

54A7

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Changes with respect to 53A6 in bold

- Torsional angle energy terms for the polypeptide ϕ and ψ dihedral angles are changed
- The choice of the C12 parameter for the interaction between O(IAC=1) and N(IAC=6)
- A new van der Waals nonbonded atom type for a charged CH3 group is added (IAC=54)
- The van der Waals parameters for the Na+(IAC=37) and CL-(IAC=38) are modified [A578]
- Two extra improper dihedral angle terms have been added to facilitate free energy calculations

Table 2.4.1

GROMOS mass atom type codes, masses and names

mass atom type code	mass in a.m.u.	mass atom name
N	ATMAS[N]	ATMASN[N]
1	1.008	H
3	13.019	CH1
4	14.027	CH2
5	15.035	CH3
6	16.043	CH4
12	12.011	C
14	14.0067	N
16	15.9994	O
19	18.9984	F
23	22.9898	NA
24	24.305	MG
28	28.08	SI
31	30.9738	P
32	32.06	S
35	35.453	CL
39	39.948	AR
40	40.08	CA
56	55.847	FE
63	63.546	CU
65	65.37	ZN
80	79.904	BR

Table 2.5.2.1

GROMOS bond-stretching parameters

Bond-type code	Force constant	Ideal bond length	Examples of usage in terms of nonbonded atom types	
	K_{b_n} $= K_{b_n}^{harm} / 2b_{0_n}^2$	b_{0_n}		$K_{b_n}^{harm}$
	10%kJmol ⁻¹ nm ⁻⁴	nm		kcalmol ⁻¹ Å ⁻²
ICBH[N] ICB[N]	CB[N]	BO[N]		
1	15.7	0.100	H - OA	750
2	18.7	0.100	H - N (all)	895
3	12.3	0.109	HC - C	700
4	37.0	0.112	C - O (CO bound to heme)	2220
5	16.6	0.123	C - O	1200
6	13.4	0.125	C - OM	1000
7	12.0	0.132	CR1 - NR (6-ring)	1000
8	8.87	0.133	H - S	750
9	10.6	0.133	C - NT, NL	900
10	11.8	0.133	C, CR1 - N, NR, CR1, C (peptide, 5-ring)	1000
11	10.5	0.134	C - N, NZ, NE	900
12	11.7	0.134	C - NR (no H) (6-ring)	1000
13	10.2	0.136	C - OA, FTfe - CTfe	900
14	11.0	0.138	C - NR (heme)	1000
15	8.66	0.139	CH2 - C, CR1 (6-ring)	800
16	10.8	0.139	C, CR1 - CH2, C, CR1 (6-ring)	1000
17	8.54	0.140	C, CR1, CH2 - NR (6-ring)	800
18	8.18	0.143	CHn - OA	800
19	9.21	0.143	CHn - OM	900
20	6.10	0.1435	CHn - OA (sugar)	600
21	8.71	0.147	CHn - N, NT, NL, NZ, NE	900
22	5.73	0.148	CHn - NR (5-ring)	600
23	7.64	0.148	CHn - NR (6-ring)	800
24	8.60	0.148	O, OM - P	900
25	8.37	0.150	O - S	900
26	5.43	0.152	CHn - CHn (sugar)	600
27	7.15	0.153	C, CHn - C, CHn	800
28	4.84	0.161	OA - P	600
29	4.72	0.163	OA - SI	600
30	2.72	0.178	FE - C (CO bound to heme)	412
31	5.94	0.178	CH3 - S	900
32	5.62	0.183	CH2 - S	900
33	3.59	0.187	CH1 - SI	600

34	0.640	0.198	NR (His) - FE (43A1)	120
35	0.628	0.200	NR (heme) - FE	120
36	5.03	0.204	S - S	1000
37	0.540	0.221	NR (His) - FE	126
38	23.2	0.100	HWat - OWat	1110
39	12.1	0.110	HChl - CChl	700
40	8.12	0.1758	CChl - CLChl	1200
41	8.04	0.153	ODmso - SDmso	900
42	4.95	0.193799	SDmso - CDmso	890
43	8.10	0.176	CCl4 - CLCl4	1200
44	13.1	0.1265	CUrea - OUrea	1000
45	10.3	0.135	CUrea - NUrea	900
46	8.71	0.163299	HWat - HWat	1110
47	2.68	0.233839	HChl - CLChl	700
48	2.98	0.290283	CLChl - CLChl	1200
49	2.39	0.279388	ODmso - CDmso	890
50	2.19	0.291189	CDmso - CDmso	890
51	3.97	0.2077	HMet - CMet	820
52	3.04	0.287407	CLCl4 - CLCl4	1200

Table 2.5.3.1

GROMOS bond-angle bending parameters

Bond-angle type code	Force constant	Ideal bond angle	Example of usage in terms of nonbonded atom types	
	K_{θ_n} $= g(K_{\theta_n}^{harm}, \theta_{n_0}, E_{k_n T})$	θ_{0_n}		$K_{\theta_n}^{harm}$
	kJmol ⁻¹	degree		kcalmol ⁻¹ rad ⁻²
ICTH[N] ICT[N]	CT[N]	(T0[N])		
1	380	90.0	NR (heme) - FE - C (CO bound to heme)	90
2	420	90.0	NR(heme) - FE - NR(heme), NR (His)	100
3	405	96.0	H - S - CH2	95
4	475	100.0	CH2 - S - CH3	110
5	420	103.0	OA - P - OA	95
6	490	104.0	CH2 - S - S	110
7	465	108.0	NR, C, CR1(5-ring)	100
8	285	109.5	CHn - CHn - CHn, NR(6-ring) (sugar)	60
9	320	109.5	CHn, OA - CHn - OA, NR(ring) (sugar)	68
10	380	109.5	H - NL, NT - H, CHn - OA - CHn(sugar)	80
11	425	109.5	H - NL - C, CHn H - NT - CHn	90
12	450	109.5	X - OA, SI - X	95
13	520	109.5	CH, C - CHn - C, CHn, OA, OM, N, NE	110
14	450	109.6	OM - P - OA	95
15	530	111.0	CHn - CHn - C, CHn, OA, NR, NT, NL	110
16	545	113.0	CHn - CH2 - S	110
17	50.0	115.0	NR(heme) - FE - NR (His) (43A1)	10
18	460	115.0	H - N - CHn	90
19	610	115.0	CHn, C - C - OA, N, NT, NL	120
20	465	116.0	H - NE - CH2	90
21	620	116.0	CH2 - N - CH1	120
22	635	117.0	CH3 - N - C, CHn - C - OM	120
23	390	120.0	H - NT, NZ, NE - C	70
24	445	120.0	H - NT, NZ - H	80
25	505	120.0	H - N - CH3, H, HC - 6-ring, H - NT - CHn	90
26	530	120.0	P, SI - OA - CHn, P	95
27	560	120.0	N, C, CR1 (6-ring, no H)	100
28	670	120.0	NZ - C - NZ, NE	120

29	780	120.0	OM - P - OM	140
30	685	121.0	O - C - CH _n , C - CH ₃ - N - CH _n	120
31	700	122.0	CH ₁ , CH ₂ - N - C	120
32	415	123.0	H - N - C	70
33	730	124.0	O - C - OA, N, NT, NL - C - NE - CH ₂	120
34	375	125.0	FE - NR - CR1 (5-ring)	60
35	750	125.0	-	120
36	575	126.0	H, HC - 5-ring	90
37	640	126.0	X(noH) - 5-ring	100
38	770	126.0	OM - C - OM	120
39	760	132.0	5, 6 ring connection	100
40	2215	155.0	SI - OA - SI	95
41	91350	180.0	Fe - C - O (CO bound to heme)	57
42	434	109.5	HWat - OWat - HWat	92
43	484	107.57	HChl - CChl - CLChl	105
44	632	111.30	CLChl - CChl - CLChl	131
45	469	97.4	CDmso - SDmso - CDmso	110
46	503	106.75	CDmso - SDmso - ODmso	110
47	443	108.53	HMet - OMet - CMet	95
48	618	109.5	CLCl ₄ - CCl ₄ - CLCl ₄	131
49	507	107.6	FTfe - CTfe - FTfe	110
50	448	109.5	HTfe - OTfe - CHTfe	95
51	524	110.3	OTfe - CHTfe - CTfe	110
52	531	111.4	CHTfe - CTfe - FTfe	110
53	636	117.2	NUrea - CUrea - NUrea	120
54	690	121.4	OUrea - CUrea - NUrea	120

Table 2.5.4.1

GROMOS improper (harmonic) dihedral angle parameters

Improper dihedral-angle type code	Force constant	Ideal improper dihedral angle	Example of usage	
	K_{ξ_n}	ξ_{0_n}		K_{ξ_n}
	kJmol ⁻¹ degree ⁻²	degree		kcalmol ⁻¹ rad ⁻²
ICQH[N] ICQ[N]	CQ[N]	(Q0[N])		
1	0.0510	0.0	planar groups	40
2	0.102	35.26439	tetrahedral centres	80
3	0.204	0.0	heme iron	160
4	0.0510	180.0	planar groups	40
5	0.102	-35.26439	tetrahedral centres	80

Table 2.5.5.1

GROMOS (trigonometric) dihedral torsional angle parameters

Dihedral-angle type code	Force constant	Phase shift	Multiplicity	Example of usage in terms of nonbonded atom types	
	K_{ϕ_n}	$\cos(\delta_n)$	m_n		K_{ϕ_n}
	kJmol^{-1}				kcalmol^{-1}
ICPH[N] ICP[N]	CP[N]	PD[N]	NP[N]		
1	2.67	-1.0	1	CHn - CHn - CHn - OA (sugar) C4 - C5 - C6 - O6 ^a	0.6
2	3.41	-1.0	1	OA - CHn - OA - CHn, H (β sugar) O5 - C1 - O1 - C1',H1	0.8
3	4.97	-1.0	1	OA - CHn - CHn - OA (sugar) C4 - C5 - C6 - O6 ^a	1.2
4	5.86	-1.0	1	N - CHn - CHn - OA (lipid)	1.4
5	9.35	-1.0	1	OA - CHn - CHn - OA (sugar) O5 - C5 - C6 - O6 ^b	2.2
6	9.45	-1.0	1	OA - CHn - OA - CHn, H (α sugar) O5 - C1 - O1 - C1',H1	2.3
7	2.79	+1.0	1	P - O5* - C5* - C4* (dna)	0.7
8	5.35	+1.0	1	O5* - C5* - C4* - O4* (dna)	1.3
9	1.53	-1.0	2	C1 - C2 - CAB - CBB (heme)	0.4
10	5.86	-1.0	2	-C-C-	1.4
11	7.11	-1.0	2	-C-OA- (at ring)	1.7
12	16.7	-1.0	2	-C-OA- (carboxyl)	4.0
13	24.0	-1.0	2	CHn - OA - C - CHn (ester lipid)	5.7
14	33.5	-1.0	2	-C-N, NT, NE, NZ,NR-	8.0
15	41.8	-1.0	2	-C-CR1- (6-ring)	10.0
16	0.0	+1.0	2	-CH1 (sugar)-NR(base)-	0.0
17	0.418	+1.0	2	O-CH1-CHn-no O	0.1
18	2.09	+1.0	2	O-CH1-CHn-O	0.5
19	3.14	+1.0	2	-OA-P-	0.75
20	5.09	+1.0	2	CHn - O - P - O (dna, phosphodiester)	1.2
21	16.7	+1.0	2	-S-S-	4.0
22	1.05	+1.0	3	-OA-P-	0.25
23	1.26	+1.0	3	-CHn-OA(no sugar)-	0.3
24	1.30	+1.0	3	HTfe - OTfe - CHTfe - CTfe	0.3
25	2.53	+1.0	3	O5* - C5* - C4* - O4* (dna)	0.6

26	2.93	+1.0	3	-CH ₂ -S-	0.7
27	3.19	+1.0	3	CH _n - O - P - O (dna, phosphodiester)	0.8
28	3.65	+1.0	3	OA - CH _n - OA - CH _n , H (α sugar) O5 - C1 - O1 - C1',H1	0.9
29	3.77	+1.0	3	-C,CH _n ,SI- NT,NL,OA(sugar)-	0.9
30	3.90	+1.0	3	CH _n - CH _n - OA - H (sugar)	0.9
31	4.18	+1.0	3	HC-C-S-	1.0
32	4.69	+1.0	3	OA - CH _n - OA - CH _n , H (β sugar) O5 - C1 - O1 - C1',H1	1.1
33	5.44	+1.0	3	HC-C-C-	1.3
34	5.92	+1.0	3	-CH _n ,SI-CH _n -	1.4
35	7.69	+1.0	3	OA - CH _n - CH _n - OA (sugar) C4 - C5 - C6 - O6 ^a	1.8
36	8.62	+1.0	3	N - CH _n - CH _n - OA (lipid)	2.1
37	9.50	+1.0	3	OA - CH _n - CH _n - OA (sugar) O5 - C5 - C6 - O6 ^b	2.3
38	0.0	+1.0	4	-NR-FE-	0.0
39	1.0	-1.0	6	-CH _n -N,NE-	0.24
40	1.0	+1.0	6	-CH _n -C,NR (ring), CR1-	0.24
41	3.77	+1.0	6	-CH _n -NT-	0.9
42	3.50	-1.0	2	-CH_n-C-	0.84
43	2.80	+1.0	3	-CH_n-N-	0.67
44	0.70	-1.0	6	-CH_n-N-	0.17
45	0.40	+1.0	6	-CH_n-C-	0.10

a) To be used if - C5 - C6 - O6 and adjacent - C4 - O4 - are axial and the other equatorial, as in galactose

b) To be used if - C5 - C6 - O6 and adjacent - C_n - O_n - H_n are both simultaneously axial or equatorial, as in glucose

Table 2.5.6.2.1

GROMOS 54A7/54B7 non-bonded atom types and integer atom codes

integer atom code	atom type	description
IAC[N]	TYPE[N]	
1	O	carbonyl oxygen (C=O)
2	OM	carboxyl oxygen (CO ⁻)
3	OA	hydroxyl or sugar oxygen
4	OE	ether or ester oxygen
5	OW	water oxygen
6	N	peptide nitrogen (NH)
7	NT	terminal nitrogen (NH ₂)
8	NL	terminal nitrogen (NH ₃)
9	NR	aromatic nitrogen
10	NZ	Arg NH (NH ₂)
11	NE	Arg NE (NH)
12	C	bare carbon
13	CH0	bare sp ³ carbon, 4 bound heavy atoms
14	CH1	aliphatic or sugar CH-group
15	CH2	aliphatic or sugar CH ₂ -group
16	CH3	aliphatic CH ₃ -group
17	CH4	methane
18	CH2r	CH ₂ -group in a ring
19	CR1	aromatic CH-group
20	HC	hydrogen bound to carbon
21	H	hydrogen not bound to carbon
22	DUM	dummy atom
23	S	sulphur
24	CU1+	copper (charge 1+)
25	CU2+	copper (charge 2+)
26	FE	iron (heme)
27	ZN2+	zinc (charge 2+)
28	MG2+	magnesium (charge 2+)
29	CA2+	calcium (charge 2+)
30	P, SI	phosphor or silicon
31	AR	argon
32	F	fluor (non-ionic)
33	CL	chlorine (non-ionic)
34	BR	bromine (non-ionic)
35	CMet	CH ₃ -group in methanol (solvent)
36	OMet	oxygen in methanol (solvent)
37	NA+	sodium (charge 1+)
38	CL-	chloride (charge 1-)
39	CChl	carbon in chloroform (solvent)
40	CLChl	chloride in chloroform (solvent)
41	HChl	hydrogen in chloroform (solvent)
42	SDmso	sulphur in DMSO (solvent)

43	CDmso	CH ₃ -group in DMSO (solvent)
44	ODmso	oxygen in DMSO (solvent)
45	CCl ₄	carbon in carbontetrachloride (solvent)
46	CLCl ₄	chloride in carbontetrachloride (solvent)
47	FTfe	fluor in trifluoroethanol
48	CTfe	carbon in trifluoroethanol
49	CHTfe	CH ₂ -group in trifluoroethanol
50	OTfe	oxygen in trifluoroethanol
51	CUrea	carbon in urea
52	OUrea	oxygen in urea
53	NUrea	nitrogen in urea
54	CH₃p	positively charged methyl

Table 2.5.6.2.2

GROMOS 54A7 normal van der Waals parameters

integer atom code	atom type	$(C6(I,I))^{1/2}$	$(C12(I,I))^{1/2}$		
		$[kJmol^{-1} nm^6]^{1/2}$	$10^{-3}[kJmol^{-1} nm^{12}]^{1/2}$		
I=IAC[N]	TYPE[N]		1	2	3
1	O	0.04756	1.000	1.130	-
2	OM	0.04756	0.8611	1.841	3.068
3	OA	0.04756	1.100	1.227	-
4	OE	0.04756	1.100	1.227	-
5	OW	0.05116	1.623	1.623	-
6	N	0.04936	1.523	1.943	-
7	NT	0.04936	1.523	2.250	-
8	NL	0.04936	1.523	3.068	-
9	NR	0.04936	1.523	1.841	-
10	NZ	0.04936	1.523	2.148	-
11	NE	0.04936	1.523	1.984	-
12	C	0.04838	2.222	-	-
13	CH0	0.04896	14.33	-	-
14	CH1	0.07790	9.850	-	-
15	CH2	0.08642	5.828	-	-
16	CH3	0.09805	5.162	-	-
17	CH4	0.1148	5.862	-	-
18	CH2r	0.08564	5.297	-	-
19	CR1	0.07425	3.888	-	-
20	HC	0.009200	0.1230	-	-
21	H	0.0	0.0	-	-
22	DUM	0.0	0.0	-	-
23	S	0.09992	3.616	-	-
24	CU1+	0.02045	0.07159	0.2250	-
25	CU2+	0.02045	0.07159	0.4091	-
26	FE	0.0	0.0	0.0	-
27	ZN2+	0.02045	0.09716	0.09716	-
28	MG2+	0.008080	0.05838	0.05838	-
29	CA2+	0.03170	0.7057	0.7057	-
30	P, SI	0.1214	4.711	4.711	-
31	AR	0.07915	3.138	-	-
32	F	0.03432	0.8722	1.227	-
33	CL	0.09362	3.911	-	-
34	BR	0.16630	8.092	-	-
35	CMet	0.09421	4.400	-	-
36	OMet	0.04756	1.525	1.525	-
37	NA+	0.0088792	0.2700	0.2700	-
38	CL-	0.11318	7.776	7.776	7.776

39	CChl	0.051292	2.0160	-	-
40	CLChl	0.091141	3.7101	-	-
41	HChl	0.0061400	0.065574	-	-
42	SDmso	0.10277	4.6366	-	-
43	CDmso	0.098050	5.1620	-	-
44	ODmso	0.047652	0.86686	1.1250	-
45	CCl4	0.051292	2.7568	-	-
46	CLCl4	0.087201	3.5732	-	-
47	FTfe	0.034320	1.0000	1.0000	-
48	CTfe	0.048380	1.8370	-	-
49	CHTfe	0.084290	5.0770	-	-
50	OTfe	0.047560	1.2270	1.2270	-
51	CUrea	0.069906	3.6864	-	-
52	OUrea	0.048620	1.2609	1.2609	-
53	NUrea	0.057903	1.9877	1.9877	-
54	CH3p	0.09805	5.162	-	-

Table 2.5.6.2.3

GROMOS 53B6 (vacuo) normal van der Waals parameters

integer atom code	atom type	$(C6(I,I))^{1/2}$	$(C12(I,I))^{1/2}$		
		$[kJmol^{-1}nm^6]^{1/2}$	$10^{-3}[kJmol^{-1}nm^{12}]^{1/2}$		
I=IAC[N]	TYPE[N]		1	2	3
2	OM	0.04756 (23.25)	0.8611 (421.0)	1.125 (550.0)	1.125 (550.0)
8	NL	0.04936 (24.13)	1.301 (636.0)	1.943 (950.0)	-

Table 2.5.6.2.4

Selection of van der Waals (repulsive) $(C12(I,I))^{1/2}$ parameters

	J	1	2	3	4	5	6	7	8	9	10	11	24	25	26	27	28	29	30	32	33	34	36	37	38	44	47	50	52	53	54
I		O	OM	OA	OE	OW	N	NT	NL	NR	NZ	NE	CU1+	CU2+	FE	ZN2+	MG2+	CA2+	P,SI	F	CL	BR	OMet	NA+	CL-	ODmso	FTfe	OTfe	OUrea	NUrea	CH3p
1	O	1	1	2	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
2	OM	1	1	2	1	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1	1	1	1	2	3
3	OA	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
4	OE	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
5	OW	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
6	N	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
7	NT	2	2	2	2	2	2	2	2	2	2	2	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	2	2	2	1
8	NL	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
9	NR	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
10	NZ	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
11	NE	2	2	2	2	2	1	2	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	2	1
24	CU1+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
25	CU2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
26	FE	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
27	ZN2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
28	MG2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
29	CA2+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
30	P,SI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
32	F	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
33	CL	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
34	BR	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
36	OMet	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1
37	NA+	2	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	1	2	1	1
38	CL-	1	1	2	1	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1	1	1	1	2	1
44	ODmso	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	2	1	2	1
47	FTfe	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	1	1	2	1
50	OTfe	1	1	2	1	2	1	2	1	2	1	1	1	1	1	1	1	1	1	1	1	1	2	1	1	2	1	2	2	2	1
52	OUrea	1	1	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1	1	2	1	2	1
53	NUrea	2	2	2	2	2	2	2	2	2	2	2	1	1	1	1	1	1	1	2	2	2	2	1	2	2	2	2	2	2	1
54	CH3p	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table 2.5.6.2.5

GROMOS 54A7 normal van der Waals parameters for mixed atom type pairs (I,J)

integer atom code	atom type	integer atom code	atom type	C6(I,J)	C12(I,J)
I		J		$10^{-3}\text{kJmol}^{-1}\text{nm}^6$	$10^{-6}\text{kJmol}^{-1}\text{nm}^{12}$
39	CChl	40	CLChl	4.6754	7.4813
39	CChl	41	HChl	0.3622	0.1745
40	CLChl	41	HChl	0.6493	0.3266

Table 2.5.6.3.1

GROMOS 54A7/54B7 third-neighbour van der Waals parameters

integer atom code	atom type	$(C6(I,I))^{1/2}$	$(C12(I,I))^{1/2}$		
		$[k]\text{mol}^{-1}\text{nm}^6]^{1/2}$	$10^{-3}[k]\text{mol}^{-1}\text{nm}^{12}]^{1/2}$		
I=IAC[N]	TYPE[N]		1	2	3
1	O	0.04756	0.8611	-	-
3	OA	0.04756	1.125	-	-
4	OE	0.04756	1.125	-	-
6	N	0.04936	1.301	-	-
7	NT	0.04936	1.301	-	-
8	NL	0.04936	1.301	-	-
9	NR	0.04936	1.301	-	-
10	NZ	0.04936	1.301	-	-
11	NE	0.04936	1.301	-	-
12	C	0.04838	1.837	-	-
13	CH0	0.04838	1.837	-	-
14	CH1	0.05396	1.933	-	-
15	CH2	0.06873	2.178	-	-
16	CH3	0.08278	2.456	-	-
18	CH2r	0.06873	2.178	-	-
19	CR1	0.07435	2.886	-	-
54	CH3p	0.08278	2.456	-	-

Table 2.5.6.5.1

GROMOS 54A7 (54B7) atomic charges and charge group definitions for amino acid residues

atom name	charge in e	occurring in
N	-0.310	all residues
H	0.310	
C	0.450	all residues
O	-0.450	
CD	0.090 (0.0)	Arg (charge +1)
NE	-0.110 (-0.240)	
HE	0.240 (0.240)	
CZ	0.340 (0.0)	
NH1/2	-0.260 (-0.480)	
HH11/12/21/22	0.240 (0.240)	
NE	-0.310	Argn (neutral)
HE	0.310	
CZ	0.266	Argn (neutral)
NH1	-0.674	
HH1	0.408	
NH2	-0.880	Argn (neutral)
HH21/22	0.440	
CG, CD	0.290	Asn, Gln
OD1, OE1	-0.450	
ND2, NE2, NZ	-0.720	Asn, Gln
HD21/22, HE21/22, HZ1/2	0.440	
CG, CD	0.270 (0.720)	Asp, Glu (charge -1)
OD1/2, OE1/2	-0.635 (-0.360)	
CG, CD	0.330	Asph, Gluh
OD1, OE1	-0.450	
OD2, OE2	-0.288	
HD2, HE2	0.408	
CB	-0.100 (0.200)	Cys (charge -.5)
SG	-0.400 (-0.200)	
CB	0.150	Cysh
SG	-0.370	
HG	0.220	
CG	0.0	Hisa (proton at D1)
ND1	-0.050	
HD1	0.310	
CD2	0.0	
HD2	0.140	
CE1	0.0	
HE1	0.140	
NE2	-0.540	
CG	0.0	Hisb (proton at E2)
ND1	-0.540	
CD2	0.0	

HD2	0.140	
CE1	0.0	
HE1	0.140	
NE2	-0.050	
HE2	0.310	
CG	-0.050 (0.0)	Hish (charge +1)
ND1	0.380 (-0.300)	
HD1	0.300 (0.300)	
CD2	-0.100 (.0)	
HD2	0.100	
CE1	-0.340 (0.0)	
HE1	0.100	
NE2	0.310 (-0.300)	
HE2	0.300 (0.300)	
CG, CB, CB	0.266	Hyp, Ser, Thr
OD1, OG, OG1	-0.674	
HD1, HG, HG1	0.408	
CE	0.127 (0.0)	Lysh (charge +1)
NZ	0.129 (-0.744)	
HZ1/2/3	0.248 (0.248)	
CE	-0.220	Lys (neutral)
NZ	-0.660	
HZ1/2	0.440	
CG /CE	0.241	Met
SD	-0.482	
CG	-0.210	Trp
CD1	-0.140	
HD1	0.140	
CD2	0.0	
NE1	-0.100	
HE1	0.310	
CE2	0.0	
CZ	0.203	Tyr
OH	-0.611	
HH	0.408	
C	-0.140	all aromatic C-H groups in Phe, Tyr, Trp
H	0.140	
C	0.0	aromatic C connected to an aliphatic CH _n in Phe, Tyr
CH2	0.0	aliphatic CH _n connected to aromatic C in Phe, Tyr

The charges for the 53B6 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

Table 2.5.6.2

GROMOS 54A7 atomic charges for various (co)solvents

atom name	charge in e	occurring in
OW	-0.82000	H ₂ O (SPC model)
HW1/2	0.41000	
OW	-0.84760	H ₂ O (SPC/E model)
HW1/2	0.42380	
OW	-0.68850	H ₂ O (SPC/L model)
HW1/2	0.34425	
CChl	0.17900	Chloroform
CLChl	-0.08700	
HChl	0.08200	
SDmso	0.12753	DMSO
CDmso	0.16000	
ODmso	-0.44753	
CMet	0.26600	Methanol
OMet	-0.67400	
HMet	0.40800	
CCl4	0.0	Carbontetrachloride
CLCl4	0.0	
FTFE	-0.17000	2,2,2-Trifluoroethanol
CTFE	0.45200	
CHTFE	0.27300	
OTFE	-0.62500	
HTFE	0.41000	
CUrea	0.14200	Urea
OUrea	-0.39000	
NUrea	-0.54200	
HUrea	0.33300	

Table 2.5.6.5.3

GROMOS 54A7 (54B7) atomic charges and charge group definitions for nucleotides

atom name	charge in e	occurring in
O3/5*	-0.360 (-0.360)	all nucleotides
P	0.990 (1.440)	
O1/2P	-0.635 (-0.360)	
C4*	0.160	all nucleotides
O4*	-0.360	
C1*	0.200	
N9, N9, N1, N1, N1	-0.200	dAde, dGua, dCyt, dThy, Ura
C4, C4	0.200	dAde, dGua
C6, C6, C6	0.100	dCyt, dThy, Ura
H6, H6, H6	0.100	dCyt, dThy, Ura
N1, N3, N7, N3, N7, N3	-0.540	dAde, dAde, dAde, dGua, dGua, dGua, dCyt
C2, C8, C8	0.440	dAde, dAde, dGua
H2, H8, H8	0.100	dAde, dAde, dGua
C6, C2, C4	0.540	dAde, dGua, dCyt
N6, N2, N4	-0.830	dAde, dGua, dCyt
H61/62, H21/22, H41/42	0.415	dAde, dGua, dCyt
N1, N3, N3	-0.310	dGua, dThy, Ura
H1, H3, H3	0.310	dGua, dThy, Ura
C6, C2, C2, C4, C2, C4	0.450	dGua, dCyt, dThy, dThy, Ura, Ura
O6, O2, O2, O4, O2, O4	-0.450	dGua, dCyt, dThy, dThy, Ura, Ura
C5, C5	-0.100	dCyt, Ura
H5, H5	0.100	dCyt, Ura

Table 2.5.6.5.4

GROMOS 54A7 (54B7) atomic charges and charge group definitions for lipids

atom name	charge in e	occurring in
C32, C33, C34, C35	0.250	dppc
N	0.0	dppc
C31	0.0	dppc
O31, O32	-0.360	dppc
O33, O34	-0.635	dppc
P	0.990	dppc
C3	0.0	dppc
C1, C2	0.160	dppc
O11, O21	-0.360	dppc
O12, O22	-0.380	dppc
C11, C21	0.580	dppc
C12, ..., C22, ...	0.0	dppc

Table 2.5.6.5.5

GROMOS 54A7 (54B7) atomic charges and charge group definitions for carbohydrates

atom name	charge in e	occurring in
C1, C2, C3, C6	0.232	glucopyranose, polyuronate, terminal - CHn - On - Hn group
O2, O3, O6	-0.642	glucopyranose, polyuronate, terminal - CHn - On - Hn group
HO2, HO3, HO6	0.410	glucopyranose, polyuronate, terminal - CHn - On - Hn group
C5	0.376	glucopyranose, polyuronate
O5	-0.480	glucopyranose, polyuronate
O1	-0.360	glucopyranose, polyuronate
C4	0.232	glucopyranose, polyuronate
C6	0.360	polyuronate
O61, O62	-0.680	polyuronate
C1	0.232	terminal - C1 - O1 - CM group
O1	-0.360	terminal - C1 - O1 - CM group
CM (methyl)	0.232	terminal - C1 - O1 - CM group

Table 4.2.1

54A7 Solute building blocks

Name	Description (charges in <i>e</i>)
<i>amino acids and analogues</i> (L if not indicated otherwise)	
ALA	Alanine
ARG	Arginine (protonated; charge +1)
ARGN	Arginine (deprotonated; neutral)
ASN	Asparagine
ASN1	Asparagine (coordinated with ZN)
ASP	Aspartic acid (deprotonated; charge -1)
ASPH	Aspartic acid (protonated; neutral)
CYS	Cysteine (deprotonated; charge -1/2)
CYSH	Cysteine (protonated; neutral)
CYS1	Cysteine (1 st member of S-S bridge)
CYS2	Cysteine (2 nd member of S-S bridge)
GLN	Glutamine
GLU	Glutamic acid (deprotonated; charge -1)
GLUH	Glutamic acid (protonated; neutral)
GLY	Glycine
HISA	Histidine (protonated at ND1; neutral)
HISB	Histidine (protonated at NE2; neutral)
HISH	Histidine (protonated at ND1 and NE2; charge +1)
HIS1	Histidine (coupled to HEME at NE2; neutral)
HIS2	Histidine (coupled to HEMC at NE2; neutral)
HYP	Hydroxyproline
ILE	Isoleucine
LEU	Leucine
LYS	Lysine (deprotonated; neutral)
LYSH	Lysine (protonated; charge +1)
MET	Methionine
PHE	Phenylalanine
PRO	Proline
SER	Serine
THR	Threonine
TRP	Tryptophan
TYR	Tyrosine
VAL	Valine
DALA	D-Alanine
ABU	L-2-amino-butanoic acid
AIB	α -methylalanine
MEBMT	(4R)-4-[(E)-2-butanyl]-4, N-dimethyl-L-threonine

MELEU	N-methyl-L-leucine
MEVAL	N-methyl-L-valine
SAR	Sarcosine or N-methylglycine

nucleotides

DADE	2'-deoxyadenosine 5'-phosphoric acid	
DGUA	2'-deoxyguanosine 5'-phosphoric acid	(DNA; charge -1)
DCYT	2'-deoxycytidine 5'-phosphoric acid	
DTHY	2'-deoxythymidine 5'-phosphoric acid	
ADE	adenosine 5'-phosphoric acid	
GUA	guanosine 5'-phosphoric acid	(RNA; charge -1)
CYT	cytidine 5'-phosphoric acid	
URA	uridine 5'-phosphoric acid	
FMNO	flavin mononucleotide (oxydized, deprotonated at FN5 and FN1; charge -1, OPOHO ₂ ⁻)	
FMNS	flavin mononucleotide (semi-reduced, protonated at FN5; charge -1, OPOHO ₂ ⁻)	
FMNR	flavin mononucleotide (reduced, protonated at FN5 and FN1; charge -1, OPOHO ₂ ⁻)	
PFN	proflavin (protonated at FN5; charge +1)	
NADP	nicotinamide adenine dinucleotide (NAD ⁺ ; charge -1)	
NADH	nicotinamide adenine dinucleotide (NADH; charge -2)	
NDPH	nicotinamide adenine dinucleotide phosphate (NADPH; charge -3, OPOHO ₂ ⁻)	
NDPP	nicotinamide adenine dinucleotide phosphate (NADP ⁺ ; charge -2, OPOHO ₂ ⁻)	
NDPHN	nicotinamide adenine dinucleotide phosphate (NADPH; neutral, OPO(OH) ₂)	

sugars

GLCA	α-D-glucopyranosyl (1-4 linkage; neutral)
GLCB	β-D-glucopyranosyl (1-4 linkage; neutral)
GALA	α-D-galactopyranosyl (1-4 linkage; neutral)
GALB	β-D-galactopyranosyl (1-4 linkage; neutral)
MANA	α-D-mannoopyranosyl (1-4 linkage; neutral)
MANB	β-D-mannoopyranosyl (1-4 linkage; neutral)
TRH	trehalose
UGLB	β-D-glucuronan (1-4 linkage; neutral)
UMNB	β-D-mannuronan (1-4 linkage; neutral)
UGAA	α-D-galacturonan (1-4 linkage; neutral)
UGUA	α-L-guluronan (1-4 linkage; neutral)

lipids

DPPC	Dipalmitoylphosphatidylcholine (neutral)
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other molecules

HEME	heme group (charge -2, acidic groups deprotonated)	
HEMC	heme group with bound CO (charge -2, acidic groups deprotonated)	
CYT*	3',5'-O-(tetra isopropyl-1,3-disiloxanediyl) cytidine (neutral)	
MTXH	methotrexate (protonated at N1; charge -2)	
FOL	folate (charge -2)	
DHF	7,8-dihydrofolate (charge -2)	
THF	5,6,7,8-tetrahydrofolate (charge -2)	
TMP	trimethoprim (deprotonated at N1; neutral)	
TMPH	trimethoprim (protonated at N1; neutral)	
TMPHP	trimethoprim (protonated at N1; charge +1)	
PDG	3-phospho-D-glycerate (charge -2)	
ATP	adenosine 5'-triphosphate (ATP; charge -3)	
PMB	p-methylbenzyl alcoholate (charge -1)	
PMBH	p-methylbenzyl alcohol (neutral)	
BA	benzoic acid	
RTOL	retinol (neutral)	
TEMP	tetramethyl pyrrolinyl (nitroxide spin label; neutral)	
ETH	ethyl alcoholate (charge -1)	
ETHH	ethyl alcohol (neutral)	
CH4	methane (united atom)	
AR	argon	

ions

SO42-	SO ₄ ²⁻ ion	(charge -2)
ZN2+	zinc ion	(charge +2)
NA+	sodium ion	(charge +1)
CL-	chlorine ion	(charge -1)
CA2+	calcium ion	(charge +2)
MG2+	magnesium ion	(charge +2)
CU1+	copper ion	(charge +1)
CU2+	copper ion	(charge +2)

(co)solvents

H2O	water (SPC model, rigid, [81.4])
H2OE	water (SPC/E model, rigid, [87.5])
CHCL3	chloroform (rigid, [94.36])
DMSO	dimethylsulfoxide (rigid, [04.6])

CH ₃ OH	methanol (rigid) [00.9]
CCL ₄	carbontetrachloride (rigid, [96.33])
TFE	2,2,2-trifluoroethanol (flexible, [00.34])
UREA	Urea (flexible, [04.5])

Table 4.2.2

54A7 Solvent building blocks

Name	Description
H2O	water (SPC model, [81.4])
H2OE	water (SPC/E model, [87.5])
H2OL	water (SPC/L model [02.18]) [*]
CHCL3	chloroform ([94.36])
DMSO	dimethylsulfoxide ([04.6])
CH3OH	methanol [00.9]
CCL4	carbontetrachloride ([96.33])

^{*}) There is no building block for SPC/L in the 53A5 force field, because it requires an additional atom type. We suggest to use atom type 22 (DUM) for the hydrogens with van der Waals parameters $C6(22,22)^{1/2} = 0.53 \text{ [kJ mol}^{-1} \text{ nm}^6]^{1/2}$ and $C12(22,22)^{1/2} = 0$. The constraints should be set to $r_{OH} = 0.11 \text{ nm}$ and $r_{HH} = 0.173952 \text{ nm}$.

Table 4.2.3

54A7 End group building blocks

Name	Description	
<i>proteins and peptides</i>		
NH3+	N-terminus	(charge +1)
NH2	N-terminus	(neutral)
NPRO	N-terminus for proline	(charge +1)
COO-	O-terminus	(charge -1)
COOH	O-terminus	(neutral)
<i>nucleic acids</i>		
D5OH	5'-terminal of DNA	(neutral)
D3OH	3'-terminal of DNA	(neutral)
3OH	3'-terminal of RNA	(neutral)
<i>sugars</i>		
C1OH	-C1-O1-H1 group for carbohydrates	(neutral)
C1OC	-C1-O1-CH3 group for carbohydrates	(neutral)
COHT	-Cn-On-Hon group for carbohydrates	(neutral)