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分子间作用力构筑的具有柔性结构的醋氯芬酸多聚物：晶体结构，热稳定性，溶解度和 DFT 计算

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Intermolecular Interaction Induced Multi-Polymers of Aceclofenac with Flexible Conformation: Crystal Structure, Thermostability, Solubility and DFT Calculations

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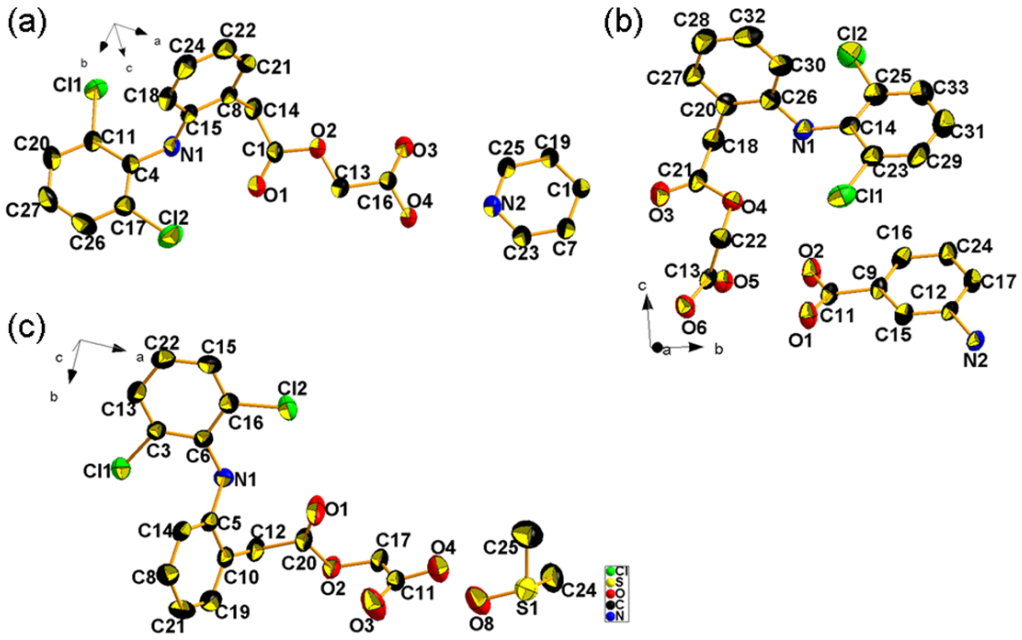

Fig.S1 ORTEP diagrams at 50% probability level for the compounds 1-3

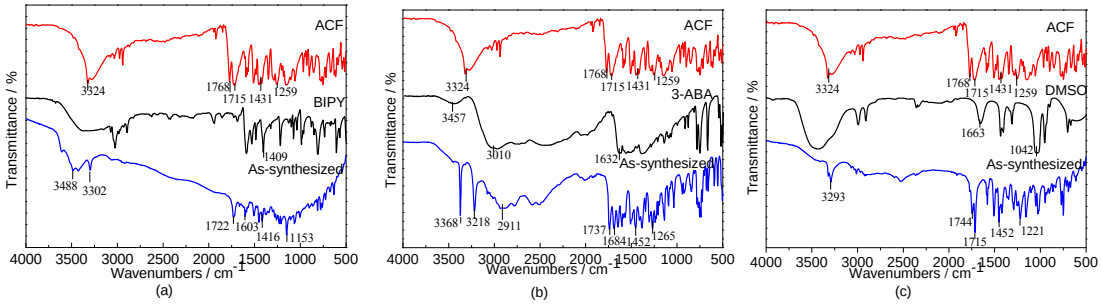

Fig.S2 IR spectra of compounds 1-3 and the starting components

(a) 1, (b) 2, (c) 3

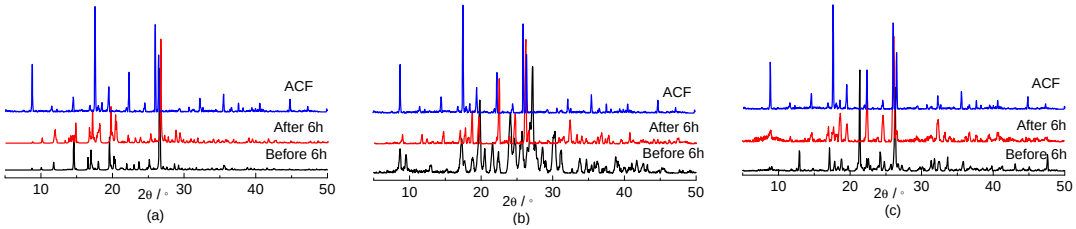

Fig.S3 PXRD patterns before and after 6h dissolution experiments in 25% ethanol-water medium for compounds 1-3 and ACF

(a) 1, (b) 2, (c) 3

Table S1 Hydrogen bonding distances (nm) and angles (°) for compounds 1-3

D–H···A	*d*(D–H)/nm	*d*(H···A)/nm	*d*(D···A)/nm	(D–H···A)/(°)
1[a]				
O(4)–H(4)···N(2)	0.0882	0.1713	0.2595	177.87
N(1)–H(1A)···O(1) #1	0.0818	0.2197	0.2935	150.20
2[b]				
N(1)-H(1B)...O(6)#1	0.091(2)	0.255(5)	0.2921(6)	105(4)
N(1)-H(1B)...O(6)#2	0.091(2)	0.194(2)	0.2822(6)	165(5)
N(1)-H(1A)...O(1)#1	0.0919(19)	0.211(3)	0.2924(7)	147(5)
O(2)–H(2A)···O(5)	0.0826(10)	0.1832(19)	0.2647(6)	168(7)
N(2)–H(2)···O(4)	0.088(2)	0.233(4)	0.3063(7)	140(5)
N(1)–H(1C)···O(5)	0.0903(3)	0.185(3)	0.2744(5)	169.3(4)
3[c]				
O(4)–H(4)···O(5) #1	0.0824(10)	0.1789(14)	0.2608(5)	173(6)
O(4)–H(4)···S(1) #1	0.0824(10)	0.290(3)	0.3616(4)	147(5)
N(1)–H(1)···O(1)	0.0899(10)	0.211(2)	0.2946(5)	130(1)

Symmetry codes: [a]#1 -*x*,-*y*+2,-z. [b]#1 -*x*+2, -*y*+1, *z*; #2 *x*+1, *y*+1, *z*; [c]#1 -*x*+1, *y*+1/2, -*z*+3/2. (D and A are hydrogen bond donors and acceptors).

Table S2 Δ*D*(C−O) of the C−O bond lengths (nm) for compounds 1-3

	1	**2**	**3**
C−O (long)/nm	0.1308(3)	0.1280(7)	0.1320(5)
C−O (short)/nm	0.1182(3)	0.1237(7)	0.1195(6)
Δ*D*(C−O)/nm	0.0126	0.0043	0.0125

Table S3 Torsion angles (°) in ACF crystal structures

Torsion Angles/(°)		**1**	**2**	**3**
τ_1	C(3)N(1)C(7)C(8)	-74.1(3)	69.7(9)	-52.1(6)
τ_2	C(4)C(13)C(14)O(4)	-74.8(3)	107.4(8)	-54.8(8)
τ_3	C(15)O(3)C(14)O(4)	2.1(4)	-2.6(9)	-2.2(8)
τ_4	O(3)C(15)C(16)O(1)	175.8(2)	-158.3(5)	-172.9(4)

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C18 C19 1.369(4) . ?

C18 H18 0.9300 . ?
C19 C20 1.370(4) . ?
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C20 C21 1.376(3) . ?
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O1 C3 C4 125.5(2) . . ?
O2 C3 C4 111.9(2) . . ?
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C8 C7 H7 120.5 . . ?
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C7 C8 H8 119.8 . . ?
C8 C9 C10 120.7(2) . . ?
C8 C9 H9 119.6 . . ?
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C9 C10 C5 119.0(2) . . ?
C9 C10 N1 121.8(2) . . ?
C5 C10 N1 119.1(2) . . ?
C16 C11 C12 115.8(2) . . ?
C16 C11 N1 122.9(2) . . ?
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C13 C12 C11 122.2(2) . . ?
C13 C12 Cl1 117.91(19) . . ?
C11 C12 Cl1 119.90(19) . . ?
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C13 C14 C15 121.0(3) . . ?
C13 C14 H14 119.5 . . ?
C15 C14 H14 119.5 . . ?
C14 C15 C16 118.4(3) . . ?
C14 C15 H15 120.8 . . ?
C16 C15 H15 120.8 . . ?
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C11 C16 Cl2 118.33(19) . . ?
C15 C16 Cl2 118.7(2) . . ?
C17 N2 C21 117.3(2) . . ?
N2 C17 C18 123.5(3) . . ?
N2 C17 H17A 118.3 . . ?
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C19 C20 C21 120.4(2) . . ?
C19 C20 H20A 119.8 . . ?

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N1 H1A O1    0.82(3) 2.20(3) 2.935(3) 150(3) .

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 '-x, -y, -z'

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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O2 O 0.3456(9) 0.4355(4) 0.1138(2) 0.0550(13) Uani 1 1 d D . .
H2A H 0.311(15) 0.3589(13) 0.108(3) 0.082 Uiso 1 1 d D . .
N1 N 1.1567(10) 0.8273(5) 0.0121(2) 0.0356(12) Uani 1 1 d D . .
H1A H 1.277(9) 0.774(4) 0.000(2) 0.043 Uiso 1 1 d D . .
H1B H 1.267(9) 0.899(3) 0.024(2) 0.043 Uiso 1 1 d D . .
H1C H 1.063(10) 0.829(5) -0.0267(14) 0.043 Uiso 1 1 d D . .
C1 C 0.5682(12) 0.4648(6) 0.0818(3) 0.0381(15) Uani 1 1 d . . .
C2 C 0.6672(11) 0.5997(5) 0.0897(3) 0.0361(15) Uani 1 1 d . . .
C3 C 0.8682(11) 0.6498(5) 0.0513(3) 0.0348(15) Uani 1 1 d . . .
H3 H 0.9381 0.5979 0.0228 0.042 Uiso 1 1 calc R . .
C4 C 0.9613(11) 0.7758(5) 0.0560(3) 0.0310(14) Uani 1 1 d . . .
C5 C 0.8648(12) 0.8549(6) 0.0987(3) 0.0451(17) Uani 1 1 d . . .
H5 H 0.9290 0.9397 0.1010 0.054 Uiso 1 1 calc R . .
C6 C 0.6697(12) 0.8065(6) 0.1385(3) 0.0457(17) Uani 1 1 d . . .
H6 H 0.6079 0.8585 0.1683 0.055 Uiso 1 1 calc R . .
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C7 C 0.5704(12) 0.6812(6) 0.1331(3) 0.0406(16) Uani 1 1 d . . .
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Cl1 Cl 0.9889(4) 0.48629(18) 0.22394(9) 0.0643(6) Uani 1 1 d . . .
Cl2 Cl 0.4593(4) 0.58732(19) 0.42856(9) 0.0744(6) Uani 1 1 d . . .
O3 O 0.2429(10) 0.0235(4) 0.2295(2) 0.0672(15) Uani 1 1 d . . .
O4 O 0.4781(8) 0.2119(4) 0.21825(18) 0.0420(11) Uani 1 1 d . . .
O5 O 0.1686(8) 0.1937(4) 0.10174(18) 0.0396(10) Uani 1 1 d . . .
O6 O 0.4321(8) 0.0566(4) 0.0659(2) 0.0475(12) Uani 1 1 d . . .
N2 N 0.5926(11) 0.4225(5) 0.3207(2) 0.0483(15) Uani 1 1 d D . .
H2 H 0.552(13) 0.396(5) 0.2807(13) 0.058 Uiso 1 1 d D . .
C8 C 0.3805(12) 0.1339(6) 0.1061(3) 0.0376(15) Uani 1 1 d . . .
C9 C 0.5863(12) 0.1601(6) 0.1639(3) 0.0437(16) Uani 1 1 d . . .
H9A H 0.6574 0.0828 0.1754 0.052 Uiso 1 1 calc R . .
H9B H 0.7416 0.2176 0.1532 0.052 Uiso 1 1 calc R . .
C10 C 0.3061(13) 0.1302(6) 0.2479(3) 0.0444(17) Uani 1 1 d . . .
C11 C 0.2236(12) 0.1911(6) 0.3068(3) 0.0465(17) Uani 1 1 d . . .
H11A H 0.1554 0.2694 0.2962 0.056 Uiso 1 1 calc R . .
H11B H 0.0733 0.1374 0.3224 0.056 Uiso 1 1 calc R . .
C12 C 0.4620(12) 0.2157(6) 0.3584(3) 0.0431(17) Uani 1 1 d . . .
C13 C 0.5147(14) 0.1225(6) 0.4013(3) 0.0543(19) Uani 1 1 d . . .
H13 H 0.4033 0.0459 0.3969 0.065 Uiso 1 1 calc R . .
C14 C 0.7286(17) 0.1424(7) 0.4499(4) 0.069(2) Uani 1 1 d . . .
H14 H 0.7617 0.0798 0.4777 0.083 Uiso 1 1 calc R . .
C15 C 0.8927(15) 0.2570(7) 0.4564(3) 0.060(2) Uani 1 1 d . . .
H15 H 1.0328 0.2721 0.4898 0.072 Uiso 1 1 calc R . .
C16 C 0.8510(13) 0.3492(7) 0.4140(3) 0.0542(19) Uani 1 1 d . . .
H16 H 0.9679 0.4243 0.4182 0.065 Uiso 1 1 calc R . .
C17 C 0.6333(12) 0.3306(6) 0.3644(3) 0.0423(16) Uani 1 1 d . . .
C18 C 0.7275(12) 0.5462(6) 0.3256(3) 0.0401(15) Uani 1 1 d . . .
C19 C 0.9077(13) 0.5892(6) 0.2815(3) 0.0486(17) Uani 1 1 d . . .
C20 C 1.0188(15) 0.7127(7) 0.2814(4) 0.064(2) Uani 1 1 d . . .
H20 H 1.1316 0.7392 0.2505 0.077 Uiso 1 1 calc R . .
C21 C 0.9636(17) 0.7965(8) 0.3268(4) 0.076(2) Uani 1 1 d . . .
H21 H 1.0412 0.8796 0.3274 0.091 Uiso 1 1 calc R . .
C22 C 0.7889(16) 0.7553(7) 0.3722(4) 0.065(2) Uani 1 1 d . . .
H22 H 0.7496 0.8109 0.4033 0.077 Uiso 1 1 calc R . .
C23 C 0.6757(13) 0.6322(7) 0.3705(3) 0.0500(18) Uani 1 1 d . . .

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O2 0.041(3) 0.039(3) 0.087(4) -0.002(3) 0.034(2) -0.007(2)
N1 0.031(3) 0.036(3) 0.040(3) 0.005(3) 0.013(3) -0.006(2)
C1 0.022(3) 0.037(4) 0.053(4) 0.010(3) 0.008(3) -0.011(3)
C2 0.028(3) 0.032(4) 0.048(4) 0.010(3) 0.006(3) -0.001(3)
C3 0.022(3) 0.036(4) 0.049(4) 0.008(3) 0.011(3) 0.004(3)
C4 0.023(3) 0.032(4) 0.038(4) 0.011(3) 0.009(3) -0.003(3)
C5 0.047(4) 0.030(4) 0.058(4) 0.001(3) 0.011(3) -0.001(3)
C6 0.044(4) 0.034(4) 0.061(5) 0.003(3) 0.022(3) -0.002(3)
C7 0.032(4) 0.043(4) 0.048(4) 0.011(3) 0.013(3) 0.002(3)
Cl1 0.0575(12) 0.0819(14) 0.0568(12) 0.0123(10) 0.0150(9) 0.0125(10)
Cl2 0.0571(12) 0.0893(15) 0.0750(14) -0.0071(11) 0.0259(10) -0.0115(11)
O3 0.090(4) 0.043(3) 0.064(3) 0.001(3) 0.022(3) -0.019(3)
O4 0.039(3) 0.047(3) 0.038(3) 0.000(2) 0.009(2) -0.004(2)
O5 0.026(2) 0.042(3) 0.051(3) 0.003(2) 0.010(2) 0.001(2)
O6 0.041(3) 0.045(3) 0.056(3) -0.009(2) 0.015(2) -0.008(2)
N2 0.049(4) 0.049(4) 0.042(3) 0.009(3) 0.001(3) -0.014(3)
C8 0.030(4) 0.040(4) 0.042(4) 0.008(3) 0.015(3) -0.011(3)
C9 0.038(4) 0.050(4) 0.043(4) -0.002(3) 0.011(3) -0.001(3)
C10 0.038(4) 0.040(4) 0.052(4) 0.011(3) 0.003(3) -0.008(3)
C11 0.034(4) 0.054(4) 0.051(4) 0.004(3) 0.016(3) -0.007(3)
C12 0.025(4) 0.053(4) 0.050(4) 0.000(3) 0.012(3) -0.007(3)
C13 0.048(5) 0.056(5) 0.057(5) 0.015(4) 0.007(4) -0.008(4)
C14 0.073(6) 0.064(6) 0.070(6) 0.019(4) -0.001(5) 0.012(5)
C15 0.048(5) 0.084(6) 0.048(5) 0.008(4) -0.003(4) 0.010(4)
C16 0.038(4) 0.073(5) 0.046(4) 0.009(4) -0.002(3) -0.013(4)
C17 0.035(4) 0.046(4) 0.045(4) 0.002(3) 0.014(3) -0.003(3)
C18 0.037(4) 0.045(4) 0.037(4) 0.007(3) -0.001(3) -0.001(3)
C19 0.047(4) 0.053(5) 0.044(4) 0.007(3) 0.005(3) -0.003(4)
C20 0.064(5) 0.059(5) 0.066(5) 0.026(4) 0.009(4) -0.009(4)
C21 0.081(6) 0.059(5) 0.079(6) 0.013(5) 0.000(5) -0.016(5)
C22 0.074(6) 0.052(5) 0.065(5) 0.001(4) 0.003(4) 0.003(4)
C23 0.034(4) 0.065(5) 0.050(4) 0.006(4) 0.007(3) -0.003(4)

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  All esds (except the esd in the dihedral angle between two l.s. planes)
  are estimated using the full covariance matrix.  The cell esds are taken
  into account individually in the estimation of esds in distances, angles
  and torsion angles; correlations between esds in cell parameters are only
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  used when they are defined by crystal symmetry.  An approximate (isotropic)
  treatment of cell esds is used for estimating esds involving l.s. planes.
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N1 C4 1.475(7) . ?
N1 H1A 0.919(19) . ?
N1 H1B 0.91(2) . ?
N1 H1C 0.904(19) . ?
C1 C2 1.478(8) . ?
C2 C3 1.408(7) . ?
C2 C7 1.410(8) . ?
C3 C4 1.379(7) . ?
C3 H3 0.9300 . ?
C4 C5 1.383(8) . ?
C5 C6 1.402(8) . ?
C5 H5 0.9300 . ?
C6 C7 1.380(8) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
Cl1 C19 1.735(7) . ?
Cl2 C23 1.746(7) . ?
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O4 C10 1.359(7) . ?
O4 C9 1.444(6) . ?
O5 C8 1.279(7) . ?
O6 C8 1.242(7) . ?
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N2 H2 0.88(2) . ?
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C9 H9B 0.9700 . ?
C10 C11 1.510(8) . ?
C11 C12 1.508(8) . ?
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C11 H11B 0.9700 . ?
C12 C17 1.405(8) . ?
C12 C13 1.409(8) . ?
C13 C14 1.384(9) . ?
C13 H13 0.9300 . ?
C14 C15 1.386(9) . ?
C14 H14 0.9300 . ?
C15 C16 1.384(9) . ?
C15 H15 0.9300 . ?
C16 C17 1.410(8) . ?
C16 H16 0.9300 . ?
C18 C23 1.376(8) . ?
C18 C19 1.401(8) . ?
C19 C20 1.378(9) . ?
C20 C21 1.372(10) . ?
C20 H20 0.9300 . ?
C21 C22 1.399(10) . ?
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C4 N1 H1B 118(4) . . ?
H1A N1 H1B 104(5) . . ?
C4 N1 H1C 109(4) . . ?
H1A N1 H1C 95(5) . . ?
H1B N1 H1C 113(5) . . ?
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O1 C1 C2 125.3(5) . . ?
O2 C1 C2 110.7(5) . . ?
C3 C2 C7 118.2(5) . . ?
C3 C2 C1 118.0(5) . . ?
C7 C2 C1 123.8(5) . . ?

C4 C3 C2 120.0(5) . . ?
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C2 C3 H3 120.0 . . ?
C3 C4 C5 121.3(5) . . ?
C3 C4 N1 118.8(5) . . ?
C5 C4 N1 119.7(5) . . ?
C4 C5 C6 119.7(6) . . ?
C4 C5 H5 120.2 . . ?
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C7 C6 C5 119.4(6) . . ?
C7 C6 H6 120.3 . . ?
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C6 C7 C2 121.4(6) . . ?
C6 C7 H7 119.3 . . ?
C2 C7 H7 119.3 . . ?
C10 O4 C9 115.1(5) . . ?
C17 N2 C18 125.7(5) . . ?
C17 N2 H2 116(4) . . ?
C18 N2 H2 111(4) . . ?
O6 C8 O5 125.2(6) . . ?
O6 C8 C9 117.1(6) . . ?
O5 C8 C9 117.7(5) . . ?
O4 C9 C8 115.1(5) . . ?
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C8 C9 H9A 108.5 . . ?
O4 C9 H9B 108.5 . . ?
C8 C9 H9B 108.5 . . ?
H9A C9 H9B 107.5 . . ?
O3 C10 O4 122.6(6) . . ?
O3 C10 C11 126.7(6) . . ?
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H11A C11 H11B 107.9 . . ?
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C21 C22 H22 120.1 . . ?
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O2 C1 C2 C7 9.8(8) . . . . ?
C7 C2 C3 C4 -1.1(8) . . . . ?
C1 C2 C3 C4 178.4(5) . . . . ?
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C5 C6 C7 C2 2.0(9) . . . . ?
C3 C2 C7 C6 -0.4(9) . . . . ?
C1 C2 C7 C6 -179.9(6) . . . . ?
C10 O4 C9 C8 73.4(7) . . . . ?
O6 C8 C9 O4 -158.4(5) . . . . ?
O5 C8 C9 O4 22.4(8) . . . . ?
C9 O4 C10 O3 -1.8(8) . . . . ?
C9 O4 C10 C11 175.5(4) . . . . ?
O3 C10 C11 C12 106.9(7) . . . . ?
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C17 C12 C13 C14 1.1(10) . . . . ?
C11 C12 C13 C14 -178.9(6) . . . . ?
C12 C13 C14 C15 0.4(11) . . . . ?
C13 C14 C15 C16 -2.2(11) . . . . ?
C14 C15 C16 C17 2.5(11) . . . . ?
C18 N2 C17 C12 172.1(6) . . . . ?
C18 N2 C17 C16 -9.9(10) . . . . ?
C13 C12 C17 N2 177.2(6) . . . . ?
C11 C12 C17 N2 -2.8(9) . . . . ?
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C11 C12 C17 C16 179.1(6) . . . . ?
C15 C16 C17 N2 -179.0(6) . . . . ?
C15 C16 C17 C12 -0.9(9) . . . . ?
C17 N2 C18 C23 -69.1(9) . . . . ?
C17 N2 C18 C19 115.3(7) . . . . ?
C23 C18 C19 C20 -2.6(10) . . . . ?
N2 C18 C19 C20 173.2(6) . . . . ?
C23 C18 C19 Cl1 179.0(5) . . . . ?
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C21 C22 C23 Cl2 -179.9(6) . . . . ?
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N2 C18 C23 C22 -174.5(6) . . . . ?
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O2 H2A O5    0.826(10) 1.832(19) 2.647(6) 168(7) .
N1 H1B O6    0.91(2) 2.55(5) 2.921(6) 105(4) 2_765
N1 H1B O6    0.91(2) 1.94(2) 2.822(6) 165(5) 1_665
N1 H1A O1    0.919(19) 2.11(3) 2.924(7) 147(5) 2_765

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 'x, -y-1/2, z-1/2'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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Cl2 Cl 0.23068(6) 0.30140(14) 0.57075(15) 0.0589(4) Uani 1 1 d . . .
O1 O 0.31397(15) 0.5285(5) 0.8123(4) 0.0786(14) Uani 1 1 d . . .
O2 O 0.36230(13) 0.6403(4) 0.9938(3) 0.0467(9) Uani 1 1 d . . .
O3 O 0.42256(19) 0.7793(4) 0.7983(4) 0.0771(13) Uani 1 1 d . . .
O4 O 0.49792(16) 0.6178(4) 0.8054(4) 0.0585(10) Uani 1 1 d D . .
H4 H 0.513(3) 0.662(6) 0.745(5) 0.088 Uiso 1 1 d D . .
N1 N 0.17579(16) 0.5143(4) 0.7474(4) 0.0419(10) Uani 1 1 d D . .
H1 H 0.2167(8) 0.490(5) 0.762(5) 0.050 Uiso 1 1 d D . .
C1 C 0.4464(2) 0.6753(5) 0.8446(5) 0.0411(12) Uani 1 1 d . . .
C2 C 0.42239(19) 0.5921(5) 0.9582(5) 0.0453(12) Uani 1 1 d . . .
H2A H 0.4184 0.4963 0.9293 0.054 Uiso 1 1 calc R . .
H2B H 0.4529 0.5962 1.0395 0.054 Uiso 1 1 calc R . .

C3 C 0.3121(2) 0.5991(6) 0.9134(5) 0.0464(13) Uani 1 1 d . . .
C4 C 0.25279(19) 0.6500(6) 0.9688(5) 0.0462(13) Uani 1 1 d . . .
H4A H 0.2642 0.7102 1.0472 0.055 Uiso 1 1 calc R . .
H4B H 0.2300 0.5718 1.0013 0.055 Uiso 1 1 calc R . .
C5 C 0.21005(19) 0.7275(5) 0.8616(5) 0.0374(11) Uani 1 1 d . . .
C6 C 0.2055(2) 0.8701(6) 0.8716(5) 0.0482(13) Uani 1 1 d . . .
H6 H 0.2301 0.9157 0.9422 0.058 Uiso 1 1 calc R . .
C7 C 0.1656(3) 0.9462(6) 0.7802(6) 0.0569(15) Uani 1 1 d . . .
H7 H 0.1630 1.0415 0.7902 0.068 Uiso 1 1 calc R . .
C8 C 0.1296(2) 0.8800(5) 0.6732(5) 0.0485(13) Uani 1 1 d . . .
H8 H 0.1030 0.9307 0.6101 0.058 Uiso 1 1 calc R . .
C9 C 0.1333(2) 0.7382(5) 0.6608(5) 0.0388(11) Uani 1 1 d . . .
H9 H 0.1094 0.6940 0.5882 0.047 Uiso 1 1 calc R . .
C10 C 0.17225(19) 0.6606(5) 0.7549(5) 0.0349(11) Uani 1 1 d . . .
C11 C 0.13172(19) 0.4327(4) 0.6685(4) 0.0331(10) Uani 1 1 d . . .
C12 C 0.06628(19) 0.4401(5) 0.6782(4) 0.0350(10) Uani 1 1 d . . .
C13 C 0.0233(2) 0.3596(5) 0.5980(5) 0.0435(12) Uani 1 1 d . . .
H13 H -0.0197 0.3712 0.6036 0.052 Uiso 1 1 calc R . .
C14 C 0.0439(2) 0.2620(5) 0.5097(5) 0.0479(13) Uani 1 1 d . . .
H14 H 0.0150 0.2086 0.4544 0.058 Uiso 1 1 calc R . .
C15 C 0.1077(2) 0.2445(5) 0.5044(5) 0.0458(12) Uani 1 1 d . . .
H15 H 0.1221 0.1761 0.4482 0.055 Uiso 1 1 calc R . .
C16 C 0.1504(2) 0.3276(5) 0.5815(5) 0.0392(11) Uani 1 1 d . . .
S1 S 0.38699(7) 0.18355(15) 0.93527(16) 0.0608(5) Uani 1 1 d . . .
O5 O 0.44581(18) 0.2417(4) 0.8861(4) 0.0698(11) Uani 1 1 d . . .
C17 C 0.3496(2) 0.0882(7) 0.7931(6) 0.078(2) Uani 1 1 d . . .
H17A H 0.3397 0.1490 0.7159 0.118 Uiso 1 1 calc R . .
H17B H 0.3114 0.0474 0.8189 0.118 Uiso 1 1 calc R . .
H17C H 0.3775 0.0167 0.7680 0.118 Uiso 1 1 calc R . .
C18 C 0.4082(3) 0.0451(7) 1.0467(6) 0.0820(19) Uani 1 1 d . . .
H18A H 0.4300 -0.0235 0.9984 0.123 Uiso 1 1 calc R . .
H18B H 0.3709 0.0052 1.0777 0.123 Uiso 1 1 calc R . .
H18C H 0.4354 0.0777 1.1249 0.123 Uiso 1 1 calc R . .

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Cl2 0.0429(7) 0.0534(9) 0.0824(10) -0.0007(8) 0.0158(7) 0.0126(6)
O1 0.0316(19) 0.125(4) 0.079(3) -0.056(3) 0.0021(18) 0.003(2)
O2 0.0296(17) 0.062(2) 0.048(2) -0.0109(18) 0.0011(15) -0.0008(16)
O3 0.080(3) 0.067(3) 0.088(3) 0.028(2) 0.025(2) 0.033(2)
O4 0.050(2) 0.061(3) 0.068(3) 0.009(2) 0.0175(18) 0.0133(19)
N1 0.030(2) 0.036(2) 0.057(3) -0.006(2) -0.0087(19) 0.0013(18)
C1 0.032(3) 0.044(3) 0.046(3) -0.006(3) 0.001(2) 0.004(2)
C2 0.027(2) 0.054(3) 0.054(3) 0.003(3) 0.001(2) 0.000(2)
C3 0.027(3) 0.064(4) 0.047(3) -0.010(3) -0.001(2) 0.001(2)
C4 0.030(2) 0.068(4) 0.041(3) -0.013(3) 0.006(2) -0.002(2)
C5 0.028(2) 0.046(3) 0.040(3) -0.007(2) 0.013(2) -0.002(2)
C6 0.048(3) 0.056(3) 0.043(3) -0.014(3) 0.014(2) -0.010(3)
C7 0.074(4) 0.037(3) 0.065(4) -0.011(3) 0.029(3) -0.011(3)
C8 0.052(3) 0.039(3) 0.057(3) 0.011(3) 0.015(3) 0.001(3)
C9 0.031(2) 0.041(3) 0.045(3) -0.001(2) 0.006(2) -0.005(2)
C10 0.030(2) 0.037(3) 0.039(3) -0.001(2) 0.009(2) -0.005(2)
C11 0.034(2) 0.031(2) 0.034(2) 0.006(2) 0.0004(19) -0.002(2)
C12 0.034(2) 0.034(3) 0.037(3) 0.003(2) 0.004(2) -0.002(2)
C13 0.032(2) 0.047(3) 0.051(3) 0.010(3) 0.002(2) -0.003(2)
C14 0.048(3) 0.044(3) 0.051(3) -0.005(3) -0.001(2) -0.007(3)
C15 0.059(3) 0.033(3) 0.047(3) -0.004(2) 0.010(2) -0.003(2)
C16 0.038(3) 0.038(3) 0.042(3) 0.006(2) 0.008(2) 0.001(2)
S1 0.0574(9) 0.0522(9) 0.0781(11) 0.0031(8) 0.0318(8) 0.0059(7)
O5 0.075(3) 0.061(3) 0.079(3) -0.010(2) 0.035(2) -0.020(2)
C17 0.053(3) 0.090(5) 0.089(5) 0.021(4) -0.011(3) -0.019(3)
C18 0.101(5) 0.080(5) 0.067(4) 0.014(4) 0.013(4) 0.001(4)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Cl1 C12 1.740(4) . ?
Cl2 C16 1.741(4) . ?
O1 C3 1.201(6) . ?
O2 C3 1.319(5) . ?
O2 C2 1.438(5) . ?
O3 C1 1.194(6) . ?
O4 C1 1.321(5) . ?
O4 H4 0.824(10) . ?
N1 C11 1.394(5) . ?
N1 C10 1.420(6) . ?
N1 H1 0.899(10) . ?
C1 C2 1.499(6) . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
C3 C4 1.506(6) . ?
C4 C5 1.509(6) . ?
C4 H4A 0.9700 . ?
C4 H4B 0.9700 . ?
C5 C6 1.388(7) . ?
C5 C10 1.404(6) . ?
C6 C7 1.376(7) . ?
C6 H6 0.9300 . ?
C7 C8 1.383(7) . ?
C7 H7 0.9300 . ?
C8 C9 1.381(6) . ?
C8 H8 0.9300 . ?
C9 C10 1.389(6) . ?
C9 H9 0.9300 . ?
C11 C16 1.407(6) . ?
C11 C12 1.408(6) . ?
C12 C13 1.379(6) . ?
C13 C14 1.379(7) . ?
C13 H13 0.9300 . ?
C14 C15 1.375(6) . ?
C14 H14 0.9300 . ?
C15 C16 1.376(6) . ?
C15 H15 0.9300 . ?
S1 O5 1.496(4) . ?
S1 C18 1.752(6) . ?
S1 C17 1.779(6) . ?
C17 H17A 0.9600 . ?
C17 H17B 0.9600 . ?
C17 H17C 0.9600 . ?

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C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?

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C3 O2 C2 116.4(4) . . ?
C1 O4 H4 113(4) . . ?
C11 N1 C10 123.9(4) . . ?
C11 N1 H1 121(3) . . ?
C10 N1 H1 108(3) . . ?
O3 C1 O4 125.4(5) . . ?
O3 C1 C2 124.5(4) . . ?
O4 C1 C2 110.1(4) . . ?
O2 C2 C1 112.5(4) . . ?
O2 C2 H2A 109.1 . . ?
C1 C2 H2A 109.1 . . ?
O2 C2 H2B 109.1 . . ?
C1 C2 H2B 109.1 . . ?
H2A C2 H2B 107.8 . . ?
O1 C3 O2 124.3(4) . . ?
O1 C3 C4 125.4(4) . . ?
O2 C3 C4 110.3(4) . . ?
C3 C4 C5 112.6(4) . . ?
C3 C4 H4A 109.1 . . ?
C5 C4 H4A 109.1 . . ?
C3 C4 H4B 109.1 . . ?
C5 C4 H4B 109.1 . . ?
H4A C4 H4B 107.8 . . ?
C6 C5 C10 118.1(4) . . ?
C6 C5 C4 119.2(4) . . ?
C10 C5 C4 122.6(4) . . ?
C7 C6 C5 122.0(5) . . ?
C7 C6 H6 119.0 . . ?
C5 C6 H6 119.0 . . ?
C6 C7 C8 119.6(5) . . ?
C6 C7 H7 120.2 . . ?
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C8 C7 H7 120.2 . . ?
C9 C8 C7 119.6(5) . . ?
C9 C8 H8 120.2 . . ?
C7 C8 H8 120.2 . . ?
C8 C9 C10 121.0(5) . . ?
C8 C9 H9 119.5 . . ?
C10 C9 H9 119.5 . . ?
C9 C10 C5 119.6(4) . . ?
C9 C10 N1 122.5(4) . . ?
C5 C10 N1 117.9(4) . . ?
N1 C11 C16 121.6(4) . . ?
N1 C11 C12 123.3(4) . . ?
C16 C11 C12 114.9(4) . . ?
C13 C12 C11 122.4(4) . . ?
C13 C12 Cl1 117.1(3) . . ?
C11 C12 Cl1 120.5(3) . . ?
C14 C13 C12 120.3(4) . . ?
C14 C13 H13 119.9 . . ?
C12 C13 H13 119.9 . . ?
C15 C14 C13 119.2(5) . . ?
C15 C14 H14 120.4 . . ?
C13 C14 H14 120.4 . . ?
C14 C15 C16 120.4(5) . . ?
C14 C15 H15 119.8 . . ?
C16 C15 H15 119.8 . . ?
C15 C16 C11 122.6(4) . . ?
C15 C16 Cl2 118.6(4) . . ?
C11 C16 Cl2 118.9(4) . . ?
O5 S1 C18 108.3(3) . . ?
O5 S1 C17 105.6(2) . . ?
C18 S1 C17 98.5(3) . . ?
S1 C17 H17A 109.5 . . ?
S1 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
S1 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
S1 C18 H18A 109.5 . . ?
S1 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
S1 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?

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  _geom_torsion_site_symmetry_2
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  _geom_torsion_site_symmetry_4
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C3 O2 C2 C1 81.2(5) . . . . ?
O3 C1 C2 O2 7.8(7) . . . . ?
O4 C1 C2 O2 -173.1(4) . . . . ?
C2 O2 C3 O1 -2.2(8) . . . . ?
C2 O2 C3 C4 176.3(4) . . . . ?
O1 C3 C4 C5 -54.7(8) . . . . ?
O2 C3 C4 C5 126.8(4) . . . . ?
C3 C4 C5 C6 -106.7(5) . . . . ?
C3 C4 C5 C10 76.3(6) . . . . ?
C10 C5 C6 C7 -0.4(7) . . . . ?
C4 C5 C6 C7 -177.6(4) . . . . ?
C5 C6 C7 C8 -1.1(7) . . . . ?
C6 C7 C8 C9 1.0(7) . . . . ?
C7 C8 C9 C10 0.7(7) . . . . ?
C8 C9 C10 C5 -2.2(6) . . . . ?
C8 C9 C10 N1 178.1(4) . . . . ?
C6 C5 C10 C9 2.0(6) . . . . ?
C4 C5 C10 C9 179.1(4) . . . . ?
C6 C5 C10 N1 -178.3(4) . . . . ?
C4 C5 C10 N1 -1.2(6) . . . . ?
C11 N1 C10 C9 -15.3(7) . . . . ?
C11 N1 C10 C5 165.0(4) . . . . ?
C10 N1 C11 C16 132.7(5) . . . . ?
C10 N1 C11 C12 -53.0(6) . . . . ?
N1 C11 C12 C13 179.2(4) . . . . ?
C16 C11 C12 C13 -6.1(6) . . . . ?
N1 C11 C12 Cl1 -2.1(6) . . . . ?
C16 C11 C12 Cl1 172.6(3) . . . . ?
C11 C12 C13 C14 3.6(7) . . . . ?
Cl1 C12 C13 C14 -175.1(4) . . . . ?
C12 C13 C14 C15 1.1(7) . . . . ?
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C13 C14 C15 C16 -2.9(7) . . . . ?
C14 C15 C16 C11 0.1(7) . . . . ?
C14 C15 C16 Cl2 -179.9(4) . . . . ?
N1 C11 C16 C15 179.0(4) . . . . ?
C12 C11 C16 C15 4.3(6) . . . . ?
N1 C11 C16 Cl2 -1.0(6) . . . . ?
C12 C11 C16 Cl2 -175.8(3) . . . . ?

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  _geom_hbond_distance_HA
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  _geom_hbond_angle_DHA
  _geom_hbond_site_symmetry_A
N1 H1 O1    0.899(10) 2.11(2) 2.946(5) 154(4) .
O4 H4 S1    0.824(10) 2.90(3) 3.616(4) 147(5) 2_656
O4 H4 O5    0.824(10) 1.789(14) 2.608(5) 173(6) 2_656

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_diffrn_measured_fraction_theta_full       0.993
_refine_diff_density_max         0.281
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