Supporting information: Crystallographic data

Experimental Section

Data Collection

A yellow crystal with approximate dimensions 0.14 x 0.08 x 0.03 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker Quazar SMART APEXII diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.96 cm.

The initial cell constants were obtained from the low temperature data collection on this crystal. The final cell constants were calculated from a set of 2725 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.83 Å. A total of 19767 data were harvested by collecting 4 sets of frames with 0.5^0 scans in ω and φ with exposure times of 100 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

The structure was also solved at 298(1) K in a similar manner.

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P\bar{1}$ and $P1$. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement [2-4].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms

were refined with anisotropic displacement coefficients. All hydrogen atoms connected to carbon atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

There are two symmetry independent molecules with similar geometries in the asymmetric unit.

The final least-squares refinement of 467 parameters against 6529 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0439 and 0.1085, respectively. The final difference Fourier map was featureless.

For the structure solved at 298K, The final least-squares refinement of 467 parameters against 6804 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0547 and 0.1602, respectively. The final difference Fourier map was featureless.

The molecular diagrams are drawn with 50% probability ellipsoids.

References

[1] Bruker-AXS. (2009) APEX2, SADABS, and SAINT Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

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[3] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. "OLEX2: a complete structure solution, refinement and analysis program". *J. Appl. Cryst.* (2009) **42**, *339-341*.

[4] Guzei, I.A. (2006-2008). Internal laboratory computer programs "Inserter", "FCF_filter", "Modicifer".

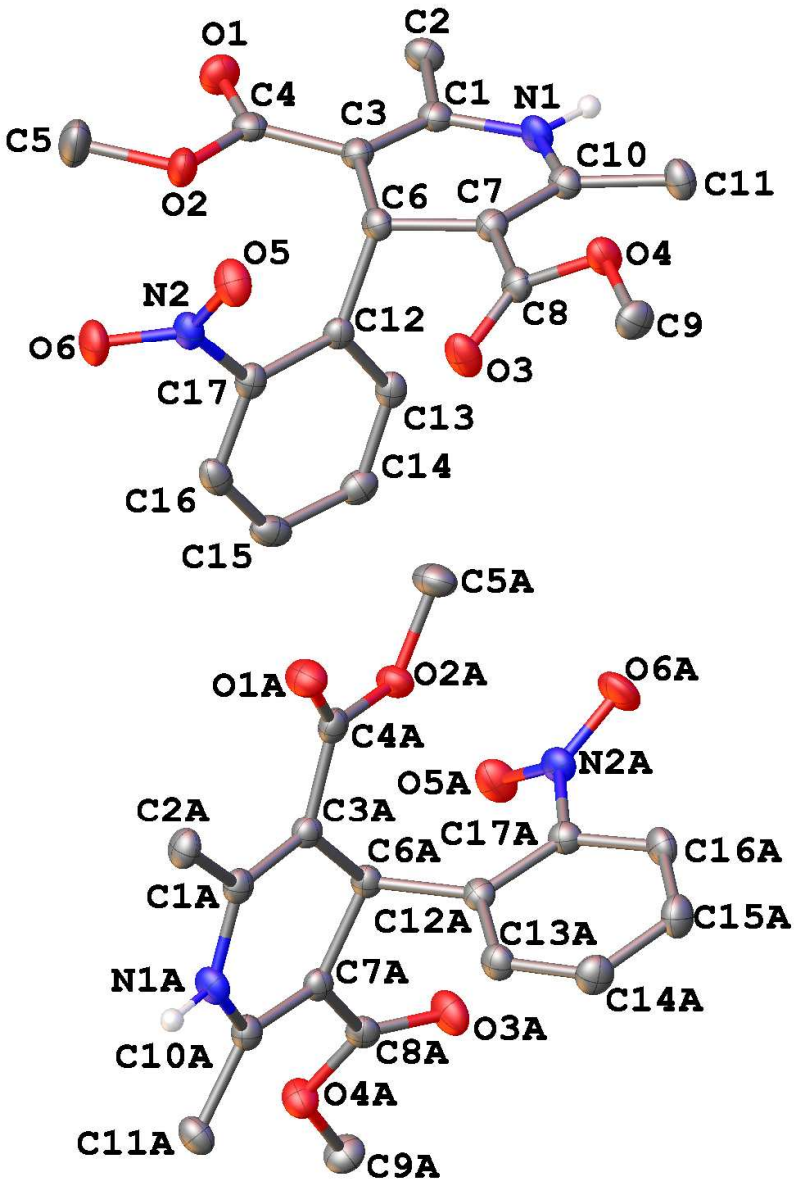

Figure S1. A molecular drawing of β NIF solved at 100 K. All H atoms connected to C atoms are omitted.

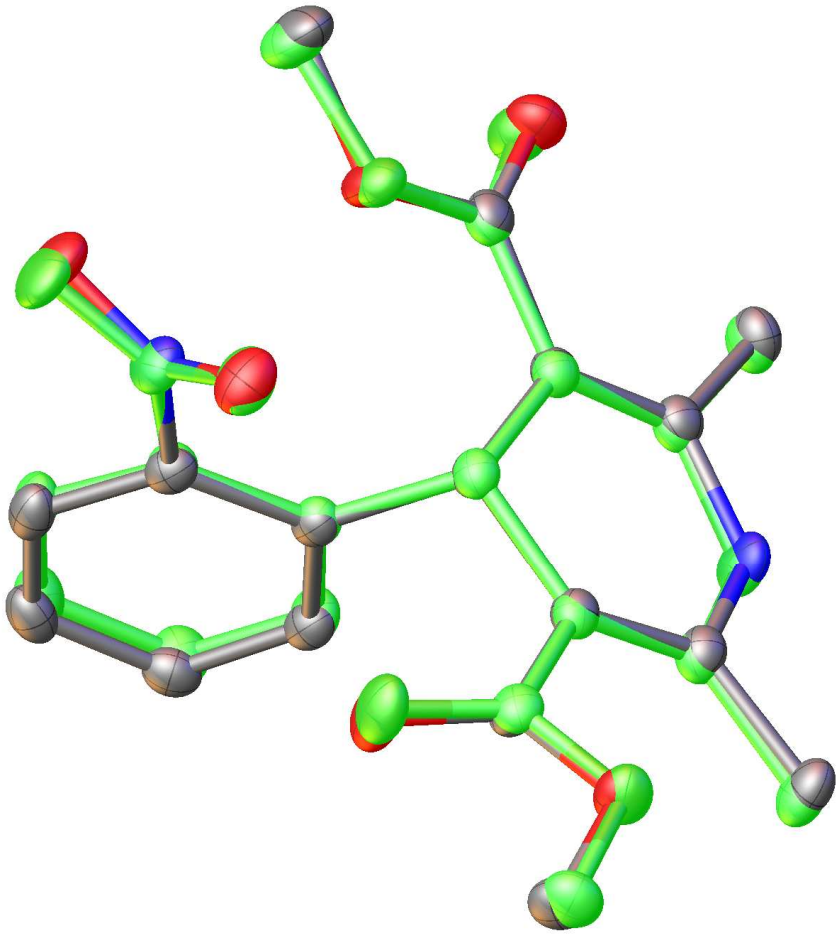

Figure S2. An overlay of the two molecules of β NIF solved at 100 K.

Table S1. Crystal data and structure refinement for β NIF solved at 100 K.

Identification code	yu03	
Empirical formula	$C_{17}\ H_{18}\ N_2\ O_6$	
Formula weight	346.33	
Temperature	100(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.6661(6) Å	α= 61.028(3)°.
	b = 13.7006(8) Å	β= 79.631(4)°.
	c = 14.1184(9) Å	γ = 81.904(4)°.
Volume	1605.89(17) $Å^3$	
Z	4	
Density (calculated)	1.432 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	728	
Crystal size	0.14 x 0.08 x 0.03 mm^3	
Theta range for data collection	1.73 to 26.43°.	
Index ranges	-12<=h<=11, -17<=k<=17, -16<=l<=17	
Reflections collected	19784	
Independent reflections	6529 [R(int) = 0.0449]	
Completeness to theta = 25.00°	99.3 %	
Absorption correction	Numerical with SADABS	
Max. and min. transmission	0.9967 and 0.9848	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6529 / 0 / 467	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.0951	
R indices (all data)	R1 = 0.0763, wR2 = 0.1085	
Largest diff. peak and hole	0.266 and -0.223 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for β NIF solved at 100 K. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-2550(2)	970(1)	7576(1)	30(1)
O(2)	-1701(1)	2232(1)	5891(1)	27(1)
O(3)	3041(2)	1523(1)	3996(1)	29(1)
O(4)	3296(1)	-230(1)	4258(1)	25(1)
O(5)	277(2)	3080(1)	3577(1)	29(1)
O(6)	-452(2)	4434(1)	3956(1)	30(1)
N(1)	970(2)	-1189(1)	7358(1)	22(1)
N(2)	267(2)	3563(1)	4116(1)	22(1)
C(1)	-148(2)	-511(2)	7495(2)	20(1)
C(2)	-1033(2)	-1050(2)	8587(2)	24(1)
C(3)	-366(2)	539(2)	6685(2)	20(1)
C(4)	-1634(2)	1222(2)	6802(2)	22(1)
C(5)	-2928(2)	2948(2)	5935(2)	40(1)
C(6)	683(2)	1047(2)	5648(2)	19(1)
C(7)	1754(2)	155(2)	5562(2)	19(1)
C(8)	2739(2)	555(2)	4545(2)	20(1)
C(9)	4358(2)	128(2)	3315(2)	26(1)
C(10)	1866(2)	-892(2)	6393(2)	20(1)
C(11)	2884(2)	-1840(2)	6422(2)	25(1)
C(12)	1417(2)	1972(2)	5642(2)	18(1)
C(13)	2336(2)	1666(2)	6412(2)	20(1)
C(14)	2993(2)	2443(2)	6506(2)	23(1)
C(15)	2729(2)	3575(2)	5833(2)	25(1)
C(16)	1814(2)	3914(2)	5071(2)	23(1)
C(17)	1198(2)	3122(2)	4973(2)	19(1)
O(1A)	4220(2)	3629(1)	7665(1)	29(1)
O(2A)	4793(1)	2494(1)	9349(1)	23(1)
O(3A)	8335(2)	3500(1)	10909(1)	30(1)
O(4A)	7854(2)	5243(1)	10671(1)	26(1)
O(5A)	6373(2)	1695(1)	11395(1)	29(1)
O(6A)	6663(2)	298(1)	11056(1)	33(1)
N(1A)	6407(2)	6092(1)	7728(1)	22(1)
N(2A)	6876(2)	1260(1)	10820(1)	22(1)
C(1A)	5670(2)	5347(2)	7656(2)	20(1)
C(2A)	4966(2)	5836(2)	6641(2)	24(1)
C(3A)	5627(2)	4279(2)	8465(2)	19(1)
C(4A)	4815(2)	3482(2)	8415(2)	21(1)
C(5A)	4155(2)	1612(2)	9334(2)	31(1)
C(6A)	6512(2)	3832(2)	9399(2)	18(1)
C(7A)	7089(2)	4785(2)	9444(2)	18(1)
C(8A)	7811(2)	4441(2)	10400(2)	20(1)
C(9A)	8663(2)	4971(2)	11544(2)	27(1)
C(10A)	7039(2)	5842(2)	8629(2)	20(1)
C(11A)	7612(2)	6841(2)	8560(2)	24(1)
C(12A)	7700(2)	3048(2)	9217(2)	18(1)
C(13A)	8691(2)	3518(2)	8297(2)	22(1)
C(14A)	9748(2)	2891(2)	7995(2)	26(1)
C(15A)	9825(2)	1738(2)	8608(2)	26(1)
C(16A)	8848(2)	1237(2)	9512(2)	23(1)
C(17A)	7830(2)	1883(2)	9816(2)	19(1)

Table S3. Bond lengths [Å] and angles [°] for β NIF solved at 100 K.

O(1)-C(4)	1.213(2)	O(1A)-C(4A)	1.213(2)
O(2)-C(4)	1.361(2)	O(2A)-C(4A)	1.357(2)
O(2)-C(5)	1.442(2)	O(2A)-C(5A)	1.443(2)
O(3)-C(8)	1.216(2)	O(3A)-C(8A)	1.219(2)
O(4)-C(8)	1.338(2)	O(4A)-C(8A)	1.335(2)
O(4)-C(9)	1.443(2)	O(4A)-C(9A)	1.445(2)
O(5)-N(2)	1.225(2)	O(5A)-N(2A)	1.223(2)
O(6)-N(2)	1.232(2)	O(6A)-N(2A)	1.231(2)
N(1)-C(1)	1.373(2)	N(1A)-C(1A)	1.375(2)
N(1)-C(10)	1.382(2)	N(1A)-C(10A)	1.381(2)
N(1)-H(1)	0.91(2)	N(1A)-H(1A)	0.86(2)
N(2)-C(17)	1.474(2)	N(2A)-C(17A)	1.473(2)
C(1)-C(3)	1.352(3)	C(1A)-C(3A)	1.352(3)
C(1)-C(2)	1.502(3)	C(1A)-C(2A)	1.503(3)
C(2)-H(2A)	0.9800	C(2A)-H(2AA)	0.9800
C(2)-H(2B)	0.9800	C(2A)-H(2AB)	0.9800
C(2)-H(2C)	0.9800	C(2A)-H(2AC)	0.9800
C(3)-C(4)	1.470(3)	C(3A)-C(4A)	1.467(3)
C(3)-C(6)	1.527(3)	C(3A)-C(6A)	1.524(3)
C(5)-H(5A)	0.9800	C(5A)-H(5AA)	0.9800
C(5)-H(5B)	0.9800	C(5A)-H(5AB)	0.9800
C(5)-H(5C)	0.9800	C(5A)-H(5AC)	0.9800
C(6)-C(7)	1.523(3)	C(6A)-C(7A)	1.523(3)
C(6)-C(12)	1.533(2)	C(6A)-C(12A)	1.533(3)
C(6)-H(6)	1.0000	C(6A)-H(6A)	1.0000
C(7)-C(10)	1.349(3)	C(7A)-C(10A)	1.345(3)
C(7)-C(8)	1.470(3)	C(7A)-C(8A)	1.470(3)
C(9)-H(9A)	0.9800	C(9A)-H(9AA)	0.9800
C(9)-H(9B)	0.9800	C(9A)-H(9AB)	0.9800
C(9)-H(9C)	0.9800	C(9A)-H(9AC)	0.9800
C(10)-C(11)	1.503(3)	C(10A)-C(11A)	1.503(3)
C(11)-H(11A)	0.9800	C(11A)-H(11D)	0.9800
C(11)-H(11B)	0.9800	C(11A)-H(11E)	0.9800
C(11)-H(11C)	0.9800	C(11A)-H(11F)	0.9800
C(12)-C(13)	1.396(3)	C(12A)-C(13A)	1.391(3)
C(12)-C(17)	1.399(3)	C(12A)-C(17A)	1.398(3)
C(13)-C(14)	1.382(3)	C(13A)-C(14A)	1.383(3)
C(13)-H(13)	0.9500	C(13A)-H(13A)	0.9500
C(14)-C(15)	1.387(3)	C(14A)-C(15A)	1.384(3)
C(14)-H(14)	0.9500	C(14A)-H(14A)	0.9500
C(15)-C(16)	1.377(3)	C(15A)-C(16A)	1.376(3)
C(15)-H(15)	0.9500	C(15A)-H(15A)	0.9500
C(16)-C(17)	1.381(3)	C(16A)-C(17A)	1.380(3)
C(16)-H(16)	0.9500	C(16A)-H(16A)	0.9500
C(4)-O(2)-C(5)	114.64(16)	C(3)-C(1)-C(2)	126.12(18)
C(8)-O(4)-C(9)	115.76(15)	N(1)-C(1)-C(2)	113.78(17)
C(1)-N(1)-C(10)	123.66(16)	C(1)-C(2)-H(2A)	109.5
C(1)-N(1)-H(1)	119.8(14)	C(1)-C(2)-H(2B)	109.5
C(10)-N(1)-H(1)	116.2(14)	H(2A)-C(2)-H(2B)	109.5
O(5)-N(2)-O(6)	123.41(16)	C(1)-C(2)-H(2C)	109.5
O(5)-N(2)-C(17)	119.28(15)	H(2A)-C(2)-H(2C)	109.5
O(6)-N(2)-C(17)	117.26(16)	H(2B)-C(2)-H(2C)	109.5
C(3)-C(1)-N(1)	120.11(18)	C(1)-C(3)-C(4)	119.60(17)

C(1)-C(3)-C(6)	121.78(17)	C(4A)-O(2A)-C(5A)	115.35(15)
C(4)-C(3)-C(6)	118.61(16)	C(8A)-O(4A)-C(9A)	116.58(15)
O(1)-C(4)-O(2)	121.26(18)	C(1A)-N(1A)-C(10A)	123.66(17)
O(1)-C(4)-C(3)	127.54(18)	C(1A)-N(1A)-H(1A)	118.0(15)
O(2)-C(4)-C(3)	111.19(16)	C(10A)-N(1A)-H(1A)	118.4(15)
O(2)-C(5)-H(5A)	109.5	O(5A)-N(2A)-O(6A)	123.14(17)
O(2)-C(5)-H(5B)	109.5	O(5A)-N(2A)-C(17A)	119.49(15)
H(5A)-C(5)-H(5B)	109.5	O(6A)-N(2A)-C(17A)	117.33(16)
O(2)-C(5)-H(5C)	109.5	C(3A)-C(1A)-N(1A)	119.72(18)
H(5A)-C(5)-H(5C)	109.5	C(3A)-C(1A)-C(2A)	126.01(18)
H(5B)-C(5)-H(5C)	109.5	N(1A)-C(1A)-C(2A)	114.27(17)
C(7)-C(6)-C(3)	111.02(15)	C(1A)-C(2A)-H(2AA)	109.5
C(7)-C(6)-C(12)	110.95(15)	C(1A)-C(2A)-H(2AB)	109.5
C(3)-C(6)-C(12)	109.32(15)	H(2AA)-C(2A)-H(2AB)	109.5
C(7)-C(6)-H(6)	108.5	C(1A)-C(2A)-H(2AC)	109.5
C(3)-C(6)-H(6)	108.5	H(2AA)-C(2A)-H(2AC)	109.5
C(12)-C(6)-H(6)	108.5	H(2AB)-C(2A)-H(2AC)	109.5
C(10)-C(7)-C(8)	122.61(17)	C(1A)-C(3A)-C(4A)	120.40(18)
C(10)-C(7)-C(6)	122.44(17)	C(1A)-C(3A)-C(6A)	121.87(17)
C(8)-C(7)-C(6)	114.72(16)	C(4A)-C(3A)-C(6A)	117.50(16)
O(3)-C(8)-O(4)	121.56(18)	O(1A)-C(4A)-O(2A)	121.39(17)
O(3)-C(8)-C(7)	123.28(17)	O(1A)-C(4A)-C(3A)	127.43(18)
O(4)-C(8)-C(7)	115.16(16)	O(2A)-C(4A)-C(3A)	111.18(16)
O(4)-C(9)-H(9A)	109.5	O(2A)-C(5A)-H(5AA)	109.5
O(4)-C(9)-H(9B)	109.5	O(2A)-C(5A)-H(5AB)	109.5
H(9A)-C(9)-H(9B)	109.5	H(5AA)-C(5A)-H(5AB)	109.5
O(4)-C(9)-H(9C)	109.5	O(2A)-C(5A)-H(5AC)	109.5
H(9A)-C(9)-H(9C)	109.5	H(5AA)-C(5A)-H(5AC)	109.5
H(9B)-C(9)-H(9C)	109.5	H(5AB)-C(5A)-H(5AC)	109.5
C(7)-C(10)-N(1)	119.62(17)	C(7A)-C(6A)-C(3A)	110.86(15)
C(7)-C(10)-C(11)	127.79(18)	C(7A)-C(6A)-C(12A)	111.64(15)
N(1)-C(10)-C(11)	112.59(16)	C(3A)-C(6A)-C(12A)	107.36(15)
C(10)-C(11)-H(11A)	109.5	C(7A)-C(6A)-H(6A)	109.0
C(10)-C(11)-H(11B)	109.5	C(3A)-C(6A)-H(6A)	109.0
H(11A)-C(11)-H(11B)	109.5	C(12A)-C(6A)-H(6A)	109.0
C(10)-C(11)-H(11C)	109.5	C(10A)-C(7A)-C(8A)	122.78(17)
H(11A)-C(11)-H(11C)	109.5	C(10A)-C(7A)-C(6A)	122.34(17)
H(11B)-C(11)-H(11C)	109.5	C(8A)-C(7A)-C(6A)	114.67(16)
C(13)-C(12)-C(17)	115.33(17)	O(3A)-C(8A)-O(4A)	122.19(18)
C(13)-C(12)-C(6)	118.28(16)	O(3A)-C(8A)-C(7A)	123.02(17)
C(17)-C(12)-C(6)	126.27(17)	O(4A)-C(8A)-C(7A)	114.78(16)
C(14)-C(13)-C(12)	122.54(18)	O(4A)-C(9A)-H(9AA)	109.5
C(14)-C(13)-H(13)	118.7	O(4A)-C(9A)-H(9AB)	109.5
C(12)-C(13)-H(13)	118.7	H(9AA)-C(9A)-H(9AB)	109.5
C(13)-C(14)-C(15)	119.97(19)	O(4A)-C(9A)-H(9AC)	109.5
C(13)-C(14)-H(14)	120.0	H(9AA)-C(9A)-H(9AC)	109.5
C(15)-C(14)-H(14)	120.0	H(9AB)-C(9A)-H(9AC)	109.5
C(16)-C(15)-C(14)	119.37(18)	C(7A)-C(10A)-N(1A)	119.63(18)
C(16)-C(15)-H(15)	120.3	C(7A)-C(10A)-C(11A)	127.35(18)
C(14)-C(15)-H(15)	120.3	N(1A)-C(10A)-C(11A)	113.02(16)
C(15)-C(16)-C(17)	119.62(18)	C(10A)-C(11A)-H(11D)	109.5
C(15)-C(16)-H(16)	120.2	C(10A)-C(11A)-H(11E)	109.5
C(17)-C(16)-H(16)	120.2	H(11D)-C(11A)-H(11E)	109.5
C(16)-C(17)-C(12)	123.12(18)	C(10A)-C(11A)-H(11F)	109.5
C(16)-C(17)-N(2)	115.73(17)	H(11D)-C(11A)-H(11F)	109.5
C(12)-C(17)-N(2)	121.15(17)	H(11E)-C(11A)-H(11F)	109.5

C(13A)-C(12A)-C(17A)	115.13(17)	C(16A)-C(15A)-C(14A)	119.12(19)
C(13A)-C(12A)-C(6A)	117.47(16)	C(16A)-C(15A)-H(15A)	120.4
C(17A)-C(12A)-C(6A)	127.08(17)	C(14A)-C(15A)-H(15A)	120.4
C(14A)-C(13A)-C(12A)	123.10(18)	C(15A)-C(16A)-C(17A)	120.08(18)
C(14A)-C(13A)-H(13A)	118.4	C(15A)-C(16A)-H(16A)	120.0
C(12A)-C(13A)-H(13A)	118.4	C(17A)-C(16A)-H(16A)	120.0
C(13A)-C(14A)-C(15A)	119.66(19)	C(16A)-C(17A)-C(12A)	122.85(18)
C(13A)-C(14A)-H(14A)	120.2	C(16A)-C(17A)-N(2A)	115.39(16)
C(15A)-C(14A)-H(14A)	120.2	C(12A)-C(17A)-N(2A)	121.76(17)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for β NIF solved at 100 K. 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)	24(1)	31(1)	29(1)	-12(1)	4(1)	-3(1)
O(2)	20(1)	20(1)	32(1)	-8(1)	-2(1)	3(1)
O(3)	38(1)	17(1)	21(1)	-3(1)	5(1)	-2(1)
O(4)	27(1)	21(1)	23(1)	-10(1)	4(1)	-3(1)
O(5)	39(1)	26(1)	20(1)	-9(1)	-9(1)	5(1)
O(6)	33(1)	19(1)	30(1)	-6(1)	-8(1)	8(1)
N(1)	27(1)	13(1)	16(1)	-1(1)	-2(1)	-1(1)
N(2)	25(1)	16(1)	17(1)	-3(1)	-1(1)	1(1)
C(1)	21(1)	20(1)	21(1)	-10(1)	-3(1)	-4(1)
C(2)	28(1)	21(1)	20(1)	-6(1)	0(1)	-6(1)
C(3)	19(1)	18(1)	20(1)	-8(1)	-4(1)	-2(1)
C(4)	21(1)	20(1)	26(1)	-10(1)	-5(1)	-4(1)
C(5)	27(1)	26(1)	50(2)	-9(1)	-1(1)	6(1)
C(6)	20(1)	16(1)	16(1)	-4(1)	-4(1)	0(1)
C(7)	20(1)	18(1)	17(1)	-8(1)	-4(1)	-1(1)
C(8)	21(1)	17(1)	19(1)	-5(1)	-5(1)	1(1)
C(9)	22(1)	30(1)	22(1)	-13(1)	3(1)	-2(1)
C(10)	22(1)	18(1)	19(1)	-7(1)	-5(1)	-1(1)
C(11)	30(1)	17(1)	22(1)	-6(1)	-3(1)	2(1)
C(12)	17(1)	18(1)	15(1)	-5(1)	1(1)	-1(1)
C(13)	20(1)	19(1)	15(1)	-5(1)	1(1)	0(1)
C(14)	19(1)	30(1)	20(1)	-12(1)	0(1)	-3(1)
C(15)	24(1)	27(1)	24(1)	-13(1)	5(1)	-10(1)
C(16)	26(1)	17(1)	20(1)	-7(1)	5(1)	-3(1)
C(17)	19(1)	20(1)	15(1)	-6(1)	0(1)	0(1)
O(1A)	33(1)	26(1)	26(1)	-9(1)	-10(1)	-3(1)
O(2A)	25(1)	18(1)	23(1)	-6(1)	-3(1)	-6(1)
O(3A)	43(1)	18(1)	24(1)	-4(1)	-13(1)	2(1)
O(4A)	32(1)	24(1)	24(1)	-12(1)	-10(1)	2(1)
O(5A)	37(1)	24(1)	18(1)	-7(1)	5(1)	-5(1)
O(6A)	42(1)	15(1)	34(1)	-5(1)	-1(1)	-9(1)
N(1A)	30(1)	15(1)	16(1)	-2(1)	-4(1)	-2(1)
N(2A)	25(1)	16(1)	19(1)	-2(1)	-4(1)	-2(1)
C(1A)	18(1)	21(1)	18(1)	-9(1)	0(1)	1(1)
C(2A)	24(1)	23(1)	20(1)	-6(1)	-6(1)	4(1)
C(3A)	17(1)	19(1)	19(1)	-9(1)	-1(1)	0(1)
C(4A)	17(1)	21(1)	22(1)	-9(1)	0(1)	2(1)
C(5A)	32(1)	25(1)	33(1)	-10(1)	-6(1)	-10(1)
C(6A)	19(1)	16(1)	16(1)	-5(1)	0(1)	-1(1)
C(7A)	17(1)	18(1)	17(1)	-8(1)	1(1)	0(1)
C(8A)	20(1)	19(1)	17(1)	-6(1)	2(1)	-4(1)
C(9A)	27(1)	33(1)	24(1)	-14(1)	-9(1)	-1(1)
C(10A)	20(1)	19(1)	19(1)	-8(1)	-2(1)	1(1)
C(11A)	32(1)	17(1)	20(1)	-6(1)	-3(1)	-2(1)
C(12A)	20(1)	18(1)	16(1)	-7(1)	-5(1)	0(1)
C(13A)	25(1)	18(1)	18(1)	-4(1)	-3(1)	-1(1)
C(14A)	25(1)	27(1)	21(1)	-9(1)	2(1)	-2(1)
C(15A)	28(1)	26(1)	25(1)	-13(1)	-2(1)	5(1)
C(16A)	28(1)	16(1)	21(1)	-5(1)	-7(1)	3(1)
C(17A)	21(1)	19(1)	16(1)	-6(1)	-3(1)	-2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for β NIF solved at 100 K.

	x	y	z	U(eq)
H(1)	1100(20)	-1900(20)	7896(19)	33(6)
H(2A)	-1969	-1157	8490	36
H(2B)	-1127	-569	8933	36
H(2C)	-580	-1776	9052	36
H(5A)	-2877	3665	5263	59
H(5B)	-2964	3075	6565	59
H(5C)	-3778	2591	6006	59
H(6)	151	1388	5003	22
H(9A)	3959	747	2685	38
H(9B)	4676	-497	3159	38
H(9C)	5159	378	3462	38
H(11A)	3020	-2368	7180	37
H(11B)	3790	-1546	6004	37
H(11C)	2506	-2224	6101	37
H(13)	2517	895	6890	24
H(14)	3625	2201	7033	28
H(15)	3175	4113	5896	30
H(16)	1608	4687	4616	27
H(1A)	6470(20)	6755(19)	7181(19)	29(6)
H(2AA)	3941	5828	6840	36
H(2AB)	5269	5390	6259	36
H(2AC)	5229	6607	6161	36
H(5AA)	4705	1426	8781	46
H(5AB)	3190	1861	9156	46
H(5AC)	4135	949	10053	46
H(6A)	5910	3393	10103	22
H(9AA)	9670	4935	11284	41
H(9AB)	8408	4246	12161	41
H(9AC)	8460	5549	11778	41
H(11D)	7755	7419	7796	36
H(11E)	8514	6621	8857	36
H(11F)	6942	7136	8983	36
H(13A)	8639	4307	7855	26
H(14A)	10418	3251	7371	31
H(15A)	10543	1298	8406	32
H(16A)	8873	445	9928	28

Table S6. Torsion angles [°] for β NIF solved at 100 K.

C(10)-N(1)-C(1)-C(3)	-4.5(3)	C(2A)-C(1A)-C(3A)-C(4A)	-1.5(3)
C(10)-N(1)-C(1)-C(2)	175.61(17)	N(1A)-C(1A)-C(3A)-C(6A)	-7.2(3)
N(1)-C(1)-C(3)-C(4)	174.63(17)	C(2A)-C(1A)-C(3A)-C(6A)	172.90(17)
C(2)-C(1)-C(3)-C(4)	-5.5(3)	C(5A)-O(2A)-C(4A)-O(1A)	6.5(3)
N(1)-C(1)-C(3)-C(6)	-6.1(3)	C(5A)-O(2A)-C(4A)-C(3A)	-173.29(16)
C(2)-C(1)-C(3)-C(6)	173.71(18)	C(1A)-C(3A)-C(4A)-O(1A)	6.4(3)
C(5)-O(2)-C(4)-O(1)	0.0(3)	C(6A)-C(3A)-C(4A)-O(1A)	-168.31(18)
C(5)-O(2)-C(4)-C(3)	179.17(17)	C(1A)-C(3A)-C(4A)-O(2A)	-173.91(17)
C(1)-C(3)-C(4)-O(1)	1.7(3)	C(6A)-C(3A)-C(4A)-O(2A)	11.4(2)
C(6)-C(3)-C(4)-O(1)	-177.61(19)	C(1A)-C(3A)-C(6A)-C(7A)	14.9(2)
C(1)-C(3)-C(4)-O(2)	-177.51(17)	C(4A)-C(3A)-C(6A)-C(7A)	-170.54(16)
C(6)-C(3)-C(4)-O(2)	3.2(2)	C(1A)-C(3A)-C(6A)-C(12A)	-107.3(2)
C(1)-C(3)-C(6)-C(7)	12.5(2)	C(4A)-C(3A)-C(6A)-C(12A)	67.3(2)
C(4)-C(3)-C(6)-C(7)	-168.21(16)	C(3A)-C(6A)-C(7A)-C(10A)	-12.3(2)
C(1)-C(3)-C(6)-C(12)	-110.2(2)	C(12A)-C(6A)-C(7A)-C(10A)	107.4(2)
C(4)-C(3)-C(6)-C(12)	69.1(2)	C(3A)-C(6A)-C(7A)-C(8A)	172.85(15)
C(3)-C(6)-C(7)-C(10)	-10.0(2)	C(12A)-C(6A)-C(7A)-C(8A)	-67.5(2)
C(12)-C(6)-C(7)-C(10)	111.8(2)	C(9A)-O(4A)-C(8A)-O(3A)	5.3(3)
C(3)-C(6)-C(7)-C(8)	175.40(16)	C(9A)-O(4A)-C(8A)-C(7A)	-174.56(16)
C(12)-C(6)-C(7)-C(8)	-62.8(2)	C(10A)-C(7A)-C(8A)-O(3A)	-151.02(19)
C(9)-O(4)-C(8)-O(3)	5.0(3)	C(6A)-C(7A)-C(8A)-O(3A)	23.8(3)
C(9)-O(4)-C(8)-C(7)	-174.70(16)	C(10A)-C(7A)-C(8A)-O(4A)	28.8(3)
C(10)-C(7)-C(8)-O(3)	-149.7(2)	C(6A)-C(7A)-C(8A)-O(4A)	-156.35(16)
C(6)-C(7)-C(8)-O(3)	24.9(3)	C(8A)-C(7A)-C(10A)-N(1A)	176.50(17)
C(10)-C(7)-C(8)-O(4)	30.0(3)	C(6A)-C(7A)-C(10A)-N(1A)	2.1(3)
C(6)-C(7)-C(8)-O(4)	-155.40(16)	C(8A)-C(7A)-C(10A)-C(11A)	-3.3(3)
C(8)-C(7)-C(10)-N(1)	175.26(17)	C(6A)-C(7A)-C(10A)-C(11A)	-177.72(18)
C(6)-C(7)-C(10)-N(1)	1.1(3)	C(1A)-N(1A)-C(10A)-C(7A)	7.8(3)
C(8)-C(7)-C(10)-C(11)	-4.9(3)	C(1A)-N(1A)-C(10A)-C(11A)	-172.43(17)
C(6)-C(7)-C(10)-C(11)	-179.02(18)	C(7A)-C(6A)-C(12A)-C(13A)	-56.7(2)
C(1)-N(1)-C(10)-C(7)	7.1(3)	C(3A)-C(6A)-C(12A)-C(13A)	65.0(2)
C(1)-N(1)-C(10)-C(11)	-172.77(17)	C(7A)-C(6A)-C(12A)-C(17A)	130.14(19)
C(7)-C(6)-C(12)-C(13)	-54.7(2)	C(3A)-C(6A)-C(12A)-C(17A)	-108.2(2)
C(3)-C(6)-C(12)-C(13)	68.1(2)	C(17A)-C(12A)-C(13A)-C(14A)	-1.0(3)
C(7)-C(6)-C(12)-C(17)	129.40(19)	C(6A)-C(12A)-C(13A)-C(14A)	-174.90(18)
C(3)-C(6)-C(12)-C(17)	-107.8(2)	C(12A)-C(13A)-C(14A)-C(15A)	1.8(3)
C(17)-C(12)-C(13)-C(14)	-0.4(3)	C(13A)-C(14A)-C(15A)-C(16A)	-0.4(3)
C(6)-C(12)-C(13)-C(14)	-176.72(17)	C(14A)-C(15A)-C(16A)-C(17A)	-1.7(3)
C(12)-C(13)-C(14)-C(15)	1.2(3)	C(15A)-C(16A)-C(17A)-C(12A)	2.6(3)
C(13)-C(14)-C(15)-C(16)	-0.2(3)	C(15A)-C(16A)-C(17A)-N(2A)	-177.67(18)
C(14)-C(15)-C(16)-C(17)	-1.4(3)	C(13A)-C(12A)-C(17A)-C(16A)	-1.2(3)
C(15)-C(16)-C(17)-C(12)	2.3(3)	C(6A)-C(12A)-C(17A)-C(16A)	172.05(18)
C(15)-C(16)-C(17)-N(2)	-178.31(17)	C(13A)-C(12A)-C(17A)-N(2A)	179.05(17)
C(13)-C(12)-C(17)-C(16)	-1.3(3)	C(6A)-C(12A)-C(17A)-N(2A)	-7.7(3)
C(6)-C(12)-C(17)-C(16)	174.66(17)	O(5A)-N(2A)-C(17A)-C(16A)	149.57(18)
C(13)-C(12)-C(17)-N(2)	179.27(16)	O(6A)-N(2A)-C(17A)-C(16A)	-28.0(2)
C(6)-C(12)-C(17)-N(2)	-4.7(3)	O(5A)-N(2A)-C(17A)-C(12A)	-30.7(3)
O(5)-N(2)-C(17)-C(16)	141.34(18)	O(6A)-N(2A)-C(17A)-C(12A)	151.76(18)
O(6)-N(2)-C(17)-C(16)	-36.1(2)		
O(5)-N(2)-C(17)-C(12)	-39.2(3)		
O(6)-N(2)-C(17)-C(12)	143.28(18)		
C(10A)-N(1A)-C(1A)-C(3A)	-5.1(3)		
C(10A)-N(1A)-C(1A)-C(2A)	174.80(17)		
N(1A)-C(1A)-C(3A)-C(4A)	178.39(17)		

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for β NIF solved at 100 K [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3A)#1	0.91(2)	2.09(2)	2.993(2)	172(2)
N(1A)-H(1A)...O(3)#2	0.86(2)	2.19(2)	3.033(2)	167(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+2 #2 -x+1,-y+1,-z+1

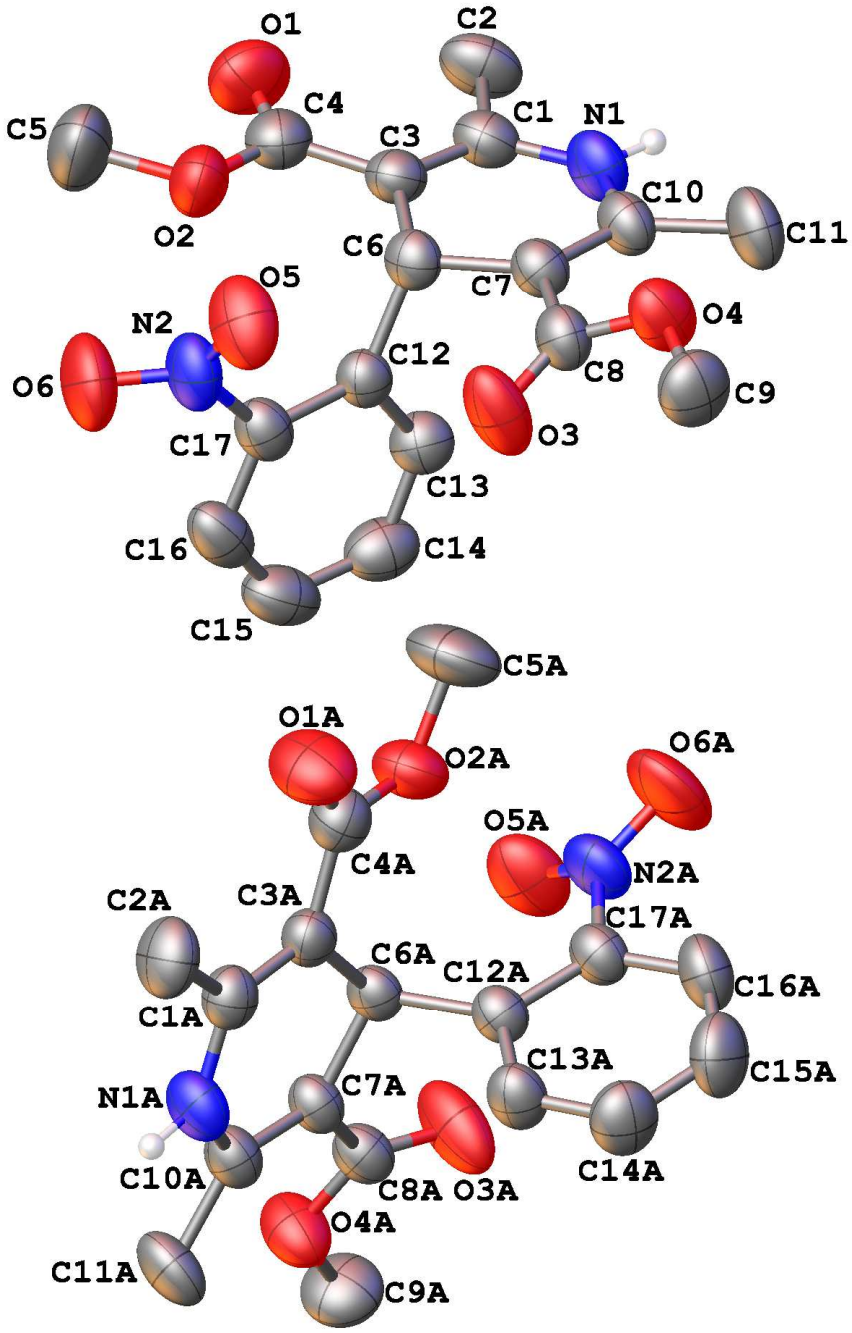

Figure S3. A molecular drawing of β NIF solved at 298 K. All H atoms connected to C atoms are omitted.

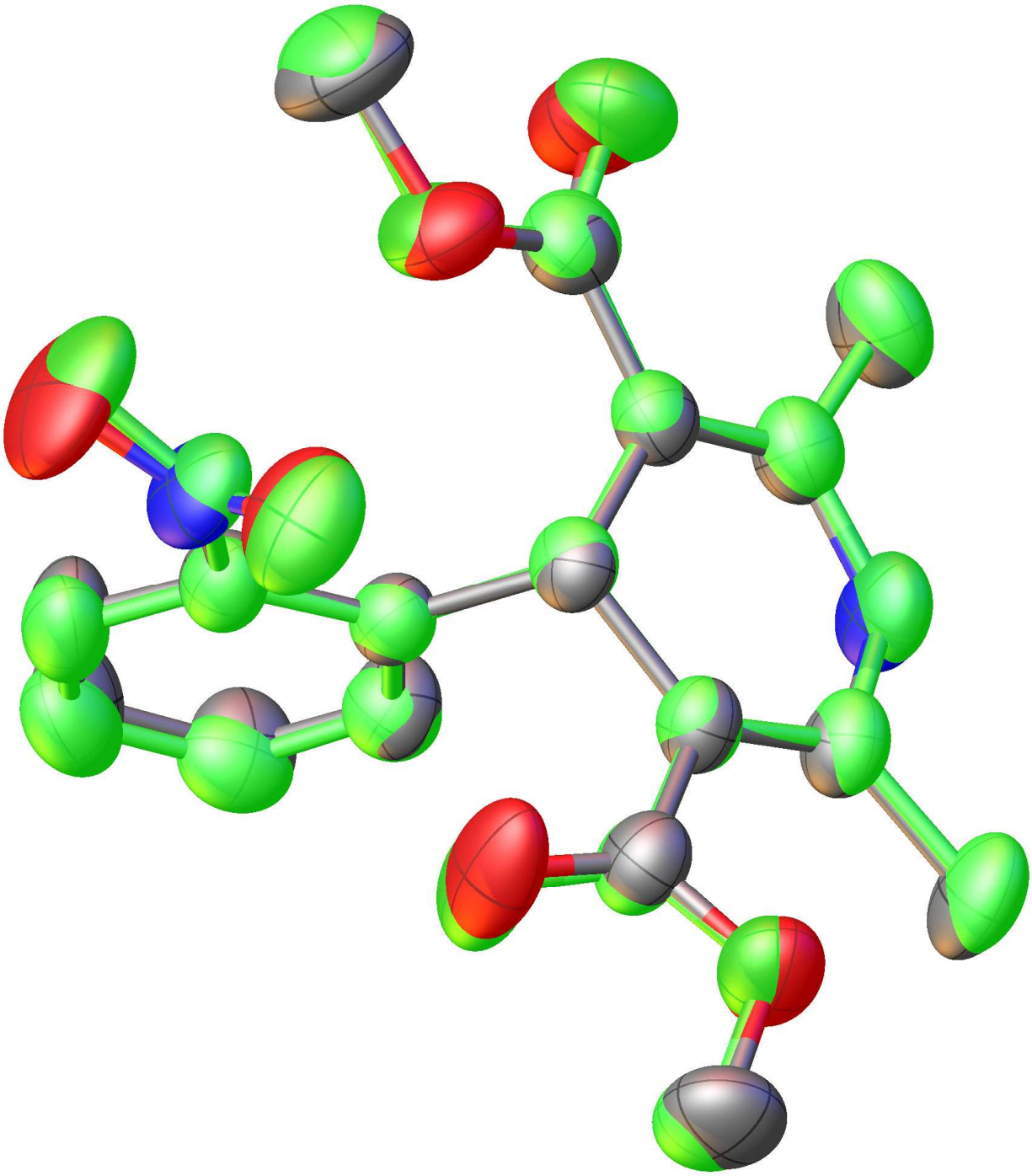

Figure S4. An overlay of the two molecules of β NIF solved at 298 K.

Table S8. Crystal data and structure refinement for β NIF solved at 298 K

Identification code	yu03rt	
Empirical formula	$C_{17}\ H_{18}\ N_2\ O_6$	
Formula weight	346.33	
Temperature	298(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.840(3) Å	α= 61.390(19)°.
	b = 13.807(4) Å	β= 79.76(2)°.
	c = 14.206(4) Å	γ = 81.99(2)°.
Volume	1664.1(9) $Å^3$	
Z	4	
Density (calculated)	1.382 Mg/m^3	
Absorption coefficient	0.106 mm^{-1}	
F(000)	728	
Crystal size	0.14 x 0.08 x 0.03 mm^3	
Theta range for data collection	1.65 to 26.56°.	
Index ranges	-12<=h<=11, -17<=k<=17, -17<=l<=17	
Reflections collected	19767	
Independent reflections	6804 [R(int) = 0.0541]	
Completeness to theta = 25.00°	99.3 %	
Absorption correction	Numerical with SADABS	
Max. and min. transmission	0.9968 and 0.9853	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6804 / 0 / 467	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0547, wR2 = 0.1263	
R indices (all data)	R1 = 0.1358, wR2 = 0.1602	
Largest diff. peak and hole	0.193 and -0.179 $e.Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for β NIF solved at 298 K. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-2431(2)	912(2)	7559(2)	89(1)
O(2)	-1654(2)	2182(2)	5902(2)	76(1)
O(3)	2950(2)	1575(2)	3938(2)	85(1)
O(4)	3300(2)	-139(2)	4202(2)	71(1)
O(5)	269(2)	3101(2)	3601(2)	85(1)
O(6)	-421(3)	4404(2)	4011(2)	96(1)
N(1)	1051(3)	-1139(2)	7274(2)	61(1)
N(2)	269(3)	3556(2)	4147(2)	65(1)
C(1)	-54(3)	-496(2)	7431(2)	55(1)
C(2)	-901(3)	-1073(2)	8526(2)	74(1)
C(3)	-298(3)	535(2)	6649(2)	51(1)
C(4)	-1547(3)	1182(3)	6788(3)	63(1)
C(5)	-2871(4)	2877(3)	5975(4)	112(1)
C(6)	718(3)	1057(2)	5624(2)	48(1)
C(7)	1779(3)	203(2)	5503(2)	48(1)
C(8)	2720(3)	617(2)	4490(2)	54(1)
C(9)	4329(3)	211(3)	3270(3)	76(1)
C(10)	1918(3)	-842(2)	6316(2)	54(1)
C(11)	2937(3)	-1761(2)	6331(2)	72(1)
C(12)	1422(3)	1968(2)	5632(2)	46(1)
C(13)	2334(3)	1656(2)	6390(2)	55(1)
C(14)	2971(3)	2418(3)	6491(3)	66(1)
C(15)	2708(3)	3530(3)	5848(3)	73(1)
C(16)	1804(3)	3874(2)	5107(3)	66(1)
C(17)	1202(3)	3098(2)	4995(2)	52(1)
O(1A)	4261(3)	3636(2)	7682(2)	92(1)
O(2A)	4798(2)	2516(2)	9340(2)	70(1)
O(3A)	8153(3)	3433(2)	10989(2)	93(1)
O(4A)	7898(2)	5158(2)	10681(2)	73(1)
O(5A)	6380(3)	1639(2)	11337(2)	87(1)
O(6A)	6730(3)	311(2)	10960(2)	110(1)
N(1A)	6427(3)	6031(2)	7780(2)	60(1)
N(2A)	6903(3)	1246(2)	10754(2)	65(1)
C(1A)	5702(3)	5310(2)	7694(2)	52(1)
C(2A)	5004(3)	5830(3)	6687(2)	73(1)
C(3A)	5658(3)	4255(2)	8476(2)	48(1)
C(4A)	4839(3)	3494(2)	8420(3)	59(1)
C(5A)	4097(4)	1668(3)	9344(3)	100(1)
C(6A)	6536(2)	3800(2)	9404(2)	44(1)
C(7A)	7082(3)	4727(2)	9478(2)	46(1)
C(8A)	7757(3)	4371(2)	10441(2)	51(1)
C(9A)	8674(3)	4878(3)	11556(3)	82(1)
C(10A)	7034(3)	5779(2)	8681(2)	52(1)
C(11A)	7576(3)	6766(2)	8623(2)	71(1)
C(12A)	7704(3)	3035(2)	9213(2)	45(1)
C(13A)	8695(3)	3518(2)	8329(2)	56(1)
C(14A)	9739(3)	2921(3)	8021(2)	70(1)
C(15A)	9820(3)	1787(3)	8595(3)	75(1)
C(16A)	8855(3)	1276(2)	9461(3)	67(1)
C(17A)	7837(3)	1890(2)	9773(2)	51(1)

Table S10. Bond lengths [Å] and angles [°] for β NIF solved at 298 K.

O(1)-C(4)	1.207(3)	O(1A)-C(4A)	1.202(3)
O(2)-C(4)	1.358(4)	O(2A)-C(4A)	1.356(3)
O(2)-C(5)	1.448(4)	O(2A)-C(5A)	1.436(3)
O(3)-C(8)	1.201(3)	O(3A)-C(8A)	1.199(3)
O(4)-C(8)	1.320(3)	O(4A)-C(8A)	1.316(3)
O(4)-C(9)	1.436(3)	O(4A)-C(9A)	1.439(3)
O(5)-N(2)	1.209(3)	O(5A)-N(2A)	1.202(3)
O(6)-N(2)	1.216(3)	O(6A)-N(2A)	1.210(3)
N(1)-C(1)	1.361(4)	N(1A)-C(1A)	1.365(4)
N(1)-C(10)	1.378(4)	N(1A)-C(10A)	1.379(4)
N(1)-H(1)	0.82(3)	N(1A)-H(1A)	0.84(3)
N(2)-C(17)	1.481(4)	N(2A)-C(17A)	1.471(4)
C(1)-C(3)	1.343(4)	C(1A)-C(3A)	1.344(4)
C(1)-C(2)	1.512(4)	C(1A)-C(2A)	1.504(4)
C(2)-H(2A)	0.9600	C(2A)-H(2AA)	0.9600
C(2)-H(2B)	0.9600	C(2A)-H(2AB)	0.9600
C(2)-H(2C)	0.9600	C(2A)-H(2AC)	0.9600
C(3)-C(4)	1.457(4)	C(3A)-C(4A)	1.449(4)
C(3)-C(6)	1.522(4)	C(3A)-C(6A)	1.530(4)
C(5)-H(5A)	0.9600	C(5A)-H(5AA)	0.9600
C(5)-H(5B)	0.9600	C(5A)-H(5AB)	0.9600
C(5)-H(5C)	0.9600	C(5A)-H(5AC)	0.9600
C(6)-C(7)	1.516(3)	C(6A)-C(7A)	1.509(3)
C(6)-C(12)	1.523(3)	C(6A)-C(12A)	1.529(3)
C(6)-H(6)	0.9800	C(6A)-H(6A)	0.9800
C(7)-C(10)	1.356(4)	C(7A)-C(10A)	1.349(4)
C(7)-C(8)	1.463(4)	C(7A)-C(8A)	1.464(4)
C(9)-H(9A)	0.9600	C(9A)-H(9AA)	0.9600
C(9)-H(9B)	0.9600	C(9A)-H(9AB)	0.9600
C(9)-H(9C)	0.9600	C(9A)-H(9AC)	0.9600
C(10)-C(11)	1.498(4)	C(10A)-C(11A)	1.493(4)
C(11)-H(11A)	0.9600	C(11A)-H(11D)	0.9600
C(11)-H(11B)	0.9600	C(11A)-H(11E)	0.9600
C(11)-H(11C)	0.9600	C(11A)-H(11F)	0.9600
C(12)-C(17)	1.387(4)	C(12A)-C(13A)	1.384(3)
C(12)-C(13)	1.393(4)	C(12A)-C(17A)	1.386(3)
C(13)-C(14)	1.372(4)	C(13A)-C(14A)	1.370(4)
C(13)-H(13)	0.9300	C(13A)-H(13A)	0.9300
C(14)-C(15)	1.375(4)	C(14A)-C(15A)	1.374(4)
C(14)-H(14)	0.9300	C(14A)-H(14A)	0.9300
C(15)-C(16)	1.364(4)	C(15A)-C(16A)	1.361(4)
C(15)-H(15)	0.9300	C(15A)-H(15A)	0.9300
C(16)-C(17)	1.378(4)	C(16A)-C(17A)	1.373(4)
C(16)-H(16)	0.9300	C(16A)-H(16A)	0.9300
C(4)-O(2)-C(5)	115.1(3)		
C(8)-O(4)-C(9)	117.2(2)	C(3)-C(1)-C(2)	126.8(3)
C(1)-N(1)-C(10)	124.4(3)	N(1)-C(1)-C(2)	113.1(3)
C(1)-N(1)-H(1)	120(2)	C(1)-C(2)-H(2A)	109.5
C(10)-N(1)-H(1)	115(2)	C(1)-C(2)-H(2B)	109.5
O(5)-N(2)-O(6)	123.4(3)	H(2A)-C(2)-H(2B)	109.5
O(5)-N(2)-C(17)	119.1(2)	C(1)-C(2)-H(2C)	109.5
O(6)-N(2)-C(17)	117.4(3)	H(2A)-C(2)-H(2C)	109.5
C(3)-C(1)-N(1)	120.1(3)	H(2B)-C(2)-H(2C)	109.5

C(1)-C(3)-C(4)	119.6(3)	C(12)-C(17)-N(2)	121.6(3)
C(1)-C(3)-C(6)	121.4(2)	C(4A)-O(2A)-C(5A)	116.1(2)
C(4)-C(3)-C(6)	118.9(2)	C(8A)-O(4A)-C(9A)	117.6(2)
O(1)-C(4)-O(2)	120.8(3)	C(1A)-N(1A)-C(10A)	123.9(3)
O(1)-C(4)-C(3)	127.6(3)	C(1A)-N(1A)-H(1A)	121(2)
O(2)-C(4)-C(3)	111.6(3)	C(10A)-N(1A)-H(1A)	115(2)
O(2)-C(5)-H(5A)	109.5	O(5A)-N(2A)-O(6A)	122.4(3)
O(2)-C(5)-H(5B)	109.5	O(5A)-N(2A)-C(17A)	120.0(2)
H(5A)-C(5)-H(5B)	109.5	O(6A)-N(2A)-C(17A)	117.5(3)
O(2)-C(5)-H(5C)	109.5	C(3A)-C(1A)-N(1A)	119.8(3)
H(5A)-C(5)-H(5C)	109.5	C(3A)-C(1A)-C(2A)	126.9(3)
H(5B)-C(5)-H(5C)	109.5	N(1A)-C(1A)-C(2A)	113.3(3)
C(7)-C(6)-C(3)	111.5(2)	C(1A)-C(2A)-H(2AA)	109.5
C(7)-C(6)-C(12)	110.9(2)	C(1A)-C(2A)-H(2AB)	109.5
C(3)-C(6)-C(12)	109.6(2)	H(2AA)-C(2A)-H(2AB)	109.5
C(7)-C(6)-H(6)	108.2	C(1A)-C(2A)-H(2AC)	109.5
C(3)-C(6)-H(6)	108.2	H(2AA)-C(2A)-H(2AC)	109.5
C(12)-C(6)-H(6)	108.2	H(2AB)-C(2A)-H(2AC)	109.5
C(10)-C(7)-C(8)	122.6(2)	C(1A)-C(3A)-C(4A)	120.4(3)
C(10)-C(7)-C(6)	122.0(2)	C(1A)-C(3A)-C(6A)	121.6(2)
C(8)-C(7)-C(6)	115.1(2)	C(4A)-C(3A)-C(6A)	117.9(2)
O(3)-C(8)-O(4)	121.2(3)	O(1A)-C(4A)-O(2A)	120.6(3)
O(3)-C(8)-C(7)	123.5(3)	O(1A)-C(4A)-C(3A)	128.1(3)
O(4)-C(8)-C(7)	115.3(2)	O(2A)-C(4A)-C(3A)	111.3(3)
O(4)-C(9)-H(9A)	109.5	O(2A)-C(5A)-H(5AA)	109.5
O(4)-C(9)-H(9B)	109.5	O(2A)-C(5A)-H(5AB)	109.5
H(9A)-C(9)-H(9B)	109.5	H(5AA)-C(5A)-H(5AB)	109.5
O(4)-C(9)-H(9C)	109.5	O(2A)-C(5A)-H(5AC)	109.5
H(9A)-C(9)-H(9C)	109.5	H(5AA)-C(5A)-H(5AC)	109.5
H(9B)-C(9)-H(9C)	109.5	H(5AB)-C(5A)-H(5AC)	109.5
C(7)-C(10)-N(1)	118.9(3)	C(7A)-C(6A)-C(12A)	111.9(2)
C(7)-C(10)-C(11)	128.2(3)	C(7A)-C(6A)-C(3A)	110.9(2)
N(1)-C(10)-C(11)	112.9(2)	C(12A)-C(6A)-C(3A)	107.8(2)
C(10)-C(11)-H(11A)	109.5	C(7A)-C(6A)-H(6A)	108.7
C(10)-C(11)-H(11B)	109.5	C(12A)-C(6A)-H(6A)	108.7
H(11A)-C(11)-H(11B)	109.5	C(3A)-C(6A)-H(6A)	108.7
C(10)-C(11)-H(11C)	109.5	C(10A)-C(7A)-C(8A)	123.3(2)
H(11A)-C(11)-H(11C)	109.5	C(10A)-C(7A)-C(6A)	122.2(2)
H(11B)-C(11)-H(11C)	109.5	C(8A)-C(7A)-C(6A)	114.4(2)
C(17)-C(12)-C(13)	115.4(3)	O(3A)-C(8A)-O(4A)	121.2(3)
C(17)-C(12)-C(6)	126.8(2)	O(3A)-C(8A)-C(7A)	123.5(3)
C(13)-C(12)-C(6)	117.7(2)	O(4A)-C(8A)-C(7A)	115.3(2)
C(14)-C(13)-C(12)	122.0(3)	O(4A)-C(9A)-H(9AA)	109.5
C(14)-C(13)-H(13)	119.0	O(4A)-C(9A)-H(9AB)	109.5
C(12)-C(13)-H(13)	119.0	H(9AA)-C(9A)-H(9AB)	109.5
C(13)-C(14)-C(15)	120.4(3)	O(4A)-C(9A)-H(9AC)	109.5
C(13)-C(14)-H(14)	119.8	H(9AA)-C(9A)-H(9AC)	109.5
C(15)-C(14)-H(14)	119.8	H(9AB)-C(9A)-H(9AC)	109.5
C(16)-C(15)-C(14)	119.6(3)	C(7A)-C(10A)-N(1A)	119.4(3)
C(16)-C(15)-H(15)	120.2	C(7A)-C(10A)-C(11A)	128.2(3)
C(14)-C(15)-H(15)	120.2	N(1A)-C(10A)-C(11A)	112.5(2)
C(15)-C(16)-C(17)	119.3(3)	C(10A)-C(11A)-H(11D)	109.5
C(15)-C(16)-H(16)	120.4	C(10A)-C(11A)-H(11E)	109.5
C(17)-C(16)-H(16)	120.4	H(11D)-C(11A)-H(11E)	109.5
C(16)-C(17)-C(12)	123.3(3)	C(10A)-C(11A)-H(11F)	109.5
C(16)-C(17)-N(2)	115.1(3)	H(11D)-C(11A)-H(11F)	109.5

H(11E)-C(11A)-H(11F)	109.5	C(16A)-C(15A)-C(14A)	119.3(3)
C(13A)-C(12A)-C(17A)	115.2(2)	C(16A)-C(15A)-H(15A)	120.4
C(13A)-C(12A)-C(6A)	117.1(2)	C(14A)-C(15A)-H(15A)	120.4
C(17A)-C(12A)-C(6A)	127.5(2)	C(15A)-C(16A)-C(17A)	120.2(3)
C(14A)-C(13A)-C(12A)	123.1(3)	C(15A)-C(16A)-H(16A)	119.9
C(14A)-C(13A)-H(13A)	118.4	C(17A)-C(16A)-H(16A)	119.9
C(12A)-C(13A)-H(13A)	118.4	C(16A)-C(17A)-C(12A)	122.6(3)
C(13A)-C(14A)-C(15A)	119.6(3)	C(16A)-C(17A)-N(2A)	115.1(2)
C(13A)-C(14A)-H(14A)	120.2	C(12A)-C(17A)-N(2A)	122.3(2)
C(15A)-C(14A)-H(14A)	120.2		

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for β NIF solved at 298 K. 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)	71(2)	99(2)	90(2)	-46(2)	16(1)	-16(1)
O(2)	56(1)	62(1)	96(2)	-30(1)	-7(1)	7(1)
O(3)	123(2)	44(1)	62(1)	-12(1)	18(1)	-4(1)
O(4)	80(1)	59(1)	68(1)	-31(1)	14(1)	-8(1)
O(5)	122(2)	71(2)	59(1)	-25(1)	-37(1)	20(1)
O(6)	116(2)	58(1)	98(2)	-27(1)	-33(2)	33(1)
N(1)	80(2)	39(2)	48(2)	-6(1)	-9(1)	-2(1)
N(2)	80(2)	43(2)	54(2)	-10(1)	-10(1)	10(1)
C(1)	62(2)	50(2)	52(2)	-21(2)	-7(2)	-12(2)
C(2)	89(2)	65(2)	60(2)	-19(2)	6(2)	-31(2)
C(3)	50(2)	48(2)	54(2)	-22(2)	-6(1)	-9(1)
C(4)	57(2)	62(2)	73(2)	-32(2)	-11(2)	-7(2)
C(5)	72(2)	84(3)	155(4)	-45(3)	-2(2)	15(2)
C(6)	54(2)	43(2)	41(2)	-13(1)	-10(1)	-1(1)
C(7)	56(2)	43(2)	42(2)	-17(1)	-6(1)	-4(1)
C(8)	62(2)	44(2)	52(2)	-18(2)	-11(2)	3(1)
C(9)	70(2)	82(2)	70(2)	-37(2)	11(2)	-4(2)
C(10)	67(2)	39(2)	50(2)	-14(1)	-15(2)	-1(1)
C(11)	96(2)	43(2)	65(2)	-18(2)	-17(2)	12(2)
C(12)	49(2)	43(2)	42(2)	-17(1)	-2(1)	-3(1)
C(13)	58(2)	57(2)	46(2)	-21(1)	-6(1)	-6(1)
C(14)	60(2)	85(3)	63(2)	-41(2)	-5(2)	-12(2)
C(15)	75(2)	76(3)	82(2)	-47(2)	6(2)	-26(2)
C(16)	77(2)	49(2)	67(2)	-28(2)	12(2)	-14(2)
C(17)	60(2)	44(2)	46(2)	-18(1)	0(1)	-4(1)
O(1A)	110(2)	88(2)	85(2)	-34(1)	-42(2)	-14(1)
O(2A)	76(1)	61(1)	72(2)	-26(1)	-10(1)	-22(1)
O(3A)	162(2)	45(1)	66(2)	-12(1)	-52(2)	5(1)
O(4A)	98(2)	59(1)	70(1)	-30(1)	-36(1)	1(1)
O(5A)	118(2)	64(2)	56(1)	-14(1)	16(1)	-24(1)
O(6A)	142(2)	45(1)	117(2)	-19(1)	13(2)	-34(1)
N(1A)	82(2)	40(2)	47(2)	-9(1)	-14(1)	-3(1)
N(2A)	82(2)	39(2)	58(2)	-7(1)	-8(1)	-14(1)
C(1A)	53(2)	51(2)	46(2)	-20(2)	-5(1)	3(1)
C(2A)	79(2)	66(2)	61(2)	-18(2)	-25(2)	15(2)
C(3A)	46(2)	45(2)	49(2)	-20(1)	-4(1)	-1(1)
C(4A)	57(2)	59(2)	60(2)	-27(2)	-9(2)	-1(2)
C(5A)	117(3)	78(2)	106(3)	-33(2)	-19(2)	-44(2)
C(6A)	51(2)	37(1)	38(2)	-11(1)	-2(1)	-6(1)
C(7A)	56(2)	37(2)	39(2)	-15(1)	-3(1)	-4(1)
C(8A)	62(2)	44(2)	44(2)	-16(2)	-3(1)	-9(1)
C(9A)	88(2)	96(3)	75(2)	-42(2)	-32(2)	-7(2)
C(10A)	62(2)	41(2)	49(2)	-17(1)	-4(1)	-4(1)
C(11A)	107(3)	37(2)	64(2)	-17(2)	-15(2)	-9(2)
C(12A)	54(2)	40(2)	38(2)	-15(1)	-6(1)	-4(1)
C(13A)	63(2)	45(2)	48(2)	-14(1)	2(2)	-5(1)
C(14A)	69(2)	71(2)	61(2)	-28(2)	7(2)	-3(2)
C(15A)	81(2)	70(2)	76(2)	-41(2)	-7(2)	18(2)
C(16A)	84(2)	44(2)	68(2)	-25(2)	-14(2)	10(2)
C(17A)	61(2)	41(2)	46(2)	-15(1)	-9(1)	-4(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for β NIF solved at 298 K.

	x	y	z	U(eq)
H(1)	1190(30)	-1780(20)	7750(20)	62(9)
H(2A)	-978	-634	8893	112
H(2B)	-456	-1783	8946	112
H(2C)	-1808	-1169	8433	112
H(5A)	-2835	3580	5336	168
H(5B)	-2899	2984	6598	168
H(5C)	-3685	2528	6040	168
H(6)	197	1393	5003	58
H(9A)	5086	485	3398	114
H(9B)	3930	787	2654	114
H(9C)	4661	-403	3134	114
H(11A)	3771	-1457	5869	108
H(11B)	2548	-2180	6077	108
H(11C)	3143	-2234	7055	108
H(13)	2516	908	6841	66
H(14)	3585	2181	6998	80
H(15)	3143	4045	5917	88
H(16)	1597	4625	4682	79
H(1A)	6510(30)	6680(30)	7280(20)	73(10)
H(2AA)	5258	5402	6306	110
H(2AB)	5290	6569	6232	110
H(2AC)	4019	5851	6881	110
H(5AA)	4606	1443	8831	149
H(5AB)	3185	1950	9151	149
H(5AC)	4033	1045	10053	149
H(6A)	5957	3366	10083	53
H(9AA)	9646	4880	11302	123
H(9AB)	8457	4157	12129	123
H(9AC)	8435	5412	11819	123
H(11D)	7731	7320	7881	107
H(11E)	8431	6556	8928	107
H(11F)	6914	7058	9021	107
H(13A)	8649	4284	7926	68
H(14A)	10389	3282	7426	84
H(15A)	10526	1374	8395	91
H(16A)	8887	508	9843	80

Table S13. Torsion angles [°] for β NIF solved at 298 K.

C(10)-N(1)-C(1)-C(3)	-5.0(4)	C(10A)-N(1A)-C(1A)-C(3A)	-6.3(4)
C(10)-N(1)-C(1)-C(2)	174.6(3)	C(10A)-N(1A)-C(1A)-C(2A)	173.0(2)
N(1)-C(1)-C(3)-C(4)	174.8(2)	N(1A)-C(1A)-C(3A)-C(4A)	177.1(2)
C(2)-C(1)-C(3)-C(4)	-4.7(4)	C(2A)-C(1A)-C(3A)-C(4A)	-2.1(4)
N(1)-C(1)-C(3)-C(6)	-6.6(4)	N(1A)-C(1A)-C(3A)-C(6A)	-7.1(4)
C(2)-C(1)-C(3)-C(6)	173.9(3)	C(2A)-C(1A)-C(3A)-C(6A)	173.7(2)
C(5)-O(2)-C(4)-O(1)	1.0(4)	C(5A)-O(2A)-C(4A)-O(1A)	3.1(4)
C(5)-O(2)-C(4)-C(3)	179.9(3)	C(5A)-O(2A)-C(4A)-C(3A)	-175.6(2)
C(1)-C(3)-C(4)-O(1)	1.4(5)	C(1A)-C(3A)-C(4A)-O(1A)	8.6(5)
C(6)-C(3)-C(4)-O(1)	-177.3(3)	C(6A)-C(3A)-C(4A)-O(1A)	-167.3(3)
C(1)-C(3)-C(4)-O(2)	-177.4(2)	C(1A)-C(3A)-C(4A)-O(2A)	-172.7(2)
C(6)-C(3)-C(4)-O(2)	4.0(4)	C(6A)-C(3A)-C(4A)-O(2A)	11.3(3)
C(1)-C(3)-C(6)-C(7)	13.7(3)	C(1A)-C(3A)-C(6A)-C(7A)	15.8(3)
C(4)-C(3)-C(6)-C(7)	-167.7(2)	C(4A)-C(3A)-C(6A)-C(7A)	-168.3(2)
C(1)-C(3)-C(6)-C(12)	-109.5(3)	C(1A)-C(3A)-C(6A)-C(12A)	-107.0(3)
C(4)-C(3)-C(6)-C(12)	69.1(3)	C(4A)-C(3A)-C(6A)-C(12A)	68.8(3)
C(3)-C(6)-C(7)-C(10)	-11.0(3)	C(12A)-C(6A)-C(7A)-C(10A)	107.2(3)
C(12)-C(6)-C(7)-C(10)	111.5(3)	C(3A)-C(6A)-C(7A)-C(10A)	-13.2(3)
C(3)-C(6)-C(7)-C(8)	174.6(2)	C(12A)-C(6A)-C(7A)-C(8A)	-68.3(3)
C(12)-C(6)-C(7)-C(8)	-62.9(3)	C(3A)-C(6A)-C(7A)-C(8A)	171.3(2)
C(9)-O(4)-C(8)-O(3)	6.7(4)	C(9A)-O(4A)-C(8A)-O(3A)	6.4(4)
C(9)-O(4)-C(8)-C(7)	-174.2(2)	C(9A)-O(4A)-C(8A)-C(7A)	-174.1(2)
C(10)-C(7)-C(8)-O(3)	-152.8(3)	C(10A)-C(7A)-C(8A)-O(3A)	-158.1(3)
C(6)-C(7)-C(8)-O(3)	21.6(4)	C(6A)-C(7A)-C(8A)-O(3A)	17.4(4)
C(10)-C(7)-C(8)-O(4)	28.1(4)	C(10A)-C(7A)-C(8A)-O(4A)	22.4(4)
C(6)-C(7)-C(8)-O(4)	-157.5(2)	C(6A)-C(7A)-C(8A)-O(4A)	-162.2(2)
C(8)-C(7)-C(10)-N(1)	175.2(2)	C(8A)-C(7A)-C(10A)-N(1A)	177.2(2)
C(6)-C(7)-C(10)-N(1)	1.3(4)	C(6A)-C(7A)-C(10A)-N(1A)	2.1(4)
C(8)-C(7)-C(10)-C(11)	-4.0(5)	C(8A)-C(7A)-C(10A)-C(11A)	-2.4(4)
C(6)-C(7)-C(10)-C(11)	-178.0(3)	C(6A)-C(7A)-C(10A)-C(11A)	-177.5(3)
C(1)-N(1)-C(10)-C(7)	7.8(4)	C(1A)-N(1A)-C(10A)-C(7A)	8.9(4)
C(1)-N(1)-C(10)-C(11)	-172.9(3)	C(1A)-N(1A)-C(10A)-C(11A)	-171.4(2)
C(7)-C(6)-C(12)-C(17)	128.4(3)	C(7A)-C(6A)-C(12A)-C(13A)	-55.2(3)
C(3)-C(6)-C(12)-C(17)	-108.1(3)	C(3A)-C(6A)-C(12A)-C(13A)	67.1(3)
C(7)-C(6)-C(12)-C(13)	-55.1(3)	C(7A)-C(6A)-C(12A)-C(17A)	130.6(3)
C(3)-C(6)-C(12)-C(13)	68.5(3)	C(3A)-C(6A)-C(12A)-C(17A)	-107.1(3)
C(17)-C(12)-C(13)-C(14)	-0.2(4)	C(17A)-C(12A)-C(13A)-C(14A)	-0.2(4)
C(6)-C(12)-C(13)-C(14)	-177.1(2)	C(6A)-C(12A)-C(13A)-C(14A)	-175.2(3)
C(12)-C(13)-C(14)-C(15)	1.0(4)	C(12A)-C(13A)-C(14A)-C(15A)	0.8(5)
C(13)-C(14)-C(15)-C(16)	0.1(4)	C(13A)-C(14A)-C(15A)-C(16A)	0.2(5)
C(14)-C(15)-C(16)-C(17)	-1.9(4)	C(14A)-C(15A)-C(16A)-C(17A)	-1.8(5)
C(15)-C(16)-C(17)-C(12)	2.7(4)	C(15A)-C(16A)-C(17A)-C(12A)	2.5(5)
C(15)-C(16)-C(17)-N(2)	-178.3(3)	C(15A)-C(16A)-C(17A)-N(2A)	-176.8(3)
C(13)-C(12)-C(17)-C(16)	-1.6(4)	C(13A)-C(12A)-C(17A)-C(16A)	-1.4(4)
C(6)-C(12)-C(17)-C(16)	175.0(2)	C(6A)-C(12A)-C(17A)-C(16A)	172.9(3)
C(13)-C(12)-C(17)-N(2)	179.4(2)	C(13A)-C(12A)-C(17A)-N(2A)	177.7(2)
C(6)-C(12)-C(17)-N(2)	-4.0(4)	C(6A)-C(12A)-C(17A)-N(2A)	-7.9(4)
O(5)-N(2)-C(17)-C(16)	141.5(3)	O(5A)-N(2A)-C(17A)-C(16A)	149.9(3)
O(6)-N(2)-C(17)-C(16)	-35.6(4)	O(6A)-N(2A)-C(17A)-C(16A)	-27.8(4)
O(5)-N(2)-C(17)-C(12)	-39.5(4)	O(5A)-N(2A)-C(17A)-C(12A)	-29.3(4)
O(6)-N(2)-C(17)-C(12)	143.4(3)	O(6A)-N(2A)-C(17A)-C(12A)	153.0(3)

Symmetry transformations used to generate equivalent atoms:

Table S14. Hydrogen bonds for β NIF solved at 298 K [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3A)#1	0.82(3)	2.22(3)	3.040(3)	173(3)
N(1A)-H(1A)...O(3)#2	0.84(3)	2.26(3)	3.093(3)	170(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+2 #2 -x+1,-y+1,-z+1