Table 8.3.2.1. *Coordinates of atoms (in Å) in standard groups appearing in polypeptides and proteins; restraint relations may be determined from these coordinates using methods described by Hendrickson (1985)*

Main chain, links and terminal groups			
Main			
N	1.20134	0.84658	0.00000
Cα	0.00000	0.00000	0.00000
C	−1.25029	0.88107	0.00000
O	−2.18525	0.66029	−0.78409
C terminal			
N	1.20006	0.84799	0.00000
Cα	0.00000	0.00000	0.00000
C	−1.26095	0.86727	0.00000
O	−2.32397	0.27288	−0.29188
O_t	−1.15186	2.04837	0.35987
N amino terminal			
N	1.20134	0.84658	0.00000
Cα	0.00000	0.00000	0.00000
C	−1.25029	0.88107	0.00000
O	−2.18525	0.66029	−0.78409
N formyl terminal			
N	1.19423	0.82137	0.00000
Cα	0.00000	0.00000	0.00000
C	−1.24896	0.88255	0.00000
O	−2.10649	0.78632	−0.90439
O_t	2.46193	−0.77877	−0.93569
C_t	2.33913	0.39064	−0.53355
N acetyl terminal			
N	1.19423	0.82137	0.00000
Cα	0.00000	0.00000	0.00000
C	−1.24896	0.88255	0.00000
O	−2.10649	0.78632	−0.90439
O_t	2.46193	−0.77877	−0.93569
C_t1	2.33913	0.39064	−0.53355
C_t2	3.44659	1.39160	−0.63532
trans peptide link			
Cα	0.00000	0.00000	0.00000
C	0.57800	1.41700	0.00000
O	1.80400	1.60700	0.00001
N	−0.33500	2.37000	0.00000
Cα	0.00000	3.80100	0.00000
cis peptide link			
Cα	0.00000	0.00000	0.00000
C	1.30900	0.79200	0.00000
O	2.38500	0.17600	0.00000
N	1.23500	2.11000	0.00000
Cα	0.00000	2.90700	0.00000
trans proline link			
Cα	0.00000	0.00000	0.00000
C	0.57800	1.41700	0.00000
O	1.80400	1.60700	0.00001
N	−0.33500	2.37000	0.00000
Cα	0.00000	3.80100	0.00000
Cδ	−1.80000	2.19600	0.00000
cis proline link			
Cα	0.00000	0.00000	0.00000
C	1.30900	0.79200	0.00000
O	2.38500	0.17600	0.00000
N	1.23500	2.11000	0.00000
Cα	0.00000	2.90700	0.00000
Cδ	2.45500	2.93900	0.00000

Table 8.3.2.1 *(cont.)*

Side chains for amino acids			
Ala A			
Cβ	0.02022	−0.92681	1.20938
Arg R			
Cβ	−0.02207	−0.93780	1.20831
Cγ	−0.09067	−0.23808	2.55932
Cδ	−0.79074	−1.07410	3.57563
Nε	−0.76228	−0.46664	4.89930
Cζ	−1.57539	−0.83569	5.89157
Nη1	−2.60422	−1.65104	5.68019
Nη2	−1.38328	−0.33329	7.11065
Asn N			
Cβ	0.04600	−1.02794	1.12104
Cγ	−0.15292	−0.42844	2.50080
Oδ1	−0.39364	0.78048	2.63809
Nδ2	−0.06382	−1.27086	3.52863
Asp D			
Cβ	0.04600	−1.02794	1.12104
Cγ	−0.15292	−0.42844	2.50080
Oδ1	−0.39364	0.78048	2.63809
Oδ2	−0.06930	−1.21904	3.46540
Cys C			
Cβ	0.01317	−0.95892	1.18266
Sγ	−0.07941	−0.15367	2.80168
Gln Q			
Cβ	−0.01691	−0.98634	1.16423
Cγ	−0.08291	−0.32584	2.52866
Cδ	−0.20841	−1.31760	3.65937
Oε1	−0.48899	−2.49684	3.46331
Nε2	−0.00450	−0.81846	4.87646
Glu E			
Cβ	−0.06551	−0.87677	1.25157
Cγ	1.15947	−1.71468	1.59818
Cδ	1.40807	−2.90920	0.72611
Oε1	0.92644	−3.06007	−0.38343
Oε2	2.16269	−3.74330	1.27140
Gly G (no nonhydrogen atoms)			
His H			
Cβ	−0.06434	−0.96857	1.20324
Cγ	−0.52019	−0.29684	2.46369
Nδ1	0.26457	0.53405	3.22184
Cε1	−0.46699	1.05500	4.19371
Nε2	−1.69370	0.59727	4.09040
Cδ2	−1.75570	−0.25685	3.02097
Ile I			
Cβ	0.03196	−0.97649	1.23019
Cγ1	−0.83268	−2.22363	0.92046
Cγ2	−0.39832	−0.28853	2.54980
Cδ1	−0.77555	−3.32741	2.01167
Leu L			
Cβ	0.09835	−0.94411	1.20341
Cγ	−0.96072	−2.02814	1.32143
Cδ1	−0.89548	−2.98661	0.13861
Cδ2	−0.73340	−2.79002	2.62540
Lys K			
Cβ	−0.03606	−0.92129	1.21541
Cγ	1.19773	−1.81387	1.35938
Cδ	1.05466	−2.77178	2.53242
Cε	2.34215	−3.51295	2.82637
Nζ	2.16781	−4.42240	3.98733

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