# Crystal Structure of N,N′-Dimethyl-diketopiperazine

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The crystals belong to the monoclinic system with space group $P2_1/c$ and cell dimensions $a = 7.05_1$ Å, $b = 6.11_0$ Å, $c = 9.67_0$ Å, $\beta = 123.9_5°$. There are two molecules in the unit cell. The phase problem was solved by a computer procedure based on direct methods. The R-value arrived at by full-matrix least squares refinement was 6.6 % for 516 observed reflections. A rigid-body analysis of translational and librational motion leads to significant corrections in bond lengths. The corrected bond length between the carbonyl carbon and nitrogen is 1.34_8 Å while the corresponding value for diketopiperazine (uncorrected) is 1.32_5 Å. The molecule deviates significantly from planarity, and may be described in terms of an extremely flattened chair form.

The crystal structure determination of N,N′-dimethyl-diketopiperazine
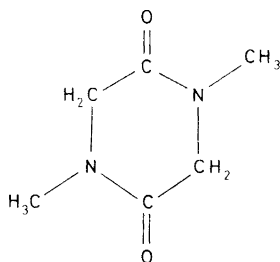
was carried out as part of a systematic study of cyclic peptides of sarcosine,[1] and in order to decide whether the substitution of methyl for hydrogen influences the degree of planarity compared to that observed for diketopiperazine.[2]

The crystals belong to the monoclinic system and the systematic absences lead to the space group $P2_1/c$. The cell parameters,[3]* measured by means of a four circle diffractometer, and their estimated standard deviations are:

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* All programs used are included in this reference.

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$a = 7.051(4)$ Å, $b = 6.110(4)$ Å, $c = 9.670(5)$ Å, $\beta = 123.95(4)°$.

The unit cell contains two molecules ($\varrho_{calc} = 1.38$ g·cm^{-3}, $\varrho_{obs} = 1.38$ g·cm^{-3}).

Intensity data were obtained by photometric measurements of integrated equiinclination Weissenberg diagrams corresponding to $h0l$, $\cdots$, $h4l$. 516 independent reflections were strong enough to be measured. No corrections have been made for absorption or secondary extinction effects.

The phase problem was solved for the $h0l$ reflections by a computer procedure based on direct methods. The three-dimensional refinement was carried out by full-matrix least squares technique. The weighting scheme:

$$\text{for } F_o \leq \text{FB}, \quad W = A1 \cdot (F_o)^{B1}; \quad \text{for } F_o > \text{FB}, \quad W = A2 \cdot (F_o)^{B2}$$

was used with: $A1 = 10.0$, $A2 = 10.0$, $B1 = 0.0$, $B2 = -0.5$ and $FB = 1.0$.

The atomic form factors were those of Hanson et al.[4]

After three cycles of isotropic refinement, anisotropic thermal parameters were introduced for the heavy atoms. One methyl hydrogen position could be localized in the difference Fourier map. The coordinates of the four other hydrogen atoms were calculated assuming C—H bond lengths of 1.03 Å. The hydrogens were included in structure factor calculations with a common B-value of 5.0 Å^2. Positional parameters only were refined. The R-value arrived

Table 1. Fractional atomic coordinates and anisotropic thermal vibration parameters with estimated standard deviations (multiplied by 10^5).[a]

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O	22672	−34310	19514	3057	3859	2028	2095	2264	1919
	32	39	25	67	119	40	111	82	84
N	10413	15452	−04312	2233	2942	1519	301	1923	352
	29	38	24	62	111	35	97	76	72
C$_1$	11627	−18950	10348	2274	2838	1448	710	1747	159
	40	49	29	67	127	39	115	81	87
C$_2$	23229	−03527	05303	2088	3120	1590	666	1799	468
	38	49	30	64	130	41	121	84	94
C$_3$	22461	30374	−08790	3452	3480	2335	−329	3579	873
	50	54	40	94	151	56	161	125	127

[a] For numbering, see Fig. 1.

Table 2. Fractional atomic coordinates for the hydrogen atoms. (H$_{m,n}$ is bonded to C$_m$).

Atom	x	y	z
H$_{2,1}$	.380	.019	.161
H$_{2,2}$	.277	−.123	−.016
H$_{3,1}$	.288	.235	−.151
H$_{3,2}$	.337	.319	.040
H$_{3,3}$	.135	.446	−.151

Table 3. Observed and calculated structure factors on 10 times absolute scale.

h	k	l	F_o	F_c
0	0	2	273	275
0	0	4	23	- 30
0	0	6	62	- 53
0	0	8	55	- 54
0	1	1	248	263
0	1	2	470	507
0	1	3	198	197
0	1	4	98	80
0	1	5	52	- 49
0	1	6	66	61
0	1	7	14	- 14
0	1	8	21	- 21
0	1	9	19	- 17
0	2	1	108	- 106
0	2	2	27	20
0	2	3	176	183
0	2	4	34	43
0	2	5	75	88
0	2	6	33	29
0	2	8	11	- 13
0	2	9	27	26
0	3	1	7	- 5
0	3	2	2	- 5
0	3	3	92	- 92
0	3	5	54	- 50
0	3	6	40	42
0	3	7	32	- 33
0	3	8	31	29
0	3	9	10	- 9
0	4	1	38	38
0	4	2	12	10
0	4	3	40	- 38
0	4	4	20	- 21
0	4	5	16	18
0	4	6	28	- 26
0	4	7	14	14
0	4	8	9	11
1	0	-8	33	- 32
1	0	-4	195	- 189
1	0	-2	327	329
1	0	0	414	416
1	0	2	12	17
1	0	4	86	85
1	0	6	59	- 60
1	1	-10	18	14
1	1	-8	8	- 1
1	1	-7	40	- 40
1	1	-6	8	5
1	1	-5	33	26
1	1	-4	103	- 99
1	1	-3	290	275
1	1	-1	123	112
1	1	0	53	49
1	1	1	127	121
1	1	2	15	- 18
1	1	3	73	- 63
1	1	4	75	78
1	1	5	49	- 48
1	1	6	34	35
1	1	7	9	8
1	2	-10	14	- 15
1	2	-8	24	22
1	2	-7	4	- 3
1	2	-6	57	50
1	2	-5	193	- 200
1	2	-4	171	173
1	2	-3	26	- 32
1	2	-2	63	42
1	2	-1	11	8
1	2	0	123	- 120
1	2	1	72	67
1	2	2	97	- 97
1	2	3	161	153
1	2	4	78	- 80
1	2	5	51	- 51
1	2	6	12	- 9
1	2	7	8	10
1	2	8	20	- 22
1	2	9	13	15
1	3	-10	4	- 4
1	3	-9	8	7
1	3	-8	35	- 30
1	3	-7	92	91
1	3	-6	16	- 15
1	3	-5	74	77
1	3	-4	5	- 5
1	3	-3	87	- 93
1	3	-2	35	36
1	3	-1	19	- 15
1	3	0	82	87
1	3	1	180	- 202
1	3	2	32	29
1	3	3	10	11
1	3	4	9	- 9
1	3	5	19	- 22
1	3	6	19	20
1	3	7	58	- 54
1	4	-9	16	- 15
1	4	-8	19	20

h	k	l	F_o	F_c
1	4	-7	18	- 18
1	4	-6	14	17
1	4	-5	95	96
1	4	-4	65	68
1	4	-3	64	64
1	4	-2	33	- 32
1	4	-1	42	37
1	4	0	52	- 50
1	4	1	11	- 13
1	4	2	9	- 10
1	4	3	28	- 26
1	4	4	71	- 74
1	4	5	49	51
1	4	6	16	- 18
1	4	7	7	- 8
2	0	-10	11	- 12
2	0	-6	56	- 68
2	0	-4	106	- 106
2	0	-2	38	37
2	0	0	459	- 463
2	0	2	4	- 8
2	0	4	36	45
2	0	6	53	49
2	0	8	33	52
2	1	-11	16	14
2	1	-10	25	20
2	1	-9	6	7
2	1	-8	6	- 10
2	1	-7	53	- 52
2	1	-6	33	27
2	1	-5	11	10
2	1	-2	98	82
2	1	-1	53	- 45
2	1	1	7	- 10
2	1	2	205	- 196
2	1	3	99	- 88
2	1	4	22	- 19
2	1	5	28	33
2	1	6	33	- 31
2	1	7	25	25
2	1	8	23	21
2	2	-11	10	9
2	2	-10	22	23
2	2	-9	60	57
2	2	-8	41	41
2	2	-7	11	- 7
2	2	-6	49	50
2	2	-5	87	- 95
2	2	-4	12	22
2	2	-3	83	- 75
2	2	-2	152	- 152
2	2	-1	211	- 223
2	2	0	26	33
2	2	1	76	81
2	2	2	53	- 51
2	2	4	47	- 50
2	2	4	29	- 30
2	2	5	54	- 52
2	2	6	28	- 24
2	2	7	11	12
2	2	8	8	- 8
2	3	-10	6	- 6
2	3	-9	35	32
2	3	-8	13	14
2	3	-7	132	139
2	3	-6	35	37
2	3	-5	45	42
2	3	-4	10	9
2	3	-3	25	17
2	3	-2	22	- 19
2	3	-1	151	- 164
2	3	0	15	- 20
2	3	1	124	- 132
2	3	2	26	- 27
2	3	3	39	35
2	3	4	5	6
2	3	5	49	- 46
2	3	7	12	- 10
2	4	-9	33	- 37
2	4	-8	12	11
2	4	-7	10	10
2	4	-6	58	55
2	4	-5	107	109
2	4	-4	55	56
2	4	-3	96	94
2	4	-2	52	- 47
2	4	0	9	- 7
2	4	1	70	- 67
2	4	2	53	- 54
2	4	4	37	- 37
2	4	5	5	6
2	4	6	5	5
3	0	-10	18	- 16
3	0	-8	51	- 57
3	0	-6	202	- 193
3	0	-4	84	75
3	0	-2	104	- 96
3	0	0	213	- 216

h	k	l	F_o	F_c
3	0	2	7	6
3	0	4	12	12
3	0	6	86	86
3	1	-11	22	22
3	1	-10	34	32
3	1	-9	16	- 16
3	1	-8	29	37
3	1	-7	34	- 33
3	1	-6	68	- 64
3	1	-5	130	- 120
3	1	-4	149	- 122
3	1	-3	263	- 245
3	1	-2	201	193
3	1	-1	6	- 4
3	1	0	89	- 78
3	1	1	53	- 54
3	1	2	74	- 64
3	1	3	34	37
3	1	4	94	- 85
3	1	5	65	63
3	1	6	34	- 32
3	1	7	19	19
3	2	-11	25	27
3	2	-10	28	27
3	2	-9	57	55
3	2	-8	30	31
3	2	-7	9	7
3	2	-6	18	15
3	2	-5	80	80
3	2	-4	147	- 161
3	2	-3	127	- 126
3	2	-2	105	- 99
3	2	-1	110	- 120
3	2	0	54	44
3	2	1	43	- 46
3	2	2	60	61
3	2	3	124	- 122
3	2	4	39	40
3	2	5	5	- 6
3	2	6	18	- 18
3	2	7	7	6
3	3	-11	11	- 11
3	3	-9	32	30
3	3	-8	38	36
3	3	-7	29	26
3	3	-6	44	45
3	3	-5	17	15
3	3	-4	22	16
3	3	-3	79	82
3	3	-2	47	- 47
3	3	-1	56	- 52
3	3	0	101	- 103
3	3	1	74	72
3	3	2	44	- 44
3	3	3	6	- 5
3	3	4	20	18
3	4	-9	31	- 26
3	4	-8	21	- 19
3	4	-7	19	21
3	4	-6	27	27
3	4	-5	9	- 5
3	4	-4	16	- 12
3	4	-3	33	34
3	4	-2	30	29
3	4	-1	7	7
3	4	0	30	29
3	4	1	10	- 10
3	4	2	34	- 33
3	4	3	38	35
3	4	4	11	11
3	4	5	5	- 6
4	0	-12	11	11
4	0	-8	112	- 103
4	0	-6	108	- 99
4	0	-4	57	59
4	0	-2	119	- 121
4	0	0	32	35
4	0	2	22	21
4	0	4	16	14
4	0	6	27	- 30
4	1	-12	18	17
4	1	-11	3	- 6
4	1	-10	38	38
4	1	-9	28	- 30
4	1	-8	49	55
4	1	-7	8	- 5
4	1	-6	78	- 75
4	1	-5	78	- 77
4	1	-4	52	47
4	1	-3	18	- 20
4	1	-2	13	10
4	1	-1	17	- 18
4	1	0	31	- 38
4	1	1	24	- 25
4	1	3	55	53
4	1	5	59	- 56
4	1	5	17	16
4	2	-11	26	26
4	2	-10	9	- 11
4	2	-8	11	7

h	k	l	F_o	F_c
4	2	-7	28	28
4	2	-6	10	- 11
4	2	-5	91	85
4	2	-4	37	- 41
4	2	-3	3	- 3
4	2	-2	58	59
4	2	-1	53	58
4	2	1	102	- 99
4	2	2	76	74
4	2	3	61	- 60
4	2	4	10	10
4	3	-8	8	- 6
4	3	-8	8	6
4	3	-7	69	- 68
4	3	-6	9	7
4	3	-5	9	13
4	3	-4	7	4
4	3	-3	35	37
4	3	-2	24	- 24
4	3	-1	120	127
4	3	0	53	- 49
4	3	1	127	126
4	3	2	4	- 2
4	3	3	20	- 17
4	3	4	10	10
4	3	5	14	- 11
4	4	-10	15	- 15
4	4	-9	9	10
4	4	-8	9	- 6
4	4	-6	10	- 13
4	4	-5	61	- 64
4	4	-3	62	- 69
4	4	-2	82	78
4	4	-1	73	- 68
4	4	0	31	29
4	4	1	66	59
4	4	2	17	16
4	4	3	46	42
4	4	4	7	10
5	0	-10	14	14
5	0	-6	114	105
5	0	-4	36	- 44
5	0	-2	59	- 62
5	0	2	37	- 43
5	0	4	9	9
5	1	-12	5	- 6
5	1	-11	16	- 17
5	1	-10	11	8
5	1	-9	4	- 3
5	1	-7	30	31
5	1	-6	49	49
5	1	-5	49	53
5	1	-4	140	129
5	1	-3	68	68
5	1	-2	23	- 17
5	1	-1	46	- 46
5	1	0	8	9
5	1	1	17	- 19
5	1	2	31	- 31
5	1	3	14	- 12
5	2	-11	3	2
5	2	-10	21	- 21
5	2	-9	28	- 28
5	2	-8	8	- 9
5	2	-7	19	18
5	2	-6	13	- 10
5	2	-5	10	9
5	2	-4	74	77
5	2	-3	107	109
5	2	-1	63	69
5	2	0	37	40
5	2	1	40	40
5	2	4	26	- 28
5	3	-11	4	- 4
5	3	-9	15	- 16
5	3	-8	10	- 12
5	3	-7	26	- 28
5	3	-6	13	- 16
5	3	-5	6	- 7
5	3	-4	7	- 5
5	3	-2	7	5
5	3	-1	127	129
5	3	0	31	29
5	3	1	46	41
5	3	2	29	26
5	3	-10	19	- 14
5	3	-9	10	9
5	3	-7	9	- 10
5	3	-6	6	8
5	3	-5	18	- 22
5	3	-3	38	36
5	3	-3	76	- 74
5	3	-2	40	39
5	3	-1	30	- 21
5	4	0	10	9
5	4	1	42	43
5	4	2	20	21

Table 3. Continued.

h	k	l	Fo	Fc		h	k	l	Fo	Fc		h	k	l	Fo	Fc		h	k	l	Fo	Fc
6	0	-12	2	- 3		6	2	-2	25	23		7	1	-9	26	25		7	4	-5	15	- 18
6	0	-10	17	13		6	2	-1	11	10		7	1	-8	24	- 24		7	4	-4	18	- 18
6	0	-8	123	118		6	2	0	14	13		7	1	-7	17	16		7	4	-3	8	- 8
6	0	-6	148	139		6	2	1	17	14		7	1	-6	27	28		7	4	-2	21	- 22
6	0	-4	29	- 30		6	2	2	27	- 29		7	1	-4	23	25		8	0	-8	9	- 10
6	0	-2	40	- 42		6	3	-10	4	2		7	1	-3	44	- 43		8	0	-6	25	- 26
6	0	0	98	- 90		6	3	-9	12	- 12		7	1	-2	46	43		8	0	-4	15	15
6	0	2	21	- 23		6	3	-8	10	9		7	1	-1	11	- 11		8	0	-2	13	13
6	1	-12	12	- 11		6	3	-7	12	9		7	1	0	5	- 5		8	1	-10	13	- 14
6	1	-11	5	8		6	3	-6	8	6		7	2	-11	18	- 20		8	1	-9	5	- 5
6	1	-10	33	- 32		6	3	-5	31	- 30		7	2	-10	18	18		8	1	-8	5	6
6	1	-9	38	39		6	3	-3	11	11		7	2	-8	20	- 20		8	1	-6	18	- 19
6	1	-8	40	- 42		6	3	-2	12	9		7	2	-7	6	8		8	1	-5	17	- 17
6	1	-7	37	37		6	3	-1	18	18		7	2	-6	31	- 32		8	1	-4	14	- 13
6	1	-5	92	95		6	3	0	38	34		7	2	-5	45	48		8	1	-3	6	- 5
6	1	-5	63	62		6	3	1	21	20		7	2	-4	37	- 37		8	1	-2	6	- 6
6	1	-4	91	93		6	4	-8	7	- 6		7	2	-3	14	14		8	2	-10	9	- 11
6	1	-2	43	46		6	4	-4	17	17		7	2	-2	15	- 12		8	2	-9	13	- 15
6	1	-1	44	- 46		6	4	-3	21	- 17		7	2	-1	12	13		8	2	-8	16	- 15
6	1	1	23	- 22		6	4	-2	19	15		7	2	0	6	- 6		8	2	-7	3	1
6	1	2	27	- 29		6	4	-1	18	20		7	3	-10	4	4		8	2	-6	10	- 11
6	2	-11	19	- 19		7	0	-12	1	- 4		7	3	-9	17	- 17		8	2	-5	15	- 15
6	2	-10	20	13		7	0	-10	6	7		7	3	-8	17	18		8	2	-4	15	- 15
6	2	-9	6	- 5		7	0	-8	76	73		7	3	-7	29	- 28		8	2	-3	19	- 22
6	2	-8	19	- 17		7	0	-6	32	34		7	3	-6	15	17		8	3	-8	4	- 3
6	2	-7	6	6		7	0	-4	10	10		7	3	-5	32	- 27		8	3	-7	40	- 43
6	2	-6	24	- 27		7	0	-2	28	- 29		7	3	-3	9	10		8	3	-6	6	- 6
6	2	-5	19	22		7	0	0	35	- 36		7	3	-1	31	- 30		8	3	-5	7	- 7
6	2	-4	27	27		7	1	-11	17	21		7	4	-8	15	- 18		8	3	-4	4	- 5
6	2	-3	91	91		7	1	-10	36	- 36		7	4	-6	8	- 9						

Table 4. The principal axes of the thermal vibration ellipsoids given by the components of a unit vector in fractional coordinates e_x, e_y, e_z; the corresponding r.m.s. amplitudes, and the B-values.

Atom	e_x	e_y	e_z	$(\overline{u^2})^{\frac{1}{2}}$ (Å)	B (Å^2)
O	.050	.120	.084	.306	7.41
	.096	.064	−.037	.265	5.56
	.133	−.091	.085	.195	3.01
N	.027	.137	.065	.242	4.60
	.003	.087	−.087	.224	3.97
	.169	−.023	.062	.196	3.02
C_1	.057	.135	−.024	.240	4.53
	.021	.073	.101	.227	4.07
	.160	−.058	.070	.192	2.91
C_2	.037	.136	.068	.249	4.93
	.017	.083	−.082	.235	4.35
	.166	−.039	.065	.186	2.74
C_3	.047	.096	.098	.290	6.64
	.132	−.100	.073	.255	5.12
	.099	.088	−.024	.213	3.58

at for 516 observed reflections was 6.6 %. The corresponding phases were used in the calculation of a final difference Fourier map which showed no larger fluctuations than ± 0.2 e·Å^{-3}.

The fractional atomic coordinates and the thermal vibration parameters are given in Tables 1 and 2; the expression for the anisotropic vibrations being

$$\exp\{-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl)\}.$$

A comparison between calculated and observed structure factors is presented in Table 3.

Table 5. Principal moments of inertia of the molecule (a.m.u. $Å^2$), unit vectors along the principal axes, L, M, N, defining the molecular coordinate system, and the rigid-body tensors referred to this coordinate system.

Axis	Moment	e_x	e_y	e_z
L	124.7	$-.020$	$-.131$	.053
M	254.3	$-.163$	.043	$-.049$
N	367.6	.049	.089	.102

$$\mathbf{T} = \begin{pmatrix} 578 & 66 & 72 \\ & 481 & 22 \\ & & 562 \end{pmatrix} \times 10^{-4} \ Å^2$$

$$\mathbf{L} = \begin{pmatrix} 117 & 3 & -7 \\ & 63 & 9 \\ & & 49 \end{pmatrix} \times 10^{-4} \ rad^2$$

	r.m.s. amplitudes	L	M	N
			Direction cosines	
$\mathbf{T}$	.258 $Å$	.7371	.4434	.5101
	.226 »	.3368	.4133	$-.8460$
	.211 »	.5859	$-.7954$	$-.1553$
$\mathbf{L}$	6.21°	$-.9945$	$-.0150$	$-.1032$
	4.68 »	$-.0306$	$-.9039$	.4267
	3.79 »	.0997	$-.4275$	$-.8985$

$(\overline{\varDelta U_{ij}{}^2})^{\frac{1}{2}} = 0.0018 \ Å^2$

The principal axes of the thermal vibration ellipsoids for oxygen, nitrogen, and carbon atoms were calculated from the temperature parameters of Table 1. Root mean square amplitudes and the corresponding B-values for the atomic anisotropic thermal vibrations along the principal axes together with the components of these axes along the crystal axes are given in Table 4.
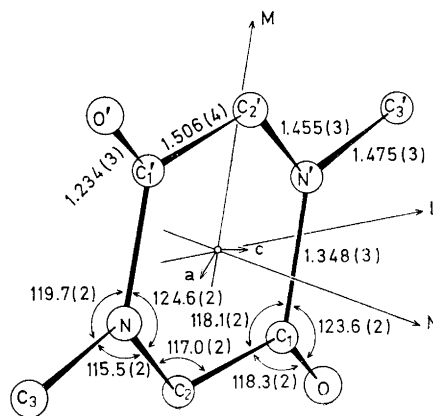
Fig. 1. Schematical drawing of the molecule viewed along [010].

The results of a rigid-body analysis of translational and librational motion of the molecule about the centre of symmetry are given in Table 5. The **T** and **L** tensors are calculated in an orthogonal coordinate system, L, M, N, defined by the principal inertial axes of the molecule. The orientation of this system with respect to crystal axes is shown in Fig. 1, where the molecule is viewed along [010]. The direction of the N-axis, corresponding to the largest moment of inertia, is approximately normal to the plane of the molecule. The largest r.m.s. amplitude of angular oscillation, 6.21°, is about a direction close to that of the L-axis, corresponding to the smallest moment of inertia. The r.m.s. discrepancy between atomic vibration tensor components, U_{ij}, calculated from the thermal parameters of Table 1, and those calculated with the rigid-body parameters, serves as a measure of the applicability of the analysis and thus of the rigidity of the molecule. The value of Table 5, 0.0018 $Å^2$, supports the assumption of regarding the molecule as an oscillating rigid body, and the fractional coordinates were accordingly corrected for librational effects.[5] Table 6 shows that some of the corrections are considerably larger than three times the corresponding standard deviation.

Table 6. Libration corrections in fractional atomic coordinates compared with estimated standard deviations in coordinates (σ's and Δ's are multiplied by 10^5).

Atom	Δx	$\sigma(x)$	Δy	$\sigma(y)$	Δz	$\sigma(z)$
O	210	32	200	39	149	25
N	75	29	79	38	−20	24
C_1	109	40	−111	49	78	29
C_2	192	38	−35	49	53	30
C_3	163	50	152	54	−41	40

Interatomic distances and bond angles (corrected for libration) with estimated standard deviations (not including cell dimension e.s.d.'s) may be found in Fig. 1. As to be expected, the largest correction in bond distance is for the $N-C_1'$ bond, which is roughly normal to the axis of maximum libration. The uncorrected value is 1.337 Å and the difference 3.7 times e.s.d.

Table 7. Comparison of bond distances and angles with those of diketopiperazine.

	diketopiperazine	present compound
C_1-C_2	1.499 Å	1.506 Å
C_1-N'	1.325 »	1.348 »
C_1-O	1.239 »	1.234 »
C_2-N	1.449 »	1.455 »
C_2-C_1-O	118.5°	118.3°
$N'-C_1-O$	122.6	123.6
C_2-C_1-N'	118.9	118.1
$C_1'-N-C_2$	126.0	124.6
$N-C_2-C_1$	115.1	117.0

Corresponding factors for the other distances range from 2.5 to 3.0. All corrections in bond angles are smaller than the corresponding standard deviations.

In Table 7 is presented a comparison of distances and angles with those of diketopiperazine.[2] The relatively large difference in the C_1—N bond lengths may be explained by the fact that no librational corrections were applied for diketopiperazine.

C—H bond lengths range from 1.03 Å to 1.05 Å. *Inter*molecular contacts correspond to van der Waals distances.

The least squares plane through the molecule, centered at (0,0,0), gives the following fit:

Atom (Fig. 1)	Distance from plane (Å)
O	0.024
N	0.031
C_1	−0.007
C_2	−0.051
C_3	0.008

This deviation from planarity is significant.

The least squares plane defined by the atoms in one half of the molecule gives a much better fit:

Atom (Fig. 1)	Distance from plane (Å)
O	−0.001
N'	0.008
C_1	−0.005
C_2	0.002
C_3'	−0.004

The distance between this plane and the (parallel) plane through O', N, C_1', C_2', C_3 is about 0.12 Å. These findings resemble what has been observed for diketopiperazine [2] although the deviation from planarity here is smaller. The authors characterize the deviation as a slight "twist" of the two (essentially planar)

$$
\begin{array}{c}
\text{N} \\
\diagdown \\
\text{C}_1\text{--O \quad groups} \\
\diagup \\
\text{C}_2
\end{array}
$$
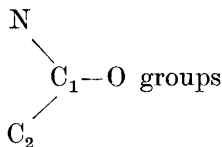
with respect to each other. However, since these groups are related by a centre of inversion, the planes are parallel, and the molecules may rather be described in terms of an extremely flattened chair form.

The dihedral angle C_2—C_1—N'—C_2' is 7.1°.

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