

Table S1. Anchor atoms for reconstructing local reference frames of heavy atoms from 20 standard residue types

Residue type	Atom type	Anchor atoms		
		A	B	C
ALA	CB	CA	N	CB
ARG	CB	CA	CB	CG
	CG	CB	CG	CD
	CD	CG	CD	NE
	NE	CD	NE	CZ
	CZ	NH1	CZ	NH2
	NH1	NE	CZ	NH1
	NH2	NE	CZ	NH2
ASN	CB	CA	CB	CG
	CG	OD1	CG	ND2
	ND2	CG	CB	ND2
	OD1	CG	CB	OD1
ASP	CB	CA	CB	CG
	CG	OD1	CG	OD2
	OD2	CG	CB	OD2
	OD1	CG	CB	OD1
CYS	CB	CA	CB	SG
	SG	CB	CA	SG
GLN	CB	CA	CB	CG
	CG	CB	CG	CD
	CD	OE1	CD	NE2
	OE1	CD	CG	OE1
	NE2	CD	CG	NE2
GLU	CB	CA	CB	CG
	CG	CB	CG	CD
	CD	OE1	CD	OE2
	OE1	CD	CG	OE1
	OE2	CD	CG	OE2
HIS	CB	CA	CB	CG
	CG	ND1	CG	CD2
	ND1	CG	ND1	CE1
	CD2	CG	CD2	NE2
	CE1	ND1	CE1	NE2
	NE2	CD2	NE2	CE1

Residue type	Atom type	Anchor atoms		
		A	B	C
ILE	CB	CA	CB	CG1
	CG1	CB	CG1	CD1
	CG2	CB	CA	CG2
	CD1	CG1	CB	CD1
LEU	CB	CA	CB	CG
	CG	CD1	CG	CD2
	CD1	CG	CB	CD1
	CD2	CG	CB	CD2
LYS	CB	CA	CB	CG
	CG	CB	CG	CD
	CD	CG	CD	CE
	CE	CD	CE	NZ
	NZ	CE	CD	NZ
MET	CB	CA	CB	CG
	CG	CB	CG	SD
	SD	CG	SD	CE
	CE	SD	CG	CE
PHE	CB	CA	CB	CG
	CG	CD1	CG	CD2
	CD1	CG	CD1	CE1
	CE1	CD1	CE1	CZ
	CD2	CG	CD2	CE2
	CE2	CD1	CE2	CZ
	CZ	CE1	CZ	CE2
PRO	CB	CA	CB	CG
	CG	CB	CG	CD
	CD	CG	CD	N
SER	CB	CA	CB	OG
	OG	CB	CA	OG
THR	CB	CA	CB	OG1
	OG1	CB	CA	OG1
	CG2	CB	CA	CG2

Residue type	Atom type	Anchor atoms		
		A	B	C
TRP	CB	CA	CB	CG
	CG	CD1	CG	CD2
	CD1	CG	CD1	NE1
	CD2	CE2	CD2	CE3
	NE1	CD1	NE1	CE2
	CE2	CD2	CE2	CZ2
	CE3	CD2	CE3	CZ3
	CZ2	CE2	CZ2	CH2
	CZ3	CE3	CZ3	CH2
CH2	CZ2	CH2	CZ3	
TYR	CB	CA	CB	CG
	CG	CD1	CG	CD2
	CD1	CG	CD1	CE1
	CE1	CD1	CE1	CZ
	CD2	CG	CD2	CE2
	CE2	CD1	CE2	CZ
	CZ	CE1	CZ	CE2
OH	CE2	CZ	CE1	
VAL	CB	CA	CB	CG1
	CG1	CB	CA	CG1
	CG2	CB	CA	CG2
all residues	N	Cprev ¹	N	CA
	CA	N	CA	C
	C	CA	C	Nnext ²
	O	CA	O	Nnext

¹ Backbone carbon of the preceding residue in the protein chain

² Backbone nitrogen of the next residue in the protein chain