Electronic Supplementary Material (ESI) for ChemComm.

A Double-Decker Cage for Allosteric Encapsulation of ATP

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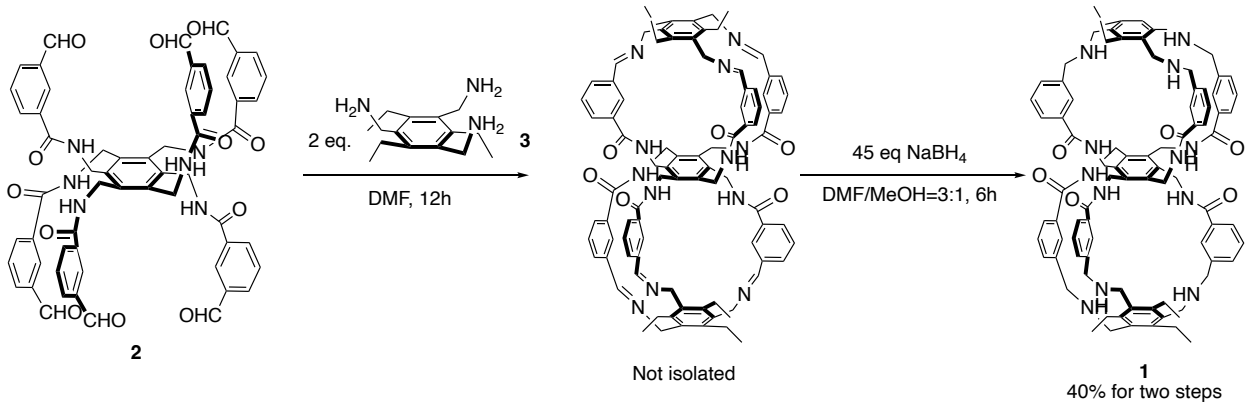
SUPPLEMENTARY INFORMATION

General Information

All chemicals were purchased from commercial sources and used as received unless stated otherwise. Chromatographic purifications were completed with silica gel 60 (SiO_2, Sorbent Technologies 40-75μm, 200 x 400 mesh). Thin-layer chromatography (TLC) studies were completed with silica-gel plates w/UV254 (200 μm). For NMR studies, we used class B glass NMR tubes (Wilmad Lab Glass). NMR experiments were completed with Bruker 400, 600, 700 and 850 MHz spectrometers. Chemical shifts are expressed in parts per million (δ, ppm) while coupling constant values (J) are given in Hertz (Hz). Residual solvent protons were used as an internal standard: for ^{1}H NMR spectra $CDCl_3$ = 7.26 ppm and $(CD_3)_2SO$ = 2.50 ppm, while for ^{13}C NMR spectra $CDCl_3$ = 77.0 ppm and $(CD_3)_2SO$ = 39.52 ppm. Deuterated solvents $CDCl_3$ and $(CD_3)_2SO$ were purchased from Cambridge Isotope Laboratories. HRMS data were obtained with a Bruker-ESI TOF instrument.

Synthetic procedures

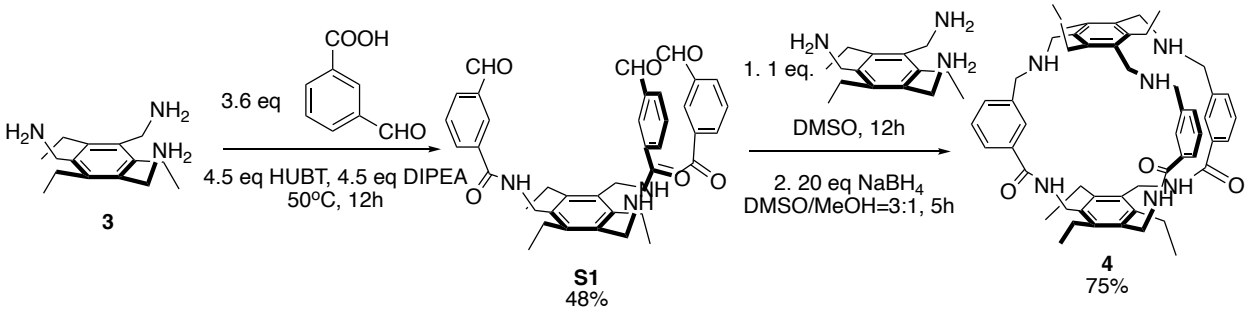


Scheme S1. A synthetic scheme describing the preparation of double-decker capsule **1**; note that hexakis-aldehyde **2** and *tris*-amine **3** were obtained following published procedures.[1, 2]

Double-decker capsule 1: To a solution of compound **2** (10 mg, 0.0096mmol) in 3.0 mL of DMF, *tris*-amine **3** (4.8 mg, 0.0192 mmol) was added. The reaction mixture was stirred at a room temperature for 24 h. Next, $NaBH_4$ (16 mg, 0.43 mmol) was added in one portion, followed by the addition of 1.0 mL pf CH_3OH. After stirring the solution overnight, the solvents were removed under reduced pressure and the crude product was washed with H_2O (3 x 5 mL). The crude product was purified by chromatography (SiO_2; CH_2Cl_2 : CH_3OH : $NH_{3(aq)}$= 60 : 5 : 1) to give **1** as a white solid (5.6 mg, 40%). ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) = 8.62 (t, 6H, J = 3.9 Hz), 7.72-7.71 (m, 12H), 7.43-7.38 (m, 12H), 4.57-4.56 (d, 6H, J = 3.9 Hz), 3.97 (s, 6H), 3.78 (s, 6H), 2.76-2.75 (d, 12H, J = 7.2 Hz), 1.18-1.15 (t, 18H, J = 7.2 Hz). ^{13}C NMR (150 MHz, DMSO-d_6): δ (ppm) =167.04, 142.44, 140.99, 138.50, 134.71, 134.03, 130.97, 128.42, 126.86, 54.31, 47.95, 38.80, 22.66, 17.35. HRMS (ESI): *m/z* calcd for $C_{90}H_{102}N_{12}O_6Na^+$: 1469.7938; found: 1469.7948. See Figure S1 for NMR spectroscopic characterization of double-decker **1**.

solvents	yield
DMSO	26%
DCM:MeOH=3:1	29%
DCM:Acetone=3:1	-
DCM:MeCN=3:1	-
MeOH:MeCN=1:1	-
DMF	40%

Table S1. The isolated yields of **1** obtained from the reductive amination reaction (Scheme S1) completed in different solvents.



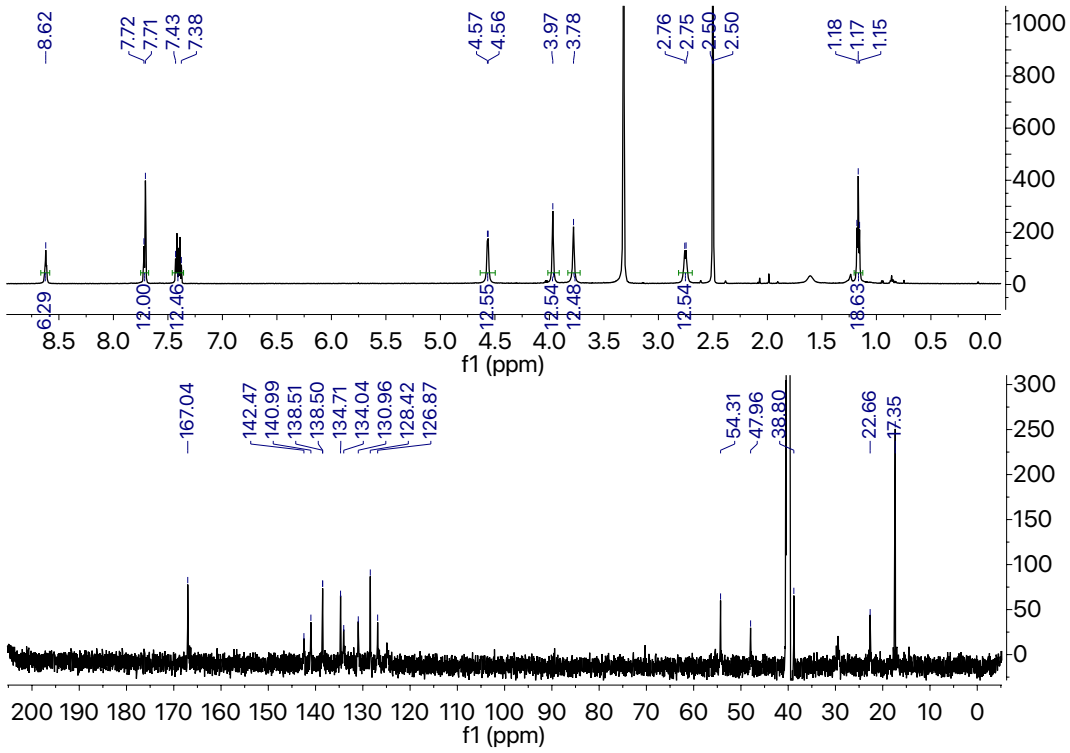
Scheme S2. A synthetic scheme describing the preparation of tripodal capsule **4**.

Compound S1: To a solution of **3** (20 mg, 0.08 mmol), 3-formylbenzoic acid (44 mg, 0.29 mmol) and HBTU (136 mg, 0.36 mmol) in 2.0 mL of dry DMF, DIPEA (64 *u*L, 0.36 mmol) was added in one portion. The reaction mixture was stirred at 50 °C and under an atmosphere of nitrogen for 12h. After its cooling to a room temperature, 20 mL of H_2O was added followed by extraction with $CH_3CO_2CH_2CH_3$ (3 x 10 mL). The organic layer was washed with H_2O (3 x 5mL), brine (10 mL) and then dried over Na_2SO_4. After the solvent removal at a low pressure, compound **S1** was isolated by chromatography (SiO_2; CH_2Cl_2 : CH_3OH= 30:1) as a white solid (25mg, 48%). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) = 10.06 (s, 3H), 8.1634 (s, 3H), 8.14-8.12 (d, 3H, J = 7.8 Hz), 7.80-7.98 (d, 3H, J = 7.6 Hz), 7.65-7.61(t, 3H, J = 7.6 Hz), 6.09 (br, 3H), 4.76-4.75 (d, 6H, J = 2.4 Hz), 2.87-2.81 (q, 6H, J = 7.5 Hz), 1.32-1.28 (t, 9H, J = 7.3 Hz). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) = 191.55, 165.78, 144.82, 136.42, 134.90, 133.40, 133.31, 132.08, 129.71, 126.56, 38.87, 23.36, 16.60. HRMS (ESI): *m/z* calcd for $C_{39}H_{39}N_3O_6Na^+$: 668.2737; found: 668.2742. See Figure S2 for $^1H/^{13}C$ NMR spectra of compound **S1**.

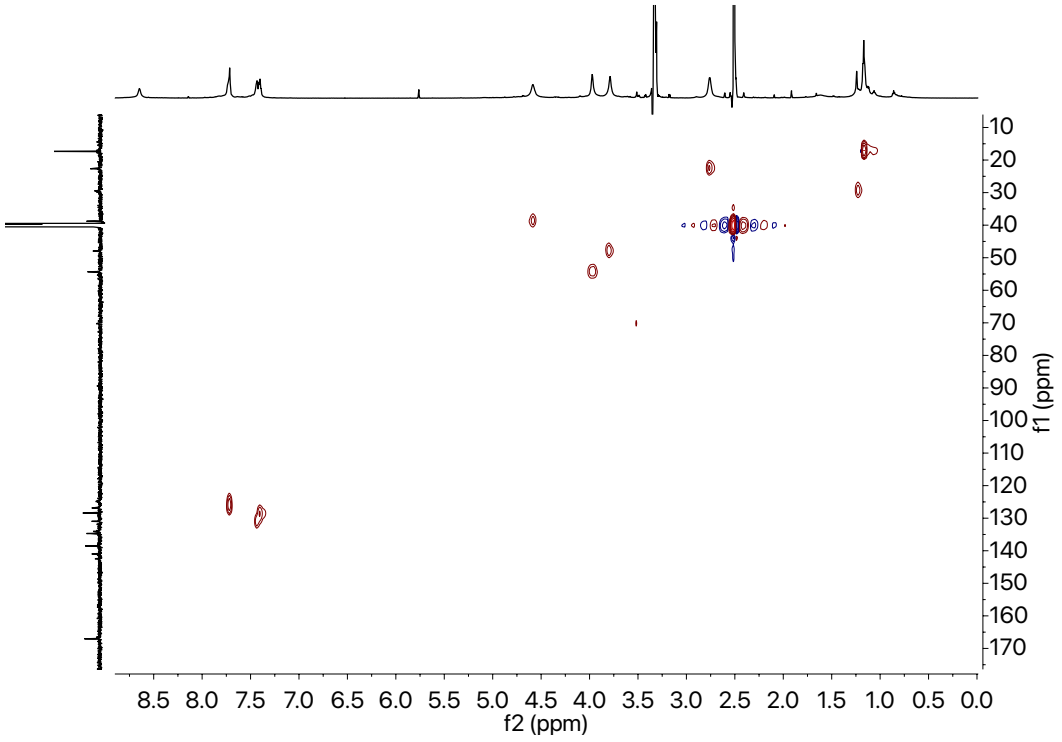
Compound 4: To a solution of compound **S1** (5 mg, 0.0078mmol) in 2.0 mL of DMSO, *tris*-amine **3** (2.0 mg, 0.008 mmol) was added. The reaction mixture was stirred at a room temperature for 24 h. Next, $NaBH_4$ (6 mg, 0.16 mmol) was added in one portion, followed by the addition of 0.5 mL of CH_3OH. After a stirring of the solution overnight, solvents were removed under reduced

pressure and the crude product was purified by chromatography (SiO_2; CH_2Cl_2 : CH_3COCH_3 : $NH_{3(aq)}$= 50 : 10: 1) to give **4** as a white solid (5 mg, 75%). ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) = 8.28-8.26 (t, 3H, J = 4.7 Hz), 7.75-7.76 (d, 3H, J = 6.5 Hz), 7.63 (s, 3H), 7.42-7.38 (m, 6H), 4.46-4.45 (d, 6H, J = 4.7 Hz), 3.95 (s, 6H, J), 3.75 (s, 6H). 2.73-2.67 (m, 12H), 1.16-1.11(m, 18H). ^{13}C NMR (150 MHz, DMSO-d_6): δ (ppm) =167.24, 144.36, 142.33, 140.89, 134.87, 133.95, 132.26, 130.79, 128.41, 127.00, 124.43, 54.30, 48.00, 38.07, 22.76, 22.64, 17.34, 16.47. HRMS (ESI): *m/z* calcd for $C_{54}H_{67}N_6O_3^+$: 847.5275; found: 847.5266. See Figure S3 for NMR spectroscopic characterization of **4**.

(A)


8.62
7.72
7.71
7.43
7.38
4.57
4.56
3.97
3.78
2.76
2.75
2.50
2.50
1.18
1.17
1.15
6.29
12.00
12.46
12.55
12.54
12.48
12.54
18.63
f1 (ppm)
167.04
142.47
140.99
138.51
138.50
134.71
134.04
130.96
128.42
126.87
54.31
47.96
38.80
22.66
17.35
f1 (ppm)

(B)


f1 (ppm)
f2 (ppm)

(C)

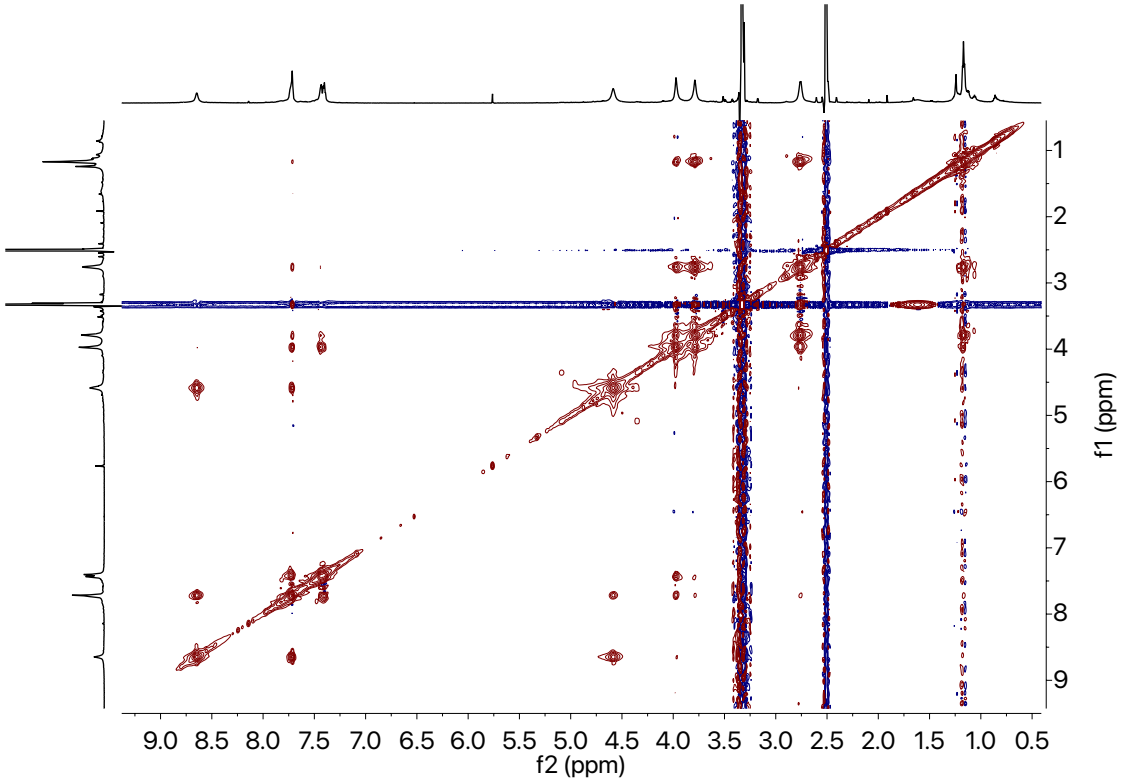


Figure S1. (A) ^{1}H NMR (700 MHz, 298 K) and ^{13}C NMR (175 MHz, 298 K), (B) ^{1}H-^{13}C HSQC NMR (700 MHz, 298K) and (C) ^{1}H-^{1}H NOESY NMR (700 MHz, 298 K) spectra of double-decker **1** in DMSO-d_6.

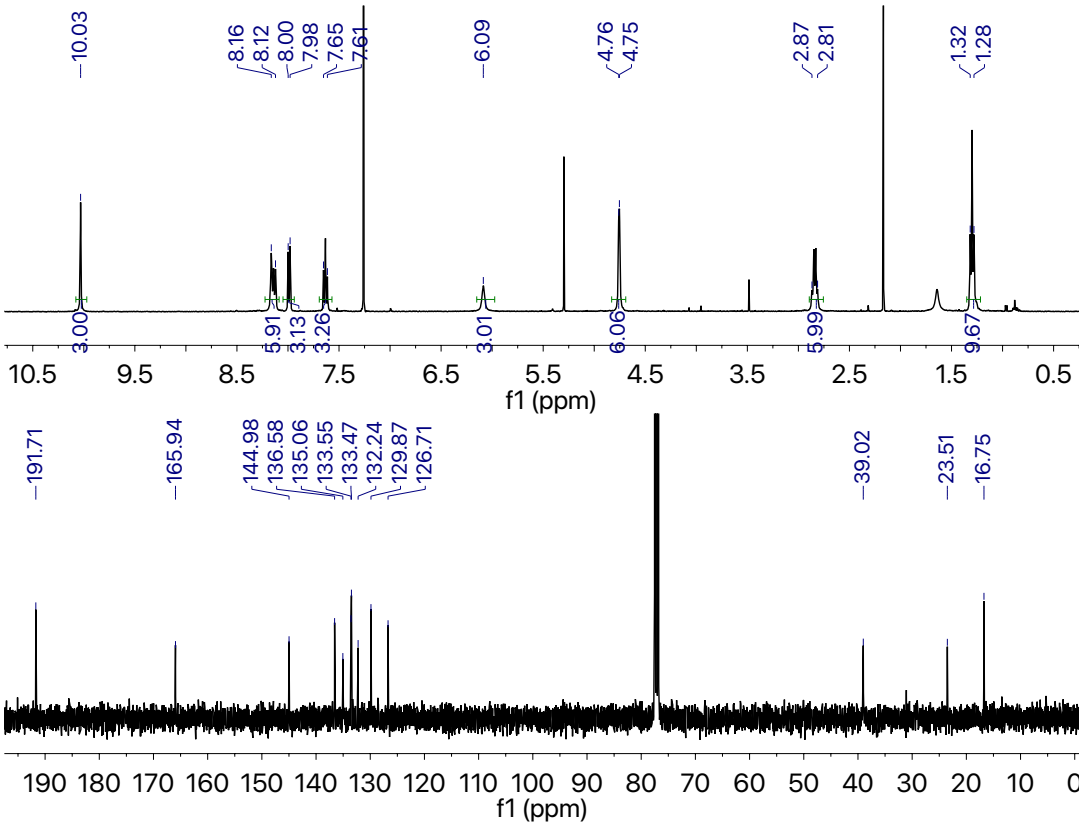
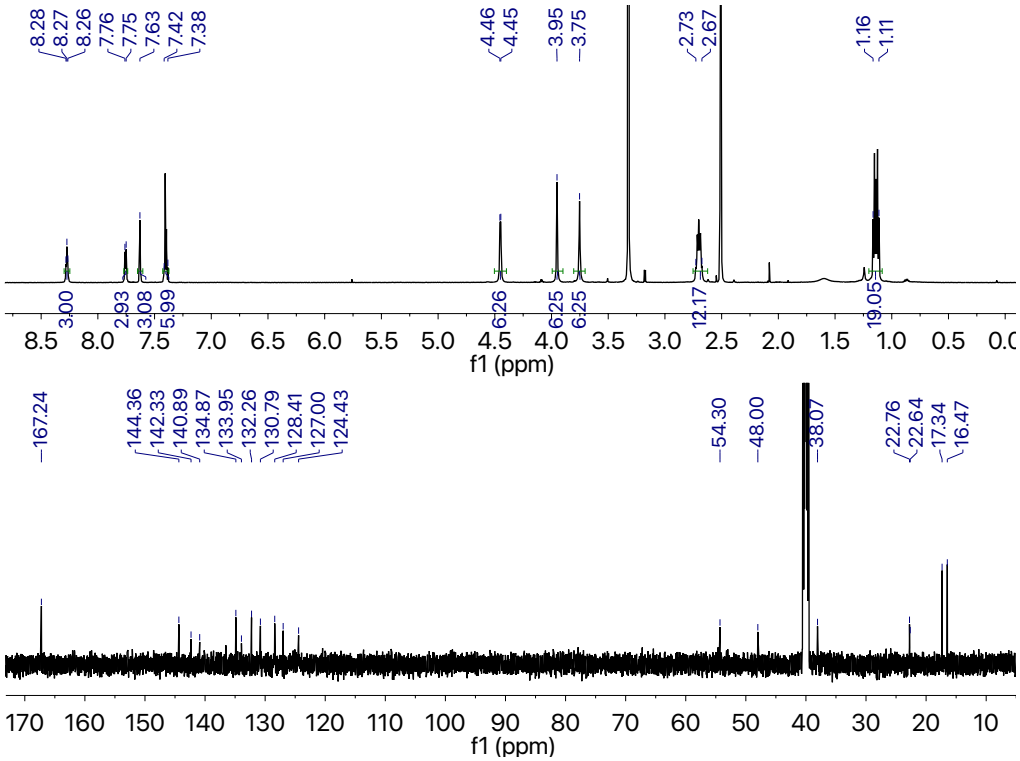
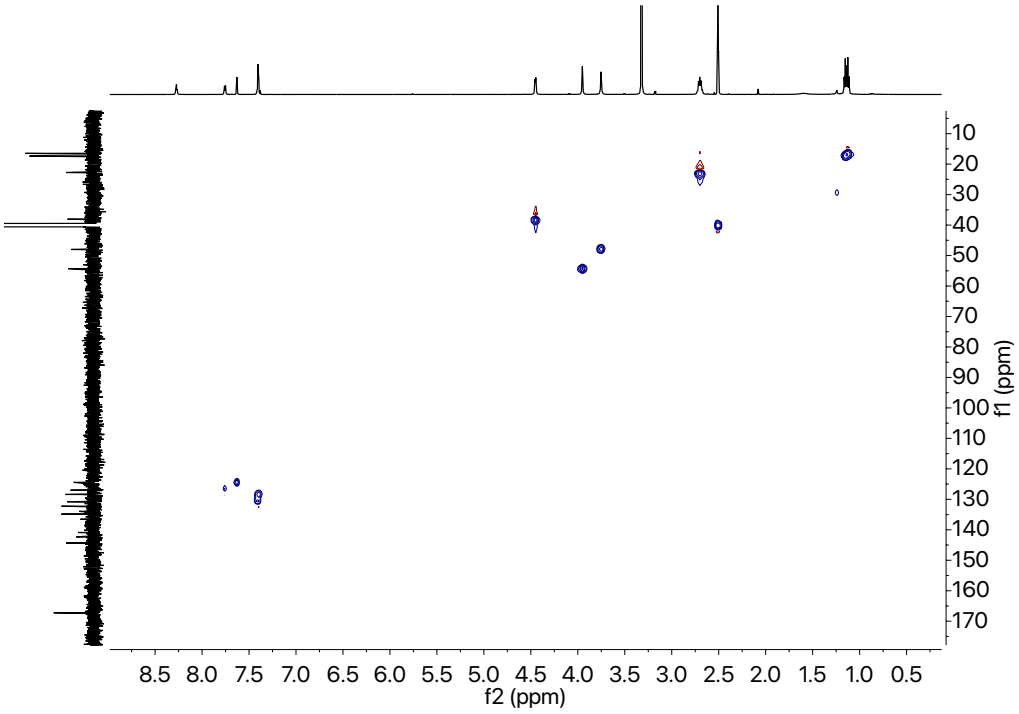


Figure S2. ^{1}H NMR (400 MHz, 298 K) and ^{13}C NMR (101 MHz, 298 K) spectra of compound **S1** in DMSO-d_6.

(A)


8.28
8.27
8.26
7.76
7.75
7.63
7.42
7.38
4.46
4.45
3.95
3.75
2.73
2.67
1.16
1.11
3.00
2.93
3.08
5.99
6.26
6.25
6.25
12.17
19.05
f1 (ppm)
167.24
144.36
142.33
140.89
134.87
133.95
132.26
130.79
128.41
127.00
124.43
54.30
48.00
38.07
22.76
22.64
17.34
16.47
f1 (ppm)

(B)


f2 (ppm)
f1 (ppm)

(C)

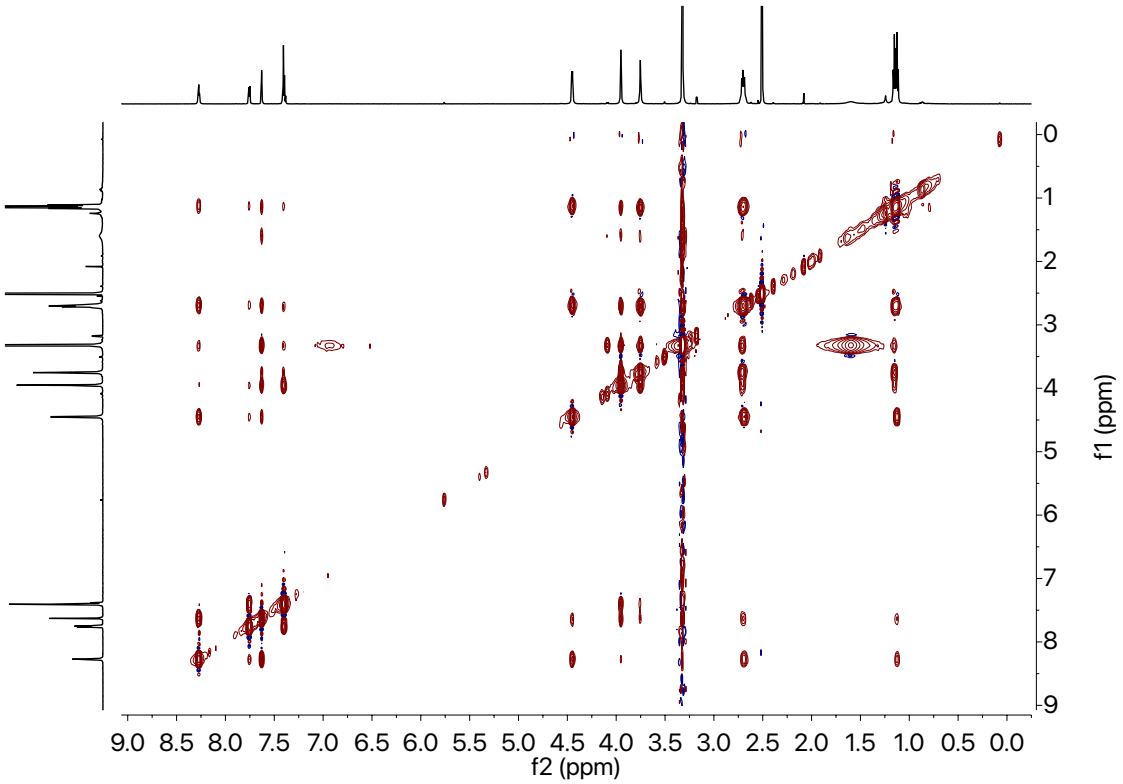


Figure S3. ^{1}H NMR (700 MHz, 298 K) and ^{13}C NMR (175 MHz, 298 K), (B) ^{1}H-^{13}C HSQC NMR (700 MHz, 298K), (C) ^{1}H-^{1}H NOESY NMR (700 MHz, 298 K) spectra of tripodal capsule **4** in DMSO-d_6.

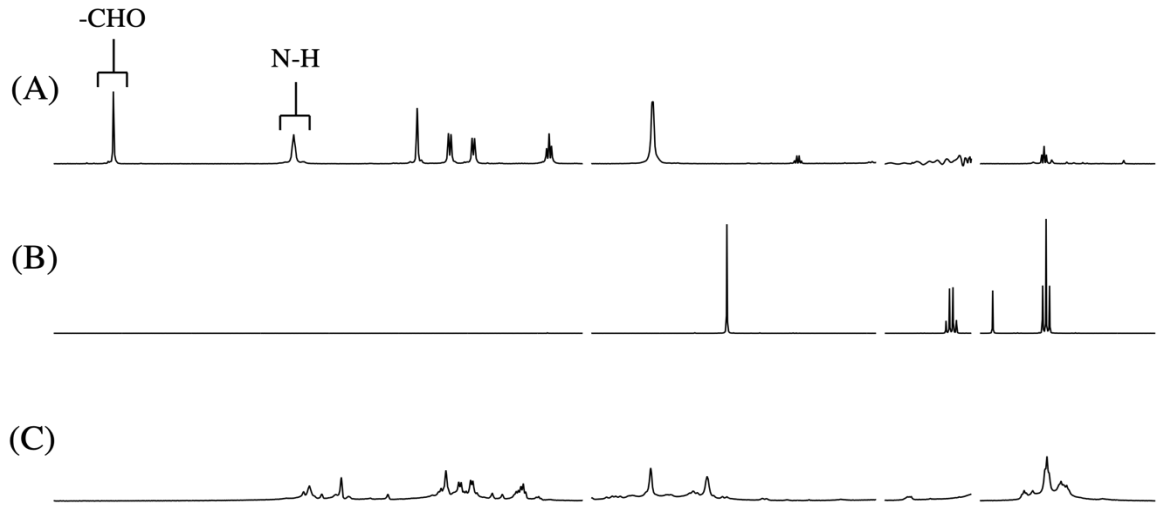


Figure S4. (A) ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of hexakis-aldehyde **2**. (B) ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of *tris*-amine **3**. (C) ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of the imine product obtained by the reaction of **2** (1.9 umol) and **3** (3.8 umol) in DMSO (500 uL).

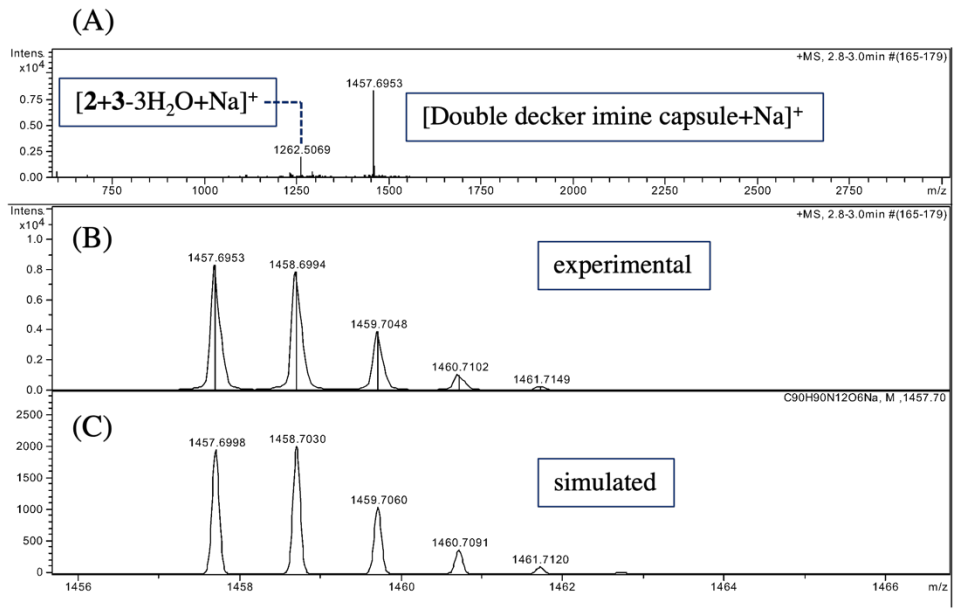


Figure S5. (A) High-resolution ESI-MS of the crude reaction mixture of hexakis-aldehyde **2** and *tris*-amine **3** showing the formation of [1+1] and [1+2] imine capsules. Experimental (B) and simulated (C) high-resolution ESI-MS of [1+2] imine capsule (Scheme S1).

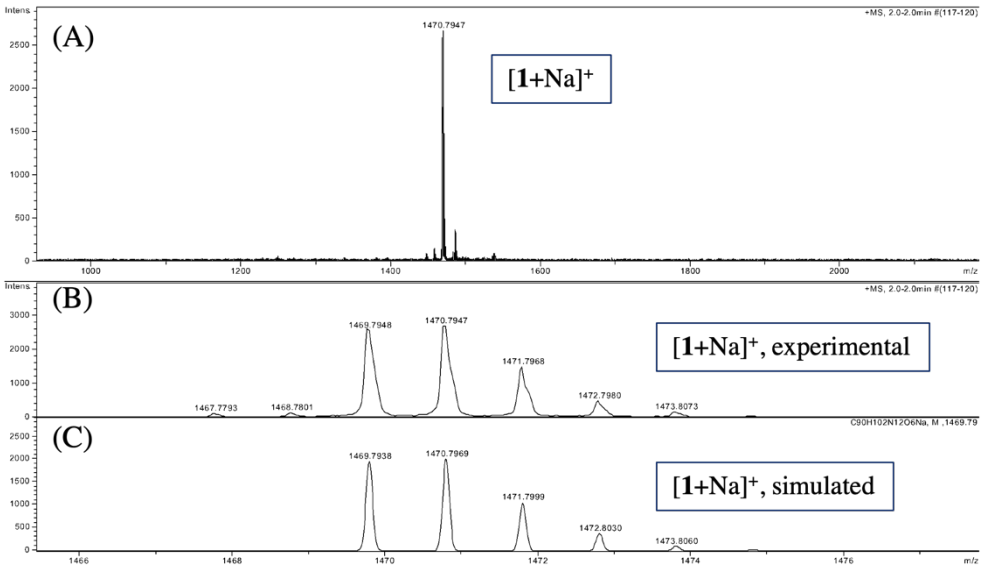
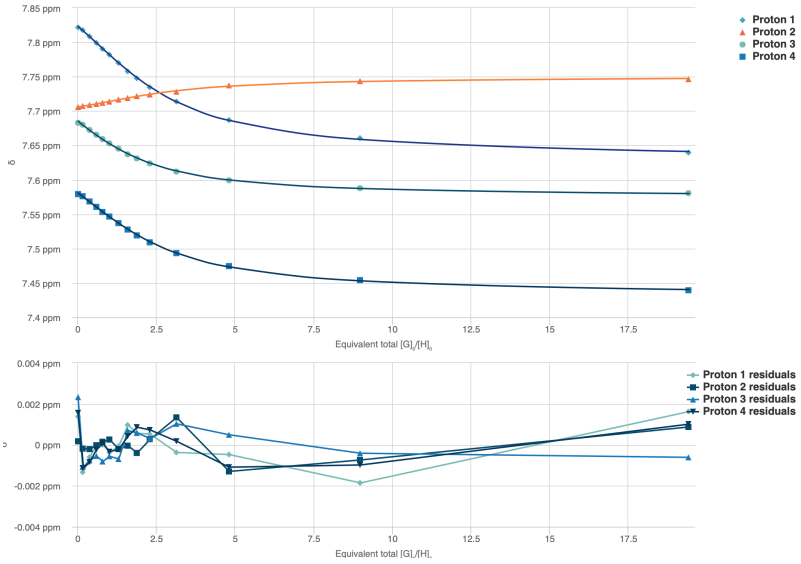


Figure S6. Experimental (A/B) and simulated (C) high-resolution ESI-MS of [**1**+Na]$^+$.



Details

Time to fit	2.2796 s
SSR	3.8443e-5
Fitted datapoints	56
Fitted params	14

Parameters

Parameter (bounds)	Optimised	Error	Initial
K_{11} (0 → ∞)	9608.21 M^{-1}	± 6.8096 %	1000.00 M^{-1}
K_{12} (0 → ∞)	2569.13 M^{-1}	± 3.5468 %	100.00 M^{-1}

Back Next

Quality of fit

Fit	RMS	Covariance
Proton 1	9.3317e-4	2.7491e-4
Proton 2	6.1367e-4	2.2761e-3
Proton 3	9.1274e-4	7.9210e-4
Proton 4	8.1575e-4	3.5367e-4
Total	**8.2854e-4**	**2.6313e-4**

Coefficients

Fit	H	HG	HG2
Proton 1	7.8231	7.7641	7.6239
Proton 2	7.7061	7.7159	7.7518
Proton 3	7.6852	7.6286	7.5730
Proton 4	7.5808	7.5284	7.4279

Figure S7. Nonlinear least-square analysis of ^{1}H NMR complexation data for the formation of ternary $[ATP_2\subset\mathbf{1}\text{-}H_6]^{2+}$ complex (1:2 fitting model; www.supramolecular.org). The data corresponds to the second of three independent titration experiments (see also Figure 3A) wherein 23.3 mM standard solution of ATP^{2-} in 27 mM HEPES buffer at pH = 3 was added to 0.35 mM $[\mathbf{1}\text{-}H_6]^{6+}$ in 450 µL of the same buffer solution. Using the change in chemical shift of $\mathbf{H}_{C/D/E/F}$ signals as a function of the overall concentration of ATP, stability constants from three measurements were found to be: K_1 = 12886 ± 13, 9608 ± 7, 18122 ± 19 M^{-1} and K_2 = 1779 ± 3 M^{-1}, 2569 ± 4, 1879 ± 4. The reported values are thus $K_1 = 1.3 \pm 0.4 \cdot 10^4$ M^{-1} and $K_2 = 2.1 \pm 0.4 \cdot 10^3$ M^{-1} (mean ± standard deviation).

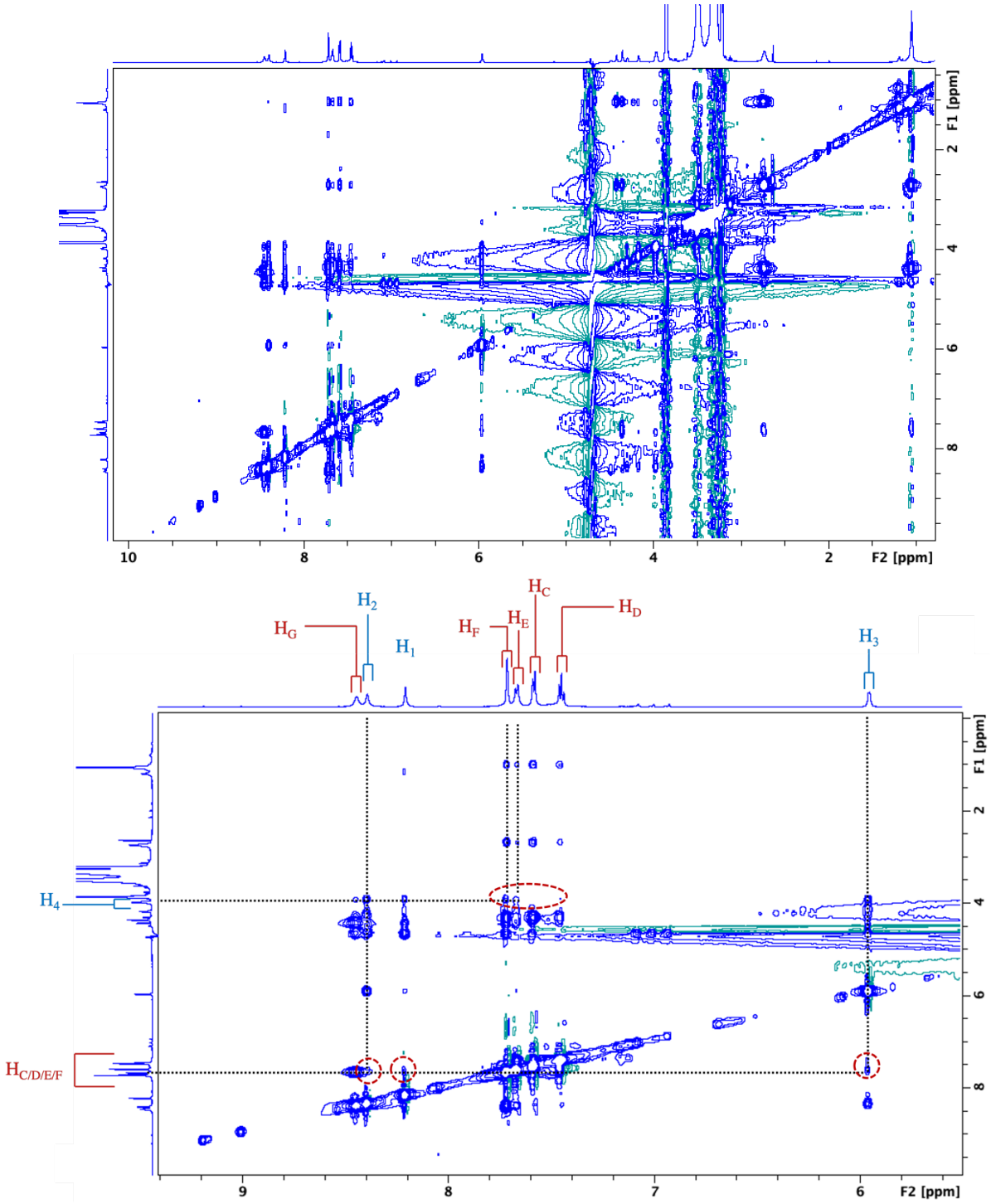
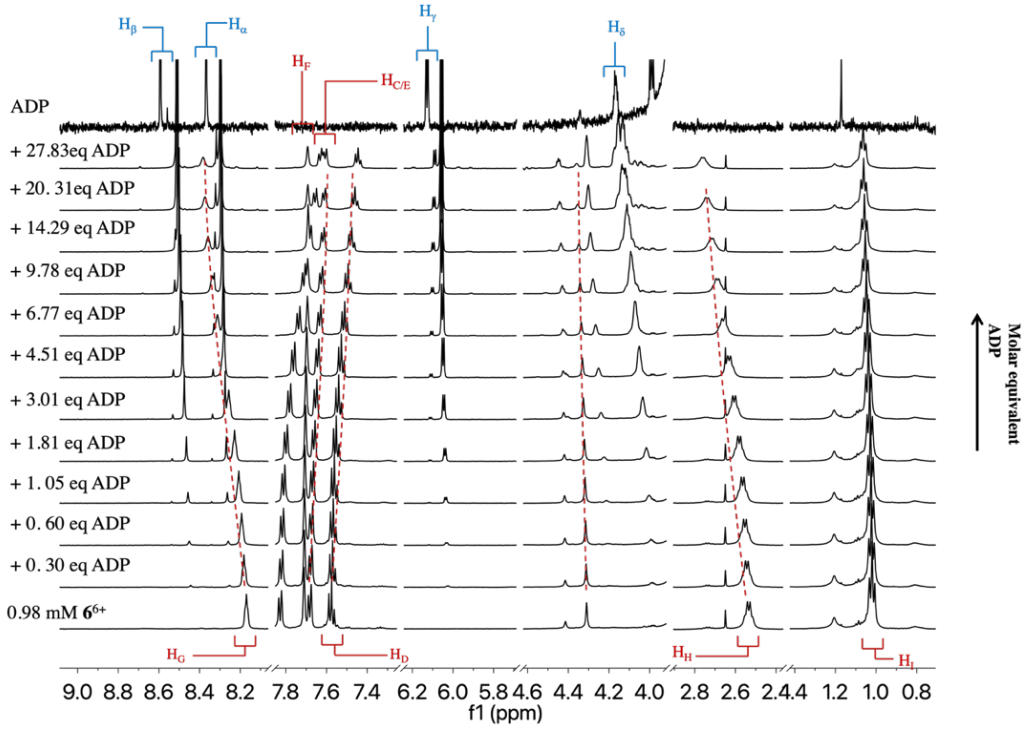
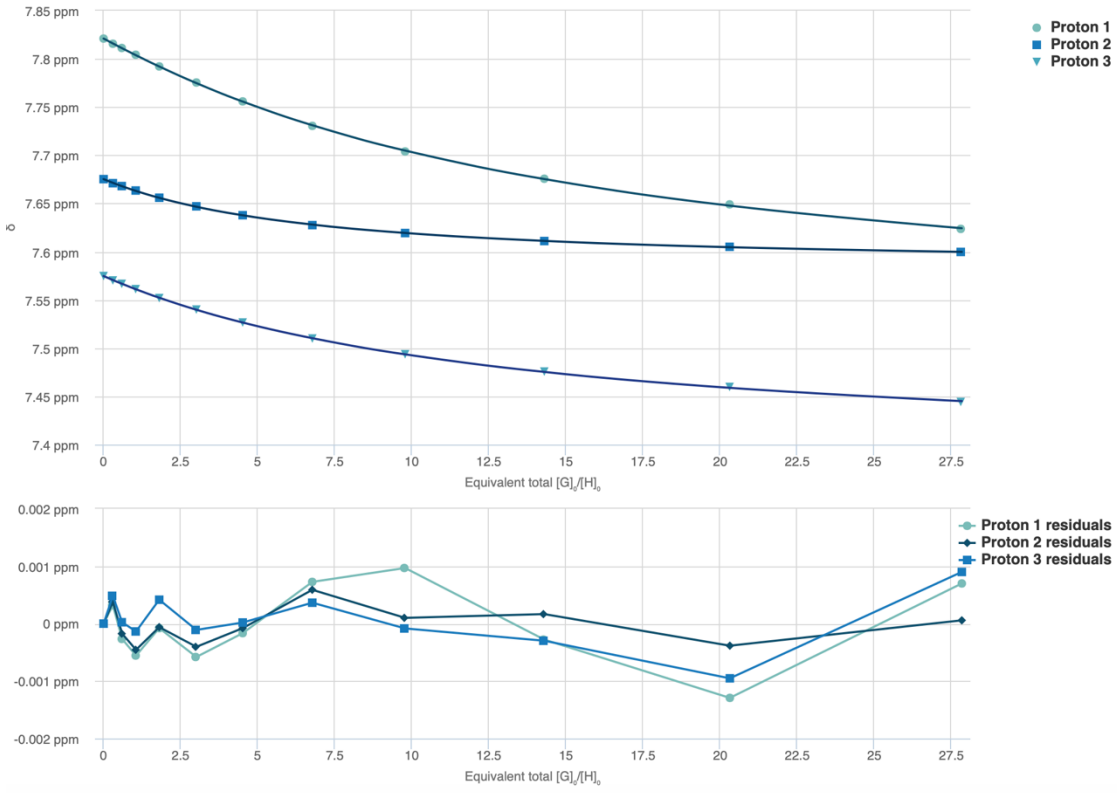


Figure S8. $^{1}H-^{1}H$ NOESY spectrum (850 MHz, 298 K) of 1.0 mM solution of [**1**-H_6]$^{6+}$ containing 2.0 mM ATP^{2-} (27 mM HEPES buffer at pH = 3.0). (Bottom) A segment from the $^{1}H-^{1}H$ NOESY spectrum with cross-correlations suggesting the formation of [ATP_2⊂**1**-H_6]$^{2+}$.

(A)


Hβ
Hα
Hγ
Hδ
HF
HC/E
ADP
+ 27.83eq ADP
+ 20. 31eq ADP
+ 14.29 eq ADP
+ 9.78 eq ADP
+ 6.77 eq ADP
+ 4.51 eq ADP
+ 3.01 eq ADP
+ 1.81 eq ADP
+ 1. 05 eq ADP
+ 0. 60 eq ADP
+ 0. 30 eq ADP
0.98 mM 6^6+
HG
HD
HH
HI
9.0 8.8 8.6 8.4 8.2 7.8 7.6 7.4 6.2 6.0 5.8 4.6 4.4 4.2 4.0 2.8 2.6 2.4 4.4 1.2 1.0 0.8
f1 (ppm)
Molar equivalent ADP

(B)


7.85 ppm
7.8 ppm
7.75 ppm
7.7 ppm
7.65 ppm
7.6 ppm
7.55 ppm
7.5 ppm
7.45 ppm
7.4 ppm
δ
0 2.5 5 7.5 10 12.5 15 17.5 20 22.5 25 27.5
Equivalent total [G]0/[H]0
Proton 1
Proton 2
Proton 3
0.002 ppm
0.001 ppm
0 ppm
-0.001 ppm
-0.002 ppm
0 2.5 5 7.5 10 12.5 15 17.5 20 22.5 25 27.5
Equivalent total [G]0/[H]0
Proton 1 residuals
Proton 2 residuals
Proton 3 residuals

Fitter: NMR 1:2 | Fit | Summary | Save

Details

Time to fit	0.9921 s
SSR	8.0288e-6
Fitted datapoints	36
Fitted params	8

Parameters

Parameter (bounds)	Optimised	Error	Initial
K_{11} (0 → ∞)	222.81 M^{-1}	± 1.7312 %	1000.00 M^{-1}
K_{12} (0 → ∞)	44.94 M^{-1}	± 1.2638 %	100.00 M^{-1}

Quality of fit

Fit	RMS	Covariance
Proton 1	6.1618e-4	8.6289e-5
Proton 2	3.0144e-4	1.3366e-4
Proton 3	4.4556e-4	1.0267e-4
Total	**4.7225e-4**	**8.6393e-5**

Coefficients

Fit	H	HG	HG2
Proton 1	7.8211	7.7259	7.4437
Proton 2	7.6753	7.6017	7.5754
Proton 3	7.5748	7.4968	7.3443

Figure S9. (A) ^{1}H NMR spectra (600 MHz, 298 K) of 0.98 mM of [**1**-H_6]$^{6+}$ in 27 mM HEPES buffer at pH = 3, obtained upon an incremental addition of 66.2 mM solution of ADP^- in the same buffer. (B) Nonlinear least-square analysis of ^{1}H NMR binding data corresponding to the formation of ternary [ADP_2⊂**1**-H_6]$^{4+}$ complex (1:2 fitting model; www.supramolecular.org). The data corresponds to one of two independent titration experiments. Using the change in chemical shift of $\mathbf{H}_{C/D/E}$ signals as a function of the overall concentration of ADP, stability constants from two measurements were found to be: K_1 = 223 ± 2, 228 ± 1 M^{-1} and K_2 = 45 ± 1, 90 ± 2 M^{-1}. The reported values are thus $K_1 = 2.25 \pm 0.03 \cdot 10^2$ M^{-1} and $K_2 = 7 \pm 3 \cdot 10^1$ M^{-1} (mean ± standard deviation).

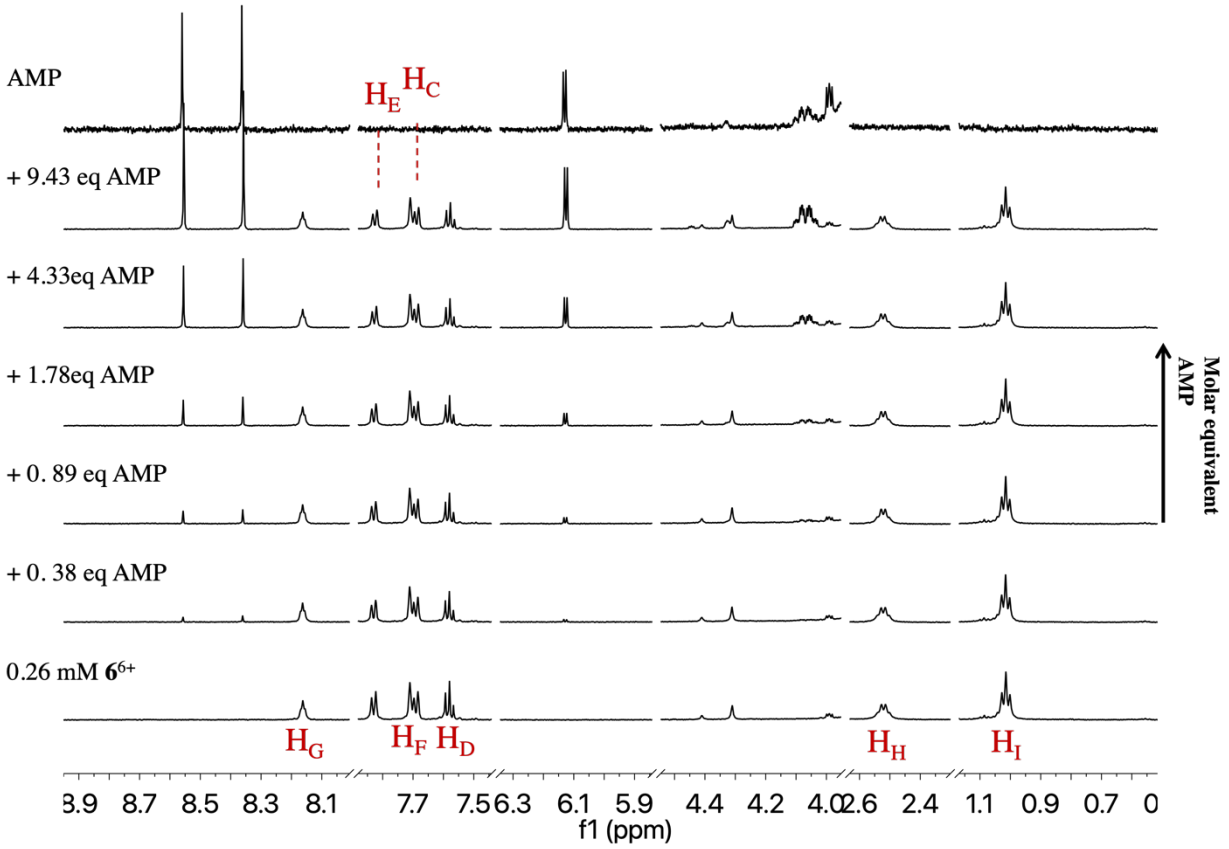
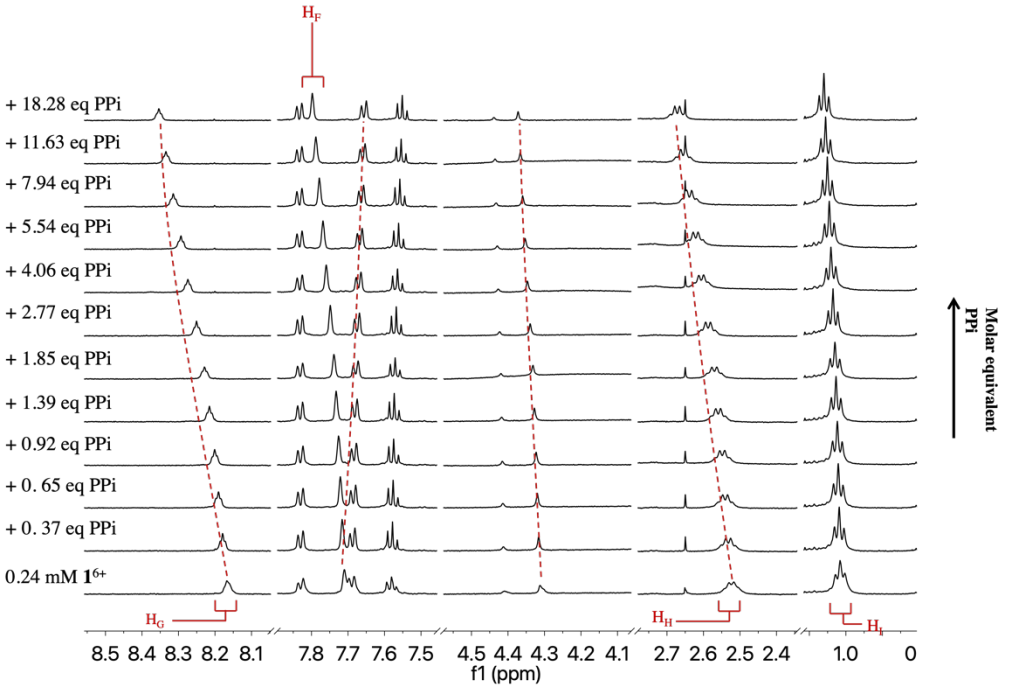
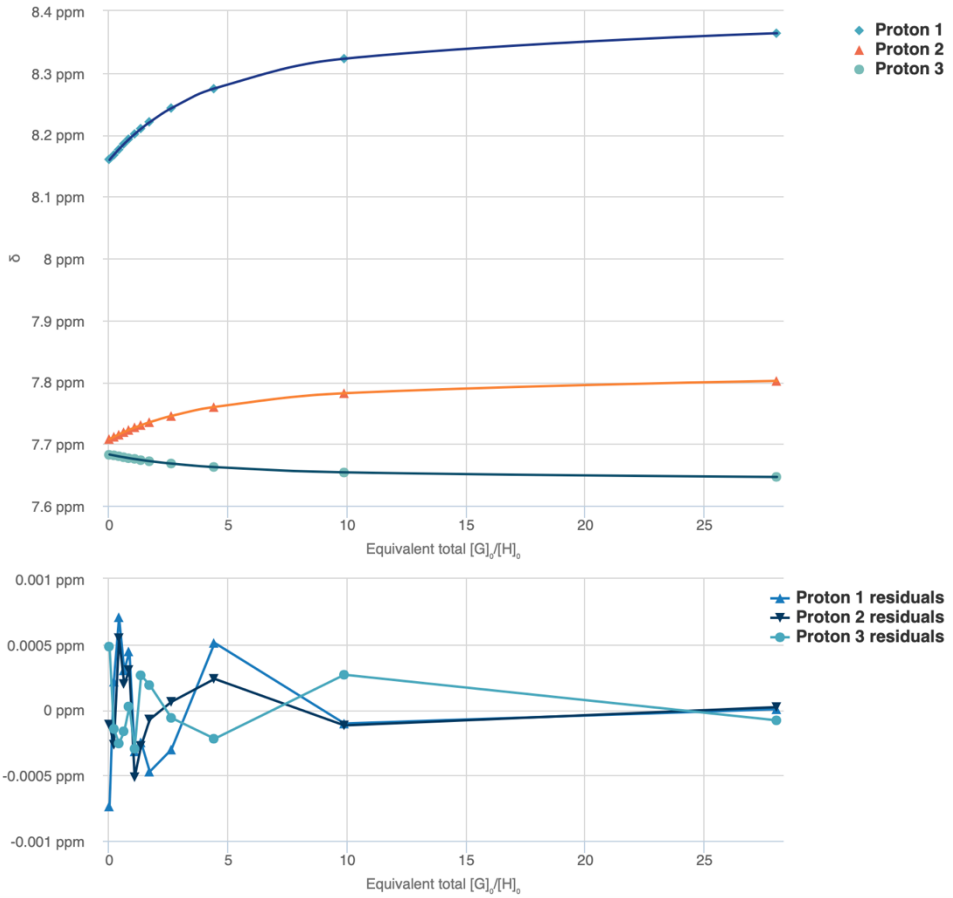


Figure S10. ^{1}H NMR spectra (600 MHz, 298 K) of 0.26 mM of [**1**-H_6]$^{6+}$ in 27 mM HEPES buffer at pH = 3, obtained upon an incremental addition of 18.0 mM solution of AMP in the same buffer. A negligible perturbation of resonances from both host and guest indicates a weak complexation.

(A)


H_F
+ 18.28 eq PPi
+ 11.63 eq PPi
+ 7.94 eq PPi
+ 5.54 eq PPi
+ 4.06 eq PPi
+ 2.77 eq PPi
+ 1.85 eq PPi
+ 1.39 eq PPi
+ 0.92 eq PPi
+ 0. 65 eq PPi
+ 0. 37 eq PPi
0.24 mM 1^6+
H_G
H_H
H_I
Molar equivalent PPi
8.5 8.4 8.3 8.2 8.1 7.8 7.7 7.6 7.5 4.5 4.4 4.3 4.2 4.1 2.7 2.6 2.5 2.4 1.0 0
f1 (ppm)

(B)


8.4 ppm
8.3 ppm
8.2 ppm
8.1 ppm
8 ppm
7.9 ppm
7.8 ppm
7.7 ppm
7.6 ppm
δ
Proton 1
Proton 2
Proton 3
0 5 10 15 20 25
Equivalent total [G]0/[H]0
0.001 ppm
0.0005 ppm
0 ppm
-0.0005 ppm
-0.001 ppm
Proton 1 residuals
Proton 2 residuals
Proton 3 residuals
0 5 10 15 20 25
Equivalent total [G]0/[H]0

Details

Time to fit	1.0384 s
SSR	3.7349e-6
Fitted datapoints	36
Fitted params	11

Parameters

Parameter (bounds)	Optimised	Error	Initial
K_{11} (0 → ∞)	1058.00 M^{-1}	± 0.9003 %	1000.00 M^{-1}
K_{12} (0 → ∞)	118.43 M^{-1}	± 6.0540 %	100.00 M^{-1}

Quality of fit

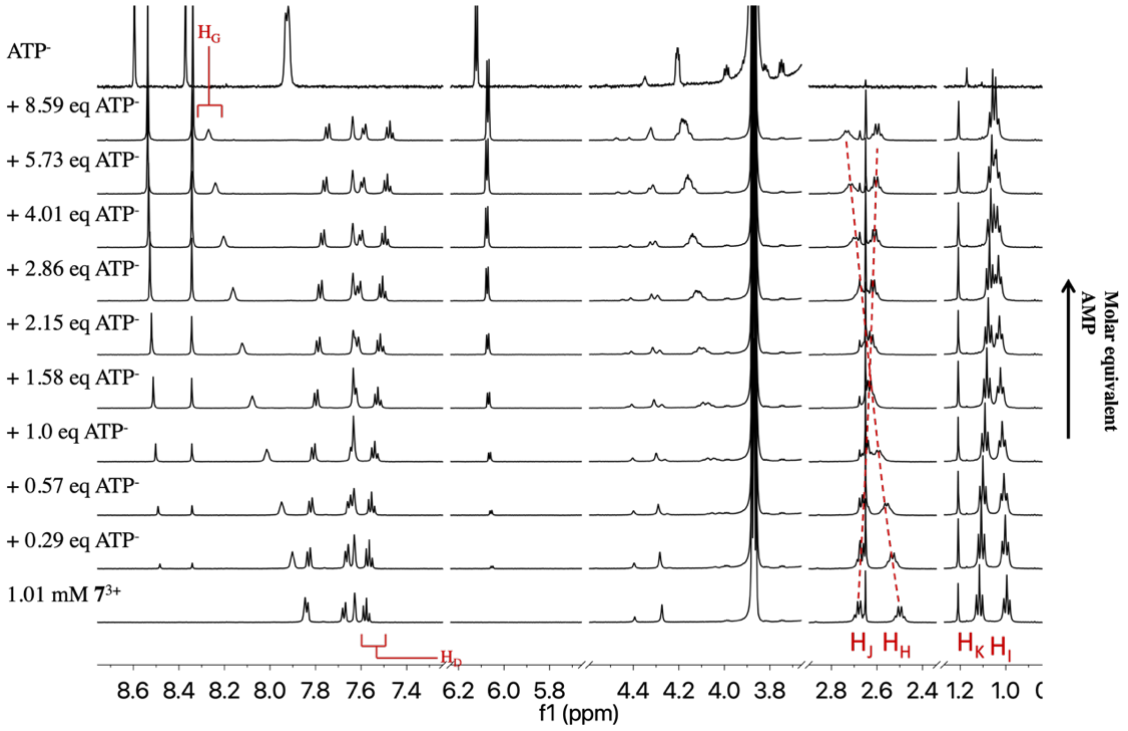
Fit	RMS	Covariance
Proton 1	4.2116e-4	4.7218e-5
Proton 2	2.7904e-4	9.8913e-5
Proton 3	2.3665e-4	4.7666e-4
Total	**3.2210e-4**	**4.0493e-5**

Coefficients

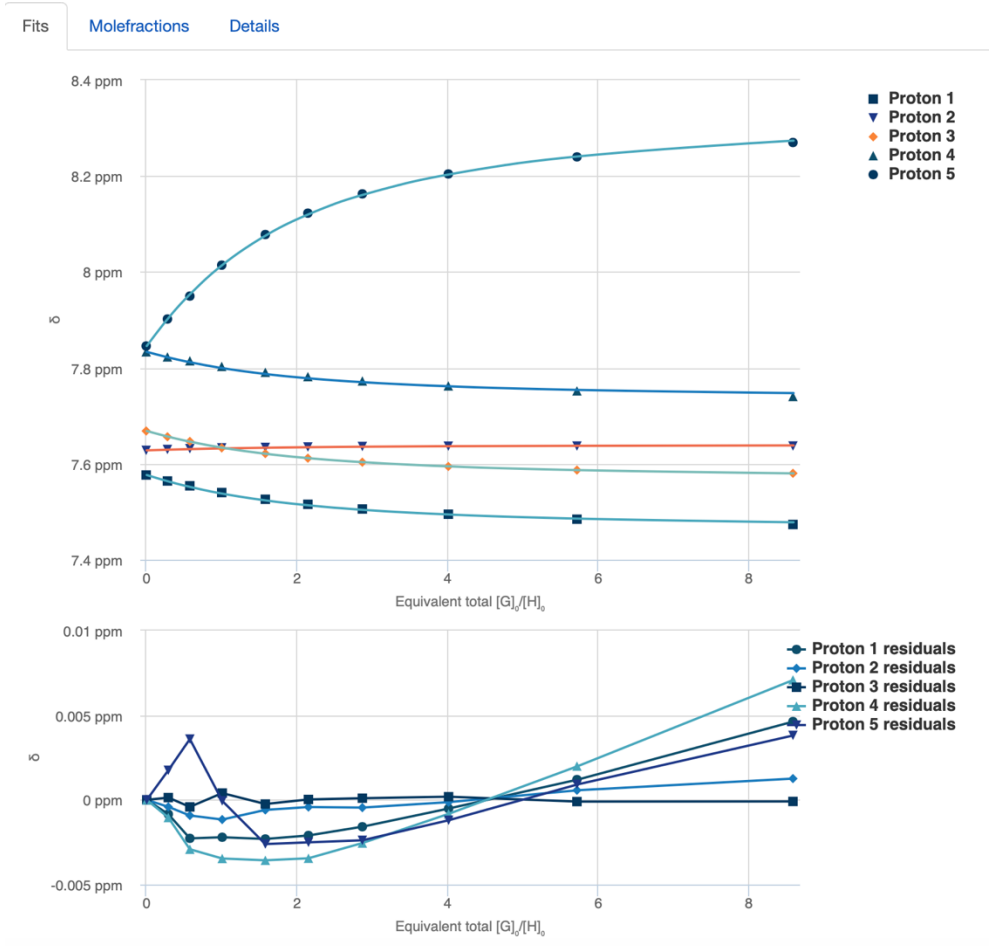
Fit	H	HG	HG2
Proton 1	8.1594	8.3839	8.3983
Proton 2	7.7077	7.8081	7.8225
Proton 3	7.6828	7.6434	7.6397

Figure S11. (A) ^{1}H NMR spectra (600 MHz, 298 K) of 0.24 mM of [**1**-H_6]$^{6+}$ in 27 mM HEPES buffer at pH = 3, obtained upon an incremental addition of 22.0 mM solution of sodium pyrophosphate (PPi) in the same buffer. (B) Nonlinear least-square analysis of ^{1}H NMR binding data corresponding to the formation of ternary [$(H_2P_2O_7)_2$⊂**1**]$^{2+}$ complex (1:2 fitting model; www.supramolecular.org). Using the change in the chemical shift of $\mathbf{H}_{G/D/F}$ as a function of the overall concentration of PPi we would, from three measurements, obtain: K_1 = 1912 ± 1, 1058 ± 1, 1264 ± 2 M^{-1} and K_2 = 527 ± 1 M^{-1}, 118 ± 6, 314 ± 5. The reported values are thus $K_1 = 1.4 \pm 0.4 \cdot 10^3$ M^{-1} and $K_2 = 3 \pm 2 \cdot 10^2$ M^{-1} (mean ± standard deviation).

(A)


ATP-
+ 8.59 eq ATP-
+ 5.73 eq ATP-
+ 4.01 eq ATP-
+ 2.86 eq ATP-
+ 2.15 eq ATP-
+ 1.58 eq ATP-
+ 1.0 eq ATP-
+ 0.57 eq ATP-
+ 0.29 eq ATP-
1.01 mM 7^3+
H_G
H_D
H_J H_H
H_K H_I
Molar equivalent AMP
8.6 8.4 8.2 8.0 7.8 7.6 7.4 6.2 6.0 5.8 4.4 4.2 4.0 3.8 2.8 2.6 2.4 1.2 1.0
f1 (ppm)

(B)


Fits
Molefractions
Details
8.4 ppm
8.2 ppm
8 ppm
7.8 ppm
7.6 ppm
7.4 ppm
δ
0
2
4
6
8
Equivalent total [G]0/[H]0
Proton 1
Proton 2
Proton 3
Proton 4
Proton 5
0.01 ppm
0.005 ppm
0 ppm
-0.005 ppm
Proton 1 residuals
Proton 2 residuals
Proton 3 residuals
Proton 4 residuals
Proton 5 residuals

Fitter: NMR 1:1 | Fit | Summary | Save

Details

Time to fit	0.2265 s
SSR	2.1080e-4
Fitted datapoints	50
Fitted params	6

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	679.01 M^{-1}	± 1.5848 %	100.00 M^{-1}

Quality of fit

Fit	RMS	Covariance
Proton 1	2.1478e-3	3.8922e-3
Proton 2	7.0951e-4	0.0502
Proton 3	2.1800e-4	5.7718e-5
Proton 4	3.2803e-3	1.1472e-2
Proton 5	2.2706e-3	2.6520e-4
Total	**2.0533e-3**	**2.5042e-4**

Coefficients

Fit	H	HG
Proton 1	7.5766	7.4585
Proton 2	7.6280	7.6403
Proton 3	7.6684	7.5625
Proton 4	7.8334	7.7304
Proton 5	7.8456	8.3585

Figure S12. (A) ^{1}H NMR spectra (600 MHz, 298 K) of 1.01 mM of [**4**-H_3]$^{3+}$ in 27 mM HEPES buffer at pH = 3, obtained upon an incremental addition of 70.0 mM solution of ATP^{2-} in the same buffer. (B) Nonlinear least-square analysis of ^{1}H NMR binding data corresponding to the formation of binary [ATP⊂**4**]$^+$ complex (1:1 fitting model; www.supramolecular.org). Using the change in chemical shift of $\mathbf{H}_{C/D/E}$ as a function of the overall concentration of ATP we would, from three measurements, obtain: K_1 = 679 ± 2, 379 ± 3 and 369 ± 3 M^{-1}. The reported value is thus $K_1 = 4.8 \pm 1.8 \cdot 10^2$ M^{-1} (mean standard ± deviation).

References

1. H. Xie, T. J. Finnegan, V. W. L. Gunawardana, R. Z. Pavlovic, C. E. Moore and J. D. Badjic, *J Am Chem Soc*, 2021, **143**, 3874-3880.
2. Q. P. B. Nguyen, T. N. Le and T. H. Kim, *B Korean Chem Soc*, 2009, **30**, 1743-1748.

Computational Studies:

General Calculation Workflow: In order to investigate the binding geometries of ATP and ADP in ternary complexes with **1** we employed a combination of conformational searches in Schrodinger's Macromodel[1] and temperature replica exchange molecular dynamics (T-REMD) simulations using AMBER.[2] All geometry optimizations were carried out using Gaussian 16[3] and frequency calculations were carried out for the final optimized molecules to confirm they were indeed minima on the potential energy surface. As a prerequisite for any MD simulation of a non-biological molecule, a single point electrostatic potential (ESP) calculation[4] must be carried out to parameterize the molecule in the AMBER gaff forcefield.[5]

Conformer Generation and Semi-Empirical Refinement: In this case, no crystal structures had been obtained for the complex, so to find low energy conformers for further optimization, frequency, and charge calculation, a conformer search with each of the individual molecules was carried out in Macromodel. For the guest molecules, ATP^{2-} and ADP^{-}, and $\mathbf{1}^{6+}$, a conformer search was carried out using the "Mixed torsional/Low-mode sampling" method with the OPLS3e forcefield[9] and the water solvation model. All default settings for this calculation were used with the exception of the maximum number of steps and the number of steps per rotatable bond which were changed to 20,000 and 180, respectively. Following this calculation, all generated conformers for the adenosine phosphates and the 30 lowest energy conformers for $\mathbf{1}^{6+}$ were exported as .xyz files. After this OPLS3e calculation (molecular mechanics), a semi-empirical refinement calculation was completed in Gaussian using the PM6 method[6] with PCM water solvation.[7] After the completion of the calculation, a Boltzmann population for each of the conformers was calculated according to the partition function at 298.15 K. Calculation of these values may easily be done using either excel spreadsheets, MATLAB[8] scripts, or python scripts.

$$Population = \frac{Q_i}{\sum_{i=1}^{100} Q_i} \qquad Q_i = e^{-E(PM6)/RT}$$

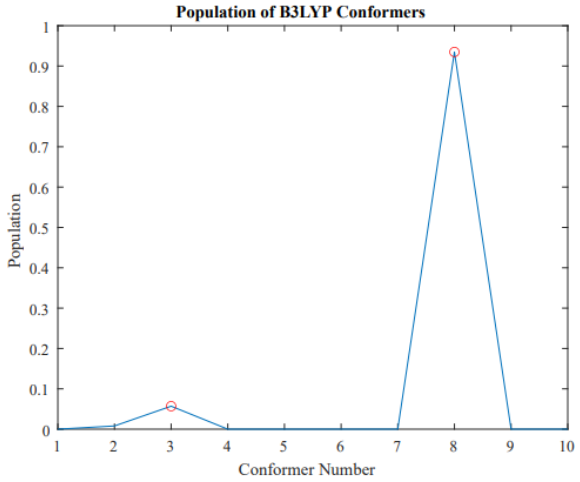
After this analysis, conformers were selected for DFT optimization under the condition that they had a predicted population (by PM6 energy) greater than 1%. Note that in this refinement step some calculations might fail under the given wall-time and in such cases these conformers were discarded.

Quantum Mechanical Calculations: Following PM6 refinement, the selected conformers were optimized in Gaussian at the B3LYP/6-31+G(d)[9-11] level of theory with PCM water solvation. Following optimization, a frequency calculation was carried out at the same level of theory to confirm the absence of imaginary frequencies confirming that the molecule is a minimum on the potential energy surface. After this calculation, the free energies of the conformers were compared and the lowest free-energy conformer was selected for charge calculation (Figure S13, S14, S15). For ESP charge generation,[12] a calculation was done at the HF/6-31G(d)[13] level of theory with Merz-Kollman charges (See Figure S16 for Gaussian file input format). This level of theory was chosen based on the calculation of charge for standard residues in the AMBER ff14SB forcefield.[14] The generated .esp file was then used to generate partial atomic charges and forcefield parameters in accordance with the RESP protocol for the GAFF forcefield using the Antechamber module in AMBER 18.[15,16]

Temperature Replica Exchange Molecular Dynamics (T-REMD) of Ternary Complexes:
Initial conformers of ternary $(ATP^{2-}/ADP^{-})_2 \subset \mathbf{1}^{6+}$ were made by docking the phosphate tails into the cavities of **1**. This was done in such a way that the final complex was C_2 symmetric (Figure S17). Next, an optimization using OPLS3e force field was done under the assumption that T-REMD equilibration and production simulations should explore the potential energy surface sufficiently. Before REMD equilibration, a standard equilibration procedure was used to prepare the input files. In short, systems were put through two minimization steps, one heating step, one density equilibration step, and four equilibrations in which restraints are slowly removed from the complex. For a detailed description of this procedure see our previously published manuscript.[17] After initial equilibration, T-REMD equilibration and production runs were completed using adapted scripts from the AMBER advanced tutorial A7.[18] A temperature distribution for T-REMD was chosen following work on the study of the association of peptide dimers.[19]

Analysis of T-REMD Complex Conformations:
Initially, T-REMD trajectories were processed using the CPPTRAJ[20] module to view stripped trajectories. In looking at these trajectories, we noticed that most of the conformational exchange in the complexes was restricted to movement of the base-pairs to form π–π contacts with the benzene rings in the "arms" of **1**. To analyze the different possible π–π contacts formed, CPPTRAJ modules were used to calculate the distance between the centroids of all benzene rings of $\mathbf{1}^{6+}$ and the base pairs of the adenosine phosphates. This data was further analyzed in MATLAB to inspect the percentage of simulation time that π–π interactions were observed and the fraction of that time that interaction occurred with each arm's benzene rings (Figures S18 and S19). Further, to create a representative model of the complex, frames were sorted based upon the different combinations of π–π interactions observed for both guest molecules and $\mathbf{1}^{6+}$. From the cluster representing the most populated π–π contacts for both arms, a single frame was chosen as a representative picture of the complex. Finally, this frame, for each ternary complex, was reoptimized in Macromodel using the OPLS3e forcefield with water solvation to give a final representative structure (Figure S20). These structures (and all others shown) were visualized using UCSF ChimeraX: developed by the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco, with support from National Institutes of Health R01-GM129325 and the Office of Cyber Infrastructure and Computational Biology, National Institute of Allergy and Infectious Diseases.[20]

(a)



(b)

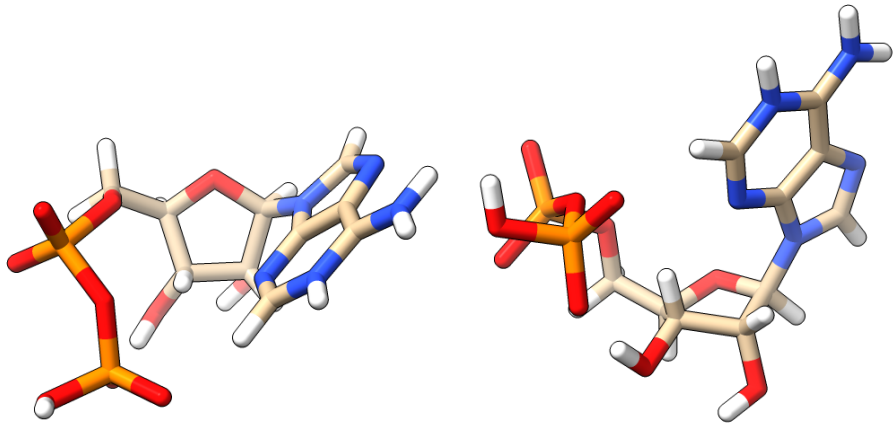
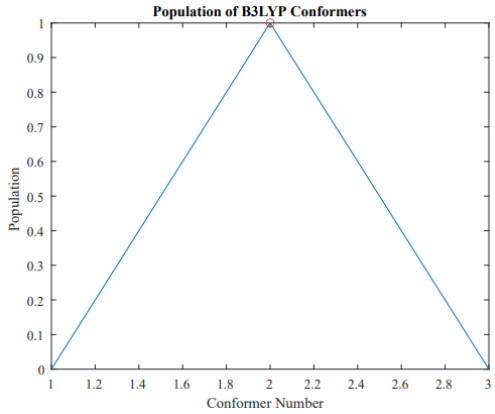


Figure S13. Summary of the DFT (B3LYP/6-31+G*, PCM water solvation) optimization and frequency calculation for the selected conformers of ADP. (a) Graph showing the populations of conformers as a line graph. In these figure peaks correspond to a conformer with a high population. (b) Structure of the lowest free energy conformer.

(a)



(b)

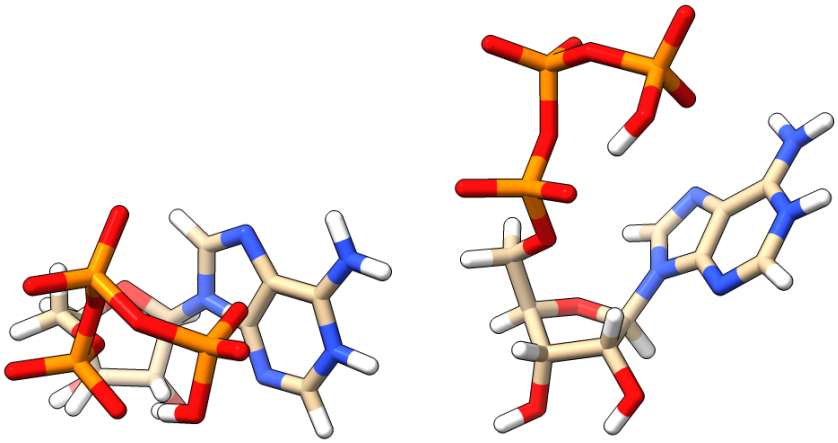
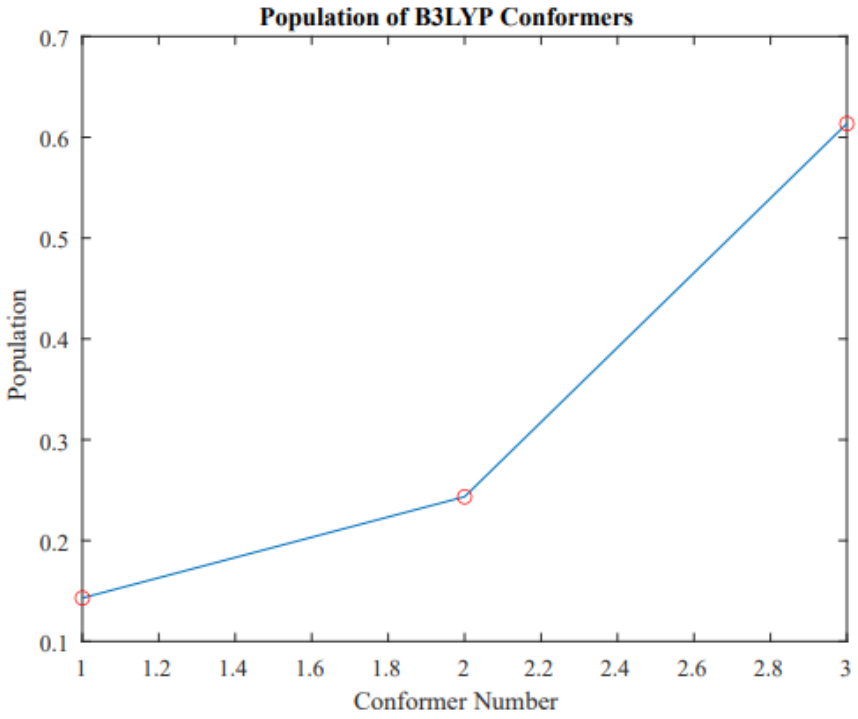


Figure S14. Summary of the DFT (B3LYP/6-31+G*, PCM water solvation) optimization and frequency calculation for the selected conformers of ATP. (a) Graph showing the populations of conformers as a line graph. In these figure peaks correspond to a conformer with a high population. (b) Structure of lowest free energy conformer.

(a)



(b)

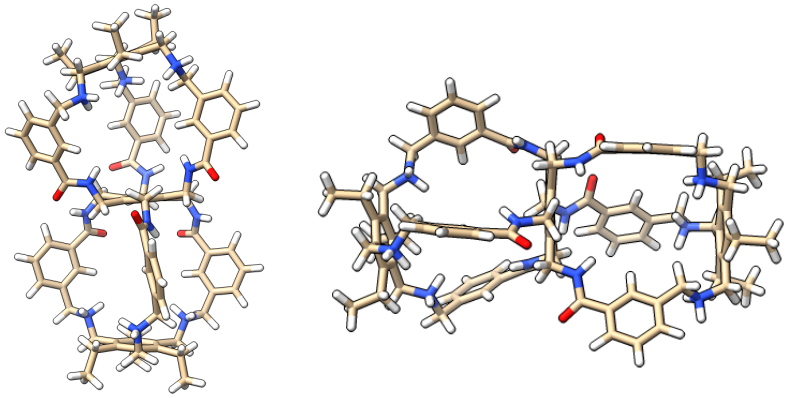


Figure S15. Summary of the DFT (B3LYP/6-31+G*, PCM water solvation) optimization and frequency calculation for the selected conformers of **1**. (a) Graph showing the populations of conformers as a line graph. In this case the lowest energy conformer had a ethyl group pointed toward the cavity so the second lowest energy conformer was taken (b) Structure of the second lowest free energy conformer.

```
%chk=atp_bp_prot_conf_1.chk
%nprocshared=28
%mem=110gb
#SP HF/6-31G* scrf=(solvent=Water, PCM) Pop=MK IOp(6/50=1) geom=allcheck

atp_bp_prot_conf_1.esp
```

Figure S16. Example of Gaussian input for ESP file generation. Note that if charges and coordinates were specified after the job control line (i.e. not using geom=allcheck), one should use the convention of a blank line with a space after the coordinates, then add [filename].esp on the next line to specify what you would like to save the ESP data to for AMBER's Antechamber. When using geom=allcheck write the [filename].esp as you would for a job title line.

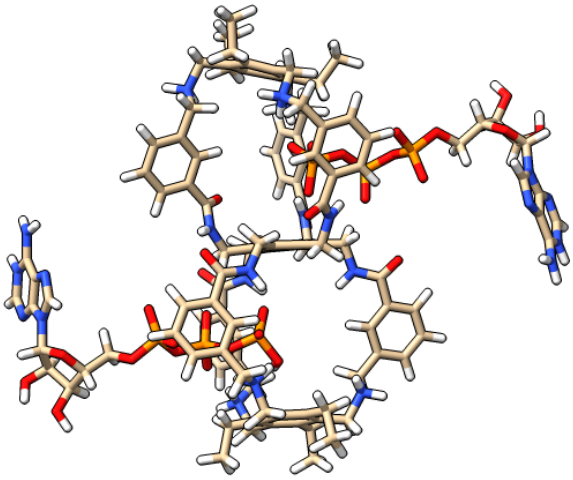
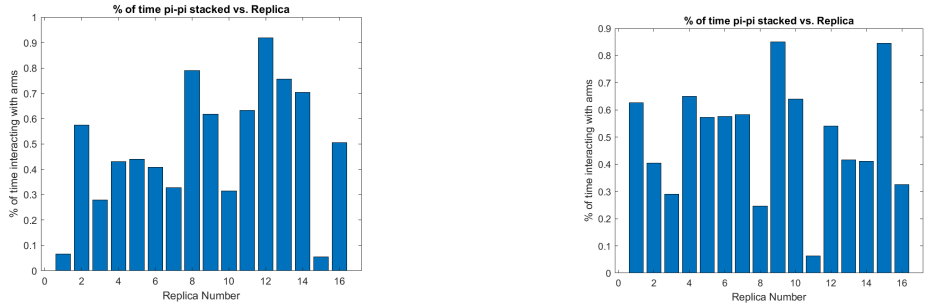


Figure S17. Initial pre-equilibration geometry of the $(ATP)_2 \subset \mathbf{1}$ complex. Note how ATP molecule occupy portals, or gaps between arms, on the opposite side of the molecules. A pseudo C_2 symmetry axis comes out of the page through the central benzene ring.

(a)



(b)

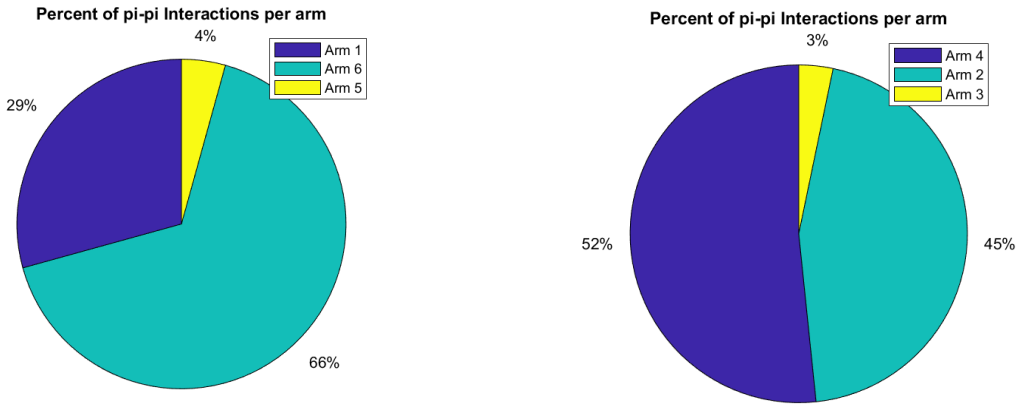
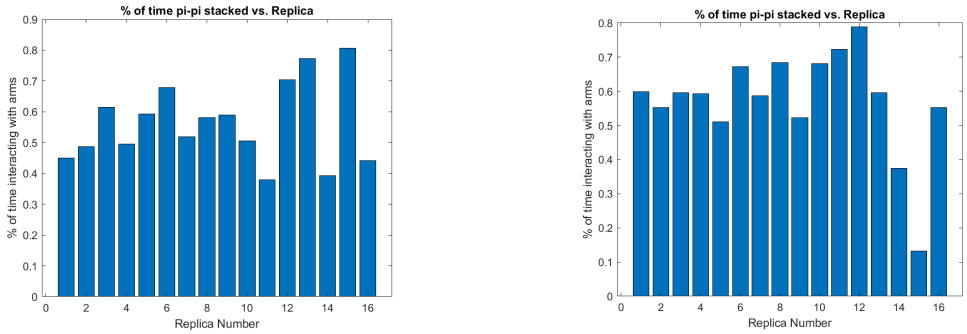


Figure S18. Summary of computed π–π interactions for $[(ADP)_2 \subset \mathbf{1}]^{2+}$ ternary complex. Corresponding graphs for individual ADP molecules are shown on the left and right sides of the figure. (a) Bar graphs showing the proportion of simulation time in which a π–π interaction was observed for each ADP molecule in the ternary complex. (b) Pie charts showing the percentage of π–π interactions that occurred different arms for each ADP molecule in the complex.

(a)



(b)

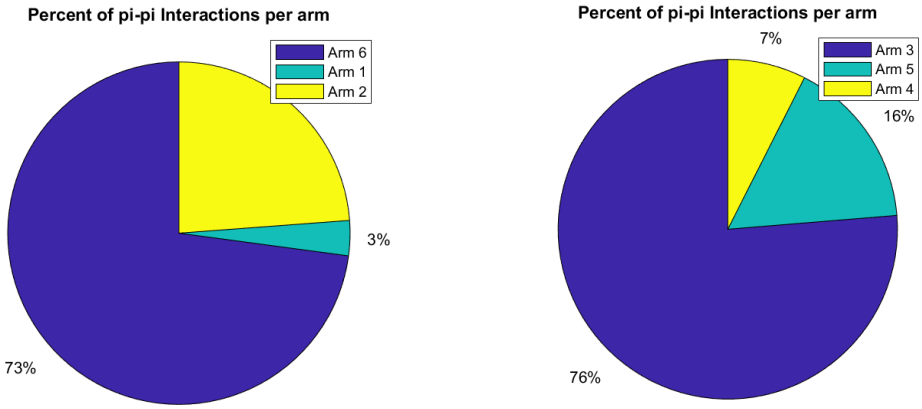
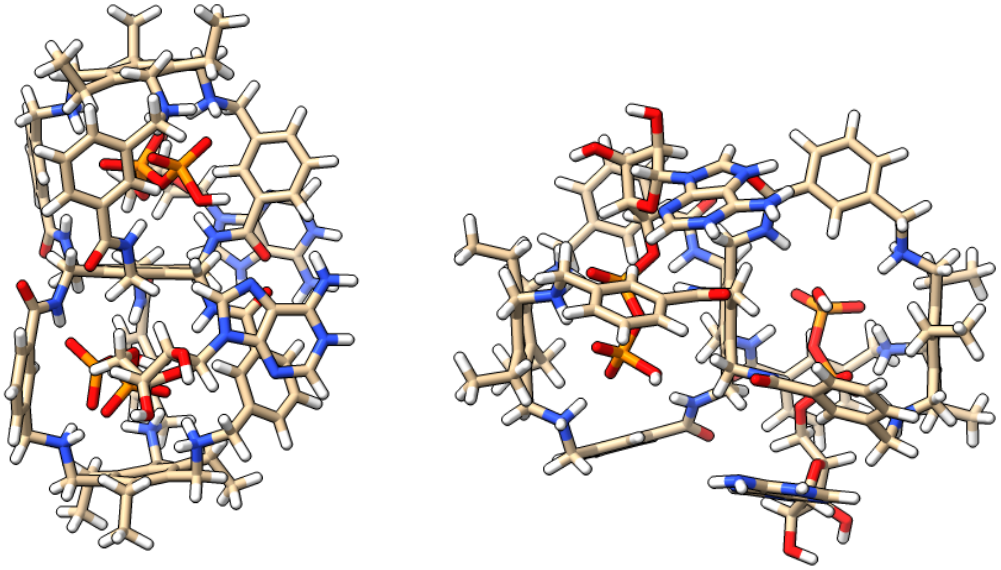


Figure S19. Summary of computed π–π interactions for $[(ATP)_2 \subset \mathbf{1}]^{4+}$ ternary complex. Corresponding graphs for individual ATP molecules are shown on the left and right sides of the figure. (a) Bar graphs showing the proportion of simulation time in which a π–π interaction was observed for each ATP molecule in the ternary complex. (b) Pie charts showing the percentage of π–π interactions that occurred different arms for each ATP molecule in the complex.

(a)



(b)

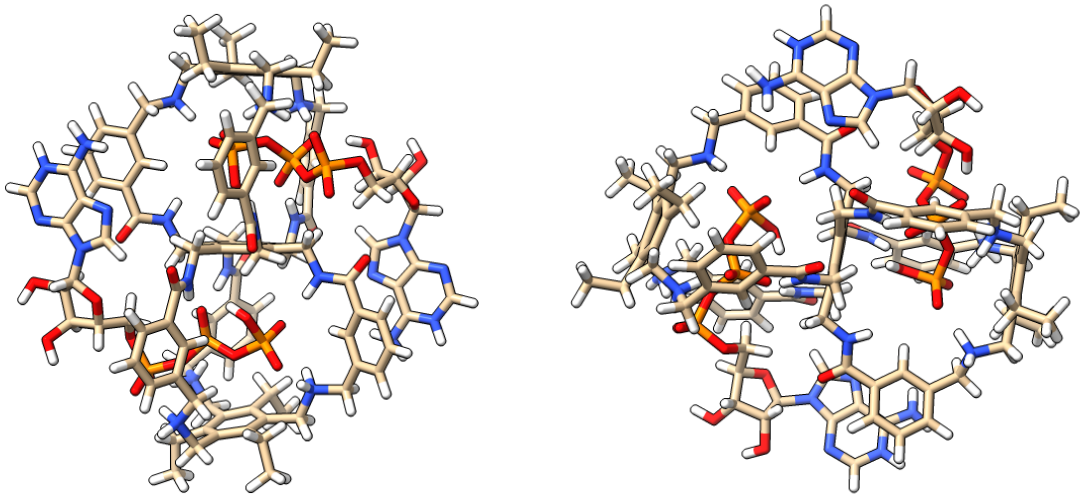


Figure S20. Representative structures for the adenosine phosphate ternary complexes after OPLS3e minimization. (a) $[(ADP)_2 \subset \mathbf{1}]^{4+}$ complex showing interaction between the ADP molecules base pairs and benzene arms of the same cavities. (b) $[(ATP)_2 \subset \mathbf{1}]^{4+}$ complex showing interaction between ATP molecules base pairs and benzene arms of opposite cavities.

Molecular Coordinates for B3LYP Optimized Structures:

1
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Number of imaginary frequencies = 0
Cartesian Coordinates:
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C -0.34100000 -2.25700000 1.80900000
C 0.25700000 -0.65000000 3.55300000
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C -0.65500000 -1.12000000 2.59000000
C 2.47600000 -0.77000000 4.76200000
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H 2.00100000 -0.26700000 5.60300000
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C -3.60900000 1.34000000 -1.96300000
C -3.58200000 2.30200000 -2.97200000
C -2.20600000 3.73500000 -1.58200000
H -1.79100000 2.99900000 0.39300000
H -4.14900000 0.40900000 -2.10300000
H -4.10400000 2.12200000 -3.90700000
H -2.85200000 4.23800000 -3.58100000
C 5.95900000 3.21200000 0.55600000
H 5.19400000 2.61600000 0.05800000
H 6.92500000 3.02800000 0.08500000
C 3.95600000 -0.93700000 -4.49900000
H 3.03400000 -0.95500000 -5.08300000
H 4.80700000 -0.84800000 -5.17600000
C -1.41200000 4.99900000 -1.36300000
H -1.61400000 5.44300000 -0.38700000
H -1.60000000 5.75000000 -2.13100000
N 5.62800000 4.67100000 0.27200000
H 6.28100000 5.26200000 0.79900000
N 3.91800000 0.35100000 -3.68100000
H 4.69000000 0.33200000 -3.00600000
C 0.84200000 5.15400000 -2.64400000
H 0.21600000 4.87100000 -3.48500000
H 0.85600000 6.24200000 -2.60900000
C 5.68300000 5.11900000 -1.19300000
H 6.67700000 4.85400000 -1.54200000
H 5.64300000 6.20700000 -1.15700000
C 3.99200000 1.64500000 -4.48400000
H 3.26100000 1.54900000 -5.28300000
H 4.97400000 1.65400000 -4.95200000
C 3.74400000 2.85100000 -3.59800000
C 3.28900000 5.12600000 -1.99100000
C 4.81800000 3.41700000 -2.87300000
C 2.43900000 3.38500000 -3.50200000

C 2.22800000 4.54000000 -2.71500000
C 4.56900000 4.52800000 -2.03500000
C 6.23600000 2.89600000 -3.07200000
C 1.29000000 2.76700000 -4.29000000
C 3.08000000 6.44500000 -1.25600000
O -3.88800000 -0.37400000 0.28200000
O 0.81600000 -4.10600000 -1.55500000
O 3.93000000 1.23400000 6.02700000
N -2.59600000 -2.98200000 0.84600000
H -3.30300000 -2.26900000 0.67900000
N -5.99900000 -5.80400000 5.30200000
H -4.97500000 -5.80600000 5.25000000
H -6.25300000 -4.81200000 5.37400000
N 0.09800000 4.70200000 -1.39000000
H 0.23700000 3.69400000 -1.26300000
H 0.53700000 5.13400000 -0.57100000
H -5.10500000 -2.05700000 8.78600000
H -1.34300000 -6.59700000 7.79300000
H 4.70200000 4.87500000 0.66500000
H 3.06800000 0.35600000 -3.10700000
H 6.81000000 2.95200000 -2.14600000
H 6.24000000 1.83300000 -3.31900000
C 6.99000000 3.66300000 -4.17900000
H 7.99900000 3.25600000 -4.29400000
H 6.47600000 3.58300000 -5.14300000
H 7.07500000 4.72900000 -3.94000000
H 0.35100000 2.86700000 -3.74100000
C 1.12100000 3.37800000 -5.69800000
H 1.42000000 1.68700000 -4.38600000
H 2.02400000 3.24500000 -6.30300000
H 0.28700000 2.89500000 -6.21700000
H 0.91700000 4.45300000 -5.64900000
H 3.71200000 6.51800000 -0.36900000
C 3.35800000 7.66500000 -2.16000000
H 2.06600000 6.52700000 -0.85900000
H 3.19100000 8.59100000 -1.59900000
H 4.39000000 7.66600000 -2.52500000
H 2.70000000 7.67200000 -3.03600000

ATP

E(RB3LYP) = -2665.941985
Number of imaginary frequencies = 0
Cartesian Coordinates:
P -12.63522200 -1.21097900 10.68192800
P -9.87890700 0.11390900 10.65258300
P -10.13226100 0.08831000 7.57928400
O -12.46385100 -2.20297600 11.80481200

O -12.72897200 -1.69571200 9.24509200
O -11.53601300 0.01036600 10.78135800
O -9.22091500 -0.93611000 11.51775400
O -9.55689400 1.57553700 10.85688700
O -9.59279100 -0.34855600 9.10239000
O -10.96901000 1.34742000 7.65520700
O -11.06099200 -1.21077800 7.23282000
O -8.92461400 0.03658300 6.66687200
O -14.00115300 -0.31893300 10.92170200
C -16.43375600 1.74918900 10.32352700
C -16.74737700 0.27760700 9.92315800
O -17.93636100 0.14728500 9.17359500
C -16.82186100 -0.44126700 11.29531900
O -18.18913200 -0.37615100 11.71962900
C -15.92082200 0.40939200 12.19657200
O -16.07985400 1.76179000 11.68522400
C -14.46480800 -0.03456700 12.24708900
N -13.92365800 2.43639600 5.83708900
C -14.94458600 1.56199000 6.12379000
N -15.50388800 1.43761600 7.29405300
C -14.97598500 2.25717200 8.23606600
C -13.94114300 3.18150900 8.04069800
C -13.37165100 3.28582900 6.75737700
N -13.65322600 3.86127300 9.19807100
C -14.49450900 3.35555800 10.07487300
N -15.31602500 2.37182000 9.55946000
N -12.42017400 4.14901500 6.41928400
H -18.65299300 0.00659700 9.82364600
H -16.48994600 -1.47960800 11.22389800
H -18.40989600 -1.16926300 12.23204700
H -14.39077500 -0.93399800 12.86858000
H -14.56262300 3.64550200 11.11266700
H -11.97691500 4.69306300 7.14948200
H -17.31227700 2.38430200 10.17617000
H -16.30423500 0.43300700 13.22045400
H -11.95985400 4.12656400 5.51776600
H -11.72174800 -1.37913900 7.96784500
H -15.92832000 -0.13562500 9.33827500
H -13.85624600 0.75761700 12.70034600
H -13.57112900 2.44122800 4.88363200
H -15.27623400 0.95602000 5.28873000

ADP
E(RB3LYP) = -2098.644828
Number of imaginary frequencies = 0
Cartesian Coordinates:

P -0.09681900 3.45539000 3.92587100
P 1.09172800 1.00290300 5.36361600
O 0.38374700 4.83972600 4.29188400
O -1.49173500 2.98857700 4.26536900
O 1.05318500 2.41784600 4.53098900
O 0.38998300 1.39133500 6.80682500
O 0.17047000 -0.03107400 4.74327900
O 2.55882700 0.70241500 5.57245600
O 0.18985000 3.27139100 2.30631900
C 1.78311200 0.75579100 -0.40910800
C 1.37317800 -0.36405000 0.57018000
O 0.62392100 -1.33262300 -0.15982800
C 0.46718200 0.37556000 1.57088300
O -0.47534200 -0.48928300 2.17302800
C -0.17210800 1.45510400 0.69296000
O 0.90378100 1.85526300 -0.19055200
C -0.74873900 2.65818800 1.41650100
N 5.63364200 2.05732900 2.74324800
C 4.40424100 1.52533100 3.05656600
N 3.50723400 1.20508200 2.16688500
C 3.88391600 1.44782200 0.89391600
C 5.10702700 1.97683300 0.47271900
C 6.05398600 2.30929700 1.46315800
N 5.15947500 2.07989300 -0.89973500
C 3.99105800 1.62354100 -1.29250900
N 3.17001900 1.21665000 -0.25667900
N 7.25498700 2.82277100 1.22135200
H -0.00336600 -1.71935800 0.48136700
H 1.09285900 0.85149300 2.32637700
H -0.31832900 -0.42097000 3.15209300
H -1.63706400 2.33308900 1.96722000
H 4.18519100 1.37480000 4.11131000
H 3.66437900 1.55269400 -2.32174300
H 7.91247300 3.05908300 1.95427500
H 1.69912900 0.40438400 -1.44126900
H -0.98352600 1.01541600 0.09382000
H 7.53572000 3.00084900 0.26471700
H 2.23722200 -0.83666900 1.04739400
H -1.05398500 3.41237200 0.68141600
H 1.01030700 1.88621900 7.36872500
H 6.25718400 2.27309100 3.51710600

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X-Ray Crystallography:

The single crystal X-ray diffraction studies were carried out on a Nonius Kappa diffractometer equipped with a Bruker APEX-II CCD and Mo K_α radiation (λ = 0.71073 Å). A 0.418 x 0.256 x 0.224 mm piece of a colorless block was mounted on a MiTeGen Micromount with CHRISTO-LUBE MCG 1024 oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 50 mm and exposure time was 30 seconds per frame using a scan width of 1.0°. Data collection was 100% complete to 25.00° in θ. A total of 180560 reflections were collected covering the indices, -32<=h<=32, -20<=k<=20, -33<=l<=33. 10288 reflections were found to be symmetry independent, with a R_{int} of 0.0514. Indexing and unit cell refinement indicated a *C*-centered, monoclinic lattice. The space group was found to be *C*2/c. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model for refinement.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. All other hydrogen atoms (H-bonding) were located in the difference map. Their relative positions were restrained using DFIX commands and their thermals freely refined. Due to unmodelable solvent disorder, OLEX2 SMTBX solvent mask was used to mask out electron density from the lattice due to the disordered solvent contribution. Solvent appeared to be a mix of DMF and diethyl ether. Four voids were found with approximately 90 electrons in each, equating to one DMF and one ether per void. Crystallographic data are summarized in Table 1.

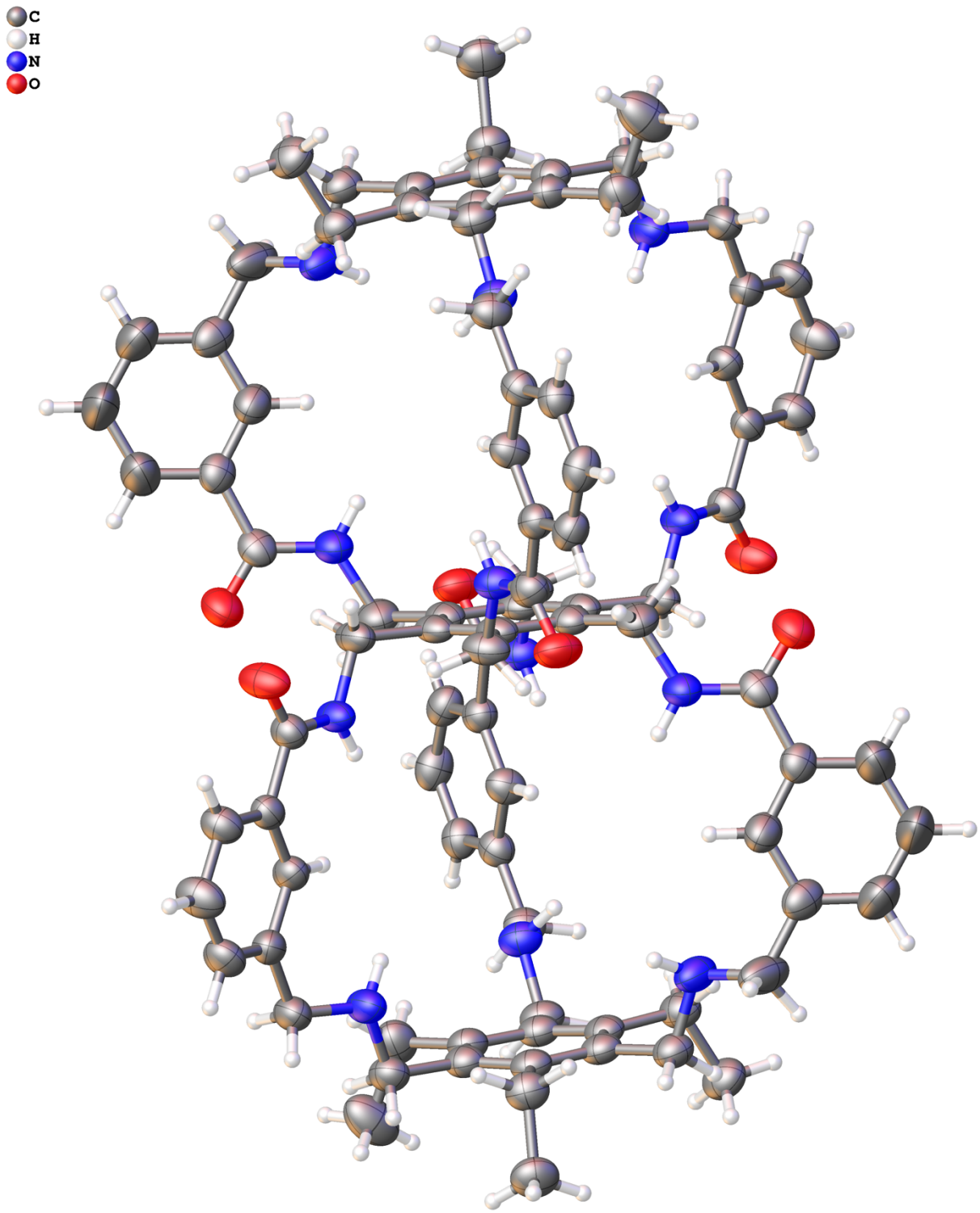
C
H
N
O

Table 1. Crystal data and structure refinement for compound **1**.

Report date	2022-02-09	
Identification code	HX20190814	
Empirical formula	C108 H144 N18 O12	
Molecular formula	C90 H102 N12 O6, 6(C3 H7 N O)	
Formula weight	1886.40	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 26.854(3) Å	α= 90°.
	b = 16.764(3) Å	β= 116.128(6)°.
	c = 27.767(4) Å	γ = 90°.
Volume	11222(3) $Å^3$	
Z	4	
Density (calculated)	1.117 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	4056	
Crystal size	0.418 x 0.256 x 0.224 mm^3	
Crystal color, habit	Colorless Block	
Theta range for data collection	1.480 to 25.365°.	
Index ranges	-32<=h<=32, -20<=k<=20, -33<=l<=33	
Reflections collected	180560	
Independent reflections	10288 [R(int) = 0.0514, R(sigma) = 0.0230]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0439 and 0.0246	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10288 / 147 / 704	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0737, wR2 = 0.2096	
R indices (all data)	R1 = 0.0974, wR2 = 0.2302	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.539 and -0.631 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6108(1)	9379(1)	3410(1)	66(1)
O(2)	9612(1)	7494(1)	5368(1)	67(1)
O(3)	6579(1)	5434(1)	5882(1)	67(1)
N(1)	6341(1)	6210(1)	2242(1)	50(1)
N(2)	6760(1)	8429(1)	3622(1)	49(1)
N(3)	8492(1)	4598(2)	3742(1)	60(1)
N(4)	8888(1)	6693(2)	5215(1)	54(1)
N(5)	6418(1)	3609(2)	3767(1)	56(1)
N(6)	6623(1)	5847(1)	5132(1)	49(1)
C(1)	6754(1)	4868(2)	2473(1)	47(1)
C(2)	7326(1)	4764(2)	2699(1)	47(1)
C(3)	7576(1)	4154(2)	3079(1)	47(1)
C(4)	7250(1)	3672(2)	3242(1)	47(1)
C(5)	6679(1)	3806(2)	3035(1)	48(1)
C(6)	6425(1)	4404(2)	2647(1)	49(1)
C(7)	6474(1)	5472(2)	2032(1)	52(1)
C(8)	6079(1)	6801(2)	1822(1)	50(1)
C(9)	5894(1)	7528(2)	2015(1)	45(1)
C(10)	6188(1)	7811(2)	2537(1)	49(1)
C(11)	6015(1)	8487(2)	2710(1)	45(1)
C(12)	5546(1)	8891(2)	2355(1)	53(1)
C(13)	5246(1)	8608(2)	1840(1)	57(1)
C(14)	5417(1)	7933(2)	1667(1)	49(1)
C(15)	6302(1)	8801(2)	3273(1)	50(1)
C(16)	7065(2)	8728(2)	4174(1)	56(1)
C(17)	7290(1)	8074(2)	4593(1)	46(1)
C(18)	7688(1)	5299(2)	2542(1)	54(1)
C(19)	7780(2)	4983(2)	2068(1)	64(1)
C(20)	8198(1)	4025(2)	3312(1)	53(1)
C(21)	9090(2)	4472(3)	3981(2)	86(1)
C(22)	9408(1)	5200(2)	4269(1)	57(1)

C(23)	9242(1)	5664(2)	4584(1)	60(1)
C(24)	9517(1)	6352(2)	4830(1)	49(1)
C(25)	9967(2)	6566(2)	4753(2)	95(1)
C(26)	10140(2)	6091(3)	4445(3)	138(3)
C(27)	9863(2)	5414(3)	4214(2)	93(1)
C(28)	9348(1)	6888(2)	5163(1)	48(1)
C(29)	8688(1)	7177(2)	5534(1)	57(1)
C(30)	8071(1)	7339(2)	5253(1)	46(1)
C(31)	7506(1)	2970(2)	3616(1)	55(1)
C(32)	7490(2)	2217(2)	3298(1)	64(1)
C(33)	6339(1)	3316(2)	3239(1)	52(1)
C(34)	6077(1)	3195(2)	3967(1)	56(1)
C(35)	6167(1)	3446(2)	4517(1)	48(1)
C(36)	6306(1)	4230(2)	4700(1)	48(1)
C(37)	6382(1)	4456(2)	5208(1)	42(1)
C(38)	6314(1)	3895(2)	5538(1)	54(1)
C(39)	6184(2)	3112(2)	5369(1)	68(1)
C(40)	6115(1)	2897(2)	4864(1)	58(1)
C(41)	6535(1)	5284(2)	5432(1)	47(1)
C(42)	6755(1)	6665(2)	5340(1)	55(1)
C(43)	7140(1)	7089(2)	5155(1)	46(1)
C(44)	5805(1)	4542(2)	2415(1)	63(1)
C(45)	5473(2)	3980(2)	1948(2)	88(1)
O(1S)	7390(1)	7106(2)	3399(1)	89(1)
N(1S)	8205(1)	7341(2)	3369(1)	72(1)
C(1S)	7853(2)	6891(2)	3466(1)	72(1)
C(2S)	8047(2)	8139(2)	3167(2)	96(2)
C(3S)	8726(2)	6994(4)	3428(2)	118(2)
O(2S)	4786(4)	5218(5)	4083(3)	134(3)
N(2S)	5011(12)	5056(17)	4961(9)	79(2)
C(4S)	4969(4)	5479(6)	4521(3)	88(2)
C(5S)	4862(4)	4241(7)	4916(5)	102(3)
C(6S)	5184(4)	5499(8)	5447(4)	99(3)
O(3S)	4478(6)	1330(9)	1636(4)	212(6)
N(3S)	5023(6)	1145(3)	2511(5)	108(2)
C(7S)	4529(5)	1190(8)	2096(4)	133(4)

C(9S)	5539(5)	1268(7)	2449(6)	140(4)
C(8S)	5008(7)	1005(11)	3024(4)	171(6)
O(4S)	8521(3)	4940(4)	5098(3)	112(2)
N(4S)	8125(8)	4042(10)	5417(5)	70(1)
C(10S)	8515(6)	4600(7)	5498(5)	96(2)
C(11S)	7794(4)	3692(6)	4900(4)	101(2)
C(12S)	8018(7)	3827(8)	5875(4)	96(2)
O(4B)	8457(3)	4261(4)	4910(3)	112(2)
N(4B)	8118(8)	3928(10)	5481(5)	70(1)
C(10B)	8441(6)	4364(7)	5352(4)	96(2)
C(11B)	7724(4)	3346(6)	5139(4)	101(2)
C(12B)	8130(7)	4076(9)	6017(4)	96(2)

Table 3. Bond lengths [Å] and angles [°] for compound **1**.

O(1)-C(15)	1.238(3)	C(7)-H(7B)	0.9900
O(2)-C(28)	1.226(3)	C(8)-H(8A)	0.9900
O(3)-C(41)	1.228(3)	C(8)-H(8B)	0.9900
N(1)-H(1)	0.930(18)	C(8)-C(9)	1.500(4)
N(1)-C(7)	1.478(4)	C(9)-C(10)	1.394(4)
N(1)-C(8)	1.454(4)	C(9)-C(14)	1.396(4)
N(2)-H(2)	0.8800	C(10)-H(10)	0.9500
N(2)-C(15)	1.339(4)	C(10)-C(11)	1.389(4)
N(2)-C(16)	1.470(4)	C(11)-C(12)	1.388(4)
N(3)-H(3)	0.944(19)	C(11)-C(15)	1.500(4)
N(3)-C(20)	1.463(4)	C(12)-H(12)	0.9500
N(3)-C(21)	1.457(4)	C(12)-C(13)	1.378(4)
N(4)-H(4)	0.8800	C(13)-H(13)	0.9500
N(4)-C(28)	1.348(4)	C(13)-C(14)	1.385(4)
N(4)-C(29)	1.466(4)	C(14)-H(14)	0.9500
N(5)-H(5)	0.925(19)	C(16)-H(16A)	0.9900
N(5)-C(33)	1.471(4)	C(16)-H(16B)	0.9900
N(5)-C(34)	1.442(4)	C(16)-C(17)	1.517(4)
N(6)-H(6)	0.8800	C(17)-C(30)#1	1.403(4)
N(6)-C(41)	1.347(3)	C(17)-C(43)#1	1.400(4)
N(6)-C(42)	1.469(3)	C(18)-H(18A)	0.9900
C(1)-C(2)	1.390(4)	C(18)-H(18B)	0.9900
C(1)-C(6)	1.413(4)	C(18)-C(19)	1.538(4)
C(1)-C(7)	1.510(4)	C(19)-H(19A)	0.9800
C(2)-C(3)	1.409(4)	C(19)-H(19B)	0.9800
C(2)-C(18)	1.521(4)	C(19)-H(19C)	0.9800
C(3)-C(4)	1.404(4)	C(20)-H(20A)	0.9900
C(3)-C(20)	1.517(4)	C(20)-H(20B)	0.9900
C(4)-C(5)	1.398(4)	C(21)-H(21A)	0.9900
C(4)-C(31)	1.520(4)	C(21)-H(21B)	0.9900
C(5)-C(6)	1.409(4)	C(21)-C(22)	1.502(5)
C(5)-C(33)	1.513(4)	C(22)-C(23)	1.383(4)
C(6)-C(44)	1.514(4)	C(22)-C(27)	1.344(5)
C(7)-H(7A)	0.9900	C(23)-H(23)	0.9500

C(23)-C(24)	1.377(4)	C(42)-C(43)	1.518(4)
C(24)-C(25)	1.364(5)	C(44)-H(44A)	0.9900
C(24)-C(28)	1.497(4)	C(44)-H(44B)	0.9900
C(25)-H(25)	0.9500	C(44)-C(45)	1.532(5)
C(25)-C(26)	1.389(6)	C(45)-H(45A)	0.9800
C(26)-H(26)	0.9500	C(45)-H(45B)	0.9800
C(26)-C(27)	1.354(6)	C(45)-H(45C)	0.9800
C(27)-H(27)	0.9500	O(1S)-C(1S)	1.228(4)
C(29)-H(29A)	0.9900	N(1S)-C(1S)	1.327(5)
C(29)-H(29B)	0.9900	N(1S)-C(2S)	1.440(5)
C(29)-C(30)	1.512(4)	N(1S)-C(3S)	1.456(5)
C(30)-C(43)#1	1.399(4)	C(1S)-H(1S)	0.9500
C(31)-H(31A)	0.9900	C(2S)-H(2SA)	0.9800
C(31)-H(31B)	0.9900	C(2S)-H(2SB)	0.9800
C(31)-C(32)	1.530(4)	C(2S)-H(2SC)	0.9800
C(32)-H(32A)	0.9800	C(3S)-H(3SA)	0.9800
C(32)-H(32B)	0.9800	C(3S)-H(3SB)	0.9800
C(32)-H(32C)	0.9800	C(3S)-H(3SC)	0.9800
C(33)-H(33A)	0.9900	O(2S)-C(4S)	1.177(10)
C(33)-H(33B)	0.9900	N(2S)-C(4S)	1.374(19)
C(34)-H(34A)	0.9900	N(2S)-C(5S)	1.41(3)
C(34)-H(34B)	0.9900	N(2S)-C(6S)	1.43(3)
C(34)-C(35)	1.497(4)	C(4S)-H(4S)	0.9500
C(35)-C(36)	1.399(4)	C(5S)-H(5SA)	0.9800
C(35)-C(40)	1.382(4)	C(5S)-H(5SB)	0.9800
C(36)-H(36)	0.9500	C(5S)-H(5SC)	0.9800
C(36)-C(37)	1.387(4)	C(6S)-H(6SA)	0.9800
C(37)-C(38)	1.381(4)	C(6S)-H(6SB)	0.9800
C(37)-C(41)	1.503(4)	C(6S)-H(6SC)	0.9800
C(38)-H(38)	0.9500	O(3S)-C(7S)	1.246(11)
C(38)-C(39)	1.386(4)	N(3S)-C(7S)	1.321(13)
C(39)-H(39)	0.9500	N(3S)-C(9S)	1.483(14)
C(39)-C(40)	1.379(5)	N(3S)-C(8S)	1.463(14)
C(40)-H(40)	0.9500	C(7S)-H(7S)	0.9500
C(42)-H(42A)	0.9900	C(9S)-H(9SA)	0.9800
C(42)-H(42B)	0.9900	C(9S)-H(9SB)	0.9800

C(9S)-H(9SC)	0.9800	C(28)-N(4)-H(4)	119.1
C(8S)-H(8SA)	0.9800	C(28)-N(4)-C(29)	121.8(2)
C(8S)-H(8SB)	0.9800	C(29)-N(4)-H(4)	119.1
C(8S)-H(8SC)	0.9800	C(33)-N(5)-H(5)	114(2)
O(4S)-C(10S)	1.255(10)	C(34)-N(5)-H(5)	120(2)
N(4S)-C(10S)	1.348(10)	C(34)-N(5)-C(33)	112.7(2)
N(4S)-C(11S)	1.438(10)	C(41)-N(6)-H(6)	120.4
N(4S)-C(12S)	1.469(9)	C(41)-N(6)-C(42)	119.3(2)
C(10S)-H(10S)	0.9500	C(42)-N(6)-H(6)	120.4
C(11S)-H(11A)	0.9800	C(2)-C(1)-C(6)	120.6(3)
C(11S)-H(11B)	0.9800	C(2)-C(1)-C(7)	120.4(3)
C(11S)-H(11C)	0.9800	C(6)-C(1)-C(7)	118.9(3)
C(12S)-H(12A)	0.9800	C(1)-C(2)-C(3)	119.8(3)
C(12S)-H(12B)	0.9800	C(1)-C(2)-C(18)	121.0(3)
C(12S)-H(12C)	0.9800	C(3)-C(2)-C(18)	119.2(3)
O(4B)-C(10B)	1.259(9)	C(2)-C(3)-C(20)	119.7(3)
N(4B)-C(10B)	1.301(10)	C(4)-C(3)-C(2)	120.0(3)
N(4B)-C(11B)	1.444(10)	C(4)-C(3)-C(20)	120.3(3)
N(4B)-C(12B)	1.494(10)	C(3)-C(4)-C(31)	120.5(3)
C(10B)-H(10B)	0.9500	C(5)-C(4)-C(3)	120.1(3)
C(11B)-H(11D)	0.9800	C(5)-C(4)-C(31)	119.3(3)
C(11B)-H(11E)	0.9800	C(4)-C(5)-C(6)	120.3(3)
C(11B)-H(11F)	0.9800	C(4)-C(5)-C(33)	119.5(3)
C(12B)-H(12D)	0.9800	C(6)-C(5)-C(33)	120.2(3)
C(12B)-H(12E)	0.9800	C(1)-C(6)-C(44)	120.5(3)
C(12B)-H(12F)	0.9800	C(5)-C(6)-C(1)	119.1(3)
		C(5)-C(6)-C(44)	120.4(3)
C(7)-N(1)-H(1)	107(2)	N(1)-C(7)-C(1)	111.2(2)
C(8)-N(1)-H(1)	110(2)	N(1)-C(7)-H(7A)	109.4
C(8)-N(1)-C(7)	111.6(2)	N(1)-C(7)-H(7B)	109.4
C(15)-N(2)-H(2)	119.7	C(1)-C(7)-H(7A)	109.4
C(15)-N(2)-C(16)	120.5(2)	C(1)-C(7)-H(7B)	109.4
C(16)-N(2)-H(2)	119.7	H(7A)-C(7)-H(7B)	108.0
C(20)-N(3)-H(3)	102(3)	N(1)-C(8)-H(8A)	109.0
C(21)-N(3)-H(3)	108(3)	N(1)-C(8)-H(8B)	109.0
C(21)-N(3)-C(20)	111.5(2)	N(1)-C(8)-C(9)	112.7(2)

H(8A)-C(8)-H(8B)	107.8	H(18A)-C(18)-H(18B)	107.6
C(9)-C(8)-H(8A)	109.0	C(19)-C(18)-H(18A)	108.7
C(9)-C(8)-H(8B)	109.0	C(19)-C(18)-H(18B)	108.7
C(10)-C(9)-C(8)	121.6(2)	C(18)-C(19)-H(19A)	109.5
C(10)-C(9)-C(14)	118.7(3)	C(18)-C(19)-H(19B)	109.5
C(14)-C(9)-C(8)	119.7(2)	C(18)-C(19)-H(19C)	109.5
C(9)-C(10)-H(10)	119.4	H(19A)-C(19)-H(19B)	109.5
C(11)-C(10)-C(9)	121.2(3)	H(19A)-C(19)-H(19C)	109.5
C(11)-C(10)-H(10)	119.4	H(19B)-C(19)-H(19C)	109.5
C(10)-C(11)-C(15)	123.4(3)	N(3)-C(20)-C(3)	110.6(2)
C(12)-C(11)-C(10)	119.2(3)	N(3)-C(20)-H(20A)	109.5
C(12)-C(11)-C(15)	117.3(3)	N(3)-C(20)-H(20B)	109.5
C(11)-C(12)-H(12)	119.9	C(3)-C(20)-H(20A)	109.5
C(13)-C(12)-C(11)	120.2(3)	C(3)-C(20)-H(20B)	109.5
C(13)-C(12)-H(12)	119.9	H(20A)-C(20)-H(20B)	108.1
C(12)-C(13)-H(13)	119.7	N(3)-C(21)-H(21A)	109.2
C(12)-C(13)-C(14)	120.7(3)	N(3)-C(21)-H(21B)	109.2
C(14)-C(13)-H(13)	119.7	N(3)-C(21)-C(22)	112.3(3)
C(9)-C(14)-H(14)	120.0	H(21A)-C(21)-H(21B)	107.9
C(13)-C(14)-C(9)	120.1(3)	C(22)-C(21)-H(21A)	109.2
C(13)-C(14)-H(14)	120.0	C(22)-C(21)-H(21B)	109.2
O(1)-C(15)-N(2)	121.4(3)	C(23)-C(22)-C(21)	121.8(3)
O(1)-C(15)-C(11)	120.1(3)	C(27)-C(22)-C(21)	119.3(3)
N(2)-C(15)-C(11)	118.5(2)	C(27)-C(22)-C(23)	118.9(3)
N(2)-C(16)-H(16A)	108.8	C(22)-C(23)-H(23)	118.9
N(2)-C(16)-H(16B)	108.8	C(24)-C(23)-C(22)	122.1(3)
N(2)-C(16)-C(17)	113.8(2)	C(24)-C(23)-H(23)	118.9
H(16A)-C(16)-H(16B)	107.7	C(23)-C(24)-C(28)	124.5(3)
C(17)-C(16)-H(16A)	108.8	C(25)-C(24)-C(23)	117.5(3)
C(17)-C(16)-H(16B)	108.8	C(25)-C(24)-C(28)	118.0(3)
C(30)#1-C(17)-C(16)	119.7(3)	C(24)-C(25)-H(25)	119.9
C(43)#1-C(17)-C(16)	120.2(3)	C(24)-C(25)-C(26)	120.2(4)
C(43)#1-C(17)-C(30)#1	120.0(3)	C(26)-C(25)-H(25)	119.9
C(2)-C(18)-H(18A)	108.7	C(25)-C(26)-H(26)	119.7
C(2)-C(18)-H(18B)	108.7	C(27)-C(26)-C(25)	120.7(4)
C(2)-C(18)-C(19)	114.1(2)	C(27)-C(26)-H(26)	119.7

C(22)-C(27)-C(26)	120.5(4)	H(34A)-C(34)-H(34B)	107.6
C(22)-C(27)-H(27)	119.8	C(35)-C(34)-H(34A)	108.7
C(26)-C(27)-H(27)	119.8	C(35)-C(34)-H(34B)	108.7
O(2)-C(28)-N(4)	121.4(3)	C(36)-C(35)-C(34)	122.1(3)
O(2)-C(28)-C(24)	121.0(3)	C(40)-C(35)-C(34)	120.2(3)
N(4)-C(28)-C(24)	117.5(2)	C(40)-C(35)-C(36)	117.8(3)
N(4)-C(29)-H(29A)	108.9	C(35)-C(36)-H(36)	119.3
N(4)-C(29)-H(29B)	108.9	C(37)-C(36)-C(35)	121.4(3)
N(4)-C(29)-C(30)	113.4(2)	C(37)-C(36)-H(36)	119.3
H(29A)-C(29)-H(29B)	107.7	C(36)-C(37)-C(41)	124.4(2)
C(30)-C(29)-H(29A)	108.9	C(38)-C(37)-C(36)	119.1(3)
C(30)-C(29)-H(29B)	108.9	C(38)-C(37)-C(41)	116.5(2)
C(17)#1-C(30)-C(29)	120.1(3)	C(37)-C(38)-H(38)	119.8
C(43)#1-C(30)-C(17)#1	119.8(3)	C(37)-C(38)-C(39)	120.5(3)
C(43)#1-C(30)-C(29)	120.2(3)	C(39)-C(38)-H(38)	119.8
C(4)-C(31)-H(31A)	109.5	C(38)-C(39)-H(39)	120.2
C(4)-C(31)-H(31B)	109.5	C(40)-C(39)-C(38)	119.5(3)
C(4)-C(31)-C(32)	110.8(2)	C(40)-C(39)-H(39)	120.2
H(31A)-C(31)-H(31B)	108.1	C(35)-C(40)-H(40)	119.2
C(32)-C(31)-H(31A)	109.5	C(39)-C(40)-C(35)	121.7(3)
C(32)-C(31)-H(31B)	109.5	C(39)-C(40)-H(40)	119.2
C(31)-C(32)-H(32A)	109.5	O(3)-C(41)-N(6)	121.4(3)
C(31)-C(32)-H(32B)	109.5	O(3)-C(41)-C(37)	119.7(2)
C(31)-C(32)-H(32C)	109.5	N(6)-C(41)-C(37)	118.8(2)
H(32A)-C(32)-H(32B)	109.5	N(6)-C(42)-H(42A)	109.0
H(32A)-C(32)-H(32C)	109.5	N(6)-C(42)-H(42B)	109.0
H(32B)-C(32)-H(32C)	109.5	N(6)-C(42)-C(43)	112.8(2)
N(5)-C(33)-C(5)	110.3(2)	H(42A)-C(42)-H(42B)	107.8
N(5)-C(33)-H(33A)	109.6	C(43)-C(42)-H(42A)	109.0
N(5)-C(33)-H(33B)	109.6	C(43)-C(42)-H(42B)	109.0
C(5)-C(33)-H(33A)	109.6	C(17)#1-C(43)-C(42)	119.8(3)
C(5)-C(33)-H(33B)	109.6	C(30)#1-C(43)-C(17)#1	120.2(2)
H(33A)-C(33)-H(33B)	108.1	C(30)#1-C(43)-C(42)	120.0(3)
N(5)-C(34)-H(34A)	108.7	C(6)-C(44)-H(44A)	109.0
N(5)-C(34)-H(34B)	108.7	C(6)-C(44)-H(44B)	109.0
N(5)-C(34)-C(35)	114.4(2)	C(6)-C(44)-C(45)	112.8(3)

H(44A)-C(44)-H(44B)	107.8	H(5SA)-C(5S)-H(5SB)	109.5
C(45)-C(44)-H(44A)	109.0	H(5SA)-C(5S)-H(5SC)	109.5
C(45)-C(44)-H(44B)	109.0	H(5SB)-C(5S)-H(5SC)	109.5
C(44)-C(45)-H(45A)	109.5	N(2S)-C(6S)-H(6SA)	109.5
C(44)-C(45)-H(45B)	109.5	N(2S)-C(6S)-H(6SB)	109.5
C(44)-C(45)-H(45C)	109.5	N(2S)-C(6S)-H(6SC)	109.5
H(45A)-C(45)-H(45B)	109.5	H(6SA)-C(6S)-H(6SB)	109.5
H(45A)-C(45)-H(45C)	109.5	H(6SA)-C(6S)-H(6SC)	109.5
H(45B)-C(45)-H(45C)	109.5	H(6SB)-C(6S)-H(6SC)	109.5
C(1S)-N(1S)-C(2S)	119.6(4)	C(7S)-N(3S)-C(9S)	121.4(11)
C(1S)-N(1S)-C(3S)	119.0(3)	C(7S)-N(3S)-C(8S)	114.3(12)
C(2S)-N(1S)-C(3S)	121.2(4)	C(8S)-N(3S)-C(9S)	124.3(11)
O(1S)-C(1S)-N(1S)	124.6(4)	O(3S)-C(7S)-N(3S)	121.3(13)
O(1S)-C(1S)-H(1S)	117.7	O(3S)-C(7S)-H(7S)	119.4
N(1S)-C(1S)-H(1S)	117.7	N(3S)-C(7S)-H(7S)	119.4
N(1S)-C(2S)-H(2SA)	109.5	N(3S)-C(9S)-H(9SA)	109.5
N(1S)-C(2S)-H(2SB)	109.5	N(3S)-C(9S)-H(9SB)	109.5
N(1S)-C(2S)-H(2SC)	109.5	N(3S)-C(9S)-H(9SC)	109.5
H(2SA)-C(2S)-H(2SB)	109.5	H(9SA)-C(9S)-H(9SB)	109.5
H(2SA)-C(2S)-H(2SC)	109.5	H(9SA)-C(9S)-H(9SC)	109.5
H(2SB)-C(2S)-H(2SC)	109.5	H(9SB)-C(9S)-H(9SC)	109.5
N(1S)-C(3S)-H(3SA)	109.5	N(3S)-C(8S)-H(8SA)	109.5
N(1S)-C(3S)-H(3SB)	109.5	N(3S)-C(8S)-H(8SB)	109.5
N(1S)-C(3S)-H(3SC)	109.5	N(3S)-C(8S)-H(8SC)	109.5
H(3SA)-C(3S)-H(3SB)	109.5	H(8SA)-C(8S)-H(8SB)	109.5
H(3SA)-C(3S)-H(3SC)	109.5	H(8SA)-C(8S)-H(8SC)	109.5
H(3SB)-C(3S)-H(3SC)	109.5	H(8SB)-C(8S)-H(8SC)	109.5
C(4S)-N(2S)-C(5S)	121(2)	C(10S)-N(4S)-C(11S)	122.9(8)
C(4S)-N(2S)-C(6S)	116(2)	C(10S)-N(4S)-C(12S)	117.3(9)
C(5S)-N(2S)-C(6S)	123.2(13)	C(11S)-N(4S)-C(12S)	119.6(8)
O(2S)-C(4S)-N(2S)	124.1(16)	O(4S)-C(10S)-N(4S)	118.6(10)
O(2S)-C(4S)-H(4S)	118.0	O(4S)-C(10S)-H(10S)	120.7
N(2S)-C(4S)-H(4S)	118.0	N(4S)-C(10S)-H(10S)	120.7
N(2S)-C(5S)-H(5SA)	109.5	N(4S)-C(11S)-H(11A)	109.5
N(2S)-C(5S)-H(5SB)	109.5	N(4S)-C(11S)-H(11B)	109.5
N(2S)-C(5S)-H(5SC)	109.5	N(4S)-C(11S)-H(11C)	109.5

H(11A)-C(11S)-H(11B)	109.5
H(11A)-C(11S)-H(11C)	109.5
H(11B)-C(11S)-H(11C)	109.5
N(4S)-C(12S)-H(12A)	109.5
N(4S)-C(12S)-H(12B)	109.5
N(4S)-C(12S)-H(12C)	109.5
H(12A)-C(12S)-H(12B)	109.5
H(12A)-C(12S)-H(12C)	109.5
H(12B)-C(12S)-H(12C)	109.5
C(10B)-N(4B)-C(11B)	125.8(9)
C(10B)-N(4B)-C(12B)	117.1(9)
C(11B)-N(4B)-C(12B)	117.0(8)
O(4B)-C(10B)-N(4B)	120.3(9)
O(4B)-C(10B)-H(10B)	119.9
N(4B)-C(10B)-H(10B)	119.9
N(4B)-C(11B)-H(11D)	109.5
N(4B)-C(11B)-H(11E)	109.5
N(4B)-C(11B)-H(11F)	109.5
H(11D)-C(11B)-H(11E)	109.5
H(11D)-C(11B)-H(11F)	109.5
H(11E)-C(11B)-H(11F)	109.5
N(4B)-C(12B)-H(12D)	109.5
N(4B)-C(12B)-H(12E)	109.5
N(4B)-C(12B)-H(12F)	109.5
H(12D)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+3/2,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	74(2)	55(1)	69(1)	-16(1)	30(1)	6(1)
O(2)	66(1)	74(2)	61(1)	-20(1)	29(1)	-22(1)
O(3)	110(2)	52(1)	47(1)	-7(1)	42(1)	-20(1)
N(1)	65(2)	44(1)	40(1)	2(1)	24(1)	5(1)
N(2)	67(2)	41(1)	41(1)	-2(1)	27(1)	-1(1)
N(3)	52(2)	70(2)	55(2)	-18(1)	22(1)	5(1)
N(4)	63(2)	52(1)	53(1)	-15(1)	32(1)	-11(1)
N(5)	76(2)	46(1)	61(2)	-12(1)	43(1)	-15(1)
N(6)	69(2)	41(1)	47(1)	-10(1)	36(1)	-13(1)
C(1)	61(2)	42(2)	40(1)	-5(1)	25(1)	2(1)
C(2)	61(2)	44(2)	40(1)	-9(1)	28(1)	-1(1)
C(3)	61(2)	44(2)	41(1)	-7(1)	27(1)	1(1)
C(4)	61(2)	44(2)	40(1)	-6(1)	25(1)	2(1)
C(5)	61(2)	44(2)	43(1)	-7(1)	27(1)	-2(1)
C(6)	58(2)	43(2)	48(2)	-6(1)	25(1)	1(1)
C(7)	68(2)	46(2)	43(2)	-2(1)	25(1)	5(1)
C(8)	54(2)	50(2)	40(1)	-1(1)	14(1)	2(1)
C(9)	49(2)	45(2)	42(1)	2(1)	20(1)	-4(1)
C(10)	49(2)	45(2)	45(2)	0(1)	14(1)	2(1)
C(11)	50(2)	43(2)	48(2)	0(1)	26(1)	-3(1)
C(12)	55(2)	53(2)	60(2)	4(1)	33(2)	5(1)
C(13)	50(2)	67(2)	55(2)	14(2)	25(1)	11(2)
C(14)	47(2)	55(2)	45(2)	7(1)	21(1)	0(1)
C(15)	61(2)	41(2)	54(2)	-1(1)	31(2)	-4(1)
C(16)	82(2)	43(2)	42(2)	-5(1)	27(2)	-7(2)
C(17)	68(2)	38(1)	37(1)	-10(1)	28(1)	-8(1)
C(18)	69(2)	49(2)	51(2)	-3(1)	33(2)	-2(1)
C(19)	82(2)	65(2)	62(2)	0(2)	45(2)	1(2)
C(20)	58(2)	54(2)	49(2)	-8(1)	26(1)	2(1)
C(21)	57(2)	97(3)	92(3)	-42(2)	21(2)	12(2)
C(22)	49(2)	69(2)	49(2)	-2(1)	17(1)	12(2)

C(23)	49(2)	74(2)	58(2)	-13(2)	26(2)	-3(2)
C(24)	43(2)	57(2)	45(2)	3(1)	17(1)	3(1)
C(25)	82(3)	70(2)	158(4)	-36(3)	76(3)	-22(2)
C(26)	124(4)	112(4)	248(7)	-78(4)	145(5)	-47(3)
C(27)	97(3)	78(3)	139(4)	-27(3)	85(3)	-7(2)
C(28)	49(2)	54(2)	35(1)	1(1)	13(1)	-5(1)
C(29)	66(2)	62(2)	47(2)	-14(1)	28(2)	-7(2)
C(30)	61(2)	43(1)	39(1)	-11(1)	26(1)	-7(1)
C(31)	65(2)	50(2)	49(2)	4(1)	24(1)	6(1)
C(32)	73(2)	49(2)	67(2)	4(2)	28(2)	12(2)
C(33)	64(2)	42(2)	55(2)	-4(1)	31(2)	-3(1)
C(34)	64(2)	49(2)	64(2)	-13(1)	36(2)	-14(1)
C(35)	46(2)	47(2)	56(2)	-9(1)	27(1)	-5(1)
C(36)	56(2)	40(1)	56(2)	-3(1)	32(1)	-6(1)
C(37)	40(1)	40(1)	47(1)	-1(1)	19(1)	-2(1)
C(38)	62(2)	47(2)	48(2)	0(1)	21(1)	-6(1)
C(39)	93(3)	52(2)	57(2)	3(2)	32(2)	-15(2)
C(40)	66(2)	41(2)	69(2)	-2(1)	31(2)	-9(1)
C(41)	53(2)	44(2)	45(2)	-2(1)	24(1)	-6(1)
C(42)	80(2)	43(2)	59(2)	-14(1)	45(2)	-18(1)
C(43)	71(2)	36(1)	42(1)	-12(1)	34(1)	-13(1)
C(44)	59(2)	53(2)	75(2)	5(2)	27(2)	4(2)
C(45)	69(2)	69(2)	92(3)	5(2)	5(2)	-3(2)
O(1S)	95(2)	85(2)	81(2)	4(1)	31(2)	28(2)
N(1S)	95(2)	68(2)	49(2)	14(1)	28(2)	12(2)
C(1S)	89(3)	63(2)	54(2)	1(2)	21(2)	21(2)
C(2S)	170(5)	60(2)	63(2)	3(2)	57(3)	14(3)
C(3S)	98(3)	140(5)	118(4)	56(4)	50(3)	30(3)
O(2S)	141(6)	167(7)	69(3)	-13(3)	22(3)	16(5)
N(2S)	57(3)	110(5)	58(4)	-3(3)	14(3)	12(3)
C(4S)	81(5)	110(5)	61(3)	-1(3)	21(3)	8(4)
C(5S)	76(6)	116(5)	104(7)	3(4)	30(5)	6(4)
C(6S)	72(5)	155(7)	70(4)	-19(4)	31(4)	-7(5)
O(3S)	212(10)	270(15)	124(5)	45(6)	47(5)	-26(10)
N(3S)	123(4)	75(3)	97(3)	16(6)	21(3)	-18(6)
C(7S)	131(5)	131(9)	106(5)	23(6)	22(4)	-12(6)

C(9S)	151(6)	104(8)	147(9)	9(7)	49(6)	-29(6)
C(8S)	165(10)	214(16)	106(5)	17(6)	33(5)	-50(10)
O(4S)	149(4)	93(3)	132(3)	8(3)	97(3)	-1(3)
N(4S)	79(2)	63(4)	80(2)	7(2)	45(2)	11(2)
C(10S)	115(3)	88(5)	110(4)	-1(3)	71(3)	-7(3)
C(11S)	103(4)	100(5)	100(4)	-7(3)	45(3)	-5(3)
C(12S)	119(5)	92(7)	91(4)	10(3)	59(4)	3(4)
O(4B)	149(4)	93(3)	132(3)	8(3)	97(3)	-1(3)
N(4B)	79(2)	63(4)	80(2)	7(2)	45(2)	11(2)
C(10B)	115(3)	88(5)	110(4)	-1(3)	71(3)	-7(3)
C(11B)	103(4)	100(5)	100(4)	-7(3)	45(3)	-5(3)
C(12B)	119(5)	92(7)	91(4)	10(3)	59(4)	3(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for compound **1**.

	x	y	z	U(eq)
H(1)	6675(10)	6400(20)	2504(12)	75
H(2)	6880	8002	3521	58
H(3)	8366(16)	4450(20)	3999(13)	90
H(4)	8701	6263	5053	65
H(5)	6464(16)	4155(12)	3810(15)	85
H(6)	6602	5726	4815	58
H(7A)	6722	5602	1863	62
H(7B)	6128	5240	1752	62
H(8A)	5753	6556	1524	60
H(8B)	6344	6963	1680	60
H(10)	6511	7538	2778	58
H(12)	5431	9364	2466	64
H(13)	4920	8880	1602	68
H(14)	5208	7745	1311	58
H(16A)	6815	9073	4258	67
H(16B)	7378	9062	4195	67
H(18A)	8053	5362	2856	64
H(18B)	7514	5833	2448	64
H(19A)	7425	4968	1745	96
H(19B)	7936	4444	2149	96
H(19C)	8038	5335	2006	96
H(20A)	8288	3476	3456	63
H(20B)	8320	4087	3027	63
H(21A)	9199	4325	3695	103
H(21B)	9188	4022	4237	103
H(23)	8927	5504	4632	72
H(25)	10162	7043	4910	114
H(26)	10456	6242	4397	166
H(27)	9991	5088	4012	111
H(29A)	8888	7692	5620	69

H(29B)	8775	6898	5876	69
H(31A)	7300	2873	3831	66
H(31B)	7895	3096	3866	66
H(32A)	7104	2081	3060	96
H(32B)	7664	1774	3546	96
H(32C)	7692	2313	3083	96
H(33A)	5942	3350	2982	63
H(33B)	6453	2749	3268	63
H(34A)	6151	2615	3973	67
H(34B)	5682	3283	3716	67
H(36)	6350	4616	4471	57
H(38)	6357	4046	5884	64
H(39)	6143	2726	5600	81
H(40)	6030	2359	4752	70
H(42A)	6931	6649	5737	66
H(42B)	6406	6974	5220	66
H(44A)	5723	5101	2289	76
H(44B)	5684	4466	2702	76
H(45A)	5592	4050	1664	132
H(45B)	5077	4103	1807	132
H(45C)	5538	3426	2075	132
H(1S)	7967	6366	3596	87
H(2SA)	8266	8524	3446	143
H(2SB)	7652	8218	3066	143
H(2SC)	8116	8217	2852	143
H(3SA)	8742	7010	3083	177
H(3SB)	8750	6439	3548	177
H(3SC)	9036	7299	3694	177
H(4S)	5095	6016	4573	106
H(5SA)	4737	4067	4543	154
H(5SB)	4561	4167	5021	154
H(5SC)	5184	3923	5151	154
H(6SA)	5566	5354	5693	149
H(6SB)	4939	5377	5614	149
H(6SC)	5165	6071	5368	149
H(7S)	4207	1114	2150	160

H(9SA)	5808	852	2646	210
H(9SB)	5695	1793	2591	210
H(9SC)	5454	1240	2068	210
H(8SA)	4622	997	2970	257
H(8SB)	5209	1432	3276	257
H(8SC)	5183	491	3172	257
H(10S)	8780	4733	5851	116
H(11A)	7872	3119	4914	152
H(11B)	7886	3944	4631	152
H(11C)	7400	3774	4804	152
H(12A)	8357	3900	6209	144
H(12B)	7901	3268	5844	144
H(12C)	7724	4170	5880	144
H(10B)	8667	4762	5592	116
H(11D)	7710	2895	5357	152
H(11E)	7839	3157	4870	152
H(11F)	7356	3591	4960	152
H(12D)	8440	4432	6226	144
H(12E)	8178	3568	6207	144
H(12F)	7781	4325	5968	144

Complex $[ATP_2 \subset 1\text{-}H_6]^{2+}$: The single crystal X-ray diffraction studies were carried out on a Bruker Kappa Photon III CPAD diffractometer equipped with Mo K_α radiation (λ = 0.71073 Å). A 0.176 x 0.134 x 0.092 mm piece of a colorless block was mounted on a Cryoloop with Paratone 24EX oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 60 mm using variable exposure time (20s-60s) depending on θ with a scan width of 1.0°. Data collection was 99.9% complete to 25.00° in θ(0.83Å). A total of 708414 reflections were collected covering the indices, -23<=h<=23, -28<=k<=28, -34<=l<=34. 90765 reflections were found to be symmetry independent, with a R_{int} of 0.0705. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be *P*1. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model for refinement.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Due to unmodelable solvent disorder, OLEX2 SMBTX mask was used to remove the electron density from the lattice due to the disordered solvent contribution. Solvent appeared to be water. One large void was found to contain approximately 875 electrons equating to 30 waters per complex of interest. The absolute stereochemistry of the molecule was established by anomalous dispersion using the Parson's method with a Flack parameter of 0.116(18), pre mask value was better, as well as due to the inclusion of known chiral ATP molecules. Crystallographic data are summarized in Table 1.

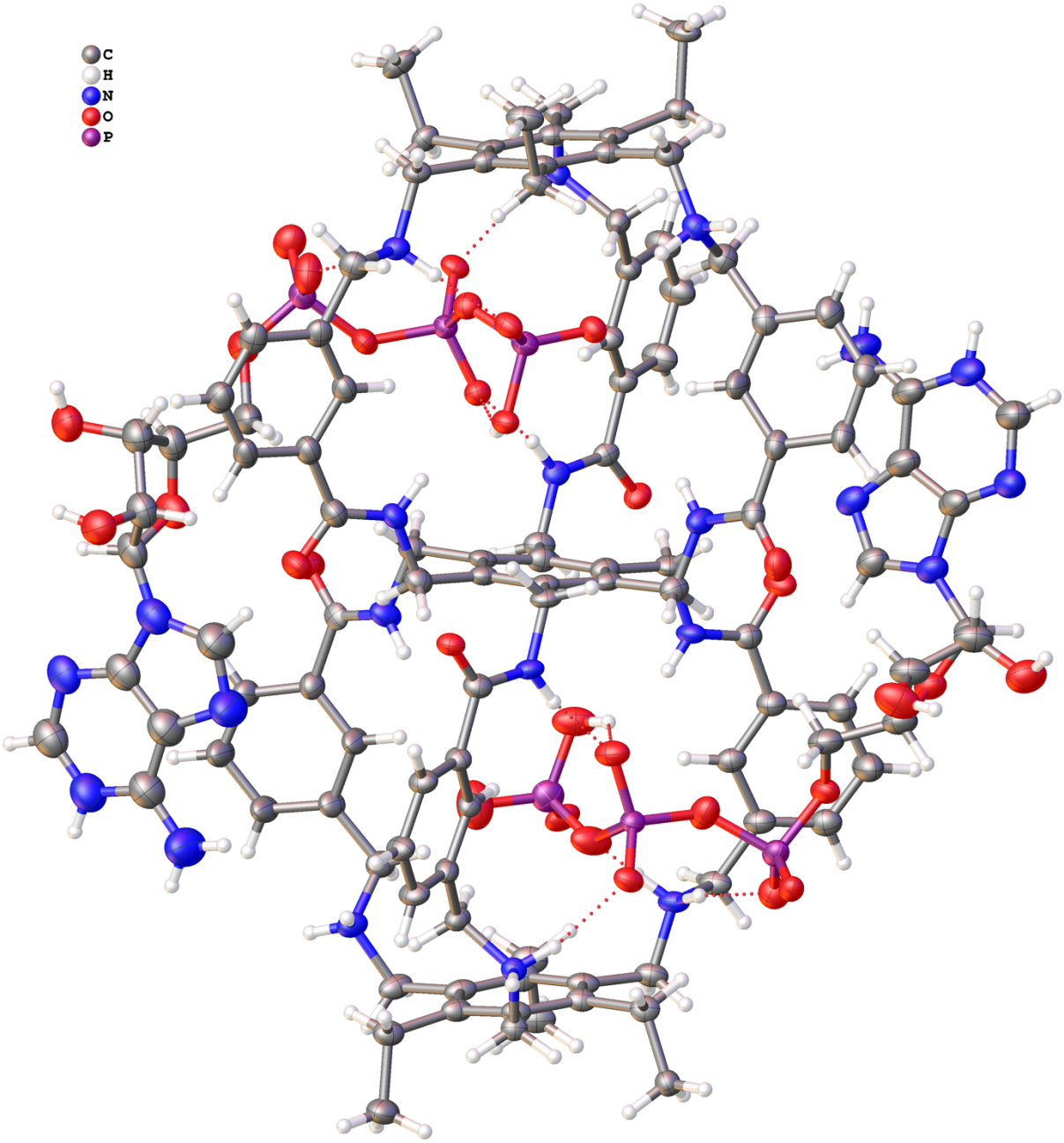
C
H
N
O
P

Table 1. Crystal data and structure refinement for **$[ATP_2 \subset 1\text{-}H_6]^{2+}$**.

Report date	2022-02-12	
Identification code	HX20220107	
Empirical formula	C110 H146 N22 O37 P6	
Molecular formula	C90 H108 N12 O6, 2(C10 H14 N5 O13 P3), 5(H2 O)	
Formula weight	2554.30	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 18.8037(15) Å	α= 86.620(3)°.
	b = 22.504(2) Å	β= 77.207(2)°.
	c = 27.891(2) Å	γ = 75.033(2)°.
Volume	11118.7(16) $Å^3$	
Z	3	
Density (calculated)	1.144 Mg/m^3	
Absorption coefficient	0.147 mm^{-1}	
F(000)	4038	
Crystal size	0.176 x 0.134 x 0.092 mm^3	
Crystal color, habit	Colorless Block	
Theta range for data collection	1.873 to 26.427°.	
Index ranges	-23<=h<=23, -28<=k<=28, -34<=l<=34	
Reflections collected	708414	
Independent reflections	90765 [R(int) = 0.0705, R(sigma) = 0.0528]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0274 and 0.0112	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	90765 / 4221 / 4823	
Goodness-of-fit on F^2	0.995	
Final R indices [I>2sigma(I)]	R1 = 0.0770, wR2 = 0.1940	
R indices (all data)	R1 = 0.1155, wR2 = 0.2244	
Absolute structure parameter	0.116(18)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.096 and -0.386 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **$[ATP_2 \subset 1\text{-}H_6]^{2+}$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1X)	-3613(2)	-2014(2)	-3508(2)	28(1)
O(2X)	-3581(3)	-1808(2)	-6531(2)	48(1)
O(3X)	1318(3)	-3136(2)	-6041(2)	41(1)
O(4X)	-4747(3)	-1183(2)	-4533(2)	44(1)
O(5X)	227(3)	-2217(2)	-6899(2)	31(1)
O(6X)	160(3)	-2313(2)	-3855(2)	42(1)
N(1X)	-2786(3)	-5198(2)	-3905(2)	24(1)
N(2X)	-2524(3)	-2587(2)	-3955(2)	28(1)
N(3X)	-3482(3)	-4961(2)	-5945(2)	36(1)
N(4X)	-3066(3)	-2281(3)	-5922(2)	36(1)
N(5X)	-132(3)	-5551(2)	-5619(2)	29(1)
N(6X)	150(3)	-3229(2)	-5686(2)	29(1)
N(7)	-3457(3)	1279(2)	-4790(2)	28(1)
N(8)	-3581(3)	-1071(3)	-4694(2)	31(1)
N(9)	-761(3)	980(2)	-6524(2)	24(1)
N(10)	-888(3)	-1659(2)	-6456(2)	26(1)
N(11)	-445(3)	793(2)	-4270(2)	32(1)
N(12)	-322(3)	-1915(3)	-4537(2)	34(1)
C(1A)	-3521(4)	-3075(3)	-3570(2)	27(1)
C(1C)	-4433(4)	-3560(3)	-3071(3)	32(1)
C(1X)	-2364(4)	-5818(3)	-4689(2)	26(1)
C(2X)	-2843(4)	-5733(3)	-5016(2)	29(1)
C(3X)	-2524(4)	-5723(3)	-5539(2)	30(1)
C(4X)	-1755(4)	-5825(3)	-5713(2)	36(1)
C(5X)	-1270(4)	-5950(3)	-5374(2)	28(1)
C(6X)	-1561(4)	-5939(3)	-4858(2)	27(1)
C(7X)	-2675(4)	-5793(3)	-4134(2)	26(1)
C(8X)	-3289(4)	-4652(3)	-4097(2)	28(1)
C(9X)	-3567(4)	-4094(3)	-3769(2)	28(1)
C(11)	-3242(3)	-3608(3)	-3888(2)	24(1)
C(12)	-4117(4)	-3061(3)	-3173(2)	30(1)

C(14)	-4142(4)	-4089(3)	-3363(3)	34(1)
C(15)	-3238(4)	-2509(3)	-3674(2)	30(1)
C(16)	-2229(4)	-2061(3)	-4151(2)	29(1)
C(17)	-1958(4)	-2094(3)	-4687(2)	27(1)
C(18)	-3682(4)	-5696(3)	-4842(2)	33(1)
C(19)	-3809(5)	-6350(3)	-4751(3)	44(2)
C(20)	-3051(4)	-5613(3)	-5888(2)	35(1)
C(21)	-3016(4)	-4580(3)	-6222(2)	34(1)
C(22)	-3480(4)	-3944(3)	-6330(2)	32(1)
C(23)	-3275(4)	-3411(3)	-6213(3)	38(2)
C(24)	-3665(4)	-2839(3)	-6338(2)	31(1)
C(25)	-4270(4)	-2791(3)	-6567(3)	34(1)
C(26)	-4523(5)	-3274(3)	-6644(3)	44(2)
C(27)	-4110(4)	-3862(3)	-6536(3)	44(2)
C(28)	-3434(3)	-2259(3)	-6248(2)	25(1)
C(29)	-2802(4)	-1745(3)	-5826(2)	31(1)
C(30)	-2204(4)	-1937(3)	-5508(2)	26(1)
C(31)	-1391(4)	-5857(3)	-6259(2)	38(2)
C(32)	-1206(5)	-6471(3)	-6490(2)	39(2)
C(33)	-421(4)	-6121(3)	-5563(2)	33(1)
C(34)	542(4)	-5622(3)	-6038(2)	32(1)
C(35)	1026(4)	-5187(3)	-6005(2)	34(1)
C(36)	701(4)	-4550(3)	-5951(2)	30(1)
C(37)	1151(4)	-4154(3)	-5949(2)	33(1)
C(38)	1939(4)	-4402(3)	-5998(3)	40(2)
C(39)	2255(4)	-5023(3)	-6067(3)	46(2)
C(40)	1791(4)	-5404(3)	-6080(2)	35(1)
C(41)	884(4)	-3477(3)	-5897(2)	29(1)
C(42)	-98(4)	-2552(3)	-5642(2)	30(1)
C(43)	-921(4)	-2342(3)	-5412(2)	30(1)
C(44)	-1054(4)	-6089(3)	-4497(2)	28(1)
C(45)	-885(4)	-6776(3)	-4375(2)	30(1)
C(46)	-2334(4)	1727(3)	-5053(2)	28(1)
C(47)	-2006(4)	1688(3)	-5553(2)	25(1)
C(48)	-1246(4)	1583(3)	-5712(2)	26(1)
C(49)	-752(4)	1505(3)	-5370(2)	26(1)

C(50)	-1089(4)	1522(3)	-4867(2)	29(1)
C(51)	-1878(4)	1640(3)	-4703(2)	27(1)
C(52)	-3168(4)	1874(3)	-4881(2)	27(1)
C(53)	-4139(4)	1367(3)	-4375(2)	35(1)
C(54)	-4542(4)	866(3)	-4361(2)	32(1)
C(55)	-4215(4)	264(3)	-4481(2)	32(1)
C(56)	-4638(4)	-173(3)	-4454(3)	34(1)
C(57)	-5419(4)	28(3)	-4272(2)	34(1)
C(58)	-5758(4)	635(3)	-4138(3)	41(2)
C(59)	-5353(4)	1056(3)	-4181(2)	35(1)
C(60)	-4306(4)	-837(3)	-4573(3)	40(2)
C(61)	-3294(4)	-1733(3)	-4781(3)	34(1)
C(62)	-2468(4)	-1933(3)	-4994(2)	27(1)
C(63)	-2528(4)	1842(3)	-5922(2)	29(1)
C(64)	-2733(4)	2538(3)	-6039(3)	38(2)
C(65)	-893(4)	1592(3)	-6269(2)	28(1)
C(66)	-236(4)	453(3)	-6303(2)	28(1)
C(67)	46(4)	-93(3)	-6652(2)	28(1)
C(68)	-232(4)	-628(3)	-6555(2)	31(1)
C(69)	61(4)	-1132(3)	-6832(2)	29(1)
C(70)	670(4)	-1144(3)	-7231(3)	41(2)
C(71)	935(4)	-636(3)	-7340(3)	43(2)
C(72)	644(4)	-101(3)	-7068(3)	42(2)
C(73)	-199(4)	-1710(3)	-6727(2)	24(1)
C(74)	-1185(4)	-2195(3)	-6272(2)	32(1)
C(75)	-1459(4)	-2164(3)	-5706(2)	30(1)
C(76)	64(4)	1509(3)	-5548(2)	26(1)
C(77)	150(4)	2177(3)	-5597(3)	41(2)
C(78)	-610(4)	1453(3)	-4493(2)	31(1)
C(79)	32(4)	327(3)	-4634(3)	37(1)
C(80)	351(4)	-260(3)	-4376(2)	33(1)
C(81)	35(4)	-757(3)	-4379(3)	40(2)
C(82)	330(4)	-1338(3)	-4160(2)	31(1)
C(83)	939(4)	-1376(3)	-3923(3)	36(1)
C(84)	1193(4)	-851(3)	-3897(3)	37(1)
C(85)	925(4)	-295(4)	-4130(3)	41(2)

C(86)	63(4)	-1888(3)	-4161(2)	31(1)
C(87)	-601(4)	-2460(3)	-4580(3)	33(1)
C(88)	-1162(4)	-2299(3)	-4898(2)	27(1)
C(89)	-2236(4)	1651(3)	-4158(2)	30(1)
C(90)	-2456(4)	2327(3)	-3958(3)	40(2)
P(1)	-1649(1)	-4166(1)	-5307(1)	40(1)
P(2)	-1217(1)	-4350(1)	-4362(1)	26(1)
P(3)	387(1)	-5053(1)	-4453(1)	33(1)
O(1)	-1331(4)	-3582(2)	-5316(2)	54(1)
O(2)	-2497(4)	-4016(3)	-5210(2)	69(2)
O(3)	-1259(3)	-4533(2)	-5755(2)	39(1)
O(4)	-1422(3)	-4549(2)	-4853(2)	52(1)
O(5)	-1444(3)	-3675(2)	-4328(2)	40(1)
O(6)	-1492(3)	-4731(2)	-3944(2)	32(1)
O(7)	-343(3)	-4519(2)	-4527(2)	47(1)
O(8)	573(3)	-5525(2)	-4862(2)	42(1)
O(9)	287(2)	-5264(2)	-3946(2)	30(1)
O(10)	1002(3)	-4673(2)	-4571(2)	37(1)
O(11)	2151(3)	-4017(2)	-4528(2)	41(1)
O(12)	1139(4)	-3685(3)	-3274(2)	66(2)
O(13)	2733(4)	-3931(3)	-3628(2)	61(1)
N(1)	2280(3)	-3032(3)	-4686(2)	42(1)
N(2)	1679(3)	-2345(3)	-5175(2)	43(1)
N(3)	3004(4)	-2401(3)	-4413(3)	48(1)
N(4)	2746(3)	-1391(3)	-4753(3)	48(1)
N(5)	1840(4)	-1030(3)	-5243(3)	64(2)
C(1)	856(4)	-4139(3)	-4251(3)	45(2)
C(2)	1591(4)	-4124(3)	-4100(3)	44(1)
C(3)	1531(5)	-3603(4)	-3760(3)	50(1)
C(4)	2292(5)	-3518(4)	-3866(3)	49(1)
C(5)	2546(4)	-3598(3)	-4421(3)	43(1)
C(6)	2517(4)	-2495(3)	-4652(3)	41(1)
C(7)	2138(4)	-2089(4)	-4978(3)	48(2)
C(8)	2223(4)	-1476(3)	-4993(3)	46(2)
C(9)	1794(4)	-2899(3)	-5000(3)	45(2)
C(10)	3103(5)	-1832(4)	-4503(4)	56(2)

P(1A)	-1907(1)	-17(1)	-5103(1)	29(1)
P(2A)	-2275(1)	68(1)	-6064(1)	28(1)
P(3A)	-3847(1)	756(1)	-6033(1)	35(1)
O(1A)	-2159(3)	-647(2)	-5061(2)	32(1)
O(2A)	-2322(2)	328(2)	-4649(2)	31(1)
O(3A)	-1077(2)	-127(2)	-5260(2)	32(1)
O(4A)	-2300(3)	348(2)	-5542(2)	32(1)
O(5A)	-1946(2)	-603(2)	-6046(2)	30(1)
O(6A)	-1947(2)	457(2)	-6465(2)	30(1)
O(7A)	-3166(3)	165(2)	-6051(2)	39(1)
O(8A)	-3738(3)	1129(3)	-6488(2)	48(1)
O(9A)	-4026(3)	1073(3)	-5563(2)	50(1)
O(10A)	-4477(3)	445(3)	-6081(3)	63(1)
O(11A)	-5300(3)	-809(3)	-6054(2)	54(1)
O(12A)	-6613(3)	363(3)	-5705(2)	56(1)
O(13A)	-6695(3)	-420(3)	-4936(2)	55(1)
N(1A)	-5759(4)	-1563(3)	-5606(3)	54(1)
N(2A)	-5125(5)	-2498(4)	-5305(3)	70(2)
N(3A)	-6539(4)	-1957(3)	-6024(2)	51(1)
N(4A)	-6342(4)	-3049(4)	-5939(3)	62(2)
N(5A)	-5535(5)	-3665(4)	-5473(3)	83(3)
C(1G)	-4530(4)	-160(4)	-5927(3)	49(2)
C(2A)	-5315(4)	-192(4)	-6002(3)	48(1)
C(3A)	-5923(4)	97(4)	-5563(3)	50(1)
C(4A)	-6031(4)	-497(4)	-5286(3)	50(1)
C(5A)	-5925(4)	-954(4)	-5717(3)	49(1)
C(6A)	-6031(4)	-2021(4)	-5758(3)	51(2)
C(7A)	-5680(5)	-2572(4)	-5555(3)	59(2)
C(8A)	-5854(5)	-3101(4)	-5645(3)	57(2)
C(9A)	-5242(5)	-1873(4)	-5316(4)	63(2)
C(10A)	-6651(5)	-2513(4)	-6113(3)	56(2)
O(1X')	-3691(2)	1354(2)	-202(2)	27(1)
O(2X')	-3596(3)	1520(2)	-3230(2)	32(1)
O(3X')	1304(2)	270(2)	-2694(2)	35(1)
O(4X')	-4768(3)	2261(2)	-1213(2)	37(1)
O(5X')	227(2)	1117(2)	-3569(2)	31(1)

O(6X')	153(2)	914(2)	-539(2)	32(1)
N(1X')	-2771(3)	-1822(2)	-571(2)	33(1)
N(2X')	-2607(3)	783(2)	-635(2)	27(1)
N(3X')	-3403(3)	-1634(3)	-2601(2)	37(1)
N(4X')	-3098(3)	1105(2)	-2603(2)	26(1)
N(5X')	-23(3)	-2194(2)	-2282(2)	25(1)
N(6X')	139(3)	133(2)	-2376(2)	30(1)
N(7')	-3369(3)	4668(2)	-1458(2)	25(1)
N(8')	-3580(3)	2324(2)	-1380(2)	26(1)
N(9')	-709(3)	4321(2)	-3220(2)	24(1)
N(10')	-882(3)	1692(2)	-3132(2)	24(1)
N(11')	-26(3)	4037(3)	-1161(2)	38(1)
N(12')	-403(3)	1381(2)	-1155(2)	28(1)
C(1X')	-2296(4)	-2448(3)	-1349(2)	28(1)
C(2X')	-2731(4)	-2388(3)	-1692(2)	31(1)
C(3X')	-2420(4)	-2363(3)	-2203(2)	30(1)
C(4X')	-1626(4)	-2470(3)	-2375(2)	31(1)
C(5X')	-1165(3)	-2596(3)	-2020(2)	25(1)
C(6X')	-1475(4)	-2575(3)	-1516(2)	27(1)
C(7X')	-2606(4)	-2424(3)	-815(2)	32(1)
C(8X')	-3309(4)	-1303(3)	-753(3)	33(1)
C(9X')	-3616(4)	-737(3)	-436(3)	31(1)
C(11')	-3586(3)	278(3)	-260(2)	26(1)
C(12')	-4183(4)	308(3)	149(2)	32(1)
C(13)	-3299(4)	-256(3)	-561(2)	26(1)
C(13')	-4477(4)	-216(3)	252(3)	38(2)
C(14')	-4185(4)	-724(3)	-34(3)	35(2)
C(15')	-3303(4)	856(3)	-370(2)	28(1)
C(16')	-2322(4)	1308(3)	-830(2)	25(1)
C(17')	-2026(3)	1269(3)	-1358(2)	22(1)
C(18')	-3568(4)	-2366(3)	-1512(3)	33(1)
C(19')	-3646(5)	-3030(4)	-1444(3)	47(2)
C(20')	-2929(4)	-2266(3)	-2560(3)	34(1)
C(21')	-2966(4)	-1218(3)	-2880(3)	34(1)
C(22')	-3469(4)	-594(3)	-2959(3)	33(1)
C(23')	-3277(4)	-52(3)	-2883(3)	36(1)

C(24')	-3705(4)	511(3)	-2990(2)	30(1)
C(25')	-4343(4)	543(3)	-3158(2)	31(1)
C(26')	-4610(4)	45(3)	-3211(3)	37(2)
C(27')	-4137(4)	-542(3)	-3136(3)	47(2)
C(28')	-3467(3)	1096(3)	-2943(2)	25(1)
C(29')	-2808(4)	1631(3)	-2530(2)	25(1)
C(30')	-2231(3)	1428(3)	-2199(2)	23(1)
C(31')	-1276(4)	-2494(3)	-2912(2)	31(1)
C(32')	-1101(4)	-3111(3)	-3139(2)	38(2)
C(33')	-304(4)	-2760(3)	-2211(2)	29(1)
C(34')	661(3)	-2270(3)	-2701(2)	27(1)
C(35')	1104(4)	-1802(3)	-2691(2)	31(1)
C(36')	751(4)	-1174(3)	-2610(2)	30(1)
C(37')	1182(4)	-748(3)	-2638(2)	29(1)
C(38')	1976(4)	-965(3)	-2737(3)	40(2)
C(39')	2318(4)	-1592(3)	-2824(3)	45(2)
C(40')	1874(4)	-2000(3)	-2797(3)	40(2)
C(41')	873(3)	-88(3)	-2581(2)	24(1)
C(42')	-128(3)	805(3)	-2303(2)	27(1)
C(43')	-974(3)	1008(3)	-2070(2)	26(1)
C(44')	-974(4)	-2729(3)	-1145(2)	31(1)
C(45')	-833(4)	-3416(3)	-1050(3)	41(2)
C(46')	-2200(3)	5077(3)	-1728(2)	26(1)
C(47')	-1900(4)	5051(3)	-2234(2)	26(1)
C(48')	-1131(4)	4915(3)	-2410(2)	24(1)
C(49')	-644(3)	4835(3)	-2071(2)	23(1)
C(50')	-946(4)	4826(3)	-1568(2)	28(1)
C(51')	-1732(3)	4952(3)	-1388(2)	23(1)
C(52')	-3051(3)	5236(3)	-1537(2)	24(1)
C(53')	-4004(4)	4739(3)	-1038(3)	38(2)
C(54')	-4454(4)	4283(3)	-1023(2)	30(1)
C(55')	-4127(4)	3653(3)	-1139(2)	30(1)
C(56')	-4608(4)	3252(3)	-1106(3)	34(1)
C(57')	-5375(4)	3476(3)	-946(2)	31(1)
C(58')	-5690(4)	4073(3)	-831(2)	36(1)
C(59')	-5261(4)	4483(3)	-853(2)	31(1)

C(60')	-4319(4)	2590(3)	-1247(3)	33(1)
C(61')	-3346(4)	1672(3)	-1479(2)	28(1)
C(62')	-2515(3)	1451(3)	-1684(2)	22(1)
C(63')	-2430(4)	5205(3)	-2590(2)	27(1)
C(64')	-2626(4)	5907(3)	-2701(3)	35(2)
C(65')	-811(4)	4929(3)	-2956(2)	28(1)
C(66')	-200(4)	3791(3)	-3003(2)	30(1)
C(67')	79(3)	3243(3)	-3344(2)	29(1)
C(68')	-190(3)	2715(3)	-3237(2)	25(1)
C(69')	99(3)	2205(3)	-3507(2)	25(1)
C(70')	694(4)	2177(3)	-3922(2)	31(1)
C(71')	971(4)	2698(3)	-4040(2)	34(1)
C(72')	679(4)	3221(3)	-3762(3)	33(1)
C(73')	-193(3)	1640(3)	-3404(2)	23(1)
C(74')	-1177(3)	1142(3)	-2951(2)	24(1)
C(75')	-1490(3)	1202(3)	-2395(2)	28(1)
C(76')	187(4)	4825(3)	-2257(2)	26(1)
C(77')	305(4)	5479(3)	-2302(3)	36(2)
C(78')	-440(4)	4735(3)	-1202(2)	30(1)
C(79')	-491(4)	3669(3)	-859(3)	38(1)
C(80')	-12(4)	3034(3)	-762(2)	36(1)
C(81')	-186(4)	2525(3)	-868(3)	36(1)
C(82')	209(4)	1947(3)	-746(2)	30(1)
C(83')	843(4)	1882(3)	-524(2)	31(1)
C(84')	1023(4)	2437(3)	-429(2)	33(1)
C(85')	601(4)	2984(3)	-529(3)	41(2)
C(86')	8(4)	1374(3)	-807(2)	29(1)
C(87')	-687(3)	837(3)	-1242(2)	25(1)
C(88')	-1207(3)	1036(3)	-1569(2)	26(1)
C(89')	-2058(4)	4930(3)	-842(2)	30(1)
C(90')	-2203(5)	5590(3)	-609(3)	41(2)
P(1B)	-1567(1)	-868(1)	-1979(1)	27(1)
P(2B)	-1202(1)	-956(1)	-1022(1)	27(1)
P(3B)	397(1)	-1588(1)	-1053(1)	28(1)
O(1B)	-1342(3)	-226(2)	-2016(2)	32(1)
O(2B)	-2405(3)	-783(2)	-1834(2)	35(1)

O(3B)	-1157(3)	-1217(2)	-2451(2)	32(1)
O(4B)	-1194(2)	-1226(2)	-1540(2)	30(1)
O(5B)	-1555(2)	-282(2)	-1019(2)	29(1)
O(6B)	-1499(2)	-1357(2)	-630(2)	30(1)
O(7B)	-348(2)	-1020(2)	-1062(2)	32(1)
O(8B)	539(3)	-1977(2)	-1494(2)	41(1)
O(9B)	312(2)	-1882(2)	-560(2)	31(1)
O(10B)	1036(2)	-1226(2)	-1153(2)	35(1)
O(11B)	2146(3)	-521(2)	-1171(2)	42(1)
O(12B)	1384(3)	-354(2)	144(2)	46(1)
O(13B)	2918(3)	-548(3)	-311(2)	67(2)
N(1B)	2294(3)	465(3)	-1288(2)	40(1)
N(2B)	1677(3)	1173(3)	-1741(2)	36(1)
N(3B)	3008(3)	1074(3)	-991(2)	39(1)
N(4B)	2717(3)	2124(3)	-1262(2)	42(1)
N(5B)	1770(3)	2511(3)	-1686(2)	47(2)
C(1B)	946(4)	-718(3)	-813(3)	41(2)
C(2B)	1669(4)	-689(3)	-716(3)	40(1)
C(3B)	1617(4)	-197(4)	-352(3)	45(1)
C(4B)	2400(5)	-87(4)	-500(3)	49(1)
C(5B)	2566(4)	-138(3)	-1061(3)	43(1)
C(6B)	2504(4)	1001(3)	-1249(3)	37(1)
C(7B)	2143(4)	1422(3)	-1531(3)	40(1)
C(8B)	2179(4)	2028(3)	-1506(3)	38(1)
C(9B)	1801(4)	612(3)	-1592(3)	40(1)
C(10B)	3093(4)	1655(3)	-1027(3)	40(2)
P(1C)	-1861(1)	3346(1)	-1791(1)	26(1)
P(2C)	-2273(1)	3439(1)	-2736(1)	25(1)
P(3C)	-3852(1)	4128(1)	-2682(1)	28(1)
O(1C)	-2081(2)	2707(2)	-1743(2)	28(1)
O(2C)	-2250(2)	3689(2)	-1327(2)	30(1)
O(3C)	-1037(2)	3251(2)	-1963(2)	30(1)
O(4C)	-2288(2)	3710(2)	-2211(2)	25(1)
O(5C)	-1930(2)	2761(2)	-2734(2)	29(1)
O(6C)	-1968(2)	3838(2)	-3130(2)	28(1)
O(7C)	-3168(2)	3526(2)	-2701(2)	28(1)

O(8C)	-3752(2)	4461(2)	-3160(2)	30(1)
O(9C)	-3998(2)	4469(2)	-2218(2)	30(1)
O(10C)	-4517(2)	3815(2)	-2699(2)	33(1)
O(11C)	-5473(3)	2988(3)	-2684(2)	48(1)
O(12C)	-6698(3)	4056(2)	-1752(2)	55(1)
O(13C)	-7192(4)	3652(3)	-2495(3)	70(2)
N(1C)	-5885(4)	2116(3)	-2363(2)	48(1)
N(2C)	-5335(4)	1362(4)	-1931(3)	59(2)
N(3C)	-6640(4)	1566(3)	-2721(2)	45(1)
N(4C)	-6413(4)	508(4)	-2503(3)	61(2)
N(5C)	-5632(5)	36(4)	-1974(3)	86(2)
C(1E)	-4952(4)	3598(4)	-2285(3)	45(2)
C(2C)	-5654(4)	3545(4)	-2405(3)	43(1)
C(3C)	-6305(4)	3462(3)	-1982(3)	53(1)
C(4C)	-6767(4)	3182(4)	-2200(3)	51(1)
C(5C)	-6102(4)	2721(4)	-2573(3)	48(1)
C(6C)	-6142(4)	1601(4)	-2445(3)	44(1)
C(7C)	-5777(5)	1119(4)	-2186(3)	57(2)
C(8C)	-5956(5)	558(4)	-2203(3)	59(2)
C(9C)	-5415(5)	1928(4)	-2057(3)	55(2)
C(10C)	-6725(5)	1015(4)	-2728(3)	60(2)
O(1X")	-3650(3)	-5357(2)	-6868(2)	30(1)
O(2X")	-3527(3)	-5184(2)	-9908(2)	34(1)
O(3X")	1363(3)	-6494(2)	-9275(2)	39(1)
O(4X")	-4758(3)	-4487(2)	-7864(2)	35(1)
O(5X")	271(2)	-5545(2)	-10240(2)	31(1)
O(6X")	110(3)	-5658(2)	-7180(2)	35(1)
N(1X")	-2804(3)	-8517(3)	-7277(2)	32(1)
N(2X")	-2552(3)	-5918(2)	-7301(2)	27(1)
N(3X")	-3028(4)	-8290(3)	-9516(2)	45(1)
N(4X")	-3114(3)	-5575(2)	-9241(2)	27(1)
N(5X")	-41(3)	-8908(2)	-8946(2)	28(1)
N(6X")	168(3)	-6562(2)	-9005(2)	26(1)
N(7")	-3515(3)	-1949(3)	-8110(2)	37(1)
N(8")	-3583(3)	-4388(2)	-8049(2)	27(1)
N(9")	-687(3)	-2357(2)	-9865(2)	27(1)

N(10")	-835(3)	-4990(2)	-9800(2)	27(1)
N(11")	-458(3)	-2556(2)	-7605(2)	34(1)
N(12")	-344(3)	-5266(2)	-7860(2)	31(1)
C(1X")	-2306(4)	-9147(3)	-8064(2)	30(1)
C(2X")	-2749(4)	-9049(3)	-8417(2)	33(1)
C(3X")	-2421(4)	-9048(3)	-8926(2)	27(1)
C(4X")	-1610(4)	-9179(3)	-9072(2)	27(1)
C(5X")	-1178(4)	-9308(3)	-8716(2)	28(1)
C(6X")	-1515(4)	-9282(3)	-8210(2)	31(1)
C(7X")	-2667(4)	-9127(3)	-7522(2)	31(1)
C(8X")	-3328(4)	-7977(3)	-7485(3)	38(1)
C(9X")	-3590(4)	-7441(3)	-7147(3)	34(1)
C(10X)	-3262(3)	-6952(3)	-7248(2)	25(1)
C(11")	-3567(3)	-6402(3)	-6940(2)	27(1)
C(12")	-4179(4)	-6385(3)	-6551(2)	32(1)
C(13")	-4473(4)	-6902(3)	-6459(3)	38(2)
C(14")	-4204(4)	-7407(3)	-6749(3)	37(2)
C(15")	-3286(4)	-5830(3)	-7030(2)	26(1)
C(16")	-2272(4)	-5377(3)	-7486(2)	30(1)
C(17")	-1972(4)	-5422(3)	-8029(2)	26(1)
C(18")	-3594(4)	-9000(3)	-8276(3)	36(1)
C(19")	-3741(5)	-9646(4)	-8240(4)	59(2)
C(20")	-2880(4)	-8925(3)	-9323(3)	38(1)
C(21")	-3514(4)	-7801(3)	-9145(3)	40(1)
C(22")	-3769(4)	-7214(3)	-9420(3)	45(2)
C(23")	-3466(4)	-6725(3)	-9399(2)	33(1)
C(24")	-3774(4)	-6151(3)	-9602(2)	30(1)
C(25")	-4337(4)	-6103(3)	-9828(2)	30(1)
C(26")	-4657(4)	-6590(3)	-9859(3)	34(1)
C(27")	-4357(4)	-7147(3)	-9660(3)	38(2)
C(28")	-3447(3)	-5592(3)	-9582(2)	25(1)
C(29")	-2784(4)	-5073(3)	-9189(2)	30(1)
C(30")	-2185(4)	-5278(3)	-8860(2)	26(1)
C(31")	-1235(4)	-9245(3)	-9618(2)	34(1)
C(32")	-1041(5)	-9875(3)	-9819(3)	41(2)
C(33")	-313(4)	-9482(3)	-8894(2)	30(1)

C(34")	634(4)	-8951(3)	-9361(2)	33(1)
C(35")	1102(4)	-8514(3)	-9299(2)	33(1)
C(36")	764(4)	-7883(3)	-9237(2)	29(1)
C(37")	1176(4)	-7489(3)	-9183(3)	38(1)
C(38")	1931(5)	-7741(4)	-9151(4)	66(3)
C(39")	2251(6)	-8356(4)	-9207(5)	85(4)
C(40")	1829(5)	-8757(4)	-9304(4)	58(2)
C(41")	896(4)	-6806(3)	-9168(2)	30(1)
C(42")	-77(3)	-5884(3)	-8974(2)	26(1)
C(43")	-924(3)	-5672(3)	-8741(2)	25(1)
C(44")	-1033(3)	-9434(3)	-7830(2)	27(1)
C(45")	-872(4)	-10126(3)	-7715(3)	38(2)
C(46")	-2304(4)	-1573(3)	-8402(2)	30(1)
C(47")	-1980(4)	-1634(3)	-8891(2)	29(1)
C(48")	-1203(4)	-1767(3)	-9056(2)	28(1)
C(49")	-731(4)	-1843(3)	-8702(2)	25(1)
C(50")	-1087(4)	-1819(3)	-8199(2)	30(1)
C(51")	-1863(4)	-1686(3)	-8046(2)	29(1)
C(52")	-3155(4)	-1397(3)	-8234(3)	33(1)
C(56")	-4636(4)	-3462(3)	-7837(3)	34(1)
C(57")	-5390(3)	-3250(3)	-7630(2)	29(1)
C(58")	-5714(4)	-2626(3)	-7546(3)	36(1)
C(60")	-4332(4)	-4141(3)	-7924(3)	36(1)
C(61")	-3313(4)	-5044(3)	-8138(2)	31(1)
C(62")	-2471(3)	-5248(3)	-8348(2)	25(1)
C(63")	-2479(4)	-1483(3)	-9278(3)	34(1)
C(64")	-2645(5)	-794(3)	-9409(3)	40(2)
C(65")	-847(4)	-1749(3)	-9595(2)	31(1)
C(66")	-147(4)	-2875(3)	-9675(2)	30(1)
C(67")	114(4)	-3440(3)	-10013(2)	30(1)
C(68")	-156(4)	-3963(3)	-9903(2)	28(1)
C(69")	85(3)	-4456(3)	-10185(2)	26(1)
C(70")	674(4)	-4463(3)	-10624(3)	36(2)
C(71")	951(4)	-3956(3)	-10749(3)	40(2)
C(72")	680(4)	-3442(4)	-10452(3)	43(2)
C(73")	-168(4)	-5026(3)	-10073(2)	27(1)

C(74")	-1141(4)	-5533(3)	-9622(2)	28(1)
C(75")	-1446(4)	-5481(3)	-9057(2)	28(1)
C(76")	97(4)	-1856(3)	-8862(2)	29(1)
C(77")	226(4)	-1205(3)	-8919(3)	41(2)
C(78")	-625(4)	-1891(3)	-7815(2)	30(1)
C(79")	29(4)	-3010(3)	-7957(2)	36(1)
C(80")	318(4)	-3616(3)	-7694(2)	34(1)
C(81")	10(4)	-4112(3)	-7709(3)	38(1)
C(82")	287(4)	-4675(3)	-7466(2)	31(1)
C(83")	888(4)	-4723(3)	-7222(3)	34(1)
C(84")	1138(4)	-4195(3)	-7196(2)	30(1)
C(85")	881(4)	-3661(3)	-7436(3)	42(2)
C(86")	31(4)	-5241(3)	-7486(2)	28(1)
C(87")	-630(4)	-5797(3)	-7917(2)	29(1)
C(88")	-1171(4)	-5628(3)	-8232(2)	28(1)
C(89")	-2242(4)	-1659(3)	-7497(2)	34(1)
C(90")	-2422(4)	-991(3)	-7281(3)	39(2)
C(53")	-4083(7)	-1985(6)	-8371(5)	36(1)
C(54")	-4503(7)	-2454(6)	-8075(6)	33(2)
C(55")	-4223(8)	-3052(7)	-8077(6)	33(2)
C(59")	-5279(8)	-2202(7)	-7777(6)	34(2)
C(54B)	-4523(7)	-2402(6)	-7728(5)	33(2)
C(53B)	-4136(8)	-1927(7)	-7730(6)	36(1)
C(55B)	-4204(8)	-3012(6)	-7809(6)	33(2)
C(59B)	-5344(7)	-2242(7)	-7528(6)	34(2)
P(1D)	-1531(1)	-7554(1)	-8675(1)	30(1)
P(2D)	-1193(1)	-7671(1)	-7708(1)	28(1)
P(3D)	391(1)	-8341(1)	-7723(1)	30(1)
O(1D)	-1268(3)	-6930(2)	-8692(2)	32(1)
O(2D)	-2366(3)	-7432(2)	-8566(2)	35(1)
O(3D)	-1095(3)	-7917(2)	-9140(2)	34(1)
O(4D)	-1218(3)	-7930(2)	-8233(2)	34(1)
O(5D)	-1506(3)	-6992(2)	-7704(2)	34(1)
O(6D)	-1503(2)	-8064(2)	-7309(2)	30(1)
O(7D)	-322(3)	-7769(2)	-7771(2)	34(1)
O(8D)	552(3)	-8782(2)	-8141(2)	38(1)

O(9D)	274(2)	-8588(2)	-7209(2)	30(1)
O(10D)	1040(2)	-7978(2)	-7817(2)	33(1)
O(11D)	2147(3)	-7256(2)	-7818(2)	39(1)
O(12D)	1251(3)	-7020(2)	-6526(2)	37(1)
O(13D)	2794(3)	-7198(2)	-6921(2)	38(1)
N(1D)	2235(3)	-6242(3)	-7941(2)	35(1)
N(2D)	1708(3)	-5574(3)	-8470(2)	40(1)
N(3D)	2925(3)	-5604(3)	-7645(2)	38(1)
N(4D)	2751(3)	-4606(3)	-8018(2)	41(1)
N(5D)	1963(4)	-4280(3)	-8601(2)	46(1)
C(1D)	923(4)	-7443(3)	-7512(3)	38(1)
C(2D)	1638(4)	-7408(3)	-7380(2)	34(1)
C(3D)	1521(4)	-6892(3)	-7020(2)	33(1)
C(4D)	2306(4)	-6758(3)	-7142(2)	36(1)
C(5D)	2494(4)	-6813(3)	-7689(2)	37(1)
C(6D)	2471(4)	-5707(3)	-7921(2)	34(1)
C(7D)	2138(4)	-5320(4)	-8256(3)	42(1)
C(8D)	2265(4)	-4724(4)	-8290(3)	44(2)
C(9D)	1802(4)	-6124(3)	-8282(2)	38(1)
C(10D)	3025(4)	-5015(3)	-7726(3)	41(2)
P(1E)	-1977(1)	-3299(1)	-8473(1)	31(1)
P(2E)	-2222(1)	-3276(1)	-9454(1)	31(1)
P(3E)	-3730(1)	-2763(1)	-9673(1)	26(1)
P(3F)	-3856(3)	-2536(3)	-9357(2)	26(1)
O(1E)	-2162(3)	-3959(2)	-8414(2)	32(1)
O(2E)	-2416(2)	-2943(2)	-8027(2)	33(1)
O(3E)	-1153(3)	-3361(2)	-8638(2)	34(1)
O(4E)	-2415(3)	-2987(2)	-8920(2)	34(1)
O(5E)	-1854(3)	-3946(2)	-9412(2)	33(1)
O(6E)	-1849(3)	-2885(2)	-9820(2)	36(1)
O(11E)	-5309(3)	-4030(2)	-9380(2)	47(1)
O(12E)	-6562(3)	-2832(3)	-9062(2)	57(1)
O(13E)	-6778(3)	-3600(3)	-8301(2)	52(1)
O(7E)	-2994(4)	-3264(3)	-9596(2)	30(1)
O(8E)	-3933(3)	-2950(3)	-10130(2)	27(1)
O(9E)	-3626(4)	-2134(3)	-9633(2)	31(1)

O(10E)	-4305(4)	-2871(3)	-9182(2)	32(1)
O(7F)	-3199(10)	-3124(8)	-9402(7)	30(1)
O(8F)	-3744(11)	-2147(9)	-9816(7)	31(1)
O(9F)	-4013(8)	-2220(7)	-8937(5)	27(1)
O(10F)	-4485(10)	-2838(9)	-9345(7)	32(1)
N(1E)	-5850(3)	-4766(3)	-8948(2)	47(1)
N(2E)	-5504(4)	-5716(3)	-8583(3)	60(2)
N(3E)	-6585(4)	-5010(3)	-9498(3)	55(2)
N(4E)	-6634(4)	-6068(4)	-9417(3)	63(2)
N(5E)	-6074(4)	-6768(3)	-8864(3)	64(2)
C(1F)	-4512(4)	-3465(3)	-9176(3)	42(1)
C(2E)	-5251(4)	-3421(4)	-9300(3)	45(1)
C(3E)	-5914(4)	-3135(4)	-8889(3)	48(1)
C(4E)	-6068(4)	-3730(4)	-8611(3)	46(1)
C(5E)	-5952(4)	-4155(4)	-9053(3)	49(1)
C(6E)	-6158(4)	-5155(4)	-9137(3)	47(1)
C(7E)	-5955(4)	-5741(4)	-8917(3)	49(1)
C(8E)	-6205(5)	-6202(4)	-9053(3)	55(2)
C(9E)	-5439(4)	-5128(4)	-8619(3)	48(2)
C(10E)	-6792(5)	-5512(5)	-9589(4)	65(2)
O(1S)	-1684(3)	-3038(2)	-7231(2)	51(1)
O(2S)	-1353(4)	-4156(3)	-6708(2)	60(2)
O(3S)	-4022(4)	-4238(3)	-5119(2)	61(2)
O(4S)	-4883(3)	-1800(3)	-2396(2)	63(2)
O(5S)	-1319(4)	-838(3)	-3373(2)	66(2)
O(6S)	-1635(3)	300(2)	-3851(2)	43(1)
O(7S)	-3951(4)	-884(3)	-1768(2)	72(2)
O(8S)	-3244(3)	392(2)	-1714(2)	42(1)
O(9S)	-219(3)	2075(2)	-2029(2)	43(1)
O(10S)	448(3)	3319(2)	-1974(2)	40(1)
O(11S)	1571(4)	3818(3)	-1343(2)	67(2)
O(12S)	-2134(5)	3305(4)	-386(3)	91(2)
O(13S)	-215(3)	-4519(2)	-8732(2)	37(1)
O(14S)	-3315(3)	-6295(2)	-8345(2)	43(1)
O(15S)	-1778(3)	-7838(3)	-9926(2)	47(1)

Table 3. Bond lengths [Å] and angles [°] for Badjic_HX20220107.

O(1X)-C(15)	1.209(8)	N(9)-H(9B)	0.9100
O(2X)-C(28)	1.261(8)	N(9)-C(65)	1.526(8)
O(3X)-C(41)	1.249(8)	N(9)-C(66)	1.530(8)
O(4X)-C(60)	1.260(8)	N(10)-H(10)	0.8800
O(5X)-C(73)	1.264(7)	N(10)-C(73)	1.328(8)
O(6X)-C(86)	1.251(8)	N(10)-C(74)	1.474(8)
N(1X)-H(1XC)	0.9100	N(11)-H(11C)	0.9100
N(1X)-H(1XD)	0.9100	N(11)-H(11D)	0.9100
N(1X)-C(7X)	1.465(8)	N(11)-C(78)	1.559(8)
N(1X)-C(8X)	1.495(8)	N(11)-C(79)	1.471(9)
N(2X)-H(2X)	0.8800	N(12)-H(12)	0.8800
N(2X)-C(15)	1.369(8)	N(12)-C(86)	1.411(9)
N(2X)-C(16)	1.462(8)	N(12)-C(87)	1.474(9)
N(3X)-H(3XC)	0.9100	C(1A)-C(11)	1.448(9)
N(3X)-H(3XD)	0.9100	C(1A)-C(12)	1.385(9)
N(3X)-C(20)	1.500(8)	C(1A)-C(15)	1.492(9)
N(3X)-C(21)	1.453(8)	C(1C)-H(1C)	0.9500
N(4X)-H(4X)	0.8800	C(1C)-C(12)	1.388(9)
N(4X)-C(28)	1.251(8)	C(1C)-C(14)	1.402(9)
N(4X)-C(29)	1.475(8)	C(1X)-C(2X)	1.392(9)
N(5X)-H(5XC)	0.9100	C(1X)-C(6X)	1.436(9)
N(5X)-H(5XD)	0.9100	C(1X)-C(7X)	1.527(8)
N(5X)-C(33)	1.506(8)	C(2X)-C(3X)	1.450(9)
N(5X)-C(34)	1.503(8)	C(2X)-C(18)	1.526(9)
N(6X)-H(6X)	0.8800	C(3X)-C(4X)	1.381(10)
N(6X)-C(41)	1.358(8)	C(3X)-C(20)	1.504(10)
N(6X)-C(42)	1.478(8)	C(4X)-C(5X)	1.423(10)
N(7)-H(7A)	0.9100	C(4X)-C(31)	1.523(9)
N(7)-H(7B)	0.9100	C(5X)-C(6X)	1.421(8)
N(7)-C(52)	1.557(8)	C(5X)-C(33)	1.519(9)
N(7)-C(53)	1.506(8)	C(6X)-C(44)	1.502(9)
N(8)-H(8)	0.8800	C(7X)-H(7XC)	0.9900
N(8)-C(60)	1.303(9)	C(7X)-H(7XD)	0.9900
N(8)-C(61)	1.464(9)	C(8X)-H(8XC)	0.9900
N(9)-H(9A)	0.9100	C(8X)-H(8XD)	0.9900

C(8X)-C(9X)	1.509(9)	C(30)-C(75)	1.360(9)
C(9X)-C(11)	1.375(9)	C(31)-H(31C)	0.9900
C(9X)-C(14)	1.378(9)	C(31)-H(31D)	0.9900
C(11)-H(11)	0.9500	C(31)-C(32)	1.485(10)
C(12)-H(12B)	0.9500	C(32)-H(32D)	0.9800
C(14)-H(14)	0.9500	C(32)-H(32E)	0.9800
C(16)-H(16C)	0.9900	C(32)-H(32F)	0.9800
C(16)-H(16D)	0.9900	C(33)-H(33C)	0.9900
C(16)-C(17)	1.468(9)	C(33)-H(33D)	0.9900
C(17)-C(62)	1.391(9)	C(34)-H(34C)	0.9900
C(17)-C(88)	1.443(9)	C(34)-H(34D)	0.9900
C(18)-H(18C)	0.9900	C(34)-C(35)	1.518(9)
C(18)-H(18D)	0.9900	C(35)-C(36)	1.408(9)
C(18)-C(19)	1.547(9)	C(35)-C(40)	1.366(10)
C(19)-H(19D)	0.9800	C(36)-H(36)	0.9500
C(19)-H(19E)	0.9800	C(36)-C(37)	1.379(9)
C(19)-H(19F)	0.9800	C(37)-C(38)	1.421(10)
C(20)-H(20C)	0.9900	C(37)-C(41)	1.481(9)
C(20)-H(20D)	0.9900	C(38)-H(38)	0.9500
C(21)-H(21C)	0.9900	C(38)-C(39)	1.376(10)
C(21)-H(21D)	0.9900	C(39)-H(39)	0.9500
C(21)-C(22)	1.524(9)	C(39)-C(40)	1.379(10)
C(22)-C(23)	1.425(9)	C(40)-H(40)	0.9500
C(22)-C(27)	1.394(9)	C(42)-H(42C)	0.9900
C(23)-H(23)	0.9500	C(42)-H(42D)	0.9900
C(23)-C(24)	1.376(9)	C(42)-C(43)	1.501(9)
C(24)-C(25)	1.402(9)	C(43)-C(75)	1.406(9)
C(24)-C(28)	1.527(9)	C(43)-C(88)	1.405(9)
C(25)-H(25)	0.9500	C(44)-H(44C)	0.9900
C(25)-C(26)	1.340(10)	C(44)-H(44D)	0.9900
C(26)-H(26)	0.9500	C(44)-C(45)	1.528(9)
C(26)-C(27)	1.405(10)	C(45)-H(45D)	0.9800
C(27)-H(27)	0.9500	C(45)-H(45E)	0.9800
C(29)-H(29C)	0.9900	C(45)-H(45F)	0.9800
C(29)-H(29D)	0.9900	C(46)-C(47)	1.392(9)
C(29)-C(30)	1.542(9)	C(46)-C(51)	1.408(9)
C(30)-C(62)	1.410(9)	C(46)-C(52)	1.489(9)

C(47)-C(48)	1.361(9)	C(66)-H(66D)	0.9900
C(47)-C(63)	1.540(9)	C(66)-C(67)	1.521(9)
C(48)-C(49)	1.446(9)	C(67)-C(68)	1.421(9)
C(48)-C(65)	1.549(9)	C(67)-C(72)	1.424(9)
C(49)-C(50)	1.406(9)	C(68)-H(68)	0.9500
C(49)-C(76)	1.506(9)	C(68)-C(69)	1.334(9)
C(50)-C(51)	1.411(9)	C(69)-C(70)	1.403(9)
C(50)-C(78)	1.499(9)	C(69)-C(73)	1.496(9)
C(51)-C(89)	1.520(9)	C(70)-H(70)	0.9500
C(52)-H(52C)	0.9900	C(70)-C(71)	1.355(10)
C(52)-H(52D)	0.9900	C(71)-H(71)	0.9500
C(53)-H(53E)	0.9900	C(71)-C(72)	1.381(10)
C(53)-H(53F)	0.9900	C(72)-H(72)	0.9500
C(53)-C(54)	1.506(10)	C(74)-H(74C)	0.9900
C(54)-C(55)	1.362(10)	C(74)-H(74D)	0.9900
C(54)-C(59)	1.453(9)	C(74)-C(75)	1.548(9)
C(55)-H(55)	0.9500	C(76)-H(76C)	0.9900
C(55)-C(56)	1.405(9)	C(76)-H(76D)	0.9900
C(56)-C(57)	1.405(9)	C(76)-C(77)	1.547(8)
C(56)-C(60)	1.489(10)	C(77)-H(77D)	0.9800
C(57)-H(57)	0.9500	C(77)-H(77E)	0.9800
C(57)-C(58)	1.384(10)	C(77)-H(77F)	0.9800
C(58)-H(58)	0.9500	C(78)-H(78C)	0.9900
C(58)-C(59)	1.347(10)	C(78)-H(78D)	0.9900
C(59)-H(59)	0.9500	C(79)-H(79C)	0.9900
C(61)-H(61C)	0.9900	C(79)-H(79D)	0.9900
C(61)-H(61D)	0.9900	C(79)-C(80)	1.515(10)
C(61)-C(62)	1.492(9)	C(80)-C(81)	1.397(10)
C(63)-H(63C)	0.9900	C(80)-C(85)	1.385(10)
C(63)-H(63D)	0.9900	C(81)-H(81)	0.9500
C(63)-C(64)	1.548(9)	C(81)-C(82)	1.438(10)
C(64)-H(64D)	0.9800	C(82)-C(83)	1.426(9)
C(64)-H(64E)	0.9800	C(82)-C(86)	1.452(10)
C(64)-H(64F)	0.9800	C(83)-H(83)	0.9500
C(65)-H(65C)	0.9900	C(83)-C(84)	1.395(10)
C(65)-H(65D)	0.9900	C(84)-H(84)	0.9500
C(66)-H(66C)	0.9900	C(84)-C(85)	1.400(10)

C(85)-H(85)	0.9500	N(4)-H(4)	0.8800
C(87)-H(87C)	0.9900	N(4)-C(8)	1.364(11)
C(87)-H(87D)	0.9900	N(4)-C(10)	1.305(11)
C(87)-C(88)	1.486(9)	N(5)-H(5A)	0.8800
C(89)-H(89C)	0.9900	N(5)-H(5B)	0.8800
C(89)-H(89D)	0.9900	N(5)-C(8)	1.334(10)
C(89)-C(90)	1.572(9)	C(1)-H(1A)	0.9900
C(90)-H(90D)	0.9800	C(1)-H(1B)	0.9900
C(90)-H(90E)	0.9800	C(1)-C(2)	1.539(11)
C(90)-H(90F)	0.9800	C(2)-H(2)	1.0000
P(1)-O(1)	1.575(6)	C(2)-C(3)	1.518(11)
P(1)-O(2)	1.507(7)	C(3)-H(3)	1.0000
P(1)-O(3)	1.478(5)	C(3)-C(4)	1.457(11)
P(1)-O(4)	1.565(6)	C(4)-H(4A)	1.0000
P(2)-O(4)	1.619(5)	C(4)-C(5)	1.521(11)
P(2)-O(5)	1.470(5)	C(5)-H(5)	1.0000
P(2)-O(6)	1.484(5)	C(6)-C(7)	1.423(11)
P(2)-O(7)	1.556(5)	C(7)-C(8)	1.426(11)
P(3)-O(7)	1.617(5)	C(9)-H(9)	0.9500
P(3)-O(8)	1.525(5)	C(10)-H(10A)	0.9500
P(3)-O(9)	1.454(5)	P(1A)-O(1A)	1.598(5)
P(3)-O(10)	1.577(5)	P(1A)-O(2A)	1.476(5)
O(1)-H(1)	0.8400	P(1A)-O(3A)	1.482(5)
O(10)-C(1)	1.470(9)	P(1A)-O(4A)	1.640(5)
O(11)-C(2)	1.460(8)	P(2A)-O(4A)	1.608(5)
O(11)-C(5)	1.422(9)	P(2A)-O(5A)	1.478(5)
O(12)-H(12D)	0.8400	P(2A)-O(6A)	1.502(4)
O(12)-C(3)	1.420(9)	P(2A)-O(7A)	1.626(5)
O(13)-H(13A)	0.8400	P(3A)-O(7A)	1.585(5)
O(13)-C(4)	1.329(10)	P(3A)-O(8A)	1.486(5)
N(1)-C(5)	1.464(9)	P(3A)-O(9A)	1.458(6)
N(1)-C(6)	1.408(10)	P(3A)-O(10A)	1.556(6)
N(1)-C(9)	1.369(10)	O(1A)-H(1AA)	0.8400
N(2)-C(7)	1.371(11)	O(10A)-C(1G)	1.425(9)
N(2)-C(9)	1.293(9)	O(11A)-C(2A)	1.397(10)
N(3)-C(6)	1.308(10)	O(11A)-C(5A)	1.431(9)
N(3)-C(10)	1.344(10)	O(12A)-H(12F)	0.8400

O(12A)-C(3A)	1.413(10)	N(1X')-H(1XF)	0.9100
O(13A)-H(13B)	0.8400	N(1X')-C(7X')	1.479(9)
O(13A)-C(4A)	1.381(9)	N(1X')-C(8X')	1.480(9)
N(1A)-C(5A)	1.358(11)	N(2X')-H(2X')	0.8800
N(1A)-C(6A)	1.385(11)	N(2X')-C(15')	1.328(8)
N(1A)-C(9A)	1.419(12)	N(2X')-C(16')	1.450(7)
N(2A)-C(7A)	1.425(12)	N(3X')-H(3XE)	0.9100
N(2A)-C(9A)	1.367(12)	N(3X')-H(3XF)	0.9100
N(3A)-C(6A)	1.310(11)	N(3X')-C(20')	1.484(9)
N(3A)-C(10A)	1.367(11)	N(3X')-C(21')	1.479(9)
N(4A)-H(4AA)	0.8800	N(4X')-H(4X')	0.8800
N(4A)-C(8A)	1.341(11)	N(4X')-C(28')	1.297(8)
N(4A)-C(10A)	1.311(11)	N(4X')-C(29')	1.466(8)
N(5A)-H(5AA)	0.8800	N(5X')-H(5XE)	0.9100
N(5A)-H(5AB)	0.8800	N(5X')-H(5XF)	0.9100
N(5A)-C(8A)	1.366(12)	N(5X')-C(33')	1.488(8)
C(1G)-H(1GA)	0.9900	N(5X')-C(34')	1.514(7)
C(1G)-H(1GB)	0.9900	N(6X')-H(6X')	0.8800
C(1G)-C(2A)	1.557(10)	N(6X')-C(41')	1.345(8)
C(2A)-H(2A)	1.0000	N(6X')-C(42')	1.476(8)
C(2A)-C(3A)	1.523(11)	N(7')-H(7'A)	0.9100
C(3A)-H(3A)	1.0000	N(7')-H(7'B)	0.9100
C(3A)-C(4A)	1.540(11)	N(7')-C(52')	1.530(7)
C(4A)-H(4AB)	1.0000	N(7')-C(53')	1.459(8)
C(4A)-C(5A)	1.575(12)	N(8')-H(8')	0.8800
C(5A)-H(5AC)	1.0000	N(8')-C(60')	1.341(8)
C(6A)-C(7A)	1.398(13)	N(8')-C(61')	1.443(8)
C(7A)-C(8A)	1.362(12)	N(9')-H(9'A)	0.9100
C(9A)-H(9AA)	0.9500	N(9')-H(9'B)	0.9100
C(10A)-H(10B)	0.9500	N(9')-C(65')	1.540(8)
O(1X')-C(15')	1.222(8)	N(9')-C(66')	1.512(8)
O(2X')-C(28')	1.218(8)	N(10')-H(10')	0.8800
O(3X')-C(41')	1.264(7)	N(10')-C(73')	1.327(8)
O(4X')-C(60')	1.242(8)	N(10')-C(74')	1.500(7)
O(5X')-C(73')	1.283(8)	N(11')-H(11E)	0.9100
O(6X')-C(86')	1.249(8)	N(11')-H(11F)	0.9100
N(1X')-H(1XE)	0.9100	N(11')-C(78')	1.571(9)

N(11')-C(79')	1.459(9)	C(18')-H(18E)	0.9900
N(12')-H(12')	0.8800	C(18')-H(18F)	0.9900
N(12')-C(86')	1.365(8)	C(18')-C(19')	1.535(10)
N(12')-C(87')	1.508(8)	C(19')-H(19G)	0.9800
C(1X')-C(2X')	1.369(9)	C(19')-H(19H)	0.9800
C(1X')-C(6X')	1.467(9)	C(19')-H(19I)	0.9800
C(1X')-C(7X')	1.473(9)	C(20')-H(20E)	0.9900
C(2X')-C(3X')	1.419(9)	C(20')-H(20F)	0.9900
C(2X')-C(18')	1.531(9)	C(21')-H(21E)	0.9900
C(3X')-C(4X')	1.425(9)	C(21')-H(21F)	0.9900
C(3X')-C(20')	1.498(10)	C(21')-C(22')	1.512(9)
C(4X')-C(5X')	1.423(9)	C(22')-C(23')	1.399(9)
C(4X')-C(31')	1.495(9)	C(22')-C(27')	1.424(9)
C(5X')-C(6X')	1.398(9)	C(23')-H(23')	0.9500
C(5X')-C(33')	1.542(9)	C(23')-C(24')	1.370(10)
C(6X')-C(44')	1.516(9)	C(24')-C(25')	1.367(9)
C(7X')-H(7XE)	0.9900	C(24')-C(28')	1.517(9)
C(7X')-H(7XF)	0.9900	C(25')-H(25')	0.9500
C(8X')-H(8XE)	0.9900	C(25')-C(26')	1.369(9)
C(8X')-H(8XF)	0.9900	C(26')-H(26')	0.9500
C(8X')-C(9X')	1.506(9)	C(26')-C(27')	1.422(10)
C(9X')-C(13)	1.358(9)	C(27')-H(27')	0.9500
C(9X')-C(14')	1.363(9)	C(29')-H(29E)	0.9900
C(11')-C(12')	1.403(9)	C(29')-H(29F)	0.9900
C(11')-C(13)	1.422(9)	C(29')-C(30')	1.541(9)
C(11')-C(15')	1.519(9)	C(30')-C(62')	1.416(8)
C(12')-H(12C)	0.9500	C(30')-C(75')	1.352(9)
C(12')-C(13')	1.415(9)	C(31')-H(31E)	0.9900
C(13)-H(13)	0.9500	C(31')-H(31F)	0.9900
C(13')-H(13')	0.9500	C(31')-C(32')	1.488(10)
C(13')-C(14')	1.353(10)	C(32')-H(32G)	0.9800
C(14')-H(14')	0.9500	C(32')-H(32H)	0.9800
C(16')-H(16E)	0.9900	C(32')-H(32I)	0.9800
C(16')-H(16F)	0.9900	C(33')-H(33E)	0.9900
C(16')-C(17')	1.452(8)	C(33')-H(33F)	0.9900
C(17')-C(62')	1.405(9)	C(34')-H(34E)	0.9900
C(17')-C(88')	1.488(9)	C(34')-H(34F)	0.9900

C(34')-C(35')	1.508(9)	C(53')-H(53G)	0.9900
C(35')-C(36')	1.406(9)	C(53')-H(53H)	0.9900
C(35')-C(40')	1.369(9)	C(53')-C(54')	1.484(9)
C(36')-H(36')	0.9500	C(54')-C(55')	1.418(9)
C(36')-C(37')	1.394(9)	C(54')-C(59')	1.444(9)
C(37')-C(38')	1.415(10)	C(55')-H(55')	0.9500
C(37')-C(41')	1.453(9)	C(55')-C(56')	1.418(9)
C(38')-H(38')	0.9500	C(56')-C(57')	1.380(9)
C(38')-C(39')	1.402(10)	C(56')-C(60')	1.493(10)
C(39')-H(39')	0.9500	C(57')-H(57')	0.9500
C(39')-C(40')	1.378(10)	C(57')-C(58')	1.346(10)
C(40')-H(40')	0.9500	C(58')-H(58')	0.9500
C(42')-H(42E)	0.9900	C(58')-C(59')	1.365(9)
C(42')-H(42F)	0.9900	C(59')-H(59')	0.9500
C(42')-C(43')	1.538(8)	C(61')-H(61E)	0.9900
C(43')-C(75')	1.440(9)	C(61')-H(61F)	0.9900
C(43')-C(88')	1.368(9)	C(61')-C(62')	1.501(9)
C(44')-H(44E)	0.9900	C(63')-H(63E)	0.9900
C(44')-H(44F)	0.9900	C(63')-H(63F)	0.9900
C(44')-C(45')	1.517(10)	C(63')-C(64')	1.555(9)
C(45')-H(45G)	0.9800	C(64')-H(64G)	0.9800
C(45')-H(45H)	0.9800	C(64')-H(64H)	0.9800
C(45')-H(45I)	0.9800	C(64')-H(64I)	0.9800
C(46')-C(47')	1.397(9)	C(65')-H(65E)	0.9900
C(46')-C(51')	1.401(9)	C(65')-H(65F)	0.9900
C(46')-C(52')	1.525(8)	C(66')-H(66E)	0.9900
C(47')-C(48')	1.378(9)	C(66')-H(66F)	0.9900
C(47')-C(63')	1.521(9)	C(66')-C(67')	1.511(9)
C(48')-C(49')	1.429(8)	C(67')-C(68')	1.400(9)
C(48')-C(65')	1.513(9)	C(67')-C(72')	1.425(9)
C(49')-C(50')	1.393(9)	C(68')-H(68')	0.9500
C(49')-C(76')	1.529(9)	C(68')-C(69')	1.332(9)
C(50')-C(51')	1.411(9)	C(69')-C(70')	1.413(9)
C(50')-C(78')	1.516(9)	C(69')-C(73')	1.500(8)
C(51')-C(89')	1.513(9)	C(70')-H(70')	0.9500
C(52')-H(52E)	0.9900	C(70')-C(71')	1.397(9)
C(52')-H(52F)	0.9900	C(71')-H(71')	0.9500

C(71')-C(72')	1.367(10)	P(1B)-O(2B)	1.503(5)
C(72')-H(72')	0.9500	P(1B)-O(3B)	1.516(5)
C(74')-H(74E)	0.9900	P(1B)-O(4B)	1.617(5)
C(74')-H(74F)	0.9900	P(2B)-O(4B)	1.595(5)
C(74')-C(75')	1.533(8)	P(2B)-O(5B)	1.490(5)
C(76')-H(76E)	0.9900	P(2B)-O(6B)	1.481(4)
C(76')-H(76F)	0.9900	P(2B)-O(7B)	1.553(5)
C(76')-C(77')	1.537(8)	P(3B)-O(7B)	1.638(5)
C(77')-H(77G)	0.9800	P(3B)-O(8B)	1.488(5)
C(77')-H(77H)	0.9800	P(3B)-O(9B)	1.483(5)
C(77')-H(77I)	0.9800	P(3B)-O(10B)	1.587(5)
C(78')-H(78E)	0.9900	O(1B)-H(1BA)	0.8400
C(78')-H(78F)	0.9900	O(10B)-C(1B)	1.479(9)
C(79')-H(79E)	0.9900	O(11B)-C(2B)	1.474(8)
C(79')-H(79F)	0.9900	O(11B)-C(5B)	1.397(9)
C(79')-C(80')	1.525(10)	O(12B)-H(12G)	0.8400
C(80')-C(81')	1.335(10)	O(12B)-C(3B)	1.408(9)
C(80')-C(85')	1.421(10)	O(13B)-H(13C)	0.8400
C(81')-H(81')	0.9500	O(13B)-C(4B)	1.395(10)
C(81')-C(82')	1.386(9)	N(1B)-C(5B)	1.479(9)
C(82')-C(83')	1.431(9)	N(1B)-C(6B)	1.379(9)
C(82')-C(86')	1.463(9)	N(1B)-C(9B)	1.358(9)
C(83')-H(83')	0.9500	N(2B)-C(7B)	1.396(9)
C(83')-C(84')	1.430(9)	N(2B)-C(9B)	1.284(9)
C(84')-H(84')	0.9500	N(3B)-C(6B)	1.356(9)
C(84')-C(85')	1.333(10)	N(3B)-C(10B)	1.353(9)
C(85')-H(85')	0.9500	N(4B)-H(4B)	0.8800
C(87')-H(87E)	0.9900	N(4B)-C(8B)	1.402(9)
C(87')-H(87F)	0.9900	N(4B)-C(10B)	1.335(9)
C(87')-C(88')	1.454(9)	N(5B)-H(5BA)	0.8800
C(89')-H(89E)	0.9900	N(5B)-H(5BB)	0.8800
C(89')-H(89F)	0.9900	N(5B)-C(8B)	1.304(9)
C(89')-C(90')	1.590(9)	C(1B)-H(1BB)	0.9900
C(90')-H(90G)	0.9800	C(1B)-H(1BC)	0.9900
C(90')-H(90H)	0.9800	C(1B)-C(2B)	1.463(10)
C(90')-H(90I)	0.9800	C(2B)-H(2B)	1.0000
P(1B)-O(1B)	1.598(4)	C(2B)-C(3B)	1.515(11)

C(3B)-H(3B)	1.0000	N(4C)-C(8C)	1.352(12)
C(3B)-C(4B)	1.520(10)	N(4C)-C(10C)	1.332(11)
C(4B)-H(4BA)	1.0000	N(5C)-H(5CA)	0.8800
C(4B)-C(5B)	1.530(11)	N(5C)-H(5CB)	0.8800
C(5B)-H(5BC)	1.0000	N(5C)-C(8C)	1.368(12)
C(6B)-C(7B)	1.339(10)	C(1E)-H(1EA)	0.9900
C(7B)-C(8B)	1.390(10)	C(1E)-H(1EB)	0.9900
C(9B)-H(9BA)	0.9500	C(1E)-C(2C)	1.466(10)
C(10B)-H(10C)	0.9500	C(2C)-H(2C)	1.0000
P(1C)-O(1C)	1.587(4)	C(2C)-C(3C)	1.543(10)
P(1C)-O(2C)	1.487(5)	C(3C)-H(3C)	1.0000
P(1C)-O(3C)	1.478(4)	C(3C)-C(4C)	1.444(11)
P(1C)-O(4C)	1.628(4)	C(4C)-H(4CA)	1.0000
P(2C)-O(4C)	1.613(4)	C(4C)-C(5C)	1.615(11)
P(2C)-O(5C)	1.494(5)	C(5C)-H(5C)	1.0000
P(2C)-O(6C)	1.488(4)	C(6C)-C(7C)	1.382(12)
P(2C)-O(7C)	1.624(4)	C(7C)-C(8C)	1.395(13)
P(3C)-O(7C)	1.604(5)	C(9C)-H(9C)	0.9500
P(3C)-O(8C)	1.489(5)	C(10C)-H(10D)	0.9500
P(3C)-O(9C)	1.481(5)	O(1X")-C(15")	1.161(7)
P(3C)-O(10C)	1.595(5)	O(2X")-C(28")	1.258(7)
O(1C)-H(1CA)	0.8400	O(3X")-C(41")	1.237(8)
O(10C)-C(1E)	1.403(8)	O(4X")-C(60")	1.233(8)
O(11C)-C(2C)	1.440(9)	O(5X")-C(73")	1.289(8)
O(11C)-C(5C)	1.429(9)	O(6X")-C(86")	1.234(8)
O(12C)-H(12H)	0.8400	N(1X")-H(1XA)	0.9100
O(12C)-C(3C)	1.457(6)	N(1X")-H(1XB)	0.9100
O(13C)-H(13D)	0.8400	N(1X")-C(7X")	1.506(8)
O(13C)-C(4C)	1.478(10)	N(1X")-C(8X")	1.527(9)
N(1C)-C(5C)	1.445(10)	N(2X")-H(2X")	0.8800
N(1C)-C(6C)	1.414(10)	N(2X")-C(15")	1.391(8)
N(1C)-C(9C)	1.337(10)	N(2X")-C(16")	1.469(8)
N(2C)-C(7C)	1.429(12)	N(3X")-H(3XA)	0.9100
N(2C)-C(9C)	1.281(11)	N(3X")-H(3XB)	0.9100
N(3C)-C(6C)	1.355(10)	N(3X")-C(20")	1.477(9)
N(3C)-C(10C)	1.294(10)	N(3X")-C(21")	1.521(9)
N(4C)-H(4C)	0.8800	N(4X")-H(4X")	0.8800

N(4X")-C(28")	1.256(8)	C(2X")-C(18")	1.527(9)
N(4X")-C(29")	1.448(8)	C(3X")-C(4X")	1.444(9)
N(5X")-H(5XA)	0.9100	C(3X")-C(20")	1.521(9)
N(5X")-H(5XB)	0.9100	C(4X")-C(5X")	1.390(9)
N(5X")-C(33")	1.495(8)	C(4X")-C(31")	1.530(9)
N(5X")-C(34")	1.503(8)	C(5X")-C(6X")	1.410(9)
N(6X")-H(6X")	0.8800	C(5X")-C(33")	1.542(9)
N(6X")-C(41")	1.321(8)	C(6X")-C(44")	1.510(9)
N(6X")-C(42")	1.477(8)	C(7X")-H(7XA)	0.9900
N(7")-H(7"C)	0.9100	C(7X")-H(7XB)	0.9900
N(7")-H(7"D)	0.9100	C(8X")-H(8XA)	0.9900
N(7")-H(7"A)	0.9100	C(8X")-H(8XB)	0.9900
N(7")-H(7"B)	0.9100	C(8X")-C(9X")	1.487(10)
N(7")-C(52")	1.549(8)	C(9X")-C(10X)	1.381(9)
N(7")-C(53")	1.439(14)	C(9X")-C(14")	1.402(9)
N(7")-C(53B)	1.384(15)	C(10X)-H(10X)	0.9500
N(8")-H(8")	0.8800	C(10X)-C(11")	1.463(9)
N(8")-C(60")	1.348(8)	C(11")-C(12")	1.390(9)
N(8")-C(61")	1.447(8)	C(11")-C(15")	1.500(8)
N(9")-H(9"A)	0.9100	C(12")-H(12A)	0.9500
N(9")-H(9"B)	0.9100	C(12")-C(13")	1.401(9)
N(9")-C(65")	1.529(8)	C(13")-H(13")	0.9500
N(9")-C(66")	1.493(8)	C(13")-C(14")	1.352(10)
N(10")-H(10")	0.8800	C(14")-H(14")	0.9500
N(10")-C(73")	1.301(8)	C(16")-H(16A)	0.9900
N(10")-C(74")	1.493(8)	C(16")-H(16B)	0.9900
N(11")-H(11A)	0.9100	C(16")-C(17")	1.495(9)
N(11")-H(11B)	0.9100	C(17")-C(62")	1.401(9)
N(11")-C(78")	1.554(8)	C(17")-C(88")	1.448(9)
N(11")-C(79")	1.444(9)	C(18")-H(18A)	0.9900
N(12")-H(12")	0.8800	C(18")-H(18B)	0.9900
N(12")-C(86")	1.395(8)	C(18")-C(19")	1.542(11)
N(12")-C(87")	1.460(8)	C(19")-H(19A)	0.9800
C(1X")-C(2X")	1.399(9)	C(19")-H(19B)	0.9800
C(1X")-C(6X")	1.409(9)	C(19")-H(19C)	0.9800
C(1X")-C(7X")	1.512(9)	C(20")-H(20A)	0.9900
C(2X")-C(3X")	1.416(9)	C(20")-H(20B)	0.9900

C(21")-H(21A)	0.9900	C(38")-C(39")	1.360(12)
C(21")-H(21B)	0.9900	C(39")-H(39")	0.9500
C(21")-C(22")	1.511(10)	C(39")-C(40")	1.418(12)
C(22")-C(23")	1.373(10)	C(40")-H(40")	0.9500
C(22")-C(27")	1.385(10)	C(42")-H(42A)	0.9900
C(23")-H(23")	0.9500	C(42")-H(42B)	0.9900
C(23")-C(24")	1.414(9)	C(42")-C(43")	1.541(9)
C(24")-C(25")	1.324(9)	C(43")-C(75")	1.431(9)
C(24")-C(28")	1.545(9)	C(43")-C(88")	1.393(9)
C(25")-H(25")	0.9500	C(44")-H(44A)	0.9900
C(25")-C(26")	1.395(9)	C(44")-H(44B)	0.9900
C(26")-H(26")	0.9500	C(44")-C(45")	1.538(9)
C(26")-C(27")	1.375(10)	C(45")-H(45A)	0.9800
C(27")-H(27")	0.9500	C(45")-H(45B)	0.9800
C(29")-H(29A)	0.9900	C(45")-H(45C)	0.9800
C(29")-H(29B)	0.9900	C(46")-C(47")	1.363(9)
C(29")-C(30")	1.570(9)	C(46")-C(51")	1.402(9)
C(30")-C(62")	1.411(9)	C(46")-C(52")	1.516(9)
C(30")-C(75")	1.343(9)	C(47")-C(48")	1.389(9)
C(31")-H(31A)	0.9900	C(47")-C(63")	1.550(9)
C(31")-H(31B)	0.9900	C(48")-C(49")	1.442(9)
C(31")-C(32")	1.481(10)	C(48")-C(65")	1.508(9)
C(32")-H(32A)	0.9800	C(49")-C(50")	1.411(9)
C(32")-H(32B)	0.9800	C(49")-C(76")	1.515(9)
C(32")-H(32C)	0.9800	C(50")-C(51")	1.384(9)
C(33")-H(33A)	0.9900	C(50")-C(78")	1.500(9)
C(33")-H(33B)	0.9900	C(51")-C(89")	1.537(9)
C(34")-H(34A)	0.9900	C(52")-H(52A)	0.9900
C(34")-H(34B)	0.9900	C(52")-H(52B)	0.9900
C(34")-C(35")	1.519(9)	C(56")-C(57")	1.376(9)
C(35")-C(36")	1.401(9)	C(56")-C(60")	1.500(10)
C(35")-C(40")	1.331(11)	C(56")-C(55")	1.402(15)
C(36")-H(36")	0.9500	C(56")-C(55B)	1.468(15)
C(36")-C(37")	1.356(9)	C(57")-H(57")	0.9500
C(37")-C(38")	1.407(11)	C(57")-C(58")	1.389(10)
C(37")-C(41")	1.490(10)	C(58")-H(58")	0.9500
C(38")-H(38")	0.9500	C(58")-H(58A)	0.9500

C(58")-C(59")	1.445(16)	C(78")-H(78B)	0.9900
C(58")-C(59B)	1.251(15)	C(79")-H(79A)	0.9900
C(61")-H(61A)	0.9900	C(79")-H(79B)	0.9900
C(61")-H(61B)	0.9900	C(79")-C(80")	1.540(9)
C(61")-C(62")	1.519(9)	C(80")-C(81")	1.390(10)
C(63")-H(63A)	0.9900	C(80")-C(85")	1.386(10)
C(63")-H(63B)	0.9900	C(81")-H(81")	0.9500
C(63")-C(64")	1.539(9)	C(81")-C(82")	1.432(9)
C(64")-H(64A)	0.9800	C(82")-C(83")	1.423(9)
C(64")-H(64B)	0.9800	C(82")-C(86")	1.479(9)
C(64")-H(64C)	0.9800	C(83")-H(83")	0.9500
C(65")-H(65A)	0.9900	C(83")-C(84")	1.396(9)
C(65")-H(65B)	0.9900	C(84")-H(84")	0.9500
C(66")-H(66A)	0.9900	C(84")-C(85")	1.371(10)
C(66")-H(66B)	0.9900	C(85")-H(85")	0.9500
C(66")-C(67")	1.535(9)	C(87")-H(87A)	0.9900
C(67")-C(68")	1.392(9)	C(87")-H(87B)	0.9900
C(67")-C(72")	1.432(9)	C(87")-C(88")	1.453(9)
C(68")-H(68")	0.9500	C(89")-H(89A)	0.9900
C(68")-C(69")	1.318(9)	C(89")-H(89B)	0.9900
C(69")-C(70")	1.456(9)	C(89")-C(90")	1.578(10)
C(69")-C(73")	1.474(9)	C(90")-H(90A)	0.9800
C(70")-H(70")	0.9500	C(90")-H(90B)	0.9800
C(70")-C(71")	1.370(10)	C(90")-H(90C)	0.9800
C(71")-H(71")	0.9500	C(53")-H(53A)	0.9900
C(71")-C(72")	1.380(10)	C(53")-H(53B)	0.9900
C(72")-H(72")	0.9500	C(53")-C(54")	1.568(18)
C(74")-H(74A)	0.9900	C(54")-C(55")	1.314(19)
C(74")-H(74B)	0.9900	C(54")-C(59")	1.50(2)
C(74")-C(75")	1.553(8)	C(55")-H(55")	0.9500
C(76")-H(76A)	0.9900	C(59")-H(59")	0.9500
C(76")-H(76B)	0.9900	C(54B)-C(53B)	1.441(19)
C(76")-C(77")	1.540(8)	C(54B)-C(55B)	1.359(19)
C(77")-H(77A)	0.9800	C(54B)-C(59B)	1.476(18)
C(77")-H(77B)	0.9800	C(53B)-H(53C)	0.9900
C(77")-H(77C)	0.9800	C(53B)-H(53D)	0.9900
C(78")-H(78A)	0.9900	C(55B)-H(55B)	0.9500

C(59B)-H(59B)	0.9500	C(2D)-H(2D)	1.0000
P(1D)-O(1D)	1.601(5)	C(2D)-C(3D)	1.521(9)
P(1D)-O(2D)	1.485(5)	C(3D)-H(3D)	1.0000
P(1D)-O(3D)	1.525(5)	C(3D)-C(4D)	1.543(10)
P(1D)-O(4D)	1.588(5)	C(4D)-H(4DA)	1.0000
P(2D)-O(4D)	1.623(5)	C(4D)-C(5D)	1.492(9)
P(2D)-O(5D)	1.489(5)	C(5D)-H(5D)	1.0000
P(2D)-O(6D)	1.490(4)	C(6D)-C(7D)	1.381(10)
P(2D)-O(7D)	1.565(5)	C(7D)-C(8D)	1.417(11)
P(3D)-O(7D)	1.626(5)	C(9D)-H(9D)	0.9500
P(3D)-O(8D)	1.504(5)	C(10D)-H(10F)	0.9500
P(3D)-O(9D)	1.497(4)	P(1E)-O(1E)	1.603(5)
P(3D)-O(10D)	1.604(5)	P(1E)-O(2E)	1.480(5)
O(1D)-H(1D)	0.8400	P(1E)-O(3E)	1.488(5)
O(10D)-C(1D)	1.457(8)	P(1E)-O(4E)	1.667(5)
O(11D)-C(2D)	1.459(8)	P(2E)-O(4E)	1.589(5)
O(11D)-C(5D)	1.427(8)	P(2E)-O(5E)	1.497(5)
O(12D)-H(12I)	0.8400	P(2E)-O(6E)	1.487(5)
O(12D)-C(3D)	1.398(8)	P(2E)-O(7E)	1.581(7)
O(13D)-H(13F)	0.8400	P(2E)-O(7F)	1.754(17)
O(13D)-C(4D)	1.384(9)	P(3E)-O(7E)	1.590(7)
N(1D)-C(5D)	1.450(9)	P(3E)-O(8E)	1.520(6)
N(1D)-C(6D)	1.394(9)	P(3E)-O(9E)	1.494(7)
N(1D)-C(9D)	1.357(9)	P(3E)-O(10E)	1.594(7)
N(2D)-C(7D)	1.352(9)	P(3F)-O(7F)	1.549(19)
N(2D)-C(9D)	1.302(9)	P(3F)-O(8F)	1.515(18)
N(3D)-C(6D)	1.339(9)	P(3F)-O(9F)	1.341(17)
N(3D)-C(10D)	1.385(9)	P(3F)-O(10F)	1.505(19)
N(4D)-H(4D)	0.8800	O(1E)-H(1E)	0.8400
N(4D)-C(8D)	1.392(10)	O(11E)-C(2E)	1.437(9)
N(4D)-C(10D)	1.274(9)	O(11E)-C(5E)	1.426(9)
N(5D)-H(5DA)	0.8800	O(12E)-H(12E)	0.8400
N(5D)-H(5DB)	0.8800	O(12E)-C(3E)	1.406(10)
N(5D)-C(8D)	1.375(10)	O(13E)-H(13E)	0.8400
C(1D)-H(1DA)	0.9900	O(13E)-C(4E)	1.389(9)
C(1D)-H(1DB)	0.9900	O(10E)-C(1F)	1.482(10)
C(1D)-C(2D)	1.493(10)	O(10F)-C(1F)	1.47(2)

N(1E)-C(5E)	1.360(10)	O(5S)-H(5SA)	0.8494
N(1E)-C(6E)	1.354(10)	O(5S)-H(5SB)	0.8510
N(1E)-C(9E)	1.417(11)	O(6S)-H(6SA)	0.913(5)
N(2E)-C(7E)	1.404(11)	O(6S)-H(6SB)	0.725(5)
N(2E)-C(9E)	1.356(10)	O(7S)-H(7SA)	0.8505
N(3E)-C(6E)	1.397(11)	O(7S)-H(7SB)	0.8499
N(3E)-C(10E)	1.340(11)	O(8S)-H(8SA)	0.8489
N(4E)-H(4E)	0.8800	O(8S)-H(8SB)	0.8496
N(4E)-C(8E)	1.404(12)	O(9S)-H(9SA)	0.845(5)
N(4E)-C(10E)	1.299(12)	O(9S)-H(9SB)	0.792(5)
N(5E)-H(5EA)	0.8800	O(10S)-H(10G)	0.905(5)
N(5E)-H(5EB)	0.8800	O(10S)-H(10H)	0.876(4)
N(5E)-C(8E)	1.332(11)	O(11S)-H(11G)	0.821(7)
C(1F)-H(1FA)	0.9900	O(11S)-H(11H)	0.921(6)
C(1F)-H(1FB)	0.9900	O(12S)-H(12J)	0.8508
C(1F)-H(1FC)	0.9900	O(12S)-H(12K)	0.8499
C(1F)-H(1FD)	0.9900	O(13S)-H(13G)	0.8496
C(1F)-C(2E)	1.485(10)	O(13S)-H(13H)	0.8486
C(2E)-H(2E)	1.0000	O(14S)-H(14A)	0.8493
C(2E)-C(3E)	1.524(11)	O(14S)-H(14B)	0.8496
C(3E)-H(3E)	1.0000	O(15S)-H(15A)	0.8497
C(3E)-C(4E)	1.566(11)	O(15S)-H(15B)	0.8493
C(4E)-H(4EA)	1.0000		
C(4E)-C(5E)	1.549(11)	H(1XC)-N(1X)-H(1XD)	107.3
C(5E)-H(5E)	1.0000	C(7X)-N(1X)-H(1XC)	108.0
C(6E)-C(7E)	1.416(12)	C(7X)-N(1X)-H(1XD)	108.0
C(7E)-C(8E)	1.349(11)	C(7X)-N(1X)-C(8X)	117.2(5)
C(9E)-H(9E)	0.9500	C(8X)-N(1X)-H(1XC)	108.0
C(10E)-H(10E)	0.9500	C(8X)-N(1X)-H(1XD)	108.0
O(1S)-H(1SA)	0.8500	C(15)-N(2X)-H(2X)	119.3
O(1S)-H(1SB)	0.8503	C(15)-N(2X)-C(16)	121.4(5)
O(2S)-H(2SA)	0.8501	C(16)-N(2X)-H(2X)	119.3
O(2S)-H(2SB)	0.8496	H(3XC)-N(3X)-H(3XD)	107.7
O(3S)-H(3SA)	0.8505	C(20)-N(3X)-H(3XC)	108.9
O(3S)-H(3SB)	0.8514	C(20)-N(3X)-H(3XD)	108.9
O(4S)-H(4SA)	0.8505	C(21)-N(3X)-H(3XC)	108.9
O(4S)-H(4SB)	0.8488	C(21)-N(3X)-H(3XD)	108.9

C(21)-N(3X)-C(20)	113.2(6)	C(86)-N(12)-H(12)	120.0
C(28)-N(4X)-H(4X)	119.6	C(86)-N(12)-C(87)	119.9(6)
C(28)-N(4X)-C(29)	120.7(6)	C(87)-N(12)-H(12)	120.0
C(29)-N(4X)-H(4X)	119.6	C(11)-C(1A)-C(15)	122.7(5)
H(5XC)-N(5X)-H(5XD)	108.1	C(12)-C(1A)-C(11)	119.4(6)
C(33)-N(5X)-H(5XC)	109.6	C(12)-C(1A)-C(15)	117.6(6)
C(33)-N(5X)-H(5XD)	109.6	C(12)-C(1C)-H(1C)	119.9
C(34)-N(5X)-H(5XC)	109.6	C(12)-C(1C)-C(14)	120.2(6)
C(34)-N(5X)-H(5XD)	109.6	C(14)-C(1C)-H(1C)	119.9
C(34)-N(5X)-C(33)	110.5(5)	C(2X)-C(1X)-C(6X)	121.6(5)
C(41)-N(6X)-H(6X)	121.5	C(2X)-C(1X)-C(7X)	120.9(6)
C(41)-N(6X)-C(42)	117.0(5)	C(6X)-C(1X)-C(7X)	117.5(5)
C(42)-N(6X)-H(6X)	121.5	C(1X)-C(2X)-C(3X)	118.7(6)
H(7A)-N(7)-H(7B)	108.0	C(1X)-C(2X)-C(18)	121.8(6)
C(52)-N(7)-H(7A)	109.4	C(3X)-C(2X)-C(18)	119.3(6)
C(52)-N(7)-H(7B)	109.4	C(2X)-C(3X)-C(20)	118.1(6)
C(53)-N(7)-H(7A)	109.4	C(4X)-C(3X)-C(2X)	120.9(6)
C(53)-N(7)-H(7B)	109.4	C(4X)-C(3X)-C(20)	120.9(6)
C(53)-N(7)-C(52)	111.0(5)	C(3X)-C(4X)-C(5X)	119.5(6)
C(60)-N(8)-H(8)	120.5	C(3X)-C(4X)-C(31)	122.7(6)
C(60)-N(8)-C(61)	119.1(6)	C(5X)-C(4X)-C(31)	117.6(6)
C(61)-N(8)-H(8)	120.5	C(4X)-C(5X)-C(33)	119.8(6)
H(9A)-N(9)-H(9B)	107.8	C(6X)-C(5X)-C(4X)	121.4(6)
C(65)-N(9)-H(9A)	109.1	C(6X)-C(5X)-C(33)	118.8(6)
C(65)-N(9)-H(9B)	109.1	C(1X)-C(6X)-C(44)	120.3(5)
C(65)-N(9)-C(66)	112.5(5)	C(5X)-C(6X)-C(1X)	117.7(6)
C(66)-N(9)-H(9A)	109.1	C(5X)-C(6X)-C(44)	121.9(6)
C(66)-N(9)-H(9B)	109.1	N(1X)-C(7X)-C(1X)	115.2(5)
C(73)-N(10)-H(10)	118.4	N(1X)-C(7X)-H(7XC)	108.5
C(73)-N(10)-C(74)	123.1(5)	N(1X)-C(7X)-H(7XD)	108.5
C(74)-N(10)-H(10)	118.4	C(1X)-C(7X)-H(7XC)	108.5
H(11C)-N(11)-H(11D)	107.8	C(1X)-C(7X)-H(7XD)	108.5
C(78)-N(11)-H(11C)	109.1	H(7XC)-C(7X)-H(7XD)	107.5
C(78)-N(11)-H(11D)	109.1	N(1X)-C(8X)-H(8XC)	108.4
C(79)-N(11)-H(11C)	109.1	N(1X)-C(8X)-H(8XD)	108.4
C(79)-N(11)-H(11D)	109.1	N(1X)-C(8X)-C(9X)	115.5(5)
C(79)-N(11)-C(78)	112.6(5)	H(8XC)-C(8X)-H(8XD)	107.5

C(9X)-C(8X)-H(8XC)	108.4	H(19E)-C(19)-H(19F)	109.5
C(9X)-C(8X)-H(8XD)	108.4	N(3X)-C(20)-C(3X)	116.8(6)
C(11)-C(9X)-C(8X)	118.7(6)	N(3X)-C(20)-H(20C)	108.1
C(11)-C(9X)-C(14)	122.7(6)	N(3X)-C(20)-H(20D)	108.1
C(14)-C(9X)-C(8X)	118.6(6)	C(3X)-C(20)-H(20C)	108.1
C(1A)-C(11)-H(11)	121.1	C(3X)-C(20)-H(20D)	108.1
C(9X)-C(11)-C(1A)	117.8(6)	H(20C)-C(20)-H(20D)	107.3
C(9X)-C(11)-H(11)	121.1	N(3X)-C(21)-H(21C)	109.2
C(1A)-C(12)-C(1C)	120.6(6)	N(3X)-C(21)-H(21D)	109.2
C(1A)-C(12)-H(12B)	119.7	N(3X)-C(21)-C(22)	112.3(6)
C(1C)-C(12)-H(12B)	119.7	H(21C)-C(21)-H(21D)	107.9
C(1C)-C(14)-H(14)	120.5	C(22)-C(21)-H(21C)	109.2
C(9X)-C(14)-C(1C)	119.0(6)	C(22)-C(21)-H(21D)	109.2
C(9X)-C(14)-H(14)	120.5	C(23)-C(22)-C(21)	119.5(6)
O(1X)-C(15)-N(2X)	122.2(6)	C(27)-C(22)-C(21)	122.1(6)
O(1X)-C(15)-C(1A)	121.6(6)	C(27)-C(22)-C(23)	118.4(6)
N(2X)-C(15)-C(1A)	116.2(6)	C(22)-C(23)-H(23)	120.2
N(2X)-C(16)-H(16C)	109.2	C(24)-C(23)-C(22)	119.6(6)
N(2X)-C(16)-H(16D)	109.2	C(24)-C(23)-H(23)	120.2
N(2X)-C(16)-C(17)	112.2(5)	C(23)-C(24)-C(25)	119.1(6)
H(16C)-C(16)-H(16D)	107.9	C(23)-C(24)-C(28)	121.3(6)
C(17)-C(16)-H(16C)	109.2	C(25)-C(24)-C(28)	119.6(6)
C(17)-C(16)-H(16D)	109.2	C(24)-C(25)-H(25)	118.4
C(62)-C(17)-C(16)	120.0(6)	C(26)-C(25)-C(24)	123.2(7)
C(62)-C(17)-C(88)	119.6(6)	C(26)-C(25)-H(25)	118.4
C(88)-C(17)-C(16)	120.4(6)	C(25)-C(26)-H(26)	121.1
C(2X)-C(18)-H(18C)	109.6	C(25)-C(26)-C(27)	117.8(7)
C(2X)-C(18)-H(18D)	109.6	C(27)-C(26)-H(26)	121.1
C(2X)-C(18)-C(19)	110.3(6)	C(22)-C(27)-C(26)	121.5(7)
H(18C)-C(18)-H(18D)	108.1	C(22)-C(27)-H(27)	119.2
C(19)-C(18)-H(18C)	109.6	C(26)-C(27)-H(27)	119.2
C(19)-C(18)-H(18D)	109.6	O(2X)-C(28)-C(24)	117.5(6)
C(18)-C(19)-H(19D)	109.5	N(4X)-C(28)-O(2X)	124.6(6)
C(18)-C(19)-H(19E)	109.5	N(4X)-C(28)-C(24)	117.7(6)
C(18)-C(19)-H(19F)	109.5	N(4X)-C(29)-H(29C)	109.6
H(19D)-C(19)-H(19E)	109.5	N(4X)-C(29)-H(29D)	109.6
H(19D)-C(19)-H(19F)	109.5	N(4X)-C(29)-C(30)	110.3(5)

H(29C)-C(29)-H(29D)	108.1	C(36)-C(37)-C(41)	125.5(6)
C(30)-C(29)-H(29C)	109.6	C(38)-C(37)-C(41)	115.8(6)
C(30)-C(29)-H(29D)	109.6	C(37)-C(38)-H(38)	119.6
C(62)-C(30)-C(29)	117.1(6)	C(39)-C(38)-C(37)	120.9(7)
C(75)-C(30)-C(29)	122.6(6)	C(39)-C(38)-H(38)	119.6
C(75)-C(30)-C(62)	120.0(6)	C(38)-C(39)-H(39)	120.6
C(4X)-C(31)-H(31C)	108.3	C(38)-C(39)-C(40)	118.8(7)
C(4X)-C(31)-H(31D)	108.3	C(40)-C(39)-H(39)	120.6
H(31C)-C(31)-H(31D)	107.4	C(35)-C(40)-C(39)	122.0(7)
C(32)-C(31)-C(4X)	115.8(6)	C(35)-C(40)-H(40)	119.0
C(32)-C(31)-H(31C)	108.3	C(39)-C(40)-H(40)	119.0
C(32)-C(31)-H(31D)	108.3	O(3X)-C(41)-N(6X)	120.1(6)
C(31)-C(32)-H(32D)	109.5	O(3X)-C(41)-C(37)	121.4(6)
C(31)-C(32)-H(32E)	109.5	N(6X)-C(41)-C(37)	118.5(6)
C(31)-C(32)-H(32F)	109.5	N(6X)-C(42)-H(42C)	109.4
H(32D)-C(32)-H(32E)	109.5	N(6X)-C(42)-H(42D)	109.4
H(32D)-C(32)-H(32F)	109.5	N(6X)-C(42)-C(43)	111.3(5)
H(32E)-C(32)-H(32F)	109.5	H(42C)-C(42)-H(42D)	108.0
N(5X)-C(33)-C(5X)	109.9(5)	C(43)-C(42)-H(42C)	109.4
N(5X)-C(33)-H(33C)	109.7	C(43)-C(42)-H(42D)	109.4
N(5X)-C(33)-H(33D)	109.7	C(75)-C(43)-C(42)	120.6(6)
C(5X)-C(33)-H(33C)	109.7	C(88)-C(43)-C(42)	120.3(6)
C(5X)-C(33)-H(33D)	109.7	C(88)-C(43)-C(75)	119.1(6)
H(33C)-C(33)-H(33D)	108.2	C(6X)-C(44)-H(44C)	109.6
N(5X)-C(34)-H(34C)	109.0	C(6X)-C(44)-H(44D)	109.6
N(5X)-C(34)-H(34D)	109.0	C(6X)-C(44)-C(45)	110.5(5)
N(5X)-C(34)-C(35)	113.0(5)	H(44C)-C(44)-H(44D)	108.1
H(34C)-C(34)-H(34D)	107.8	C(45)-C(44)-H(44C)	109.6
C(35)-C(34)-H(34C)	109.0	C(45)-C(44)-H(44D)	109.6
C(35)-C(34)-H(34D)	109.0	C(44)-C(45)-H(45D)	109.5
C(36)-C(35)-C(34)	120.3(6)	C(44)-C(45)-H(45E)	109.5
C(40)-C(35)-C(34)	119.9(6)	C(44)-C(45)-H(45F)	109.5
C(40)-C(35)-C(36)	119.4(6)	H(45D)-C(45)-H(45E)	109.5
C(35)-C(36)-H(36)	120.0	H(45D)-C(45)-H(45F)	109.5
C(37)-C(36)-C(35)	120.0(6)	H(45E)-C(45)-H(45F)	109.5
C(37)-C(36)-H(36)	120.0	C(47)-C(46)-C(51)	120.2(6)
C(36)-C(37)-C(38)	118.7(6)	C(47)-C(46)-C(52)	120.6(6)

C(51)-C(46)-C(52)	119.2(5)	C(56)-C(57)-H(57)	119.4
C(46)-C(47)-C(63)	118.3(6)	C(58)-C(57)-C(56)	121.3(6)
C(48)-C(47)-C(46)	120.8(6)	C(58)-C(57)-H(57)	119.4
C(48)-C(47)-C(63)	120.5(5)	C(57)-C(58)-H(58)	119.3
C(47)-C(48)-C(49)	121.4(6)	C(59)-C(58)-C(57)	121.3(7)
C(47)-C(48)-C(65)	120.4(6)	C(59)-C(58)-H(58)	119.3
C(49)-C(48)-C(65)	118.0(5)	C(54)-C(59)-H(59)	120.4
C(48)-C(49)-C(76)	120.7(5)	C(58)-C(59)-C(54)	119.2(7)
C(50)-C(49)-C(48)	117.0(6)	C(58)-C(59)-H(59)	120.4
C(50)-C(49)-C(76)	121.6(6)	O(4X)-C(60)-N(8)	119.7(7)
C(49)-C(50)-C(51)	121.3(6)	O(4X)-C(60)-C(56)	118.2(6)
C(49)-C(50)-C(78)	119.7(6)	N(8)-C(60)-C(56)	122.1(6)
C(51)-C(50)-C(78)	118.9(6)	N(8)-C(61)-H(61C)	108.7
C(46)-C(51)-C(50)	119.2(6)	N(8)-C(61)-H(61D)	108.7
C(46)-C(51)-C(89)	119.9(6)	N(8)-C(61)-C(62)	114.2(5)
C(50)-C(51)-C(89)	120.9(6)	H(61C)-C(61)-H(61D)	107.6
N(7)-C(52)-H(52C)	109.3	C(62)-C(61)-H(61C)	108.7
N(7)-C(52)-H(52D)	109.3	C(62)-C(61)-H(61D)	108.7
C(46)-C(52)-N(7)	111.5(5)	C(17)-C(62)-C(30)	119.9(6)
C(46)-C(52)-H(52C)	109.3	C(17)-C(62)-C(61)	120.2(6)
C(46)-C(52)-H(52D)	109.3	C(30)-C(62)-C(61)	119.8(6)
H(52C)-C(52)-H(52D)	108.0	C(47)-C(63)-H(63C)	109.3
N(7)-C(53)-H(53E)	109.2	C(47)-C(63)-H(63D)	109.3
N(7)-C(53)-H(53F)	109.2	C(47)-C(63)-C(64)	111.7(6)
H(53E)-C(53)-H(53F)	107.9	H(63C)-C(63)-H(63D)	107.9
C(54)-C(53)-N(7)	111.9(6)	C(64)-C(63)-H(63C)	109.3
C(54)-C(53)-H(53E)	109.2	C(64)-C(63)-H(63D)	109.3
C(54)-C(53)-H(53F)	109.2	C(63)-C(64)-H(64D)	109.5
C(55)-C(54)-C(53)	126.3(6)	C(63)-C(64)-H(64E)	109.5
C(55)-C(54)-C(59)	118.8(6)	C(63)-C(64)-H(64F)	109.5
C(59)-C(54)-C(53)	114.9(6)	H(64D)-C(64)-H(64E)	109.5
C(54)-C(55)-H(55)	118.9	H(64D)-C(64)-H(64F)	109.5
C(54)-C(55)-C(56)	122.3(6)	H(64E)-C(64)-H(64F)	109.5
C(56)-C(55)-H(55)	118.9	N(9)-C(65)-C(48)	113.4(5)
C(55)-C(56)-C(60)	124.3(6)	N(9)-C(65)-H(65C)	108.9
C(57)-C(56)-C(55)	117.1(7)	N(9)-C(65)-H(65D)	108.9
C(57)-C(56)-C(60)	118.4(6)	C(48)-C(65)-H(65C)	108.9

C(48)-C(65)-H(65D)	108.9	C(43)-C(75)-C(74)	118.6(6)
H(65C)-C(65)-H(65D)	107.7	C(49)-C(76)-H(76C)	109.6
N(9)-C(66)-H(66C)	109.7	C(49)-C(76)-H(76D)	109.6
N(9)-C(66)-H(66D)	109.7	C(49)-C(76)-C(77)	110.5(5)
H(66C)-C(66)-H(66D)	108.2	H(76C)-C(76)-H(76D)	108.1
C(67)-C(66)-N(9)	109.8(5)	C(77)-C(76)-H(76C)	109.6
C(67)-C(66)-H(66C)	109.7	C(77)-C(76)-H(76D)	109.6
C(67)-C(66)-H(66D)	109.7	C(76)-C(77)-H(77D)	109.5
C(68)-C(67)-C(66)	121.7(5)	C(76)-C(77)-H(77E)	109.5
C(68)-C(67)-C(72)	117.8(6)	C(76)-C(77)-H(77F)	109.5
C(72)-C(67)-C(66)	120.4(6)	H(77D)-C(77)-H(77E)	109.5
C(67)-C(68)-H(68)	118.9	H(77D)-C(77)-H(77F)	109.5
C(69)-C(68)-C(67)	122.2(6)	H(77E)-C(77)-H(77F)	109.5
C(69)-C(68)-H(68)	118.9	N(11)-C(78)-H(78C)	109.1
C(68)-C(69)-C(70)	119.6(6)	N(11)-C(78)-H(78D)	109.1
C(68)-C(69)-C(73)	123.3(6)	C(50)-C(78)-N(11)	112.6(5)
C(70)-C(69)-C(73)	117.0(6)	C(50)-C(78)-H(78C)	109.1
C(69)-C(70)-H(70)	120.2	C(50)-C(78)-H(78D)	109.1
C(71)-C(70)-C(69)	119.7(7)	H(78C)-C(78)-H(78D)	107.8
C(71)-C(70)-H(70)	120.2	N(11)-C(79)-H(79C)	109.6
C(70)-C(71)-H(71)	118.6	N(11)-C(79)-H(79D)	109.6
C(70)-C(71)-C(72)	122.8(7)	N(11)-C(79)-C(80)	110.2(5)
C(72)-C(71)-H(71)	118.6	H(79C)-C(79)-H(79D)	108.1
C(67)-C(72)-H(72)	121.1	C(80)-C(79)-H(79C)	109.6
C(71)-C(72)-C(67)	117.9(6)	C(80)-C(79)-H(79D)	109.6
C(71)-C(72)-H(72)	121.1	C(81)-C(80)-C(79)	118.3(6)
O(5X)-C(73)-N(10)	122.7(6)	C(85)-C(80)-C(79)	120.6(6)
O(5X)-C(73)-C(69)	120.1(5)	C(85)-C(80)-C(81)	121.1(7)
N(10)-C(73)-C(69)	117.2(5)	C(80)-C(81)-H(81)	119.4
N(10)-C(74)-H(74C)	109.5	C(80)-C(81)-C(82)	121.3(6)
N(10)-C(74)-H(74D)	109.5	C(82)-C(81)-H(81)	119.4
N(10)-C(74)-C(75)	110.6(5)	C(81)-C(82)-C(86)	125.6(6)
H(74C)-C(74)-H(74D)	108.1	C(83)-C(82)-C(81)	117.1(6)
C(75)-C(74)-H(74C)	109.5	C(83)-C(82)-C(86)	117.2(6)
C(75)-C(74)-H(74D)	109.5	C(82)-C(83)-H(83)	120.5
C(30)-C(75)-C(43)	122.0(6)	C(84)-C(83)-C(82)	119.0(7)
C(30)-C(75)-C(74)	119.4(6)	C(84)-C(83)-H(83)	120.5

C(83)-C(84)-H(84)	118.3	O(5)-P(2)-O(6)	120.4(3)
C(83)-C(84)-C(85)	123.4(7)	O(5)-P(2)-O(7)	105.3(3)
C(85)-C(84)-H(84)	118.3	O(6)-P(2)-O(4)	108.7(3)
C(80)-C(85)-C(84)	117.8(7)	O(6)-P(2)-O(7)	112.9(3)
C(80)-C(85)-H(85)	121.1	O(7)-P(2)-O(4)	99.1(3)
C(84)-C(85)-H(85)	121.1	O(8)-P(3)-O(7)	108.2(3)
O(6X)-C(86)-N(12)	121.3(6)	O(8)-P(3)-O(10)	107.5(3)
O(6X)-C(86)-C(82)	123.4(6)	O(9)-P(3)-O(7)	110.1(3)
N(12)-C(86)-C(82)	115.3(6)	O(9)-P(3)-O(8)	118.8(3)
N(12)-C(87)-H(87C)	110.0	O(9)-P(3)-O(10)	110.9(3)
N(12)-C(87)-H(87D)	110.0	O(10)-P(3)-O(7)	99.5(3)
N(12)-C(87)-C(88)	108.5(5)	P(1)-O(1)-H(1)	109.5
H(87C)-C(87)-H(87D)	108.4	P(1)-O(4)-P(2)	131.5(4)
C(88)-C(87)-H(87C)	110.0	P(2)-O(7)-P(3)	140.3(3)
C(88)-C(87)-H(87D)	110.0	C(1)-O(10)-P(3)	115.1(4)
C(17)-C(88)-C(87)	120.9(6)	C(5)-O(11)-C(2)	111.8(6)
C(43)-C(88)-C(17)	119.0(6)	C(3)-O(12)-H(12D)	109.5
C(43)-C(88)-C(87)	120.0(6)	C(4)-O(13)-H(13A)	109.5
C(51)-C(89)-H(89C)	109.7	C(6)-N(1)-C(5)	122.5(7)
C(51)-C(89)-H(89D)	109.7	C(9)-N(1)-C(5)	131.1(6)
C(51)-C(89)-C(90)	109.9(5)	C(9)-N(1)-C(6)	106.4(6)
H(89C)-C(89)-H(89D)	108.2	C(9)-N(2)-C(7)	103.4(7)
C(90)-C(89)-H(89C)	109.7	C(6)-N(3)-C(10)	110.3(7)
C(90)-C(89)-H(89D)	109.7	C(8)-N(4)-H(4)	119.1
C(89)-C(90)-H(90D)	109.5	C(10)-N(4)-H(4)	119.1
C(89)-C(90)-H(90E)	109.5	C(10)-N(4)-C(8)	121.8(7)
C(89)-C(90)-H(90F)	109.5	H(5A)-N(5)-H(5B)	120.0
H(90D)-C(90)-H(90E)	109.5	C(8)-N(5)-H(5A)	120.0
H(90D)-C(90)-H(90F)	109.5	C(8)-N(5)-H(5B)	120.0
H(90E)-C(90)-H(90F)	109.5	O(10)-C(1)-H(1A)	109.9
O(2)-P(1)-O(1)	113.3(4)	O(10)-C(1)-H(1B)	109.9
O(2)-P(1)-O(4)	105.9(4)	O(10)-C(1)-C(2)	109.1(6)
O(3)-P(1)-O(1)	109.0(3)	H(1A)-C(1)-H(1B)	108.3
O(3)-P(1)-O(2)	114.8(3)	C(2)-C(1)-H(1A)	109.9
O(3)-P(1)-O(4)	108.3(3)	C(2)-C(1)-H(1B)	109.9
O(4)-P(1)-O(1)	104.8(3)	O(11)-C(2)-C(1)	110.7(6)
O(5)-P(2)-O(4)	108.4(3)	O(11)-C(2)-H(2)	109.3

O(11)-C(2)-C(3)	102.3(6)	O(1A)-P(1A)-O(4A)	102.5(3)
C(1)-C(2)-H(2)	109.3	O(2A)-P(1A)-O(1A)	105.8(3)
C(3)-C(2)-C(1)	115.6(7)	O(2A)-P(1A)-O(3A)	121.0(3)
C(3)-C(2)-H(2)	109.3	O(2A)-P(1A)-O(4A)	105.4(3)
O(12)-C(3)-C(2)	112.5(6)	O(3A)-P(1A)-O(1A)	111.3(3)
O(12)-C(3)-H(3)	105.9	O(3A)-P(1A)-O(4A)	109.2(2)
O(12)-C(3)-C(4)	122.1(8)	O(4A)-P(2A)-O(7A)	101.6(3)
C(2)-C(3)-H(3)	105.9	O(5A)-P(2A)-O(4A)	107.5(3)
C(4)-C(3)-C(2)	103.3(7)	O(5A)-P(2A)-O(6A)	121.0(3)
C(4)-C(3)-H(3)	105.9	O(5A)-P(2A)-O(7A)	106.8(3)
O(13)-C(4)-C(3)	110.9(6)	O(6A)-P(2A)-O(4A)	108.6(2)
O(13)-C(4)-H(4A)	110.1	O(6A)-P(2A)-O(7A)	109.6(3)
O(13)-C(4)-C(5)	111.8(7)	O(8A)-P(3A)-O(7A)	111.1(3)
C(3)-C(4)-H(4A)	110.1	O(8A)-P(3A)-O(10A)	104.5(3)
C(3)-C(4)-C(5)	103.8(7)	O(9A)-P(3A)-O(7A)	110.9(3)
C(5)-C(4)-H(4A)	110.1	O(9A)-P(3A)-O(8A)	117.6(3)
O(11)-C(5)-N(1)	105.5(6)	O(9A)-P(3A)-O(10A)	111.4(4)
O(11)-C(5)-C(4)	103.6(6)	O(10A)-P(3A)-O(7A)	99.7(3)
O(11)-C(5)-H(5)	111.7	P(1A)-O(1A)-H(1AA)	109.5
N(1)-C(5)-C(4)	112.1(6)	P(2A)-O(4A)-P(1A)	126.4(3)
N(1)-C(5)-H(5)	111.7	P(3A)-O(7A)-P(2A)	133.2(3)
C(4)-C(5)-H(5)	111.7	C(1G)-O(10A)-P(3A)	126.9(5)
N(1)-C(6)-C(7)	102.0(7)	C(2A)-O(11A)-C(5A)	109.6(6)
N(3)-C(6)-N(1)	129.4(7)	C(3A)-O(12A)-H(12F)	109.5
N(3)-C(6)-C(7)	128.4(7)	C(4A)-O(13A)-H(13B)	109.5
N(2)-C(7)-C(6)	112.7(7)	C(5A)-N(1A)-C(6A)	128.4(8)
N(2)-C(7)-C(8)	131.5(8)	C(5A)-N(1A)-C(9A)	126.7(8)
C(6)-C(7)-C(8)	115.2(8)	C(6A)-N(1A)-C(9A)	104.8(7)
N(4)-C(8)-C(7)	115.0(7)	C(9A)-N(2A)-C(7A)	100.9(8)
N(5)-C(8)-N(4)	122.9(7)	C(6A)-N(3A)-C(10A)	111.3(8)
N(5)-C(8)-C(7)	122.0(8)	C(8A)-N(4A)-H(4AA)	119.4
N(1)-C(9)-H(9)	122.3	C(10A)-N(4A)-H(4AA)	119.4
N(2)-C(9)-N(1)	115.3(7)	C(10A)-N(4A)-C(8A)	121.3(8)
N(2)-C(9)-H(9)	122.3	H(5AA)-N(5A)-H(5AB)	120.0
N(3)-C(10)-H(10A)	115.8	C(8A)-N(5A)-H(5AA)	120.0
N(4)-C(10)-N(3)	128.4(9)	C(8A)-N(5A)-H(5AB)	120.0
N(4)-C(10)-H(10A)	115.8	O(10A)-C(1G)-H(1GA)	110.8

O(10A)-C(1G)-H(1GB)	110.8	C(7A)-C(8A)-N(5A)	123.8(9)
O(10A)-C(1G)-C(2A)	104.5(6)	N(1A)-C(9A)-H(9AA)	122.7
H(1GA)-C(1G)-H(1GB)	108.9	N(2A)-C(9A)-N(1A)	114.5(8)
C(2A)-C(1G)-H(1GA)	110.8	N(2A)-C(9A)-H(9AA)	122.7
C(2A)-C(1G)-H(1GB)	110.8	N(3A)-C(10A)-H(10B)	116.7
O(11A)-C(2A)-C(1G)	108.2(6)	N(4A)-C(10A)-N(3A)	126.6(9)
O(11A)-C(2A)-H(2A)	109.3	N(4A)-C(10A)-H(10B)	116.7
O(11A)-C(2A)-C(3A)	110.9(6)	H(1XE)-N(1X')-H(1XF)	107.3
C(1G)-C(2A)-H(2A)	109.3	C(7X')-N(1X')-H(1XE)	108.0
C(3A)-C(2A)-C(1G)	109.6(7)	C(7X')-N(1X')-H(1XF)	108.0
C(3A)-C(2A)-H(2A)	109.3	C(7X')-N(1X')-C(8X')	117.0(6)
O(12A)-C(3A)-C(2A)	111.0(7)	C(8X')-N(1X')-H(1XE)	108.0
O(12A)-C(3A)-H(3A)	113.6	C(8X')-N(1X')-H(1XF)	108.0
O(12A)-C(3A)-C(4A)	105.2(6)	C(15')-N(2X')-H(2X')	119.4
C(2A)-C(3A)-H(3A)	113.6	C(15')-N(2X')-C(16')	121.1(5)
C(2A)-C(3A)-C(4A)	98.7(7)	C(16')-N(2X')-H(2X')	119.4
C(4A)-C(3A)-H(3A)	113.6	H(3XE)-N(3X')-H(3XF)	107.9
O(13A)-C(4A)-C(3A)	114.2(7)	C(20')-N(3X')-H(3XE)	109.1
O(13A)-C(4A)-H(4AB)	107.9	C(20')-N(3X')-H(3XF)	109.1
O(13A)-C(4A)-C(5A)	116.0(6)	C(21')-N(3X')-H(3XE)	109.1
C(3A)-C(4A)-H(4AB)	107.9	C(21')-N(3X')-H(3XF)	109.1
C(3A)-C(4A)-C(5A)	102.5(7)	C(21')-N(3X')-C(20')	112.3(5)
C(5A)-C(4A)-H(4AB)	107.9	C(28')-N(4X')-H(4X')	118.7
O(11A)-C(5A)-C(4A)	100.5(6)	C(28')-N(4X')-C(29')	122.5(5)
O(11A)-C(5A)-H(5AC)	109.8	C(29')-N(4X')-H(4X')	118.7
N(1A)-C(5A)-O(11A)	110.0(6)	H(5XE)-N(5X')-H(5XF)	108.0
N(1A)-C(5A)-C(4A)	116.6(7)	C(33')-N(5X')-H(5XE)	109.4
N(1A)-C(5A)-H(5AC)	109.8	C(33')-N(5X')-H(5XF)	109.4
C(4A)-C(5A)-H(5AC)	109.8	C(33')-N(5X')-C(34')	111.2(5)
N(1A)-C(6A)-C(7A)	106.9(8)	C(34')-N(5X')-H(5XE)	109.4
N(3A)-C(6A)-N(1A)	127.5(8)	C(34')-N(5X')-H(5XF)	109.4
N(3A)-C(6A)-C(7A)	125.6(8)	C(41')-N(6X')-H(6X')	121.7
C(6A)-C(7A)-N(2A)	112.3(8)	C(41')-N(6X')-C(42')	116.6(5)
C(8A)-C(7A)-N(2A)	128.5(9)	C(42')-N(6X')-H(6X')	121.7
C(8A)-C(7A)-C(6A)	119.0(9)	H(7'A)-N(7')-H(7'B)	107.9
N(4A)-C(8A)-N(5A)	120.0(8)	C(52')-N(7')-H(7'A)	109.2
N(4A)-C(8A)-C(7A)	116.2(9)	C(52')-N(7')-H(7'B)	109.2

C(53')-N(7')-H(7'A)	109.2	C(6X')-C(5X')-C(4X')	121.8(6)
C(53')-N(7')-H(7'B)	109.2	C(6X')-C(5X')-C(33')	120.5(6)
C(53')-N(7')-C(52')	111.9(5)	C(1X')-C(6X')-C(44')	120.1(5)
C(60')-N(8')-H(8')	120.8	C(5X')-C(6X')-C(1X')	118.9(6)
C(60')-N(8')-C(61')	118.3(5)	C(5X')-C(6X')-C(44')	120.9(6)
C(61')-N(8')-H(8')	120.8	N(1X')-C(7X')-H(7XE)	108.0
H(9'A)-N(9')-H(9'B)	108.0	N(1X')-C(7X')-H(7XF)	108.0
C(65')-N(9')-H(9'A)	109.4	C(1X')-C(7X')-N(1X')	117.0(5)
C(65')-N(9')-H(9'B)	109.4	C(1X')-C(7X')-H(7XE)	108.0
C(66')-N(9')-H(9'A)	109.4	C(1X')-C(7X')-H(7XF)	108.0
C(66')-N(9')-H(9'B)	109.4	H(7XE)-C(7X')-H(7XF)	107.3
C(66')-N(9')-C(65')	111.3(5)	N(1X')-C(8X')-H(8XE)	108.1
C(73')-N(10')-H(10')	118.8	N(1X')-C(8X')-H(8XF)	108.1
C(73')-N(10')-C(74')	122.3(5)	N(1X')-C(8X')-C(9X')	116.9(6)
C(74')-N(10')-H(10')	118.8	H(8XE)-C(8X')-H(8XF)	107.3
H(11E)-N(11')-H(11F)	107.6	C(9X')-C(8X')-H(8XE)	108.1
C(78')-N(11')-H(11E)	108.7	C(9X')-C(8X')-H(8XF)	108.1
C(78')-N(11')-H(11F)	108.7	C(13)-C(9X')-C(8X')	117.8(6)
C(79')-N(11')-H(11E)	108.7	C(13)-C(9X')-C(14')	122.4(6)
C(79')-N(11')-H(11F)	108.7	C(14')-C(9X')-C(8X')	119.9(6)
C(79')-N(11')-C(78')	114.3(5)	C(12')-C(11')-C(13)	120.9(6)
C(86')-N(12')-H(12')	118.9	C(12')-C(11')-C(15')	115.9(6)
C(86')-N(12')-C(87')	122.1(5)	C(13)-C(11')-C(15')	123.1(5)
C(87')-N(12')-H(12')	118.9	C(11')-C(12')-H(12C)	121.3
C(2X')-C(1X')-C(6X')	118.9(6)	C(11')-C(12')-C(13')	117.4(6)
C(2X')-C(1X')-C(7X')	123.5(6)	C(13')-C(12')-H(12C)	121.3
C(6X')-C(1X')-C(7X')	117.6(6)	C(9X')-C(13)-C(11')	117.8(6)
C(1X')-C(2X')-C(3X')	121.7(6)	C(9X')-C(13)-H(13)	121.1
C(1X')-C(2X')-C(18')	118.2(6)	C(11')-C(13)-H(13)	121.1
C(3X')-C(2X')-C(18')	120.1(6)	C(12')-C(13')-H(13')	119.6
C(2X')-C(3X')-C(4X')	120.0(6)	C(14')-C(13')-C(12')	120.7(6)
C(2X')-C(3X')-C(20')	119.5(6)	C(14')-C(13')-H(13')	119.6
C(4X')-C(3X')-C(20')	120.4(6)	C(9X')-C(14')-H(14')	119.6
C(3X')-C(4X')-C(31')	121.4(6)	C(13')-C(14')-C(9X')	120.8(6)
C(5X')-C(4X')-C(3X')	118.1(6)	C(13')-C(14')-H(14')	119.6
C(5X')-C(4X')-C(31')	120.4(6)	O(1X')-C(15')-N(2X')	122.5(6)
C(4X')-C(5X')-C(33')	117.7(5)	O(1X')-C(15')-C(11')	121.0(6)

N(2X')-C(15')-C(11')	116.4(6)	C(22')-C(23')-H(23')	119.5
N(2X')-C(16')-H(16E)	109.1	C(24')-C(23')-C(22')	121.0(6)
N(2X')-C(16')-H(16F)	109.1	C(24')-C(23')-H(23')	119.5
N(2X')-C(16')-C(17')	112.7(5)	C(23')-C(24')-C(28')	121.1(6)
H(16E)-C(16')-H(16F)	107.8	C(25')-C(24')-C(23')	119.4(6)
C(17')-C(16')-H(16E)	109.1	C(25')-C(24')-C(28')	119.5(6)
C(17')-C(16')-H(16F)	109.1	C(24')-C(25')-H(25')	117.9
C(16')-C(17')-C(88')	121.7(5)	C(24')-C(25')-C(26')	124.1(7)
C(62')-C(17')-C(16')	120.3(5)	C(26')-C(25')-H(25')	117.9
C(62')-C(17')-C(88')	118.0(5)	C(25')-C(26')-H(26')	121.8
C(2X')-C(18')-H(18E)	110.1	C(25')-C(26')-C(27')	116.3(7)
C(2X')-C(18')-H(18F)	110.1	C(27')-C(26')-H(26')	121.8
C(2X')-C(18')-C(19')	108.1(6)	C(22')-C(27')-H(27')	119.6
H(18E)-C(18')-H(18F)	108.4	C(26')-C(27')-C(22')	120.8(6)
C(19')-C(18')-H(18E)	110.1	C(26')-C(27')-H(27')	119.6
C(19')-C(18')-H(18F)	110.1	O(2X')-C(28')-N(4X')	122.9(6)
C(18')-C(19')-H(19G)	109.5	O(2X')-C(28')-C(24')	120.2(6)
C(18')-C(19')-H(19H)	109.5	N(4X')-C(28')-C(24')	116.8(6)
C(18')-C(19')-H(19I)	109.5	N(4X')-C(29')-H(29E)	110.0
H(19G)-C(19')-H(19H)	109.5	N(4X')-C(29')-H(29F)	110.0
H(19G)-C(19')-H(19I)	109.5	N(4X')-C(29')-C(30')	108.7(5)
H(19H)-C(19')-H(19I)	109.5	H(29E)-C(29')-H(29F)	108.3
N(3X')-C(20')-C(3X')	117.0(6)	C(30')-C(29')-H(29E)	110.0
N(3X')-C(20')-H(20E)	108.0	C(30')-C(29')-H(29F)	110.0
N(3X')-C(20')-H(20F)	108.0	C(62')-C(30')-C(29')	117.3(5)
C(3X')-C(20')-H(20E)	108.0	C(75')-C(30')-C(29')	121.0(5)
C(3X')-C(20')-H(20F)	108.0	C(75')-C(30')-C(62')	121.5(6)
H(20E)-C(20')-H(20F)	107.3	C(4X')-C(31')-H(31E)	108.7
N(3X')-C(21')-H(21E)	109.3	C(4X')-C(31')-H(31F)	108.7
N(3X')-C(21')-H(21F)	109.3	H(31E)-C(31')-H(31F)	107.6
N(3X')-C(21')-C(22')	111.6(5)	C(32')-C(31')-C(4X')	114.4(6)
H(21E)-C(21')-H(21F)	108.0	C(32')-C(31')-H(31E)	108.7
C(22')-C(21')-H(21E)	109.3	C(32')-C(31')-H(31F)	108.7
C(22')-C(21')-H(21F)	109.3	C(31')-C(32')-H(32G)	109.5
C(23')-C(22')-C(21')	121.2(6)	C(31')-C(32')-H(32H)	109.5
C(23')-C(22')-C(27')	118.0(6)	C(31')-C(32')-H(32I)	109.5
C(27')-C(22')-C(21')	120.7(6)	H(32G)-C(32')-H(32H)	109.5

H(32G)-C(32')-H(32I)	109.5	N(6X')-C(42')-C(43')	112.2(5)
H(32H)-C(32')-H(32I)	109.5	H(42E)-C(42')-H(42F)	107.9
N(5X')-C(33')-C(5X')	110.5(5)	C(43')-C(42')-H(42E)	109.2
N(5X')-C(33')-H(33E)	109.5	C(43')-C(42')-H(42F)	109.2
N(5X')-C(33')-H(33F)	109.5	C(75')-C(43')-C(42')	117.8(5)
C(5X')-C(33')-H(33E)	109.5	C(88')-C(43')-C(42')	119.6(6)
C(5X')-C(33')-H(33F)	109.5	C(88')-C(43')-C(75')	122.4(6)
H(33E)-C(33')-H(33F)	108.1	C(6X')-C(44')-H(44E)	110.3
N(5X')-C(34')-H(34E)	109.0	C(6X')-C(44')-H(44F)	110.3
N(5X')-C(34')-H(34F)	109.0	C(6X')-C(44')-C(45')	107.0(6)
H(34E)-C(34')-H(34F)	107.8	H(44E)-C(44')-H(44F)	108.6
C(35')-C(34')-N(5X')	113.0(5)	C(45')-C(44')-H(44E)	110.3
C(35')-C(34')-H(34E)	109.0	C(45')-C(44')-H(44F)	110.3
C(35')-C(34')-H(34F)	109.0	C(44')-C(45')-H(45G)	109.5
C(36')-C(35')-C(34')	121.8(6)	C(44')-C(45')-H(45H)	109.5
C(40')-C(35')-C(34')	117.8(6)	C(44')-C(45')-H(45I)	109.5
C(40')-C(35')-C(36')	120.2(6)	H(45G)-C(45')-H(45H)	109.5
C(35')-C(36')-H(36')	119.9	H(45G)-C(45')-H(45I)	109.5
C(37')-C(36')-C(35')	120.2(6)	H(45H)-C(45')-H(45I)	109.5
C(37')-C(36')-H(36')	119.9	C(47')-C(46')-C(51')	121.4(6)
C(36')-C(37')-C(38')	118.5(6)	C(47')-C(46')-C(52')	120.0(5)
C(36')-C(37')-C(41')	124.5(6)	C(51')-C(46')-C(52')	118.7(5)
C(38')-C(37')-C(41')	116.9(6)	C(46')-C(47')-C(63')	119.5(6)
C(37')-C(38')-H(38')	119.8	C(48')-C(47')-C(46')	120.3(6)
C(39')-C(38')-C(37')	120.3(6)	C(48')-C(47')-C(63')	120.2(5)
C(39')-C(38')-H(38')	119.8	C(47')-C(48')-C(49')	119.5(6)
C(38')-C(39')-H(39')	120.2	C(47')-C(48')-C(65')	120.0(6)
C(40')-C(39')-C(38')	119.5(7)	C(49')-C(48')-C(65')	120.0(5)
C(40')-C(39')-H(39')	120.2	C(48')-C(49')-C(76')	120.1(5)
C(35')-C(40')-C(39')	121.1(7)	C(50')-C(49')-C(48')	119.4(5)
C(35')-C(40')-H(40')	119.4	C(50')-C(49')-C(76')	120.2(5)
C(39')-C(40')-H(40')	119.4	C(49')-C(50')-C(51')	120.8(6)
O(3X')-C(41')-N(6X')	120.5(6)	C(49')-C(50')-C(78')	120.5(6)
O(3X')-C(41')-C(37')	119.9(6)	C(51')-C(50')-C(78')	118.5(6)
N(6X')-C(41')-C(37')	119.4(5)	C(46')-C(51')-C(50')	118.2(6)
N(6X')-C(42')-H(42E)	109.2	C(46')-C(51')-C(89')	121.1(6)
N(6X')-C(42')-H(42F)	109.2	C(50')-C(51')-C(89')	120.7(6)

N(7')-C(52')-H(52E)	109.0	C(62')-C(61')-H(61E)	109.1
N(7')-C(52')-H(52F)	109.0	C(62')-C(61')-H(61F)	109.1
C(46')-C(52')-N(7')	112.9(5)	C(17')-C(62')-C(30')	120.8(5)
C(46')-C(52')-H(52E)	109.0	C(17')-C(62')-C(61')	119.0(5)
C(46')-C(52')-H(52F)	109.0	C(30')-C(62')-C(61')	120.2(5)
H(52E)-C(52')-H(52F)	107.8	C(47')-C(63')-H(63E)	109.5
N(7')-C(53')-H(53G)	108.8	C(47')-C(63')-H(63F)	109.5
N(7')-C(53')-H(53H)	108.8	C(47')-C(63')-C(64')	110.6(5)
N(7')-C(53')-C(54')	113.8(6)	H(63E)-C(63')-H(63F)	108.1
H(53G)-C(53')-H(53H)	107.7	C(64')-C(63')-H(63E)	109.5
C(54')-C(53')-H(53G)	108.8	C(64')-C(63')-H(63F)	109.5
C(54')-C(53')-H(53H)	108.8	C(63')-C(64')-H(64G)	109.5
C(55')-C(54')-C(53')	123.2(6)	C(63')-C(64')-H(64H)	109.5
C(55')-C(54')-C(59')	118.3(6)	C(63')-C(64')-H(64I)	109.5
C(59')-C(54')-C(53')	118.3(6)	H(64G)-C(64')-H(64H)	109.5
C(54')-C(55')-H(55')	120.6	H(64G)-C(64')-H(64I)	109.5
C(54')-C(55')-C(56')	118.8(6)	H(64H)-C(64')-H(64I)	109.5
C(56')-C(55')-H(55')	120.6	N(9')-C(65')-H(65E)	108.8
C(55')-C(56')-C(60')	122.7(6)	N(9')-C(65')-H(65F)	108.8
C(57')-C(56')-C(55')	119.7(6)	C(48')-C(65')-N(9')	113.9(5)
C(57')-C(56')-C(60')	117.6(6)	C(48')-C(65')-H(65E)	108.8
C(56')-C(57')-H(57')	119.1	C(48')-C(65')-H(65F)	108.8
C(58')-C(57')-C(56')	121.8(6)	H(65E)-C(65')-H(65F)	107.7
C(58')-C(57')-H(57')	119.1	N(9')-C(66')-H(66E)	109.4
C(57')-C(58')-H(58')	119.2	N(9')-C(66')-H(66F)	109.4
C(57')-C(58')-C(59')	121.5(7)	H(66E)-C(66')-H(66F)	108.0
C(59')-C(58')-H(58')	119.2	C(67')-C(66')-N(9')	111.1(5)
C(54')-C(59')-H(59')	120.2	C(67')-C(66')-H(66E)	109.4
C(58')-C(59')-C(54')	119.7(6)	C(67')-C(66')-H(66F)	109.4
C(58')-C(59')-H(59')	120.2	C(68')-C(67')-C(66')	121.4(6)
O(4X')-C(60')-N(8')	118.3(6)	C(68')-C(67')-C(72')	117.3(6)
O(4X')-C(60')-C(56')	119.8(6)	C(72')-C(67')-C(66')	121.0(6)
N(8')-C(60')-C(56')	121.7(6)	C(67')-C(68')-H(68')	118.8
N(8')-C(61')-H(61E)	109.1	C(69')-C(68')-C(67')	122.4(6)
N(8')-C(61')-H(61F)	109.1	C(69')-C(68')-H(68')	118.8
N(8')-C(61')-C(62')	112.6(5)	C(68')-C(69')-C(70')	121.0(6)
H(61E)-C(61')-H(61F)	107.8	C(68')-C(69')-C(73')	123.1(5)

C(70')-C(69')-C(73')	115.9(6)	C(50')-C(78')-H(78E)	109.4
C(69')-C(70')-H(70')	121.0	C(50')-C(78')-H(78F)	109.4
C(71')-C(70')-C(69')	117.9(6)	H(78E)-C(78')-H(78F)	108.0
C(71')-C(70')-H(70')	121.0	N(11')-C(79')-H(79E)	109.5
C(70')-C(71')-H(71')	119.4	N(11')-C(79')-H(79F)	109.5
C(72')-C(71')-C(70')	121.3(6)	N(11')-C(79')-C(80')	110.7(6)
C(72')-C(71')-H(71')	119.4	H(79E)-C(79')-H(79F)	108.1
C(67')-C(72')-H(72')	119.9	C(80')-C(79')-H(79E)	109.5
C(71')-C(72')-C(67')	120.1(6)	C(80')-C(79')-H(79F)	109.5
C(71')-C(72')-H(72')	119.9	C(81')-C(80')-C(79')	120.9(7)
O(5X')-C(73')-N(10')	121.3(5)	C(81')-C(80')-C(85')	119.6(7)
O(5X')-C(73')-C(69')	119.9(5)	C(85')-C(80')-C(79')	119.4(6)
N(10')-C(73')-C(69')	118.8(5)	C(80')-C(81')-H(81')	119.3
N(10')-C(74')-H(74E)	109.9	C(80')-C(81')-C(82')	121.4(7)
N(10')-C(74')-H(74F)	109.9	C(82')-C(81')-H(81')	119.3
N(10')-C(74')-C(75')	109.0(5)	C(81')-C(82')-C(83')	120.2(6)
H(74E)-C(74')-H(74F)	108.3	C(81')-C(82')-C(86')	124.5(6)
C(75')-C(74')-H(74E)	109.9	C(83')-C(82')-C(86')	115.2(6)
C(75')-C(74')-H(74F)	109.9	C(82')-C(83')-H(83')	121.6
C(30')-C(75')-C(43')	119.0(6)	C(84')-C(83')-C(82')	116.7(6)
C(30')-C(75')-C(74')	122.4(6)	C(84')-C(83')-H(83')	121.6
C(43')-C(75')-C(74')	118.6(5)	C(83')-C(84')-H(84')	119.6
C(49')-C(76')-H(76E)	109.3	C(85')-C(84')-C(83')	120.8(7)
C(49')-C(76')-H(76F)	109.3	C(85')-C(84')-H(84')	119.6
C(49')-C(76')-C(77')	111.5(5)	C(80')-C(85')-H(85')	119.4
H(76E)-C(76')-H(76F)	108.0	C(84')-C(85')-C(80')	121.2(7)
C(77')-C(76')-H(76E)	109.3	C(84')-C(85')-H(85')	119.4
C(77')-C(76')-H(76F)	109.3	O(6X')-C(86')-N(12')	120.8(6)
C(76')-C(77')-H(77G)	109.5	O(6X')-C(86')-C(82')	123.1(6)
C(76')-C(77')-H(77H)	109.5	N(12')-C(86')-C(82')	116.0(6)
C(76')-C(77')-H(77I)	109.5	N(12')-C(87')-H(87E)	110.2
H(77G)-C(77')-H(77H)	109.5	N(12')-C(87')-H(87F)	110.2
H(77G)-C(77')-H(77I)	109.5	H(87E)-C(87')-H(87F)	108.5
H(77H)-C(77')-H(77I)	109.5	C(88')-C(87')-N(12')	107.5(5)
N(11')-C(78')-H(78E)	109.4	C(88')-C(87')-H(87E)	110.2
N(11')-C(78')-H(78F)	109.4	C(88')-C(87')-H(87F)	110.2
C(50')-C(78')-N(11')	111.0(5)	C(43')-C(88')-C(17')	118.1(6)

C(43')-C(88')-C(87')	122.4(6)	C(3B)-O(12B)-H(12G)	109.5
C(87')-C(88')-C(17')	119.4(5)	C(4B)-O(13B)-H(13C)	109.5
C(51')-C(89')-H(89E)	109.8	C(6B)-N(1B)-C(5B)	127.4(6)
C(51')-C(89')-H(89F)	109.8	C(9B)-N(1B)-C(5B)	128.1(6)
C(51')-C(89')-C(90')	109.5(5)	C(9B)-N(1B)-C(6B)	104.5(6)
H(89E)-C(89')-H(89F)	108.2	C(9B)-N(2B)-C(7B)	103.8(6)
C(90')-C(89')-H(89E)	109.8	C(10B)-N(3B)-C(6B)	111.8(6)
C(90')-C(89')-H(89F)	109.8	C(8B)-N(4B)-H(4B)	120.3
C(89')-C(90')-H(90G)	109.5	C(10B)-N(4B)-H(4B)	120.3
C(89')-C(90')-H(90H)	109.5	C(10B)-N(4B)-C(8B)	119.3(6)
C(89')-C(90')-H(90I)	109.5	H(5BA)-N(5B)-H(5BB)	120.0
H(90G)-C(90')-H(90H)	109.5	C(8B)-N(5B)-H(5BA)	120.0
H(90G)-C(90')-H(90I)	109.5	C(8B)-N(5B)-H(5BB)	120.0
H(90H)-C(90')-H(90I)	109.5	O(10B)-C(1B)-H(1BB)	109.3
O(1B)-P(1B)-O(4B)	103.7(3)	O(10B)-C(1B)-H(1BC)	109.3
O(2B)-P(1B)-O(1B)	111.8(3)	H(1BB)-C(1B)-H(1BC)	108.0
O(2B)-P(1B)-O(3B)	117.3(3)	C(2B)-C(1B)-O(10B)	111.6(6)
O(2B)-P(1B)-O(4B)	108.5(3)	C(2B)-C(1B)-H(1BB)	109.3
O(3B)-P(1B)-O(1B)	107.3(2)	C(2B)-C(1B)-H(1BC)	109.3
O(3B)-P(1B)-O(4B)	107.4(2)	O(11B)-C(2B)-H(2B)	109.5
O(5B)-P(2B)-O(4B)	108.4(3)	O(11B)-C(2B)-C(3B)	104.1(5)
O(5B)-P(2B)-O(7B)	105.6(2)	C(1B)-C(2B)-O(11B)	109.6(6)
O(6B)-P(2B)-O(4B)	108.1(2)	C(1B)-C(2B)-H(2B)	109.5
O(6B)-P(2B)-O(5B)	120.4(3)	C(1B)-C(2B)-C(3B)	114.6(6)
O(6B)-P(2B)-O(7B)	111.6(3)	C(3B)-C(2B)-H(2B)	109.5
O(7B)-P(2B)-O(4B)	101.0(3)	O(12B)-C(3B)-C(2B)	114.5(6)
O(8B)-P(3B)-O(7B)	108.3(3)	O(12B)-C(3B)-H(3B)	108.1
O(8B)-P(3B)-O(10B)	106.1(3)	O(12B)-C(3B)-C(4B)	116.2(7)
O(9B)-P(3B)-O(7B)	109.0(2)	C(2B)-C(3B)-H(3B)	108.1
O(9B)-P(3B)-O(8B)	118.8(3)	C(2B)-C(3B)-C(4B)	101.3(6)
O(9B)-P(3B)-O(10B)	112.5(3)	C(4B)-C(3B)-H(3B)	108.1
O(10B)-P(3B)-O(7B)	100.6(2)	O(13B)-C(4B)-C(3B)	110.4(6)
P(1B)-O(1B)-H(1BA)	109.5	O(13B)-C(4B)-H(4BA)	111.3
P(2B)-O(4B)-P(1B)	127.8(3)	O(13B)-C(4B)-C(5B)	109.8(7)
P(2B)-O(7B)-P(3B)	136.0(3)	C(3B)-C(4B)-H(4BA)	111.3
C(1B)-O(10B)-P(3B)	117.1(4)	C(3B)-C(4B)-C(5B)	102.3(6)
C(5B)-O(11B)-C(2B)	109.9(6)	C(5B)-C(4B)-H(4BA)	111.3

O(11B)-C(5B)-N(1B)	106.3(6)	O(9C)-P(3C)-O(10C)	111.5(3)
O(11B)-C(5B)-C(4B)	106.9(6)	O(10C)-P(3C)-O(7C)	100.0(2)
O(11B)-C(5B)-H(5BC)	110.8	P(1C)-O(1C)-H(1CA)	109.5
N(1B)-C(5B)-C(4B)	111.1(7)	P(2C)-O(4C)-P(1C)	126.2(3)
N(1B)-C(5B)-H(5BC)	110.8	P(3C)-O(7C)-P(2C)	132.0(3)
C(4B)-C(5B)-H(5BC)	110.8	C(1E)-O(10C)-P(3C)	124.3(4)
N(3B)-C(6B)-N(1B)	126.1(6)	C(5C)-O(11C)-C(2C)	109.1(5)
C(7B)-C(6B)-N(1B)	107.0(6)	C(3C)-O(12C)-H(12H)	109.5
C(7B)-C(6B)-N(3B)	126.9(7)	C(4C)-O(13C)-H(13D)	109.5
C(6B)-C(7B)-N(2B)	110.1(6)	C(6C)-N(1C)-C(5C)	125.6(7)
C(6B)-C(7B)-C(8B)	118.5(7)	C(9C)-N(1C)-C(5C)	128.0(7)
C(8B)-C(7B)-N(2B)	130.3(7)	C(9C)-N(1C)-C(6C)	106.4(7)
N(5B)-C(8B)-N(4B)	117.2(7)	C(9C)-N(2C)-C(7C)	106.7(7)
N(5B)-C(8B)-C(7B)	126.9(7)	C(10C)-N(3C)-C(6C)	111.9(7)
C(7B)-C(8B)-N(4B)	115.9(6)	C(8C)-N(4C)-H(4C)	121.0
N(1B)-C(9B)-H(9BA)	122.7	C(10C)-N(4C)-H(4C)	121.0
N(2B)-C(9B)-N(1B)	114.5(7)	C(10C)-N(4C)-C(8C)	117.9(8)
N(2B)-C(9B)-H(9BA)	122.7	H(5CA)-N(5C)-H(5CB)	120.0
N(3B)-C(10B)-H(10C)	116.8	C(8C)-N(5C)-H(5CA)	120.0
N(4B)-C(10B)-N(3B)	126.4(7)	C(8C)-N(5C)-H(5CB)	120.0
N(4B)-C(10B)-H(10C)	116.8	O(10C)-C(1E)-H(1EA)	109.9
O(1C)-P(1C)-O(4C)	103.4(2)	O(10C)-C(1E)-H(1EB)	109.9
O(2C)-P(1C)-O(1C)	106.9(2)	O(10C)-C(1E)-C(2C)	108.9(6)
O(2C)-P(1C)-O(4C)	105.4(2)	H(1EA)-C(1E)-H(1EB)	108.3
O(3C)-P(1C)-O(1C)	110.5(2)	C(2C)-C(1E)-H(1EA)	109.9
O(3C)-P(1C)-O(2C)	119.7(3)	C(2C)-C(1E)-H(1EB)	109.9
O(3C)-P(1C)-O(4C)	109.7(2)	O(11C)-C(2C)-C(1E)	106.8(6)
O(4C)-P(2C)-O(7C)	100.5(2)	O(11C)-C(2C)-H(2C)	109.3
O(5C)-P(2C)-O(4C)	108.1(2)	O(11C)-C(2C)-C(3C)	103.0(5)
O(5C)-P(2C)-O(7C)	106.4(2)	C(1E)-C(2C)-H(2C)	109.3
O(6C)-P(2C)-O(4C)	108.6(2)	C(1E)-C(2C)-C(3C)	118.7(7)
O(6C)-P(2C)-O(5C)	120.9(3)	C(3C)-C(2C)-H(2C)	109.3
O(6C)-P(2C)-O(7C)	110.4(2)	O(12C)-C(3C)-C(2C)	109.2(6)
O(8C)-P(3C)-O(7C)	109.5(2)	O(12C)-C(3C)-H(3C)	109.1
O(8C)-P(3C)-O(10C)	103.5(3)	C(2C)-C(3C)-H(3C)	109.1
O(9C)-P(3C)-O(7C)	110.7(3)	C(4C)-C(3C)-O(12C)	114.2(7)
O(9C)-P(3C)-O(8C)	119.6(3)	C(4C)-C(3C)-C(2C)	105.8(6)

C(4C)-C(3C)-H(3C)	109.1	H(3XA)-N(3X")-H(3XB)	107.5
O(13C)-C(4C)-H(4CA)	113.5	C(20")-N(3X")-H(3XA)	108.5
O(13C)-C(4C)-C(5C)	108.2(7)	C(20")-N(3X")-H(3XB)	108.5
C(3C)-C(4C)-O(13C)	108.6(7)	C(20")-N(3X")-C(21")	115.0(6)
C(3C)-C(4C)-H(4CA)	113.5	C(21")-N(3X")-H(3XA)	108.5
C(3C)-C(4C)-C(5C)	98.3(6)	C(21")-N(3X")-H(3XB)	108.5
C(5C)-C(4C)-H(4CA)	113.5	C(28")-N(4X")-H(4X")	118.8
O(11C)-C(5C)-N(1C)	109.8(6)	C(28")-N(4X")-C(29")	122.4(5)
O(11C)-C(5C)-C(4C)	107.1(6)	C(29")-N(4X")-H(4X")	118.8
O(11C)-C(5C)-H(5C)	109.3	H(5XA)-N(5X")-H(5XB)	107.9
N(1C)-C(5C)-C(4C)	112.1(6)	C(33")-N(5X")-H(5XA)	109.2
N(1C)-C(5C)-H(5C)	109.3	C(33")-N(5X")-H(5XB)	109.2
C(4C)-C(5C)-H(5C)	109.3	C(33")-N(5X")-C(34")	112.1(5)
N(3C)-C(6C)-N(1C)	128.4(7)	C(34")-N(5X")-H(5XA)	109.2
N(3C)-C(6C)-C(7C)	125.5(8)	C(34")-N(5X")-H(5XB)	109.2
C(7C)-C(6C)-N(1C)	106.1(7)	C(41")-N(6X")-H(6X")	121.7
C(6C)-C(7C)-N(2C)	107.0(8)	C(41")-N(6X")-C(42")	116.6(5)
C(6C)-C(7C)-C(8C)	116.5(9)	C(42")-N(6X")-H(6X")	121.7
C(8C)-C(7C)-N(2C)	136.3(8)	H(7"C)-N(7")-H(7"D)	106.7
N(4C)-C(8C)-N(5C)	117.8(9)	H(7"A)-N(7")-H(7"B)	107.3
N(4C)-C(8C)-C(7C)	118.3(8)	C(52")-N(7")-H(7"C)	106.8
N(5C)-C(8C)-C(7C)	123.5(10)	C(52")-N(7")-H(7"D)	106.8
N(1C)-C(9C)-H(9C)	123.1	C(52")-N(7")-H(7"A)	108.1
N(2C)-C(9C)-N(1C)	113.7(8)	C(52")-N(7")-H(7"B)	108.1
N(2C)-C(9C)-H(9C)	123.1	C(53")-N(7")-H(7"A)	108.1
N(3C)-C(10C)-N(4C)	129.5(9)	C(53")-N(7")-H(7"B)	108.1
N(3C)-C(10C)-H(10D)	115.2	C(53")-N(7")-C(52")	116.8(7)
N(4C)-C(10C)-H(10D)	115.2	C(53B)-N(7")-H(7"C)	106.8
H(1XA)-N(1X")-H(1XB)	107.5	C(53B)-N(7")-H(7"D)	106.8
C(7X")-N(1X")-H(1XA)	108.5	C(53B)-N(7")-C(52")	122.0(8)
C(7X")-N(1X")-H(1XB)	108.5	C(60")-N(8")-H(8")	120.7
C(7X")-N(1X")-C(8X")	115.2(5)	C(60")-N(8")-C(61")	118.6(5)
C(8X")-N(1X")-H(1XA)	108.5	C(61")-N(8")-H(8")	120.7
C(8X")-N(1X")-H(1XB)	108.5	H(9"A)-N(9")-H(9"B)	107.7
C(15")-N(2X")-H(2X")	120.5	C(65")-N(9")-H(9"A)	108.8
C(15")-N(2X")-C(16")	119.0(5)	C(65")-N(9")-H(9"B)	108.8
C(16")-N(2X")-H(2X")	120.5	C(66")-N(9")-H(9"A)	108.8

C(66")-N(9")-H(9"B)	108.8	H(7XA)-C(7X")-H(7XB)	107.5
C(66")-N(9")-C(65")	114.0(5)	N(1X")-C(8X")-H(8XA)	109.4
C(73")-N(10")-H(10")	117.8	N(1X")-C(8X")-H(8XB)	109.4
C(73")-N(10")-C(74")	124.4(6)	H(8XA)-C(8X")-H(8XB)	108.0
C(74")-N(10")-H(10")	117.8	C(9X")-C(8X")-N(1X")	111.3(6)
H(11A)-N(11")-H(11B)	107.7	C(9X")-C(8X")-H(8XA)	109.4
C(78")-N(11")-H(11A)	108.8	C(9X")-C(8X")-H(8XB)	109.4
C(78")-N(11")-H(11B)	108.8	C(10X)-C(9X")-C(8X")	119.5(6)
C(79")-N(11")-H(11A)	108.8	C(10X)-C(9X")-C(14")	119.8(6)
C(79")-N(11")-H(11B)	108.8	C(14")-C(9X")-C(8X")	120.5(6)
C(79")-N(11")-C(78")	113.9(5)	C(9X")-C(10X)-H(10X)	120.4
C(86")-N(12")-H(12")	119.3	C(9X")-C(10X)-C(11")	119.2(6)
C(86")-N(12")-C(87")	121.4(5)	C(11")-C(10X)-H(10X)	120.4
C(87")-N(12")-H(12")	119.3	C(10X)-C(11")-C(15")	124.1(5)
C(2X")-C(1X")-C(6X")	120.2(6)	C(12")-C(11")-C(10X)	119.2(6)
C(2X")-C(1X")-C(7X")	120.6(6)	C(12")-C(11")-C(15")	116.6(6)
C(6X")-C(1X")-C(7X")	119.1(6)	C(11")-C(12")-H(12A)	120.6
C(1X")-C(2X")-C(3X")	121.2(6)	C(11")-C(12")-C(13")	118.8(6)
C(1X")-C(2X")-C(18")	121.6(6)	C(13")-C(12")-H(12A)	120.6
C(3X")-C(2X")-C(18")	116.9(6)	C(12")-C(13")-H(13")	118.9
C(2X")-C(3X")-C(4X")	118.0(6)	C(14")-C(13")-C(12")	122.3(6)
C(2X")-C(3X")-C(20")	123.2(6)	C(14")-C(13")-H(13")	118.9
C(4X")-C(3X")-C(20")	118.8(6)	C(9X")-C(14")-H(14")	119.7
C(3X")-C(4X")-C(31")	119.2(6)	C(13")-C(14")-C(9X")	120.6(6)
C(5X")-C(4X")-C(3X")	119.8(6)	C(13")-C(14")-H(14")	119.7
C(5X")-C(4X")-C(31")	120.6(6)	O(1X")-C(15")-N(2X")	123.0(6)
C(4X")-C(5X")-C(6X")	121.4(6)	O(1X")-C(15")-C(11")	122.0(6)
C(4X")-C(5X")-C(33")	117.5(5)	N(2X")-C(15")-C(11")	114.9(5)
C(6X")-C(5X")-C(33")	121.1(6)	N(2X")-C(16")-H(16A)	109.5
C(1X")-C(6X")-C(5X")	119.2(6)	N(2X")-C(16")-H(16B)	109.5
C(1X")-C(6X")-C(44")	120.3(5)	N(2X")-C(16")-C(17")	110.5(5)
C(5X")-C(6X")-C(44")	120.4(6)	H(16A)-C(16")-H(16B)	108.1
N(1X")-C(7X")-C(1X")	115.0(5)	C(17")-C(16")-H(16A)	109.5
N(1X")-C(7X")-H(7XA)	108.5	C(17")-C(16")-H(16B)	109.5
N(1X")-C(7X")-H(7XB)	108.5	C(62")-C(17")-C(16")	119.6(6)
C(1X")-C(7X")-H(7XA)	108.5	C(62")-C(17")-C(88")	119.3(5)
C(1X")-C(7X")-H(7XB)	108.5	C(88")-C(17")-C(16")	121.0(6)

C(2X")-C(18")-H(18A)	109.6	C(27")-C(26")-C(25")	118.2(7)
C(2X")-C(18")-H(18B)	109.6	C(27")-C(26")-H(26")	120.9
C(2X")-C(18")-C(19")	110.1(6)	C(22")-C(27")-H(27")	119.7
H(18A)-C(18")-H(18B)	108.1	C(26")-C(27")-C(22")	120.7(7)
C(19")-C(18")-H(18A)	109.6	C(26")-C(27")-H(27")	119.7
C(19")-C(18")-H(18B)	109.6	O(2X")-C(28")-C(24")	118.2(6)
C(18")-C(19")-H(19A)	109.5	N(4X")-C(28")-O(2X")	123.9(6)
C(18")-C(19")-H(19B)	109.5	N(4X")-C(28")-C(24")	117.9(6)
C(18")-C(19")-H(19C)	109.5	N(4X")-C(29")-H(29A)	109.6
H(19A)-C(19")-H(19B)	109.5	N(4X")-C(29")-H(29B)	109.6
H(19A)-C(19")-H(19C)	109.5	N(4X")-C(29")-C(30")	110.2(5)
H(19B)-C(19")-H(19C)	109.5	H(29A)-C(29")-H(29B)	108.1
N(3X")-C(20")-C(3X")	115.4(6)	C(30")-C(29")-H(29A)	109.6
N(3X")-C(20")-H(20A)	108.4	C(30")-C(29")-H(29B)	109.6
N(3X")-C(20")-H(20B)	108.4	C(62")-C(30")-C(29")	116.0(5)
C(3X")-C(20")-H(20A)	108.4	C(75")-C(30")-C(29")	121.8(5)
C(3X")-C(20")-H(20B)	108.4	C(75")-C(30")-C(62")	122.3(6)
H(20A)-C(20")-H(20B)	107.5	C(4X")-C(31")-H(31A)	108.4
N(3X")-C(21")-H(21A)	110.0	C(4X")-C(31")-H(31B)	108.4
N(3X")-C(21")-H(21B)	110.0	H(31A)-C(31")-H(31B)	107.5
H(21A)-C(21")-H(21B)	108.4	C(32")-C(31")-C(4X")	115.4(6)
C(22")-C(21")-N(3X")	108.3(6)	C(32")-C(31")-H(31A)	108.4
C(22")-C(21")-H(21A)	110.0	C(32")-C(31")-H(31B)	108.4
C(22")-C(21")-H(21B)	110.0	C(31")-C(32")-H(32A)	109.5
C(23")-C(22")-C(21")	120.3(7)	C(31")-C(32")-H(32B)	109.5
C(23")-C(22")-C(27")	119.4(7)	C(31")-C(32")-H(32C)	109.5
C(27")-C(22")-C(21")	120.1(6)	H(32A)-C(32")-H(32B)	109.5
C(22")-C(23")-H(23")	119.9	H(32A)-C(32")-H(32C)	109.5
C(22")-C(23")-C(24")	120.1(7)	H(32B)-C(32")-H(32C)	109.5
C(24")-C(23")-H(23")	119.9	N(5X")-C(33")-C(5X")	108.9(5)
C(23")-C(24")-C(28")	121.2(6)	N(5X")-C(33")-H(33A)	109.9
C(25")-C(24")-C(23")	118.8(6)	N(5X")-C(33")-H(33B)	109.9
C(25")-C(24")-C(28")	120.0(6)	C(5X")-C(33")-H(33A)	109.9
C(24")-C(25")-H(25")	118.6	C(5X")-C(33")-H(33B)	109.9
C(24")-C(25")-C(26")	122.8(7)	H(33A)-C(33")-H(33B)	108.3
C(26")-C(25")-H(25")	118.6	N(5X")-C(34")-H(34A)	109.1
C(25")-C(26")-H(26")	120.9	N(5X")-C(34")-H(34B)	109.1

N(5X")-C(34")-C(35")	112.6(5)	H(44A)-C(44")-H(44B)	108.2
H(34A)-C(34")-H(34B)	107.8	C(45")-C(44")-H(44A)	109.7
C(35")-C(34")-H(34A)	109.1	C(45")-C(44")-H(44B)	109.7
C(35")-C(34")-H(34B)	109.1	C(44")-C(45")-H(45A)	109.5
C(36")-C(35")-C(34")	119.8(6)	C(44")-C(45")-H(45B)	109.5
C(40")-C(35")-C(34")	117.4(7)	C(44")-C(45")-H(45C)	109.5
C(40")-C(35")-C(36")	122.8(7)	H(45A)-C(45")-H(45B)	109.5
C(35")-C(36")-H(36")	119.8	H(45A)-C(45")-H(45C)	109.5
C(37")-C(36")-C(35")	120.4(7)	H(45B)-C(45")-H(45C)	109.5
C(37")-C(36")-H(36")	119.8	C(47")-C(46")-C(51")	121.1(6)
C(36")-C(37")-C(38")	117.6(7)	C(47")-C(46")-C(52")	120.2(6)
C(36")-C(37")-C(41")	124.8(7)	C(51")-C(46")-C(52")	118.7(6)
C(38")-C(37")-C(41")	117.6(6)	C(46")-C(47")-C(48")	121.3(6)
C(37")-C(38")-H(38")	119.4	C(46")-C(47")-C(63")	120.1(6)
C(39")-C(38")-C(37")	121.2(8)	C(48")-C(47")-C(63")	118.3(6)
C(39")-C(38")-H(38")	119.4	C(47")-C(48")-C(49")	119.2(6)
C(38")-C(39")-H(39")	119.8	C(47")-C(48")-C(65")	121.4(6)
C(38")-C(39")-C(40")	120.4(9)	C(49")-C(48")-C(65")	119.0(6)
C(40")-C(39")-H(39")	119.8	C(48")-C(49")-C(76")	121.0(5)
C(35")-C(40")-C(39")	117.2(8)	C(50")-C(49")-C(48")	117.6(6)
C(35")-C(40")-H(40")	121.4	C(50")-C(49")-C(76")	120.9(6)
C(39")-C(40")-H(40")	121.4	C(49")-C(50")-C(78")	119.9(6)
O(3X")-C(41")-N(6X")	122.9(6)	C(51")-C(50")-C(49")	121.7(6)
O(3X")-C(41")-C(37")	118.2(6)	C(51")-C(50")-C(78")	118.2(6)
N(6X")-C(41")-C(37")	118.6(6)	C(46")-C(51")-C(89")	120.1(6)
N(6X")-C(42")-H(42A)	109.5	C(50")-C(51")-C(46")	118.8(6)
N(6X")-C(42")-H(42B)	109.5	C(50")-C(51")-C(89")	121.1(6)
N(6X")-C(42")-C(43")	110.5(5)	N(7")-C(52")-H(52A)	108.6
H(42A)-C(42")-H(42B)	108.1	N(7")-C(52")-H(52B)	108.6
C(43")-C(42")-H(42A)	109.5	C(46")-C(52")-N(7")	114.6(5)
C(43")-C(42")-H(42B)	109.5	C(46")-C(52")-H(52A)	108.6
C(75")-C(43")-C(42")	118.6(5)	C(46")-C(52")-H(52B)	108.6
C(88")-C(43")-C(42")	120.6(6)	H(52A)-C(52")-H(52B)	107.6
C(88")-C(43")-C(75")	120.7(6)	C(57")-C(56")-C(60")	117.7(6)
C(6X")-C(44")-H(44A)	109.7	C(57")-C(56")-C(55")	120.0(8)
C(6X")-C(44")-H(44B)	109.7	C(57")-C(56")-C(55B)	112.6(8)
C(6X")-C(44")-C(45")	109.8(6)	C(55")-C(56")-C(60")	120.1(8)

C(55B)-C(56")-C(60")	127.1(7)	C(48")-C(65")-H(65A)	108.7
C(56")-C(57")-H(57")	119.5	C(48")-C(65")-H(65B)	108.7
C(56")-C(57")-C(58")	120.9(6)	H(65A)-C(65")-H(65B)	107.6
C(58")-C(57")-H(57")	119.5	N(9")-C(66")-H(66A)	109.1
C(57")-C(58")-H(58")	121.2	N(9")-C(66")-H(66B)	109.1
C(57")-C(58")-H(58A)	118.1	N(9")-C(66")-C(67")	112.3(5)
C(57")-C(58")-C(59")	117.5(8)	H(66A)-C(66")-H(66B)	107.9
C(59")-C(58")-H(58")	121.2	C(67")-C(66")-H(66A)	109.1
C(59B)-C(58")-C(57")	123.7(9)	C(67")-C(66")-H(66B)	109.1
C(59B)-C(58")-H(58A)	118.1	C(68")-C(67")-C(66")	122.9(6)
O(4X")-C(60")-N(8")	118.6(6)	C(68")-C(67")-C(72")	118.0(6)
O(4X")-C(60")-C(56")	121.0(6)	C(72")-C(67")-C(66")	119.1(6)
N(8")-C(60")-C(56")	120.3(6)	C(67")-C(68")-H(68")	118.5
N(8")-C(61")-H(61A)	108.9	C(69")-C(68")-C(67")	122.9(6)
N(8")-C(61")-H(61B)	108.9	C(69")-C(68")-H(68")	118.5
N(8")-C(61")-C(62")	113.3(5)	C(68")-C(69")-C(70")	119.0(6)
H(61A)-C(61")-H(61B)	107.7	C(68")-C(69")-C(73")	124.5(6)
C(62")-C(61")-H(61A)	108.9	C(70")-C(69")-C(73")	116.4(6)
C(62")-C(61")-H(61B)	108.9	C(69")-C(70")-H(70")	120.0
C(17")-C(62")-C(30")	119.5(6)	C(71")-C(70")-C(69")	120.0(7)
C(17")-C(62")-C(61")	119.7(5)	C(71")-C(70")-H(70")	120.0
C(30")-C(62")-C(61")	120.8(6)	C(70")-C(71")-H(71")	120.1
C(47")-C(63")-H(63A)	109.4	C(70")-C(71")-C(72")	119.8(6)
C(47")-C(63")-H(63B)	109.4	C(72")-C(71")-H(71")	120.1
H(63A)-C(63")-H(63B)	108.0	C(67")-C(72")-H(72")	119.9
C(64")-C(63")-C(47")	111.1(6)	C(71")-C(72")-C(67")	120.2(6)
C(64")-C(63")-H(63A)	109.4	C(71")-C(72")-H(72")	119.9
C(64")-C(63")-H(63B)	109.4	O(5X")-C(73")-N(10")	121.5(6)
C(63")-C(64")-H(64A)	109.5	O(5X")-C(73")-C(69")	120.0(6)
C(63")-C(64")-H(64B)	109.5	N(10")-C(73")-C(69")	118.5(6)
C(63")-C(64")-H(64C)	109.5	N(10")-C(74")-H(74A)	109.9
H(64A)-C(64")-H(64B)	109.5	N(10")-C(74")-H(74B)	109.9
H(64A)-C(64")-H(64C)	109.5	N(10")-C(74")-C(75")	109.1(5)
H(64B)-C(64")-H(64C)	109.5	H(74A)-C(74")-H(74B)	108.3
N(9")-C(65")-H(65A)	108.7	C(75")-C(74")-H(74A)	109.9
N(9")-C(65")-H(65B)	108.7	C(75")-C(74")-H(74B)	109.9
C(48")-C(65")-N(9")	114.4(5)	C(30")-C(75")-C(43")	119.5(6)

C(30")-C(75")-C(74")	121.7(6)	C(84")-C(83")-H(83")	121.1
C(43")-C(75")-C(74")	118.7(5)	C(83")-C(84")-H(84")	118.7
C(49")-C(76")-H(76A)	109.2	C(85")-C(84")-C(83")	122.6(7)
C(49")-C(76")-H(76B)	109.2	C(85")-C(84")-H(84")	118.7
C(49")-C(76")-C(77")	112.1(5)	C(80")-C(85")-H(85")	120.0
H(76A)-C(76")-H(76B)	107.9	C(84")-C(85")-C(80")	120.0(7)
C(77")-C(76")-H(76A)	109.2	C(84")-C(85")-H(85")	120.0
C(77")-C(76")-H(76B)	109.2	O(6X")-C(86")-N(12")	120.9(6)
C(76")-C(77")-H(77A)	109.5	O(6X")-C(86")-C(82")	123.0(6)
C(76")-C(77")-H(77B)	109.5	N(12")-C(86")-C(82")	116.1(5)
C(76")-C(77")-H(77C)	109.5	N(12")-C(87")-H(87A)	109.9
H(77A)-C(77")-H(77B)	109.5	N(12")-C(87")-H(87B)	109.9
H(77A)-C(77")-H(77C)	109.5	H(87A)-C(87")-H(87B)	108.3
H(77B)-C(77")-H(77C)	109.5	C(88")-C(87")-N(12")	108.9(5)
N(11")-C(78")-H(78A)	109.2	C(88")-C(87")-H(87A)	109.9
N(11")-C(78")-H(78B)	109.2	C(88")-C(87")-H(87B)	109.9
C(50")-C(78")-N(11")	112.2(5)	C(17")-C(88")-C(87")	121.4(6)
C(50")-C(78")-H(78A)	109.2	C(43")-C(88")-C(17")	118.6(6)
C(50")-C(78")-H(78B)	109.2	C(43")-C(88")-C(87")	120.0(6)
H(78A)-C(78")-H(78B)	107.9	C(51")-C(89")-H(89A)	109.2
N(11")-C(79")-H(79A)	109.6	C(51")-C(89")-H(89B)	109.2
N(11")-C(79")-H(79B)	109.6	C(51")-C(89")-C(90")	111.8(5)
N(11")-C(79")-C(80")	110.3(5)	H(89A)-C(89")-H(89B)	107.9
H(79A)-C(79")-H(79B)	108.1	C(90")-C(89")-H(89A)	109.2
C(80")-C(79")-H(79A)	109.6	C(90")-C(89")-H(89B)	109.2
C(80")-C(79")-H(79B)	109.6	C(89")-C(90")-H(90A)	109.5
C(81")-C(80")-C(79")	120.2(6)	C(89")-C(90")-H(90B)	109.5
C(85")-C(80")-C(79")	119.5(6)	C(89")-C(90")-H(90C)	109.5
C(85")-C(80")-C(81")	120.3(6)	H(90A)-C(90")-H(90B)	109.5
C(80")-C(81")-H(81")	120.1	H(90A)-C(90")-H(90C)	109.5
C(80")-C(81")-C(82")	119.8(6)	H(90B)-C(90")-H(90C)	109.5
C(82")-C(81")-H(81")	120.1	N(7")-C(53")-H(53A)	110.6
C(81")-C(82")-C(86")	124.1(6)	N(7")-C(53")-H(53B)	110.6
C(83")-C(82")-C(81")	119.2(6)	N(7")-C(53")-C(54")	105.7(10)
C(83")-C(82")-C(86")	116.5(6)	H(53A)-C(53")-H(53B)	108.7
C(82")-C(83")-H(83")	121.1	C(54")-C(53")-H(53A)	110.6
C(84")-C(83")-C(82")	117.8(6)	C(54")-C(53")-H(53B)	110.6

C(55")-C(54")-C(53")	124.5(12)	O(8D)-P(3D)-O(10D)	108.3(3)
C(55")-C(54")-C(59")	117.8(13)	O(9D)-P(3D)-O(7D)	109.2(3)
C(59")-C(54")-C(53")	117.7(12)	O(9D)-P(3D)-O(8D)	118.3(3)
C(56")-C(55")-H(55")	118.5	O(9D)-P(3D)-O(10D)	110.6(3)
C(54")-C(55")-C(56")	123.0(12)	O(10D)-P(3D)-O(7D)	99.1(2)
C(54")-C(55")-H(55")	118.5	P(1D)-O(1D)-H(1D)	109.5
C(58")-C(59")-C(54")	118.9(12)	P(1D)-O(4D)-P(2D)	128.2(3)
C(58")-C(59")-H(59")	120.5	P(2D)-O(7D)-P(3D)	136.4(3)
C(54")-C(59")-H(59")	120.5	C(1D)-O(10D)-P(3D)	117.7(4)
C(53B)-C(54B)-C(59B)	117.2(12)	C(5D)-O(11D)-C(2D)	108.5(5)
C(55B)-C(54B)-C(53B)	126.8(12)	C(3D)-O(12D)-H(12I)	109.5
C(55B)-C(54B)-C(59B)	114.9(12)	C(4D)-O(13D)-H(13F)	109.5
N(7")-C(53B)-C(54B)	116.1(12)	C(6D)-N(1D)-C(5D)	125.2(6)
N(7")-C(53B)-H(53C)	108.3	C(9D)-N(1D)-C(5D)	129.4(6)
N(7")-C(53B)-H(53D)	108.3	C(9D)-N(1D)-C(6D)	105.0(6)
C(54B)-C(53B)-H(53C)	108.3	C(9D)-N(2D)-C(7D)	103.0(6)
C(54B)-C(53B)-H(53D)	108.3	C(6D)-N(3D)-C(10D)	110.3(6)
H(53C)-C(53B)-H(53D)	107.4	C(8D)-N(4D)-H(4D)	120.0
C(56")-C(55B)-H(55B)	118.3	C(10D)-N(4D)-H(4D)	120.0
C(54B)-C(55B)-C(56")	123.5(11)	C(10D)-N(4D)-C(8D)	119.9(7)
C(54B)-C(55B)-H(55B)	118.3	H(5DA)-N(5D)-H(5DB)	120.0
C(58")-C(59B)-C(54B)	119.6(12)	C(8D)-N(5D)-H(5DA)	120.0
C(58")-C(59B)-H(59B)	120.2	C(8D)-N(5D)-H(5DB)	120.0
C(54B)-C(59B)-H(59B)	120.2	O(10D)-C(1D)-H(1DA)	109.4
O(2D)-P(1D)-O(1D)	111.3(3)	O(10D)-C(1D)-H(1DB)	109.4
O(2D)-P(1D)-O(3D)	117.6(3)	O(10D)-C(1D)-C(2D)	111.4(6)
O(2D)-P(1D)-O(4D)	109.3(3)	H(1DA)-C(1D)-H(1DB)	108.0
O(3D)-P(1D)-O(1D)	107.6(3)	C(2D)-C(1D)-H(1DA)	109.4
O(3D)-P(1D)-O(4D)	106.0(3)	C(2D)-C(1D)-H(1DB)	109.4
O(4D)-P(1D)-O(1D)	104.0(3)	O(11D)-C(2D)-C(1D)	109.2(6)
O(5D)-P(2D)-O(4D)	108.1(3)	O(11D)-C(2D)-H(2D)	110.0
O(5D)-P(2D)-O(6D)	120.9(3)	O(11D)-C(2D)-C(3D)	104.8(5)
O(5D)-P(2D)-O(7D)	105.2(3)	C(1D)-C(2D)-H(2D)	110.0
O(6D)-P(2D)-O(4D)	108.6(3)	C(1D)-C(2D)-C(3D)	112.6(6)
O(6D)-P(2D)-O(7D)	112.1(3)	C(3D)-C(2D)-H(2D)	110.0
O(7D)-P(2D)-O(4D)	100.0(3)	O(12D)-C(3D)-C(2D)	115.7(5)
O(8D)-P(3D)-O(7D)	109.7(3)	O(12D)-C(3D)-H(3D)	108.0

O(12D)-C(3D)-C(4D)	115.7(6)	O(4E)-P(2E)-O(7F)	86.3(6)
C(2D)-C(3D)-H(3D)	108.0	O(5E)-P(2E)-O(4E)	107.4(3)
C(2D)-C(3D)-C(4D)	100.9(5)	O(5E)-P(2E)-O(7E)	104.3(3)
C(4D)-C(3D)-H(3D)	108.0	O(5E)-P(2E)-O(7F)	113.1(6)
O(13D)-C(4D)-C(3D)	109.3(5)	O(6E)-P(2E)-O(4E)	110.2(3)
O(13D)-C(4D)-H(4DA)	111.2	O(6E)-P(2E)-O(5E)	120.2(3)
O(13D)-C(4D)-C(5D)	112.5(6)	O(6E)-P(2E)-O(7E)	106.5(3)
C(3D)-C(4D)-H(4DA)	111.2	O(6E)-P(2E)-O(7F)	114.1(6)
C(5D)-C(4D)-C(3D)	100.9(6)	O(7E)-P(2E)-O(4E)	107.5(3)
C(5D)-C(4D)-H(4DA)	111.2	O(7E)-P(3E)-O(10E)	99.6(4)
O(11D)-C(5D)-N(1D)	108.1(6)	O(8E)-P(3E)-O(7E)	106.7(4)
O(11D)-C(5D)-C(4D)	108.0(5)	O(8E)-P(3E)-O(10E)	112.2(3)
O(11D)-C(5D)-H(5D)	108.9	O(9E)-P(3E)-O(7E)	109.7(4)
N(1D)-C(5D)-C(4D)	113.8(6)	O(9E)-P(3E)-O(8E)	120.4(4)
N(1D)-C(5D)-H(5D)	108.9	O(9E)-P(3E)-O(10E)	106.3(4)
C(4D)-C(5D)-H(5D)	108.9	O(8F)-P(3F)-O(7F)	109.7(11)
N(3D)-C(6D)-N(1D)	127.5(7)	O(9F)-P(3F)-O(7F)	115.5(10)
N(3D)-C(6D)-C(7D)	128.6(7)	O(9F)-P(3F)-O(8F)	113.9(10)
C(7D)-C(6D)-N(1D)	103.9(6)	O(9F)-P(3F)-O(10F)	107.8(10)
N(2D)-C(7D)-C(6D)	112.9(7)	O(10F)-P(3F)-O(7F)	98.2(10)
N(2D)-C(7D)-C(8D)	131.8(7)	O(10F)-P(3F)-O(8F)	110.5(11)
C(6D)-C(7D)-C(8D)	115.1(7)	P(1E)-O(1E)-H(1E)	109.5
N(4D)-C(8D)-C(7D)	117.6(7)	P(2E)-O(4E)-P(1E)	123.5(3)
N(5D)-C(8D)-N(4D)	120.0(7)	C(5E)-O(11E)-C(2E)	110.5(6)
N(5D)-C(8D)-C(7D)	122.3(7)	C(3E)-O(12E)-H(12E)	109.5
N(1D)-C(9D)-H(9D)	122.4	C(4E)-O(13E)-H(13E)	109.5
N(2D)-C(9D)-N(1D)	115.2(6)	P(2E)-O(7E)-P(3E)	137.6(5)
N(2D)-C(9D)-H(9D)	122.4	C(1F)-O(10E)-P(3E)	113.4(5)
N(3D)-C(10D)-H(10F)	115.9	P(3F)-O(7F)-P(2E)	135.2(11)
N(4D)-C(10D)-N(3D)	128.2(7)	C(1F)-O(10F)-P(3F)	126.9(14)
N(4D)-C(10D)-H(10F)	115.9	C(5E)-N(1E)-C(9E)	129.4(7)
O(1E)-P(1E)-O(4E)	101.3(3)	C(6E)-N(1E)-C(5E)	125.5(8)
O(2E)-P(1E)-O(1E)	106.6(2)	C(6E)-N(1E)-C(9E)	105.1(7)
O(2E)-P(1E)-O(3E)	121.0(3)	C(9E)-N(2E)-C(7E)	103.8(7)
O(2E)-P(1E)-O(4E)	104.9(3)	C(10E)-N(3E)-C(6E)	108.5(8)
O(3E)-P(1E)-O(1E)	111.2(3)	C(8E)-N(4E)-H(4E)	120.4
O(3E)-P(1E)-O(4E)	109.9(3)	C(10E)-N(4E)-H(4E)	120.4

C(10E)-N(4E)-C(8E)	119.2(8)	N(1E)-C(5E)-C(4E)	115.8(7)
H(5EA)-N(5E)-H(5EB)	120.0	N(1E)-C(5E)-H(5E)	108.7
C(8E)-N(5E)-H(5EA)	120.0	C(4E)-C(5E)-H(5E)	108.7
C(8E)-N(5E)-H(5EB)	120.0	N(1E)-C(6E)-N(3E)	125.8(8)
O(10E)-C(1F)-H(1FA)	108.5	N(1E)-C(6E)-C(7E)	108.5(8)
O(10E)-C(1F)-H(1FB)	108.5	N(3E)-C(6E)-C(7E)	125.7(7)
O(10E)-C(1F)-C(2E)	114.9(6)	N(2E)-C(7E)-C(6E)	109.5(7)
O(10F)-C(1F)-H(1FC)	112.9	C(8E)-C(7E)-N(2E)	132.1(9)
O(10F)-C(1F)-H(1FD)	112.9	C(8E)-C(7E)-C(6E)	118.4(9)
O(10F)-C(1F)-C(2E)	94.2(9)	N(5E)-C(8E)-N(4E)	118.6(8)
H(1FA)-C(1F)-H(1FB)	107.5	N(5E)-C(8E)-C(7E)	124.4(9)
H(1FC)-C(1F)-H(1FD)	110.3	C(7E)-C(8E)-N(4E)	117.0(9)
C(2E)-C(1F)-H(1FA)	108.5	N(1E)-C(9E)-H(9E)	123.5
C(2E)-C(1F)-H(1FB)	108.5	N(2E)-C(9E)-N(1E)	113.1(7)
C(2E)-C(1F)-H(1FC)	112.9	N(2E)-C(9E)-H(9E)	123.5
C(2E)-C(1F)-H(1FD)	112.9	N(3E)-C(10E)-H(10E)	114.5
O(11E)-C(2E)-C(1F)	108.8(6)	N(4E)-C(10E)-N(3E)	131.1(10)
O(11E)-C(2E)-H(2E)	109.4	N(4E)-C(10E)-H(10E)	114.5
O(11E)-C(2E)-C(3E)	107.2(6)	H(1SA)-O(1S)-H(1SB)	104.4
C(1F)-C(2E)-H(2E)	109.4	H(2SA)-O(2S)-H(2SB)	104.4
C(1F)-C(2E)-C(3E)	112.6(7)	H(3SA)-O(3S)-H(3SB)	104.3
C(3E)-C(2E)-H(2E)	109.4	H(4SA)-O(4S)-H(4SB)	104.5
O(12E)-C(3E)-C(2E)	112.9(7)	H(5SA)-O(5S)-H(5SB)	104.5
O(12E)-C(3E)-H(3E)	111.8	H(6SA)-O(6S)-H(6SB)	109.7(6)
O(12E)-C(3E)-C(4E)	107.8(6)	H(7SA)-O(7S)-H(7SB)	104.4
C(2E)-C(3E)-H(3E)	111.8	H(8SA)-O(8S)-H(8SB)	104.6
C(2E)-C(3E)-C(4E)	100.3(6)	H(9SA)-O(9S)-H(9SB)	110.3(6)
C(4E)-C(3E)-H(3E)	111.8	H(10G)-O(10S)-H(10H)	97.8(5)
O(13E)-C(4E)-C(3E)	110.6(6)	H(11G)-O(11S)-H(11H)	100.8(6)
O(13E)-C(4E)-H(4EA)	109.8	H(12J)-O(12S)-H(12K)	104.5
O(13E)-C(4E)-C(5E)	116.4(6)	H(13G)-O(13S)-H(13H)	104.5
C(3E)-C(4E)-H(4EA)	109.8	H(14A)-O(14S)-H(14B)	104.6
C(5E)-C(4E)-C(3E)	100.1(6)	H(15A)-O(15S)-H(15B)	104.5
C(5E)-C(4E)-H(4EA)	109.8		
O(11E)-C(5E)-C(4E)	102.9(6)		
O(11E)-C(5E)-H(5E)	108.7		
N(1E)-C(5E)-O(11E)	111.7(6)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **$[ATP_2 \subset 1\text{-}H_6]^{2+}$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1X)	33(2)	24(2)	28(2)	-1(2)	-4(2)	-11(2)
O(2X)	60(3)	41(2)	55(3)	9(2)	-33(2)	-21(2)
O(3X)	37(2)	28(2)	55(3)	-7(2)	2(2)	-10(2)
O(4X)	35(2)	39(2)	61(3)	3(2)	-9(2)	-17(2)
O(5X)	33(2)	24(2)	32(2)	-6(2)	-8(2)	-2(2)
O(6X)	35(3)	51(2)	42(2)	6(2)	-14(2)	-12(2)
N(1X)	27(2)	24(2)	22(2)	-2(2)	-4(2)	-8(2)
N(2X)	36(2)	17(2)	31(2)	1(2)	-6(2)	-7(2)
N(3X)	46(3)	25(2)	40(3)	2(2)	-16(2)	-9(2)
N(4X)	47(3)	36(3)	35(2)	3(2)	-15(2)	-21(2)
N(5X)	37(2)	21(2)	28(2)	-1(2)	1(2)	-10(2)
N(6X)	34(2)	19(2)	33(3)	0(2)	-1(2)	-10(1)
N(7)	32(2)	23(2)	28(2)	0(2)	-5(2)	-8(2)
N(8)	30(2)	32(2)	34(3)	1(2)	-10(2)	-14(1)
N(9)	24(2)	25(2)	25(2)	-1(2)	-7(2)	-10(2)
N(10)	33(2)	25(2)	20(2)	-4(2)	-6(2)	-6(2)
N(11)	32(2)	33(2)	33(2)	-1(2)	-6(2)	-11(2)
N(12)	41(3)	28(2)	36(2)	-1(2)	-17(2)	-7(2)
C(1A)	29(2)	24(2)	28(2)	-5(2)	-5(2)	-7(2)
C(1C)	29(3)	24(2)	39(3)	-4(2)	0(2)	-4(2)
C(1X)	36(2)	23(3)	19(2)	0(2)	-3(1)	-11(2)
C(2X)	43(2)	23(3)	25(2)	0(2)	-10(1)	-12(2)
C(3X)	46(2)	21(3)	23(2)	-1(2)	-8(1)	-8(2)
C(4X)	47(2)	38(3)	23(2)	-2(2)	-6(1)	-12(2)
C(5X)	43(2)	22(3)	21(2)	-2(2)	-3(1)	-14(2)
C(6X)	36(2)	24(3)	21(2)	-4(2)	-4(1)	-11(2)
C(7X)	30(3)	26(2)	21(2)	-2(2)	-4(2)	-8(2)
C(8X)	33(3)	23(2)	30(2)	-1(2)	-12(2)	-6(2)
C(9X)	26(2)	25(2)	34(2)	-6(2)	-10(2)	-6(2)
C(11)	26(2)	23(2)	24(2)	-4(2)	-10(2)	-5(2)
C(12)	33(2)	22(2)	32(2)	-4(2)	-1(2)	-5(2)

C(14)	37(3)	21(2)	39(2)	-6(2)	-2(2)	-5(2)
C(15)	36(2)	27(2)	27(3)	-3(2)	-6(2)	-11(2)
C(16)	43(3)	16(2)	29(2)	-1(2)	-6(2)	-9(2)
C(17)	37(2)	18(3)	28(2)	-1(2)	-7(1)	-9(2)
C(18)	44(2)	29(3)	30(3)	-2(2)	-10(2)	-12(2)
C(19)	51(4)	32(3)	54(4)	2(3)	-18(3)	-18(3)
C(20)	54(3)	24(2)	28(3)	-3(2)	-15(2)	-6(2)
C(21)	42(3)	29(2)	33(3)	-2(2)	-14(2)	-8(2)
C(22)	38(3)	31(2)	33(3)	-1(2)	-17(2)	-11(2)
C(23)	43(3)	29(2)	54(4)	-1(2)	-30(3)	-10(2)
C(24)	31(2)	31(2)	33(3)	-2(2)	-11(2)	-7(2)
C(25)	38(3)	33(2)	35(3)	4(2)	-16(2)	-11(2)
C(26)	50(3)	34(2)	61(4)	6(2)	-34(3)	-14(2)
C(27)	52(3)	32(2)	61(4)	4(2)	-37(3)	-16(2)
C(28)	18(2)	30(2)	22(2)	-8(2)	5(2)	-4(2)
C(29)	38(3)	30(3)	30(3)	1(2)	-10(2)	-12(2)
C(30)	36(2)	19(3)	28(2)	2(2)	-8(1)	-14(2)
C(31)	54(4)	34(3)	25(2)	-3(2)	-1(2)	-16(3)
C(32)	59(4)	35(3)	23(3)	-2(2)	0(3)	-16(3)
C(33)	44(2)	29(3)	27(3)	0(2)	-1(2)	-16(2)
C(34)	40(2)	26(3)	26(3)	-5(2)	3(2)	-11(2)
C(35)	40(2)	26(2)	33(3)	-1(2)	-1(2)	-10(2)
C(36)	37(2)	26(2)	24(3)	1(2)	-4(2)	-8(2)
C(37)	36(2)	28(2)	33(3)	-1(2)	-4(2)	-9(1)
C(38)	37(2)	35(2)	47(4)	1(2)	-6(2)	-9(2)
C(39)	38(2)	36(2)	63(5)	-2(2)	-6(2)	-10(2)
C(40)	39(2)	32(2)	30(3)	1(2)	-2(2)	-10(2)
C(41)	34(2)	28(2)	27(3)	-1(2)	-7(2)	-8(1)
C(42)	37(2)	19(2)	34(3)	-3(2)	-7(2)	-10(2)
C(43)	38(2)	23(3)	28(2)	-2(2)	-8(1)	-8(2)
C(44)	35(3)	29(3)	17(2)	-6(2)	-1(2)	-8(2)
C(45)	28(3)	30(3)	33(3)	-1(2)	-8(3)	-8(2)
C(46)	34(2)	21(3)	27(2)	2(2)	-6(1)	-8(2)
C(47)	35(2)	11(2)	28(2)	3(2)	-7(1)	-6(2)
C(48)	35(2)	19(3)	26(2)	1(2)	-6(1)	-9(2)
C(49)	36(2)	14(3)	29(2)	0(2)	-6(1)	-10(2)

C(50)	38(2)	22(3)	29(2)	2(2)	-6(1)	-12(2)
C(51)	37(2)	20(3)	27(2)	4(2)	-6(1)	-13(2)
C(52)	34(2)	21(2)	25(3)	-2(2)	-5(2)	-8(2)
C(53)	35(2)	38(3)	31(3)	3(2)	-3(2)	-12(2)
C(54)	31(2)	36(2)	27(3)	8(2)	-6(2)	-10(2)
C(55)	26(2)	37(2)	32(3)	5(2)	-6(2)	-11(2)
C(56)	28(2)	38(2)	37(3)	6(2)	-8(2)	-12(2)
C(57)	27(2)	43(2)	35(3)	11(2)	-8(2)	-12(2)
C(58)	33(2)	45(2)	44(4)	9(2)	-5(2)	-9(2)
C(59)	32(2)	43(3)	27(3)	6(2)	-4(2)	-8(2)
C(60)	30(2)	39(2)	53(4)	1(2)	-8(2)	-14(2)
C(61)	37(2)	35(2)	36(3)	-2(2)	-10(2)	-14(2)
C(62)	37(2)	19(3)	29(2)	2(2)	-9(1)	-12(2)
C(63)	32(3)	28(3)	25(2)	3(2)	-7(2)	-4(2)
C(64)	46(4)	28(3)	32(3)	6(2)	-7(3)	3(2)
C(65)	36(3)	23(2)	28(2)	0(2)	-6(2)	-12(2)
C(66)	29(3)	26(2)	30(2)	-2(2)	-9(2)	-5(2)
C(67)	27(2)	26(2)	30(2)	-3(2)	-4(2)	-7(2)
C(68)	32(3)	27(2)	32(3)	-5(2)	-2(2)	-7(2)
C(69)	31(2)	26(2)	28(2)	-4(2)	-1(2)	-6(2)
C(70)	42(3)	38(3)	38(3)	-8(2)	9(3)	-14(2)
C(71)	42(3)	39(3)	44(3)	-6(2)	9(3)	-16(2)
C(72)	42(3)	39(3)	40(3)	-5(2)	8(2)	-17(2)
C(73)	32(2)	23(2)	17(2)	-1(2)	-7(2)	-5(1)
C(74)	43(3)	30(3)	24(2)	-1(2)	-6(2)	-12(2)
C(75)	38(2)	29(3)	25(2)	2(2)	-7(1)	-12(2)
C(76)	35(2)	23(3)	23(3)	-2(2)	-6(2)	-11(2)
C(77)	45(4)	23(3)	54(4)	-7(2)	2(3)	-15(2)
C(78)	37(3)	27(2)	31(2)	-2(2)	-8(2)	-9(2)
C(79)	38(3)	38(2)	35(3)	-1(2)	-8(2)	-8(2)
C(80)	31(2)	37(2)	29(3)	-6(2)	-6(2)	-6(2)
C(81)	39(3)	37(2)	50(4)	3(2)	-28(3)	-9(2)
C(82)	27(2)	36(2)	30(3)	-4(2)	-10(2)	-2(2)
C(83)	28(3)	41(3)	38(3)	-4(2)	-14(2)	-3(2)
C(84)	35(3)	41(2)	36(3)	-7(2)	-14(3)	-5(2)
C(85)	41(3)	43(3)	43(3)	-2(2)	-17(3)	-11(2)

C(86)	24(3)	36(2)	30(2)	-7(2)	-6(2)	-3(2)
C(87)	39(3)	30(3)	31(3)	0(2)	-11(2)	-8(2)
C(88)	37(2)	16(3)	28(2)	1(2)	-9(1)	-9(2)
C(89)	36(3)	31(3)	27(2)	3(2)	-5(2)	-18(2)
C(90)	55(4)	31(3)	32(3)	-1(2)	1(3)	-17(3)
P(1)	46(1)	46(1)	30(1)	5(1)	-9(1)	-12(1)
P(2)	28(1)	23(1)	28(1)	0(1)	-8(1)	-8(1)
P(3)	28(1)	32(1)	35(1)	8(1)	-3(1)	-7(1)
O(1)	83(3)	42(2)	38(3)	2(2)	-3(2)	-26(2)
O(2)	57(2)	96(4)	53(3)	-16(3)	-12(2)	-14(2)
O(3)	56(3)	30(2)	30(2)	9(2)	-14(2)	-6(2)
O(4)	82(3)	46(2)	42(2)	8(2)	-27(2)	-33(2)
O(5)	45(2)	28(2)	43(3)	0(2)	0(2)	-10(2)
O(6)	39(2)	31(2)	31(2)	3(2)	-10(2)	-16(2)
O(7)	35(2)	48(2)	51(2)	14(2)	-5(1)	-6(1)
O(8)	40(2)	44(2)	41(2)	2(2)	-6(2)	-12(2)
O(9)	25(2)	30(2)	33(2)	9(2)	-5(1)	-8(2)
O(10)	32(2)	30(2)	47(2)	5(2)	-3(2)	-12(2)
O(11)	43(2)	33(2)	47(2)	8(2)	-7(2)	-10(2)
O(12)	82(4)	73(4)	49(2)	6(2)	-2(2)	-42(3)
O(13)	72(3)	51(3)	60(3)	14(2)	-16(2)	-18(2)
N(1)	40(3)	35(2)	47(3)	10(2)	-4(2)	-9(2)
N(2)	39(3)	36(2)	47(3)	8(2)	0(2)	-5(2)
N(3)	37(3)	37(2)	66(3)	6(2)	-6(2)	-10(2)
N(4)	40(3)	34(2)	63(3)	2(2)	2(2)	-6(2)
N(5)	71(4)	36(3)	83(4)	14(3)	-21(3)	-11(3)
C(1)	54(3)	29(3)	53(3)	3(2)	-8(2)	-13(2)
C(2)	51(3)	31(3)	47(2)	8(2)	-7(2)	-14(2)
C(3)	65(3)	36(3)	50(2)	4(2)	-6(2)	-19(2)
C(4)	65(3)	40(3)	46(2)	7(2)	-9(2)	-22(2)
C(5)	48(3)	31(2)	49(2)	9(2)	-12(2)	-12(2)
C(6)	32(3)	33(2)	51(3)	7(2)	3(2)	-7(2)
C(7)	45(3)	35(2)	59(3)	9(2)	-5(3)	-8(2)
C(8)	40(3)	32(2)	59(3)	7(2)	2(3)	-7(2)
C(9)	42(3)	39(2)	49(3)	9(2)	-5(3)	-8(2)
C(10)	50(3)	40(3)	79(4)	10(3)	-13(3)	-14(2)

P(1A)	31(1)	27(1)	31(1)	0(1)	-6(1)	-11(1)
P(2A)	24(1)	25(1)	33(1)	2(1)	-5(1)	-8(1)
P(3A)	30(1)	38(1)	38(1)	4(1)	-6(1)	-12(1)
O(1A)	29(2)	25(2)	41(2)	0(2)	-4(2)	-8(2)
O(2A)	29(2)	30(2)	33(2)	-5(2)	0(2)	-12(2)
O(3A)	28(2)	32(2)	36(2)	1(2)	-4(1)	-10(1)
O(4A)	34(2)	29(2)	32(2)	-2(1)	-5(1)	-6(2)
O(5A)	30(2)	28(2)	33(2)	2(1)	-8(2)	-8(1)
O(6A)	34(2)	28(2)	31(2)	-2(2)	-7(2)	-15(2)
O(7A)	31(2)	33(2)	57(3)	5(2)	-14(1)	-15(1)
O(8A)	44(3)	52(3)	43(2)	9(2)	-7(2)	-10(2)
O(9A)	37(3)	64(3)	47(2)	-8(2)	-13(2)	-3(2)
O(10A)	45(2)	49(2)	100(4)	12(2)	-26(2)	-17(2)
O(11A)	41(2)	58(2)	62(3)	-4(2)	1(2)	-17(2)
O(12A)	40(2)	59(3)	67(3)	5(3)	-10(2)	-13(2)
O(13A)	46(2)	52(3)	61(3)	2(2)	-3(2)	-12(2)
N(1A)	47(3)	60(2)	56(3)	-5(2)	-4(2)	-20(2)
N(2A)	75(4)	59(3)	87(5)	-3(3)	-37(4)	-20(2)
N(3A)	39(3)	65(3)	45(3)	-9(2)	3(2)	-15(2)
N(4A)	61(3)	65(3)	66(4)	-5(2)	-20(3)	-21(2)
N(5A)	96(5)	67(3)	106(6)	11(3)	-57(5)	-28(3)
C(1G)	35(2)	43(3)	68(4)	5(2)	-12(2)	-10(2)
C(2A)	37(2)	56(3)	52(3)	2(2)	-10(2)	-14(2)
C(3A)	41(2)	54(2)	56(3)	0(2)	-8(2)	-12(2)
C(4A)	41(3)	56(3)	54(2)	0(2)	-9(2)	-14(2)
C(5A)	32(3)	60(2)	56(3)	-4(2)	-3(2)	-17(2)
C(6A)	43(3)	61(2)	48(3)	-6(2)	0(3)	-19(2)
C(7A)	61(4)	62(2)	58(4)	-3(2)	-16(3)	-22(2)
C(8A)	55(4)	63(3)	58(4)	-2(2)	-13(3)	-22(2)
C(9A)	66(4)	60(3)	70(4)	-4(3)	-22(4)	-21(2)
C(10A)	48(4)	66(3)	55(4)	-6(2)	-7(3)	-19(2)
O(1X')	35(2)	26(2)	21(2)	4(1)	-8(2)	-9(2)
O(2X')	42(3)	33(2)	24(2)	2(2)	-13(2)	-12(2)
O(3X')	29(2)	33(2)	41(3)	-10(2)	7(2)	-13(2)
O(4X')	27(2)	35(2)	50(3)	-6(2)	-4(2)	-10(2)
O(5X')	32(2)	26(2)	33(2)	-6(2)	-7(2)	-6(2)

O(6X')	27(2)	31(2)	39(2)	6(2)	-12(2)	-10(2)
N(1X')	32(3)	29(2)	34(2)	-3(2)	0(2)	-5(2)
N(2X')	31(2)	18(2)	32(2)	8(2)	-4(2)	-9(2)
N(3X')	45(3)	31(2)	39(3)	-5(2)	-11(2)	-11(2)
N(4X')	35(2)	19(2)	28(2)	0(2)	-11(2)	-7(2)
N(5X')	21(2)	25(2)	27(2)	-1(2)	-1(2)	-2(2)
N(6X')	27(2)	20(2)	39(3)	-1(2)	2(2)	-8(1)
N(7')	31(2)	21(2)	27(2)	2(2)	-12(2)	-8(2)
N(8')	28(2)	28(2)	22(2)	2(2)	-4(2)	-9(1)
N(9')	27(2)	27(2)	21(2)	-2(2)	-7(2)	-11(2)
N(10')	26(2)	24(2)	25(2)	-3(2)	-7(2)	-11(2)
N(11')	43(3)	43(2)	35(3)	4(2)	-24(2)	-12(2)
N(12')	30(2)	25(2)	31(2)	1(2)	-12(2)	-7(2)
C(1X')	30(2)	26(3)	30(2)	1(2)	-3(1)	-12(2)
C(2X')	33(2)	30(3)	32(2)	-2(2)	-6(1)	-11(2)
C(3X')	34(2)	26(3)	31(2)	-2(2)	-6(1)	-12(2)
C(4X')	34(2)	36(3)	26(2)	0(2)	-9(1)	-13(2)
C(5X')	28(2)	25(3)	24(2)	1(2)	-6(1)	-10(2)
C(6X')	29(2)	29(3)	24(2)	-1(2)	-6(1)	-10(2)
C(7X')	37(3)	25(2)	31(2)	-1(2)	-1(2)	-7(2)
C(8X')	34(3)	28(2)	37(3)	-4(2)	-5(2)	-8(2)
C(9X')	30(2)	26(2)	36(2)	-1(2)	-3(2)	-8(2)
C(11')	25(2)	26(2)	28(2)	4(2)	-10(2)	-7(2)
C(12')	33(3)	29(2)	33(2)	3(2)	-5(2)	-12(2)
C(13)	30(3)	27(2)	25(2)	4(2)	-12(2)	-8(2)
C(13')	36(3)	32(2)	42(3)	-4(2)	7(2)	-15(2)
C(14')	34(3)	30(2)	40(3)	-1(2)	1(2)	-12(2)
C(15')	32(2)	27(2)	27(3)	2(2)	-6(2)	-11(2)
C(16')	33(3)	21(2)	25(2)	3(2)	-7(2)	-11(2)
C(17')	29(2)	17(2)	25(2)	2(2)	-7(1)	-11(2)
C(18')	30(2)	33(3)	38(3)	-5(2)	-6(2)	-10(2)
C(19')	51(4)	38(3)	58(5)	-2(3)	-12(4)	-20(3)
C(20')	40(3)	29(2)	36(3)	-6(2)	-11(2)	-10(2)
C(21')	38(3)	31(2)	38(3)	-3(2)	-15(2)	-10(2)
C(22')	35(2)	28(2)	43(3)	-2(2)	-18(2)	-12(2)
C(23')	40(3)	29(2)	48(4)	-3(2)	-21(3)	-12(2)

C(24')	33(2)	28(2)	30(3)	-4(2)	-8(2)	-9(2)
C(25')	32(2)	33(2)	30(3)	-2(2)	-7(2)	-10(2)
C(26')	39(3)	32(2)	45(4)	3(2)	-20(3)	-10(2)
C(27')	47(3)	30(2)	79(5)	3(2)	-40(3)	-14(2)
C(28')	28(3)	25(2)	22(2)	-4(2)	-4(2)	-7(2)
C(29')	31(2)	20(2)	26(2)	1(2)	-7(2)	-10(2)
C(30')	29(2)	19(3)	24(2)	-1(2)	-6(1)	-9(2)
C(31')	33(3)	38(3)	26(2)	2(2)	-11(2)	-11(2)
C(32')	51(4)	41(3)	25(3)	-1(2)	-2(3)	-20(3)
C(33')	29(2)	29(3)	29(3)	4(2)	-5(2)	-9(2)
C(34')	26(2)	28(2)	25(3)	-7(2)	2(2)	-7(2)
C(35')	28(2)	30(2)	34(3)	-6(2)	-2(2)	-8(2)
C(36')	28(2)	30(2)	30(3)	-6(2)	0(2)	-9(2)
C(37')	34(2)	29(2)	27(3)	-4(2)	-6(2)	-10(1)
C(38')	35(2)	37(2)	48(4)	-5(2)	-8(2)	-10(2)
C(39')	26(2)	38(2)	70(5)	-9(2)	-4(2)	-9(2)
C(40')	30(2)	35(3)	54(4)	-5(2)	-5(2)	-9(2)
C(41')	26(2)	29(2)	18(3)	-2(2)	-5(2)	-10(1)
C(42')	25(2)	21(2)	35(3)	-1(2)	-3(2)	-10(2)
C(43')	26(2)	24(3)	28(2)	2(2)	-5(1)	-10(2)
C(44')	30(3)	40(3)	26(2)	5(2)	-8(2)	-11(2)
C(45')	48(4)	40(3)	32(3)	7(2)	-6(3)	-9(2)
C(46')	30(2)	22(3)	27(2)	1(2)	-10(1)	-6(2)
C(47')	35(2)	16(3)	29(2)	1(2)	-11(1)	-8(2)
C(48')	35(2)	14(3)	25(2)	0(2)	-12(1)	-7(2)
C(49')	32(2)	14(3)	26(2)	2(2)	-13(1)	-7(2)
C(50')	33(2)	29(3)	26(2)	2(2)	-12(1)	-11(2)
C(51')	32(2)	13(2)	29(2)	3(2)	-12(1)	-9(2)
C(52')	30(2)	20(2)	23(2)	0(2)	-9(2)	-6(2)
C(53')	41(2)	34(3)	40(3)	-2(2)	-3(2)	-13(2)
C(54')	39(2)	32(2)	20(3)	3(2)	-8(2)	-11(2)
C(55')	29(2)	34(2)	30(3)	-1(2)	-6(2)	-12(2)
C(56')	29(2)	35(2)	39(3)	-5(2)	-2(2)	-11(2)
C(57')	28(2)	38(2)	27(3)	-3(2)	-4(2)	-10(2)
C(58')	35(2)	39(2)	32(3)	-6(2)	-2(2)	-9(2)
C(59')	40(2)	37(2)	18(3)	3(2)	-9(2)	-10(2)

C(60')	26(2)	35(2)	37(3)	-4(2)	-4(2)	-10(1)
C(61')	30(2)	28(2)	26(3)	0(2)	-5(2)	-7(2)
C(62')	28(2)	16(2)	24(2)	-2(1)	-5(1)	-7(2)
C(63')	35(3)	20(3)	28(2)	3(2)	-13(2)	-6(2)
C(64')	50(4)	22(3)	29(3)	3(2)	-7(3)	-2(2)
C(65')	36(3)	27(2)	26(2)	0(2)	-13(2)	-10(2)
C(66')	31(3)	30(2)	32(2)	2(2)	-8(2)	-9(2)
C(67')	25(2)	29(2)	34(2)	-1(2)	-6(2)	-10(2)
C(68')	21(2)	29(2)	27(2)	0(2)	-6(2)	-9(2)
C(69')	23(2)	28(2)	24(2)	1(2)	-5(2)	-10(2)
C(70')	27(2)	35(2)	30(2)	-2(2)	-1(2)	-13(2)
C(71')	34(3)	39(2)	30(3)	-6(2)	3(2)	-19(2)
C(72')	30(3)	38(3)	34(2)	-5(2)	-2(2)	-15(2)
C(73')	26(2)	26(2)	21(2)	-1(2)	-9(2)	-9(1)
C(74')	25(2)	21(2)	26(2)	-2(2)	-5(2)	-8(2)
C(75')	28(2)	27(3)	27(2)	-1(2)	-5(1)	-7(2)
C(76')	35(2)	19(3)	29(3)	0(2)	-12(2)	-8(2)
C(77')	42(4)	25(3)	43(4)	-2(2)	-7(3)	-14(2)
C(78')	35(3)	32(2)	32(2)	5(2)	-17(2)	-16(2)
C(79')	43(3)	35(2)	36(3)	-2(2)	-12(2)	-8(2)
C(80')	39(3)	37(2)	32(3)	-1(2)	-7(2)	-7(2)
C(81')	38(3)	33(2)	38(3)	0(2)	-15(3)	-3(2)
C(82')	30(2)	31(2)	33(3)	1(2)	-13(2)	-7(2)
C(83')	34(2)	29(2)	32(3)	3(2)	-15(2)	-6(2)
C(84')	32(3)	34(2)	35(3)	-2(2)	-8(2)	-10(2)
C(85')	45(3)	35(2)	43(4)	1(2)	-16(3)	-8(2)
C(86')	32(3)	29(2)	29(2)	1(2)	-11(2)	-8(2)
C(87')	27(2)	21(2)	28(2)	-2(2)	-7(2)	-4(2)
C(88')	27(2)	24(3)	29(2)	2(2)	-7(1)	-7(2)
C(89')	40(3)	21(3)	30(2)	4(2)	-12(2)	-7(2)
C(90')	68(5)	25(3)	32(3)	1(2)	-9(3)	-18(3)
P(1B)	32(1)	21(1)	29(1)	4(1)	-6(1)	-10(1)
P(2B)	27(1)	26(1)	28(1)	-1(1)	-5(1)	-9(1)
P(3B)	28(1)	30(1)	29(1)	3(1)	-6(1)	-10(1)
O(1B)	39(2)	25(2)	34(2)	3(2)	-5(2)	-14(2)
O(2B)	34(2)	33(2)	37(2)	0(2)	-6(2)	-9(2)

O(3B)	46(2)	20(2)	27(2)	5(1)	-7(2)	-5(2)
O(4B)	34(2)	26(2)	28(1)	1(1)	-6(1)	-7(2)
O(5B)	27(2)	28(2)	33(2)	-2(1)	-9(2)	-10(1)
O(6B)	30(2)	29(2)	32(2)	0(2)	-7(2)	-13(2)
O(7B)	29(1)	31(2)	36(2)	8(2)	-8(1)	-10(1)
O(8B)	46(3)	43(2)	32(2)	-4(2)	-5(2)	-9(2)
O(9B)	34(2)	26(2)	32(2)	4(2)	-6(2)	-6(2)
O(10B)	30(2)	30(2)	44(2)	5(2)	-7(2)	-8(2)
O(11B)	36(2)	47(2)	47(2)	4(2)	-3(2)	-24(2)
O(12B)	51(3)	44(3)	49(2)	4(2)	-10(2)	-22(2)
O(13B)	60(3)	69(3)	79(4)	38(3)	-24(2)	-31(2)
N(1B)	31(2)	43(2)	51(3)	13(2)	-12(2)	-18(2)
N(2B)	29(2)	40(2)	39(3)	9(2)	-8(2)	-11(2)
N(3B)	35(3)	41(2)	46(3)	11(2)	-13(2)	-17(2)
N(4B)	37(3)	42(2)	52(3)	13(2)	-15(2)	-15(2)
N(5B)	35(3)	49(3)	62(4)	22(2)	-19(3)	-20(2)
C(1B)	31(2)	37(3)	54(3)	-7(2)	-2(2)	-12(2)
C(2B)	36(2)	40(3)	47(2)	5(2)	-5(2)	-19(2)
C(3B)	49(3)	42(3)	50(2)	5(2)	-10(2)	-23(2)
C(4B)	54(3)	49(3)	54(2)	12(2)	-17(2)	-28(2)
C(5B)	38(3)	41(2)	56(2)	14(2)	-17(2)	-18(2)
C(6B)	31(3)	44(2)	40(3)	10(2)	-8(2)	-16(2)
C(7B)	36(3)	46(2)	44(3)	13(2)	-11(2)	-18(2)
C(8B)	32(3)	45(2)	39(3)	13(2)	-7(2)	-16(2)
C(9B)	31(3)	43(2)	48(3)	12(2)	-11(2)	-14(2)
C(10B)	38(3)	41(2)	45(3)	11(2)	-13(3)	-15(2)
P(1C)	30(1)	25(1)	24(1)	0(1)	-7(1)	-9(1)
P(2C)	28(1)	24(1)	26(1)	0(1)	-7(1)	-9(1)
P(3C)	27(1)	29(1)	30(1)	2(1)	-7(1)	-11(1)
O(1C)	32(2)	27(2)	26(2)	2(2)	-10(2)	-9(2)
O(2C)	32(2)	31(2)	29(2)	-4(2)	-5(2)	-10(2)
O(3C)	29(2)	22(2)	40(2)	4(2)	-9(1)	-8(1)
O(4C)	29(2)	22(2)	24(1)	-3(1)	-6(1)	-3(1)
O(5C)	30(2)	24(2)	33(2)	0(1)	-4(2)	-10(1)
O(6C)	30(2)	28(2)	27(2)	-1(2)	-6(2)	-11(2)
O(7C)	29(1)	24(2)	35(2)	1(1)	-12(1)	-12(1)

O(8C)	30(2)	29(2)	33(2)	4(2)	-9(2)	-10(2)
O(9C)	28(2)	29(2)	37(2)	-2(2)	-12(2)	-8(2)
O(10C)	32(2)	36(2)	34(2)	-1(2)	-8(2)	-15(2)
O(11C)	45(2)	59(2)	42(2)	-1(2)	-5(2)	-20(2)
O(12C)	37(2)	60(3)	73(3)	-19(2)	-9(2)	-17(2)
O(13C)	79(3)	53(3)	87(4)	-4(3)	-38(3)	-17(3)
N(1C)	43(3)	57(2)	46(3)	4(2)	-11(2)	-17(2)
N(2C)	57(3)	65(3)	53(3)	8(2)	-16(3)	-14(2)
N(3C)	41(3)	53(3)	42(3)	2(2)	-4(2)	-16(2)
N(4C)	66(4)	55(3)	62(4)	7(2)	-7(3)	-20(3)
N(5C)	100(5)	73(3)	75(5)	17(3)	-16(4)	-11(3)
C(1E)	41(2)	64(4)	37(3)	10(2)	-11(2)	-25(3)
C(2C)	37(2)	51(3)	44(3)	3(2)	-15(2)	-14(2)
C(3C)	47(2)	60(3)	54(3)	-7(2)	-5(2)	-21(2)
C(4C)	42(2)	53(3)	61(3)	-4(2)	-9(2)	-17(2)
C(5C)	45(2)	55(2)	47(3)	2(2)	-11(2)	-18(2)
C(6C)	40(3)	56(2)	33(3)	3(2)	0(2)	-16(2)
C(7C)	59(4)	63(2)	48(4)	9(2)	-13(3)	-15(2)
C(8C)	56(4)	63(3)	50(4)	3(2)	2(3)	-14(2)
C(9C)	51(3)	65(3)	49(3)	5(2)	-14(3)	-15(2)
C(10C)	69(4)	54(3)	63(4)	4(2)	-16(4)	-25(3)
O(1X")	37(2)	26(2)	25(2)	0(2)	-4(2)	-9(2)
O(2X")	45(3)	37(2)	30(2)	9(2)	-19(2)	-20(2)
O(3X")	35(2)	35(2)	48(3)	-5(2)	-5(2)	-11(2)
O(4X")	34(2)	34(2)	41(3)	-1(2)	-11(2)	-10(2)
O(5X")	31(2)	31(2)	34(2)	-6(2)	-10(2)	-7(2)
O(6X")	41(3)	32(2)	37(2)	7(2)	-14(2)	-12(2)
N(1X")	35(3)	34(2)	26(2)	-6(2)	4(2)	-13(2)
N(2X")	31(2)	23(2)	28(2)	0(2)	-3(2)	-11(2)
N(3X")	58(3)	38(2)	45(3)	-3(2)	-22(2)	-10(2)
N(4X")	32(2)	23(2)	27(2)	2(2)	-11(2)	-5(2)
N(5X")	31(2)	29(2)	21(2)	4(2)	-3(2)	-8(2)
N(6X")	34(2)	24(2)	24(2)	2(2)	-9(2)	-10(1)
N(7")	33(2)	34(3)	49(3)	6(2)	-14(2)	-12(2)
N(8")	29(2)	27(2)	26(3)	-1(2)	-6(2)	-8(1)
N(9")	29(2)	29(2)	24(2)	4(2)	-7(2)	-11(2)

N(10")	31(2)	28(2)	24(2)	-1(2)	-10(2)	-9(2)
N(11")	39(3)	30(2)	36(2)	2(2)	-13(2)	-8(2)
N(12")	41(3)	22(2)	33(2)	4(2)	-15(2)	-10(2)
C(1X")	33(2)	32(3)	24(2)	-1(2)	-5(1)	-11(2)
C(2X")	36(2)	34(3)	30(2)	-3(2)	-8(1)	-10(2)
C(3X")	30(2)	25(3)	30(2)	-3(2)	-8(1)	-11(2)
C(4X")	31(2)	29(3)	24(2)	1(2)	-7(1)	-11(2)
C(5X")	33(2)	27(3)	25(2)	2(2)	-8(1)	-10(2)
C(6X")	34(2)	35(3)	24(2)	4(2)	-8(1)	-10(2)
C(7X")	37(3)	33(2)	22(2)	-4(2)	-3(2)	-10(2)
C(8X")	40(3)	34(2)	42(3)	-7(2)	-7(2)	-14(2)
C(9X")	30(2)	33(2)	40(3)	-8(2)	-5(2)	-13(2)
C(10X)	23(2)	27(2)	27(2)	-4(2)	-10(2)	-6(2)
C(11")	26(2)	26(2)	31(2)	-3(2)	-7(2)	-8(2)
C(12")	31(2)	29(2)	36(3)	-8(2)	-4(2)	-10(2)
C(13")	35(3)	31(2)	47(3)	-11(2)	1(2)	-12(2)
C(14")	37(3)	28(2)	45(3)	-9(2)	4(2)	-17(2)
C(15")	31(2)	27(2)	23(2)	-1(2)	-7(2)	-10(2)
C(16")	39(3)	30(3)	27(2)	2(2)	-9(2)	-18(2)
C(17")	33(2)	22(3)	26(2)	4(2)	-7(1)	-12(2)
C(18")	35(2)	45(3)	29(3)	-8(2)	-6(2)	-13(2)
C(19")	44(4)	48(4)	89(7)	-10(3)	-7(4)	-20(3)
C(20")	44(3)	35(2)	40(3)	-2(2)	-19(2)	-13(2)
C(21")	47(3)	34(2)	46(3)	-4(2)	-21(2)	-12(2)
C(22")	51(3)	35(2)	58(4)	2(2)	-28(3)	-14(2)
C(23")	38(3)	31(2)	31(3)	-3(2)	-12(2)	-7(2)
C(24")	32(2)	30(2)	29(3)	-1(2)	-8(2)	-8(2)
C(25")	30(2)	34(2)	27(3)	3(2)	-7(2)	-12(2)
C(26")	32(3)	35(2)	40(3)	0(2)	-9(2)	-13(2)
C(27")	44(3)	36(2)	42(3)	1(2)	-18(3)	-16(2)
C(28")	27(3)	26(2)	22(2)	-1(2)	-4(2)	-5(2)
C(29")	37(2)	27(2)	30(3)	4(2)	-13(2)	-12(2)
C(30")	32(2)	24(3)	24(2)	2(2)	-8(1)	-11(2)
C(31")	41(3)	40(3)	22(2)	2(2)	-6(2)	-13(2)
C(32")	53(4)	41(3)	24(3)	-1(2)	-1(3)	-10(3)
C(33")	36(2)	31(3)	26(3)	7(2)	-7(2)	-12(2)

C(34")	37(2)	29(3)	28(3)	-2(2)	5(2)	-10(2)
C(35")	38(2)	33(2)	26(3)	-2(2)	3(2)	-12(2)
C(36")	34(2)	32(2)	21(3)	-2(2)	0(2)	-11(2)
C(37")	39(2)	32(2)	48(4)	-2(2)	-14(2)	-11(2)
C(38")	45(3)	35(3)	127(8)	0(3)	-35(3)	-11(2)
C(39")	55(3)	38(3)	172(11)	-5(3)	-42(4)	-11(2)
C(40")	41(2)	38(3)	93(6)	-3(3)	-11(3)	-11(2)
C(41")	35(2)	32(2)	24(3)	-1(2)	-8(2)	-10(1)
C(42")	30(2)	23(2)	27(3)	4(2)	-6(2)	-13(2)
C(43")	31(2)	23(3)	25(2)	4(2)	-8(1)	-12(2)
C(44")	25(2)	35(3)	20(2)	-1(2)	-1(2)	-6(2)
C(45")	45(4)	38(3)	33(3)	3(2)	-15(3)	-9(2)
C(46")	36(2)	26(3)	32(2)	3(2)	-11(1)	-10(2)
C(47")	38(2)	22(3)	30(2)	4(2)	-11(1)	-9(2)
C(48")	38(2)	19(3)	29(2)	2(2)	-10(1)	-10(2)
C(49")	36(2)	14(3)	28(2)	3(2)	-10(1)	-9(2)
C(50")	37(2)	26(3)	29(2)	4(2)	-11(1)	-10(2)
C(51")	38(2)	22(3)	30(2)	6(2)	-11(1)	-12(2)
C(52")	35(2)	31(3)	37(3)	1(2)	-13(2)	-10(2)
C(56")	26(2)	32(2)	42(3)	-2(2)	-4(2)	-8(1)
C(57")	26(2)	37(2)	25(3)	4(2)	-8(2)	-6(2)
C(58")	27(2)	38(2)	43(3)	1(2)	-10(2)	-5(2)
C(60")	28(2)	33(2)	44(4)	-5(2)	-6(2)	-7(1)
C(61")	32(2)	29(2)	31(3)	-1(2)	-5(2)	-6(2)
C(62")	31(2)	21(3)	25(2)	1(2)	-7(1)	-9(2)
C(63")	46(3)	24(3)	35(3)	1(2)	-18(2)	-9(2)
C(64")	64(4)	23(3)	28(3)	0(2)	-10(3)	-4(2)
C(65")	33(3)	31(2)	31(2)	2(2)	-9(2)	-11(2)
C(66")	32(3)	30(2)	29(2)	4(2)	-10(2)	-8(2)
C(67")	30(2)	30(2)	30(2)	3(2)	-7(2)	-9(2)
C(68")	30(3)	30(2)	25(2)	3(2)	-9(2)	-8(2)
C(69")	26(2)	30(2)	25(2)	3(2)	-12(2)	-7(2)
C(70")	39(3)	37(3)	34(2)	-2(2)	-1(2)	-17(2)
C(71")	44(3)	41(3)	35(3)	-5(2)	5(3)	-21(2)
C(72")	47(3)	41(3)	40(3)	-5(2)	5(2)	-23(2)
C(73")	32(2)	30(2)	22(2)	1(2)	-11(2)	-9(2)

C(74")	38(3)	27(3)	21(2)	1(2)	-9(2)	-12(2)
C(75")	33(2)	31(3)	22(2)	2(2)	-8(1)	-10(2)
C(76")	36(2)	22(3)	32(3)	-1(2)	-9(2)	-10(2)
C(77")	47(4)	24(3)	52(4)	-7(3)	-1(3)	-17(3)
C(78")	33(3)	29(2)	28(2)	2(2)	-8(2)	-8(2)
C(79")	43(3)	33(2)	34(3)	-1(2)	-13(2)	-8(2)
C(80")	38(3)	32(2)	28(3)	-2(2)	-5(2)	-6(2)
C(81")	35(3)	31(2)	48(3)	3(2)	-17(3)	-5(2)
C(82")	33(3)	26(2)	36(3)	-2(2)	-13(2)	-5(2)
C(83")	35(3)	30(2)	39(3)	1(2)	-17(3)	-7(2)
C(84")	29(3)	30(2)	30(3)	-2(2)	-6(2)	-6(2)
C(85")	49(3)	35(2)	46(3)	7(2)	-21(3)	-13(2)
C(86")	31(3)	26(2)	29(2)	-1(2)	-9(2)	-5(2)
C(87")	36(2)	23(2)	28(2)	1(2)	-10(2)	-8(2)
C(88")	33(2)	27(3)	25(2)	4(2)	-8(1)	-10(2)
C(89")	45(3)	31(3)	30(2)	6(2)	-10(2)	-15(2)
C(90")	47(4)	33(3)	40(3)	1(2)	-14(3)	-13(3)
C(53")	32(2)	33(3)	46(3)	3(2)	-12(2)	-10(2)
C(54")	28(2)	31(2)	40(3)	-2(2)	-8(2)	-7(2)
C(55")	25(2)	32(2)	42(4)	-1(2)	-4(2)	-8(2)
C(59")	28(2)	37(2)	36(4)	1(2)	-9(2)	-6(2)
C(54B)	28(2)	31(2)	40(3)	-2(2)	-8(2)	-7(2)
C(53B)	32(2)	33(3)	46(3)	3(2)	-12(2)	-10(2)
C(55B)	25(2)	32(2)	42(4)	-1(2)	-4(2)	-8(2)
C(59B)	28(2)	37(2)	36(4)	1(2)	-9(2)	-6(2)
P(1D)	34(1)	27(1)	31(1)	2(1)	-11(1)	-10(1)
P(2D)	28(1)	28(1)	31(1)	0(1)	-8(1)	-10(1)
P(3D)	30(1)	36(1)	26(1)	4(1)	-5(1)	-11(1)
O(1D)	42(2)	26(2)	33(2)	1(2)	-12(2)	-14(2)
O(2D)	35(2)	37(2)	33(2)	1(2)	-9(2)	-10(2)
O(3D)	46(2)	28(2)	29(2)	0(2)	-7(2)	-12(2)
O(4D)	43(2)	27(2)	33(2)	2(1)	-14(1)	-9(2)
O(5D)	31(2)	28(2)	42(2)	0(1)	-7(2)	-9(1)
O(6D)	33(2)	28(2)	31(2)	1(2)	-8(2)	-12(2)
O(7D)	32(1)	38(2)	34(2)	6(2)	-9(1)	-12(1)
O(8D)	43(2)	42(2)	31(2)	1(2)	-8(2)	-16(2)

O(9D)	23(2)	40(2)	27(2)	4(2)	-4(1)	-10(2)
O(10D)	32(2)	35(2)	32(2)	-1(2)	-3(2)	-12(2)
O(11D)	43(2)	43(2)	33(2)	-6(2)	1(2)	-22(2)
O(12D)	54(3)	30(2)	27(2)	1(2)	-4(2)	-16(2)
O(13D)	45(2)	39(2)	34(2)	2(2)	-9(2)	-16(2)
N(1D)	36(2)	43(2)	30(2)	1(2)	-4(2)	-18(2)
N(2D)	40(3)	48(2)	37(2)	6(2)	-8(2)	-19(2)
N(3D)	40(3)	44(2)	35(2)	0(2)	-7(2)	-18(2)
N(4D)	37(3)	47(3)	46(3)	9(2)	-13(2)	-20(2)
N(5D)	49(3)	50(3)	47(3)	6(2)	-19(3)	-19(2)
C(1D)	40(2)	37(3)	40(3)	-2(2)	-6(2)	-14(2)
C(2D)	37(2)	33(3)	32(2)	-2(2)	-2(2)	-12(2)
C(3D)	43(2)	29(3)	28(2)	1(2)	-5(2)	-11(2)
C(4D)	43(2)	36(3)	30(2)	-1(2)	-5(2)	-13(2)
C(5D)	44(3)	42(2)	31(2)	0(2)	-7(2)	-21(2)
C(6D)	29(3)	41(2)	30(2)	-4(2)	1(2)	-13(2)
C(7D)	40(3)	50(2)	40(3)	4(2)	-9(2)	-19(2)
C(8D)	39(3)	49(2)	48(3)	6(2)	-13(3)	-17(2)
C(9D)	41(3)	46(2)	30(3)	3(2)	-7(2)	-19(2)
C(10D)	43(3)	42(2)	44(3)	3(2)	-13(3)	-15(2)
P(1E)	35(1)	24(1)	35(1)	1(1)	-5(1)	-10(1)
P(2E)	29(1)	29(1)	39(1)	10(1)	-12(1)	-12(1)
P(3E)	26(1)	28(1)	26(1)	3(1)	-8(1)	-10(1)
P(3F)	26(1)	28(1)	26(1)	3(1)	-8(1)	-10(1)
O(1E)	34(2)	25(2)	34(2)	3(2)	-3(2)	-9(2)
O(2E)	30(2)	31(2)	38(2)	1(2)	-3(2)	-12(2)
O(3E)	35(2)	28(2)	38(2)	0(2)	-4(2)	-12(2)
O(4E)	36(2)	28(2)	36(2)	4(1)	-9(1)	-6(2)
O(5E)	34(2)	30(2)	37(2)	5(1)	-7(2)	-11(1)
O(6E)	38(2)	39(2)	37(2)	9(2)	-13(2)	-18(2)
O(11E)	41(2)	56(2)	45(2)	-7(2)	1(2)	-20(2)
O(12E)	46(2)	59(3)	65(3)	2(2)	-13(2)	-12(2)
O(13E)	47(2)	53(3)	54(3)	-12(2)	2(2)	-16(2)
O(7E)	30(1)	28(2)	34(3)	4(2)	-10(1)	-10(1)
O(8E)	24(2)	30(2)	28(2)	2(1)	-8(1)	-9(2)
O(9E)	39(3)	31(2)	29(2)	4(2)	-13(2)	-14(2)

O(10E)	32(2)	37(2)	30(2)	1(2)	-7(1)	-13(2)
O(7F)	30(1)	28(2)	34(3)	4(2)	-10(1)	-10(1)
O(8F)	39(3)	31(2)	29(2)	4(2)	-13(2)	-14(2)
O(9F)	24(2)	30(2)	28(2)	2(1)	-8(1)	-9(2)
O(10F)	32(2)	37(2)	30(2)	1(2)	-7(1)	-13(2)
N(1E)	35(3)	57(2)	50(3)	-7(2)	0(2)	-19(2)
N(2E)	64(4)	57(3)	65(3)	-4(2)	-13(3)	-23(2)
N(3E)	45(3)	63(3)	63(3)	-10(2)	-11(3)	-21(2)
N(4E)	59(3)	67(3)	62(3)	-18(2)	2(3)	-24(3)
N(5E)	71(4)	66(3)	54(4)	-15(2)	6(3)	-30(3)
C(1F)	44(2)	40(2)	46(3)	3(2)	-10(2)	-17(2)
C(2E)	43(2)	51(2)	45(3)	-1(2)	-8(2)	-17(2)
C(3E)	43(2)	53(2)	47(3)	-2(2)	-9(2)	-12(2)
C(4E)	43(3)	51(2)	44(2)	-6(2)	-4(2)	-13(2)
C(5E)	42(3)	57(2)	49(3)	-8(2)	1(2)	-19(2)
C(6E)	32(3)	60(2)	49(3)	-9(2)	5(2)	-20(2)
C(7E)	39(3)	60(2)	45(3)	-11(2)	9(2)	-19(2)
C(8E)	44(3)	66(3)	52(3)	-16(2)	15(2)	-26(2)
C(9E)	38(3)	54(3)	49(3)	-11(2)	2(3)	-14(2)
C(10E)	58(4)	69(3)	76(4)	-13(3)	-10(4)	-30(3)
O(1S)	58(4)	35(3)	56(4)	3(3)	-1(3)	-15(3)
O(2S)	68(4)	56(4)	48(3)	13(3)	-16(3)	-1(3)
O(3S)	95(5)	44(3)	50(3)	3(3)	-27(3)	-20(3)
O(4S)	43(3)	88(5)	69(4)	-10(3)	-8(3)	-35(3)
O(5S)	68(4)	65(4)	50(3)	4(3)	-13(3)	7(3)
O(6S)	46(3)	31(3)	51(3)	5(2)	-10(2)	-13(2)
O(7S)	119(6)	45(4)	62(4)	3(3)	-36(4)	-25(4)
O(8S)	62(3)	27(3)	35(3)	8(2)	-3(3)	-15(2)
O(9S)	51(3)	39(3)	31(3)	-1(2)	-6(2)	2(2)
O(10S)	37(3)	48(3)	32(3)	-11(2)	-1(2)	-9(2)
O(11S)	74(4)	49(4)	80(4)	2(3)	-22(3)	-16(3)
O(12S)	116(7)	81(6)	53(4)	12(4)	-7(4)	2(4)
O(13S)	51(3)	29(3)	31(2)	-4(2)	-23(2)	5(2)
O(14S)	58(3)	31(3)	44(3)	3(2)	-5(3)	-24(2)
O(15S)	46(3)	61(4)	40(3)	1(3)	-8(2)	-25(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **$[ATP_2⊂1\text{-}H_6]^{2+}$**.

	x	y	z	U(eq)
H(1XC)	-2327	-5120	-3936	29
H(1XD)	-2977	-5232	-3578	29
H(2X)	-2236	-2961	-4018	34
H(3XC)	-3860	-4960	-6099	43
H(3XD)	-3695	-4794	-5641	43
H(4X)	-2963	-2619	-5748	44
H(5XC)	-502	-5221	-5675	35
H(5XD)	-2	-5481	-5335	35
H(6X)	-164	-3462	-5580	35
H(7A)	-3576	1180	-5069	33
H(7B)	-3085	962	-4718	33
H(8)	-3268	-834	-4723	37
H(9A)	-559	1017	-6849	29
H(9B)	-1212	888	-6499	29
H(10)	-1182	-1289	-6382	31
H(11C)	-212	789	-4016	39
H(11D)	-889	692	-4148	39
H(12)	-396	-1607	-4744	41
H(1C)	-4848	-3542	-2802	38
H(7XC)	-3164	-5904	-4067	31
H(7XD)	-2325	-6108	-3977	31
H(8XC)	-3731	-4776	-4156	34
H(8XD)	-3013	-4535	-4419	34
H(11)	-2847	-3622	-4170	29
H(12B)	-4311	-2707	-2970	36
H(14)	-4337	-4441	-3283	40
H(16C)	-1810	-2044	-3995	35
H(16D)	-2631	-1677	-4066	35
H(18C)	-3957	-5485	-5094	40
H(18D)	-3883	-5455	-4535	40

H(19D)	-3717	-6556	-5067	65
H(19E)	-4329	-6320	-4574	65
H(19F)	-3461	-6587	-4554	65
H(20C)	-2755	-5767	-6216	42
H(20D)	-3419	-5864	-5776	42
H(21C)	-2734	-4786	-6536	40
H(21D)	-2645	-4535	-6033	40
H(23)	-2871	-3452	-6050	46
H(25)	-4512	-2396	-6674	41
H(26)	-4968	-3220	-6768	53
H(27)	-4263	-4213	-6605	52
H(29C)	-3234	-1423	-5653	38
H(29D)	-2583	-1571	-6141	38
H(31C)	-1735	-5562	-6435	45
H(31D)	-921	-5719	-6306	45
H(32D)	-959	-6446	-6837	59
H(32E)	-1670	-6602	-6468	59
H(32F)	-867	-6769	-6319	59
H(33C)	-178	-6408	-5329	40
H(33D)	-294	-6331	-5884	40
H(34C)	367	-5547	-6351	38
H(34D)	853	-6051	-6043	38
H(36)	173	-4393	-5917	36
H(38)	2252	-4136	-5984	48
H(39)	2783	-5186	-6104	55
H(40)	2009	-5829	-6143	42
H(42C)	0	-2365	-5973	36
H(42D)	198	-2411	-5440	36
H(44C)	-1301	-5849	-4192	33
H(44D)	-577	-5974	-4637	33
H(45D)	-568	-7010	-4664	45
H(45E)	-1359	-6902	-4279	45
H(45F)	-621	-6856	-4103	45
H(52C)	-3407	2132	-5130	32
H(52D)	-3315	2113	-4572	32
H(53E)	-3982	1370	-4059	42

H(53F)	-4491	1770	-4412	42
H(55)	-3683	136	-4588	38
H(57)	-5720	-258	-4240	41
H(58)	-6287	756	-4013	50
H(59)	-5595	1473	-4095	42
H(61C)	-3568	-1858	-5007	41
H(61D)	-3405	-1952	-4465	41
H(63C)	-2996	1710	-5784	35
H(63D)	-2275	1610	-6230	35
H(64D)	-3052	2617	-6282	57
H(64E)	-2271	2671	-6173	57
H(64F)	-3005	2768	-5738	57
H(65C)	-1229	1916	-6430	34
H(65D)	-405	1702	-6313	34
H(66C)	197	591	-6246	34
H(66D)	-509	329	-5983	34
H(68)	-639	-627	-6284	37
H(70)	894	-1506	-7422	49
H(71)	1339	-648	-7616	52
H(72)	836	251	-7156	50
H(74C)	-785	-2578	-6363	38
H(74D)	-1608	-2203	-6426	38
H(76C)	263	1301	-5871	32
H(76D)	360	1279	-5313	32
H(77D)	-251	2434	-5746	62
H(77E)	642	2182	-5805	62
H(77F)	112	2337	-5271	62
H(78C)	-868	1753	-4225	38
H(78D)	-126	1550	-4649	38
H(79C)	450	486	-4832	44
H(79D)	-270	242	-4858	44
H(81)	-383	-711	-4530	47
H(83)	1168	-1753	-3784	43
H(84)	1567	-871	-3713	45
H(85)	1130	47	-4119	49
H(87C)	-838	-2589	-4251	40

H(87D)	-177	-2805	-4727	40
H(89C)	-1878	1382	-3977	36
H(89D)	-2692	1492	-4105	36
H(90D)	-2744	2603	-4171	60
H(90E)	-1997	2455	-3954	60
H(90F)	-2763	2343	-3623	60
H(1)	-1349	-3485	-5026	81
H(12D)	1449	-3798	-3091	99
H(13A)	2819	-3760	-3395	91
H(4)	2847	-1028	-4768	58
H(5A)	1920	-660	-5257	76
H(5B)	1506	-1104	-5393	76
H(1A)	465	-4169	-3955	55
H(1B)	671	-3756	-4428	55
H(2)	1794	-4526	-3945	52
H(3)	1213	-3228	-3890	60
H(4A)	2282	-3093	-3773	59
H(5)	3105	-3764	-4523	51
H(9)	1559	-3192	-5084	54
H(10A)	3481	-1738	-4367	68
H(1AA)	-2110	-782	-5344	48
H(12F)	-6779	727	-5602	83
H(13B)	-7045	-175	-5043	82
H(4AA)	-6458	-3380	-6017	74
H(5AA)	-5651	-3995	-5555	100
H(5AB)	-5215	-3700	-5280	100
H(1GA)	-4498	-227	-5578	58
H(1GB)	-4122	-473	-6130	58
H(2A)	-5418	38	-6308	57
H(3A)	-5764	380	-5369	60
H(4AB)	-5603	-651	-5115	60
H(5AC)	-6380	-845	-5866	59
H(9AA)	-4998	-1662	-5144	76
H(10B)	-6987	-2511	-6323	67
H(1XE)	-2329	-1715	-601	40
H(1XF)	-2954	-1871	-245	40

H(2X')	-2313	410	-693	33
H(3XE)	-3780	-1650	-2752	45
H(3XF)	-3618	-1479	-2293	45
H(4X')	-3018	784	-2409	32
H(5XE)	101	-2110	-2001	30
H(5XF)	-394	-1871	-2347	30
H(6X')	-167	-110	-2291	36
H(7'A)	-3521	4600	-1734	30
H(7'B)	-2999	4333	-1410	30
H(8')	-3245	2541	-1405	31
H(9'A)	-1167	4242	-3194	29
H(9'B)	-508	4358	-3545	29
H(10')	-1175	2062	-3056	29
H(11E)	138	3874	-1469	45
H(11F)	387	4011	-1034	45
H(12')	-506	1715	-1335	34
H(7XE)	-2244	-2724	-655	39
H(7XF)	-3077	-2561	-752	39
H(8XE)	-3740	-1453	-798	40
H(8XF)	-3058	-1182	-1080	40
H(12C)	-4382	665	349	38
H(13)	-2899	-275	-841	32
H(13')	-4884	-211	525	46
H(14')	-4379	-1076	47	42
H(16E)	-1917	1338	-665	30
H(16F)	-2733	1688	-755	30
H(18E)	-3856	-2149	-1755	40
H(18F)	-3768	-2142	-1196	40
H(19G)	-3423	-3254	-1755	71
H(19H)	-4181	-3027	-1347	71
H(19I)	-3385	-3233	-1189	71
H(20E)	-2613	-2392	-2890	41
H(20F)	-3266	-2546	-2468	41
H(21E)	-2692	-1405	-3203	41
H(21F)	-2588	-1168	-2699	41
H(23')	-2842	-74	-2755	43

H(25')	-4620	937	-3244	37
H(26')	-5084	89	-3294	45
H(27')	-4269	-903	-3204	57
H(29E)	-3227	1974	-2374	30
H(29F)	-2564	1776	-2851	30
H(31E)	-1621	-2198	-3086	37
H(31F)	-803	-2359	-2961	37
H(32G)	-745	-3122	-3455	57
H(32H)	-1567	-3192	-3190	57
H(32I)	-878	-3426	-2920	57
H(33E)	-58	-3035	-1972	35
H(33F)	-172	-2982	-2527	35
H(34E)	994	-2687	-2685	33
H(34F)	495	-2233	-3017	33
H(36')	216	-1039	-2536	36
H(38')	2279	-685	-2744	48
H(39')	2851	-1736	-2902	54
H(40')	2107	-2425	-2852	48
H(42E)	-28	1014	-2624	32
H(42F)	159	934	-2088	32
H(44E)	-1224	-2498	-836	38
H(44F)	-491	-2618	-1278	38
H(45G)	-451	-3637	-1323	61
H(45H)	-1303	-3540	-1022	61
H(45I)	-655	-3513	-743	61
H(52E)	-3296	5515	-1774	29
H(52F)	-3177	5458	-1221	29
H(53G)	-4338	5158	-1046	46
H(53H)	-3811	4702	-732	46
H(55')	-3596	3501	-1236	36
H(57')	-5691	3201	-916	37
H(58')	-6222	4211	-732	43
H(59')	-5493	4898	-757	38
H(61E)	-3623	1578	-1717	34
H(61F)	-3481	1446	-1171	34
H(63E)	-2898	5078	-2445	32

H(63F)	-2188	4975	-2900	32
H(64G)	-3043	6011	-2873	53
H(64H)	-2184	6016	-2907	53
H(64I)	-2774	6137	-2391	53
H(65E)	-317	5029	-3010	34
H(65F)	-1151	5263	-3107	34
H(66E)	236	3922	-2943	37
H(66F)	-480	3672	-2684	37
H(68')	-593	2720	-2962	30
H(70')	899	1814	-4116	37
H(71')	1371	2690	-4318	41
H(72')	876	3571	-3848	40
H(74E)	-766	762	-3024	29
H(74F)	-1580	1118	-3119	29
H(76E)	374	4622	-2582	32
H(76F)	484	4583	-2027	32
H(77G)	56	5706	-2555	54
H(77H)	846	5456	-2394	54
H(77I)	90	5691	-1986	54
H(78E)	-746	4886	-875	36
H(78F)	-62	4978	-1306	36
H(79E)	-885	3626	-1029	45
H(79F)	-744	3881	-542	45
H(81')	-590	2560	-1029	44
H(83')	1129	1490	-445	37
H(84')	1450	2416	-293	40
H(85')	710	3348	-442	49
H(87E)	-260	496	-1393	30
H(87F)	-947	690	-926	30
H(89E)	-1703	4623	-682	36
H(89F)	-2538	4806	-787	36
H(90G)	-2519	5898	-788	61
H(90H)	-1720	5692	-633	61
H(90I)	-2459	5586	-263	61
H(1BA)	-1588	-11	-1769	48
H(12G)	1465	-738	171	69

H(13C)	2898	-467	-17	100
H(4B)	2805	2490	-1263	51
H(5BA)	1427	2470	-1842	56
H(5BB)	1836	2878	-1651	56
H(1BB)	712	-324	-957	49
H(1BC)	605	-779	-499	49
H(2B)	1928	-1099	-599	48
H(3B)	1246	184	-426	54
H(4BA)	2403	330	-396	59
H(5BC)	3116	-311	-1195	52
H(9BA)	1567	324	-1686	48
H(10C)	3456	1737	-869	48
H(1CA)	-2075	2586	-2024	41
H(12H)	-6848	4006	-1449	83
H(13D)	-7648	3755	-2350	105
H(4C)	-6501	152	-2547	74
H(5CA)	-5724	-317	-2024	103
H(5CB)	-5332	54	-1777	103
H(1EA)	-5067	3886	-2007	54
H(1EB)	-4669	3191	-2186	54
H(2C)	-5843	3905	-2612	51
H(3C)	-6094	3175	-1731	63
H(4CA)	-7093	2967	-1957	61
H(5C)	-6273	2685	-2883	57
H(9C)	-5163	2190	-1944	66
H(10D)	-7060	963	-2923	72
H(1XA)	-2353	-8426	-7302	38
H(1XB)	-3003	-8555	-6951	38
H(2X")	-2259	-6291	-7362	32
H(3XA)	-3258	-8275	-9773	54
H(3XB)	-2579	-8196	-9635	54
H(4X")	-3079	-5878	-9027	32
H(5XA)	82	-8838	-8661	33
H(5XB)	-419	-8584	-9000	33
H(6X")	-154	-6792	-8919	32
H(7"C)	-3642	-2039	-8388	45

H(7"D)	-3145	-2276	-8049	45
H(7"A)	-3140	-2302	-8168	45
H(7"B)	-3723	-1938	-7782	45
H(8")	-3264	-4156	-8075	33
H(9"A)	-1129	-2463	-9841	32
H(9"B)	-498	-2300	-10190	32
H(10")	-1126	-4622	-9714	32
H(11A)	-240	-2562	-7343	41
H(11B)	-902	-2661	-7494	41
H(12")	-410	-4956	-8066	37
H(7XA)	-3155	-9236	-7479	37
H(7XB)	-2339	-9445	-7351	37
H(8XA)	-3058	-7856	-7807	45
H(8XB)	-3769	-8107	-7538	45
H(10X)	-2842	-6973	-7515	30
H(12A)	-4394	-6029	-6351	38
H(13")	-4876	-6899	-6184	46
H(14")	-4432	-7742	-6682	44
H(16A)	-1868	-5348	-7320	36
H(16B)	-2687	-5000	-7408	36
H(18A)	-3845	-8754	-8526	43
H(18B)	-3810	-8787	-7956	43
H(19A)	-3571	-9840	-8565	89
H(19B)	-4281	-9611	-8123	89
H(19C)	-3463	-9898	-8010	89
H(20A)	-2611	-9209	-9601	45
H(20B)	-3369	-9024	-9189	45
H(21A)	-3957	-7938	-8958	48
H(21B)	-3220	-7731	-8909	48
H(23")	-3049	-6773	-9248	39
H(25")	-4529	-5721	-9975	35
H(26")	-5072	-6538	-10013	41
H(27")	-4554	-7489	-9686	46
H(29A)	-3185	-4716	-9038	36
H(29B)	-2541	-4947	-9518	36
H(31A)	-1577	-8969	-9807	41

H(31B)	-768	-9101	-9672	41
H(32A)	-709	-9891	-10146	61
H(32B)	-1503	-9984	-9846	61
H(32C)	-783	-10166	-9600	61
H(33A)	-77	-9763	-8654	36
H(33B)	-172	-9696	-9214	36
H(34A)	462	-8856	-9674	40
H(34B)	953	-9377	-9382	40
H(36")	242	-7732	-9232	35
H(38")	2224	-7479	-9090	79
H(39")	2760	-8517	-9181	103
H(40")	2055	-9181	-9369	69
H(42A)	23	-5706	-9308	31
H(42B)	216	-5735	-8774	31
H(44A)	-1298	-9197	-7526	33
H(44B)	-553	-9317	-7956	33
H(45A)	-438	-10348	-7958	57
H(45B)	-1314	-10275	-7726	57
H(45C)	-762	-10198	-7385	57
H(52A)	-3374	-1150	-8496	40
H(52B)	-3292	-1134	-7939	40
H(57")	-5694	-3534	-7543	35
H(58")	-6202	-2484	-7345	43
H(58A)	-6246	-2484	-7500	43
H(61A)	-3583	-5160	-8370	37
H(61B)	-3434	-5265	-7826	37
H(63A)	-2218	-1728	-9579	40
H(63B)	-2959	-1598	-9147	40
H(64A)	-2945	-713	-9663	59
H(64B)	-2170	-678	-9533	59
H(64C)	-2926	-552	-9115	59
H(65A)	-368	-1628	-9631	37
H(65B)	-1186	-1427	-9756	37
H(66A)	-390	-2993	-9344	36
H(66B)	299	-2735	-9643	36
H(68")	-530	-3966	-9612	33

H(70")	866	-4821	-10825	43
H(71")	1328	-3957	-11039	48
H(72")	869	-3089	-10539	51
H(74A)	-738	-5917	-9701	33
H(74B)	-1552	-5545	-9787	33
H(76A)	307	-2075	-9180	35
H(76B)	370	-2087	-8616	35
H(77A)	-56	-970	-9155	61
H(77B)	765	-1233	-9039	61
H(77C)	52	-997	-8600	61
H(78A)	-897	-1600	-7543	35
H(78B)	-142	-1786	-7960	35
H(79A)	461	-2855	-8137	43
H(79B)	-252	-3085	-8199	43
H(81")	-383	-4077	-7881	45
H(83")	1112	-5101	-7082	40
H(84")	1501	-4208	-7004	36
H(85")	1090	-3320	-7426	50
H(87A)	-209	-6144	-8064	34
H(87B)	-875	-5930	-7591	34
H(89A)	-1906	-1949	-7313	41
H(89B)	-2716	-1790	-7452	41
H(90A)	-2788	-709	-7443	58
H(90B)	-1957	-852	-7339	58
H(90C)	-2631	-998	-6926	58
H(53A)	-3848	-2131	-8711	43
H(53B)	-4437	-1576	-8384	43
H(55")	-3719	-3215	-8247	40
H(59")	-5484	-1771	-7739	41
H(53C)	-4500	-1523	-7744	43
H(53D)	-3972	-1946	-7415	43
H(55B)	-3673	-3155	-7849	40
H(59B)	-5591	-1848	-7387	41
H(1D)	-1482	-6731	-8432	49
H(12I)	1203	-7382	-6501	56
H(13F)	2930	-7030	-6707	58

H(4D)	2869	-4250	-8047	49
H(5DA)	2077	-3923	-8627	56
H(5DB)	1656	-4355	-8773	56
H(1DA)	543	-7467	-7207	46
H(1DB)	725	-7065	-7691	46
H(2D)	1880	-7810	-7241	41
H(3D)	1153	-6525	-7119	40
H(4DA)	2279	-6334	-7037	44
H(5D)	3053	-6962	-7802	45
H(9D)	1582	-6423	-8377	45
H(10F)	3336	-4901	-7541	49
H(1E)	-2093	-4111	-8694	47
H(12E)	-6612	-3042	-9286	85
H(13E)	-7026	-3249	-8367	78
H(4E)	-6794	-6357	-9526	75
H(5EA)	-5808	-6860	-8635	76
H(5EB)	-6253	-7049	-8969	76
H(1FA)	-4518	-3648	-8844	51
H(1FB)	-4115	-3748	-9411	51
H(1FC)	-4526	-3522	-8819	51
H(1FD)	-4098	-3786	-9366	51
H(2E)	-5286	-3172	-9607	54
H(3E)	-5774	-2863	-8674	57
H(4EA)	-5675	-3901	-8415	55
H(5E)	-6396	-4017	-9211	59
H(9E)	-5147	-4975	-8442	58
H(10E)	-7110	-5450	-9819	78
H(1SA)	-1937	-3129	-7421	77
H(1SB)	-1608	-3349	-7043	77
H(2SA)	-1510	-4381	-6473	90
H(2SB)	-1150	-3930	-6577	90
H(3SA)	-4129	-3869	-5021	92
H(3SB)	-4416	-4361	-4995	92
H(4SA)	-4968	-2004	-2132	94
H(4SB)	-5177	-1872	-2565	94
H(5SA)	-1587	-1083	-3391	99

H(5SB)	-1410	-754	-3068	99
H(6SA)	-1853	281	-4110	64
H(6SB)	-1661	38	-3690	64
H(7SA)	-4204	-510	-1750	108
H(7SB)	-4209	-1067	-1548	108
H(8SA)	-3051	12	-1774	63
H(8SB)	-3709	444	-1712	63
H(9SA)	-368	2452	-2095	64
H(9SB)	161	1924	-2216	64
H(10G)	-4	3298	-2024	60
H(10H)	704	3250	-2277	60
H(11G)	1907	3790	-1192	100
H(11H)	1475	4229	-1425	100
H(12J)	-1834	3538	-454	136
H(12K)	-2158	3185	-663	136
H(13G)	-412	-4175	-8850	56
H(13H)	-409	-4773	-8837	56
H(14A)	-3058	-6659	-8422	65
H(14B)	-3745	-6336	-8195	65
H(15A)	-1884	-7741	-9624	70
H(15B)	-1463	-7636	-10060	70