========== From crysol.txt (CRYSOL ver. 2.7)

Table 1. Possible values for IATYPE

	C	CH	CH2	CH3	N	NH	NH2	NH3	O	OH	S	SH	P	FE	CU	CA	MG	MN	ZN
IATYPE	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19

Table 2. Protein atoms

	N	CA	C	CB	CG	CD	CE	CZ	CH	N	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX	
									O													
ALA	6,	2,	1,	9,	4,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	ALA
ARG	6,	2,	1,	9,	3,	3,	3,	0,	1,	0,	0,	6,	0,	7,	0,	0,	0,	0,	0,	0,	9,	ARG
ASN	6,	2,	1,	9,	3,	1,	0,	0,	0,	0,	7,	0,	0,	0,	0,	9,	0,	0,	0,	0,	9,	ASN
ASP	6,	2,	1,	9,	3,	1,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	0,	0,	0,	0,	9,	ASP
CYS	6,	2,	1,	9,	3,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,11,	0,	9,	CYS
GLN	6,	2,	1,	9,	3,	3,	1,	0,	0,	0,	0,	7,	0,	0,	0,	0,	9,	0,	0,	0,	9,	GLN
GLU	6,	2,	1,	9,	3,	3,	1,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	0,	0,	0,	9,	GLU
GLY	6,	3,	1,	9,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	GLY
HIS	6,	2,	1,	9,	3,	1,	2,	2,	0,	0,	5,	6,	0,	0,	0,	0,	0,	0,	0,	0,	9,	HIS
ILE	6,	2,	1,	9,	2,−1,	4,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	ILE
LEU	6,	2,	1,	9,	3,	2,	4,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	LEU
LYS	6,	2,	1,	9,	3,	3,	3,	3,	0,	0,	0,	0,	8,	0,	0,	0,	0,	0,	0,	0,	9,	LYS
MET	6,	2,	1,	9,	3,	3,	0,	4,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,12,	9,	MET
PHE	6,	2,	1,	9,	3,	1,	2,	2,	2,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	PHE
PRO	5,	2,	1,	9,	3,	3,	3,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9,	PRO
SER	6,	2,	1,	9,	3,	0,	0,	0,	0,	0,	0,	0,	0,	0,10,	0,	0,	0,	0,	0,	0,	9,	SER
THR	6,	2,	1,	9,	2,	4,	0,	0,	0,	0,	0,	0,	0,	0,10,	0,	0,	0,	0,	0,	0,	9,	THR
TRP	6,	2,	1,	9,	3,	1,	1,	2,	2,	2,	0,	6,	0,	0,	0,	0,	0,	0,	0,	0,	9,	TRP
TYR	6,	2,	1,	9,	3,	1,	2,	2,	1,	0,	0,	0,	0,	0,	0,	0,	0,10,	0,	0,	0,	9,	TYR
VAL	6,	2,	1,	9,	2,	4,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	0,	9	VAL
	N	CA	C	CB	CG	CD	CE	CZ	CH	N	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX	
									O													

========== myTest with two-atom models (9-10Dec2013)

f_invacuo(q=0) = sqrt(I_invacuo(q=0)/4)

I_invacuo: 3rd column in the crysol *.int file

pdb file: contains two atoms (having same ATYPE/RTYPE, but different coordinates: 0,0,0 and 50,0,0)

Values below: f_invacuo(q=0) ~ total valence electrons within an atomic group

(actual Atomic Group, actual IATYPE)

ALA	N	CA*	C	CB*	O	CG*	CD	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	8.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH3,4)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
ARG	N	CA*	C	CB*	O	CG	CD	CE*	CZ	CH	ND	NE	NZ	NH*	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	7.9991	7.9991	5.9992	5.9992	5.9992	6.9946	7.9945	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH2,3)	(CH2,3)	(C,1)	(C,1)	(C,1)	(N,5)	(NH,6)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
ASN	N	CA*	C	CB*	O	CG*	CD	CE	CZ	CH	ND*	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)

ASP	N	CA*	C	CB*	O	CG*	CD	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
CYS	N	CA*	C	CB*	O	CG*	CD	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG*	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	16.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(SH,12)	(S,11)	(O,9)
GLN	N	CA*	C	CB*	O	CG	CD*	CE	CZ	CH	ND	NE*	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	7.9991	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH2,3)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
GLU	N	CA*	C	CB*	O	CG	CD*	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	7.9991	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH2,3)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
GLY	N	CA*	C	CB*	O	CG	CD	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	5.9992	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(C,1)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
HIS	N	CA*	C	CB*	O	CG*	CD	CE*	CZ*	CH	ND	NE*	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
ILE	N	CA*	C	CB*	O	CG*	CD	CE*	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	6.9992	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH,2)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
LEU	N	CA*	C	CB*	O	CG*	CD*	CE*	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	6.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH,2)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
LYS	N	CA*	C	CB*	O	CG	CD	CE	CZ*	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	7.9991	7.9991	7.9991	5.9992	5.9992	6.9946	6.9946	9.9945	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH2,3)	(CH2,3)	(CH2,3)	(C,1)	(C,1)	(N,5)	(N,5)	(NH3,8)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
MET	N	CA*	C	CB*	O	CG	CD*	CE*	CZ*	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD*	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	7.9991	5.9992	8.9991	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH2,3)	(C,1)	(CH3,4)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
PHE	N	CA*	C	CB*	O	CG*	CD	CE*	CZ	CH*	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	6.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(CH,2)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
PRO	N	CA*	C	CB*	O	CG	CD	CE*	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	6.9946	12.7783	5.9992	7.9991	7.9994	7.9991	7.9991	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(N,5)	(?,?)	(C,1)	(CH2,3)	(O,9)	(CH2,3)	(CH2,3)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
SER	N	CA*	C	CB*	O	CG*	CD	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	8.9993	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(OH,10)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)

THR	N	CA*	C	CB*	O	CG*	CD*	CE	CZ	CH	ND	NE	NZ	NH	OG*	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	6.9992	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH,2)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
TRP	N	CA*	C	CB*	O	CG*	CD	CE	CZ*	CH*	ND	NE*	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
TYR	N	CA*	C	CB*	O	CG*	CD	CE*	CZ*	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	8.9993	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)
VAL	N	CA*	C	CB*	O	CG*	CD*	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	6.9992	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH,2)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)

*IATYPE different from Table 2
 According to crysol.txt, if IATYPE = 0, actual IATYPE is assigned from the columns 13-14.

========== myTest with two-atom models: RTYPE - DAM (10Dec2013)

DAM	N	CA	C	CB	O	CG	CD	CE	CZ	CH	ND	NE	NZ	NH	OG	OD	OE	OH	SG	SD	OX
	7.9945	12.7783	5.9992	7.9991	7.9994	5.9992	5.9992	5.9992	5.9992	5.9992	6.9946	6.9946	6.9946	6.9946	7.9994	7.9994	7.9994	7.9994	15.9998	15.9998	7.9994
	(NH,6)	(?,?)	(C,1)	(CH2,3)	(O,9)	(C,1)	(C,1)	(C,1)	(C,1)	(C,1)	(N,5)	(N,5)	(N,5)	(N,5)	(O,9)	(O,9)	(O,9)	(O,9)	(S,11)	(S,11)	(O,9)