |
| H14C  | 0.33684 | -0.16778| 0.63991 | 3.632            |
| H15A  | 0.59940 | 0.11069 | 0.87049 | 2.479            |
| H15B  | 0.66813 | 0.02094 | 0.87708 | 2.479            |
| H15C  | 0.63384 | 0.10564 | 0.80777 | 2.479            |
| H16A  | 0.54341 | -0.15139| 0.72365 | 2.673            |
| H16B  | 0.60040 | -0.05144| 0.71976 | 2.673            |
| H16C  | 0.63469 | -0.13614| 0.78906 | 2.673            |
| H17A  | 0.48859 | -0.14528| 0.82650 | 2.910            |
| H17B  | 0.58218 | -0.13031| 0.88759 | 2.910            |
| H17C  | 0.51347 | -0.04173| 0.88289 | 2.910            |
| H21A  | 0.33795 | 0.33230 | 0.40520 | 3.210            |
| H21B  | 0.37451 | 0.39675 | 0.48386 | 3.210            |
| H21C  | 0.33950 | 0.27315 | 0.47858 | 3.210            |
| H22A  | 0.54906 | 0.32574 | 0.44800 | 3.332            |
| H22B  | 0.45879 | 0.35173 | 0.38370 | 3.332            |
| H22C  | 0.49748 | 0.42885 | 0.45684 | 3.332            |
| H23A  | 0.49663 | 0.12461 | 0.45542 | 3.788            |
| H23B  | 0.41463 | 0.11227 | 0.46832 | 3.788            |
| H23C  | 0.40908 | 0.16061 | 0.39058 | 3.788            |
| H24A  | 0.69543 | 0.17059 | 0.58110 | 3.350            |
Table S9-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogens/$B_{\text{eq}}$ (continued)

| atom | x      | y      | z      | $B_{\text{eq}}$ |
|------|--------|--------|--------|-----------------|
| H24B | 0.60987| 0.10390| 0.54689| 3.350           |
| H24C | 0.62122| 0.21182| 0.50476| 3.350           |
| H25A | 0.70523| 0.35647| 0.63547| 2.775           |
| H25B | 0.62760| 0.40507| 0.56457| 2.775           |
| H25C | 0.62935| 0.41011| 0.64646| 2.775           |
| H26A | 0.68968| 0.18271| 0.69892| 2.731           |
| H26B | 0.61536| 0.24218| 0.70939| 2.731           |
| H26C | 0.60157| 0.12294| 0.66990| 2.731           |
| H27  | 0.29906| 0.43537| 0.69516| 1.774           |
| H30  | 0.57539| 0.46188| 0.84836| 1.721           |
| H48  | 0.4211(14)| 0.2929(17)| 0.5829(12)| 0.9(4)          |
Table S9-3. Anisotropic displacement parameters

| atom | U11    | U22    | U33    | U12    | U13    | U23    |
|------|--------|--------|--------|--------|--------|--------|
| Nb1  | 0.01444(11) | 0.01243(9) | 0.01284(9) | 0.00077(6) | 0.00601(7) | 0.00059(6) |
| F1   | 0.0457(9)  | 0.0380(8)  | 0.0526(9)  | -0.0169(7) | 0.0270(7)  | -0.0039(7) |
| F2   | 0.0302(8)  | 0.0487(9)  | 0.0315(7)  | -0.0058(6) | 0.0102(6)  | -0.0191(6) |
| F3   | 0.0170(7)  | 0.0582(10) | 0.0503(9)  | 0.0033(7)  | 0.0108(6)  | -0.0163(7) |
| F4   | 0.0364(8)  | 0.0262(7)  | 0.0419(8)  | -0.0064(6) | 0.0172(6)  | 0.0015(6)  |
| F5   | 0.0482(9)  | 0.0310(7)  | 0.0771(12) | 0.0214(7)  | 0.0339(9)  | 0.0110(7)  |
| F6   | 0.0600(10) | 0.0437(8)  | 0.0235(7)  | 0.0068(7)  | 0.0100(7)  | 0.0130(6)  |
| F7   | 0.0354(8)  | 0.0231(7)  | 0.0452(9)  | -0.0014(6) | 0.0003(7)  | 0.0101(6)  |
| F8   | 0.0240(7)  | 0.0581(9)  | 0.0358(8)  | 0.0123(7)  | 0.0099(6)  | -0.0040(7) |
| F9   | 0.0273(7)  | 0.0335(7)  | 0.0240(6)  | -0.0037(6) | -0.0019(5) | -0.0035(5) |
| F10  | 0.0294(7)  | 0.0351(7)  | 0.0377(7)  | -0.0071(6) | 0.0186(6)  | 0.0056(6)  |
| F11  | 0.0436(8)  | 0.0199(6)  | 0.0278(7)  | -0.0046(6) | 0.0056(6)  | -0.0049(5) |
| F12  | 0.0253(7)  | 0.0251(6)  | 0.0296(6)  | 0.0022(5)  | 0.0077(5)  | 0.0071(5)  |
| O1   | 0.0162(7)  | 0.0214(7)  | 0.0171(6)  | 0.0043(6)  | 0.0070(5)  | 0.0016(5)  |
| O2   | 0.0177(7)  | 0.0202(7)  | 0.0159(6)  | -0.0034(5) | 0.0066(5)  | -0.0025(5) |
| N1   | 0.0188(9)  | 0.0160(7)  | 0.0150(7)  | 0.0015(6)  | 0.0066(6)  | 0.0008(6)  |
| N2   | 0.0208(9)  | 0.0164(8)  | 0.0170(8)  | 0.0007(6)  | 0.0090(7)  | 0.0011(6)  |
| N3   | 0.0156(9)  | 0.0204(8)  | 0.0179(8)  | -0.0008(7) | 0.0076(7)  | -0.0013(6) |
| C1   | 0.0147(9)  | 0.0220(9)  | 0.0143(8)  | -0.0024(7) | 0.0066(7)  | -0.0017(7) |
| C2   | 0.0171(10) | 0.0243(10) | 0.0186(9)  | 0.0011(8)  | 0.0066(8)  | -0.0024(7) |
| C3   | 0.0243(11) | 0.0288(11) | 0.0213(10) | 0.0027(9)  | 0.0091(8)  | -0.0054(8) |
| C4   | 0.0285(12) | 0.0442(13) | 0.0178(9)  | 0.0014(10) | 0.0126(9)  | -0.0062(9) |
| C5   | 0.0299(12) | 0.0345(12) | 0.0176(9)  | -0.0028(9) | 0.0123(9)  | 0.0017(8)  |
| C6   | 0.0207(11) | 0.0244(10) | 0.0165(9)  | -0.0017(8) | 0.0071(8)  | -0.0000(7) |
| C7   | 0.0426(14) | 0.0225(10) | 0.0227(10) | -0.0013(9) | 0.0155(10) | 0.0041(8)  |
| C8   | 0.0313(12) | 0.0203(9)  | 0.0262(10) | 0.0019(9)  | 0.0142(9)  | -0.0017(8) |
| C9   | 0.0228(11) | 0.0168(9)  | 0.0169(9)  | 0.0015(8)  | 0.0112(8)  | -0.0001(7) |
| C10  | 0.0251(11) | 0.0198(9)  | 0.0228(10) | -0.0042(8) | 0.0092(8)  | -0.0008(8) |
| C11  | 0.0248(11) | 0.0171(9)  | 0.0239(10) | 0.0032(8)  | 0.0110(8)  | 0.0041(8)  |
| C12  | 0.0326(13) | 0.0393(13) | 0.0209(10) | -0.0102(10)| 0.0070(9)  | -0.0017(9) |
| C13  | 0.0279(12) | 0.0464(14) | 0.0292(11) | -0.0088(11)| 0.0128(10)| -0.0049(10)|
| C14  | 0.0418(15) | 0.0265(12) | 0.0400(13) | -0.0060(11)| 0.0111(11)| -0.0062(10)|
| C15  | 0.0250(12) | 0.0256(10) | 0.0235(10) | 0.0040(9)  | 0.0062(9)  | 0.0043(8)  |
| C16  | 0.0312(12) | 0.0192(10) | 0.0349(12) | 0.0062(9)  | 0.0148(10)| 0.0024(8)  |
| C17  | 0.0395(13) | 0.0249(10) | 0.0281(11) | 0.0043(10)| 0.0148(10)| 0.0109(9)  |
| C18  | 0.0227(11) | 0.0144(8)  | 0.0188(9)  | -0.0006(8) | 0.0101(8)  | -0.0015(7) |
| C19  | 0.0231(11) | 0.0353(11) | 0.0166(9)  | -0.0013(9) | 0.0090(8)  | -0.0032(8) |
Table S9-3. Anisotropic displacement parameters (continued)

| atom | U_{11}   | U_{22}   | U_{33}   | U_{12}   | U_{13}   | U_{23}   |
|------|----------|----------|----------|----------|----------|----------|
| C20  | 0.0214(11)| 0.0240(10)| 0.0239(10)| 0.0033(8)| 0.0125(8)| 0.0004(8)|
| C21  | 0.0255(12)| 0.0567(15)| 0.0172(10)| 0.0035(11)| 0.0070(9)| 0.0023(10)|
| C22  | 0.0333(13)| 0.0526(15)| 0.0219(11)| 0.0029(11)| 0.0141(10)| 0.0081(10)|
| C23  | 0.0395(15)| 0.0505(15)| 0.0319(12)| -0.0104(12)| 0.0171(11)| -0.0218(11)|
| C24  | 0.0338(14)| 0.0427(14)| 0.0345(13)| 0.0111(11)| 0.0192(11)| -0.0034(10)|
| C25  | 0.0207(11)| 0.0323(12)| 0.0323(12)| -0.0035(9)| 0.0089(9)| 0.0014(9)|
| C26  | 0.0266(12)| 0.0323(11)| 0.0281(11)| 0.0121(9)| 0.0121(9)| 0.0077(9)|
| C27  | 0.0170(10)| 0.0211(9)| 0.0181(9)| 0.0035(8)| 0.0075(8)| -0.0009(7)|
| C28  | 0.0223(12)| 0.0309(11)| 0.0298(11)| -0.0016(9)| 0.0124(9)| -0.0068(9)|
| C29  | 0.0302(12)| 0.0238(10)| 0.0302(11)| 0.0070(9)| 0.0131(9)| 0.0026(9)|
| C30  | 0.0185(10)| 0.0185(9)| 0.0156(8)| -0.0026(8)| 0.0055(7)| -0.0018(7)|
| C31  | 0.0239(11)| 0.0247(10)| 0.0224(10)| -0.0025(9)| 0.0055(8)| -0.0015(8)|
| C32  | 0.0202(10)| 0.0221(10)| 0.0209(9)| -0.0035(8)| 0.0064(8)| -0.0000(8)|

The general temperature factor expression: exp(-2π²(a²U_{11}h² + b²U_{22}k² + c²U_{33}l² + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))
Table S9-4. Bond lengths (Å)

| atom | atom | distance  | atom | atom | distance |
|------|------|-----------|------|------|----------|
| Nb1  | O1   | 1.9986(12)| Nb1  | O2   | 1.9879(14) |
| Nb1  | N1   | 1.790(2)  | Nb1  | N2   | 1.9399(16) |
| Nb1  | N3   | 2.440(2)  | F1   | C28  | 1.340(3)  |
| F2   | C28  | 1.339(3)  | F3   | C28  | 1.339(3)  |
| F4   | C29  | 1.339(3)  | F5   | C29  | 1.332(3)  |
| F6   | C29  | 1.339(3)  | F7   | C31  | 1.336(3)  |
| F8   | C31  | 1.330(3)  | F9   | C31  | 1.343(2)  |
| F10  | C32  | 1.345(3)  | F11  | C32  | 1.345(2)  |
| F12  | C32  | 1.336(2)  | O1   | C27  | 1.376(3)  |
| C10  | C30  | 1.383(2)  | N1   | C1   | 1.403(3)  |
| N2   | C9   | 1.266(2)  | N3   | C18  | 1.295(3)  |
| C1   | C2   | 1.411(3)  | C1   | C6   | 1.417(3)  |
| C2   | C3   | 1.400(4)  | C2   | C8   | 1.511(3)  |
| C3   | C4   | 1.378(3)  | C4   | C5   | 1.383(3)  |
| C5   | C6   | 1.399(4)  | C6   | C7   | 1.503(3)  |
| C9   | C10  | 1.569(3)  | C9   | C11  | 1.558(3)  |
| C10  | C12  | 1.540(3)  | C10  | C13  | 1.537(4)  |
| C10  | C14  | 1.547(3)  | C11  | C15  | 1.536(3)  |
| C11  | C16  | 1.545(4)  | C11  | C17  | 1.546(4)  |
| C18  | C19  | 1.553(2)  | C18  | C20  | 1.531(3)  |
| C19  | C21  | 1.540(4)  | C19  | C22  | 1.542(4)  |
| C19  | C23  | 1.552(4)  | C20  | C24  | 1.541(4)  |
| C20  | C25  | 1.548(3)  | C20  | C26  | 1.537(3)  |
| C27  | C28  | 1.527(3)  | C27  | C29  | 1.536(3)  |
| C30  | C31  | 1.531(3)  | C30  | C32  | 1.528(3)  |
Table S9-5. Bond lengths involving hydrogens (Å)

| atom | atom | distance  | atom | atom | distance |
|------|------|-----------|------|------|----------|
| N3   | H48  | 0.86(2)   | C3   | H3   | 0.950    |
| C4   | H4   | 0.950     | C5   | H5   | 0.950    |
| C7   | H7A  | 0.980     | C7   | H7B  | 0.980    |
| C7   | H7C  | 0.980     | C8   | H8A  | 0.980    |
| C8   | H8B  | 0.980     | C8   | H8C  | 0.980    |
| C12  | H12A | 0.980     | C12  | H12B | 0.980    |
| C12  | H12C | 0.980     | C13  | H13A | 0.980    |
| C13  | H13B | 0.980     | C13  | H13C | 0.980    |
| C14  | H14A | 0.980     | C14  | H14B | 0.980    |
| C14  | H14C | 0.980     | C15  | H15A | 0.980    |
| C15  | H15B | 0.980     | C15  | H15C | 0.980    |
| C16  | H16A | 0.980     | C16  | H16B | 0.980    |
| C16  | H16C | 0.980     | C17  | H17A | 0.980    |
| C17  | H17B | 0.980     | C17  | H17C | 0.980    |
| C21  | H21A | 0.980     | C21  | H21B | 0.980    |
| C21  | H21C | 0.980     | C22  | H22A | 0.980    |
| C22  | H22B | 0.980     | C22  | H22C | 0.980    |
| C23  | H23A | 0.980     | C23  | H23B | 0.980    |
| C23  | H23C | 0.980     | C24  | H24A | 0.980    |
| C24  | H24B | 0.980     | C24  | H24C | 0.980    |
| C25  | H25A | 0.980     | C25  | H25B | 0.980    |
| C25  | H25C | 0.980     | C26  | H26A | 0.980    |
| C26  | H26B | 0.980     | C26  | H26C | 0.980    |
| C27  | H27  | 1.000     | C30  | H30  | 1.000    |
| atom | atom | atom | angle  | atom | atom | atom | angle |
|------|------|------|--------|------|------|------|-------|
| O1   | Nb1  | O2   | 117.89(6) | O1   | Nb1  | N1   | 98.64(7) |
| O1   | Nb1  | N2   | 116.07(6) | O1   | Nb1  | N3   | 72.16(6) |
| O2   | Nb1  | N1   | 98.38(7)  | O2   | Nb1  | N2   | 119.13(6) |
| O2   | Nb1  | N3   | 83.62(6)  | N1   | Nb1  | N2   | 99.42(8)  |
| N1   | Nb1  | N3   | 170.26(6) | N2   | Nb1  | N3   | 87.78(7)  |
| Nb1  | O1   | C27  | 134.76(12)| Nb1  | O2   | C30  | 129.15(15) |
| Nb1  | N1   | C1   | 177.89(14)| Nb1  | N2   | C9   | 174.01(12) |
| Nb1  | N3   | C18  | 157.30(12)| N1   | C1   | C2   | 120.96(19) |
| N1   | C1   | C6   | 118.54(18)| C2   | C1   | C6   | 120.5(2)  |
| C1   | C2   | C3   | 118.6(2)  | C1   | C2   | C8   | 122.1(2)  |
| C3   | C2   | C8   | 119.29(19)| C2   | C3   | C4   | 121.1(2)  |
| C3   | C4   | C5   | 120.3(2)  | C4   | C5   | C6   | 121.0(2)  |
| C1   | C6   | C5   | 118.41(19)| C1   | C6   | C7   | 120.3(2)  |
| C5   | C6   | C7   | 121.2(2)  | N2   | C9   | C10  | 116.48(15) |
| N2   | C9   | C11  | 119.45(15)| C10  | C9   | C11  | 123.97(16) |
| C9   | C10  | C12  | 108.59(18)| C9   | C10  | C13  | 107.28(17) |
| C9   | C10  | C14  | 117.07(18)| C12  | C10  | C13  | 108.91(18) |
| C12  | C10  | C14  | 105.87(18)| C13  | C10  | C14  | 108.9(2)  |
| C9   | C11  | C15  | 110.08(16)| C9   | C11  | C16  | 111.06(16) |
| C9   | C11  | C17  | 110.7(2)  | C15  | C11  | C16  | 107.3(2)  |
| C15  | C11  | C17  | 107.28(17)| C16  | C11  | C17  | 110.37(17) |
| N3   | C18  | C19  | 118.65(18)| N3   | C18  | C20  | 117.86(16) |
| C19  | C18  | C20  | 123.5(2)  | C18  | C19  | C21  | 111.4(2)  |
| C18  | C19  | C22  | 112.72(17)| C18  | C19  | C23  | 108.42(17) |
| C21  | C19  | C22  | 106.63(19)| C21  | C19  | C23  | 106.93(19) |
| C22  | C19  | C23  | 110.6(2)  | C18  | C20  | C24  | 115.60(16) |
| C18  | C20  | C25  | 107.85(16)| C18  | C20  | C26  | 109.7(2)  |
| C24  | C20  | C25  | 109.3(2)  | C24  | C20  | C26  | 106.34(18) |
| C25  | C20  | C26  | 107.77(16)| O1   | C27  | C29  | 111.77(15) |
| O1   | C27  | C29  | 109.4(2)  | C28  | C27  | C29  | 111.77(15) |
| F1   | C28  | F2   | 106.65(18)| F1   | C28  | F3   | 107.0(2)  |
| F1   | C28  | C27  | 109.31(15)| F2   | C28  | F3   | 107.46(15) |
| F2   | C28  | C27  | 113.1(2)  | F3   | C28  | C27  | 112.97(18) |
| F4   | C29  | F5   | 106.90(17)| F4   | C29  | F6   | 106.8(2)  |
| F4   | C29  | C27  | 109.74(15)| F5   | C29  | F6   | 108.04(17) |
| F5   | C29  | C27  | 112.2(2)  | F6   | C29  | C27  | 112.89(17) |
| O2   | C30  | C31  | 108.95(16)| O2   | C30  | C32  | 109.51(15) |
Table S9-6. Bond angles (°) (continued)

| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| C31  | C30  | C32  | 112.69(17) | F7   | C31  | F8   | 107.87(19) |
| F7   | C31  | F9   | 106.92(16)  | F7   | C31  | C30  | 109.20(18)  |
| F8   | C31  | F9   | 107.47(18)  | F8   | C31  | C30  | 112.86(17)  |
| F9   | C31  | C30  | 112.26(17)  | F10  | C32  | F11  | 107.20(17)  |
| F10  | C32  | F12  | 106.95(17)  | F10  | C32  | C30  | 113.36(18)  |
| F11  | C32  | F12  | 107.16(17)  | F11  | C32  | C30  | 111.65(17)  |
| F12  | C32  | C30  | 110.21(16)  |
| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| Nb1  | N3   | H48  | 91.8(18)| C18  | N3   | H48  | 110.5(18) |
| C2   | C3   | H3   | 119.4   | C4   | C3   | H3   | 119.5   |
| C3   | C4   | H4   | 119.8   | C5   | C4   | H4   | 119.8   |
| C4   | C5   | H5   | 119.5   | C6   | C5   | H5   | 119.5   |
| C6   | C7   | H7A  | 109.5   | C6   | C7   | H7B  | 109.5   |
| C6   | C7   | H7C  | 109.5   | H7A  | C7   | H7B  | 109.5   |
| H7A  | C7   | H7C  | 109.5   | H7B  | C7   | H7C  | 109.5   |
| C2   | C8   | H8A  | 109.5   | C2   | C8   | H8B  | 109.5   |
| C2   | C8   | H8C  | 109.5   | H8A  | C8   | H8B  | 109.5   |
| H8A  | C8   | H8C  | 109.5   | H8B  | C8   | H8C  | 109.5   |
| C10  | C12  | H12A | 109.5   | C10  | C12  | H12B | 109.5   |
| C10  | C12  | H12C | 109.5   | H12A | C12  | H12B | 109.5   |
| H12A | C12  | H12C | 109.5   | H12B | C12  | H12C | 109.5   |
| C10  | C13  | H13A | 109.5   | C10  | C13  | H13B | 109.5   |
| C10  | C13  | H13C | 109.5   | H13A | C13  | H13B | 109.5   |
| H13A | C13  | H13C | 109.5   | H13B | C13  | H13C | 109.5   |
| C10  | C14  | H14A | 109.5   | C10  | C14  | H14B | 109.5   |
| C10  | C14  | H14C | 109.5   | H14A | C14  | H14B | 109.5   |
| H14A | C14  | H14C | 109.5   | H14B | C14  | H14C | 109.5   |
| C11  | C15  | H15A | 109.5   | C11  | C15  | H15B | 109.5   |
| C11  | C15  | H15C | 109.5   | H15A | C15  | H15B | 109.5   |
| H15A | C15  | H15C | 109.5   | H15B | C15  | H15C | 109.5   |
| C11  | C16  | H16A | 109.5   | C11  | C16  | H16B | 109.5   |
| C11  | C16  | H16C | 109.5   | H16A | C16  | H16B | 109.5   |
| H16A | C16  | H16C | 109.5   | H16B | C16  | H16C | 109.5   |
| C11  | C17  | H17A | 109.5   | C11  | C17  | H17B | 109.5   |
| C11  | C17  | H17C | 109.5   | H17A | C17  | H17B | 109.5   |
| H17A | C17  | H17C | 109.5   | H17B | C17  | H17C | 109.5   |
| C19  | C21  | H21A | 109.5   | C19  | C21  | H21B | 109.5   |
| C19  | C21  | H21C | 109.5   | H21A | C21  | H21B | 109.5   |
| H21A | C21  | H21C | 109.5   | H21B | C21  | H21C | 109.5   |
| C19  | C22  | H22A | 109.5   | C19  | C22  | H22B | 109.5   |
| C19  | C22  | H22C | 109.5   | H22A | C22  | H22B | 109.5   |
| H22A | C22  | H22C | 109.5   | H22B | C22  | H22C | 109.5   |
| C19  | C23  | H23A | 109.5   | C19  | C23  | H23B | 109.5   |
| C19  | C23  | H23C | 109.5   | H23A | C23  | H23B | 109.5   |
| H23A | C23  | H23C | 109.5   | H23B | C23  | H23C | 109.5   |
Table S9-7. Bond angles involving hydrogens (°) (continued)

| atom  | atom   | atom | angle | atom  | atom   | atom | angle |
|-------|--------|------|-------|-------|--------|------|-------|
| C20   | C24    | H24A | 109.5 | C20   | C24    | H24B | 109.5 |
| C20   | C24    | H24C | 109.5 | H24A  | C24    | H24B | 109.5 |
| H24A  | C24    | H24C | 109.5 | H24B  | C24    | H24C | 109.5 |
| C20   | C25    | H25A | 109.5 | C20   | C25    | H25B | 109.5 |
| C20   | C25    | H25C | 109.5 | H25A  | C25    | H25B | 109.5 |
| H25A  | C25    | H25C | 109.5 | H25B  | C25    | H25C | 109.5 |
| C20   | C26    | H26A | 109.5 | C20   | C26    | H26B | 109.5 |
| C20   | C26    | H26C | 109.5 | H26A  | C26    | H26B | 109.5 |
| H26A  | C26    | H26C | 109.5 | H26B  | C26    | H26C | 109.5 |
| O1    | C27    | H27  | 108.8 | C28   | C27    | H27  | 108.8 |
| C29   | C27    | H27  | 108.8 | O2    | C30    | H30  | 108.5 |
| C31   | C30    | H30  | 108.5 | C32   | C30    | H30  | 108.5 |
Table S9-8. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle     | atom1 | atom2 | atom3 | atom4 | angle     |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|-----------|
| O1    | Nb1   | O2    | C30   | 107.25(10)| O2    | Nb1   | O1    | C27   | -98.08(14)|
| N1    | Nb1   | O1    | C27   | 6.23(14)  | N2    | Nb1   | O1    | C27   | 111.22(13)|
| O1    | Nb1   | N3    | C18   | 155.3(3)  | N3    | Nb1   | O1    | C27   | -170.48(14)|
| N1    | Nb1   | O2    | C30   | 2.78(11)  | N2    | Nb1   | O2    | C30   | -102.97(12)|
| O2    | Nb1   | N3    | C18   | 33.2(3)   | N3    | Nb1   | O2    | C30   | 173.17(11)|
| N2    | Nb1   | N3    | C18   | -86.4(3)  | Nb1   | O1    | C27   | C28   | -120.51(13)|
| Nb1   | O1    | C27   | C29   | 116.92(15)| Nb1   | O2    | C30   | C31   | 113.42(15)|
| Nb1   | O2    | C30   | C32   | -122.91(14)| Nb1   | N3    | C18   | C19   | -169.1(2)|
| Nb1   | N3    | C18   | C20   | 10.4(4)   | N1    | C1    | C2    | C3    | 178.19(14)|
| N1    | C1    | C2    | C8    | -2.1(2)   | N1    | C1    | C6    | C5    | -177.27(14)|
| N1    | C1    | C6    | C7    | 3.9(2)    | C2    | C1    | C6    | C5    | 3.0(3)    |
| C2    | C1    | C6    | C7    | -175.87(14)| C6    | C1    | C2    | C3    | -2.0(2)   |
| C6    | C1    | C2    | C8    | 177.64(15)| C8    | C2    | C3    | C4    | -0.2(3)   |
| C8    | C2    | C3    | C4    | -179.88(15)| C3    | C4    | C5    | 1.5(3)   |
| C3    | C4    | C5    | C6    | -0.5(3)   | C4    | C5    | C6    | C1    | -1.7(3)   |
| C4    | C5    | C6    | C7    | 177.13(17)| N2    | C9    | C10   | C12   | 42.4(3)   |
| N2    | C9    | C10   | C13   | -75.2(2)  | N2    | C9    | C10   | C14   | 162.11(19)|
| N2    | C9    | C11   | C15   | 0.6(3)    | N2    | C9    | C11   | C16   | -118.1(2)|
| N2    | C9    | C11   | C17   | 119.0(2)  | N2    | C9    | C11   | C15   | -175.67(19)|
| C10   | C9    | C11   | C16   | 65.7(3)   | C10   | C9    | C11   | C17   | -57.3(3)  |
| C11   | C9    | C10   | C12   | -141.3(2) | C11   | C9    | C10   | C13   | 101.2(2)  |
| C11   | C9    | C10   | C14   | -21.6(3)  | N3    | C18   | C19   | C21   | 13.3(2)   |
| N3    | C18   | C19   | C22   | 133.08(18)| N3    | C18   | C19   | C23   | -104.1(2)|
| N3    | C18   | C20   | C24   | 147.59(16)| N3    | C18   | C20   | C25   | -89.8(2)  |
| N3    | C18   | C20   | C26   | 27.4(2)   | C19   | C18   | C20   | C24   | -33.0(3)  |
| C19   | C18   | C20   | C25   | 89.7(2)   | C19   | C18   | C20   | C26   | -153.18(16)|
| C20   | C18   | C19   | C21   | -166.17(15)| C20   | C18   | C19   | C22   | -46.4(2)  |
| C20   | C18   | C19   | C23   | 76.5(2)   | O1    | C27   | C28   | F1    | 69.6(2)   |
| O1    | C27   | C28   | F2    | -49.1(2)  | O1    | C27   | C28   | F3    | -171.40(16)|
| O1    | C27   | C29   | F4    | -50.3(2)  | O1    | C27   | C29   | F5    | -168.96(13)|
| O1    | C27   | C29   | F6    | 68.7(2)   | C28   | C27   | C29   | F4    | -171.27(19)|
| C28   | C27   | C29   | F5    | 70.0(2)   | C28   | C27   | C29   | F6    | -52.3(3)  |
| C29   | C27   | C28   | F1    | -169.30(19)| C29   | C27   | C28   | F2    | 72.1(2)   |
| C29   | C27   | C28   | F3    | -50.3(3)  | O2    | C30   | C31   | F7    | -64.7(2)  |
| O2    | C30   | C31   | F8    | 55.3(2)   | O2    | C30   | C31   | F9    | 176.89(17)|
| O2    | C30   | C32   | F10   | -66.89(19)| O2    | C30   | C32   | F11   | 171.90(16)|
| O2    | C30   | C32   | F12   | 52.9(2)   | C31   | C30   | C32   | F10   | 54.5(2)   |
Table S9-8. Torsion angles (°) (continued)

| atom1 | atom2 | atom3 | atom4 | angle     | atom1 | atom2 | atom3 | atom4 | angle     |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|-----------|
| C31   | C30   | C32   | F11   | -66.7(2)  | C31   | C30   | C32   | F12   | 174.37(17) |
| C32   | C30   | C31   | F7    | 173.53(17)| C32   | C30   | C31   | F8    | -66.5(2)  |
| C32   | C30   | C31   | F9    | 55.1(3)   |       |       |       |       |           |
Table S9-9. Intramolecular contacts less than 3.60 Å

| atom | atom | distance  | atom | atom | distance |
|------|------|-----------|------|------|----------|
| F1   | O1   | 2.829(2)  | F2   | F6   | 2.790(2) |
| F2   | O1   | 2.7150(17)| F2   | C29  | 3.056(3) |
| F3   | F5   | 2.732(2)  | F3   | F6   | 3.182(3) |
| F3   | O1   | 3.554(2)  | F3   | C29  | 2.857(3) |
| F4   | F12  | 3.0437(16)| F4   | O1   | 2.6757(18)|
| F4   | C8   | 3.432(3)  | F5   | O1   | 3.546(2) |
| F5   | C28  | 3.021(3)  | F6   | O1   | 2.8907(18)|
| F6   | C28  | 2.876(3)  | F7   | O2   | 2.7828(18)|
| F7   | C15  | 3.190(2)  | F8   | F10  | 2.7623(19)|
| F8   | O2   | 2.7602(19)| F8   | C32  | 3.011(3) |
| F9   | F10  | 3.3140(18)| F9   | F11  | 2.7241(17)|
| F9   | O2   | 3.5629(16)| F9   | C32  | 2.905(2) |
| F10  | O2   | 2.886(2)  | F10  | C31  | 2.920(2) |
| F11  | O2   | 3.5593(18)| F11  | C31  | 2.999(2) |
| F12  | O2   | 2.7039(18)| F12  | C8   | 3.318(3) |
| O2   | C26  | 3.334(3)  | N1   | C7   | 2.849(3) |
| N1   | C8   | 2.937(3)  | N1   | C27  | 3.335(2) |
| N1   | C30  | 3.200(3)  | N2   | C7   | 3.564(3) |
| N2   | C12  | 2.804(2)  | N2   | C13  | 3.050(3) |
| N2   | C15  | 2.730(2)  | N2   | C16  | 3.504(3) |
| N2   | C17  | 3.506(3)  | N2   | C26  | 3.577(4) |
| N3   | C21  | 2.766(2)  | N3   | C23  | 3.372(3) |
| N3   | C25  | 3.206(3)  | N3   | C26  | 2.740(3) |
| C1   | C4   | 2.787(3)  | C2   | C5   | 2.799(3) |
| C3   | C6   | 2.800(3)  | C10  | C16  | 3.342(3) |
| C10  | C17  | 3.261(3)  | C11  | C13  | 3.598(3) |
| C11  | C14  | 3.184(3)  | C13  | C17  | 3.556(3) |
| C14  | C16  | 3.173(4)  | C14  | C17  | 3.409(3) |
| C19  | C24  | 3.148(3)  | C19  | C25  | 3.467(3) |
| C20  | C22  | 3.179(3)  | C20  | C23  | 3.355(3) |
| C22  | C24  | 3.335(3)  | C22  | C25  | 3.351(3) |
| C23  | C24  | 3.195(3)  |      |      |          |
Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H7A  | 3.213    | Nb1  | H8A  | 3.273    |
| Nb1  | H12C | 3.172    | Nb1  | H26B | 2.991    |
| Nb1  | H27  | 3.142    | Nb1  | H30  | 3.016    |
| F1   | H12C | 3.079    | F1   | H13B | 3.019    |
| F1   | H27  | 2.487    | F2   | H12C | 3.241    |
| F2   | H21C | 3.073    | F2   | H27  | 3.214    |
| F2   | H48  | 3.54(3)  | F3   | H27  | 2.691    |
| F4   | H8A  | 2.704    | F4   | H8B  | 3.319    |
| F4   | H27  | 2.637    | F5   | H8B  | 3.394    |
| F5   | H27  | 2.549    | F6   | H21B | 2.892    |
| F6   | H21C | 3.590    | F6   | H27  | 3.224    |
| F7   | H15A | 2.756    | F7   | H15B | 3.489    |
| F7   | H15C | 2.861    | F7   | H26B | 3.320    |
| F7   | H30  | 2.509    | F8   | H25A | 3.550    |
| F8   | H25C | 3.199    | F8   | H26A | 3.390    |
| F8   | H26B | 2.988    | F8   | H30  | 3.210    |
| F9   | H30  | 2.647    | F10  | H25C | 2.942    |
| F10  | H30  | 3.227    | F11  | H8C  | 3.511    |
| F11  | H30  | 2.557    | F12  | H8A  | 2.652    |
| F12  | H8C  | 3.108    | F12  | H30  | 2.609    |
| O1   | H8A  | 3.295    | O1   | H12C | 2.935    |
| O1   | H21B | 3.331    | O1   | H21C | 3.326    |
| O1   | H48  | 2.15(3)  | O2   | H8A  | 3.384    |
| O2   | H25C | 2.817    | O2   | H26B | 2.392    |
| O2   | H48  | 3.486(19)| N1   | H7A  | 2.361    |
| N1   | H7B  | 3.513    | N1   | H7C  | 3.498    |
| N1   | H8A  | 2.476    | N1   | H8B  | 3.586    |
| N1   | H8C  | 3.600    | N1   | H27  | 2.799    |
| N1   | H30  | 2.594    | N2   | H7A  | 2.592    |
| N2   | H12A | 3.021    | N2   | H12C | 2.498    |
| N2   | H13A | 3.390    | N2   | H13B | 2.770    |
| N2   | H15A | 2.634    | N2   | H15C | 2.652    |
| N2   | H16B | 3.439    | N2   | H17C | 3.441    |
| N2   | H26B | 3.083    | N2   | H26C | 3.164    |
| N2   | H48  | 3.33(2)  | N3   | H12A | 3.306    |
| N3   | H12C | 3.101    | N3   | H21B | 2.714    |
| N3   | H21C | 2.656    | N3   | H23B | 3.222    |
Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| N3    | H25B  | 3.554    | N3    | H25C  | 2.994    |
| N3    | H26B  | 2.511    | N3    | H26C  | 2.826    |
| C1    | H3    | 3.275    | C1    | H5    | 3.279    |
| C1    | H7A   | 2.563    | C1    | H7B   | 3.149    |
| C1    | H7C   | 3.162    | C1    | H8A   | 2.601    |
| C1    | H8B   | 3.176    | C1    | H8C   | 3.173    |
| C1    | H27   | 3.246    | C1    | H30   | 3.040    |
| C2    | H4    | 3.273    | C2    | H27   | 3.290    |
| C2    | H30   | 3.290    | C3    | H5    | 3.248    |
| C3    | H8A   | 3.311    | C3    | H8B   | 2.753    |
| C3    | H8C   | 2.753    | C5    | H3    | 3.248    |
| C5    | H7A   | 3.321    | C5    | H7B   | 2.777    |
| C5    | H7C   | 2.777    | C6    | H4    | 3.276    |
| C7    | H5    | 2.686    | C7    | H13A  | 3.573    |
| C7    | H13B  | 3.450    | C7    | H15A  | 3.139    |
| C7    | H17C  | 2.958    | C8    | H3    | 2.652    |
| C8    | H27   | 2.954    | C8    | H30   | 3.151    |
| C9    | H7A   | 2.963    | C9    | H12A  | 2.728    |
| C9    | H12B  | 3.378    | C9    | H12C  | 2.674    |
| C9    | H13A  | 2.694    | C9    | H13B  | 2.652    |
| C9    | H13C  | 3.361    | C9    | H14A  | 2.853    |
| C9    | H14B  | 2.878    | C9    | H14C  | 3.476    |
| C9    | H15A  | 2.712    | C9    | H15B  | 3.384    |
| C9    | H15C  | 2.726    | C9    | H16A  | 2.743    |
| C9    | H16B  | 2.748    | C9    | H16C  | 3.401    |
| C9    | H17A  | 2.738    | C9    | H17B  | 3.398    |
| C9    | H17C  | 2.740    | C9    | H26C  | 3.336    |
| C10   | H16A  | 3.032    | C10   | H17A  | 2.940    |
| C10   | H17C  | 3.487    | C11   | H7A   | 3.374    |
| C11   | H13A  | 3.398    | C11   | H14A  | 3.198    |
| C11   | H14B  | 2.999    | C11   | H26C  | 3.468    |
| C12   | H13A  | 3.354    | C12   | H13B  | 2.686    |
| C12   | H13C  | 2.686    | C12   | H14A  | 2.659    |
| C12   | H14B  | 3.324    | C12   | H14C  | 2.612    |
| C12   | H48   | 3.42(2)  | C13   | H7A   | 3.452    |
| C13   | H7C   | 3.503    | C13   | H12A  | 3.354    |
| C13   | H12B  | 2.686    | C13   | H12C  | 2.686    |
Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C13  | H14A | 3.359    | C13  | H14B | 2.693    |
| C13  | H14C | 2.693    | C13  | H17A | 3.169    |
| C13  | H17C | 3.416    | C14  | H12A | 2.657    |
| C14  | H12B | 2.610    | C14  | H12C | 3.325    |
| C14  | H13A | 2.729    | C14  | H13B | 3.359    |
| C14  | H13C | 2.653    | C14  | H16A | 2.453    |
| C14  | H17A | 2.758    | C15  | H7A  | 3.267    |
| C15  | H16A | 3.337    | C15  | H16B | 2.658    |
| C15  | H16C | 2.659    | C15  | H17A | 3.338    |
| C15  | H17B | 2.660    | C15  | H17C | 2.660    |
| C15  | H26B | 3.378    | C15  | H26C | 3.351    |
| C16  | H14A | 2.748    | C16  | H14B | 3.055    |
| C16  | H15A | 3.338    | C16  | H15B | 2.656    |
| C16  | H15C | 2.656    | C16  | H17A | 2.751    |
| C16  | H17B | 2.700    | C16  | H17C | 3.382    |
| C16  | H26C | 3.193    | C17  | H7A  | 3.399    |
| C17  | H13A | 2.956    | C17  | H14B | 2.808    |
| C17  | H15A | 2.668    | C17  | H15B | 2.646    |
| C17  | H15C | 3.340    | C17  | H16A | 2.750    |
| C17  | H16B | 3.382    | C17  | H16C | 2.700    |
| C18  | H21A | 3.395    | C18  | H21B | 2.715    |
| C18  | H21C | 2.771    | C18  | H22A | 2.752    |
| C18  | H22B | 3.412    | C18  | H22C | 2.788    |
| C18  | H23A | 2.696    | C18  | H23B | 2.699    |
| C18  | H23C | 3.371    | C18  | H24A | 3.422    |
| C18  | H24B | 2.807    | C18  | H24C | 2.807    |
| C18  | H25A | 3.341    | C18  | H25B | 2.669    |
| C18  | H25C | 2.669    | C18  | H26A | 3.355    |
| C18  | H26B | 2.695    | C18  | H26C | 2.695    |
| C19  | H24B | 3.258    | C19  | H24C | 2.892    |
| C19  | H25B | 3.207    | C19  | H48  | 2.41(3)  |
| C20  | H22A | 2.859    | C20  | H22B | 2.645    |
| C20  | H23A | 3.059    | C20  | H22C | 3.388    |
| C21  | H22A | 3.330    | C21  | H22B | 2.645    |
| C21  | H22C | 2.645    | C21  | H23A | 3.341    |
| C21  | H23B | 2.660    | C21  | H23C | 2.660    |
| C21  | H48  | 2.23(2)  | C22  | H21A | 2.590    |
Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| C22   | H21B  | 2.702    | C22   | H21C  | 3.327    |
| C22   | H23A  | 2.765    | C22   | H23B  | 3.385    |
| C22   | H23C  | 2.702    | C22   | H24C  | 2.692    |
| C22   | H25B  | 2.691    | C23   | H21A  | 2.701    |
| C23   | H21B  | 3.341    | C23   | H21C  | 2.614    |
| C23   | H22A  | 2.761    | C23   | H22B  | 2.701    |
| C23   | H22C  | 3.387    | C23   | H24B  | 2.873    |
| C23   | H24C  | 2.966    | C23   | H48   | 3.33(3)  |
| C24   | H22A  | 2.674    | C24   | H23A  | 2.492    |
| C24   | H25A  | 2.656    | C24   | H25B  | 2.753    |
| C24   | H25C  | 3.365    | C24   | H26A  | 2.593    |
| C24   | H26B  | 3.322    | C24   | H26C  | 2.682    |
| C25   | H22A  | 2.990    | C25   | H22C  | 3.167    |
| C25   | H24A  | 2.688    | C25   | H24B  | 3.369    |
| C25   | H24C  | 2.716    | C25   | H26A  | 2.690    |
| C25   | H26B  | 2.647    | C25   | H26C  | 3.347    |
| C26   | H15C  | 2.772    | C26   | H16B  | 3.188    |
| C26   | H24A  | 2.622    | C26   | H24B  | 2.654    |
| C26   | H24C  | 3.323    | C26   | H25A  | 2.683    |
| C26   | H25B  | 3.345    | C26   | H25C  | 2.659    |
| C26   | H48   | 3.59(2)  | C27   | H8A   | 3.124    |
| C27   | H8B   | 3.597    | C27   | H48   | 3.39(3)  |
| C28   | H12C  | 3.544    | C29   | H8A   | 3.330    |
| C30   | H8A   | 3.268    | C30   | H26B  | 3.428    |
| C31   | H26B  | 3.404    | C32   | H8A   | 3.399    |
| H3    | H4    | 2.317    | H3    | H8A   | 3.586    |
| H3    | H8B   | 2.688    | H3    | H8C   | 2.689    |
| H4    | H5    | 2.324    | H5    | H7B   | 2.743    |
| H5    | H7C   | 2.719    | H7A   | H13A  | 3.225    |
| H7A   | H13B  | 2.962    | H7A   | H15A  | 2.472    |
| H7A   | H17C  | 2.649    | H7B   | H15A  | 2.940    |
| H7B   | H17C  | 2.830    | H7C   | H13A  | 3.013    |
| H7C   | H13B  | 3.086    | H7C   | H17C  | 2.893    |
| H8A   | H27   | 2.502    | H8A   | H30   | 2.690    |
| H8B   | H27   | 2.795    | H8C   | H30   | 3.089    |
| H12A  | H13B  | 3.581    | H12A  | H13C  | 3.581    |
| H12A  | H14A  | 2.479    | H12A  | H14B  | 3.565    |
Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H12A  | H14C  | 2.907    | H12A  | H21C  | 3.497    |
| H12A  | H23B  | 2.790    | H12A  | H48   | 3.196    |
| H12B  | H13A  | 3.582    | H12B  | H13B  | 2.967    |
| H12B  | H13C  | 2.498    | H12B  | H14A  | 2.908    |
| H12B  | H14B  | 3.506    | H12B  | H14C  | 2.377    |
| H12C  | H13A  | 3.582    | H12C  | H13B  | 2.498    |
| H12C  | H13C  | 2.967    | H12C  | H14A  | 3.567    |
| H12C  | H14C  | 3.509    | H12C  | H21C  | 3.322    |
| H12C  | H48   | 2.758    | H13A  | H14B  | 2.546    |
| H13A  | H14C  | 3.027    | H13A  | H17A  | 2.530    |
| H13A  | H17C  | 2.720    | H13B  | H14C  | 3.569    |
| H13C  | H14A  | 3.557    | H13C  | H14B  | 2.916    |
| H13C  | H14C  | 2.466    | H14A  | H16A  | 1.938    |
| H14A  | H16B  | 3.020    | H14A  | H16C  | 3.531    |
| H14A  | H17A  | 3.189    | H14B  | H16A  | 2.340    |
| H14B  | H17A  | 1.998    | H14B  | H17B  | 3.448    |
| H14B  | H17C  | 3.388    | H14C  | H16A  | 3.349    |
| H14C  | H17A  | 3.522    | H15A  | H16B  | 3.558    |
| H15A  | H16C  | 3.559    | H15A  | H17A  | 3.565    |
| H15A  | H17B  | 2.951    | H15A  | H17C  | 2.473    |
| H15B  | H16A  | 3.555    | H15B  | H16B  | 2.934    |
| H15B  | H16C  | 2.459    | H15B  | H17A  | 3.548    |
| H15B  | H17B  | 2.449    | H15B  | H17C  | 2.919    |
| H15C  | H16A  | 3.555    | H15C  | H16B  | 2.459    |
| H15C  | H16C  | 2.934    | H15C  | H17B  | 3.555    |
| H15C  | H17C  | 3.565    | H15C  | H26A  | 2.879    |
| H15C  | H26B  | 2.452    | H15C  | H26C  | 2.531    |
| H16A  | H17A  | 2.602    | H16A  | H17B  | 3.008    |
| H16B  | H17B  | 3.585    | H16B  | H26A  | 3.351    |
| H16B  | H26B  | 3.556    | H16B  | H26C  | 2.321    |
| H16C  | H17A  | 3.008    | H16C  | H17B  | 2.493    |
| H16C  | H17C  | 3.585    | H21A  | H22A  | 3.504    |
| H21A  | H22B  | 2.387    | H21A  | H22C  | 2.838    |
| H21A  | H23A  | 3.591    | H21A  | H23B  | 2.997    |
| H21A  | H23C  | 2.508    | H21A  | H48   | 3.198    |
| H21B  | H22A  | 3.590    | H21B  | H22B  | 3.002    |
| H21B  | H22C  | 2.507    | H21B  | H23B  | 3.538    |
Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom     | atom     | distance | atom     | atom     | distance |
|----------|----------|----------|----------|----------|----------|
| H21B     | H23C     | 3.579    | H21B     | H48      | 2.161    |
| H21C     | H22B     | 3.516    | H21C     | H22C     | 3.568    |
| H21C     | H23A     | 3.524    | H21C     | H23B     | 2.415    |
| H21C     | H23C     | 2.870    | H21C     | H48      | 1.960    |
| H22A     | H23A     | 2.623    | H22A     | H23C     | 3.014    |
| H22A     | H24A     | 3.368    | H22A     | H24B     | 3.208    |
| H22A     | H24C     | 1.887    | H22A     | H25A     | 3.570    |
| H22A     | H25B     | 2.322    | H22B     | H23A     | 3.018    |
| H22B     | H23B     | 3.583    | H22B     | H23C     | 2.491    |
| H22B     | H24C     | 3.323    | H22C     | H23C     | 3.586    |
| H22C     | H24C     | 3.291    | H22C     | H25B     | 2.404    |
| H22C     | H25C     | 3.467    | H23A     | H24A     | 3.400    |
| H23A     | H24B     | 2.071    | H23A     | H24C     | 2.273    |
| H23B     | H24B     | 3.161    | H23B     | H48      | 3.100    |
| H23C     | H24C     | 3.542    | H24A     | H25A     | 2.454    |
| H24A     | H25B     | 3.034    | H24A     | H25C     | 3.560    |
| H24A     | H26A     | 2.370    | H24A     | H26B     | 3.504    |
| H24A     | H26C     | 2.954    | H24B     | H25A     | 3.556    |
| H24B     | H26A     | 2.871    | H24B     | H26B     | 3.571    |
| H24B     | H26C     | 2.500    | H24C     | H25A     | 2.933    |
| H24C     | H25B     | 2.587    | H24C     | H26A     | 3.497    |
| H24C     | H26C     | 3.581    | H25A     | H26A     | 2.512    |
| H25A     | H26B     | 2.934    | H25A     | H26C     | 3.589    |
| H25B     | H26A     | 3.589    | H25B     | H26B     | 3.544    |
| H25C     | H26A     | 2.961    | H25C     | H26B     | 2.439    |
| H25C     | H26C     | 3.550    | H26B     | H48      | 3.355    |
| H26C     | H48      | 3.581    |          |          |          |
| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| F1   | C3   | 3.570(3) | F1   | C8   | 3.398(3) |
| F2   | F7   | 3.096(2) | F3   | C13  | 3.600(3) |
| F4   | C14  | 3.381(3) | F4   | C22  | 3.559(4) |
| F5   | C5   | 3.553(3) | F5   | C6   | 3.515(3) |
| F5   | C7   | 3.283(3) | F7   | F2   | 3.096(2) |
| F7   | C21  | 3.435(3) | F8   | C23  | 3.495(3) |
| F9   | C12  | 3.406(2) | F9   | C24  | 3.271(3) |
| F11  | C16  | 3.531(2) | F11  | C24  | 3.586(3) |
| F12  | C16  | 3.516(2) | F12  | C22  | 3.461(3) |
| C3   | F1   | 3.570(3) | C5   | F5   | 3.553(3) |
| C6   | F5   | 3.515(3) | C7   | F5   | 3.283(3) |
| C8   | F1   | 3.398(3) | C12  | F9   | 3.406(2) |
| C13  | F3   | 3.600(3) | C14  | F4   | 3.381(3) |
| C16  | F11  | 3.531(2) | C16  | F12  | 3.516(2) |
| C21  | F7   | 3.435(3) | C22  | F4   | 3.559(4) |
| C22  | F12  | 3.461(3) | C23  | F8   | 3.495(3) |
| C24  | F9   | 3.271(3) | C24  | F11  | 3.586(3) |

Symmetry Operators:

1. \(-X+1/2,Y+1/2,-Z+1/2+1\)
2. \(X,-Y+1,Z\)
3. \(-X+1/2,Y+1/2,-Z+1/2+1\)
4. \(X,Y+1,Z\)
5. \(-X+1,-Y+1,-Z+1\)
6. \(X+1,-Y+1,Z+1\)
7. \(-X+1/2+1,Y+1/2,-Z+1/2+1\)
8. \(X,Y-1,Z\)
9. \(-X+1/2+1,Y+1/2-1,-Z+1/2+1\)
Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom | atom  | distance | atom | atom  | distance |
|------|------|----------|------|------|----------|
| F1   | H3\(^1\) | 2.800    | F1   | H8B\(^1\) | 2.699 |
| F1   | H8C\(^1\) | 3.352    | F1   | H13A\(^2\) | 3.314 |
| F2   | H3\(^1\) | 3.196    | F2   | H7B\(^3\) | 3.313 |
| F2   | H15A\(^3\) | 3.145    | F2   | H15B\(^3\) | 3.545 |
| F3   | H7B\(^3\) | 2.824    | F3   | H7C\(^2\) | 2.771 |
| F3   | H13A\(^2\) | 2.700    | F3   | H17A\(^2\) | 3.514 |
| F3   | H17C\(^2\) | 3.169    | F4   | H14A\(^4\) | 3.378 |
| F4   | H14B\(^4\) | 3.189    | F4   | H14C\(^4\) | 3.021 |
| F4   | H22A\(^5\) | 2.953    | F4   | H22B\(^5\) | 3.498 |
| F5   | H5\(^2\) | 3.309    | F5   | H7C\(^2\) | 2.417 |
| F5   | H13A\(^2\) | 3.592    | F5   | H13B\(^2\) | 3.566 |
| F5   | H14C\(^4\) | 3.260    | F6   | H15B\(^3\) | 2.813 |
| F6   | H17B\(^3\) | 3.539    | F6   | H25B\(^5\) | 3.292 |
| F7   | H21A\(^6\) | 3.180    | F7   | H21C\(^6\) | 2.798 |
| F8   | H16B\(^7\) | 3.461    | F8   | H21A\(^6\) | 3.284 |
| F8   | H21C\(^6\) | 3.445    | F8   | H23B\(^6\) | 3.242 |
| F8   | H23C\(^6\) | 2.879    | F9   | H4\(^8\) | 2.766 |
| F9   | H12A\(^6\) | 3.206    | F9   | H12B\(^6\) | 2.841 |
| F9   | H21C\(^6\) | 3.373    | F9   | H23B\(^6\) | 3.063 |
| F9   | H24A\(^7\) | 2.707    | F9   | H24B\(^7\) | 2.996 |
| F10  | H16C\(^4\) | 3.428    | F10  | H21A\(^5\) | 3.322 |
| F10  | H22B\(^5\) | 2.766    | F10  | H24A\(^7\) | 3.273 |
| F10  | H26A\(^7\) | 2.667    | F11  | H4\(^8\) | 2.829 |
| F11  | H5\(^8\) | 3.330    | F11  | H16A\(^4\) | 3.395 |
| F11  | H16C\(^4\) | 2.840    | F11  | H17A\(^4\) | 3.593 |
| F11  | H17B\(^4\) | 3.064    | F11  | H24A\(^7\) | 2.607 |
| F11  | H26A\(^7\) | 3.551    | F12  | H14A\(^4\) | 3.463 |
| F12  | H14B\(^4\) | 3.158    | F12  | H16A\(^4\) | 2.818 |
| F12  | H16C\(^4\) | 3.339    | F12  | H17A\(^4\) | 3.538 |
| F12  | H22A\(^5\) | 3.544    | F12  | H22B\(^5\) | 2.627 |
| C1   | H13C\(^2\) | 3.465    | C2   | H13C\(^2\) | 2.975 |
| C3   | H12B\(^2\) | 3.182    | C3   | H13C\(^2\) | 3.041 |
| C4   | H8C\(^8\) | 3.393    | C4   | H12B\(^2\) | 3.142 |
| C4   | H13C\(^2\) | 3.565    | C4   | H30\(^8\) | 3.313 |
| C5   | H8C\(^8\) | 3.306    | C5   | H17B\(^9\) | 3.468 |
| C8   | H13C\(^2\) | 3.400    | C8   | H14B\(^4\) | 3.550 |
| C13  | H8B\(^1\) | 3.346    | C13  | H27\(^1\) | 3.335 |
Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom     | distance | atom   | atom     | distance |
|--------|----------|----------|--------|----------|----------|
| C14    | H24C<sup>10</sup> | 3.515    | C16    | H23C<sup>10</sup> | 2.976    |
| C16    | H25A<sup>11</sup> | 3.481    | C17    | H5<sup>9</sup> | 3.194    |
| C21    | H25B<sup>5</sup> | 3.299    | C22    | H14A<sup>10</sup> | 3.563    |
| C22    | H22C<sup>5</sup> | 3.308    | C22    | H25C<sup>5</sup> | 3.553    |
| C23    | H14A<sup>10</sup> | 3.507    | C23    | H16A<sup>10</sup> | 3.435    |
| C23    | H16B<sup>10</sup> | 3.257    | C23    | H24B<sup>10</sup> | 3.309    |
| C24    | H23B<sup>10</sup> | 3.582    | C24    | H16C<sup>7</sup> | 3.572    |
| C25    | H21B<sup>5</sup> | 3.362    | C25    | H22C<sup>5</sup> | 3.388    |
| C27    | H13A<sup>2</sup> | 3.596    | C27    | H3<sup>1</sup> | 3.519    |
| C28    | H13A<sup>2</sup> | 3.348    | C28    | H7C<sup>2</sup> | 3.593    |
| C30    | H4<sup>8</sup> | 3.157    | C30    | H4<sup>8</sup> | 3.502    |
| C31    | H21C<sup>6</sup> | 3.431    | C31    | H4<sup>8</sup> | 3.502    |
| C32    | H16A<sup>4</sup> | 3.522    | C32    | H16C<sup>4</sup> | 3.438    |
| C32    | H22B<sup>5</sup> | 3.261    | C32    | H24A<sup>7</sup> | 3.427    |
| H3     | F1<sup>2</sup> | 2.800    | H3     | F2<sup>2</sup> | 3.196    |
| H3     | C28<sup>8</sup> | 3.519    | H3     | H12B<sup>2</sup> | 3.058    |
| H3     | H13C<sup>2</sup> | 3.267    | H3     | F9<sup>8</sup> | 2.766    |
| H4     | F11<sup>8</sup> | 3.289    | H4     | C30<sup>8</sup> | 3.157    |
| H4     | C31<sup>8</sup> | 3.355    | H4     | C32<sup>8</sup> | 3.502    |
| H4     | H8C<sup>8</sup> | 3.235    | H4     | H12B<sup>2</sup> | 2.972    |
| H4     | H30<sup>8</sup> | 2.490    | H5     | F5<sup>1</sup> | 3.309    |
| H5     | F11<sup>8</sup> | 3.330    | H5     | C17<sup>9</sup> | 3.194    |
| H5     | H8C<sup>8</sup> | 3.070    | H5     | H17A<sup>9</sup> | 3.260    |
| H5     | H17B<sup>9</sup> | 2.520    | H5     | H17C<sup>9</sup> | 3.336    |
| H7B    | F2<sup>6</sup> | 3.313    | H7B    | F3<sup>6</sup> | 2.824    |
| H7B    | H17C<sup>9</sup> | 3.563    | H7B    | F3<sup>1</sup> | 2.771    |
| H7C    | F5<sup>1</sup> | 2.417    | H7C    | C29<sup>1</sup> | 3.593    |
| H8A    | H14B<sup>4</sup> | 3.481    | H8B    | F1<sup>2</sup> | 2.699    |
| H8B    | H13C<sup>2</sup> | 3.346    | H8B    | H13B<sup>2</sup> | 2.939    |
| H8B    | H13C<sup>2</sup> | 2.901    | H8B    | H14B<sup>4</sup> | 3.349    |
| H8C    | F1<sup>2</sup> | 3.352    | H8C    | C4<sup>8</sup> | 3.393    |
| H8C    | C5<sup>8</sup> | 3.306    | H8C    | H4<sup>8</sup> | 3.235    |
| H8C    | H5<sup>8</sup> | 3.070    | H8C    | H14B<sup>4</sup> | 3.237    |
| H8C    | H17A<sup>4</sup> | 2.866    | H12A   | F9<sup>8</sup> | 3.206    |
| H12A   | H23A<sup>10</sup> | 3.196    | H12A   | H24B<sup>10</sup> | 3.161    |
| H12A   | H24C<sup>10</sup> | 3.446    | H12B   | F9<sup>8</sup> | 2.841    |
| H12B   | C3<sup>1</sup> | 3.182    | H12B   | C4<sup>1</sup> | 3.142    |
Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H12B | H3$^1$ | 3.058 | H12B | H4$^1$ | 2.972 |
| H13A | F1$^1$ | 3.314 | H13A | F3$^1$ | 2.700 |
| H13A | F5$^1$ | 3.592 | H13A | C27$^1$ | 3.596 |
| H13A | C28$^1$ | 3.348 | H13A | H27$^1$ | 3.015 |
| H13B | F5$^1$ | 3.566 | H13B | H8B$^1$ | 2.939 |
| H13B | H27$^1$ | 3.482 | H13C | C1$^1$ | 3.465 |
| H13C | C2$^1$ | 2.975 | H13C | C3$^1$ | 3.041 |
| H13C | C4$^1$ | 3.565 | H13C | C8$^1$ | 3.400 |
| H13C | H3$^1$ | 3.267 | H13C | H8B$^1$ | 2.901 |
| H13C | H27$^1$ | 3.980 | H14A | F4$^{12}$ | 3.378 |
| H14A | F12$^{12}$ | 3.463 | H14A | C22$^{10}$ | 3.563 |
| H14A | C23$^{10}$ | 3.507 | H14A | H22A$^{10}$ | 2.968 |
| H14A | H22B$^{10}$ | 3.364 | H14A | H23A$^{10}$ | 2.902 |
| H14A | H23C$^{10}$ | 3.304 | H14A | H24C$^{10}$ | 2.857 |
| H14B | F4$^{12}$ | 3.199 | H14B | F12$^{12}$ | 3.158 |
| H14B | C8$^{12}$ | 3.550 | H14B | H8A$^{12}$ | 3.481 |
| H14B | H8B$^{12}$ | 3.349 | H14B | H8C$^{12}$ | 3.237 |
| H14C | F4$^{12}$ | 3.021 | H14C | F5$^{12}$ | 3.260 |
| H14C | H24C$^{10}$ | 3.285 | H15A | F2$^6$ | 3.145 |
| H15B | F2$^6$ | 3.545 | H15B | F6$^6$ | 2.813 |
| H15B | H21A$^6$ | 3.351 | H15B | H21B$^6$ | 3.522 |
| H15B | H25A$^{11}$ | 3.099 | H15C | H21A$^6$ | 3.404 |
| H16A | F11$^{12}$ | 3.395 | H16A | F12$^{12}$ | 2.818 |
| H16A | C23$^{10}$ | 3.435 | H16A | C32$^{12}$ | 3.522 |
| H16A | H22B$^{10}$ | 3.196 | H16A | H23A$^{10}$ | 3.299 |
| H16A | H23C$^{10}$ | 2.727 | H16B | F8$^{11}$ | 3.461 |
| H16B | C23$^{10}$ | 3.257 | H16B | H23A$^{10}$ | 2.520 |
| H16B | H23C$^{10}$ | 2.482 | H16C | F10$^{12}$ | 3.428 |
| H16C | F11$^{12}$ | 2.840 | H16C | F12$^{12}$ | 3.339 |
| H16C | C25$^{11}$ | 3.572 | H16C | C32$^{12}$ | 3.438 |
| H16C | H23C$^{10}$ | 3.292 | H16C | H25A$^{11}$ | 2.605 |
| H17A | F3$^1$ | 3.514 | H17A | F11$^{12}$ | 3.593 |
| H17A | F12$^{12}$ | 3.538 | H17A | H5$^9$ | 3.260 |
| H17A | H8C$^{12}$ | 2.866 | H17B | F6$^6$ | 3.539 |
| H17B | F11$^{12}$ | 3.064 | H17B | C5$^9$ | 3.468 |
| H17B | H5$^9$ | 2.520 | H17C | F3$^1$ | 3.169 |
| H17C | H5$^9$ | 3.336 | H17C | H7B$^9$ | 3.563 |
Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H21A  | F7$^3$| 3.180    | H21A  | F8$^3$| 3.284    |
| H21A  | F10$^5$| 3.322   | H21A  | H15B$^3$| 3.351 |
| H21A  | H15C$^3$| 3.404  | H21A  | H25B$^5$| 3.227 |
| H21A  | H25C$^5$| 3.391   | H21B  | C25$^5$| 3.362    |
| H21B  | H15B$^3$| 3.522   | H21B  | H22C$^5$| 2.955 |
| H21B  | H25B$^5$| 2.563   | H21B  | H25C$^5$| 3.441    |
| H21C  | F7$^3$| 2.798    | H21C  | F8$^3$| 3.445    |
| H21C  | F9$^3$| 3.373    | H21C  | C31$^3$| 3.431    |
| H22A  | F4$^5$| 2.953    | H22A  | F12$^5$| 3.544    |
| H22A  | H14A$^{10}$| 2.968 | H22B  | F4$^5$| 3.498    |
| H22B  | F10$^5$| 2.766    | H22B  | F12$^5$| 2.627    |
| H22B  | C32$^5$| 3.261    | H22B  | H14A$^{10}$| 3.364 |
| H22B  | H16A$^{10}$| 3.196 | H22B  | H25C$^5$| 3.203    |
| H22C  | C22$^5$| 3.308    | H22C  | C25$^5$| 3.388    |
| H22C  | H21B$^5$| 2.955   | H22C  | H22C$^5$| 2.387    |
| H22C  | H25B$^5$| 2.895   | H22C  | H25C$^5$| 3.016    |
| H23A  | H12A$^{10}$| 3.196 | H23A  | H14A$^{10}$| 2.902 |
| H23A  | H16A$^{10}$| 3.299   | H23A  | H16B$^{10}$| 3.250 |
| H23A  | H23A$^{10}$| 3.451   | H23A  | H23B$^{10}$| 3.296 |
| H23A  | H24B$^{10}$| 3.336   | H23B  | F8$^3$| 3.242    |
| H23B  | F9$^3$| 3.063    | H23B  | C24$^{10}$| 3.582 |
| H23B  | H23A$^{10}$| 3.296   | H23B  | H24B$^{10}$| 2.634 |
| H23C  | F8$^3$| 2.879    | H23C  | C16$^{10}$| 2.976    |
| H23C  | H14A$^{10}$| 3.304   | H23C  | H16A$^{10}$| 2.727 |
| H23C  | H16B$^{10}$| 2.482   | H23C  | H16C$^{10}$| 3.292 |
| H23C  | H24B$^{10}$| 3.482   | H23C  | H26C$^{10}$| 3.593 |
| H24A  | F9$^{11}$| 2.707   | H24A  | F10$^{11}$| 3.273    |
| H24A  | F11$^{11}$| 2.607   | H24A  | C32$^{11}$| 3.427    |
| H24B  | F9$^{11}$| 2.996    | H24B  | C23$^{10}$| 3.309    |
| H24B  | H12A$^{10}$| 3.161   | H24B  | H23A$^{10}$| 3.336 |
| H24B  | H23B$^{10}$| 2.634   | H24B  | H23C$^{10}$| 3.482 |
| H24C  | C14$^{10}$| 3.515    | H24C  | H12A$^{10}$| 3.446 |
| H24C  | H14A$^{10}$| 2.857   | H24C  | H14C$^{10}$| 3.285 |
| H25A  | C16$^7$| 3.481    | H25A  | H15B$^7$| 3.099 |
| H25A  | H16C$^7$| 2.605    | H25B  | F6$^6$| 3.292    |
| H25B  | C21$^5$| 3.299    | H25B  | H21A$^5$| 3.227 |
| H25B  | H21B$^5$| 2.563    | H25B  | H22C$^5$| 2.895 |
### Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H25C   | C22$^5$| 3.553    | H25C   | H21A$^5$| 3.391    |
| H25C   | H21B$^5$| 3.441    | H25C   | H22B$^5$| 3.203    |
| H25C   | H22C$^5$| 3.016    | H26A   | F10$^{11}$| 2.667    |
| H26A   | F11$^{11}$| 3.551    | H26C   | H23C$^{10}$| 3.593    |
| H27    | C13$^2$| 3.335    | H27    | H13A$^2$| 3.015    |
| H27    | H13B$^2$| 3.482    | H27    | H13C$^2$| 2.980    |
| H30    | C4$^8$ | 3.313    | H30    | H4$^8$ | 2.490    |

Symmetry Operators:

(1) $-X+1/2,Y+1/2,-Z+1/2+1$

(2) $-X+1/2,Y+1/2,-Z+1/2+1$

(3) $X,-Y+1,Z$

(4) $X,Y+1,Z$

(5) $-X+1,-Y+1,-Z+1$

(6) $X+1,-Y+1,Z+1$

(7) $-X+1/2+1,Y+1/2,-Z+1/2+1$

(8) $-X+1,-Y+1,-Z+2$

(9) $-X+1,-Y,-Z+2$

(10) $-X+1,-Y,-Z+1$

(11) $-X+1/2+1,Y+1/2-1,-Z+1/2+1$

(12) $X,Y-1,Z$
X-ray Structure Report

for

\[ \text{Nb(N}-2,6-\text{Mes}_{2}\text{C}_{6}\text{H}_{3})(\text{N}^{}=\text{C}^{}=\text{Bu}^{}_{2})_{2}^{\text{x}}(\text{OC}_{6}\text{F}_{5})(\text{HN}^{}=\text{C}^{}=\text{Bu}^{}_{2}) \] (11)

December 25, 2017
Experimental

Data Collection

A yellow block crystal of C_{41}H_{64}F_{5}N_{4}NbO having approximate dimensions of 0.180 x 0.170 x 0.140 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 45.00 mm.

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

\[
\begin{align*}
    a &= 11.903(3) \text{ Å} \\
    b &= 18.130(5) \text{ Å} \\
    c &= 20.798(6) \text{ Å} \\
    V &= 4349(2) \text{ Å}^3
\end{align*}
\]

For Z = 4 and F.W. = 816.88, the calculated density is 1.247 g/cm³. The reflection conditions of:

- h0l: h+l = 2n
- 0k0: k = 2n

uniquely determine the space group to be:

P2_1/n (#14)

The data were collected at a temperature of -180 ± 1°C to a maximum 2θ value of 55.0°. A total of 1620 oscillation images were collected. A sweep of data was done using θ scans from -103.0 to 77.0° in 0.25° step, at θ=22.0° and θ = -180.0°. The exposure rate was 20.0 [sec./°]. The detector swing angle was -13.08°. A second sweep was performed using θ scans from -103.0 to 77.0° in 0.25° step, at θ=55.0° and θ = 108.0°. The exposure rate was 20.0 [sec./°]. The detector swing angle was -13.08°. Another sweep was
performed using \( \square \) scans from \(-103.0^\circ \) to \(-58.0^\circ \) in \(0.25^\circ\) step, at \( \square = 33.0^\circ \) and \( \square = 144.0^\circ \). The exposure rate was \(20.0 \text{ sec.}/^\circ\). The detector swing angle was \(-13.08^\circ\). The crystal-to-detector distance was \(45.00\) mm. Readout was performed in the \(0.172\) mm pixel mode.

**Data Reduction**

Of the 41166 reflections were collected, where 9916 were unique (\(R_{\text{int}} = 0.0968\)); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku). \(^1\)

The linear absorption coefficient, \(\mu\), for Mo-K\(\alpha\) radiation is \(3.320\) \(\text{cm}^{-1}\). An empirical absorption correction was applied which resulted in transmission factors ranging from \(0.310\) to \(0.955\). The data were corrected for Lorentz and polarization effects.

**Structure Solution and Refinement**

The structure was solved by direct methods\(^2\) and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model. The final cycle of full-matrix least-squares refinement\(^3\) on \(F^2\) was based on 9916 observed reflections and 473 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

\[
R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} = 0.0736
\]

\[
wR2 = \left[ \frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum w(F_o^2)^2} \right]^{1/2} = 0.2163
\]

The goodness of fit\(^4\) was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to \(2.57\) and \(-1.82\) \(e^{-}/\text{Å}^3\), respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 \(^5\). Anomalous dispersion effects were included in \(F_{\text{calc}}\); the values for \(|f^e|\) and \(|f^o|\) were
those of Creagh and McAuley\textsuperscript{7}. The values for the mass attenuation coefficients are those of Creagh and Hubbell\textsuperscript{8}. All calculations were performed using the CrystalStructure\textsuperscript{9} crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7\textsuperscript{10}.

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998–2015). Tokyo 196-8666, Japan.

(2) SHELXT Version 2014/5: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

\[ \sum w(F_o^2 - F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.} \]

(4) Goodness of fit is defined as:

\[ \left[ \sum w(F_o^2 - F_c^2)^2/(N_o - N_V) \right]^{1/2} \]

where: \( N_o = \text{number of observations} \quad N_V = \text{number of variables} \)

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000–2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula \( \text{C}_{41}\text{H}_{64}\text{F}_{5}\text{N}_{4}\text{NbO} \)

Formula Weight 816.88

Crystal Color, Habit yellow, block

Crystal Dimensions 0.180 X 0.170 X 0.140 mm

Crystal System monoclinic

Lattice Type Primitive

Lattice Parameters
\begin{align*}
    a &= 11.903(3) \text{ Å} \\
    b &= 18.130(5) \text{ Å} \\
    c &= 20.798(6) \text{ Å} \\
    \beta &= 104.299(5) ^\circ \\
    V &= 4349(2) \text{ Å}^3
\end{align*}

Space Group \( \text{P2}_1/n \) (#14)

Z value 4

\( \text{D}_{\text{calc}} \) 1.247 g/cm\(^3\)

\( \text{F}_{000} \) 1728.00

\( \mu(\text{MoK}\alpha) \) 3.320 cm\(^{-1}\)
B. Intensity Measurements

| Parameter                        | Details |
|----------------------------------|---------|
| Diffractometer                   | XtaLAB P200 |
| Radiation                        | MoKα (λ = 0.71075 Å) multi-layer mirror monochromated |
| Voltage, Current                 | 50kV, 24mA |
| Temperature                      | -180.0°C |
| Detector Aperture                | 83.8 x 70.0 mm |
| Data Images                      | 1620 exposures |
| ω oscillation Range (χ=22.0, φ=-180.0) | -103.0 - 77.0° |
| Exposure Rate                    | 20.0 sec./° |
| Detector Swing Angle             | -13.08° |
| ω oscillation Range (χ=55.0, φ=108.0) | -103.0 - 77.0° |
| Exposure Rate                    | 20.0 sec./° |
| Detector Swing Angle             | -13.08° |
| ω oscillation Range (χ=33.0, φ=144.0) | -103.0 - -58.0° |
| Exposure Rate                    | 20.0 sec./° |
| Detector Swing Angle             | -13.08° |
| Parameter                  | Value               |
|---------------------------|---------------------|
| Detector Position         | 45.00 mm            |
| Pixel Size                | 0.172 mm            |
| $2\theta_{\text{max}}$    | 55.0°               |
| No. of Reflections Measured |                    |
| Total: 41166              | Unique: 9916 ($R_{\text{int}} = 0.0968$) |
| Corrections               | Lorentz-polarization |
|                           | Absorption          |
|                           | (trans. factors: 0.310 - 0.955) |
C. Structure Solution and Refinement

Structure Solution
Direct Methods (SHELXT Version 2014/5)

Refinement
Full-matrix least-squares on $F^2$

Function Minimized
$\sum w (F_o^2 - F_c^2)^2$

Least Squares Weights
$w = 1/ [ \sigma^2(F_o^2) + (0.1428 \cdot P)^2 + 0.0000 \cdot P ]$
where $P = (\text{Max}(F_o^2,0) + 2F_c^2)/3$

$2\theta_{\text{max}}$ cutoff
55.0°

Anomalous Dispersion
All non-hydrogen atoms

No. Observations (All reflections)
9916

No. Variables
473

Reflection/Parameter Ratio
20.96

Residuals: $R_1$ ($I > 2.00\sigma(I)$)
0.0736

Residuals: $R$ (All reflections)
0.1009

Residuals: $wR^2$ (All reflections)
0.2163

Goodness of Fit Indicator
1.058

Max Shift/Error in Final Cycle
0.001

Maximum peak in Final Diff. Map
2.57 e$^-/\text{Å}^3$

Minimum peak in Final Diff. Map
-1.82 e$^-/\text{Å}^3$
Table S10-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$

| atom | x          | y          | z          | $B_{\text{eq}}$ |
|------|------------|------------|------------|-----------------|
| Nb1  | 0.29980(3) | 0.31492(2) | 0.61776(2) | 1.726(11)       |
| F1   | 0.5484(2)  | 0.38078(13)| 0.57252(12)| 2.83(4)         |
| F2   | 0.6884(2)  | 0.49819(15)| 0.60651(13)| 3.16(5)         |
| F3   | 0.5987(2)  | 0.63481(14)| 0.61499(13)| 3.33(5)         |
| F4   | 0.3636(2)  | 0.65304(14)| 0.58174(15)| 3.51(5)         |
| F5   | 0.2217(2)  | 0.53519(14)| 0.54845(13)| 3.05(5)         |
| O1   | 0.3093(2)  | 0.39524(15)| 0.54882(13)| 2.24(5)         |
| N1   | 0.4051(3)  | 0.35915(18)| 0.68326(15)| 1.97(5)         |
| N2   | 0.3788(3)  | 0.22414(19)| 0.60204(16)| 2.16(5)         |
| N3   | 0.1649(3)  | 0.32028(18)| 0.65620(17)| 2.15(6)         |
| N4   | 0.1564(3)  | 0.2841(2)  | 0.51531(16)| 2.15(6)         |
| C1   | 0.4817(3)  | 0.4042(2)  | 0.72708(18)| 2.07(6)         |
| C2   | 0.4402(4)  | 0.4682(2)  | 0.75236(19)| 2.38(7)         |
| C3   | 0.5186(4)  | 0.5135(3)  | 0.7953(2)  | 3.01(8)         |
| C4   | 0.6350(4)  | 0.4966(3)  | 0.8136(2)  | 3.53(9)         |
| C5   | 0.6750(4)  | 0.4333(3)  | 0.7903(2)  | 3.33(9)         |
| C6   | 0.6008(3)  | 0.3858(3)  | 0.7471(2)  | 2.57(7)         |
| C7   | 0.3139(4)  | 0.4868(3)  | 0.7331(2)  | 2.78(7)         |
| C8   | 0.6449(4)  | 0.3172(3)  | 0.7218(2)  | 2.95(8)         |
| C9   | 0.4330(4)  | 0.1684(2)  | 0.5888(2)  | 2.21(7)         |
| C10  | 0.4460(4)  | 0.0995(2)  | 0.6348(2)  | 2.53(7)         |
| C11  | 0.4884(4)  | 0.1735(2)  | 0.5280(2)  | 2.71(8)         |
| C12  | 0.4105(4)  | 0.1200(3)  | 0.6986(2)  | 3.02(8)         |
| C13  | 0.3645(4)  | 0.0370(2)  | 0.6017(2)  | 3.16(8)         |
| C14  | 0.5726(4)  | 0.0714(3)  | 0.6559(3)  | 3.89(10)        |
| C15  | 0.4224(4)  | 0.2305(3)  | 0.4791(2)  | 3.08(8)         |
| C16  | 0.6134(4)  | 0.2009(3)  | 0.5526(3)  | 3.55(9)         |
| C17  | 0.4866(5)  | 0.1018(3)  | 0.4893(3)  | 3.72(10)        |
| C18  | 0.0801(3)  | 0.3242(2)  | 0.68188(19)| 1.99(6)         |
| C19  | 0.0785(3)  | 0.2742(2)  | 0.74311(19)| 2.30(7)         |
| C20  | -0.0191(3) | 0.3796(2)  | 0.65206(19)| 2.26(7)         |
| C21  | 0.1668(4)  | 0.2124(3)  | 0.7477(2)  | 2.61(7)         |
| C22  | -0.0393(4) | 0.2390(3)  | 0.7408(3)  | 3.21(8)         |
| C23  | 0.1180(5)  | 0.3203(3)  | 0.8073(2)  | 3.24(9)         |
| C24  | 0.0238(4)  | 0.4365(3)  | 0.6078(2)  | 2.97(8)         |
| C25  | -0.1198(4) | 0.3377(3)  | 0.6055(2)  | 2.77(7)         |
| C26  | -0.0627(4) | 0.4235(3)  | 0.7044(2)  | 2.92(8)         |
Table S10-1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

| atom | x        | y        | z        | $B_{\text{eq}}$ |
|------|----------|----------|----------|-----------------|
| C27  | 0.0769(3)| 0.2499(2)| 0.47402(19) | 2.18(6)        |
| C28  | 0.0228(4)| 0.2849(3)| 0.4055(2)  | 2.61(7)        |
| C29  | 0.0389(4)| 0.1735(2)| 0.4943(2)  | 2.61(7)        |
| C30  | 0.1042(5)| 0.3446(3)| 0.3884(2)  | 3.88(10)       |
| C31  | -0.0898(5)| 0.3247(3)| 0.4085(3)  | 3.91(10)       |
| C32  | -0.0006(4)| 0.2308(3)| 0.3474(2)  | 3.20(8)        |
| C33  | 0.0790(4)| 0.1643(3)| 0.5697(2)  | 2.69(7)        |
| C34  | -0.0932(4)| 0.1612(3)| 0.4760(3)  | 3.76(10)       |
| C35  | 0.0994(5)| 0.1130(3)| 0.4626(2)  | 3.41(9)        |
| C36  | 0.3797(3)| 0.4534(2)| 0.56177(18)| 2.07(6)        |
| C37  | 0.5005(3)| 0.4476(2)| 0.57521(18)| 2.17(6)        |
| C38  | 0.5730(3)| 0.5072(2)| 0.59255(19)| 2.41(7)        |
| C39  | 0.5280(4)| 0.5763(2)| 0.5962(2)  | 2.42(7)        |
| C40  | 0.4087(4)| 0.5852(2)| 0.5796(2)  | 2.51(7)        |
| C41  | 0.3376(3)| 0.5252(2)| 0.56253(19)| 2.26(7)        |

$B_{\text{eq}} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$
Table S10-2. Atomic coordinates and $B_{iso}$ involving hydrogen atoms

| atom | x       | y        | z        | $B_{iso}$ |
|------|---------|----------|----------|-----------|
| H1   | 0.164(4)| 0.3219(16)| 0.5017(10)| 0.8(8)   |
| H3   | 0.49145 | 0.55675  | 0.81237  | 3.615    |
| H4   | 0.68762 | 0.52877  | 0.84224  | 4.231    |
| H5   | 0.75526 | 0.42174  | 0.80400  | 3.997    |
| H7A  | 0.27205 | 0.44901  | 0.70273  | 3.331    |
| H7B  | 0.28389 | 0.48855  | 0.77288  | 3.331    |
| H7C  | 0.30312 | 0.53492  | 0.71099  | 3.331    |
| H8A  | 0.58019 | 0.29108  | 0.69225  | 3.535    |
| H8B  | 0.70253 | 0.33027  | 0.69729  | 3.535    |
| H8C  | 0.68069 | 0.28522  | 0.75926  | 3.535    |
| H12A | 0.46038 | 0.15984  | 0.72138  | 3.625    |
| H12B | 0.32955 | 0.13639  | 0.68743  | 3.625    |
| H12C | 0.41892 | 0.07677  | 0.72769  | 3.625    |
| H13A | 0.38413 | 0.02207  | 0.56053  | 3.795    |
| H13B | 0.37343 | -0.00529 | 0.63193  | 3.795    |
| H13C | 0.28407 | 0.05433  | 0.59167  | 3.795    |
| H14A | 0.59865 | 0.05770  | 0.61636  | 4.673    |
| H14B | 0.62263 | 0.11046  | 0.67999  | 4.673    |
| H14C | 0.57650 | 0.02821  | 0.68471  | 4.673    |
| H15A | 0.42136 | 0.27764  | 0.50192  | 3.699    |
| H15B | 0.46071 | 0.23690  | 0.44280  | 3.699    |
| H15C | 0.34265 | 0.21348  | 0.46100  | 3.699    |
| H16A | 0.65819 | 0.16528  | 0.58428  | 4.265    |
| H16B | 0.64838 | 0.20604  | 0.51485  | 4.265    |
| H16C | 0.61364 | 0.24878  | 0.57445  | 4.265    |
| H17A | 0.52825 | 0.06343  | 0.51903  | 4.468    |
| H17B | 0.40612 | 0.08628  | 0.47116  | 4.468    |
| H17C | 0.52418 | 0.10969  | 0.45296  | 4.468    |
| H21A | 0.24317 | 0.23353  | 0.74926  | 3.127    |
| H21B | 0.17069 | 0.18347  | 0.78802  | 3.127    |
| H21C | 0.14325 | 0.18028  | 0.70876  | 3.127    |
| H22A | -0.09772| 0.27773  | 0.73782  | 3.849    |
| H22B | -0.06146| 0.20673  | 0.70190  | 3.849    |
| H22C | -0.03401| 0.20992  | 0.78115  | 3.849    |
| H23A | 0.06338 | 0.36098  | 0.80645  | 3.889    |
| H23B | 0.11991 | 0.28887  | 0.84585  | 3.889    |
| H23C | 0.19553 | 0.34030  | 0.81015  | 3.889    |
Table S10-2. Atomic coordinates and $B_{\text{iso}}$ involving hydrogens/$B_{\text{eq}}$ (continued)

| atom   | x       | y       | z       | $B_{\text{eq}}$ |
|--------|---------|---------|---------|-----------------|
| H24A   | 0.05234 | 0.41045 | 0.57371 | 3.560           |
| H24B   | -0.04043| 0.46898 | 0.58650 | 3.560           |
| H24C   | 0.08663 | 0.46600 | 0.63525 | 3.560           |
| H25A   | -0.09028| 0.31011 | 0.57260 | 3.326           |
| H25B   | -0.15423| 0.30328 | 0.63159 | 3.326           |
| H25C   | -0.17875| 0.37291 | 0.58284 | 3.326           |
| H26A   | 0.00243 | 0.44975 | 0.73342 | 3.499           |
| H26B   | -0.12139| 0.45918 | 0.68219 | 3.499           |
| H26C   | -0.09688| 0.38954 | 0.73094 | 3.499           |
| H30A   | 0.12255 | 0.38120 | 0.42408 | 4.662           |
| H30B   | 0.17598 | 0.32127 | 0.38352 | 4.662           |
| H30C   | 0.06558 | 0.36887 | 0.34669 | 4.662           |
| H31A   | -0.07394| 0.35923 | 0.44589 | 4.692           |
| H31B   | -0.11990| 0.35183 | 0.36707 | 4.692           |
| H31C   | -0.14731| 0.28833 | 0.41444 | 4.692           |
| H32A   | 0.07168 | 0.20575 | 0.34587 | 3.840           |
| H32B   | -0.05789| 0.19424 | 0.35318 | 3.840           |
| H32C   | -0.03048| 0.25775 | 0.30582 | 3.840           |
| H33A   | 0.16312 | 0.17163 | 0.58401 | 3.223           |
| H33B   | 0.04002 | 0.20083 | 0.59136 | 3.223           |
| H33C   | 0.05972 | 0.11458 | 0.58199 | 3.223           |
| H34A   | -0.12349| 0.16656 | 0.42796 | 4.509           |
| H34B   | -0.11030| 0.11154 | 0.48955 | 4.509           |
| H34C   | -0.12999| 0.19780 | 0.49891 | 4.509           |
| H35A   | 0.07550 | 0.11736 | 0.41419 | 4.097           |
| H35B   | 0.18368 | 0.11901 | 0.47764 | 4.097           |
| H35C   | 0.07746 | 0.06432 | 0.47596 | 4.097           |
Table S10-3. Anisotropic displacement parameters

| atom | U_{11}   | U_{22}   | U_{33}   | U_{12}  | U_{13}  | U_{23}  |
|------|----------|----------|----------|---------|---------|---------|
| Nb1  | 0.01033(19) | 0.0289(2) | 0.0278(2) | 0.00174(13) | 0.00729(13) | -0.00088(13) |
| F1   | 0.0222(12) | 0.0364(13) | 0.0511(14) | 0.0063(10) | 0.0137(11) | 0.0029(11) |
| F2   | 0.0130(11) | 0.0504(15) | 0.0560(15) | 0.0001(11) | 0.0070(10) | 0.0086(12) |
| F3   | 0.0323(15) | 0.0405(14) | 0.0544(15) | -0.0123(11) | 0.0123(12) | -0.0021(12) |
| F4   | 0.0352(15) | 0.0324(13) | 0.0717(18) | 0.0012(11) | 0.0245(13) | -0.0022(13) |
| F5   | 0.0155(12) | 0.0398(14) | 0.0620(16) | 0.0056(10) | 0.0123(11) | 0.0042(12) |
| O1   | 0.0165(13) | 0.0322(14) | 0.0357(14) | -0.0004(11) | 0.0051(11) | -0.0002(12) |
| N1   | 0.0120(15) | 0.0345(18) | 0.0300(16) | 0.0013(13) | 0.0085(12) | -0.0003(13) |
| N2   | 0.0139(15) | 0.0356(18) | 0.0343(17) | 0.0018(13) | 0.0096(13) | -0.0015(14) |
| N3   | 0.0119(15) | 0.0359(18) | 0.0330(17) | 0.0004(13) | 0.0036(13) | -0.0053(14) |
| N4   | 0.0185(17) | 0.0329(19) | 0.0309(17) | 0.0013(14) | 0.0073(13) | 0.0009(15) |
| C1   | 0.0153(18) | 0.038(2)   | 0.0270(18) | -0.0043(16) | 0.0088(14) | 0.0039(16) |
| C2   | 0.022(2)   | 0.038(2)   | 0.033(2)   | -0.0059(17) | 0.0117(16) | -0.0015(17) |
| C3   | 0.030(2)   | 0.043(2)   | 0.043(2)   | -0.011(2)   | 0.0139(19) | -0.004(2)   |
| C4   | 0.026(2)   | 0.065(3)   | 0.042(2)   | -0.021(2)   | 0.0070(19) | -0.009(2)   |
| C5   | 0.0132(19) | 0.069(3)   | 0.044(2)   | -0.010(2)   | 0.0057(17) | -0.001(2)   |
| C6   | 0.0140(18) | 0.051(3)   | 0.035(2)   | -0.0059(18) | 0.0094(15) | 0.0027(18)  |
| C7   | 0.024(2)   | 0.040(2)   | 0.043(2)   | 0.0023(18)  | 0.0113(17) | -0.0078(19) |
| C8   | 0.0133(19) | 0.055(3)   | 0.045(2)   | 0.0041(18)  | 0.0084(17) | 0.003(2)    |
| C9   | 0.0186(19) | 0.033(2)   | 0.037(2)   | 0.0030(16)  | 0.0143(16) | 0.0003(16)  |
| C10  | 0.023(2)   | 0.034(2)   | 0.044(2)   | 0.0098(17)  | 0.0175(17) | 0.0057(18)  |
| C11  | 0.032(2)   | 0.035(2)   | 0.045(2)   | 0.0050(18)  | 0.026(2)   | -0.0006(18) |
| C12  | 0.036(3)   | 0.041(2)   | 0.042(2)   | 0.008(2)    | 0.0181(19) | 0.006(2)    |
| C13  | 0.043(3)   | 0.033(2)   | 0.051(3)   | 0.002(2)    | 0.024(2)   | 0.001(2)    |
| C14  | 0.030(3)   | 0.055(3)   | 0.069(3)   | 0.017(2)    | 0.025(2)   | 0.021(3)    |
| C15  | 0.043(3)   | 0.041(3)   | 0.041(2)   | 0.003(2)    | 0.025(2)   | -0.0007(19) |
| C16  | 0.029(3)   | 0.050(3)   | 0.064(3)   | 0.005(2)    | 0.027(2)   | 0.009(2)    |
| C17  | 0.059(3)   | 0.040(3)   | 0.053(3)   | 0.005(2)    | 0.035(3)   | -0.001(2)   |
| C18  | 0.0126(18) | 0.035(2)   | 0.0288(18) | -0.0029(15) | 0.0060(14) | -0.0044(15) |
| C19  | 0.0152(18) | 0.041(2)   | 0.034(2)   | 0.0029(16)  | 0.0117(15) | 0.0001(17)  |
| C20  | 0.0147(18) | 0.040(2)   | 0.0317(19) | 0.0043(16)  | 0.0070(15) | -0.0035(17) |
| C21  | 0.020(2)   | 0.043(2)   | 0.036(2)   | 0.0051(18)  | 0.0075(16) | 0.0028(18)  |
| C22  | 0.020(2)   | 0.053(3)   | 0.053(3)   | 0.001(2)    | 0.0165(19) | 0.010(2)    |
| C23  | 0.042(3)   | 0.050(3)   | 0.031(2)   | 0.008(2)    | 0.0093(19) | 0.0014(19)  |
| C24  | 0.021(2)   | 0.043(2)   | 0.048(2)   | 0.0072(18)  | 0.0077(18) | 0.006(2)    |
| C25  | 0.016(2)   | 0.049(2)   | 0.038(2)   | 0.0027(18)  | 0.0019(16) | -0.0046(19) |
| C26  | 0.022(2)   | 0.048(3)   | 0.041(2)   | 0.0089(19)  | 0.0077(17) | -0.010(2)   |
Table S10-3. Anisotropic displacement parameters (continued)

| atom | U11     | U22     | U33     | U12     | U13     | U23     |
|------|---------|---------|---------|---------|---------|---------|
| C27  | 0.0154(18) | 0.036(2) | 0.0337(19) | 0.0025(16) | 0.0096(15) | -0.0040(17) |
| C28  | 0.021(2)   | 0.040(2) | 0.036(2) | 0.0025(18) | 0.0036(16) | 0.0003(18) |
| C29  | 0.024(2)   | 0.040(2) | 0.036(2) | -0.0029(17) | 0.0092(17) | -0.0049(18) |
| C30  | 0.044(3)   | 0.060(3) | 0.037(2) | -0.013(3)  | -0.001(2)  | 0.009(2)  |
| C31  | 0.033(3)   | 0.072(4) | 0.040(3) | 0.016(2)   | 0.001(2)   | -0.004(2) |
| C32  | 0.039(3)   | 0.049(3) | 0.034(2) | 0.002(2)   | 0.0107(19) | -0.003(2) |
| C33  | 0.030(2)   | 0.040(2) | 0.033(2) | -0.0063(19) | 0.0099(18) | -0.0020(18) |
| C34  | 0.032(3)   | 0.066(3) | 0.044(3) | -0.019(2)  | 0.008(2)   | -0.002(2) |
| C35  | 0.050(3)   | 0.038(2) | 0.044(2) | 0.000(2)   | 0.017(2)   | -0.006(2) |
| C36  | 0.0204(19) | 0.033(2) | 0.0269(17) | -0.0011(16) | 0.0090(14) | 0.0001(15) |
| C37  | 0.0218(19) | 0.031(2) | 0.0307(19) | 0.0046(16) | 0.0084(15) | 0.0044(16) |
| C38  | 0.0164(19) | 0.045(2) | 0.0327(19) | -0.0007(17) | 0.0098(15) | 0.0082(17) |
| C39  | 0.023(2)   | 0.035(2) | 0.036(2) | -0.0065(17) | 0.0097(16) | -0.0005(17) |
| C40  | 0.029(2)   | 0.031(2) | 0.040(2) | 0.0034(17) | 0.0169(18) | 0.0043(17) |
| C41  | 0.0175(19) | 0.037(2) | 0.0339(19) | 0.0029(16) | 0.0104(15) | 0.0025(17) |

The general temperature factor expression: $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2abU_{12}ilk + 2acU_{13}ihk + 2bcU_{23}hkl))$
Table S10-4. Bond lengths (Å)

| atom | atom | distance  | atom | atom | distance  |
|------|------|-----------|------|------|-----------|
| Nb1  | O1   | 2.066(3)  | Nb1  | N1   | 1.796(3)  |
| Nb1  | N2   | 1.963(4)  | Nb1  | N3   | 1.965(4)  |
| Nb1  | N4   | 2.443(3)  | F1   | C37  | 1.347(5)  |
| F2   | C38  | 1.342(5)  | F3   | C39  | 1.350(5)  |
| F4   | C40  | 1.347(5)  | F5   | C41  | 1.350(5)  |
| O1   | C36  | 1.333(5)  | N1   | C1   | 1.385(5)  |
| N2   | C9   | 1.265(5)  | N3   | C18  | 1.255(6)  |
| N4   | C27  | 1.271(5)  | C1   | C2   | 1.413(6)  |
| C1   | C6   | 1.416(5)  | C2   | C3   | 1.389(6)  |
| C2   | C7   | 1.495(6)  | C3   | C4   | 1.377(6)  |
| C4   | C5   | 1.377(8)  | C5   | C6   | 1.392(6)  |
| C6   | C8   | 1.495(7)  | C9   | C10  | 1.557(6)  |
| C9   | C11  | 1.567(7)  | C10  | C12  | 1.534(7)  |
| C10  | C13  | 1.540(6)  | C10  | C14  | 1.548(6)  |
| C11  | C15  | 1.525(6)  | C11  | C16  | 1.532(7)  |
| C11  | C17  | 1.525(7)  | C18  | C19  | 1.566(6)  |
| C18  | C20  | 1.559(5)  | C19  | C21  | 1.524(6)  |
| C19  | C22  | 1.531(6)  | C19  | C23  | 1.546(6)  |
| C20  | C24  | 1.550(7)  | C20  | C25  | 1.542(5)  |
| C20  | C26  | 1.538(7)  | C27  | C28  | 1.548(6)  |
| C27  | C29  | 1.548(6)  | C28  | C30  | 1.551(7)  |
| C28  | C31  | 1.536(7)  | C28  | C32  | 1.528(6)  |
| C29  | C33  | 1.531(6)  | C29  | C34  | 1.540(7)  |
| C29  | C35  | 1.547(7)  | C36  | C37  | 1.399(6)  |
| C36  | C41  | 1.396(6)  | C37  | C38  | 1.373(6)  |
| C38  | C39  | 1.373(6)  | C39  | C40  | 1.386(6)  |
| C40  | C41  | 1.370(6)  |
Table S10-5. Bond lengths involving hydrogens (Å)

| atom  | atom | distance | atom  | atom | distance |
|-------|------|----------|-------|------|----------|
| N4    | H1   | 0.76(3)  | C3    | H3   | 0.950    |
| C4    | H4   | 0.950    | C5    | H5   | 0.950    |
| C7    | H7A  | 0.980    | C7    | H7B  | 0.980    |
| C7    | H7C  | 0.980    | C8    | H8A  | 0.980    |
| C8    | H8B  | 0.980    | C8    | H8C  | 0.980    |
| C12   | H12A | 0.980    | C12   | H12B | 0.980    |
| C12   | H12C | 0.980    | C13   | H13A | 0.980    |
| C13   | H13B | 0.980    | C13   | H13C | 0.980    |
| C14   | H14A | 0.980    | C14   | H14B | 0.980    |
| C14   | H14C | 0.980    | C15   | H15A | 0.980    |
| C15   | H15B | 0.980    | C15   | H15C | 0.980    |
| C16   | H16A | 0.980    | C16   | H16B | 0.980    |
| C16   | H16C | 0.980    | C17   | H17A | 0.980    |
| C17   | H17B | 0.980    | C17   | H17C | 0.980    |
| C21   | H21A | 0.980    | C21   | H21B | 0.980    |
| C21   | H21C | 0.980    | C22   | H22A | 0.980    |
| C22   | H22B | 0.980    | C22   | H22C | 0.980    |
| C23   | H23A | 0.980    | C23   | H23B | 0.980    |
| C23   | H23C | 0.980    | C24   | H24A | 0.980    |
| C24   | H24B | 0.980    | C24   | H24C | 0.980    |
| C25   | H25A | 0.980    | C25   | H25B | 0.980    |
| C25   | H25C | 0.980    | C26   | H26A | 0.980    |
| C26   | H26B | 0.980    | C26   | H26C | 0.980    |
| C30   | H30A | 0.980    | C30   | H30B | 0.980    |
| C30   | H30C | 0.980    | C31   | H31A | 0.980    |
| C31   | H31B | 0.980    | C31   | H31C | 0.980    |
| C32   | H32A | 0.980    | C32   | H32B | 0.980    |
| C32   | H32C | 0.980    | C33   | H33A | 0.980    |
| C33   | H33B | 0.980    | C33   | H33C | 0.980    |
| C34   | H34A | 0.980    | C34   | H34B | 0.980    |
| C34   | H34C | 0.980    | C35   | H35A | 0.980    |
| C35   | H35B | 0.980    | C35   | H35C | 0.980    |
Table S10-6. Bond angles (°)

| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| O1   | Nb1  | N1   | 93.68(13) | O1   | Nb1  | N2   | 111.40(13) |
| O1   | Nb1  | N3   | 115.97(12) | O1   | Nb1  | N4   | 72.68(11) |
| N1   | Nb1  | N2   | 103.15(13) | N1   | Nb1  | N3   | 99.00(15)  |
| N1   | Nb1  | N4   | 165.90(13) | N2   | Nb1  | N3   | 125.63(14) |
| N2   | Nb1  | N4   | 85.60(12)  | N3   | Nb1  | N4   | 84.32(13)  |
| Nb1  | O1   | C36  | 123.9(2)   | Nb1  | N1   | C1   | 170.1(3)   |
| Nb1  | N2   | C9   | 175.6(3)   | Nb1  | N3   | C18  | 178.8(3)   |
| Nb1  | N4   | C27  | 160.7(3)   | N1   | C1   | C2   | 119.7(3)   |
| N1   | C1   | C6   | 120.3(4)   | C2   | C1   | C6   | 120.1(3)   |
| C1   | C2   | C3   | 118.9(4)   | C1   | C2   | C7   | 120.4(3)   |
| C3   | C2   | C7   | 120.7(4)   | C2   | C3   | C4   | 121.1(4)   |
| C3   | C4   | C5   | 120.0(4)   | C4   | C5   | C6   | 121.6(4)   |
| C1   | C6   | C5   | 118.3(4)   | C1   | C6   | C8   | 120.3(3)   |
| C5   | C6   | C8   | 121.4(4)   | N2   | C9   | C10  | 119.1(4)   |
| N2   | C9   | C11  | 117.9(4)   | C10  | C9   | C11  | 123.0(4)   |
| C9   | C10  | C12  | 109.3(4)   | C9   | C10  | C13  | 111.2(3)   |
| C9   | C10  | C14  | 112.4(4)   | C12  | C10  | C13  | 106.6(4)   |
| C12  | C10  | C14  | 106.9(4)   | C13  | C10  | C14  | 110.2(4)   |
| C9   | C11  | C15  | 109.2(4)   | C9   | C11  | C16  | 108.5(4)   |
| C9   | C11  | C17  | 115.0(4)   | C15  | C11  | C16  | 107.5(4)   |
| C15  | C11  | C17  | 106.7(4)   | C16  | C11  | C17  | 109.8(4)   |
| N3   | C18  | C19  | 119.0(3)   | N3   | C18  | C20  | 118.5(4)   |
| C19  | C18  | C20  | 122.4(4)   | C18  | C19  | C21  | 109.3(4)   |
| C18  | C19  | C22  | 114.2(3)   | C18  | C19  | C23  | 109.1(3)   |
| C21  | C19  | C22  | 107.8(4)   | C21  | C19  | C23  | 106.6(3)   |
| C22  | C19  | C23  | 109.5(4)   | C18  | C20  | C24  | 109.7(3)   |
| C18  | C20  | C25  | 109.0(3)   | C18  | C20  | C26  | 114.0(3)   |
| C24  | C20  | C25  | 105.9(3)   | C24  | C20  | C26  | 107.1(4)   |
| C25  | C20  | C26  | 110.7(3)   | N4   | C27  | C28  | 119.5(4)   |
| N4   | C27  | C29  | 118.1(3)   | C28  | C27  | C29  | 122.4(3)   |
| C27  | C28  | C30  | 110.8(3)   | C27  | C28  | C31  | 108.9(4)   |
| C27  | C28  | C32  | 114.7(4)   | C30  | C28  | C31  | 106.4(4)   |
| C30  | C28  | C32  | 105.5(4)   | C31  | C28  | C32  | 110.1(4)   |
| C27  | C29  | C33  | 109.8(3)   | C27  | C29  | C34  | 114.3(4)   |
| C27  | C29  | C35  | 108.7(4)   | C33  | C29  | C34  | 106.2(4)   |
| C33  | C29  | C35  | 107.4(3)   | C34  | C29  | C35  | 110.3(4)   |
| O1   | C36  | C37  | 123.0(4)   | O1   | C36  | C41  | 122.0(3)   |
Table S10-6. Bond angles (°) (continued)

| atom | atom | atom | angle   | atom | atom | atom | angle   |
|------|------|------|---------|------|------|------|---------|
| C37  | C36  | C41  | 114.9(4)| F1   | C37  | C36  | 119.0(3)|
| F1   | C37  | C38  | 118.2(4)| C36  | C37  | C38  | 122.8(4)|
| F2   | C38  | C37  | 120.3(4)| F2   | C38  | C39  | 119.4(4)|
| C37  | C38  | C39  | 120.2(4)| F3   | C39  | C38  | 120.6(4)|
| F3   | C39  | C40  | 120.5(4)| C38  | C39  | C40  | 118.8(4)|
| F4   | C40  | C39  | 119.3(4)| F4   | C40  | C41  | 120.5(4)|
| C39  | C40  | C41  | 120.1(4)| F5   | C41  | C36  | 118.3(3)|
| F5   | C41  | C40  | 118.8(4)| C36  | C41  | C40  | 122.9(4)|
Table S10-7. Bond angles involving hydrogens (°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| Nb1  | N4   | H1   | 90(2) | C27  | N4   | H1   | 109(2) |
| C2   | C3   | H3   | 119.4 | C4   | C3   | H3   | 119.4 |
| C3   | C4   | H4   | 120.0 | C5   | C4   | H4   | 120.0 |
| C4   | C5   | H5   | 119.2 | C6   | C5   | H5   | 119.2 |
| C2   | C7   | H7A  | 109.5 | C2   | C7   | H7B  | 109.5 |
| C2   | C7   | H7C  | 109.5 | H7A  | C7   | H7B  | 109.5 |
| C6   | C8   | H8A  | 109.5 | C6   | C8   | H8B  | 109.5 |
| C6   | C8   | H8C  | 109.5 | H8A  | C8   | H8B  | 109.5 |
| H8A  | C8   | H8C  | 109.5 | H8B  | C8   | H8C  | 109.5 |
| C10  | C12  | H12A | 109.5 | C10  | C12  | H12B | 109.5 |
| C10  | C12  | H12C | 109.5 | H12A | C12  | H12B | 109.5 |
| H12A | C12  | H12C | 109.5 | H12B | C12  | H12C | 109.5 |
| C10  | C13  | H13A | 109.5 | C10  | C13  | H13B | 109.5 |
| C10  | C13  | H13C | 109.5 | H13A | C13  | H13B | 109.5 |
| H13A | C13  | H13C | 109.5 | H13B | C13  | H13C | 109.5 |
| C10  | C14  | H14A | 109.5 | C10  | C14  | H14B | 109.5 |
| C10  | C14  | H14C | 109.5 | H14A | C14  | H14B | 109.5 |
| H14A | C14  | H14C | 109.5 | H14B | C14  | H14C | 109.5 |
| C11  | C15  | H15A | 109.5 | C11  | C15  | H15B | 109.5 |
| C11  | C15  | H15C | 109.5 | H15A | C15  | H15B | 109.5 |
| H15A | C15  | H15C | 109.5 | H15B | C15  | H15C | 109.5 |
| C11  | C16  | H16A | 109.5 | C11  | C16  | H16B | 109.5 |
| C11  | C16  | H16C | 109.5 | H16A | C16  | H16B | 109.5 |
| H16A | C16  | H16C | 109.5 | H16B | C16  | H16C | 109.5 |
| C11  | C17  | H17A | 109.5 | C11  | C17  | H17B | 109.5 |
| C11  | C17  | H17C | 109.5 | H17A | C17  | H17B | 109.5 |
| H17A | C17  | H17C | 109.5 | H17B | C17  | H17C | 109.5 |
| C19  | C21  | H21A | 109.5 | C19  | C21  | H21B | 109.5 |
| C19  | C21  | H21C | 109.5 | H21A | C21  | H21B | 109.5 |
| H21A | C21  | H21C | 109.5 | H21B | C21  | H21C | 109.5 |
| C19  | C22  | H22A | 109.5 | C19  | C22  | H22B | 109.5 |
| C19  | C22  | H22C | 109.5 | H22A | C22  | H22B | 109.5 |
| H22A | C22  | H22C | 109.5 | H22B | C22  | H22C | 109.5 |
| C19  | C23  | H23A | 109.5 | C19  | C23  | H23B | 109.5 |
| C19  | C23  | H23C | 109.5 | H23A | C23  | H23B | 109.5 |
| H23A | C23  | H23C | 109.5 | H23B | C23  | H23C | 109.5 |
Table S10-7. Bond angles involving hydrogens (°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|------|------|------|-------|------|------|------|-------|
| C20  | C24  | H24A | 109.5 | C20  | C24  | H24B | 109.5 |
| C20  | C24  | H24C | 109.5 | H24A | C24  | H24B | 109.5 |
| H24A | C24  | H24C | 109.5 | H24B | C24  | H24C | 109.5 |
| C20  | C25  | H25A | 109.5 | C20  | C25  | H25B | 109.5 |
| C20  | C25  | H25C | 109.5 | H25A | C25  | H25B | 109.5 |
| H25A | C25  | H25C | 109.5 | H25B | C25  | H25C | 109.5 |
| C20  | C26  | H26A | 109.5 | C26  | H26B | C26  | 109.5 |
| C20  | C26  | H26C | 109.5 | H26A | C26  | H26B | 109.5 |
| H26A | C26  | H26C | 109.5 | H26B | C26  | H26C | 109.5 |
| C28  | C30  | H30A | 109.5 | H30A | C30  | H30B | 109.5 |
| C28  | C30  | H30C | 109.5 | H30B | C30  | H30C | 109.5 |
| C28  | C31  | H31A | 109.5 | C28  | C31  | H31B | 109.5 |
| C28  | C31  | H31C | 109.5 | H31A | C31  | H31B | 109.5 |
| H31A | C31  | H31C | 109.5 | H31B | C31  | H31C | 109.5 |
| C28  | C32  | H32A | 109.5 | C28  | C32  | H32B | 109.5 |
| C28  | C32  | H32C | 109.5 | H32A | C32  | H32B | 109.5 |
| H32A | C32  | H32C | 109.5 | H32B | C32  | H32C | 109.5 |
| C29  | C33  | H33A | 109.5 | C29  | C33  | H33B | 109.5 |
| C29  | C33  | H33C | 109.5 | H33A | C33  | H33B | 109.5 |
| H33A | C33  | H33C | 109.5 | H33B | C33  | H33C | 109.5 |
| C29  | C34  | H34A | 109.5 | C29  | C34  | H34B | 109.5 |
| C29  | C34  | H34C | 109.5 | H34A | C34  | H34B | 109.5 |
| H34A | C34  | H34C | 109.5 | H34B | C34  | H34C | 109.5 |
| C29  | C35  | H35A | 109.5 | C29  | C35  | H35B | 109.5 |
| C29  | C35  | H35C | 109.5 | H35A | C35  | H35B | 109.5 |
| H35A | C35  | H35C | 109.5 | H35B | C35  | H35C | 109.5 |
Table S10-8. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

| atom1 | atom2 | atom3 | atom4 | angle  | atom1 | atom2 | atom3 | atom4 | angle  |
|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|
| N1    | Nb1   | O1    | C36   | 1.4(2) | N2    | Nb1   | O1    | C36   | -104.3(2) |
| N3    | Nb1   | O1    | C36   | 103.2(2) | N4    | Nb1   | O1    | C36   | 177.7(2) |
| Nb1   | O1    | C36   | C37   | 67.6(4) | Nb1   | O1    | C36   | C41   | -112.7(3) |
| N1    | C1    | C2    | C3    | -178.8(3) | N1    | C1    | C2    | C7    | 1.2(6) |
| N1    | C1    | C6    | C5    | 178.8(3) | N1    | C1    | C6    | C8    | -0.7(6) |
| C2    | C1    | C6    | C5    | -1.9(6) | C2    | C1    | C6    | C8    | 178.6(3) |
| C6    | C1    | C2    | C3    | 1.9(6) | C6    | C1    | C2    | C7    | -178.1(3) |
| C1    | C2    | C3    | C4    | -0.3(6) | C7    | C2    | C3    | C4    | 179.7(4) |
| C2    | C3    | C4    | C5    | -1.3(7) | C3    | C4    | C5    | C6    | 1.3(7) |
| C4    | C5    | C6    | C1    | 0.3(7) | C4    | C5    | C6    | C8    | 179.8(4) |
| N2    | C9    | C10   | C12   | -12.5(5) | N2    | C9    | C10   | C13   | 105.0(4) |
| N2    | C9    | C10   | C14   | -131.0(4) | N2    | C9    | C11   | C15   | -25.1(5) |
| N2    | C9    | C11   | C16   | 91.8(4) | N2    | C9    | C11   | C17   | -144.9(3) |
| C10   | C9    | C11   | C15   | 157.3(3) | C10   | C9    | C11   | C16   | -85.8(4) |
| C10   | C9    | C11   | C17   | 37.5(5) | C11   | C9    | C10   | C12   | 165.1(3) |
| C11   | C9    | C10   | C13   | -77.5(4) | C11   | C9    | C10   | C14   | 46.6(5) |
| N3    | C18   | C19   | C21   | -16.9(4) | N3    | C18   | C19   | C22   | -137.8(3) |
| N3    | C18   | C19   | C23   | 99.4(4) | N3    | C18   | C20   | C24   | -16.5(4) |
| N3    | C18   | C20   | C25   | 99.1(4) | N3    | C18   | C20   | C26   | -136.6(3) |
| C19   | C18   | C20   | C24   | 162.6(3) | C19   | C18   | C20   | C25   | -81.8(4) |
| C19   | C18   | C20   | C26   | 42.5(5) | C20   | C18   | C19   | C21   | 164.0(3) |
| C20   | C18   | C19   | C22   | 43.1(5) | C20   | C18   | C19   | C23   | -79.7(4) |
| N4    | C27   | C28   | C30   | 20.1(5) | N4    | C27   | C28   | C31   | -96.6(4) |
| N4    | C27   | C28   | C32   | 139.5(4) | N4    | C27   | C29   | C33   | 17.8(5) |
| N4    | C27   | C29   | C34   | 137.0(4) | N4    | C27   | C29   | C35   | -99.4(4) |
| C28   | C27   | C29   | C33   | -163.0(3) | C28   | C27   | C29   | C34   | -43.8(5) |
| C28   | C27   | C29   | C35   | 79.9(4) | C29   | C27   | C28   | C30   | -159.1(4) |
| C29   | C27   | C28   | C31   | 84.2(5) | C29   | C27   | C28   | C32   | -39.7(5) |
| O1    | C36   | C37   | F1    | 2.7(6) | O1    | C36   | C37   | C38   | -175.9(3) |
| O1    | C36   | C41   | F5    | -1.2(6) | O1    | C36   | C41   | C40   | 176.0(3) |
| C37   | C36   | C41   | F5    | 178.5(3) | C37   | C36   | C41   | C40   | -4.3(6) |
| C41   | C36   | C37   | F1    | -177.0(3) | C41   | C36   | C37   | C38   | 4.5(5) |
| F1    | C37   | C38   | F2    | -0.2(6) | F1    | C37   | C38   | C39   | -179.7(3) |
| C36   | C37   | C38   | F2    | 178.4(3) | C36   | C37   | C38   | C39   | -1.2(6) |
| F2    | C38   | C39   | F3    | -1.4(6) | F2    | C38   | C39   | C40   | 177.9(3) |
| C37   | C38   | C39   | F3    | 178.2(3) | C37   | C38   | C39   | C40   | -2.6(6) |
| F3    | C39   | C40   | F4    | 0.5(6) | F3    | C39   | C40   | C41   | -178.0(3) |
Table S10-8. Torsion angles (°) (continued)

| atom1 | atom2 | atom3 | atom4 | angle   | atom1 | atom2 | atom3 | atom4 | angle   |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| C38   | C39   | C40   | F4    | -178.7(4) | C38   | C39   | C40   | C41   | 2.7(6)  |
| F4    | C40   | C41   | F5    | -0.4(6)  | F4    | C40   | C41   | C36   | -177.7(3) |
| C39   | C40   | C41   | F5    | 178.0(4) | C39   | C40   | C41   | C36   | 0.8(6)  |
Table S10-9. Intramolecular contacts less than 3.60 Å

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | F1   | 3.528(3) | F1   | F2   | 2.688(3) |
| F1   | O1   | 2.778(4) | F1   | N1   | 3.211(4) |
| F1   | C1   | 3.522(5) | F1   | C6   | 3.531(5) |
| F1   | C8   | 3.244(5) | F1   | C15  | 3.466(5) |
| F1   | C16  | 3.401(6) | F1   | C39  | 3.596(5) |
| F1   | C41  | 3.597(5) | F2   | F3   | 2.720(4) |
| F3   | F4   | 2.731(4) | F4   | F5   | 2.705(4) |
| F5   | O1   | 2.743(4) | F5   | C24  | 3.422(6) |
| F5   | C37  | 3.595(5) | N1   | C7   | 2.856(6) |
| N1   | C8   | 2.870(5) | N1   | C36  | 3.003(5) |
| N1   | C37  | 3.190(5) | N2   | C12  | 2.714(6) |
| N2   | C13  | 3.397(6) | N2   | C15  | 2.735(6) |
| N2   | C16  | 3.233(7) | N3   | C21  | 2.726(6) |
| N3   | C23  | 3.324(6) | N3   | C24  | 2.727(5) |
| N3   | C25  | 3.306(5) | N3   | C33  | 3.372(5) |
| N4   | C15  | 3.566(6) | N4   | C30  | 2.783(6) |
| N4   | C31  | 3.293(6) | N4   | C33  | 2.712(6) |
| N4   | C35  | 3.304(6) | C1   | C4   | 2.785(6) |
| C1   | C36  | 3.468(5) | C1   | C37  | 3.316(6) |
| C2   | C5   | 2.784(6) | C3   | C6   | 2.794(7) |
| C10  | C16  | 3.456(8) | C10  | C17  | 3.179(8) |
| C11  | C13  | 3.430(7) | C11  | C14  | 3.191(7) |
| C13  | C17  | 3.261(8) | C14  | C16  | 3.298(8) |
| C14  | C17  | 3.406(8) | C19  | C25  | 3.427(5) |
| C19  | C26  | 3.183(6) | C20  | C22  | 3.191(7) |
| C20  | C23  | 3.411(6) | C22  | C25  | 3.271(7) |
| C22  | C26  | 3.426(7) | C23  | C26  | 3.229(6) |
| C28  | C34  | 3.176(8) | C28  | C35  | 3.380(6) |
| C29  | C31  | 3.419(7) | C29  | C32  | 3.151(6) |
| C31  | C34  | 3.284(8) | C32  | C34  | 3.380(8) |
| C32  | C35  | 3.212(6) | C36  | C39  | 2.823(6) |
| C37  | C40  | 2.733(6) | C38  | C41  | 2.736(6) |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| Nb1  | H7A  | 3.071    | Nb1  | H8A  | 3.342    |
| Nb1  | H12B | 3.528    | Nb1  | H15A | 3.174    |
| Nb1  | H21A | 3.320    | Nb1  | H24A | 3.344    |
| Nb1  | H33A | 3.054    | F1   | H8A  | 2.919    |
| F1   | H8B  | 2.930    | F1   | H15A | 2.616    |
| F1   | H16C | 2.513    | F2   | H8B  | 3.564    |
| F5   | H7A  | 3.485    | F5   | H7C  | 3.279    |
| F5   | H24A | 3.159    | F5   | H24C | 2.975    |
| O1   | H1   | 2.21(3)  | O1   | H7A  | 3.478    |
| O1   | H15A | 2.814    | O1   | H24A | 3.238    |
| O1   | H30A | 2.981    | N1   | H7B  | 3.519    |
| N1   | H7B  | 3.519    | N1   | H7C  | 3.508    |
| N1   | H8A  | 2.390    | N1   | H8B  | 3.519    |
| N1   | H8C  | 3.535    | N1   | H21A | 3.477    |
| N2   | H1   | 3.38(3)  | N2   | H8A  | 2.919    |
| N2   | H12A | 2.697    | N2   | H12B | 2.558    |
| N2   | H13C | 3.267    | N2   | H15A | 2.461    |
| N2   | H15C | 2.864    | N2   | H16A | 3.597    |
| N2   | H16C | 3.022    | N2   | H33A | 2.676    |
| N2   | H35B | 3.571    | N3   | H7A  | 2.720    |
| N3   | H7A  | 2.720    | N3   | H21A | 2.489    |
| N3   | H21C | 2.801    | N3   | H23C | 3.153    |
| N3   | H24A | 2.505    | N3   | H24C | 2.800    |
| N3   | H25A | 3.111    | N3   | H33A | 3.083    |
| N3   | H33B | 2.780    | N4   | H15A | 3.236    |
| N4   | H15C | 3.011    | N4   | H24A | 3.000    |
| N4   | H25A | 3.463    | N4   | H30A | 2.546    |
| N4   | H30B | 2.888    | N4   | H31A | 3.082    |
| N4   | H33A | 2.480    | N4   | H33B | 2.789    |
| N4   | H35B | 3.131    | C1   | H3   | 3.273    |
| C1   | H5   | 3.270    | C1   | H7A  | 2.554    |
| C1   | H7B  | 3.146    | C1   | H7C  | 3.146    |
| C1   | H8A  | 2.554    | C1   | H8B  | 3.145    |
| C1   | H8C  | 3.150    | C2   | H4   | 3.264    |
| C3   | H5   | 3.238    | C3   | H7A  | 3.301    |
| C3   | H7B  | 2.754    | C3   | H7C  | 2.754    |
| C5   | H3   | 3.239    | C5   | H8A  | 3.308    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C5   | H8B  | 2.766    | C5   | H8C  | 2.766    |
| C6   | H4   | 3.270    | C7   | H3   | 2.659    |
| C7   | H23C | 3.567    | C7   | H24C | 2.980    |
| C8   | H5   | 2.671    | C8   | H12A | 3.598    |
| C8   | H16C | 3.241    | C9   | H8A  | 3.283    |
| C9   | H12A | 2.699    | C9   | H13A | 2.749    |
| C9   | H12C | 3.372    | C9   | H13B | 2.735    |
| C9   | H13B | 3.397    | C9   | H14A | 2.777    |
| C9   | H14C | 3.417    | C9   | H15A | 2.661    |
| C9   | H15B | 3.372    | C9   | H15C | 2.735    |
| C9   | H16A | 2.706    | C9   | H16B | 3.369    |
| C9   | H16C | 2.674    | C9   | H17A | 2.798    |
| C9   | H17B | 2.815    | C9   | H17C | 3.437    |
| C9   | H33A | 3.190    | C9   | H35B | 3.401    |
| C10  | H16A | 3.196    | C10  | H17A | 2.889    |
| C10  | H17B | 3.326    | C10  | H33A | 3.522    |
| C11  | H13A | 3.154    | C11  | H14A | 2.883    |
| C11  | H14B | 3.370    | C12  | H13A | 3.324    |
| C12  | H13B | 2.640    | C12  | H13C | 2.641    |
| C12  | H14A | 3.333    | C12  | H14B | 2.653    |
| C12  | H14C | 2.653    | C12  | H21A | 3.218    |
| C12  | H21C | 3.419    | C12  | H33A | 3.429    |
| C13  | H12A | 3.325    | C13  | H12B | 2.639    |
| C13  | H12C | 2.639    | C13  | H14A | 2.754    |
| C13  | H14B | 3.376    | C13  | H14C | 2.687    |
| C13  | H17A | 2.940    | C13  | H17B | 3.014    |
| C13  | H33A | 3.377    | C13  | H35B | 3.280    |
| C14  | H12A | 2.666    | C14  | H12B | 3.335    |
| C14  | H12C | 2.633    | C14  | H13A | 2.751    |
| C14  | H13B | 2.686    | C14  | H13C | 3.377    |
| C14  | H16A | 2.628    | C14  | H17A | 2.768    |
| C15  | H16A | 3.321    | C15  | H16B | 2.645    |
| C15  | H16C | 2.645    | C15  | H17A | 3.307    |
| C15  | H17B | 2.623    | C15  | H17C | 2.624    |
| C15  | H30B | 3.519    | C15  | H35B | 3.481    |
| C16  | H8A  | 3.440    | C16  | H14A | 2.939    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C16  | H14B | 3.094    | C16  | H15A | 2.662    |
| C16  | H15B | 2.626    | C16  | H15C | 3.322    |
| C16  | H17A | 2.715    | C16  | H17B | 3.348    |
| C16  | H17C | 2.659    | C17  | H13A | 2.581    |
| C17  | H14A | 2.767    | C17  | H15A | 3.307    |
| C17  | H15B | 2.624    | C17  | H15C | 2.623    |
| C17  | H16A | 2.721    | C17  | H16B | 2.657    |
| C17  | H16C | 3.346    | C17  | H35B | 3.567    |
| C18  | H7A  | 3.169    | C18  | H21A | 2.663    |
| C18  | H21B | 3.372    | C18  | H21C | 2.734    |
| C18  | H22A | 2.786    | C18  | H22B | 2.810    |
| C18  | H22C | 3.433    | C18  | H23A | 2.730    |
| C18  | H23B | 3.386    | C18  | H23C | 2.698    |
| C18  | H24A | 2.692    | C18  | H24B | 3.388    |
| C18  | H24C | 2.756    | C18  | H25A | 2.658    |
| C18  | H25B | 2.753    | C18  | H25C | 3.374    |
| C18  | H26A | 2.770    | C18  | H26B | 3.428    |
| C18  | H26C | 2.819    | C18  | H33B | 2.886    |
| C19  | H25B | 3.187    | C19  | H26A | 3.301    |
| C19  | H26C | 2.921    | C19  | H33B | 3.351    |
| C20  | H7A  | 3.592    | C20  | H22A | 2.880    |
| C20  | H22B | 3.379    | C20  | H23A | 3.136    |
| C21  | H12B | 2.902    | C21  | H22A | 3.323    |
| C21  | H22B | 2.650    | C21  | H22C | 2.650    |
| C21  | H23A | 3.318    | C21  | H23B | 2.639    |
| C21  | H23C | 2.639    | C21  | H33A | 3.473    |
| C21  | H33B | 3.235    | C22  | H21A | 3.324    |
| C22  | H21B | 2.648    | C22  | H21C | 2.648    |
| C22  | H23A | 2.725    | C22  | H23B | 2.672    |
| C22  | H23C | 3.358    | C22  | H25B | 2.618    |
| C22  | H26C | 2.810    | C22  | H33B | 3.532    |
| C23  | H21A | 2.653    | C23  | H21B | 2.614    |
| C23  | H21C | 3.322    | C23  | H22A | 2.728    |
| C23  | H22B | 3.360    | C23  | H22C | 2.662    |
| C23  | H26A | 2.952    | C23  | H26C | 2.937    |
| C24  | H7A  | 3.130    | C24  | H25A | 2.672    |
| C24  | H25B | 3.329    | C24  | H25C | 2.606    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom | distance |
|-------|------|----------|
| C24   | H26A | 2.697    |
| C24   | H26C | 3.341    |
| C25   | H22A | 2.909    |
| C25   | H24A | 2.654    |
| C25   | H24C | 3.329    |
| C25   | H26B | 2.722    |
| C25   | H31A | 3.517    |
| C25   | H34C | 3.351    |
| C26   | H23A | 2.543    |
| C26   | H24B | 2.661    |
| C26   | H25A | 3.377    |
| C26   | H25C | 2.723    |
| C27   | H25A | 3.372    |
| C27   | H30B | 2.776    |
| C27   | H31A | 2.641    |
| C27   | H31C | 2.740    |
| C27   | H32B | 2.814    |
| C27   | H33A | 2.672    |
| C27   | H33C | 3.366    |
| C27   | H34B | 3.423    |
| C27   | H35A | 2.704    |
| C27   | H35C | 3.365    |
| C28   | H34A | 2.874    |
| C28   | H35A | 3.098    |
| C29   | H25A | 3.519    |
| C29   | H32A | 3.259    |
| C30   | H1   | 2.32(2)  |
| C30   | H31B | 2.597    |
| C30   | H32A | 2.664    |
| C30   | H32C | 2.576    |
| C31   | H25A | 3.425    |
| C31   | H30B | 3.330    |
| C31   | H32A | 3.358    |
| C31   | H32C | 2.697    |
| C31   | H34C | 3.082    |
| C32   | H30B | 2.625    |
| C32   | H31A | 3.356    |

| atom  | atom | distance |
|-------|------|----------|
| C24   | H26B | 2.621    |
| C24   | H31A | 3.567    |
| C25   | H22B | 3.074    |
| C25   | H24B | 2.627    |
| C25   | H26A | 3.378    |
| C25   | H26C | 2.722    |
| C25   | H33B | 3.184    |
| C26   | H22A | 2.790    |
| C26   | H24A | 3.340    |
| C26   | H24C | 2.661    |
| C26   | H25B | 2.723    |
| C27   | H30A | 2.705    |
| C27   | H30C | 3.392    |
| C27   | H31B | 3.358    |
| C27   | H32A | 2.769    |
| C27   | H32B | 3.418    |
| C27   | H33B | 2.733    |
| C27   | H34A | 2.786    |
| C27   | H34C | 2.803    |
| C27   | H35B | 2.684    |
| C28   | H34C | 3.365    |
| C28   | H1   | 2.37(3)  |
| C29   | H1   | 3.06(3)  |
| C29   | H31C | 3.192    |
| C29   | H32B | 2.901    |
| C30   | H31A | 2.693    |
| C30   | H31C | 3.332    |
| C30   | H32B | 3.315    |
| C30   | H32B | 3.315    |
| C30   | H31B | 3.16(4)  |
| C31   | H30A | 2.672    |
| C31   | H30C | 2.624    |
| C31   | H32B | 2.697    |
| C31   | H34A | 2.937    |
| C31   | H30A | 3.312    |
| C32   | H30C | 2.625    |
| C32   | H31B | 2.699    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| C32  | H31C | 2.699    | C32  | H34A | 2.742    |
| C32  | H35A | 2.522    | C33  | H1   | 3.45(3)  |
| C33  | H12B | 3.396    | C33  | H13C | 3.097    |
| C33  | H21C | 2.818    | C33  | H25A | 3.334    |
| C33  | H34A | 3.316    | C33  | H34B | 2.630    |
| C33  | H34C | 2.630    | C33  | H35A | 3.335    |
| C33  | H35B | 2.659    | C33  | H35C | 2.659    |
| C34  | H25A | 3.359    | C34  | H31C | 2.638    |
| C34  | H32B | 2.756    | C34  | H33A | 3.317    |
| C34  | H33B | 2.628    | C34  | H33C | 2.628    |
| C34  | H35A | 2.756    | C34  | H35B | 3.376    |
| C34  | H35C | 2.686    | C35  | H13C | 3.202    |
| C35  | H15C | 3.428    | C35  | H32A | 2.904    |
| C35  | H32B | 2.958    | C35  | H33A | 2.671    |
| C35  | H33B | 3.338    | C35  | H33C | 2.640    |
| C35  | H34A | 2.749    | C35  | H34B | 2.690    |
| C35  | H34C | 3.378    | C36  | H1   | 3.50(3)  |
| C36  | H7A  | 3.478    | C36  | H15A | 3.501    |
| C37  | H15A | 3.464    | C40  | H7C  | 3.403    |
| C41  | H7A  | 3.484    | C41  | H7C  | 3.219    |
| H1   | H15A | 3.165    | H1   | H15C | 3.160    |
| H1   | H24A | 2.752    | H1   | H30A | 1.900    |
| H1   | H30B | 2.496    | H1   | H30C | 3.259    |
| H1   | H31A | 2.864    | H1   | H33A | 3.220    |
| H1   | H33B | 3.441    | H3   | H4   | 2.319    |
| H3   | H7A  | 3.591    | H3   | H7B  | 2.703    |
| H3   | H7C  | 2.701    | H4   | H5   | 2.316    |
| H5   | H8B  | 2.717    | H5   | H8C  | 2.715    |
| H7A  | H23C | 3.273    | H7A  | H24A | 3.326    |
| H7A  | H24C | 2.325    | H7A  | H26A | 3.423    |
| H7B  | H23C | 3.055    | H7B  | H24C | 3.249    |
| H7B  | H26A | 3.322    | H7C  | H24C | 2.946    |
| H8A  | H12A | 2.914    | H8A  | H14B | 3.333    |
| H8A  | H16A | 3.484    | H8A  | H16C | 2.689    |
| H8B  | H16C | 2.914    | H8C  | H12A | 3.412    |
| H8C  | H14B | 3.560    | H12A | H13B | 3.542    |
| H12A | H13C | 3.542    | H12A | H14A | 3.562    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom  | atom  | distance | atom  | atom  | distance |
|-------|-------|----------|-------|-------|----------|
| H12A  | H14B  | 2.469    | H12A  | H14C  | 2.951    |
| H12A  | H21A  | 3.090    | H12B  | H13A  | 3.540    |
| H12B  | H13B  | 2.916    | H12B  | H13C  | 2.437    |
| H12B  | H14B  | 3.561    | H12B  | H14C  | 3.546    |
| H12B  | H21A  | 2.543    | H12B  | H21B  | 3.261    |
| H12B  | H21C  | 2.497    | H12B  | H33A  | 2.618    |
| H12B  | H33C  | 3.435    | H12C  | H13A  | 3.540    |
| H12C  | H13B  | 2.437    | H12C  | H13C  | 2.916    |
| H12C  | H14A  | 3.536    | H12C  | H14B  | 2.903    |
| H12C  | H14C  | 2.433    | H13A  | H14A  | 2.612    |
| H13A  | H14C  | 3.001    | H13A  | H17A  | 2.232    |
| H13A  | H17B  | 2.262    | H13A  | H17C  | 3.486    |
| H13A  | H35B  | 3.118    | H13B  | H14A  | 3.004    |
| H13B  | H14B  | 3.569    | H13B  | H14C  | 2.471    |
| H13B  | H17A  | 3.550    | H13C  | H14C  | 3.572    |
| H13C  | H17A  | 3.595    | H13C  | H17B  | 3.244    |
| H13C  | H33A  | 2.551    | H13C  | H33C  | 2.846    |
| H13C  | H35B  | 2.651    | H13C  | H35C  | 2.991    |
| H14A  | H16A  | 2.233    | H14A  | H16B  | 3.558    |
| H14A  | H16C  | 3.587    | H14A  | H17A  | 1.993    |
| H14A  | H17B  | 3.350    | H14A  | H17C  | 3.426    |
| H14B  | H16A  | 2.355    | H14B  | H16C  | 3.317    |
| H14B  | H17A  | 3.367    | H14C  | H16A  | 3.534    |
| H14C  | H17A  | 3.411    | H15A  | H16A  | 3.556    |
| H15A  | H16B  | 2.950    | H15A  | H16C  | 2.466    |
| H15A  | H17B  | 3.524    | H15A  | H17C  | 3.524    |
| H15A  | H30B  | 3.416    | H15B  | H16A  | 3.529    |
| H15B  | H16B  | 2.428    | H15B  | H16C  | 2.897    |
| H15B  | H17A  | 3.524    | H15B  | H17B  | 2.901    |
| H15B  | H17C  | 2.420    | H15C  | H16B  | 3.536    |
| H15C  | H16C  | 3.553    | H15C  | H17A  | 3.524    |
| H15C  | H17B  | 2.420    | H15C  | H17C  | 2.901    |
| H15C  | H30B  | 2.962    | H15C  | H32A  | 3.513    |
| H15C  | H35A  | 3.545    | H15C  | H35B  | 2.638    |
| H16A  | H17A  | 2.570    | H16A  | H17C  | 2.978    |
| H16B  | H17A  | 2.966    | H16B  | H17B  | 3.544    |
| H16B  | H17C  | 2.440    | H16C  | H17C  | 3.542    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H17B | H35B | 2.749    | H21A | H22B | 3.548    |
| H21A | H22C | 3.548    | H21A | H23A | 3.548    |
| H21A | H23B | 2.941    | H21A | H23C | 2.455    |
| H21A | H33A | 3.516    | H21B | H22A | 3.545    |
| H21B | H22B | 2.929    | H21B | H22C | 2.453    |
| H21B | H23A | 3.518    | H21B | H23B | 2.413    |
| H21B | H23C | 2.884    | H21C | H22A | 3.545    |
| H21C | H22B | 2.453    | H21C | H22C | 2.929    |
| H21C | H23B | 3.532    | H21C | H23C | 3.550    |
| H21C | H33A | 2.667    | H21C | H33B | 2.476    |
| H21C | H33C | 2.840    | H22A | H23A | 2.577    |
| H22A | H23B | 2.987    | H22A | H25A | 3.509    |
| H22A | H25B | 2.194    | H22A | H25C | 3.572    |
| H22A | H26A | 3.348    | H22A | H26B | 3.475    |
| H22A | H26C | 2.032    | H22B | H23B | 3.557    |
| H22B | H25A | 3.226    | H22B | H25B | 2.372    |
| H22B | H26C | 3.414    | H22B | H33B | 2.851    |
| H22B | H33C | 3.587    | H22C | H23A | 2.970    |
| H22C | H23B | 2.449    | H22C | H23C | 3.550    |
| H22C | H25B | 3.520    | H22C | H26C | 3.445    |
| H23A | H26A | 2.209    | H23A | H26B | 3.446    |
| H23A | H26C | 2.212    | H23B | H26C | 3.557    |
| H23C | H26A | 3.155    | H23C | H26C | 3.577    |
| H24A | H25A | 2.484    | H24A | H25B | 3.568    |
| H24A | H25C | 2.885    | H24A | H26A | 3.587    |
| H24A | H26B | 3.529    | H24A | H30A | 3.457    |
| H24A | H31A | 2.866    | H24B | H25A | 2.941    |
| H24B | H25B | 3.517    | H24B | H25C | 2.385    |
| H24B | H26A | 2.991    | H24B | H26B | 2.422    |
| H24B | H26C | 3.542    | H24B | H31A | 3.478    |
| H24C | H25A | 3.573    | H24C | H25C | 3.509    |
| H24C | H26A | 2.504    | H24C | H26B | 2.880    |
| H24C | H26C | 3.578    | H25A | H31A | 2.834    |
| H25A | H31C | 3.215    | H25A | H33B | 2.487    |
| H25A | H34C | 2.522    | H25B | H26B | 3.008    |
| H25B | H26C | 2.546    | H25B | H33B | 3.233    |
| H25B | H34C | 3.428    | H25C | H26B | 2.547    |
Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H25C | H26C | 3.008    | H25C | H31A | 3.389    |
| H30A | H31A | 2.522    | H30A | H31B | 2.886    |
| H30A | H31C | 3.588    | H30A | H32A | 3.556    |
| H30A | H32C | 3.488    | H30B | H31A | 3.593    |
| H30B | H31B | 3.497    | H30B | H32A | 2.462    |
| H30B | H32B | 3.547    | H30B | H32C | 2.831    |
| H30C | H31A | 2.956    | H30C | H31B | 2.369    |
| H30C | H31C | 3.508    | H30C | H32A | 2.958    |
| H30C | H32B | 3.507    | H30C | H32C | 2.368    |
| H31A | H32B | 3.589    | H31A | H32C | 3.589    |
| H31A | H34A | 3.547    | H31A | H34C | 3.254    |
| H31B | H32A | 3.592    | H31B | H32B | 2.983    |
| H31B | H32C | 2.517    | H31B | H34A | 3.594    |
| H31C | H32A | 3.593    | H31C | H32B | 2.517    |
| H31C | H32C | 2.983    | H31C | H34A | 2.235    |
| H31C | H34B | 3.545    | H31C | H34C | 2.376    |
| H32A | H34A | 3.283    | H32A | H35A | 2.135    |
| H32A | H35B | 3.155    | H32B | H34A | 1.970    |
| H32B | H34B | 3.399    | H32B | H34C | 3.348    |
| H32B | H35A | 2.254    | H32B | H35C | 3.554    |
| H32C | H34A | 3.435    | H32B | H35C | 3.427    |
| H33A | H34B | 3.533    | H33A | H34C | 3.533    |
| H33A | H35A | 3.565    | H33A | H35B | 2.476    |
| H33A | H35C | 2.957    | H33B | H34A | 3.529    |
| H33B | H34B | 2.904    | H33B | H34C | 2.423    |
| H33B | H35B | 3.566    | H33B | H35C | 3.551    |
| H33C | H34A | 3.529    | H33C | H34B | 2.423    |
| H33C | H34C | 2.904    | H33C | H35A | 3.541    |
| H33C | H35B | 2.911    | H33C | H35C | 2.443    |
| H34A | H35A | 2.612    | H34A | H35C | 2.996    |
| H34B | H35A | 3.012    | H34B | H35B | 3.571    |
| H34B | H35C | 2.474    | H34C | H35C | 3.573    |
Table S10-11. Intermolecular contacts less than 3.60 Å

| atom  | atom       | distance  | atom  | atom       | distance  |
|-------|------------|-----------|-------|------------|-----------|
| F1    | C39\(^1\)  | 3.489(5)  | F1    | C40\(^1\)  | 3.383(5)  |
| F2    | C26\(^2\)  | 3.432(5)  | F2    | C36\(^4\)  | 3.504(5)  |
| F2    | C41\(^1\)  | 3.478(5)  | F3    | C15\(^1\)  | 3.100(5)  |
| F3    | C30\(^1\)  | 3.574(7)  | F4    | C31\(^3\)  | 3.340(7)  |
| F5    | C31\(^3\)  | 3.228(6)  | C1    | C32\(^4\)  | 3.469(6)  |
| C6    | C32\(^4\)  | 3.393(7)  | C8    | C32\(^4\)  | 3.579(7)  |
| C15   | F3\(^1\)   | 3.100(5)  | C26   | F2\(^5\)   | 3.432(5)  |
| C30   | F3\(^1\)   | 3.574(7)  | C31   | F4\(^3\)   | 3.340(7)  |
| C31   | F5\(^3\)   | 3.228(6)  | C32   | C1\(^6\)   | 3.469(6)  |
| C32   | C6\(^6\)   | 3.393(7)  | C32   | C8\(^6\)   | 3.579(7)  |
| C36   | F2\(^1\)   | 3.504(5)  | C36   | C38\(^1\)  | 3.467(6)  |
| C37   | C38\(^1\)  | 3.479(5)  | C37   | C39\(^1\)  | 3.524(6)  |
| C38   | C36\(^1\)  | 3.467(6)  | C38   | C37\(^1\)  | 3.479(5)  |
| C39   | F1\(^1\)   | 3.489(5)  | C39   | C37\(^1\)  | 3.524(6)  |
| C40   | F1\(^1\)   | 3.383(5)  | C41   | F2\(^1\)   | 3.478(5)  |

Symmetry Operators:

(1) \(-X+1, -Y+1, -Z+1\)  
(2) \(X+1, Y, Z\)  
(3) \(-X, -Y+1, -Z+1\)  
(4) \(X+1, -Y+1, Z+1\)  
(5) \(X-1, Y, Z\)  
(6) \(X, -Y+1, Z\)
Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens

| atom | atom   | distance | atom | atom   | distance |
|------|--------|----------|------|--------|----------|
| F1   | H25C¹  | 3.204    | F2   | H2AB¹  | 3.396    |
| F2   | H2C¹   | 2.879    | F2   | H26B¹  | 2.519    |
| F2   | H30A²  | 3.310    | F3   | H15A²  | 2.864    |
| F3   | H15B²  | 2.633    | F3   | H15C²  | 3.331    |
| F3   | H22C³  | 2.817    | F3   | H30B²  | 2.791    |
| F4   | H15B²  | 3.024    | F4   | H22C³  | 3.233    |
| F4   | H21B³  | 2.890    | F4   | H31A⁴  | 3.360    |
| F4   | H23B³  | 2.868    | F4   | H31C⁴  | 2.804    |
| F4   | H31B⁴  | 3.329    | F4   | H25C⁴  | 3.131    |
| F5   | H31A⁴  | 2.622    | N1   | H32B⁵  | 3.585    |
| C1   | H32C⁵  | 3.258    | C1   | H32A⁵  | 3.149    |
| C3   | H32B⁵  | 3.300    | C3   | H32C⁵  | 3.382    |
| C3   | H21C³  | 3.575    | C3   | H22B³  | 3.539    |
| C3   | H33C³  | 3.452    | C3   | H35A⁵  | 3.372    |
| C4   | H14A⁶  | 3.335    | C4   | H14B⁶  | 3.523    |
| C4   | H14C⁶  | 3.473    | C4   | H35A⁵  | 3.144    |
| C5   | H14C⁶  | 3.349    | C5   | H26C¹  | 3.343    |
| C5   | H32A⁵  | 3.148    | C5   | H35A⁵  | 3.224    |
| C6   | H32A⁵  | 2.728    | C6   | H32B⁵  | 3.549    |
| C6   | H32C⁵  | 3.413    | C6   | H35A⁵  | 3.561    |
| C7   | H12C³  | 3.482    | C8   | H22A¹  | 3.083    |
| C8   | H25B¹  | 3.394    | C8   | H26C¹  | 3.304    |
| C8   | H32A⁵  | 2.950    | C8   | H32C⁵  | 3.325    |
| C12  | H7B⁷   | 3.473    | C12  | H26A⁷  | 3.446    |
| C12  | H30C⁵  | 3.182    | C12  | H32C⁵  | 3.100    |
| C13  | H17A⁸  | 3.582    | C13  | H17C⁸  | 3.296    |
| C14  | H4⁹    | 2.948    | C14  | H5⁹    | 3.379    |
| C14  | H26A⁷  | 3.461    | C16  | H25B¹  | 3.399    |
| C16  | H34C¹  | 3.502    | C17  | H13A⁸  | 3.046    |
| C17  | H17A⁸  | 3.004    | C17  | H37    | 3.450    |
| C21  | H7C⁷   | 3.326    | C21  | H31B⁵  | 3.294    |
| C21  | H32C⁵  | 3.548    | C22  | H37    | 3.574    |
| C22  | H8B¹⁰  | 3.410    | C22  | H8C¹⁰  | 3.549    |
| C23  | H13B³  | 3.398    | C23  | H34A⁵  | 3.466    |
| C25  | H8B¹⁰  | 3.182    | C25  | H16C¹⁰ | 3.474    |
Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom    | distance | atom   | atom    | distance |
|--------|---------|----------|--------|---------|----------|
| C26    | H5\(^{10}\) | 3.347    | C26    | H8B\(^{10}\) | 3.238    |
| C26    | H12C\(^3\) | 3.384    | C26    | H14C\(^3\) | 3.023    |
| C30    | H12A\(^{11}\) | 3.473    | C30    | H24B\(^4\) | 3.532    |
| C31    | H21A\(^{11}\) | 3.575    | C31    | H21B\(^{11}\) | 3.301    |
| C32    | H8C\(^{11}\) | 3.170    | C32    | H12A\(^{11}\) | 3.227    |
| C32    | H21A\(^{11}\) | 3.288    | C33    | H3\(^7\) | 3.397    |
| C34    | H16B\(^{10}\) | 3.464    | C39    | H15A\(^2\) | 3.485    |
| C39    | H15B\(^2\) | 3.492    | C39    | H22C\(^3\) | 3.505    |
| C40    | H21B\(^3\) | 3.597    | H3\(^3\) | C21\(^3\) | 3.450    |
| H3\(^3\) | C22\(^3\) | 3.574    | H3\(^3\) | C33\(^3\) | 3.397    |
| H3\(^3\) | H21B\(^3\) | 3.372    | H3\(^3\) | H21C\(^3\) | 2.726    |
| H3\(^3\) | H22B\(^3\) | 2.881    | H3\(^3\) | H22C\(^3\) | 3.498    |
| H3\(^3\) | H33B\(^3\) | 3.368    | H3\(^3\) | H33C\(^3\) | 2.638    |
| H4\(^3\) | C14\(^6\) | 2.948    | H4\(^3\) | H14A\(^6\) | 2.531    |
| H4\(^3\) | H14B\(^6\) | 2.833    | H4\(^3\) | H14C\(^6\) | 2.996    |
| H4\(^3\) | H16A\(^6\) | 3.232    | H4\(^3\) | H22B\(^3\) | 3.581    |
| H4\(^3\) | H35A\(^5\) | 3.468    | H5\(^3\) | C14\(^6\) | 3.379    |
| H5\(^3\) | C26\(^1\) | 3.347    | H5\(^3\) | H14A\(^6\) | 3.228    |
| H5\(^3\) | H14C\(^6\) | 2.749    | H5\(^3\) | H17B\(^5\) | 3.500    |
| H5\(^3\) | H26B\(^1\) | 3.297    | H5\(^3\) | H26C\(^1\) | 2.659    |
| H5\(^3\) | H32A\(^5\) | 3.437    | H5\(^3\) | H35A\(^5\) | 3.571    |
| H7B\(^3\) | C12\(^3\) | 3.473    | H7B\(^3\) | H12B\(^3\) | 3.200    |
| H7B\(^3\) | H12C\(^3\) | 2.893    | H7B\(^3\) | H13B\(^3\) | 3.045    |
| H7B\(^3\) | H13C\(^3\) | 3.337    | H7B\(^3\) | H21C\(^3\) | 3.580    |
| H7C\(^3\) | C21\(^3\) | 3.326    | H7C\(^3\) | H12B\(^3\) | 3.463    |
| H7C\(^3\) | H12C\(^3\) | 3.294    | H7C\(^3\) | H21B\(^3\) | 2.711    |
| H7C\(^3\) | H21C\(^3\) | 3.100    | H7C\(^3\) | H31B\(^4\) | 3.140    |
| H8A\(^3\) | H32A\(^5\) | 3.222    | H8A\(^3\) | H32C\(^5\) | 3.104    |
| H8B\(^3\) | C22\(^1\) | 3.410    | H8B\(^3\) | C25\(^1\) | 3.182    |
| H8B\(^3\) | C26\(^1\) | 3.238    | H8B\(^3\) | H22A\(^1\) | 2.506    |
| H8B\(^3\) | H22B\(^1\) | 3.576    | H8B\(^3\) | H25B\(^1\) | 2.483    |
| H8B\(^3\) | H25C\(^1\) | 3.150    | H8B\(^3\) | H26B\(^1\) | 3.206    |
| H8B\(^3\) | H26C\(^1\) | 2.553    | H8C\(^3\) | C22\(^1\) | 3.549    |
| H8C\(^3\) | C32\(^5\) | 3.170    | H8C\(^3\) | H22A\(^1\) | 2.785    |
| H8C\(^3\) | H22C\(^1\) | 3.583    | H8C\(^3\) | H26C\(^1\) | 3.421    |
| H8C\(^3\) | H30B\(^5\) | 3.237    | H8C\(^3\) | H32A\(^5\) | 2.472    |
| H8C\(^3\) | H32C\(^5\) | 3.011    | H12A\(^3\) | C30\(^8\) | 3.473    |
Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom | distance | atom | atom | distance |
|------|------|----------|------|------|----------|
| H12A | C32$^5$ | 3.227 | H12A | H30C$^5$ | 2.649 |
| H12A | H31B$^5$ | 3.401 | H12A | H32A$^5$ | 3.564 |
| H12A | H32C$^5$ | 2.288 | H12B | H7B$^7$ | 3.200 |
| H12B | H7C$^7$ | 3.463 | H12B | H32C$^5$ | 3.240 |
| H12C | C7$^7$ | 3.482 | H12C | C26$^7$ | 3.384 |
| H12C | H7B$^7$ | 2.893 | H12C | H7C$^7$ | 3.294 |
| H12C | H24C$^7$ | 3.501 | H12C | H26A$^7$ | 2.542 |
| H12C | H26B$^7$ | 3.411 | H12C | H30C$^5$ | 2.830 |
| H12C | H31B$^5$ | 3.310 | H12C | H32C$^5$ | 3.394 |
| H13A | C17$^8$ | 3.046 | H13A | H17A$^8$ | 2.661 |
| H13A | H17B$^8$ | 3.367 | H13A | H17C$^8$ | 2.670 |
| H13B | C23$^7$ | 3.398 | H13B | H7B$^7$ | 3.045 |
| H13B | H17C$^8$ | 3.041 | H13B | H23A$^7$ | 2.759 |
| H13B | H23C$^7$ | 3.233 | H13B | H26A$^7$ | 2.940 |
| H13C | H7B$^7$ | 3.337 | H14A | C4$^9$ | 3.335 |
| H14A | H4$^9$ | 2.531 | H14A | H5$^9$ | 3.228 |
| H14A | H17A$^8$ | 3.596 | H14A | H17B$^8$ | 3.175 |
| H14A | H17C$^8$ | 3.519 | H14B | C4$^9$ | 3.523 |
| H14B | H4$^9$ | 2.833 | H14C | C4$^9$ | 3.473 |
| H14C | C5$^9$ | 3.349 | H14C | C26$^7$ | 3.023 |
| H14C | H4$^9$ | 2.996 | H14C | H5$^9$ | 2.749 |
| H14C | H23A$^7$ | 3.486 | H14C | H26A$^7$ | 2.568 |
| H14C | H26B$^7$ | 2.964 | H14C | H26C$^7$ | 3.041 |
| H15A | F3$^2$ | 2.864 | H15A | C39$^2$ | 3.485 |
| H15B | F3$^2$ | 2.633 | H15B | F4$^2$ | 3.024 |
| H15B | C39$^2$ | 3.492 | H15B | H22C$^{12}$ | 3.513 |
| H15B | H23B$^{12}$ | 3.124 | H15C | F3$^2$ | 3.331 |
| H16A | H4$^9$ | 3.232 | H16A | H25B$^1$ | 3.336 |
| H16A | H34C$^1$ | 3.474 | H16B | F4$^2$ | 3.231 |
| H16B | C34$^1$ | 3.464 | H16B | H25B$^1$ | 3.448 |
| H16B | H25A$^1$ | 3.582 | H16B | H25B$^1$ | 3.421 |
| H16B | H34B$^1$ | 3.494 | H16B | H34C$^1$ | 2.743 |
| H16C | C25$^1$ | 3.474 | H16C | H25B$^1$ | 2.898 |
| H16C | H25C$^1$ | 3.315 | H17A | C13$^8$ | 3.582 |
| H17A | C17$^8$ | 3.004 | H17A | H13A$^8$ | 2.661 |
| H17A | H14A$^8$ | 3.596 | H17A | H17A$^8$ | 2.471 |
| H17A | H17B$^8$ | 2.818 | H17A | H17C$^8$ | 3.280 |
Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom   | atom   | distance | atom   | atom   | distance |
|--------|--------|----------|--------|--------|----------|
| H17B   | H5\textsuperscript{11} | 3.500    | H17B   | H13A\textsuperscript{8} | 3.367    |
| H17B   | H14A\textsuperscript{8} | 3.175    | H17B   | H17A\textsuperscript{8} | 2.818    |
| H17C   | C13\textsuperscript{8} | 3.296    | H17C   | H13A\textsuperscript{8} | 2.670    |
| H17C   | H13B\textsuperscript{8} | 3.041    | H17C   | H14A\textsuperscript{8} | 3.519    |
| H17C   | H17A\textsuperscript{8} | 3.280    | H17C   | H23A\textsuperscript{12} | 3.238    |
| H17C   | H23B\textsuperscript{12} | 3.301    | H21A   | C31\textsuperscript{5} | 3.575    |
| H21A   | C32\textsuperscript{5} | 3.288    | H21A   | H31B\textsuperscript{5} | 3.014    |
| H21A   | H31C\textsuperscript{5} | 3.383    | H21A   | H32B\textsuperscript{5} | 3.077    |
| H21A   | H32C\textsuperscript{5} | 2.665    | H21B   | F4\textsuperscript{7} | 2.890    |
| H21B   | C31\textsuperscript{5} | 3.301    | H21B   | C40\textsuperscript{7} | 3.597    |
| H21B   | H3\textsuperscript{7} | 3.372    | H21B   | H7C\textsuperscript{7} | 2.711    |
| H21B   | H31B\textsuperscript{5} | 2.702    | H21B   | H31C\textsuperscript{5} | 3.009    |
| H21C   | C3\textsuperscript{7} | 3.575    | H21C   | H3\textsuperscript{7} | 2.726    |
| H21C   | H7B\textsuperscript{7} | 3.580    | H21C   | H7C\textsuperscript{7} | 3.100    |
| H22A   | C8\textsuperscript{10} | 3.083    | H22A   | H8B\textsuperscript{10} | 2.506    |
| H22A   | H8C\textsuperscript{10} | 2.785    | H22B   | H4\textsuperscript{7} | 3.581    |
| H22B   | H3\textsuperscript{7} | 2.881    | H22B   | H4\textsuperscript{7} | 3.581    |
| H22B   | H8B\textsuperscript{10} | 3.576    | H22C   | F3\textsuperscript{7} | 2.817    |
| H22C   | F4\textsuperscript{7} | 3.233    | H22C   | C39\textsuperscript{7} | 3.505    |
| H22C   | H3\textsuperscript{7} | 3.498    | H22C   | H8C\textsuperscript{10} | 3.583    |
| H22C   | H15B\textsuperscript{13} | 3.513    | H22A   | H13B\textsuperscript{3} | 2.759    |
| H23A   | H14C\textsuperscript{3} | 3.486    | H23A   | H17C\textsuperscript{13} | 3.238    |
| H23B   | F4\textsuperscript{7} | 2.868    | H23B   | H15B\textsuperscript{13} | 3.124    |
| H23B   | H16B\textsuperscript{13} | 3.448    | H23B   | H17C\textsuperscript{13} | 3.301    |
| H23B   | H31C\textsuperscript{5} | 3.117    | H23B   | H34A\textsuperscript{5} | 3.213    |
| H23C   | H13B\textsuperscript{3} | 3.233    | H23C   | H31C\textsuperscript{5} | 3.411    |
| H23C   | H32B\textsuperscript{5} | 2.917    | H23C   | H34A\textsuperscript{5} | 2.838    |
| H24B   | F2\textsuperscript{10} | 3.396    | H24B   | F5\textsuperscript{4} | 3.090    |
| H24B   | C30\textsuperscript{4} | 3.532    | H24B   | H30A\textsuperscript{4} | 2.877    |
| H24B   | H30C\textsuperscript{4} | 3.297    | H24B   | H31A\textsuperscript{4} | 3.530    |
| H24C   | H12C\textsuperscript{3} | 3.501    | H24C   | H30C\textsuperscript{4} | 3.567    |
| H24C   | H31A\textsuperscript{4} | 3.576    | H24C   | H31B\textsuperscript{4} | 3.328    |
| H25A   | H16B\textsuperscript{10} | 3.582    | H25B   | C8\textsuperscript{10} | 3.394    |
| H25B   | C16\textsuperscript{10} | 3.399    | H25B   | H8B\textsuperscript{10} | 2.483    |
| H25B   | H16A\textsuperscript{10} | 3.336    | H25B   | H16B\textsuperscript{10} | 3.421    |
| H25B   | H16C\textsuperscript{10} | 2.898    | H25C   | F1\textsuperscript{10} | 3.204    |
| H25C   | F2\textsuperscript{10} | 2.879    | H25C   | F5\textsuperscript{4} | 3.131    |
Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom | atom   | distance | atom | atom   | distance |
|------|--------|----------|------|--------|----------|
| H25C | H8B<sup>10</sup> | 3.150    | H25C | H16C<sup>10</sup> | 3.315    |
| H26A | C12<sup>3</sup>  | 3.446    | H26A | C14<sup>4</sup>  | 3.461    |
| H26A | H12C<sup>3</sup> | 2.542    | H26A | H13B<sup>3</sup> | 2.940    |
| H26A | H14C<sup>3</sup> | 2.568    | H26B | F2<sup>10</sup> | 2.519    |
| H26B | H5<sup>10</sup>  | 3.297    | H26B | H8B<sup>10</sup> | 3.206    |
| H26B | H12C<sup>3</sup> | 3.411    | H26B | H14C<sup>3</sup> | 2.964    |
| H26B | H30C<sup>4</sup> | 3.274    | H26C | C5<sup>10</sup>  | 3.343    |
| H26C | C8<sup>10</sup>  | 3.304    | H26C | H5<sup>10</sup>  | 2.659    |
| H26C | H8B<sup>10</sup> | 2.553    | H26C | H8C<sup>10</sup> | 3.421    |
| H26C | H14C<sup>3</sup> | 3.041    | H30A | F2<sup>2</sup>  | 3.310    |
| H30A | H24B<sup>4</sup> | 2.877    | H30A | F3<sup>2</sup>  | 2.791    |
| H30B | H8C<sup>11</sup> | 3.237    | H30B | C12<sup>11</sup> | 3.182    |
| H30C | H12A<sup>11</sup> | 2.649   | H30C | H12C<sup>11</sup> | 2.830    |
| H30C | H24B<sup>4</sup> | 3.297    | H30C | H24C<sup>4</sup> | 3.567    |
| H30C | H26B<sup>4</sup> | 3.274    | H31A | F4<sup>4</sup>  | 3.360    |
| H31A | F5<sup>4</sup>  | 2.622    | H31A | H24B<sup>4</sup> | 3.530    |
| H31A | H24C<sup>4</sup> | 3.576    | H31B | F4<sup>4</sup>  | 3.329    |
| H31B | F5<sup>4</sup>  | 3.131    | H31B | C21<sup>11</sup> | 3.294    |
| H31B | H7C<sup>4</sup>  | 3.140    | H31B | H12A<sup>11</sup> | 3.401    |
| H31B | H12C<sup>11</sup> | 3.310   | H31B | H21A<sup>11</sup> | 3.014    |
| H31B | H21B<sup>11</sup> | 2.702   | H31B | H24C<sup>4</sup> | 3.328    |
| H31C | F4<sup>4</sup>  | 2.804    | H31C | F5<sup>4</sup>  | 3.458    |
| H31C | H21A<sup>11</sup> | 3.383   | H31C | H21B<sup>11</sup> | 3.009    |
| H31C | H23B<sup>11</sup> | 3.117   | H31C | H23C<sup>11</sup> | 3.411    |
| H32A | C1<sup>11</sup>  | 3.149    | H32A | C5<sup>11</sup>  | 3.148    |
| H32A | G6<sup>11</sup>  | 2.728    | H32A | C8<sup>11</sup>  | 2.950    |
| H32A | H5<sup>11</sup>  | 3.437    | H32A | H8A<sup>11</sup> | 3.222    |
| H32A | H8C<sup>11</sup> | 2.472    | H32A | H12A<sup>11</sup> | 3.564    |
| H32B | N1<sup>11</sup>  | 3.585    | H32B | C1<sup>11</sup>  | 3.300    |
| H32B | C6<sup>11</sup>  | 3.549    | H32B | H21A<sup>11</sup> | 3.077    |
| H32B | H23C<sup>11</sup> | 2.917   | H32C | N1<sup>11</sup>  | 3.258    |
| H32C | C1<sup>11</sup>  | 3.382    | H32C | C6<sup>11</sup>  | 3.413    |
| H32C | C8<sup>11</sup>  | 3.325    | H32C | C12<sup>11</sup> | 3.100    |
| H32C | C21<sup>11</sup> | 3.548    | H32C | H8A<sup>11</sup> | 3.104    |
| H32C | H8C<sup>11</sup> | 3.011    | H32C | H12A<sup>11</sup> | 2.288    |
| H32C | H12B<sup>11</sup> | 3.240   | H32C | H12C<sup>11</sup> | 3.394    |
| H32C | H21A<sup>11</sup> | 2.665   | H33B | H3<sup>7</sup>  | 3.368    |
Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

| atom      | atom     | distance | atom      | atom     | distance |
|-----------|----------|----------|-----------|----------|----------|
| H33C      | C3<sup>7</sup> | 3.452    | H33C      | H3<sup>7</sup> | 2.638    |
| H34A      | C23<sup>11</sup> | 3.466    | H34A      | H23B<sup>11</sup> | 3.213    |
| H34A      | H23C<sup>11</sup> | 2.838    | H34B      | H16B<sup>10</sup> | 3.494    |
| H34B      | H35C<sup>14</sup> | 3.270    | H34C      | C16<sup>10</sup> | 3.502    |
| H34C      | H16A<sup>10</sup> | 3.474    | H34C      | H16B<sup>10</sup> | 2.743    |
| H35A      | C3<sup>11</sup> | 3.372    | H35A      | C4<sup>11</sup> | 3.144    |
| H35A      | C5<sup>11</sup> | 3.224    | H35A      | C6<sup>11</sup> | 3.561    |
| H35A      | H4<sup>11</sup> | 3.468    | H35A      | H5<sup>11</sup> | 3.571    |
| H35C      | H34B<sup>14</sup> | 3.270    | H35C      | H35C<sup>14</sup> | 3.279    |

Symmetry Operators:

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