Table 8.3.2.1 (*cont.*)

Met M			
Cβ	0.02044	−0.96506	1.17716
Cγ	−1.00916	−2.05384	1.00286
Sδ	−0.77961	−3.24454	2.37236
Cε	−2.08622	−4.42220	1.97795
Phe F			
Cβ	0.00662	−1.03603	1.11081
Cγ	0.03254	−0.49711	2.50951
Cδ1	−1.15813	−0.12084	3.13467
Cε1	−1.15720	0.38038	4.42732
Cζ	0.05385	0.51332	5.11032
Cε2	1.26137	0.11613	4.50975
Cδ2	1.23668	−0.38351	3.20288
Pro P			
Cβ	0.12372	−0.78264	1.31393
Cγ	0.89489	0.13845	2.22063
Cδ	1.87411	0.86170	1.30572
Ser S			
Cβ	−0.00255	−0.96014	1.17670
Oγ	−0.19791	−0.28358	2.40542
Thr T			
Cβ	−0.00660	−0.98712	1.23470
Oγ1	0.04119	−0.14519	2.43011
Cγ2	1.12889	−2.01366	1.21493
Trp W			
Cβ	0.02501	−0.98461	1.16268
Cγ	0.03297	−0.36560	2.51660
Cδ1	−1.03107	0.15011	3.20411
Nε1	−0.62445	0.62417	4.42903
Cε2	0.72100	0.41985	4.55667
Cζ2	1.57452	0.72329	5.60758
Cη2	2.91029	0.38415	5.45120
Cη3	3.37037	−0.23008	4.28944
Cε3	2.51952	−0.53303	3.24549
Cδ2	1.17472	−0.20516	3.37412
Tyr Y			
Cβ	0.00470	−0.95328	1.20778
Cγ	−0.18427	−0.27254	2.54372
Cδ1	0.89731	0.26132	3.25049
Cε1	0.72371	0.85064	4.50059
Cζ	−0.54776	0.88971	5.06861
Cε2	−1.63905	0.38287	4.37622
Cδ2	−1.44975	−0.19374	3.12415
Oη	−0.76405	1.40409	6.31652
Val V			
Cβ	0.05260	−0.99339	1.17429
Cγ1	−0.13288	−0.31545	2.52668
Cγ2	−0.94265	−2.12930	0.99811

$$\Delta_n = (d_{\min} - d_{\text{model}})^4/\sigma_n^4, \tag{8.3.2.6}$$

which are included only when $d_{\text{model}} < d_{\min}$. Macromolecules usually gain flexibility by relatively unrestricted rotation about single bonds. There are, nevertheless, significant restrictions on these torsion angles, which may, therefore, be restrained by terms of the form

$$\Delta_t = (\chi_{\text{ideal}} - \chi_{\text{model}})^2/\sigma_t^2, \tag{8.3.2.7}$$

Table 8.3.2.2. *Ideal values for distances (Å), torsion angles (°), etc. for a glycine–alanine dipeptide with a trans peptide bond; distance type 1 is a bond, type 2 a next-nearest-neighbour distance involving a bond angle*

Interatomic distances

Number				Distance	Type
1	N(1)	to	C(1)α	1.470	1
2	Cα(1)	to	C(1)	1.530	1
3	C(1)	to	O(1)	1.240	1
4	N(1)	to	C(1)	2.452	2
5	C(1)α	to	O(1)	2.414	2
6	N(2)	to	C(2)α	1.469	1
7	C(2)α	to	C(2)	1.530	1
8	C(2)	to	O(2)	1.252	1
9	N(2)	to	C(2)	2.461	2
10	C(2)α	to	O(2)	2.358	2
11	C(2)β	to	C(2)α	1.524	1
12	C(2)β	to	C(2)	2.515	2
13	C(2)β	to	N(2)	2.450	2
14	C(2)	to	$O(2)_t$	1.240	1
15	O(2)	to	$O(2)_t$	2.225	2
16	C(2)α	to	$O(2)_t$	2.377	2
17	N(2)	to	C(1)	1.320	1
18	N(2)	to	O(1)	2.271	2
19	N(2)	to	C(1)α	2.394	2
20	C(2)α	to	C(1)	2.453	2

Planar groups

1	CTRM	C(2)α	C(2)	O(2)	O(2)	
2	LINK	C(1)α	C(1)	O(1)	N(2)	C(2)α

Chiral centres

		Central atom				Chiral volume (Å^3)
1	Ala	C(2)α	N(2)	C(2)	C(2)β	2.492

Possible nonbonded contacts

Number				Distance
1	N(1)	to	O(1)	3.050
2	N(2)	to	O(2)	3.050
3	O(2)	to	C(2)β	3.350
4	N(2)	to	$O(2)_t$	3.050
5	$O(2)_t$	to	C(2)β	3.350

Torsion angles

N(1)	C(1)α	C(1)	N(2)	0.0
C(1)α	C(1)	N(2)	C(2)α	180.0
C(1)	N(2)	C(2)α	C(2)	0.0
N(2)	C(2)α	C(2)	$O(2)_t$	0.0

where χ_{ideal} and χ_{model} are dihedral angles between planar groups at opposite ends of the bond.

Interatomic distances are independent of the handedness of an enantiomorphous group. If $\mathbf{r}_c$ is the position vector of a central atom and $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are the positions of three atoms bonded to it, such that the four atoms are not coplanar, the *chiral volume* is defined by

$$V_c = (\mathbf{r}_1 - \mathbf{r}_c) \cdot [(\mathbf{r}_2 - \mathbf{r}_c) \times (\mathbf{r}_3 - \mathbf{r}_c)], \tag{8.3.2.8}$$

where × indicates the vector product. The chiral volume may be either positive or negative, depending on the handedness of the group. It may be restrained by including terms of the form

$$\Delta_c = (V_{\text{ideal}} - V_{\text{model}})^2/\sigma_c^2. \tag{8.3.2.9}$$

Table 8.3.2.1 gives ideal coordinates, in an orthonormal coordinate system measured in Å, of various groups that are

references