

Table 1. Crystal data and structure refinement for ctf25n.

Identification code	ctf25n
Empirical formula	C ₃₈ H ₇₁ N ₇ O ₁₁
Formula weight	802.02
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.435(2) Å alpha = 68.4(1) deg. b = 20.878(3) Å beta = 89.1(1) deg. c = 24.207(3) Å gamma = 82.8(1) deg.
Volume	4862.1(13) Å ³
Z, Calculated density	4, 1.096 Mg/m ³
Absorption coefficient	0.660 mm ⁻¹
F(000)	1744
Crystal size	0.4 x 0.4 x 0.2 mm
Theta range for data collection	2.30 to 50.00 deg.
Limiting indices	-10 ≤ h ≤ 10, -18 ≤ k ≤ 20, 0 ≤ l ≤ 24
Reflections collected / unique	9347 / 9311 [R(int) = 0.0264]
Completeness to theta = 50.00	93.2 %
Absorption correction	None
Refinement method	Full-matrix-block least-squares on F ²
Data / restraints / parameters	9311 / 268 / 1070
Goodness-of-fit on F ²	0.896
Final R indices [I > 2σ(I)]	R ₁ = 0.0834, wR ₂ = 0.2063
R indices (all data)	R ₁ = 0.1749, wR ₂ = 0.2472
Largest diff. peak and hole	0.424 and -0.307 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ctf25n. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C01	6235 (7)	9504 (4)	-4432 (3)	116 (3)
C0	7098 (6)	9135 (4)	-3884 (3)	82 (2)
O0	6917 (4)	9255 (2)	-3427 (2)	89 (2)
N1	8075 (5)	8685 (3)	-3930 (2)	83 (2)
CA1	9043 (6)	8301 (3)	-3455 (2)	66 (2)
CB11	9878 (6)	8759 (4)	-3308 (3)	76 (2)
CG11	11084 (6)	8949 (4)	-3685 (3)	85 (2)
CD11	10729 (7)	9410 (4)	-4323 (3)	100 (3)
CD21	11922 (8)	9294 (4)	-3395 (3)	115 (3)
ND1	11826 (5)	8280 (3)	-3672 (2)	90 (2)
OD1	13005 (5)	8315 (3)	-3839 (3)	138 (2)
CG21	11309 (6)	7610 (4)	-3484 (3)	76 (2)
CD31	11972 (7)	7202 (4)	-3839 (3)	110 (3)
CD41	11600 (6)	7214 (4)	-2825 (3)	94 (2)
CB21	9867 (6)	7767 (4)	-3666 (3)	81 (2)
C1	8339 (6)	7889 (3)	-2878 (3)	73 (2)
O1	8866 (4)	7753 (2)	-2391 (2)	80 (1)
N2	7218 (5)	7686 (3)	-2944 (2)	76 (2)
CA2	6511 (6)	7282 (4)	-2416 (3)	80 (2)
CB12	5181 (7)	7239 (5)	-2642 (3)	115 (3)
CB22	7249 (8)	6552 (4)	-2093 (3)	116 (3)
C2	6275 (6)	7668 (4)	-1987 (3)	74 (2)
O2	6032 (4)	7334 (2)	-1470 (2)	89 (2)
N3	6288 (4)	8359 (3)	-2207 (2)	70 (2)
CA3	6126 (5)	8775 (3)	-1830 (3)	63 (2)
CB13	6558 (7)	9483 (3)	-2186 (3)	89 (2)
CB23	4710 (6)	8841 (4)	-1660 (3)	95 (2)
C3	7007 (6)	8440 (3)	-1264 (3)	69 (2)
O3	6720 (4)	8539 (3)	-807 (2)	87 (2)
N4	8152 (4)	8089 (2)	-1304 (2)	64 (2)
CA4	9101 (5)	7786 (3)	-816 (2)	62 (2)
CB14	9597 (6)	8339 (4)	-639 (3)	77 (2)
CG14	10903 (6)	8566 (3)	-887 (3)	71 (2)
CD14	10877 (7)	8929 (4)	-1569 (3)	97 (3)
CD24	11326 (7)	9032 (4)	-593 (3)	96 (2)
ND4	11842 (5)	7915 (3)	-702 (2)	69 (2)
OD4	12969 (4)	7915 (2)	-503 (2)	92 (2)
CG24	11561 (6)	7268 (4)	-762 (3)	71 (2)
CD34	12546 (6)	7094 (4)	-1182 (3)	105 (3)
CD44	11749 (7)	6690 (3)	-151 (3)	87 (2)
CB24	10194 (5)	7363 (3)	-1027 (3)	69 (2)
C4	8473 (6)	7274 (4)	-270 (3)	77 (2)
O4	8806 (4)	7183 (2)	235 (2)	91 (2)
N5	7634 (5)	6916 (3)	-384 (2)	91 (2)
CA5	6902 (8)	6421 (4)	80 (3)	110 (3)
CB15	6325 (9)	5959 (5)	-181 (4)	145 (4)
CB25	5928 (10)	6798 (6)	332 (5)	189 (5)
C5	7999 (12)	5923 (6)	456 (4)	174 (5)
O5	9010 (8)	5714 (3)	325 (4)	202 (4)
OTA6	7664 (12)	5694 (8)	1024 (4)	209 (8)
CT1A6	8784 (18)	5139 (9)	1420 (8)	192 (6)
CT2A6	10073 (13)	5423 (8)	1387 (6)	134 (6)

CT4A6	8244 (18)	4986 (9)	2035 (6)	190 (8)
OTX6	7950 (16)	5745 (11)	1045 (5)	209 (6)
CT1X6	9150 (20)	5186 (12)	1321 (11)	192 (6)
CT2X6	10130 (20)	4957 (11)	924 (8)	186 (7)
CT3X6	9870 (20)	5538 (13)	1628 (10)	162 (11)
CT4X6	8570 (30)	4580 (11)	1669 (10)	190 (7)
C10110	6564 (9)	9523 (5)	606 (3)	130 (4)
C10010	5940 (7)	9082 (4)	1170 (3)	89 (2)
O10010	6103 (5)	9151 (2)	1644 (2)	98 (2)
N11	5191 (5)	8644 (3)	1098 (2)	79 (2)
CA11	4436 (6)	8218 (3)	1582 (2)	66 (2)
CB111	3870 (6)	7717 (4)	1347 (3)	80 (2)
CG111	2484 (6)	7581 (4)	1509 (3)	79 (2)
CD111	2027 (8)	7195 (4)	1141 (3)	117 (3)
CD211	2330 (7)	7167 (4)	2174 (3)	103 (3)
ND11	1684 (5)	8258 (3)	1346 (2)	91 (2)
OD11	526 (5)	8318 (3)	1146 (3)	140 (2)
CG211	2102 (7)	8874 (4)	1404 (3)	84 (2)
CD311	2228 (8)	9423 (4)	769 (3)	107 (3)
CD411	1059 (7)	9167 (4)	1735 (3)	119 (3)
CB211	3354 (6)	8667 (4)	1763 (3)	80 (2)
C11	5324 (6)	7789 (3)	2136 (3)	72 (2)
O11	4913 (4)	7638 (2)	2637 (2)	82 (2)
N12	6549 (5)	7583 (3)	2039 (2)	81 (2)
CA12	7441 (7)	7151 (4)	2536 (3)	87 (2)
CB112	8806 (7)	7063 (5)	2291 (4)	128 (3)
CB212	7031 (9)	6432 (4)	2848 (4)	137 (4)
C12	7566 (6)	7501 (4)	2982 (3)	78 (2)
O12	7977 (4)	7148 (3)	3494 (2)	101 (2)
N13	7292 (5)	8181 (3)	2798 (2)	73 (2)
CA13	7367 (6)	8595 (4)	3173 (3)	76 (2)
CB113	8754 (6)	8605 (4)	3355 (3)	110 (3)
CB213	6687 (8)	9330 (4)	2840 (3)	101 (3)
C13	6584 (6)	8281 (3)	3747 (3)	72 (2)
O13	6830 (4)	8392 (3)	4194 (2)	95 (2)
N14	5590 (4)	7957 (3)	3701 (2)	68 (2)
CA14	4778 (6)	7659 (4)	4216 (3)	70 (2)
CB114	3894 (6)	7235 (4)	4026 (3)	78 (2)
CG114	2557 (6)	7146 (4)	4304 (3)	79 (2)
CD114	1698 (7)	6934 (4)	3914 (3)	114 (3)
CD214	2678 (7)	6614 (4)	4937 (3)	100 (3)
ND14	1961 (5)	7816 (3)	4319 (2)	75 (2)
OD14	822 (4)	7831 (3)	4520 (2)	98 (2)
CG214	2603 (6)	8452 (4)	4116 (3)	73 (2)
CD314	2522 (7)	8799 (4)	3436 (3)	101 (3)
CD414	1946 (7)	8953 (4)	4380 (3)	106 (3)
CB214	3982 (6)	8240 (3)	4376 (3)	76 (2)
C14	5662 (7)	7174 (4)	4746 (3)	84 (2)
O14	5393 (5)	7127 (3)	5257 (2)	97 (2)
N15	6651 (5)	6788 (3)	4639 (2)	101 (2)
CA15	7568 (8)	6318 (5)	5096 (3)	122 (3)
CB115	8423 (9)	6718 (6)	5305 (4)	177 (5)
CB215	8366 (10)	5830 (5)	4843 (4)	172 (5)
C15	6789 (14)	5917 (8)	5595 (5)	144 (8)
O15	5950 (11)	5644 (5)	5549 (4)	157 (6)
C'15	6810 (30)	5736 (17)	5414 (9)	200 (20)
O'15	5810 (20)	5591 (12)	5245 (8)	167 (10)
OTB16	7281 (9)	5752 (6)	6140 (4)	182 (6)
CT1B16	6391 (14)	5236 (8)	6567 (6)	156 (5)
CT2B16	6308 (17)	4555 (8)	6484 (6)	175 (5)
CT3B16	4938 (16)	5601 (11)	6504 (6)	209 (7)
CT4B16	7012 (16)	5128 (8)	7128 (6)	190 (6)
QTY16	6733 (17)	5663 (11)	5998 (7)	182 (5)

CT2Y16	4870 (20)	4927 (13)	5967 (10)	175 (6)
CT3Y16	6550 (30)	4532 (14)	6724 (10)	209 (7)
CT4Y16	4910 (30)	5533 (16)	6661 (13)	190 (6)
O1W20	8695 (4)	8627 (3)	-5119 (2)	115 (2)
O2W21	5612 (5)	7897 (4)	-4023 (2)	145 (2)
O3W22	4664 (4)	8645 (3)	-91 (2)	95 (2)
O4W23	8065 (6)	7970 (4)	936 (3)	154 (3)

Table 3. Bond lengths [Å] and angles [deg] for ctf25n.

C01-C0	1.508 (9)
C0-O0	1.230 (7)
C0-N1	1.329 (8)
N1-CA1	1.463 (8)
CA1-CB11	1.507 (8)
CA1-CB21	1.552 (9)
CA1-C1	1.573 (9)
CB11-CG11	1.548 (9)
CG11-ND1	1.499 (9)
CG11-CD11	1.512 (9)
CG11-CD21	1.526 (9)
ND1-OD1	1.291 (7)
ND1-CG21	1.472 (9)
CG21-CD31	1.523 (9)
CG21-CD41	1.518 (8)
CG21-CB21	1.535 (9)
C1-O1	1.226 (6)
C1-N2	1.324 (7)
N2-CA2	1.492 (8)
CA2-CB12	1.525 (9)
CA2-C2	1.531 (9)
CA2-CB22	1.541 (10)
C2-O2	1.229 (7)
C2-N3	1.343 (8)
N3-CA3	1.468 (7)
CA3-CB13	1.533 (9)
CA3-CB23	1.531 (8)
CA3-C3	1.544 (8)
C3-O3	1.224 (7)
C3-N4	1.343 (7)
N4-CA4	1.451 (7)
CA4-CB14	1.520 (8)
CA4-CB24	1.549 (8)
CA4-C4	1.559 (9)
CB14-CG14	1.539 (9)
CG14-ND4	1.497 (8)
CG14-CD24	1.506 (8)
CG14-CD14	1.543 (8)
ND4-OD4	1.279 (6)
ND4-CG24	1.474 (8)
CG24-CD44	1.522 (9)
CG24-CB24	1.533 (8)
CG24-CD34	1.539 (9)
C4-O4	1.217 (7)
C4-N5	1.312 (8)
N5-CA5	1.494 (9)
CA5-CB25	1.470 (12)
CA5-CB15	1.517 (11)
CA5-C5	1.502 (14)
C5-O5	1.174 (13)
C5-OTX6	1.337 (10)
C5-OTA6	1.336 (10)
OTA6-CT1A6	1.583 (10)
CT1A6-CT3A6	1.515 (19)
CT1A6-CT2A6	1.527 (19)
CT1A6-CT4A6	1.518 (19)
OTX6-CT1X6	1.569 (11)
CT1X6-CT2X6	1.54 (2)
CT1X6-CT4X6	1.44 (2)

C10110-C10010	1.527(9)
C10010-O10010	1.225(7)
C10010-N11	1.332(8)
N11-CA11	1.471(7)
CA11-CB211	1.539(9)
CA11-CB111	1.539(8)
CA11-C11	1.551(9)
CB111-CG111	1.526(9)
CG111-ND11	1.468(9)
CG111-CD111	1.521(9)
CG111-CD211	1.539(8)
ND11-OD11	1.283(7)
ND11-CG211	1.462(9)
CG211-CB211	1.506(9)
CG211-CD411	1.538(9)
CG211-CD311	1.558(9)
C11-O11	1.221(6)
C11-N12	1.342(8)
N12-CA12	1.468(9)
CA12-CB212	1.524(10)
CA12-C12	1.524(9)
CA12-CB112	1.550(9)
C12-O12	1.237(7)
C12-N13	1.315(8)
N13-CA13	1.477(8)
CA13-CB113	1.524(9)
CA13-CB213	1.531(10)
CA13-C13	1.567(9)
C13-O13	1.223(6)
C13-N14	1.334(7)
N14-CA14	1.480(7)
CA14-CB114	1.539(8)
CA14-C14	1.539(9)
CA14-CB214	1.547(9)
CB114-CG114	1.541(9)
CG114-ND14	1.471(8)
CG114-CD214	1.522(9)
CG114-CD114	1.524(9)
ND14-OD14	1.279(6)
ND14-CG214	1.480(8)
CG214-CD414	1.507(9)
CG214-CB214	1.526(9)
CG214-CD314	1.533(8)
C14-O14	1.234(7)
C14-N15	1.311(8)
N15-CA15	1.450(9)
CA15-CB115	1.502(12)
CA15-C15	1.488(16)
CA15-C'15	1.49(2)
CA15-CB215	1.529(12)
C15-OTB16	1.329(10)
C15-O15	1.131(18)
C'15-O'15	1.236(19)
C'15-OTY16	1.368(11)
OTB16-CT1B16	1.577(10)
CT1B16-CT4B16	1.444(16)
CT1B16-CT2B16	1.521(17)
CT1B16-CT3B16	1.592(19)
OTY16-CT1Y16	1.550(11)
CT1Y16-CT2Y16	1.45(2)
CT1Y16-CT4Y16	1.53(3)
CT1Y16-CT3Y16	1.54(3)

O0-C0-C01	121.6 (7)
N1-C0-C01	116.2 (7)
C0-N1-CA1	123.9 (5)
N1-CA1-CB11	113.5 (6)
N1-CA1-CB21	106.2 (5)
CB11-CA1-CB21	111.2 (5)
N1-CA1-C1	109.1 (5)
CB11-CA1-C1	108.5 (5)
CB21-CA1-C1	108.2 (6)
CA1-CB11-CG11	117.3 (5)
ND1-CG11-CD11	108.9 (6)
ND1-CG11-CD21	108.7 (6)
CD11-CG11-CD21	111.1 (7)
ND1-CG11-CB11	106.9 (6)
CD11-CG11-CB11	112.3 (6)
CD21-CG11-CB11	108.8 (6)
OD1-ND1-CG21	119.5 (6)
OD1-ND1-CG11	115.5 (6)
CG21-ND1-CG11	124.9 (6)
ND1-CG21-CD31	107.6 (6)
ND1-CG21-CD41	109.7 (6)
CD31-CG21-CD41	109.9 (6)
ND1-CG21-CB21	107.3 (6)
CD31-CG21-CB21	107.4 (6)
CD41-CG21-CB21	114.7 (6)
CG21-CB21-CA1	116.5 (5)
O1-C1-N2	123.2 (7)
O1-C1-CA1	118.9 (6)
N2-C1-CA1	117.8 (6)
C1-N2-CA2	120.6 (5)
N2-CA2-CB12	106.9 (6)
N2-CA2-C2	111.1 (6)
CB12-CA2-C2	106.3 (6)
N2-CA2-CB22	110.9 (6)
CB12-CA2-CB22	111.1 (7)
C2-CA2-CB22	110.5 (6)
O2-C2-N3	123.7 (7)
O2-C2-CA2	118.3 (7)
N3-C2-CA2	117.9 (6)
C2-N3-CA3	122.3 (6)
N3-CA3-CB13	107.4 (5)
N3-CA3-CB23	109.2 (5)
CB13-CA3-CB23	112.0 (6)
N3-CA3-C3	111.1 (5)
CB13-CA3-C3	107.3 (6)
CB23-CA3-C3	110.0 (5)
O3-C3-N4	120.8 (6)
O3-C3-CA3	121.1 (6)
N4-C3-CA3	117.8 (6)
C3-N4-CA4	123.3 (5)
N4-CA4-CB14	111.5 (6)
N4-CA4-CB24	106.4 (5)
CB14-CA4-CB24	112.3 (5)
N4-CA4-C4	109.2 (5)
CB14-CA4-C4	109.0 (5)
CB24-CA4-C4	108.3 (6)
CA4-CB14-CG14	116.7 (5)
ND4-CG14-CD24	108.4 (5)
ND4-CG14-CB14	105.8 (5)
CD24-CG14-CB14	108.9 (6)
ND4-CG14-CD14	109.5 (5)
CD24-CG14-CD14	110.6 (6)
CB14-CG14-CD14	113.5 (5)

OD4-ND4-CG14	119.4 (5)
CG24-ND4-CG14	123.4 (5)
ND4-CG24-CD44	108.0 (5)
ND4-CG24-CB24	110.5 (5)
CD44-CG24-CB24	112.4 (6)
ND4-CG24-CD34	108.1 (6)
CD44-CG24-CD34	108.7 (6)
CB24-CG24-CD34	109.1 (5)
CG24-CB24-CA4	118.1 (5)
O4-C4-N5	122.1 (7)
O4-C4-CA4	121.2 (6)
N5-C4-CA4	116.6 (6)
C4-N5-CA5	124.1 (6)
CB25-CA5-N5	110.6 (7)
CB25-CA5-CB15	112.9 (8)
N5-CA5-CB15	109.5 (7)
CB25-CA5-C5	121.5 (9)
N5-CA5-C5	100.5 (7)
CB15-CA5-C5	100.7 (8)
O5-C5-OTX6	110.5 (13)
O5-C5-OTA6	119.8 (13)
O5-C5-CA5	131.0 (9)
OTX6-C5-CA5	117.7 (13)
OTA6-C5-CA5	109.2 (11)
C5-OTA6-CT1A6	109.6 (12)
CT3A6-CT1A6-CT2A6	106.6 (14)
CT3A6-CT1A6-CT4A6	109.7 (14)
CT2A6-CT1A6-CT4A6	110.1 (15)
CT3A6-CT1A6-OTA6	116.2 (15)
CT2A6-CT1A6-OTA6	113.5 (13)
CT4A6-CT1A6-OTA6	100.6 (13)
C5-OTX6-CT1X6	106.5 (14)
CT2X6-CT1X6-CT4X6	107 (2)
CT2X6-CT1X6-CT3X6	106.0 (19)
CT4X6-CT1X6-CT3X6	119 (2)
CT2X6-CT1X6-OTX6	121.4 (18)
CT4X6-CT1X6-OTX6	103.2 (17)
CT3X6-CT1X6-OTX6	101.5 (17)
O10010-C10010-N11	123.8 (6)
O10010-C10010-C10110	121.2 (7)
N11-C10010-C10110	115.0 (6)
C10010-N11-CA11	122.5 (5)
N11-CA11-CB211	111.7 (6)
N11-CA11-CB111	106.2 (5)
CB211-CA11-CB111	110.8 (6)
N11-CA11-C11	110.5 (5)
CB211-CA11-C11	108.6 (5)
CB111-CA11-C11	109.0 (6)
CG111-CB111-CA11	116.8 (6)
ND11-CG111-CD111	108.9 (6)
ND11-CG111-CB111	107.5 (6)
CD111-CG111-CB111	108.3 (6)
ND11-CG111-CD211	108.6 (6)
CD111-CG111-CD211	109.9 (6)
CB111-CG111-CD211	113.6 (6)
OD11-ND11-CG211	117.0 (7)
OD11-ND11-CG111	118.3 (6)
CG211-ND11-CG111	124.7 (6)
ND11-CG211-CB211	109.1 (6)
ND11-CG211-CD411	108.0 (6)
CB211-CG211-CD411	109.1 (6)
ND11-CG211-CD311	108.4 (6)
CB211-CG211-CD311	112.5 (6)

CG211-CB211-CA11	117.2 (5)
O11-C11-N12	121.9 (7)
O11-C11-CA11	121.0 (6)
N12-C11-CA11	117.1 (6)
C11-N12-CA12	120.7 (6)
N12-CA12-CB212	111.6 (7)
N12-CA12-C12	111.5 (6)
CB212-CA12-C12	110.1 (6)
N12-CA12-CB112	108.6 (6)
CB212-CA12-CB112	108.3 (7)
C12-CA12-CB112	106.5 (6)
O12-C12-N13	121.9 (8)
O12-C12-CA12	119.7 (7)
N13-C12-CA12	118.4 (7)
C12-N13-CA13	124.9 (6)
N13-CA13-CB113	112.3 (6)
N13-CA13-CB213	108.7 (5)
CB113-CA13-CB213	111.5 (7)
N13-CA13-C13	108.9 (6)
CB113-CA13-C13	108.9 (5)
CB213-CA13-C13	106.2 (6)
O13-C13-N14	123.1 (6)
O13-C13-CA13	119.6 (6)
N14-C13-CA13	117.0 (6)
C13-N14-CA14	120.8 (5)
N14-CA14-CB114	105.6 (5)
N14-CA14-C14	108.6 (5)
CB114-CA14-C14	109.8 (6)
N14-CA14-CB214	110.8 (6)
CB114-CA14-CB214	111.4 (5)
C14-CA14-CB214	110.5 (5)
CA14-CB114-CG114	118.4 (6)
ND14-CG114-CD214	108.4 (6)
ND14-CG114-CD114	108.2 (6)
CD214-CG114-CD114	111.2 (6)
ND14-CG114-CB114	109.1 (6)
CD214-CG114-CB114	111.0 (6)
CD114-CG114-CB114	108.9 (6)
OD14-ND14-CG114	116.4 (5)
OD14-ND14-CG214	119.9 (6)
CG114-ND14-CG214	123.7 (5)
ND14-CG214-CD414	109.0 (6)
ND14-CG214-CB214	106.7 (6)
CD414-CG214-CB214	107.1 (6)
ND14-CG214-CD314	110.9 (6)
CD414-CG214-CD314	109.1 (6)
CB214-CG214-CD314	113.9 (6)
CG214-CB214-CA14	115.2 (5)
O14-C14-N15	121.8 (7)
O14-C14-CA14	120.2 (6)
N15-C14-CA14	117.9 (6)
C14-N15-CA15	123.4 (7)
N15-CA15-CB115	110.6 (8)
N15-CA15-C15	106.3 (9)
CB115-CA15-C15	110.1 (10)
N15-CA15-C'15	102.3 (14)
CB115-CA15-C'15	133.3 (11)
N15-CA15-CB215	108.5 (7)
CB115-CA15-CB215	111.0 (8)
C15-CA15-CB215	110.2 (10)
C'15-CA15-CB215	87.8 (14)
OTB16-C15-O15	116.9 (15)
OTB16-C15-CA15	116.4 (15)

O'15-C'15-OTY16	110.3 (19)
O'15-C'15-CA15	129 (2)
OTY16-C'15-CA15	109.0 (17)
C15-OTB16-CT1B16	105.6 (12)
CT4B16-CT1B16-CT2B16	111.9 (13)
CT4B16-CT1B16-CT3B16	112.9 (15)
CT2B16-CT1B16-CT3B16	105.1 (13)
CT4B16-CT1B16-OTB16	98.8 (11)
CT2B16-CT1B16-OTB16	117.9 (13)
CT3B16-CT1B16-OTB16	110.4 (12)
C'15-OTY16-CT1Y16	109.1 (15)
CT2Y16-CT1Y16-CT4Y16	111 (2)
CT2Y16-CT1Y16-CT3Y16	106 (2)
CT4Y16-CT1Y16-CT3Y16	109 (2)
CT2Y16-CT1Y16-OTY16	123.3 (19)
CT4Y16-CT1Y16-OTY16	105 (2)
CT3Y16-CT1Y16-OTY16	101.6 (18)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ctf25n. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C01	82 (6)	143 (8)	96 (6)	-25 (5)	-38 (5)	29 (6)
C0	63 (5)	92 (6)	72 (5)	-14 (5)	-6 (4)	10 (4)
O0	85 (4)	101 (4)	67 (3)	-21 (3)	11 (3)	11 (3)
N1	60 (4)	125 (5)	61 (4)	-37 (4)	-10 (3)	2 (4)
CA1	47 (4)	101 (6)	53 (4)	-34 (4)	1 (3)	-2 (4)
CB11	62 (5)	106 (6)	62 (4)	-37 (4)	-3 (4)	2 (4)
CG11	66 (5)	106 (7)	74 (5)	-26 (5)	8 (4)	-7 (5)
CD11	101 (6)	94 (6)	79 (5)	-9 (5)	19 (4)	7 (5)
CD21	96 (7)	149 (8)	109 (7)	-47 (6)	22 (5)	-51 (6)
ND1	60 (4)	107 (5)	91 (5)	-25 (4)	10 (3)	0 (4)
OD1	68 (4)	138 (5)	175 (6)	-22 (4)	39 (4)	-5 (4)
CG21	57 (5)	95 (6)	73 (5)	-32 (5)	3 (4)	1 (4)
CD31	93 (6)	127 (7)	116 (7)	-58 (6)	19 (5)	6 (5)
CD41	61 (5)	111 (7)	85 (6)	-11 (5)	-11 (4)	6 (4)
CB21	62 (5)	115 (6)	75 (5)	-44 (5)	0 (4)	-10 (4)
C1	50 (5)	94 (6)	72 (5)	-31 (4)	-19 (4)	8 (4)
O1	48 (3)	120 (4)	67 (3)	-31 (3)	-5 (2)	-2 (3)
N2	51 (4)	98 (5)	76 (4)	-30 (3)	-13 (3)	-3 (3)
CA2	62 (5)	92 (6)	81 (5)	-24 (5)	-5 (4)	-22 (4)
CB12	87 (6)	158 (8)	120 (7)	-65 (6)	0 (5)	-48 (6)
CB22	117 (8)	80 (6)	130 (7)	-21 (5)	-17 (6)	7 (5)
C2	36 (4)	95 (6)	78 (5)	-16 (5)	-8 (4)	-12 (4)
O2	68 (3)	100 (4)	81 (3)	-7 (3)	5 (3)	-30 (3)
N3	51 (4)	78 (4)	63 (4)	-6 (3)	3 (3)	-10 (3)
CA3	39 (4)	79 (5)	71 (5)	-30 (4)	6 (3)	4 (4)
CB13	104 (6)	69 (5)	81 (5)	-13 (4)	19 (4)	-9 (5)
CB23	49 (5)	130 (7)	88 (5)	-27 (5)	3 (4)	8 (4)
C3	47 (5)	81 (5)	71 (5)	-19 (4)	3 (4)	-7 (4)
O3	60 (3)	126 (4)	74 (3)	-38 (3)	11 (2)	-8 (3)
N4	41 (3)	78 (4)	65 (3)	-19 (3)	5 (3)	-7 (3)
CA4	38 (4)	83 (5)	62 (4)	-23 (4)	0 (3)	-9 (4)
CB14	56 (5)	103 (6)	73 (5)	-36 (4)	2 (4)	-8 (4)
CG14	54 (5)	87 (6)	67 (5)	-22 (4)	1 (4)	-13 (4)
CD14	90 (6)	102 (6)	83 (6)	-14 (5)	13 (4)	-18 (5)
CD24	81 (6)	101 (6)	113 (6)	-44 (5)	-8 (5)	-19 (5)
ND4	44 (4)	86 (4)	71 (4)	-23 (3)	-6 (3)	-11 (3)
OD4	53 (3)	113 (4)	107 (4)	-35 (3)	-11 (3)	-15 (3)
CG24	53 (5)	92 (6)	73 (5)	-37 (4)	-6 (4)	-3 (4)
CD34	63 (5)	150 (8)	111 (6)	-67 (6)	-2 (4)	10 (5)
CD44	82 (6)	66 (5)	96 (6)	-10 (4)	-14 (4)	-1 (4)
CB24	50 (4)	82 (5)	78 (5)	-32 (4)	-5 (3)	-11 (4)
C4	60 (5)	93 (6)	71 (5)	-24 (5)	-4 (4)	-11 (4)
O4	86 (4)	108 (4)	68 (3)	-18 (3)	3 (3)	-18 (3)
N5	80 (5)	102 (5)	77 (4)	-10 (4)	1 (3)	-30 (4)
CA5	93 (7)	101 (7)	81 (6)	29 (5)	-27 (5)	-11 (6)
CB15	130 (9)	148 (9)	139 (8)	-11 (7)	-27 (6)	-76 (7)
CB25	132 (10)	184 (11)	255 (13)	-79 (10)	131 (9)	-60 (8)
C5	174 (12)	138 (10)	194 (11)	-27 (8)	9 (9)	-73 (9)
O5	154 (7)	109 (5)	297 (10)	-24 (6)	-97 (7)	4 (5)
OTA6	198 (12)	214 (13)	156 (11)	26 (8)	-75 (9)	-92 (10)
CT1A6	189 (11)	209 (10)	158 (10)	-48 (10)	-56 (11)	-10 (12)
CT2A6	131 (10)	144 (10)	96 (9)	-26 (9)	-36 (9)	41 (10)

OTX6	198 (8)	214 (9)	156 (10)	26 (11)	-75 (10)	-92 (10)
CT1X6	189 (10)	209 (11)	158 (12)	-48 (10)	-56 (10)	-10 (9)
CT2X6	297 (11)	105 (11)	103 (11)	27 (12)	-94 (14)	-23 (16)
CT3X6	210 (20)	179 (19)	134 (16)	-92 (15)	-49 (14)	-31 (16)
CT4X6	252 (10)	151 (10)	126 (10)	-29 (11)	54 (11)	53 (11)
C10110	156 (9)	152 (9)	78 (6)	-12 (5)	24 (5)	-103 (7)
C10010	111 (7)	92 (6)	69 (5)	-22 (5)	6 (5)	-55 (5)
O10010	117 (4)	95 (4)	84 (4)	-26 (3)	-7 (3)	-50 (3)
N11	86 (4)	107 (5)	55 (4)	-30 (3)	23 (3)	-48 (4)
CA11	64 (5)	82 (5)	54 (4)	-24 (4)	15 (4)	-24 (4)
CB111	72 (5)	97 (6)	80 (5)	-35 (4)	14 (4)	-32 (4)
CG111	72 (5)	79 (6)	75 (5)	-10 (4)	7 (4)	-32 (4)
CD111	109 (7)	125 (8)	120 (7)	-34 (6)	-4 (5)	-58 (6)
CD211	81 (6)	113 (7)	84 (6)	4 (5)	20 (4)	-29 (5)
ND11	67 (4)	101 (5)	85 (4)	-9 (4)	-4 (3)	-22 (4)
OD11	87 (4)	142 (5)	169 (6)	-31 (4)	-31 (4)	-14 (4)
CG211	77 (6)	107 (7)	63 (5)	-25 (5)	0 (4)	-16 (5)
CD311	129 (7)	96 (6)	76 (6)	-6 (5)	1 (5)	-24 (5)
CD411	93 (7)	154 (9)	105 (6)	-56 (6)	-3 (5)	31 (6)
CB211	87 (6)	100 (6)	57 (4)	-32 (4)	14 (4)	-17 (5)
C11	50 (5)	90 (6)	80 (5)	-32 (5)	22 (4)	-27 (4)
O11	61 (3)	116 (4)	65 (3)	-24 (3)	22 (2)	-22 (3)
N12	71 (4)	96 (5)	79 (4)	-32 (4)	23 (3)	-23 (4)
CA12	65 (5)	95 (6)	96 (6)	-30 (5)	34 (4)	-9 (5)
CB112	84 (6)	145 (8)	144 (8)	-47 (6)	47 (6)	7 (6)
CB212	137 (9)	91 (7)	168 (9)	-28 (6)	47 (7)	-25 (6)
C12	45 (5)	76 (6)	87 (6)	-6 (5)	15 (4)	6 (4)
O12	62 (3)	105 (4)	99 (4)	-2 (3)	4 (3)	11 (3)
N13	61 (4)	87 (5)	58 (4)	-11 (3)	3 (3)	-8 (3)
CA13	54 (5)	104 (6)	65 (5)	-21 (4)	-5 (4)	-24 (4)
CB113	66 (6)	162 (8)	93 (6)	-30 (5)	-2 (4)	-36 (5)
CB213	125 (7)	89 (6)	77 (5)	-16 (5)	-12 (5)	-11 (5)
C13	44 (4)	98 (6)	71 (5)	-26 (4)	-11 (4)	-7 (4)
O13	67 (3)	137 (5)	81 (4)	-38 (3)	-8 (3)	-18 (3)
N14	43 (3)	93 (4)	65 (4)	-25 (3)	3 (3)	-14 (3)
CA14	48 (4)	103 (6)	62 (5)	-34 (4)	11 (4)	-11 (4)
CB114	61 (5)	94 (6)	79 (5)	-30 (4)	13 (4)	-20 (4)
CG114	58 (5)	91 (6)	94 (6)	-39 (5)	23 (4)	-20 (4)
CD114	83 (6)	158 (8)	145 (7)	-93 (7)	32 (5)	-57 (6)
CD214	95 (6)	76 (6)	112 (6)	-17 (5)	32 (5)	-12 (5)
ND14	58 (4)	90 (5)	76 (4)	-27 (3)	18 (3)	-18 (4)
OD14	55 (3)	122 (4)	111 (4)	-37 (3)	26 (3)	-7 (3)
CG214	51 (5)	100 (6)	65 (5)	-30 (4)	0 (4)	2 (4)
CD314	74 (6)	122 (7)	86 (6)	-17 (5)	-5 (4)	-8 (5)
CD414	86 (6)	116 (7)	120 (7)	-51 (6)	26 (5)	-6 (5)
CB214	69 (5)	92 (6)	72 (5)	-36 (4)	16 (4)	-16 (4)
C14	68 (5)	96 (6)	76 (5)	-18 (5)	-1 (4)	-7 (5)
O14	94 (4)	117 (4)	65 (3)	-18 (3)	3 (3)	-5 (3)
N15	71 (4)	107 (5)	86 (5)	-3 (4)	3 (4)	23 (4)
CA15	85 (6)	136 (8)	95 (6)	10 (6)	16 (5)	5 (6)
CB115	105 (8)	211 (11)	177 (9)	-32 (8)	-61 (7)	3 (8)
CB215	131 (8)	143 (9)	170 (9)	6 (7)	40 (7)	44 (7)
C15	130 (14)	114 (12)	129 (12)	9 (10)	73 (11)	25 (10)
O15	172 (11)	78 (7)	156 (10)	24 (6)	91 (8)	-4 (7)
C'15	190 (30)	180 (30)	230 (30)	-80 (20)	21 (19)	15 (18)
O'15	176 (18)	197 (18)	136 (15)	-58 (13)	2 (13)	-71 (14)
OTB16	110 (8)	242 (12)	107 (7)	30 (7)	-4 (6)	5 (7)
CT1B16	120 (9)	190 (10)	150 (9)	-53 (9)	-51 (9)	-15 (9)
CT2B16	180 (10)	191 (10)	99 (9)	-8 (9)	2 (9)	39 (10)
CT3B16	182 (10)	255 (11)	105 (9)	17 (9)	71 (9)	20 (10)
CT4B16	188 (11)	164 (10)	183 (11)	-23 (10)	-42 (10)	-12 (10)
OTY16	110 (7)	242 (6)	107 (7)	30 (9)	-4 (10)	5 (9)
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CT3Y16	182 (9)	255 (9)	105 (10)	17 (11)	71 (10)	20 (11)
CT4Y16	188 (10)	164 (10)	183 (10)	-23 (3)	-42 (5)	-12 (4)
O1W20	73 (3)	189 (5)	98 (4)	-76 (4)	-10 (3)	-1 (4)
O2W21	85 (4)	244 (7)	130 (5)	-98 (5)	-5 (3)	-15 (4)
O3W22	68 (3)	150 (5)	76 (3)	-48 (3)	17 (2)	-29 (3)
O4W23	119 (5)	249 (8)	133 (5)	-107 (5)	59 (4)	-55 (5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ctf25n.

	x	y	z	U(eq)
H01A	6535	9348	-4743	174
H01B	6253	9996	-4558	174
H01C	5366	9403	-4341	174
H01	8143	8615	-4259	99
HB1A1	10166	8531	-2895	91
HB1B1	9342	9188	-3344	91
HD1A1	10200	9183	-4495	150
HD1B1	11502	9499	-4544	150
HD1C1	10260	9842	-4336	150
HD2A1	12679	9409	-3623	173
HD2B1	12176	8981	-2998	173
HD2C1	11439	9710	-3380	173
HD3A1	11784	7456	-4255	165
HD3B1	11660	6759	-3722	165
HD3C1	12889	7134	-3763	165
HD4A1	11185	7476	-2603	141
HD4B1	12517	7143	-2748	141
HD4C1	11281	6772	-2705	141
HB2A1	9496	7334	-3513	98
HB2B1	9792	7935	-4096	98
H02	6895	7788	-3295	91
HB1A2	4744	7699	-2844	172
HB1B2	4683	6993	-2313	172
HB1C2	5277	6997	-2913	172
HB2A2	8084	6593	-1958	174
HB2B2	7353	6309	-2362	174
HB2C2	6771	6299	-1759	174
H03	6395	8565	-2581	84
HB1A3	7447	9420	-2285	133
HB1B3	6466	9769	-1951	133
HB1C3	6033	9705	-2543	133
HB2A3	4475	8388	-1440	142
HB2B3	4170	9059	-2014	142
HB2C3	4597	9119	-1418	142
H04	8331	8041	-1636	76
HB1A4	9669	8169	-209	92
HB1B4	8953	8747	-766	92
HD1A4	10613	8624	-1749	146
HD1B4	11724	9041	-1696	146
HD1C4	10277	9347	-1687	146
HD2A4	12146	9171	-741	145
HD2B4	11405	8785	-171	145
HD2C4	10697	9436	-681	145
HD3A4	12436	7456	-1569	157
HD3B4	12411	6661	-1210	157
HD3C4	13406	7058	-1029	157
HD4A4	11142	6794	115	131
HD4B4	12612	6652	-2	131
HD4C4	11610	6258	-183	131
HB2A4	9946	6905	-945	83
HB2B4	10233	7586	-1455	83
H05	7497	6971	-749	110
HB1A5	6991	5747	-361	218
HB1B5	5670	6233	-476	218

HB2A5	6344	7080	493	283
HB2B5	5497	6471	643	283
HB2C5	5309	7089	27	283
HT2A6	10388	5538	991	200
HT2B6	10688	5078	1663	200
HT2C6	9955	5832	1484	200
HT3A6	9390	4571	911	163
HT3B6	8273	4267	1328	163
HT3C6	9684	4153	1591	163
HT4A6	7425	4817	2048	286
HT4B6	8131	5404	2119	286
HT4C6	8834	4641	2325	286
HT2D6	10351	5360	605	279
HT2E6	9759	4662	765	279
HT2F6	10898	4708	1157	279
HT3D6	10091	5967	1343	244
HT3E6	10646	5242	1815	244
HT3F6	9340	5632	1924	244
HT4D6	8231	4383	1411	286
HT4E6	7888	4708	1893	286
HT4F6	9215	4245	1937	286
H10A10	6331	9397	281	195
H10B10	7487	9442	665	195
H10C10	6268	10005	517	195
H011	5148	8610	756	95
HB1A11	3911	7900	917	97
HB1B11	4422	7275	1494	97
HD1A11	2129	7455	726	176
HD1B11	1133	7139	1211	176
HD1C11	2531	6746	1251	176
HD2A11	2623	7413	2404	154
HD2B11	2835	6718	2285	154
HD2C11	1437	7110	2248	154
HD3A11	1408	9540	558	161
HD3B11	2858	9234	558	161
HD3C11	2496	9833	799	161
HD4A11	261	9305	1505	179
HD4B11	1329	9562	1792	179
HD4C11	935	8816	2114	179
HB2A11	3164	8416	2175	96
HB2B11	3684	9088	1746	96
H012	6815	7705	1681	97
HB1A12	9084	7511	2096	193
HB1B12	8777	6836	2012	193
HB1C12	9401	6787	2614	193
HB2A12	6974	6212	2566	206
HB2B12	6203	6475	3019	206
HB2C12	7657	6156	3157	206
H013	7051	8400	2431	88
HB1A13	9149	8137	3566	164
HB1B13	8755	8868	3606	164
HB1C13	9231	8814	3006	164
HB2A13	5814	9307	2737	152
HB2B13	7139	9548	2485	152
HB2C13	6682	9597	3090	152
H014	5420	7921	3368	81
HB1A14	4359	6774	4112	93
HB1B14	3758	7449	3598	93
HD1A14	1652	7274	3516	171
HD1B14	847	6907	4070	171
HD1C14	2056	6490	3910	171
HD2A14	3224	6759	5173	149
		6171	4934	149

HD3A14	2954	8486	3265	151
HD3B14	2928	9215	3315	151
HD3C14	1631	8914	3303	151
HD4A14	1071	9098	4227	159
HD4B14	2400	9352	4277	159
HD4C14	1948	8729	4805	159
HB2A14	3948	8086	4806	91
HB2B14	4434	8647	4240	91
H015	6762	6816	4279	121
HB1A15	7902	7020	5462	265
HB1B15	8895	6990	4977	265
HB1C15	9019	6400	5609	265
HB2A15	7797	5594	4700	258
HB2B15	8938	5495	5149	258
HB2C15	8863	6094	4522	258
HT2A16	5987	4649	6089	263
HT2B16	5734	4293	6767	263
HT2C16	7152	4292	6544	263
HT3A16	4578	5669	6121	314
HT3B16	4921	6042	6545	314
HT3C16	4437	5311	6809	314
HT4A16	7024	5568	7169	286
HT4B16	7882	4908	7142	286
HT4C16	6542	4837	7447	286
HT2D16	4371	5315	5670	263
HT2E16	4300	4642	6235	263
HT2F16	5389	4658	5778	263
HT3D16	7081	4312	6499	314
HT3E16	6010	4212	6974	314
HT3F16	7098	4670	6965	314
HT4D16	4374	5937	6399	286
HT4E16	5473	5669	6895	286
HT4F16	4367	5217	6920	286
H1WA20	8127	8592	-5338	172
H1WB20	9278	8294	-5004	172
H2WA21	5736	7696	-4264	218
H2WB21	4871	8092	-4030	218
H3WA22	5386	8483	-157	142
H3WB22	4049	8497	-204	142
H4WA23	8175	7717	736	231
H4WB23	8408	8329	809	231

Table 6. Torsion angles [deg] for ctf25n.

O0-C0-N1-CA1	-1.4 (11)
C01-C0-N1-CA1	177.3 (7)
C0-N1-CA1-CB11	-65.5 (8)
C0-N1-CA1-CB21	172.0 (7)
C0-N1-CA1-C1	55.7 (9)
N1-CA1-CB11-CG11	-85.6 (7)
CB21-CA1-CB11-CG11	34.1 (8)
C1-CA1-CB11-CG11	153.0 (6)
CA1-CB11-CG11-ND1	-52.2 (8)
CA1-CB11-CG11-CD11	67.2 (9)
CA1-CB11-CG11-CD21	-169.5 (6)
CD11-CG11-ND1-OD1	74.5 (8)
CD21-CG11-ND1-OD1	-46.6 (8)
CB11-CG11-ND1-OD1	-164.0 (6)
CD11-CG11-ND1-CG21	-105.9 (7)
CD21-CG11-ND1-CG21	133.0 (7)
CB11-CG11-ND1-CG21	15.6 (8)
OD1-ND1-CG21-CD31	-31.8 (8)
CG11-ND1-CG21-CD31	148.6 (6)
OD1-ND1-CG21-CD41	87.7 (7)
CG11-ND1-CG21-CD41	-91.9 (7)
OD1-ND1-CG21-CB21	-147.1 (6)
CG11-ND1-CG21-CB21	33.3 (8)
ND1-CG21-CB21-CA1	-52.9 (8)
CD31-CG21-CB21-CA1	-168.3 (6)
CD41-CG21-CB21-CA1	69.2 (9)
N1-CA1-CB21-CG21	145.0 (6)
CB11-CA1-CB21-CG21	21.1 (8)
C1-CA1-CB21-CG21	-98.0 (7)
N1-CA1-C1-O1	-153.0 (6)
CB11-CA1-C1-O1	-28.9 (8)
CB21-CA1-C1-O1	91.9 (7)
N1-CA1-C1-N2	29.1 (8)
CB11-CA1-C1-N2	153.2 (6)
CB21-CA1-C1-N2	-86.0 (7)
O1-C1-N2-CA2	1.1 (10)
CA1-C1-N2-CA2	178.9 (6)
C1-N2-CA2-CB12	170.9 (6)
C1-N2-CA2-C2	55.4 (8)
C1-N2-CA2-CB22	-67.9 (8)
N2-CA2-C2-O2	-160.5 (5)
CB12-CA2-C2-O2	83.7 (7)
CB22-CA2-C2-O2	-36.9 (8)
N2-CA2-C2-N3	22.5 (8)
CB12-CA2-C2-N3	-93.4 (7)
CB22-CA2-C2-N3	146.0 (6)
O2-C2-N3-CA3	5.7 (9)
CA2-C2-N3-CA3	-177.4 (5)
C2-N3-CA3-CB13	164.8 (6)
C2-N3-CA3-CB23	-73.6 (7)
C2-N3-CA3-C3	47.8 (7)
N3-CA3-C3-O3	-153.3 (6)
CB13-CA3-C3-O3	89.6 (7)
CB23-CA3-C3-O3	-32.4 (9)
N3-CA3-C3-N4	32.5 (8)
CB13-CA3-C3-N4	-84.6 (7)
CB23-CA3-C3-N4	153.4 (6)
O3-C3-N4-CA4	2.0 (10)
CA2-C2-N3-CA3	176.2 (6)

C3-N4-CA4-CB24	173.8(6)
C3-N4-CA4-C4	57.1(8)
N4-CA4-CB14-CG14	-98.9(7)
CB24-CA4-CB14-CG14	20.4(8)
C4-CA4-CB14-CG14	140.4(6)
CA4-CB14-CG14-ND4	-55.4(7)
CA4-CB14-CG14-CD24	-171.6(6)
CA4-CB14-CG14-CD14	64.7(8)
CD24-CG14-ND4-OD4	-20.3(8)
CB14-CG14-ND4-OD4	-137.0(5)
CD14-CG14-ND4-OD4	100.3(6)
CD24-CG14-ND4-CG24	162.5(6)
CB14-CG14-ND4-CG24	45.9(7)
CD14-CG14-ND4-CG24	-76.8(7)
OD4-ND4-CG24-CD44	58.8(7)
CG14-ND4-CG24-CD44	-124.0(6)
OD4-ND4-CG24-CB24	-177.9(5)
CG14-ND4-CG24-CB24	-0.7(8)
OD4-ND4-CG24-CD34	-58.6(7)
CG14-ND4-CG24-CD34	118.6(6)
ND4-CG24-CB24-CA4	-40.0(8)
CD44-CG24-CB24-CA4	80.7(8)
CD34-CG24-CB24-CA4	-158.6(6)
N4-CA4-CB24-CG24	152.1(6)
CB14-CA4-CB24-CG24	29.8(8)
C4-CA4-CB24-CG24	-90.6(7)
N4-CA4-C4-O4	-148.5(6)
CB14-CA4-C4-O4	-26.4(9)
CB24-CA4-C4-O4	96.0(8)
N4-CA4-C4-N5	35.8(8)
CB14-CA4-C4-N5	157.8(6)
CB24-CA4-C4-N5	-79.7(7)
O4-C4-N5-CA5	6.5(12)
CA4-C4-N5-CA5	-177.8(6)
C4-N5-CA5-CB25	70.9(10)
C4-N5-CA5-CB15	-164.1(7)
C4-N5-CA5-C5	-58.7(10)
CB25-CA5-C5-O5	-158.3(12)
N5-CA5-C5-O5	-36.1(16)
CB15-CA5-C5-O5	76.3(14)
CB25-CA5-C5-OTX6	11(2)
N5-CA5-C5-OTX6	133.0(19)
CB15-CA5-C5-OTX6	-114.7(19)
CB25-CA5-C5-OTA6	23.8(16)
N5-CA5-C5-OTA6	146.0(13)
CB15-CA5-C5-OTA6	-101.7(14)
O5-C5-OTA6-CT1A6	-1(2)
CA5-C5-OTA6-CT1A6	177.0(12)
C5-OTA6-CT1A6-CT3A6	-65(2)
C5-OTA6-CT1A6-CT2A6	59(2)
C5-OTA6-CT1A6-CT4A6	176.8(17)
O5-C5-OTX6-CT1X6	-13(3)
CA5-C5-OTX6-CT1X6	175.8(14)
C5-OTX6-CT1X6-CT2X6	2(3)
C5-OTX6-CT1X6-CT4X6	-117(2)
C5-OTX6-CT1X6-CT3X6	119(2)
O10010-C10010-N11-CA11	2.7(12)
C10110-C10010-N11-CA11	-175.3(7)
C10010-N11-CA11-CB211	66.9(8)
C10010-N11-CA11-CB111	-172.2(7)
C10010-N11-CA11-C11	-54.2(9)
N11-CA11-CB111-CG111	-140.1(6)
CB211-CA11-CB111-CG111	-18.5(8)

CA11-CB111-CG111-ND11	51.6 (8)
CA11-CB111-CG111-CD111	169.1 (6)
CA11-CB111-CG111-CD211	-68.6 (9)
CD111-CG111-ND11-OD11	27.3 (9)
CB111-CG111-ND11-OD11	144.3 (6)
CD211-CG111-ND11-OD11	-92.4 (7)
CD111-CG111-ND11-CG211	-153.8 (6)
CB111-CG111-ND11-CG211	-36.8 (9)
CD211-CG111-ND11-CG211	86.5 (7)
OD11-ND11-CG211-CB211	167.8 (6)
CG111-ND11-CG211-CB211	-11.1 (9)
OD11-ND11-CG211-CD411	49.3 (8)
CG111-ND11-CG211-CD411	-129.6 (7)
OD11-ND11-CG211-CD311	-69.3 (8)
CG111-ND11-CG211-CD311	111.8 (7)
ND11-CG211-CB211-CA11	49.2 (8)
CD411-CG211-CB211-CA11	167.0 (6)
CD311-CG211-CB211-CA11	-71.3 (9)
N11-CA11-CB211-CG211	84.1 (8)
CB111-CA11-CB211-CG211	-34.1 (8)
C11-CA11-CB211-CG211	-153.8 (6)
N11-CA11-C11-O11	149.2 (6)
CB211-CA11-C11-O11	26.3 (9)
CB111-CA11-C11-O11	-94.5 (7)
N11-CA11-C11-N12	-31.9 (8)
CB211-CA11-C11-N12	-154.8 (6)
CB111-CA11-C11-N12	84.4 (7)
O11-C11-N12-CA12	1.3 (10)
CA11-C11-N12-CA12	-177.6 (6)
C11-N12-CA12-CB212	66.4 (9)
C11-N12-CA12-C12	-57.3 (8)
C11-N12-CA12-CB112	-174.3 (7)
N12-CA12-C12-O12	160.3 (6)
CB212-CA12-C12-O12	35.9 (9)
CB112-CA12-C12-O12	-81.4 (8)
N12-CA12-C12-N13	-23.1 (8)
CB212-CA12-C12-N13	-147.6 (7)
CB112-CA12-C12-N13	95.2 (7)
O12-C12-N13-CA13	-3.4 (10)
CA12-C12-N13-CA13	-179.9 (5)
C12-N13-CA13-CB113	68.9 (8)
C12-N13-CA13-CB213	-167.2 (6)
C12-N13-CA13-C13	-51.9 (8)
N13-CA13-C13-O13	157.3 (6)
CB113-CA13-C13-O13	34.5 (9)
CB213-CA13-C13-O13	-85.8 (7)
N13-CA13-C13-N14	-28.8 (8)
CB113-CA13-C13-N14	-151.7 (7)
CB213-CA13-C13-N14	88.1 (7)
O13-C13-N14-CA14	-5.0 (10)
CA13-C13-N14-CA14	-178.6 (6)
C13-N14-CA14-CB114	-171.1 (6)
C13-N14-CA14-C14	-53.4 (8)
C13-N14-CA14-CB214	68.1 (8)
N14-CA14-CB114-CG114	-151.5 (6)
C14-CA14-CB114-CG114	91.6 (8)
CB214-CA14-CB114-CG114	-31.2 (9)
CA14-CB114-CG114-ND14	43.2 (8)
CA14-CB114-CG114-CD214	-76.2 (8)
CA14-CB114-CG114-CD114	161.0 (6)
CD214-CG114-ND14-OD14	-61.4 (7)
CD114-CG114-ND14-OD14	59.3 (7)
CB114-CG114-ND14-OD14	177.6 (5)

CD114-CG114-ND14-CG214	-120.4 (6)
CB114-CG114-ND14-CG214	-2.1 (9)
OD14-ND14-CG214-CD414	19.4 (8)
CG114-ND14-CG214-CD414	-160.9 (6)
OD14-ND14-CG214-CB214	134.7 (6)
CG114-ND14-CG214-CB214	-45.6 (8)
OD14-ND14-CG214-CD314	-100.7 (7)
CG114-ND14-CG214-CD314	79.0 (7)
ND14-CG214-CB214-CA14	56.6 (7)
CD414-CG214-CB214-CA14	173.2 (6)
CD314-CG214-CB214-CA14	-66.1 (8)
N14-CA14-CB214-CG214	96.3 (7)
CB114-CA14-CB214-CG214	-20.9 (8)
C14-CA14-CB214-CG214	-143.2 (6)
N14-CA14-C14-O14	145.3 (6)
CB114-CA14-C14-O14	-99.7 (7)
CB214-CA14-C14-O14	23.5 (9)
N14-CA14-C14-N15	-38.7 (9)
CB114-CA14-C14-N15	76.3 (8)
CB214-CA14-C14-N15	-160.4 (7)
O14-C14-N15-CA15	-5.0 (12)
CA14-C14-N15-CA15	179.0 (7)
C14-N15-CA15-CB115	-72.2 (10)
C14-N15-CA15-C15	47.2 (13)
C14-N15-CA15-C'15	74.0 (14)
C14-N15-CA15-CB215	165.8 (8)
N15-CA15-C15-OTB16	-145.0 (15)
CB115-CA15-C15-OTB16	-25.2 (19)
CB215-CA15-C15-OTB16	97.6 (17)
N15-CA15-C15-O15	49.4 (18)
CB115-CA15-C15-O15	169.2 (14)
CB215-CA15-C15-O15	-68.0 (17)
N15-CA15-C'15-O'15	17 (4)
CB115-CA15-C'15-O'15	152 (2)
CB215-CA15-C'15-O'15	-91 (3)
N15-CA15-C'15-OTY16	-121 (2)
CB115-CA15-C'15-OTY16	13 (4)
CB215-CA15-C'15-OTY16	131 (2)
O15-C15-OTB16-CT1B16	-4 (2)
CA15-C15-OTB16-CT1B16	-171.1 (14)
C15-OTB16-CT1B16-CT4B16	-178.1 (14)
C15-OTB16-CT1B16-CT2B16	61.2 (18)
C15-OTB16-CT1B16-CT3B16	-59.6 (19)
O'15-C'15-OTY16-CT1Y16	21 (4)
CA15-C'15-OTY16-CT1Y16	167.5 (19)
C'15-OTY16-CT1Y16-CT2Y16	-7 (3)
C'15-OTY16-CT1Y16-CT4Y16	-135 (2)
C'15-OTY16-CT1Y16-CT3Y16	112 (3)

Table 7. Hydrogen bonds for ctf25n [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N3-H03...O0	0.86	2.13	2.972(7)	164.4
N4-H04...O1	0.86	2.17	3.022(7)	171.2
N5-H05...O2	0.86	2.18	2.922(8)	143.7
N13-H013...O10010	0.86	2.13	2.959(8)	161.7
N14-H014...O11	0.86	2.15	3.004(7)	169.2
N15-H015...O12	0.86	2.21	2.961(8)	146.2
N1-H01...O1W20	0.86	2.14	2.981(7)	164.6
N2-H02...O2W21	0.86	2.16	2.988(8)	162.6
N11-H011...O3W22	0.86	2.09	2.938(7)	168.0
N12-H012...O4W23	0.86	2.15	2.979(8)	161.4
O1W20-H1WA20...O13#1	0.83	1.96	2.782(7)	173.3
O1W20-H1WB20...OD14#2	0.83	2.29	2.922(7)	133.6
O2W21-H2WA21...O14#1	0.84	2.00	2.800(8)	159.0
O2W21-H2WB21...OD1#3	0.83	2.03	2.831(8)	163.2
O3W22-H3WA22...O3	0.83	2.06	2.777(7)	144.2
O3W22-H3WB22...OD4#3	0.84	2.07	2.880(7)	162.9
O4W23-H4WA23...O4	0.83	1.98	2.806(8)	167.8
O4W23-H4WB23...OD11#4	0.83	2.36	2.856(9)	119.1

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x+1,y,z-1 #3 x-1,y,z #4 x+1,y,z