Supporting Information

L-DOPA and Droxidopa: from force development to molecular docking into Human β_2-Adrenergic Receptor

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adrenaline.itp: OPLS AA force field parameters of adrenaline generated with JOYCE.

dopa.itp: OPLS AA force field parameters of L-DOPA generated with JOYCE.

droxidopa.itp: OPLS AA force field parameters of Droxidopa generated with JOYCE.

Calculation of torsional profiles with subtracted Coulomb and Lennard-Jones contributions

The combination rule for the OPLS AA force field is a geometric average of C6 and C12 values in the topology file, which correspond to sigma (in nm) and epsilon (in kJ/mol) values in the ffnonbonded.itp file, as expressed by the following equations:

$$\sigma_{ij} = \left(\sigma_{ii}\sigma_{jj}\right)^{1/2} \quad \text{(S1)}$$

$$\varepsilon_{ij} = \left(\varepsilon_{ii}\varepsilon_{jj}\right)^{1/2} \quad \text{(S2)}$$

which have been used to estimate Coulomb (electrostatic) and Lennard-Jones (van der Waals) contributions to torsional profiles of dihedral angles of adrenaline, L-DOPA and Droxidopa molecules. The Coulomb and Lennard-Jones energy contributions were calculated using the following equations:

$$Vc\left(r_{ij}\right) = \frac{q_i q_j}{4\pi\varepsilon_0\varepsilon_r r_{ij}} \quad \text{(S3)}$$

$$V_{LJ}\left(r_{ij}\right) = 4\varepsilon_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - 4\varepsilon_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6} \quad \text{(S4)}$$

equations S1 and S2, and the distance matrices obtained as output from Gaussian QM calculations for each dihedral. Minimum and maximum values of electrostatic and LJ energies for each dihedral of adrenaline, L-DOPA and Droxidopa are reported in **Table S4**. Then, electrostatic and Lennard-Jones terms estimated from equations S3 and S4 were subtracted from QM profiles energetic deltas with the fudge (0.5 for QQ and 0.5 for LJ interactions) applied only to 1-4 interactions, which is in good agreement with the usual treatment of these interactions in the OPLS AA force field, using the following equation for the torsional energy rescaling:

$$E\_new = (QM\_E - QM\ min) - (Q\_E - Q\_E(QM\_min)) - (Q\_LJ - Q\_LJ(QM\_min)) \quad \text{(S5)}$$

where QM_E is the QM torsional profile energy, QM min is the minimum energy in the QM profile, and Q_E and Q_LJ are eletrostatic and van der Waals contributions, respectively. Finally, these new energetic profiles were used to generate new force field parameters for adrenaline, L-DOPA and Droxidopa molecules by fitting them with linear combinations of cosine functions, depending on the multiplicity of the dihedral angle of interest.

Figure S1

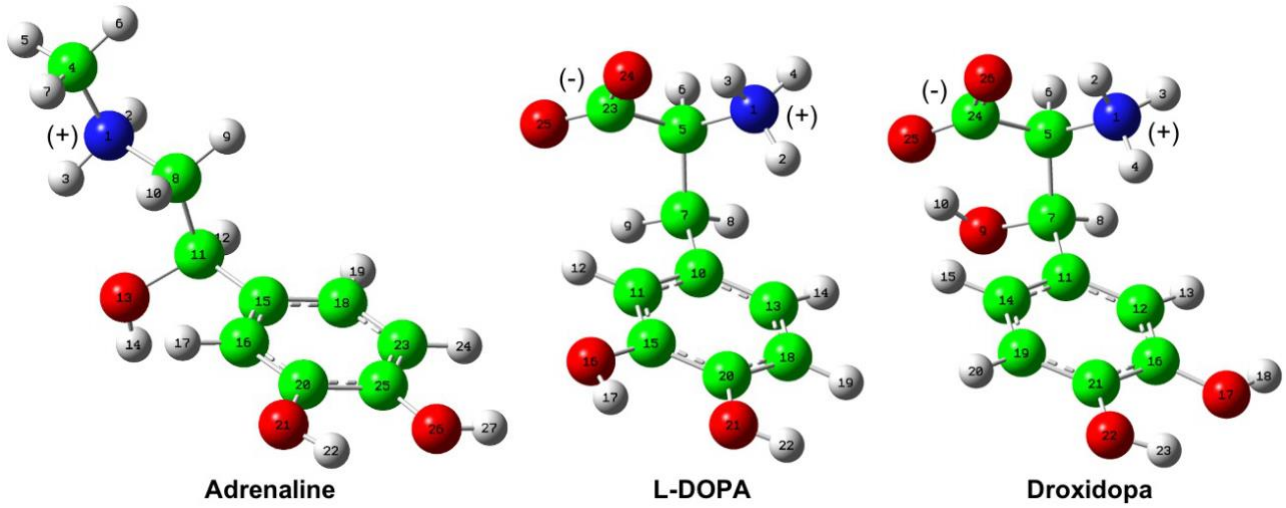


Figure S1 Geometry optimized chemical structures of protonated adrenaline, zwitterionic L-DOPA and Droxidopa with atom numbers used for the force field development.

Figure S2

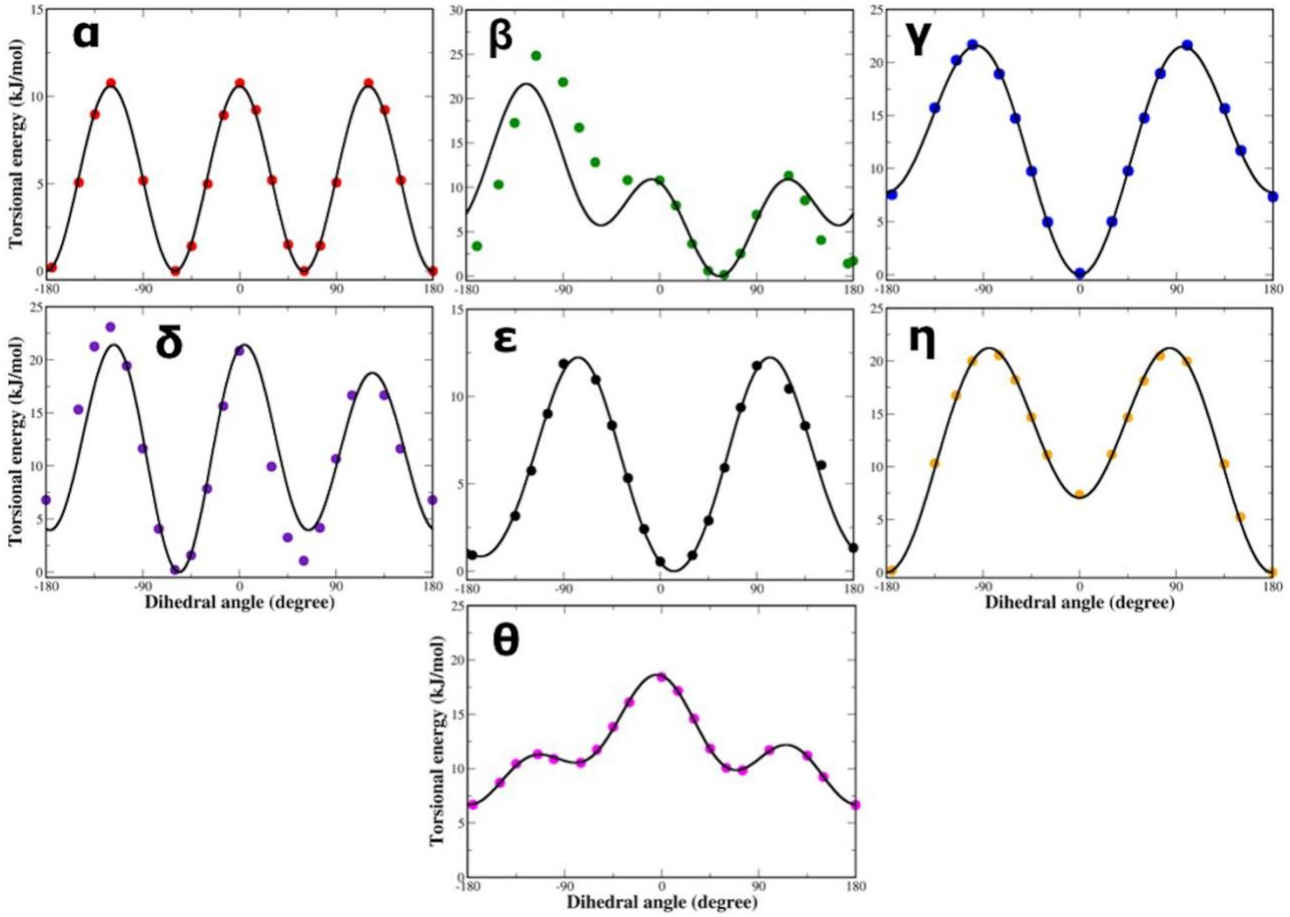


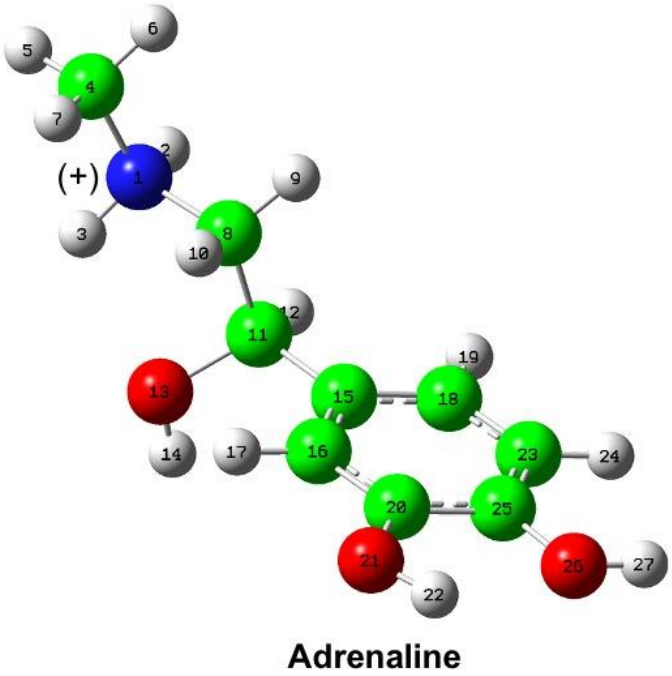
Figure S2 Torsional profiles derived from QM calculations (dots) and JOYCE (lines) for protonated adrenaline. Each panel refers to dihedral angles defined in Figure 1. Energies are reported in kilojoules per mole (1 kJ/mol = 0.24 kcal/mol).

Table S1

Partial atomic charges and OPLS AA force field Lennard-Jones parameters of Adrenaline (ALE).

Atom number	Atom name	Atom type	Adrenaline			
			Mass (u)	Charge (e)	σ (nm)	ε (kJ/mol)
1	N	N	14.0027	-0.446343	0.325	0.71128
2	H1	H	1.00800	0.382023	0	0
3	H2	H	1.00800	0.363936	0	0
4	C1	C	12.0110	-0.076781	0.35	0.276144
5	H3	H	1.00800	0.137222	0	0
6	H4	H	1.00800	0.135202	0	0
7	H5	H	1.00800	0.135338	0	0
8	CA	CA	12.0110	-0.024055	0.35	0.276144
9	HA1	HA	1.00800	0.138286	0.25	0.12552
10	HA2	HA	1.00800	0.133064	0.25	0.12552
11	CB	CB	12.0110	0.027731	0.35	0.276144
12	HB1	HC	1.00800	0.117273	0.25	0.12552
13	OG	OH	15.9994	-0.422795	0.307	0.71128
14	HG	HH	1.00800	0.347155	0	0
15	CG	CC	12.0110	-0.029545	0.355	0.29288
16	CD1	CC	12.0110	-0.104846	0.355	0.29288
17	HD1	HC	1.00800	0.107227	0.242	0.12552
18	CD2	CC	12.0110	-0.101815	0.355	0.29288
19	HD2	HC	1.00800	0.103567	0.242	0.12552
20	CE1	CC	12.0110	0.073348	0.355	0.29288
21	OE1	OH	15.9994	-0.394652	0.307	0.71128
22	HE1	HH	1.00800	0.340755	0	0
23	CE2	CC	12.0110	-0.107124	0.355	0.29288
24	HE2	HC	1.00800	0.112182	0.242	0.12552
25	CZ	CZ	12.0110	0.071847	0.355	0.29288
26	OH	OH	15.9994	-0.381798	0.307	0.71128
27	HH	HH	1.00800	0.363632	0	0

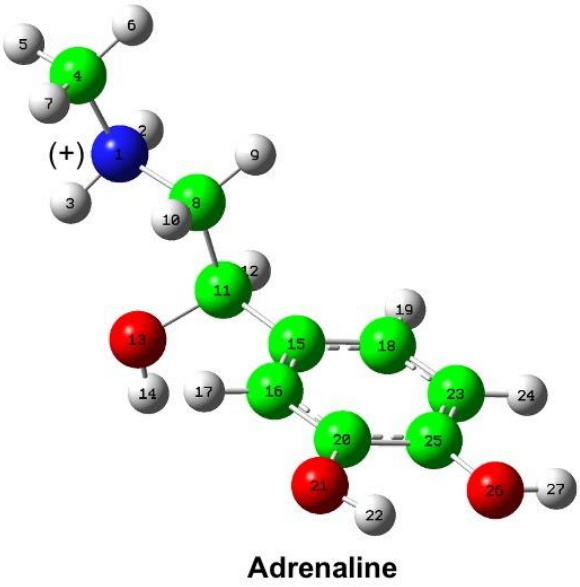
Figure S3



a_i	a_j	type	r_{eq} (nm)	k_r (kJ/mol nm^2)
1	2	1	0.1025	393683.477
1	4	1	0.1496	196521.091
4	5	1	0.1094	328457.447
1	8	1	0.1501	179667.704
8	9	1	0.1094	323493.654
8	11	1	0.1524	182391.941
11	12	1	0.1102	301357.367
11	13	1	0.1436	199950.22
13	14	1	0.0966	486572.973
11	15	1	0.1512	205697.663
15	16	1	0.1403	339484.191
16	17	1	0.109	332540.269
20	21	1	0.1368	307423.405
21	22	1	0.0969	480865.258
25	26	1	0.1372	306132.262

Figure S3 OPLS AA force field parameters of adrenaline: bond lengths and force constants. For clarity, only a selection of the most representative bonds is reported in the table. A complete list of bonds parameters can be found in the attached adrenaline.itp file.

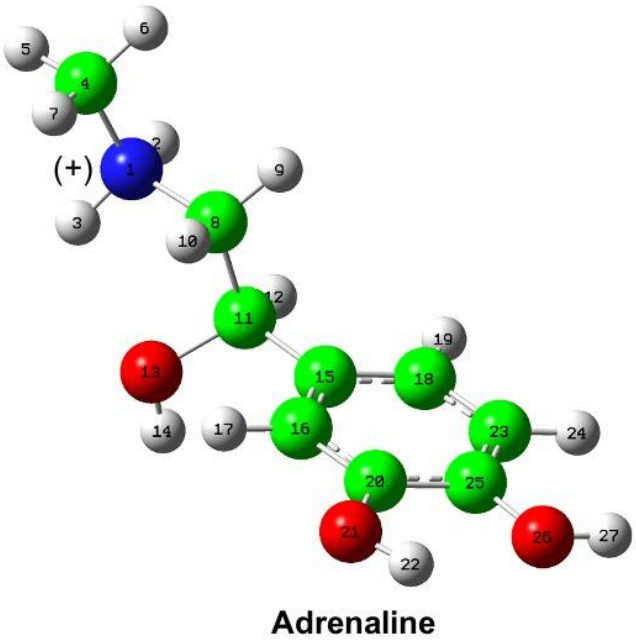
Figure S4



a_i	a_j	a_k	type	θ_{eq} (dgr)	k_θ (kJ/mol rad^2)
2	1	3	1	105.8	366.874
2	1	4	1	109.51	373.8285
2	1	8	1	109.42	381.2262
1	4	5	1	108.48	468.3697
4	1	8	1	114.27	472.0079
5	4	6	1	110.52	309.0556
1	8	9	1	108.31	451.2013
1	8	11	1	109.59	643.5652
11	15	16	1	120.12	588.9987
15	16	17	1	120.97	293.3534
15	16	20	1	120.2	495.6412
16	20	21	1	119.58	534.1722
16	20	25	1	119.91	361.9651
20	21	22	1	108.56	522.9635
21	20	25	1	120.51	771.4094

Figure S4 OPLS AA force field parameters of adrenaline: bond angles and force constants. For clarity, only a selection of the most representative angles is reported in the table. A complete list of angles parameters can be found in the attached adrenaline.itp file.

Figure S5



a_i	a_j	a_k	a_l	type	δ_{eq} (dgr)	k_δ (kJ/mol)	n
3	1	4	6	1	1.11	5.3	3
2	1	8	9	1	270.19	5.179	1
2	1	8	9	1	-171.66	2.193	2
2	1	8	9	1	1.25	3.196	3
20	25	26	27	1	-179.55	3.882	1
20	25	26	27	1	179.73	8.726	2
9	8	11	12	1	-162.12	2.055	1
9	8	11	12	1	63.42	1.109	2
9	8	11	12	1	-0.25	8.553	3
9	8	11	12	1	-6.16	0.163	4
12	11	15	18	1	180.84	0.004	1
12	11	15	18	1	-152.83	5.737	2
12	11	15	18	1	161.46	0.004	3
12	11	15	18	1	17.84	0.217	4
16	20	21	22	1	-0.56	3.524	1

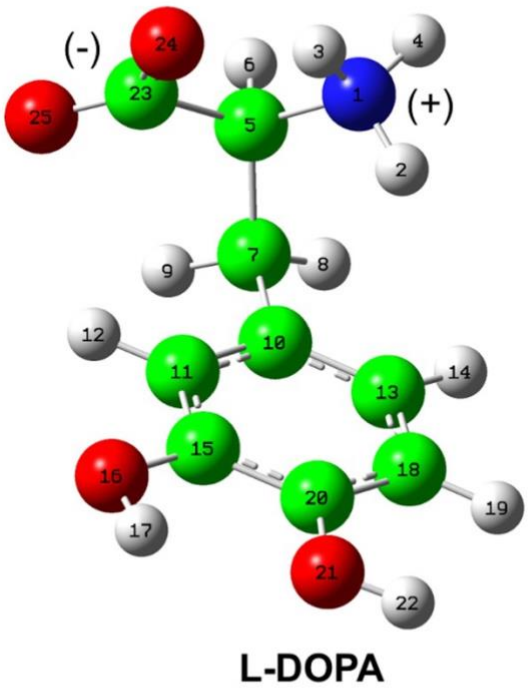
Figure S5 OPLS AA force field parameters of adrenaline: dihedral angles, force constants and multiplicity.

Table S2

Partial atomic charges and OPLS AA force field Lennard-Jones parameters of L-DOPA (DAH).

Atom number	Atom name	Atom type	L-DOPA			
			Mass (u)	Charge (e)	σ (nm)	ε (kJ/mol)
1	N	N	14.0027	-0.564145	0.325	0.71128
2	H1	H	1.00800	0.38029	0	0
3	H2	H	1.00800	0.371986	0	0
4	H3	H	1.00800	0.328559	0	0
5	CA	CA	12.0110	0.028023	0.35	0.276144
6	HA	HA	1.00800	0.12435	0.25	0.12552
7	CB	CB	12.0110	-0.134714	0.35	0.276144
8	HB1	HA	1.00800	0.102968	0.25	0.12552
9	HB2	HA	1.00800	0.10481	0.25	0.12552
10	CG	CC	12.0110	-0.022917	0.355	0.29288
11	CD1	CC	12.0110	-0.109878	0.355	0.29288
12	HD1	HC	1.00800	0.104159	0.242	0.12552
13	CD2	CC	12.0110	-0.109974	0.355	0.29288
14	HD2	HC	1.00800	0.100022	0.242	0.12552
15	CE1	CC	12.0110	0.067123	0.355	0.29288
16	OE1	OH	15.9994	-0.399226	0.307	0.71128
17	HE1	HH	1.00800	0.338272	0	0
18	CE2	CC	12.0110	-0.11227	0.355	0.29288
19	HE2	HC	1.00800	0.108509	0.242	0.12552
20	CZ	CZ	12.0110	0.062947	0.355	0.29288
21	OH	OH	15.9994	-0.388243	0.307	0.71128
22	HH	HH	1.00800	0.360275	0	0
23	C	C	12.0110	0.185232	0.375	0.43932
24	O1	O	15.9994	-0.468657	0.296	0.87864
25	O2	O	15.9994	-0.457493	0.296	0.87864

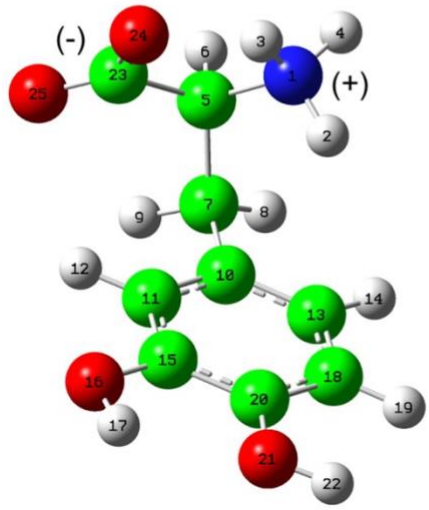
Figure S6



a_i	a_j	type	r_{eq} (nm)	k_r (kJ/mol nm^2)
1	2	1	0.1026	368489.034
1	5	1	0.1506	180341.536
5	6	1	0.1095	318058.259
5	7	1	0.1536	180195.043
7	8	1	0.1098	314597.457
7	10	1	0.1512	214106.063
10	11	1	0.1405	332239.63
11	12	1	0.109	331723.534
15	16	1	0.1368	305030.302
16	17	1	0.0969	480979.109
15	20	1	0.1408	309763.805
20	21	1	0.1374	305476.385
21	22	1	0.0966	480979.109
5	23	1	0.156	136630.345
23	24	1	0.1269	478155.015

Figure S6 OPLS AA force field parameters of L-DOPA: bond lengths and force constants. For clarity, only a selection of the most representative bonds is reported in the table. A complete list of bonds parameters can be found in the attached dopa.itp file.

Figure S7

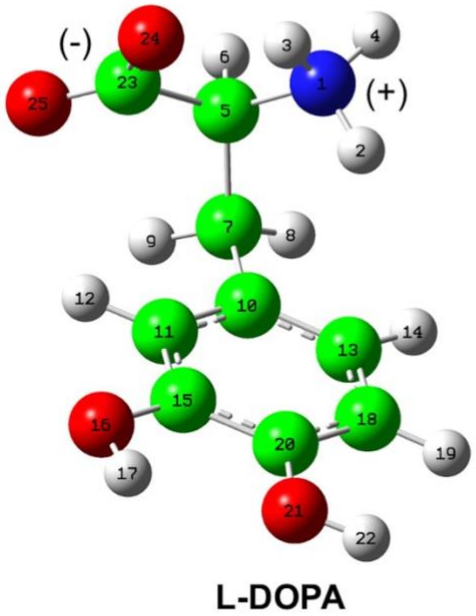


L-DOPA

a_i	a_j	a_k	type	θ_{eq} (dgr)	k_θ (kJ/mol rad^2)
2	1	3	1	108.76	338.0992
2	1	5	1	111.79	354.8638
1	5	6	1	107.34	467.6459
1	5	7	1	111.77	482.7422
1	5	23	1	105.54	528.7628
6	5	7	1	109.7	396.4863
6	5	23	1	107.64	316.9483
5	7	8	1	109.02	342.6356
5	7	10	1	112.82	622.4218
7	5	23	1	114.51	523.3779
9	7	10	1	111.11	348.8275
7	10	11	1	120.42	495.9408
10	11	12	1	120.47	295.1435
11	10	13	1	118.84	539.073
11	15	16	1	119.53	574.6185
11	15	20	1	120.05	379.8506
15	16	17	1	108.53	518.3672
16	15	20	1	120.42	796.0599
13	18	19	1	120.37	295.1435
13	18	20	1	119.76	379.8506
19	18	20	1	119.86	327.6687
15	20	18	1	119.9	99.2215
15	20	21	1	115.28	699.1805
20	21	22	1	110.6	449.2292
5	23	24	1	114.7	372.9536
24	23	25	1	128.67	683.7864

Figure S7 OPLS AA force field parameters of L-DOPA: bond angles and force constants. For clarity, only a selection of the most representative angles is reported in the table. A complete list of angles parameters can be found in the attached dopa.itp file.

Figure S8



a_i	a_j	a_k	a_l	type	δ_{eq} (dgr)	k_δ (kJ/mol)	n
6	5	23	24	1	320.79	9.731	2
6	5	23	25	1	318.43	9.731	2
2	1	5	6	1	127.76	2.482	3
3	1	5	6	1	140.68	2.482	3
18	20	21	22	1	0	3.251	1
18	20	21	22	1	179.99	8.441	2
6	5	7	8	1	-193.73	5.697	1
6	5	7	8	1	-94.39	1.592	2
6	5	7	8	1	-14.05	6.757	3
6	5	7	8	1	8.32	0.158	4
8	7	10	13	1	242.4	0.135	1
8	7	10	13	1	199.06	8.06	2
8	7	10	13	1	252.02	0.038	3
8	7	10	13	1	-62.1	2.03	4
8	7	10	11	1	242.4	0.135	1
8	7	10	11	1	199.06	8.06	2
8	7	10	11	1	252.02	0.038	3
8	7	10	11	1	-62.1	2.03	4
11	15	16	17	1	359.82	3.153	1
11	15	16	17	1	179.64	9.114	2

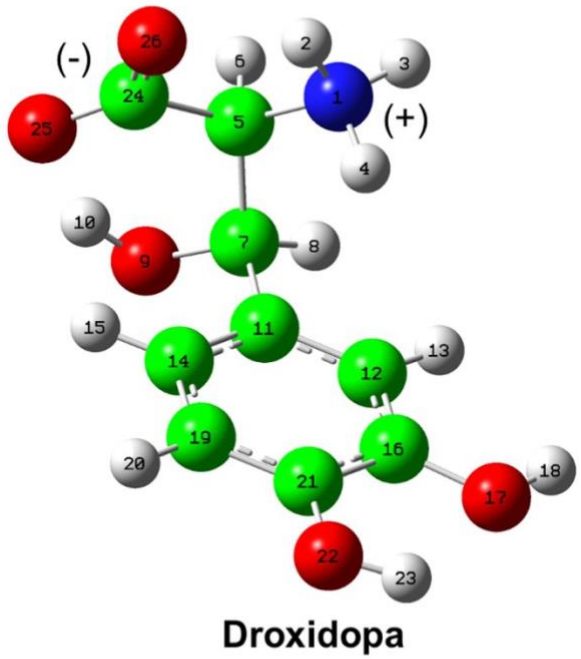
Figure S8 OPLS AA force field parameters of L-DOPA: dihedral angles, force constants and multiplicity.

Table S3

Partial atomic charges and OPLS AA force field Lennard-Jones parameters of Droxidopa (DRO).

Atom number	Atom name	Atom type	Droxidopa			
			Mass (u)	Charge (e)	σ (nm)	ε (kJ/mol)
1	N	N	14.0027	-0.563874	0.325	0.71128
2	H1	H	1.00800	0.334884	0	0
3	H2	H	1.00800	0.383193	0	0
4	H3	H	1.00800	0.347978	0	0
5	CA	CA	12.0110	0.025501	0.35	0.276144
6	HA	HA	1.00800	0.138072	0.25	0.12552
7	CB	CB	12.0110	0.018493	0.35	0.276144
8	HB1	HA	1.00800	0.11258	0.25	0.12552
9	OG	OH	15.9994	-0.469561	0.307	0.71128
10	HG	HO	1.00800	0.286741	0	0
11	CG	CC	12.0110	-0.037767	0.355	0.29288
12	CD1	CC	12.0110	-0.106979	0.355	0.29288
13	HD1	HC	1.00800	0.113467	0.242	0.12552
14	CD2	CC	12.0110	-0.106878	0.355	0.29288
15	HD2	HC	1.00800	0.096655	0.242	0.12552
16	CE1	CC	12.0110	0.071455	0.355	0.29288
17	OE1	OH	15.9994	-0.382444	0.307	0.71128
18	HE1	HH	1.00800	0.363284	0	0
19	CE2	CC	12.0110	-0.103248	0.355	0.29288
20	HE2	HC	1.00800	0.108686	0.242	0.12552
21	CZ	CZ	12.0110	0.073032	0.355	0.29288
22	OH	OH	15.9994	-0.393531	0.307	0.71128
23	HH	HH	1.00800	0.341308	0	0
24	C	C	12.0110	0.201167	0.375	0.43932
25	O1	O	15.9994	-0.421581	0.296	0.87864
26	O2	O	15.9994	-0.430621	0.296	0.87864

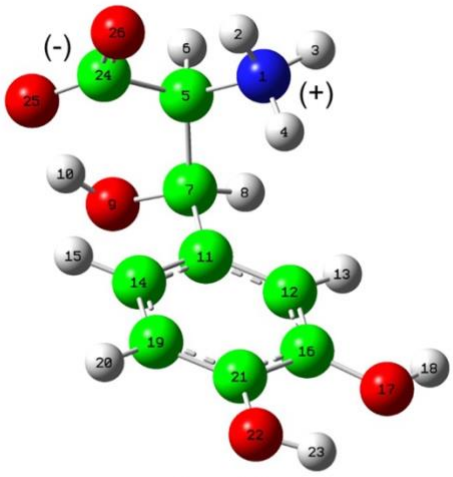
Figure S9



a_i	a_j	type	r_{eq} (nm)	k_r (kJ/mol nm^2)
1	2	1	0.1048	373470.846
1	5	1	0.1499	207081.212
5	6	1	0.1096	317299.775
5	7	1	0.1551	154162.502
7	8	1	0.1099	305252.01
7	9	1	0.142	225968.096
9	10	1	0.0987	383776.997
7	11	1	0.152	208485.422
11	12	1	0.1404	316021.4
12	13	1	0.1093	332268.673
16	17	1	0.1372	289583.572
17	18	1	0.0966	481033.117
16	21	1	0.1404	321359.557
5	24	1	0.1558	132339.541
24	25	1	0.1259	479501.584

Figure S9 OPLS AA force field parameters of Droxidopa: bond lengths and force constants. For clarity, only a selection of the most representative bonds is reported in the table. A complete list of bonds parameters can be found in the attached droxidopa.itp file.

Figure S10

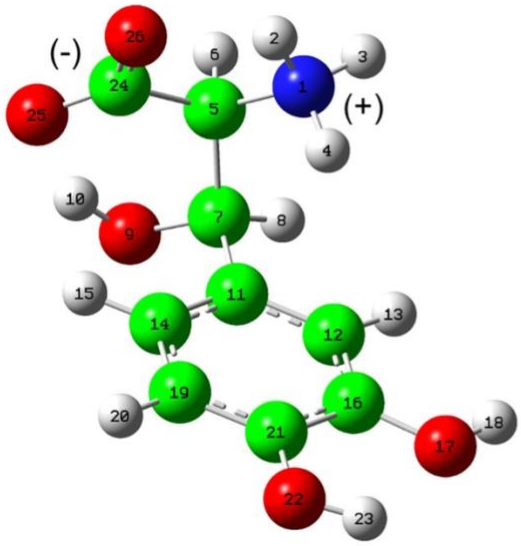


Droxidopa

a_i	a_j	a_k	type	θ_{eq} (dgr)	k_θ (kJ/mol rad^2)
2	1	3	1	111.49	343.4745
2	1	5	1	102.59	361.7045
1	5	6	1	107.66	519.9423
1	5	7	1	111.87	553.7967
1	5	24	1	105.89	484.0496
6	5	7	1	108.85	417.8032
6	5	24	1	107.9	291.6417
5	7	8	1	107.6	419.7621
5	7	9	1	108.48	744.6744
5	7	11	1	111.66	365.07
7	5	24	1	114.39	468.9387
8	7	9	1	106.95	492.3242
8	7	11	1	107.98	276.5572
7	9	10	1	105.6	632.6532
9	7	11	1	113.89	449.8951
7	11	12	1	119.34	687.2295
11	12	13	1	120.26	298.4541
12	11	14	1	119.01	496.0446
12	16	17	1	124.4	731.9646
12	16	21	1	120.09	377.2683
16	17	18	1	110.69	453.9904
17	16	21	1	115.5	634.4644
20	19	21	1	118.8	323.2446
16	21	19	1	119.52	209.44
16	21	22	1	120.77	671.056
21	22	23	1	108.62	481.9262
5	24	25	1	116.12	324.2452
25	24	26	1	128.37	813.2475

Figure S10 OPLS AA force field parameters of Droxidopa: bond angles and force constants. For clarity, only a selection of the most representative angles is reported in the table. A complete list of angles parameters can be found in the attached droxidopa.itp file.

Figure S11



a_i	a_j	a_k	a_l	type	δ_{eq} (dgr)	k_δ (kJ/mol)	n
6	5	24	25	1	328.39	10.451	2
6	5	24	26	1	330.59	10.451	2
2	1	5	6	1	125.59	2.547	3
3	1	5	6	1	123.45	2.547	3
19	21	22	23	1	359.86	3.272	1
19	21	22	23	1	179.73	8.853	2
6	5	7	8	1	-218.42	3.367	1
6	5	7	8	1	-87.74	9.305	2
6	5	7	8	1	-25.06	9.134	3
6	5	7	8	1	-144.67	0.009	4
8	7	11	14	1	-120.9	0.702	1
8	7	11	14	1	185.55	10.437	2
8	7	11	14	1	41.83	0.182	3
8	7	11	14	1	0	0.042	4
8	7	11	12	1	-120.9	0.702	1
8	7	11	12	1	185.55	10.437	2
8	7	11	12	1	41.83	0.182	3
8	7	11	12	1	0	0.042	4
12	16	17	18	1	0	3.272	1
12	16	17	18	1	179.99	8.853	2
5	7	9	10	1	-215.05	12.202	1
5	7	9	10	1	128.96	6.72	2
5	7	9	10	1	777.43	2.465	3
5	7	9	10	1	43.77	0.432	4

Figure S11 OPLS AA force field parameters of Droxidopa: dihedral angles, force constants and multiplicity.

Figure S12

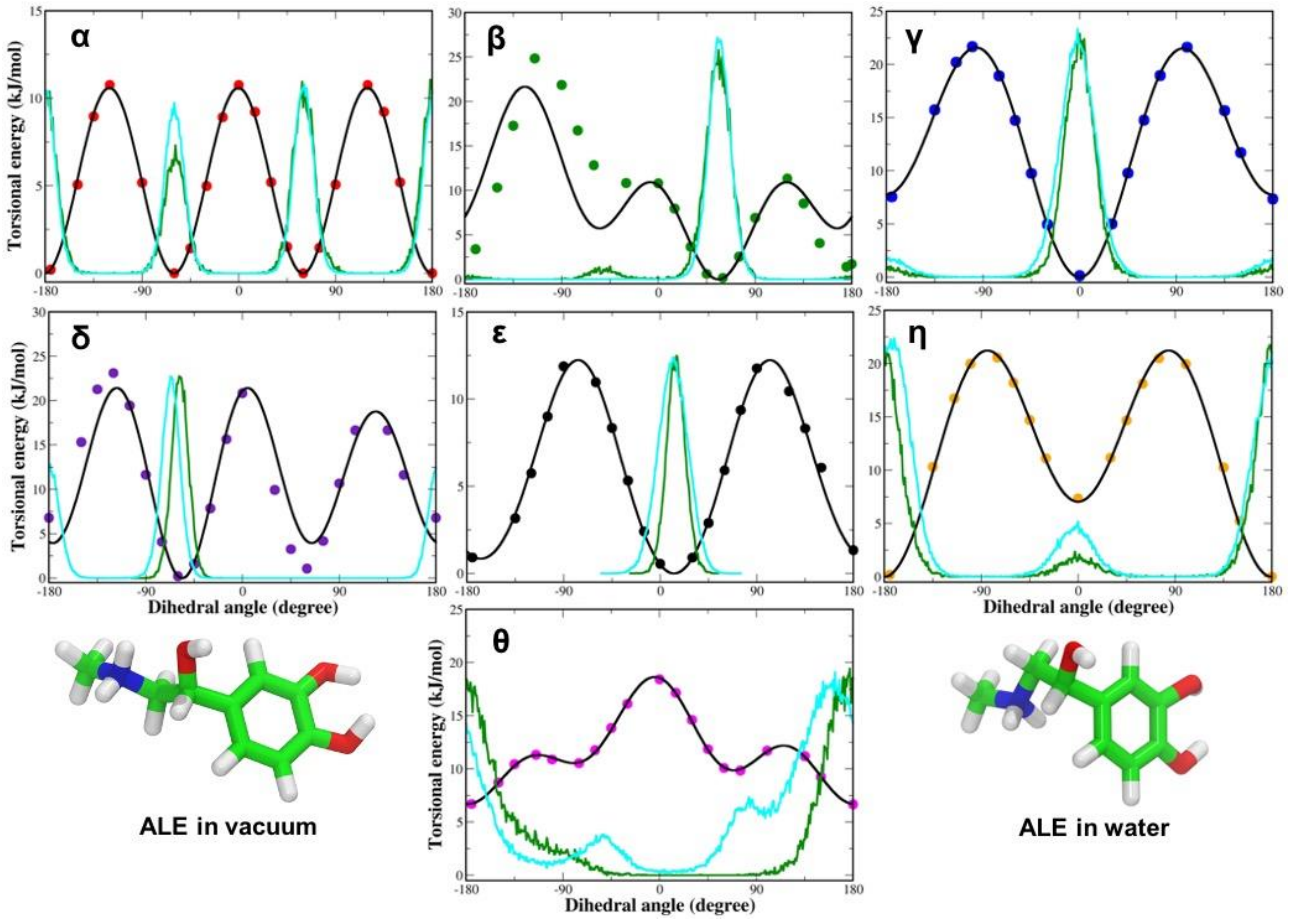


Figure S12 (Top) Dihedrals distributions in vacuum (green) and water (cyan) are compared to torsional profiles obtained by QM calculations (dots) and JOYCE (lines) for protonated adrenaline. Each panel refers to dihedral angles defined in Figure 1. (Bottom) Adrenaline structures simulated for 20 ns and 100 ns in vacuum and water, respectively. Energies are reported in kilojoules per mole (1 kJ/mol = 0.24 kcal/mol).

Table S4

Minimum and maximum values of Coulomb (V_C) and Lennard-Jones (V_{LJ}) energies of each dihedral of Adrenaline, L-DOPA and Droxidopa molecules.

Ligand	Dihedral	V_C (kJ/mol)	V_{LJ} (kJ/mol)
Adrenaline	α	1.28 ÷ 1.30	-30.8 ÷ -30.1
	β	1.23 ÷ 1.47	-32.6 ÷ -29.4
	γ	1.34 ÷ 1.66	-31.1 ÷ -29.6
	δ	1.04 ÷ 1.71	-41.6 ÷ -26.8
	ε	1.29 ÷ 1.44	-37.5 ÷ -30.6
	η	1.29 ÷ 1.66	-31.2 ÷ -29.4
	θ	1.63 ÷ 1.93	-27.2 ÷ -25.8
L-DOPA	α	-3.7 ÷ -4.2	-27.4 ÷ -41.4
	β	-3.8 ÷ -4.2	-37.3 ÷ -41.7
	γ	-4.1 ÷ -4.5	-41.0 ÷ -42.5
	δ	-3.9 ÷ -4.5	-35.0 ÷ -44.5
	ε	-4.1 ÷ -4.4	-39.5 ÷ -50.5
	η	-4.1 ÷ -4.2	-40.5 ÷ -42.5
Droxidopa	α	-3.4 ÷ -3.8	-36.4 ÷ -50.7
	β	-3.5 ÷ -3.9	-48.7 ÷ -51.2
	γ	-3.6 ÷ -3.8	-50.0 ÷ -51.3
	δ	-3.6 ÷ -4.6	-36.6 ÷ -59.2
	ε	-3.6 ÷ -4.1	-50.8 ÷ -61.5
	η	-3.6 ÷ -4.0	-49.6 ÷ -51.3
	θ	-3.4 ÷ -4.1	-45.6 ÷ -51.5

Figure S13

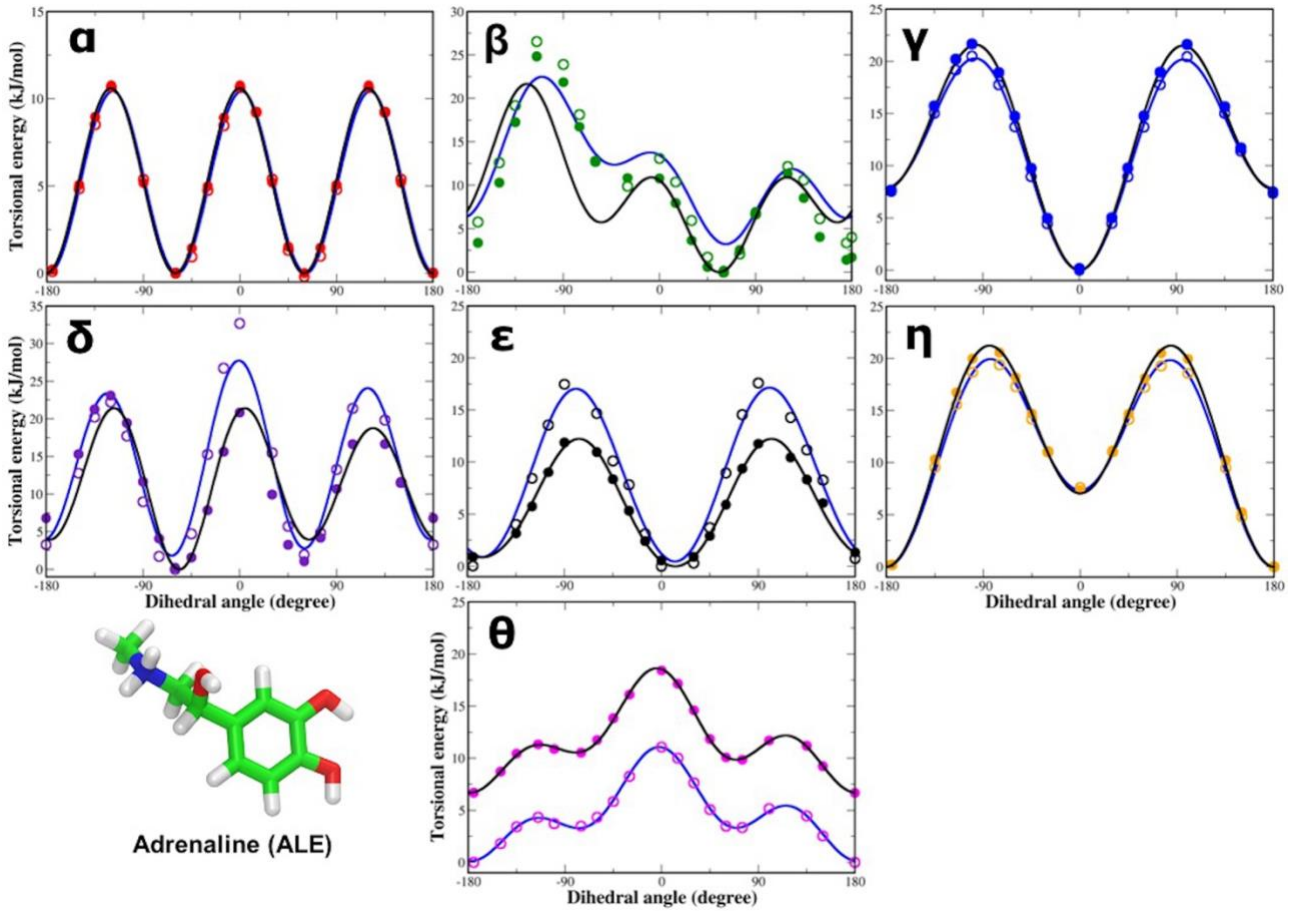


Figure S13 Comparison of protonated adrenaline dihedral angles torsional energy profiles from QM (closed circles), JOYCE (black lines), QM after the subtraction of electrostatic and Lennard-Jones energy contributions (open circles) and fittings (blue lines) calculations. Energies are reported in kilojoules per mole (1 kJ/mol = 0.24 kcal/mol).

Figure S14

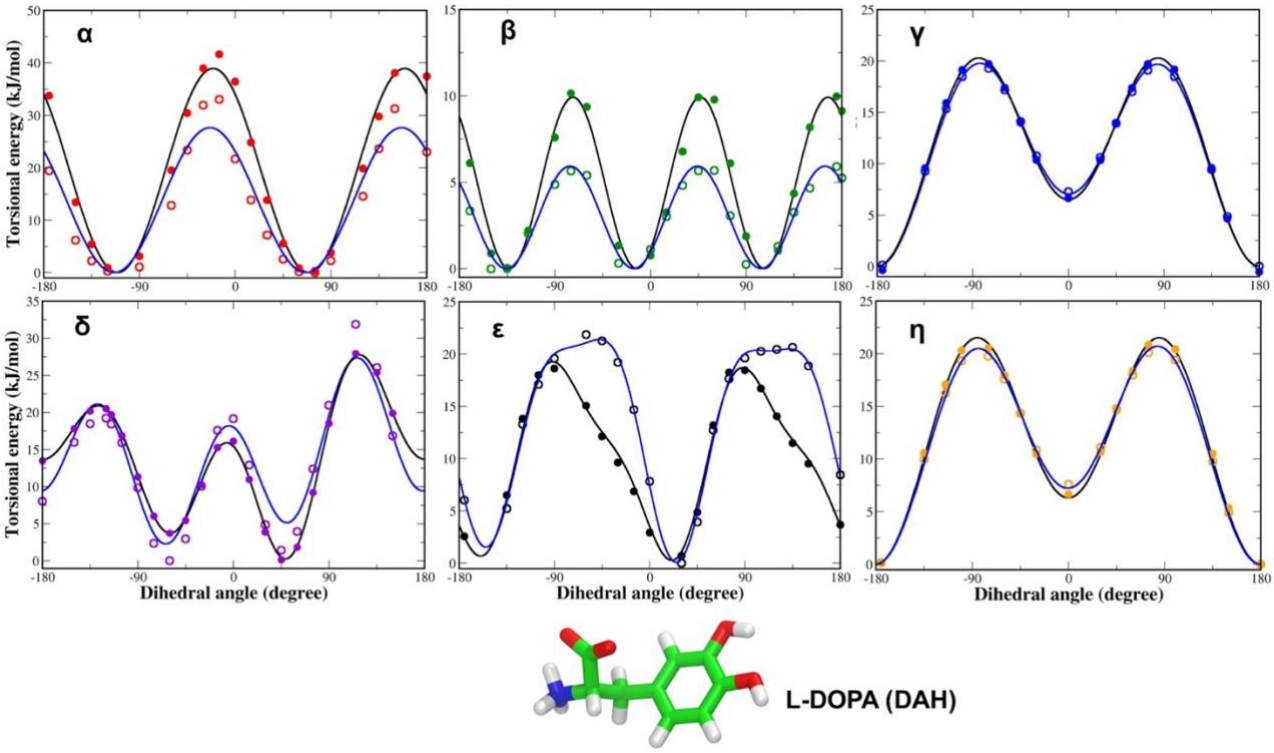


Figure S14 Comparison of zwitterionic L-DOPA dihedral angles torsional energy profiles from QM (closed circles), JOYCE (black lines), QM after the subtraction of electrostatic and Lennard-Jones energy contributions (open circles) and fittings (blue lines) calculations. Energies are reported in kilojoules per mole (1 kJ/mol = 0.24 kcal/mol).

Figure S15

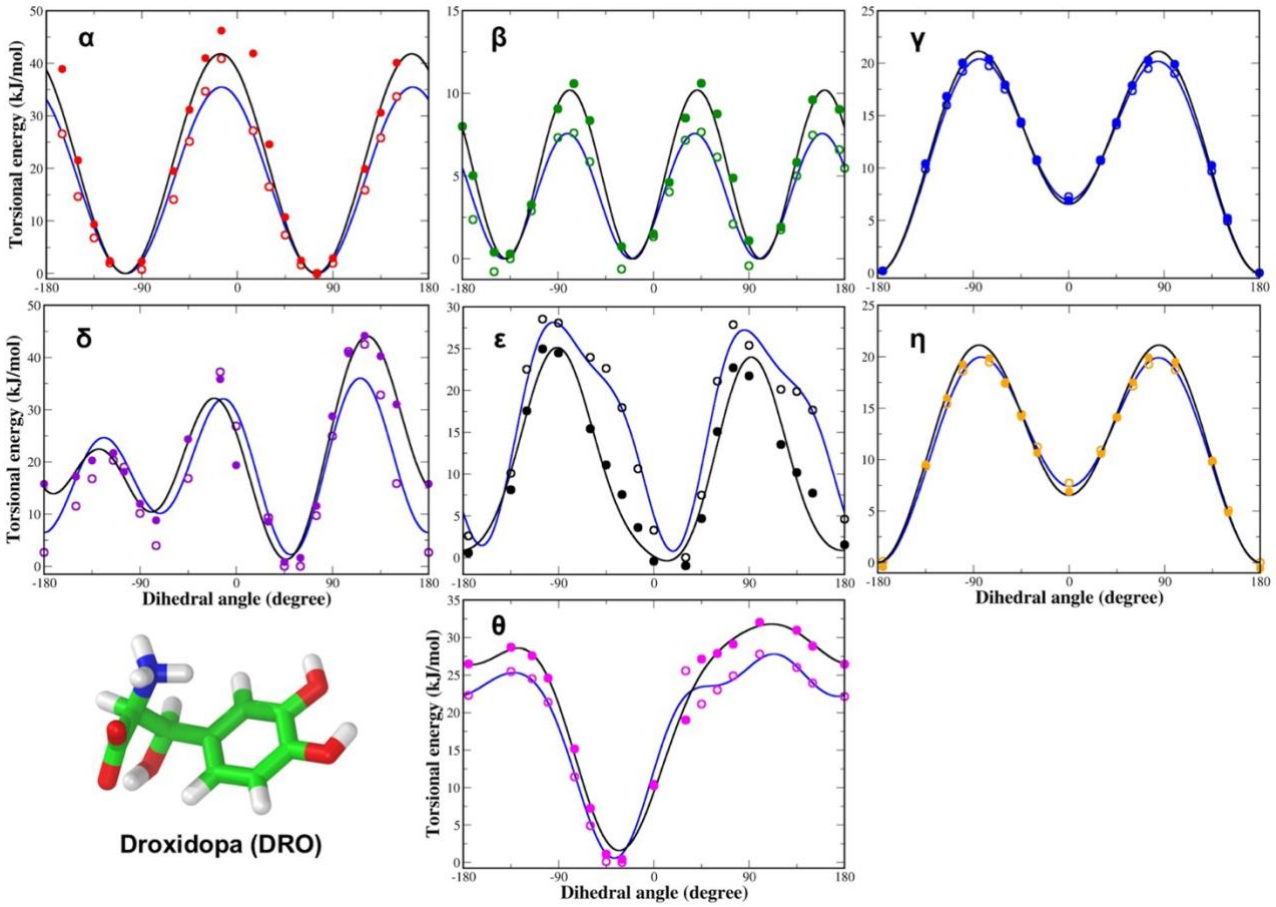


Figure S15 Comparison of zwitterionic Droxidopa dihedral angles torsional energy profiles from QM (closed circles), JOYCE (black lines), QM after the subtraction of electrostatic and Lennard-Jones energy contributions (open circles) and fittings (blue lines) calculations. Energies are reported in kilojoules per mole (1 kJ/mol = 0.24 kcal/mol).

Figure S16

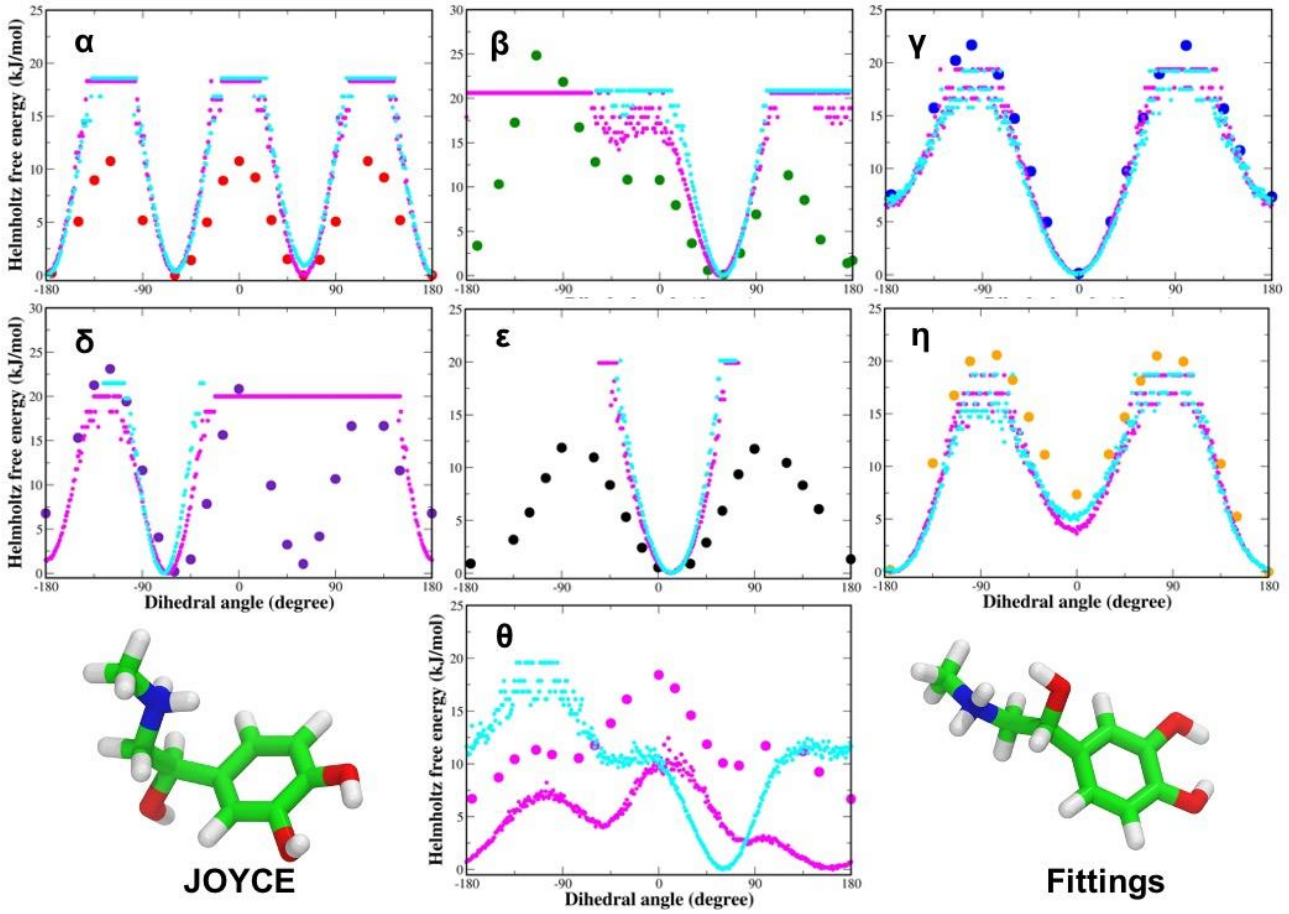
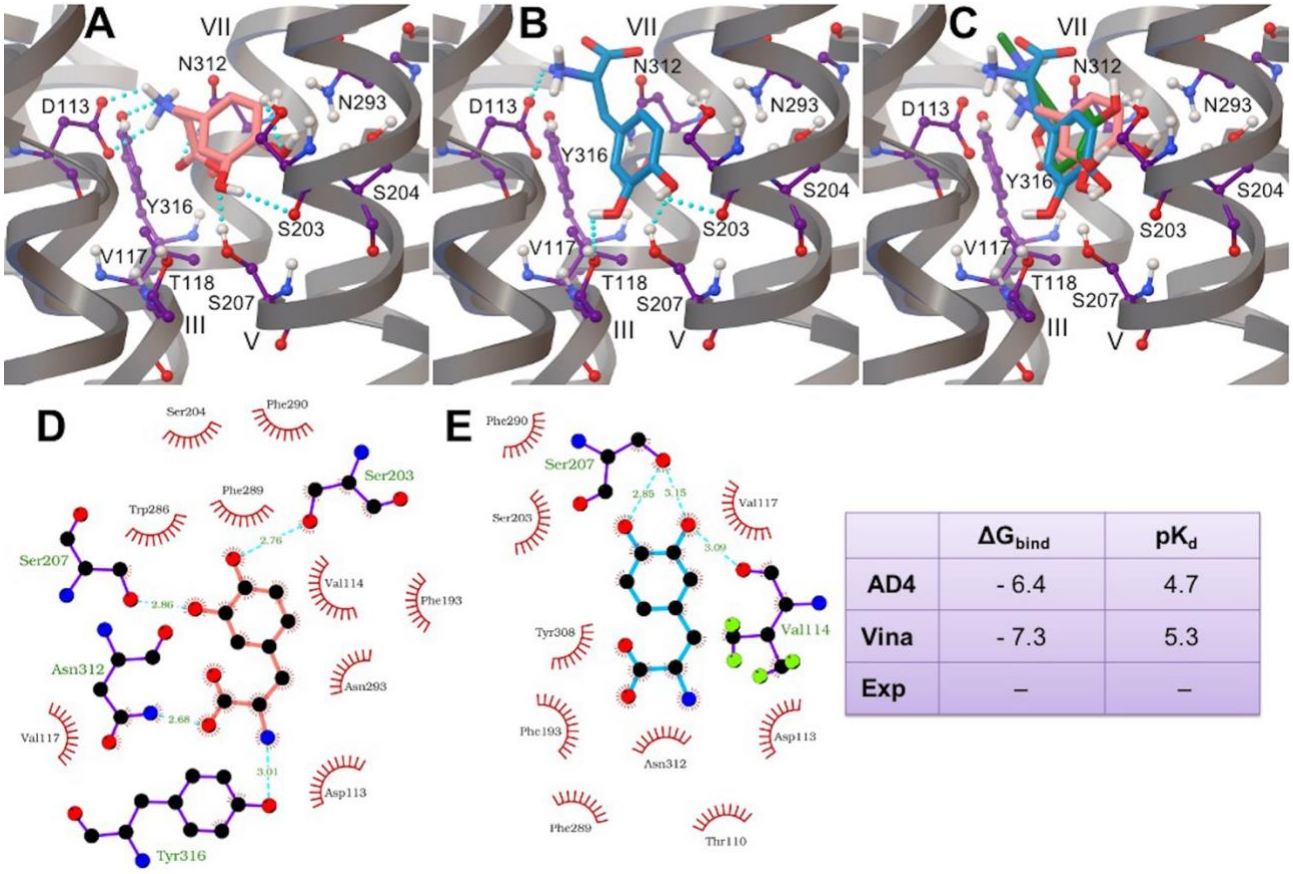


Figure S16 (Top) Protonated adrenaline QM torsional energy profiles (circles) compared with Helmholtz free energy variations as a function of the dihedral angle, as obtained from MD simulations performed using JOYCE (magenta dots) and OPLS (cyan dots) FFs. (Bottom) 100 ns structures of adrenaline from MD simulations using JOYCE and OPLS (Fittings) FF parameters, respectively. Energies are reported in kilojoules per mole (1 kJ/mol = 0.24 kcal/mol).

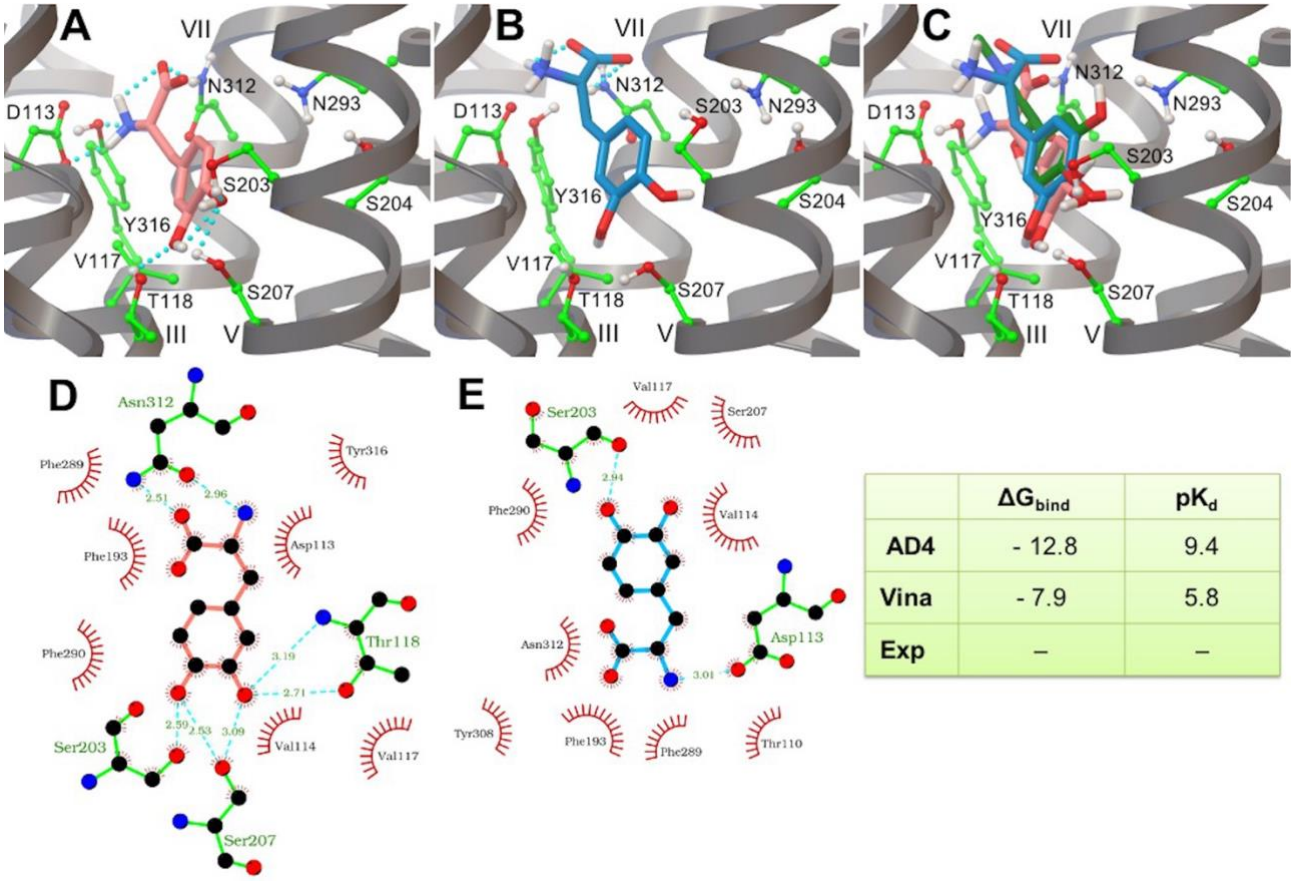
Figure S17



	ΔG_{bind}	pK_d
AD4	- 6.4	4.7
Vina	- 7.3	5.3
Exp	–	–

Figure S17 Lowest energy conformations of L-DOPA obtained from the docking of the ligand into rigid β_2AR models performed with molecular docking software packages AutoDock4.2 and AutoDock Vina are shown in magenta (A, AD4) and skyblue (B, Vina), respectively. (C) Lowest energy poses of L-DOPA are compared to adrenaline's conformation in the X-ray crystal structure (PDB ID: 4LDO, ligand in dark green). Color code and view point as in Figure 9. Hydrogen bond network of L-DOPA lowest energy conformations generated by (D) AD4 and (E) Vina calculations. Free energies of binding (in kcal/mol) and binding affinities estimated by AD4 and Vina calculations are compared to experimental results.

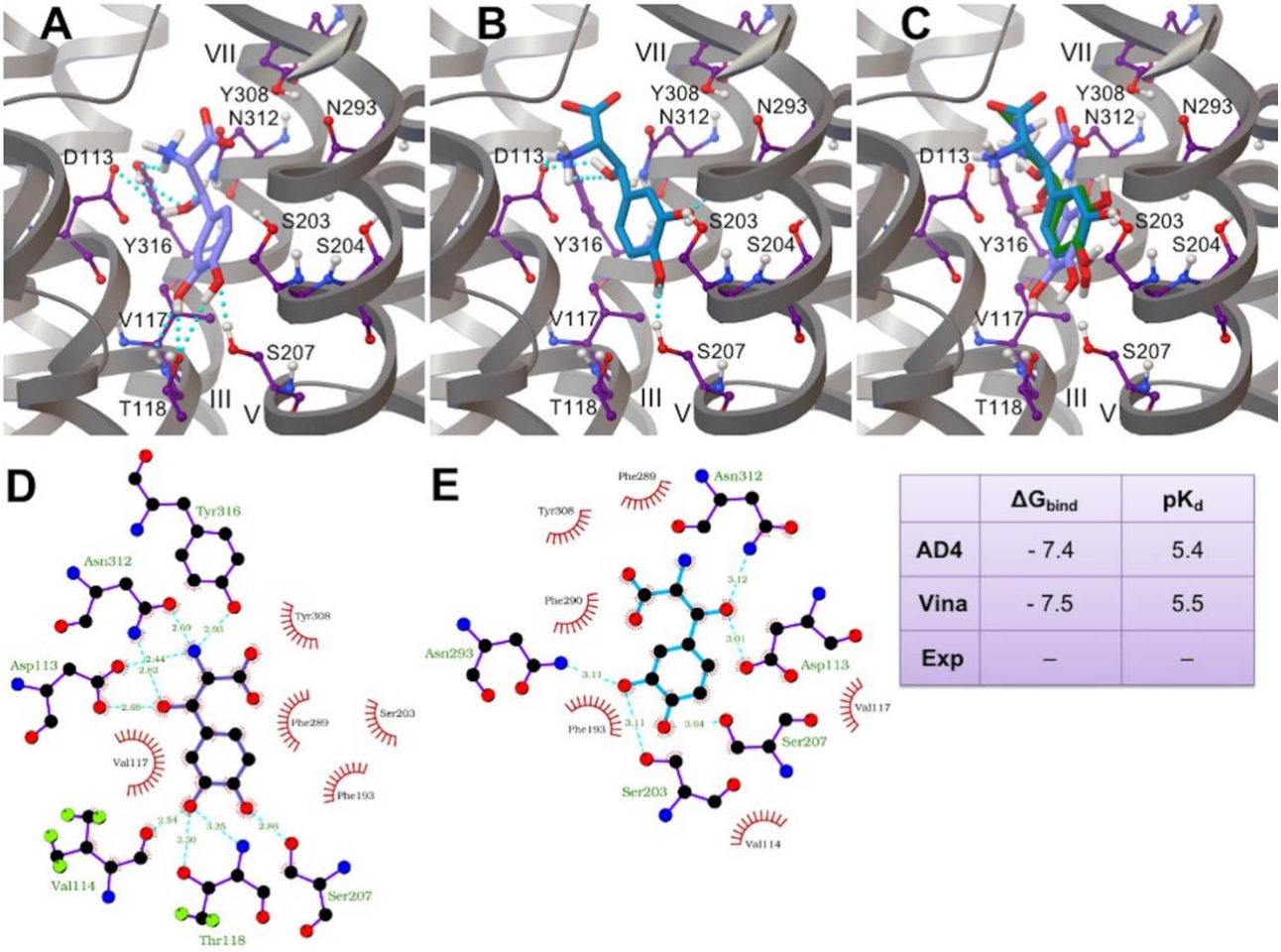
Figure S18



	ΔG_{bind}	pK_d
AD4	- 12.8	9.4
Vina	- 7.9	5.8
Exp	–	–

Figure S18 Lowest energy conformations of L-DOPA obtained from the docking of the ligand into flexible β_2AR models performed with molecular docking software packages AutoDock4.2 and AutoDock Vina are shown in magenta (A, AD4) and skyblue (B, Vina), respectively. (C) Lowest energy poses of L-DOPA are compared to adrenaline's conformation in the X-ray crystal structure (PDB ID: 4LDO, ligand in dark green). Color code and view point as in Figure 9. Hydrogen bond network of L-DOPA lowest energy conformations generated by (D) AD4 and (E) Vina calculations. Free energies of binding (in kcal/mol) and binding affinities estimated by AD4 and Vina calculations are compared to experimental results.

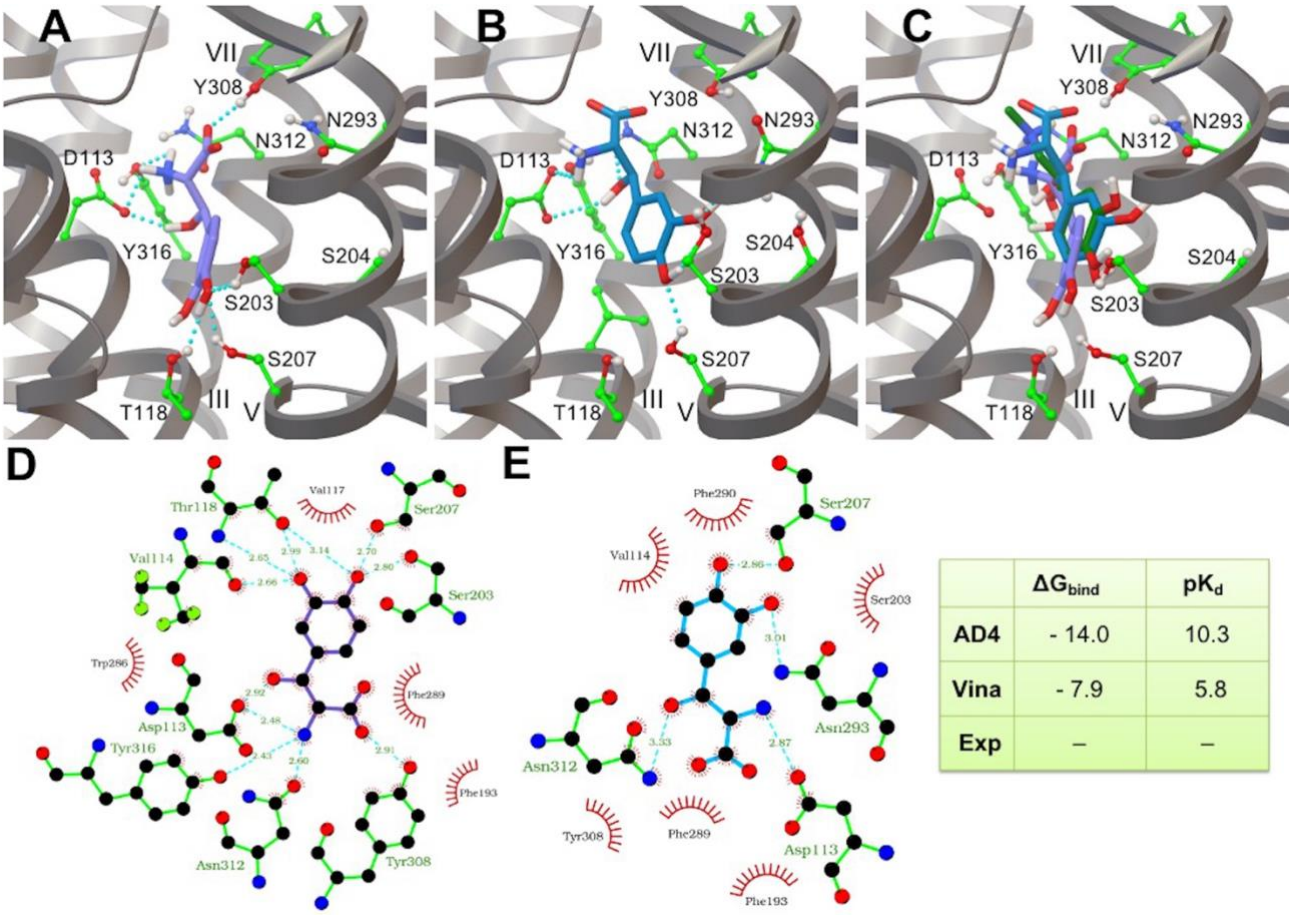
Figure S19



	ΔG_{bind}	pK_d
AD4	- 7.4	5.4
Vina	- 7.5	5.5
Exp	–	–

Figure S19 Lowest energy conformations of Droxidopa obtained from the docking of the ligand into rigid β_2AR models performed with molecular docking software packages AutoDock4.2 and AutoDock Vina are shown in violet (A, AD4) and skyblue (B, Vina), respectively. (C) Lowest energy poses of Droxidopa are compared to adrenaline's conformation in the X-ray crystal structure (PDB ID: 4LDO, ligand in dark green). Color code and view point as in Figure 9. Hydrogen bond network of Droxidopa lowest energy conformations generated by (D) AD4 and (E) Vina calculations. Free energies of binding (in kcal/mol) and binding affinities estimated by AD4 and Vina calculations are compared to experimental results.

Figure S20



	ΔG_{bind}	pK_d
AD4	- 14.0	10.3
Vina	- 7.9	5.8
Exp	–	–

Figure S20 Lowest energy conformations of Droxidopa obtained from the docking of the ligand into flexible β_2AR models performed with molecular docking software packages AutoDock4.2 and AutoDock Vina are shown in violet (A, AD4) and skyblue (B, Vina), respectively. (C) Lowest energy poses of Droxidopa are compared to adrenaline's conformation in the X-ray crystal structure (PDB ID: 4LDO, ligand in dark green). Color code and view point as in Figure 9. Hydrogen bond network of Droxidopa lowest energy conformations generated by (D) AD4 and (E) Vina calculations. Free energies of binding (in kcal/mol) and binding affinities estimated by AD4 and Vina calculations are compared to experimental results.

Table S5

Percentage of hydrogen bond formation for different β_2AR-Ligand complexes from 1 μs all atom MD simulations performed with CHARMM and OPLS AA FF parameters. The analysis was performed over the whole trajectory for adrenaline (ALE), L-DOPA (DAH) and Droxidopa (DRO) ligands.

Hydrogen bonds (β_2AR-Ligand)	**Percentage of H-bond formation (%)**					
	CHARMM			**OPLS**		
	ALE	**DAH**	**DRO**	**ALE**	**DAH**	**DRO**
OG (S203) - O (para)	23.6	28.4	11.9	12.6	3.5	7.4
OG (S203) - O (meta)	**54.3**	15.3	12.4	**4.4**	0.3	20.7
OG (S204) - O (para)	0.1	11.4	2.4	0.6	0.3	0.8
OG (S204) - O (meta)	1.3	31.9	20.9	0	0	39.9
OG (S207) - O (para)	**47.9**	32.0	44.3	**19.3**	21.4	7.6
OG (S207) - O (meta)	0	11.2	7.6	9.1	7.2	0.9
ND2 (N293) - O (para)	0	0	0.4	3.0	0.1	0
ND2 (N293) - O (meta)	**4.1**	4.9	16.7	**0**	0	13.5
OG1 (T118) - O (para)	1.1	0.8	18.9	1.1	1.1	28.6
OG1 (T118) - O (meta)	0	3.4	4.4	25.4	4.9	0
OD1 (D113) - N (amino)	72.6	47.3	38.6	75.7	50.9	55.0
OD2 (D113) - N (amino)	**97.7**	88.0	36.1	**76.3**	52.6	55.3
OD1 (D113) - O (β-OH)	**46.6**	-[a]	16.9	**59.6**	-	0
OD2 (D113) - O (β-OH)	**37.0**	-	18.0	**60.9**	-	0
OH (Y308) - O1 (-COO^-)	- -[c]	29.0	1.1	- -	0.2	1.5
OH (Y308) - O2 (-COO^-)	- -	76.6	8.1	- -	0.7	0.2
ND2 (N312) - O (β-OH)	**47.9**	-	21.2	**71.7**	-	18.5
OD1 (N312) - N (amino)	**66.4**	82.8	26.6	**87.3**	0.9	23.9
ND2 (N312) - O1 (-COO^-)	- -	0	0.2	- -	3.8	0
ND2 (N312) - O2 (-COO^-)	- -	12.9	3.7	- -	2.4	0
OH (Y316) - O (β-OH)	0.2	-	1.0	45.5	-	0
OH (Y316) - N (amino)	0	3.3	0	5.0	1.8	12.0

[a] Hydrogen bonds formed by adrenaline's conformation in the β_2AR X-ray crystal structure (PDB ID: 4LDO) are highlighted in bold.
[b] β-OH group is absent in the L-DOPA ligand.
[c] -COO^- group is absent in the endogenous ligand.

Figure S21

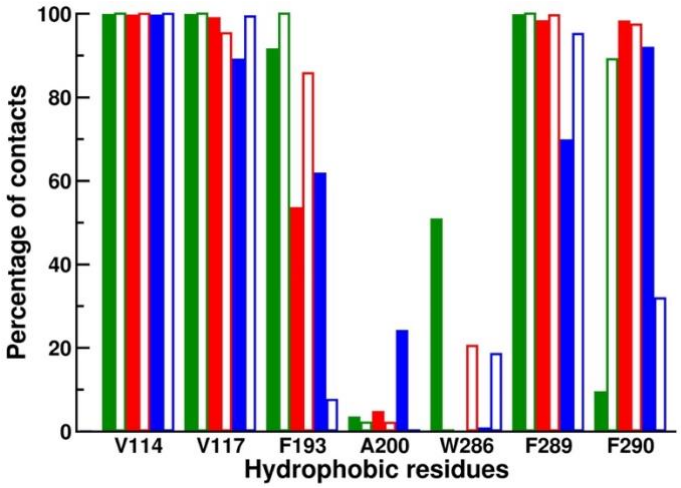


Figure S21 Percentage of contacts of ligands with the receptor hydrophobic residues extracted from MD simulations of β_2AR-catecholamine complexes performed with CHARMM (closed bars) and OPLS (open bars) AA FFs. Adrenaline, L-DOPA and Droxidopa percentages of contacts with β_2AR hydrophobic residues are shown with green, red and blue bars, respectively. This analysis was performed over the whole 1 μs trajectory.

Figure S22

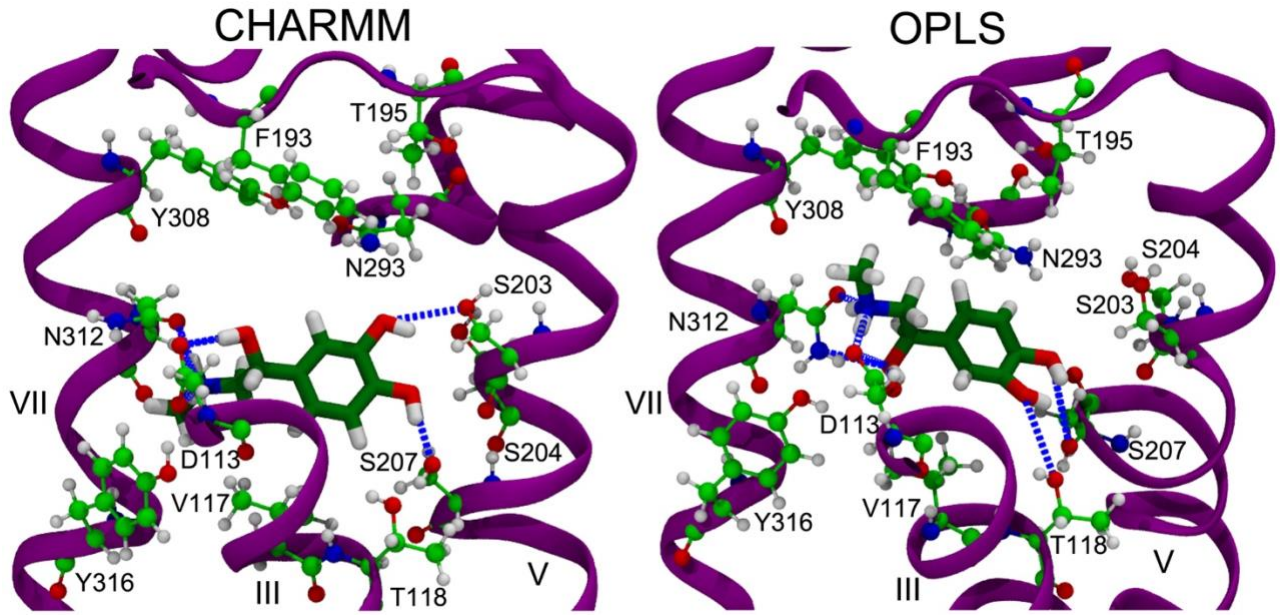


Figure S22 Snapshots of MD simulations of β_2AR-adrenaline complexes show the hydrogen bond network of the endogenous ligand with key amino acids of the receptor binding pocket using CHARMM and OPLS AA FFs. Hydrogen bonds are highlighted with dashed blue lines. View point and color code as in Figure 5 of Biswas et al. 2021.

Figure S23

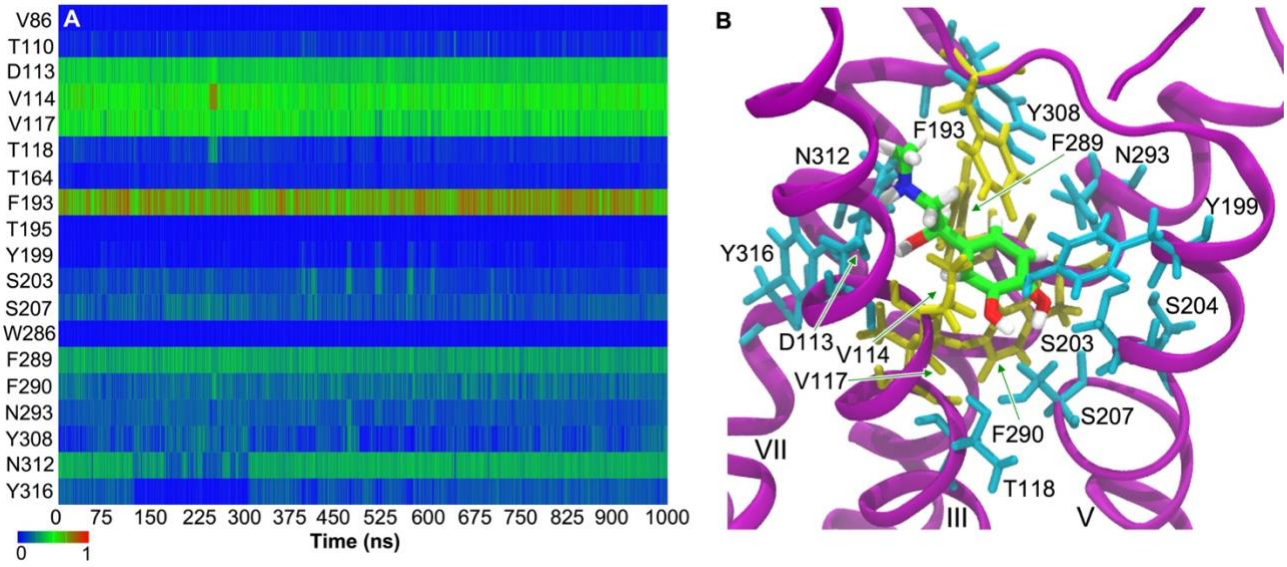


Figure S23 (A) Normalized number of contacts of adrenaline with the receptor residues extracted from the 1 μs all atom MD simulation of the β_2AR-adrenaline complex performed with the OPLS AA FF. (B) A snapshot from the MD simulation shows β_2AR hydrophilic (cyan) and hydrophobic (yellow) residues interacting with the adrenaline ligand. For clarity, only β_2AR residues displaying the largest percentages of contacts with the ligand are shown. Sidechains of some residues are indicated by green arrows. This analysis was performed over the whole 1 μs trajectory.

Figure S24

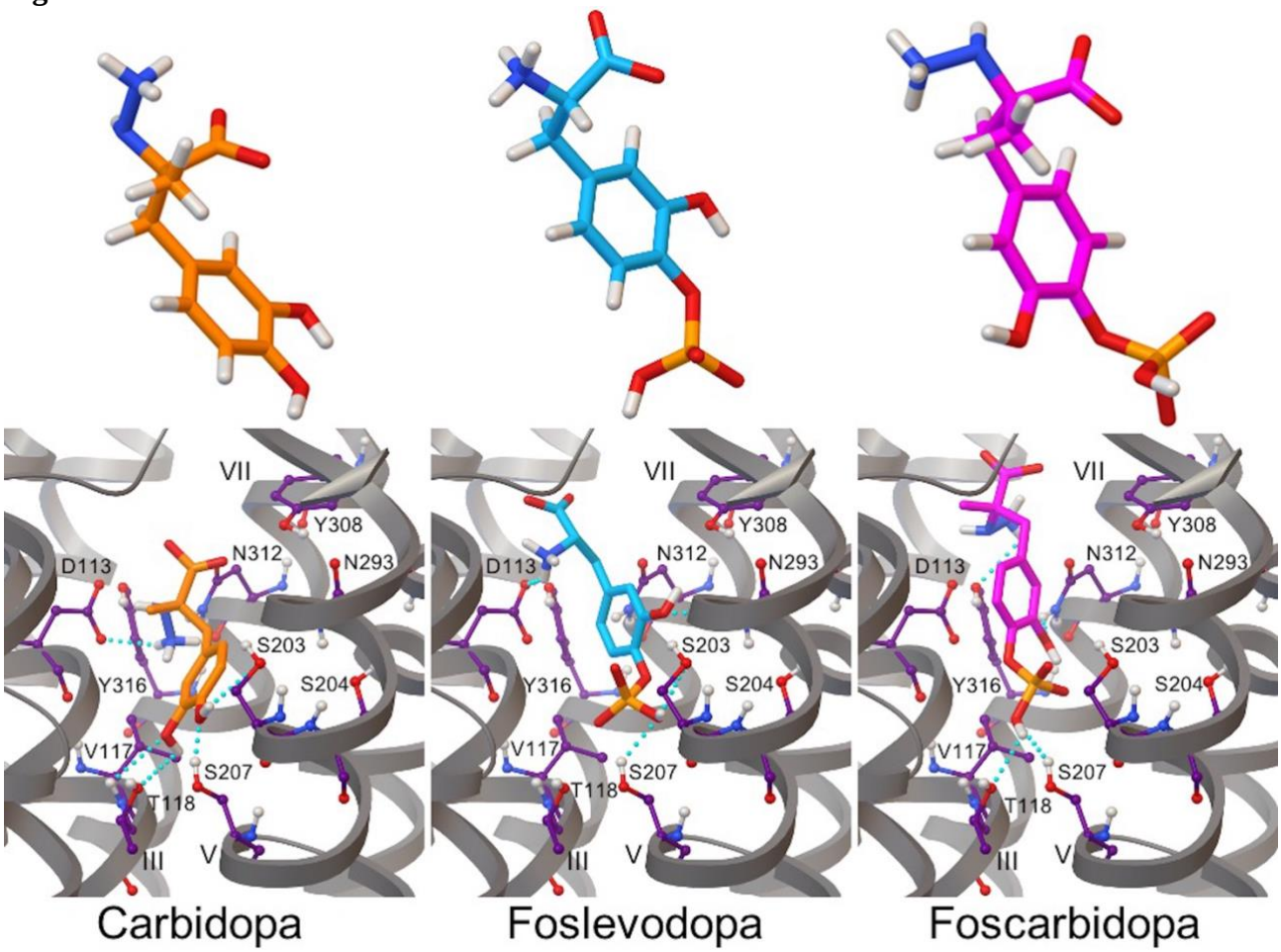


Figure S24 (top) Chemical structures of protonated Carbidopa (orange), Foslevodopa (celestial blue) and Foscarbidopa (magenta). (bottom) Lowest energy conformations and hydrogen bond network obtained from the docking of each ligand into a rigid β_2AR model performed with the molecular docking software package AutoDock Vina v. 1.2.3. Color code and view point as in Figure 9.

adrenaline.itp

```
;       OPLS AA force field parameters of Adrenaline generated with JOYCE

[ moleculetype ]
; Name            nrexcl
ALE     3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
; residue   1 ALE rtp ALE  q +1.0
     1   oplsm_309      1    ALE      N      1   -0.446343    14.0027
     2   oplsm_310      1    ALE     H1      1    0.382023     1.008
     3   oplsm_310      1    ALE     H2      1    0.363936     1.008
     4   oplsm_149      1    ALE     C1      1   -0.076781    12.011
     5   oplsm_140    1    ALE     H3      1    0.137222     1.008
     6   oplsm_140    1    ALE     H4      1    0.135202     1.008
     7   oplsm_140    1    ALE     H5      1    0.135338     1.008
     8   oplsm_293      1    ALE     CA      1   -0.024055    12.011
     9   oplsm_140      1    ALE    HA1      1    0.138286     1.008
    10   oplsm_140      1    ALE    HA2      1    0.133064     1.008
    11   oplsm_149      1    ALE     CB      2    0.027731    12.011
    12   oplsm_140      1    ALE    HB1      2    0.117273     1.008
    13   oplsm_154      1    ALE     OG      3   -0.422795    15.9994
    14   oplsm_155      1    ALE     HG      3    0.347155     1.008
    15   oplsm_145      1    ALE     CG      3   -0.029545    12.011
    16   oplsm_145      1    ALE    CD1      4   -0.104846    12.011
    17   oplsm_146      1    ALE    HD1      4    0.107227     1.008
    18   oplsm_145      1    ALE    CD2      5   -0.101815    12.011
    19   oplsm_146      1    ALE    HD2      5    0.103567     1.008
    20   oplsm_166      1    ALE    CE1      6    0.073348    12.011
    21   oplsm_167      1    ALE    OE1      6   -0.394652    15.9994
    22   oplsm_168      1    ALE    HE1      6    0.340755     1.008
    23   oplsm_145      1    ALE    CE2      7   -0.107124    12.011
    24   oplsm_146      1    ALE    HE2      7    0.112182     1.008
    25   oplsm_166      1    ALE     CZ      8    0.071847    12.011
    26   oplsm_167      1    ALE     OH      8   -0.381798    15.9994
    27   oplsm_168      1    ALE     HH      8    0.363632     1.008   ; qtot 1.000033

; Stretchings
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     1    3   1    0.1028    393683.477
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     4    5   1    0.1094    328457.447
     4    6   1    0.1094    328457.447
     4    7   1    0.1093    328457.447
     1    8   1    0.1501    179667.704
     8    9   1    0.1094    323493.654
     8   10   1    0.1095    323493.654
     8   11   1    0.1524    182391.941
    11   12   1    0.1102    301357.367
    11   13   1    0.1436    199950.220
    13   14   1    0.0966    486572.973
    11   15   1    0.1512    205697.663
    15   16   1    0.1403    339484.191
    16   17   1    0.1090    332540.269
    15   18   1    0.1397    339484.191
    18   19   1    0.1091    332540.269
    16   20   1    0.1391    339484.191
```

```
    20    21   1    0.1368    307423.405
    21    22   1    0.0969    480865.258
    18    23   1    0.1400    339484.191
    23    24   1    0.1091    332540.269
    20    25   1    0.1408    311404.166
    23    25   1    0.1393    311404.166
    25    26   1    0.1372    306132.262
    26    27   1    0.0966    480865.258

; Bendings
[ angles ]
     2    1    3   1    105.80     366.8740
     2    1    4   1    109.51     373.8285
     2    1    8   1    109.42     381.2262
     3    1    4   1    110.55     373.8285
     3    1    8   1    106.93     381.2262
     1    4    5   1    108.48     468.3697
     1    4    6   1    108.40     468.3697
     1    4    7   1    108.25     468.3697
     4    1    8   1    114.27     472.0079
     5    4    6   1    110.52     309.0556
     5    4    7   1    110.50     309.0556
     6    4    7   1    110.60     309.0556
     1    8    9   1    108.31     451.2013
     1    8   10   1    106.94     451.2013
     1    8   11   1    109.59     643.5652
     9    8   10   1    109.67     292.8912
     9    8   11   1    111.50     292.9588
    10    8   11   1    110.69     292.9588
     8   11   12   1    109.16     383.0963
     8   11   13   1    104.55     660.4204
     8   11   15   1    110.97     474.4008
    12   11   13   1    109.73     388.2702
    12   11   15   1    108.71     325.9046
    11   13   14   1    108.97     469.7023
    13   11   15   1    113.61     557.7615
    11   15   16   1    120.12     588.9987
    11   15   18   1    120.26     588.9987
    15   16   17   1    120.97     293.3534
    16   15   18   1    119.62     495.6412
    15   16   20   1    120.20     495.6412
    17   16   20   1    118.83     293.3534
    15   18   19   1    120.08     293.3534
    15   18   23   1    120.43     495.6412
    19   18   23   1    119.49     293.3534
    16   20   21   1    119.58     534.1722
    16   20   25   1    119.91     361.9651
    20   21   22   1    108.56     522.9635
    21   20   25   1    120.51     771.4094
    18   23   24   1    120.43     293.3534
    18   23   25   1    119.76     361.9651
    24   23   25   1    119.80     320.3130
    20   25   23   1    120.09     115.1701
    20   25   26   1    115.22     699.2490
    23   25   26   1    124.69     699.2490
    25   26   27   1    110.64     448.1807

; Torsions - Proper dihedral angles
[ dihedrals ]
;  ai    aj    ak    al funct           c0           c1           c2           c3           c4           c5
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  3   1   4   6   1     1.11      5.300   3
  3   1   4   7   1     1.11      5.300   3
  2   1   8   9   1   270.19      5.179   1
  2   1   8   9   1  -171.66      2.193   2
  2   1   8   9   1     1.25      3.196   3
  2   1   8  10   1   270.19      5.179   1
  2   1   8  10   1  -171.66      2.193   2
  2   1   8  10   1     1.25      3.196   3
 20  25  26  27   1  -179.55      3.882   1
 20  25  26  27   1   179.73      8.726   2
  9   8  11  12   1  -162.12      2.055   1
  9   8  11  12   1    63.42      1.109   2
  9   8  11  12   1    -0.25      8.553   3
  9   8  11  12   1    -6.16      0.163   4
 12  11  15  18   1   180.84      0.004   1
 12  11  15  18   1  -152.83      5.737   2
 12  11  15  18   1   161.46      0.004   3
 12  11  15  18   1    17.84      0.217   4
 12  11  15  16   1   180.84      0.004   1
 12  11  15  16   1  -152.83      5.737   2
 12  11  15  16   1   161.46      0.004   3
 12  11  15  16   1    17.84      0.217   4
 16  20  21  22   1    -0.56      3.524   1
 16  20  21  22   1   180.05      8.762   2
  8  11  13  14   1    22.00      9.094   1
  8  11  13  14   1    70.38      1.057   2
  8  11  13  14   1    73.83      1.153   2
  8  11  13  14   1    -4.18      0.700   3

; Nonbonded terms
[ pairs ]
; 1-4 interactions
  1  12   2   0.500   -0.446   0.117   0.2875   0.14940   # N   - HA
  1  13   2   0.500   -0.446  -0.423   0.3160   0.35564   # N   - OH
  1  15   2   0.500   -0.446  -0.030   0.3400   0.22821   # N   - CC
  2   5   2   0.500    0.382   0.137   0.1250   0.00000   # H   - HA
  2   6   2   0.500    0.382   0.135   0.1250   0.00000   # H   - HA
  2   7   2   0.500    0.382   0.135   0.1250   0.00000   # H   - HA
  2   9   2   0.500    0.382   0.138   0.1250   0.00000   # H   - HA
  2  10   2   0.500    0.382   0.133   0.1250   0.00000   # H   - HA
  2  11   2   0.500    0.382   0.028   0.1750   0.00000   # H   - CB
  3   5   2   0.500    0.364   0.137   0.1250   0.00000   # H   - HA
  3   6   2   0.500    0.364   0.135   0.1250   0.00000   # H   - HA
  3   7   2   0.500    0.364   0.135   0.1250   0.00000   # H   - HA
  3   9   2   0.500    0.364   0.138   0.1250   0.00000   # H   - HA
  3  10   2   0.500    0.364   0.133   0.1250   0.00000   # H   - HA
  3  11   2   0.500    0.364   0.028   0.1750   0.00000   # H   - CB
  4   9   2   0.500   -0.077   0.138   0.3125   0.11741   # C   - HA
  4  10   2   0.500   -0.077   0.133   0.3125   0.11741   # C   - HA
  4  11   2   0.500   -0.077   0.028   0.3625   0.17415   # C   - CB
  5   8   2   0.500    0.137  -0.024   0.3000   0.09309   # HA  - CA
  6   8   2   0.500    0.135  -0.024   0.3000   0.09309   # HA  - CA
  7   8   2   0.500    0.135  -0.024   0.3000   0.09309   # HA  - CA
  8  14   2   0.500   -0.024   0.347   0.1750   0.00000   # CA  - HO
  8  16   2   0.500   -0.024  -0.105   0.3525   0.14219   # CA  - CC
  8  18   2   0.500   -0.024  -0.102   0.3525   0.14219   # CA  - CC
  9  12   2   0.500    0.138   0.117   0.2500   0.06276   # HA  - HA
  9  13   2   0.500    0.138  -0.423   0.2785   0.14940   # HA  - OH
  9  15   2   0.500    0.138  -0.030   0.3025   0.09587   # HA  - CC
 10  12   2   0.500    0.133   0.117   0.2500   0.06276   # HA  - HA
```

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10 13  2   0.500   0.133  -0.423   0.2785   0.14940   # HA  - OH
10 15  2   0.500   0.133  -0.030   0.3025   0.09587   # HA  - CC
11 17  2   0.500   0.028   0.107   0.2960   0.09309   # CB  - HC
11 19  2   0.500   0.028   0.104   0.2960   0.09309   # CB  - HC
11 20  2   0.500   0.028   0.073   0.3525   0.14219   # CB  - CC
11 23  2   0.500   0.028  -0.107   0.3525   0.14219   # CB  - CC
12 14  2   0.500   0.117   0.347   0.1250   0.00000   # HA  - HO
12 16  2   0.500   0.117  -0.105   0.3025   0.09587   # HA  - CC
12 18  2   0.500   0.117  -0.102   0.3025   0.09587   # HA  - CC
13 16  2   0.500  -0.423  -0.105   0.3310   0.22821   # OH  - CC
13 18  2   0.500  -0.423  -0.102   0.3310   0.22821   # OH  - CC
14 15  2   0.500   0.347  -0.030   0.1775   0.00000   # HO  - CC
15 21  2   0.500  -0.030  -0.395   0.3310   0.22821   # CC  - OH
15 24  2   0.500  -0.030   0.112   0.2985   0.09587   # CC  - HC
15 25  2   0.500  -0.030   0.072   0.3550   0.14644   # CC  - CZ
16 19  2   0.500  -0.105   0.104   0.2985   0.09587   # CC  - HC
16 22  2   0.500  -0.105   0.341   0.1775   0.00000   # CC  - HH
16 23  2   0.500  -0.105  -0.107   0.3550   0.14644   # CC  - CC
16 26  2   0.500  -0.105  -0.382   0.3310   0.22821   # CC  - OH
17 18  2   0.500   0.107  -0.102   0.2985   0.09587   # HC  - CC
17 21  2   0.500   0.107  -0.395   0.2745   0.14940   # HC  - OH
17 25  2   0.500   0.107   0.072   0.2985   0.09587   # HC  - CZ
18 20  2   0.500  -0.102   0.073   0.3550   0.14644   # CC  - CC
18 26  2   0.500  -0.102  -0.382   0.3310   0.22821   # CC  - OH
19 24  2   0.500   0.104   0.112   0.2420   0.06276   # HC  - HC
19 25  2   0.500   0.104   0.072   0.2985   0.09587   # HC  - CZ
20 24  2   0.500   0.073   0.112   0.2985   0.09587   # CC  - HC
20 27  2   0.500   0.073   0.364   0.1775   0.00000   # CC  - HH
21 23  2   0.500  -0.395  -0.107   0.3310   0.22821   # OH  - CC
21 26  2   0.500  -0.395  -0.382   0.3070   0.35564   # OH  - OH
22 25  2   0.500   0.341   0.072   0.1775   0.00000   # HH  - CZ
23 27  2   0.500  -0.107   0.364   0.1775   0.00000   # CC  - HH
24 26  2   0.500   0.112  -0.382   0.2745   0.14940   # HC  - OH
 1 14  2   0.500  -0.446   0.347   0.1625   0.00000   # N   - HO
 1 16  2   0.500  -0.446  -0.105   0.3400   0.45642   # N   - CC
 1 17  2   0.500  -0.446   0.107   0.2835   0.29880   # N   - HC
 1 18  2   0.500  -0.446  -0.102   0.3400   0.45642   # N   - CC
 1 19  2   0.500  -0.446   0.104   0.2835   0.29880   # N   - HC
 1 20  2   0.500  -0.446   0.073   0.3400   0.45642   # N   - CC
 1 21  2   0.500  -0.446  -0.395   0.3160   0.71128   # N   - OH
 1 22  2   0.500  -0.446   0.341   0.1625   0.00000   # N   - HH
 1 23  2   0.500  -0.446  -0.107   0.3400   0.45642   # N   - CC
 1 24  2   0.500  -0.446   0.112   0.2835   0.29880   # N   - HC
 1 25  2   0.500  -0.446   0.072   0.3400   0.45642   # N   - CZ
 1 26  2   0.500  -0.446  -0.382   0.3160   0.71128   # N   - OH
 1 27  2   0.500  -0.446   0.364   0.1625   0.00000   # N   - HH
 2 12  2   0.500   0.382   0.117   0.1250   0.00000   # H   - HA
 2 13  2   0.500   0.382  -0.423   0.1535   0.00000   # H   - OH
 2 14  2   0.500   0.382   0.347   0.0000   0.00000   # H   - HO
 2 15  2   0.500   0.382  -0.030   0.1775   0.00000   # H   - CC
 2 16  2   0.500   0.382  -0.105   0.1775   0.00000   # H   - CC
 2 17  2   0.500   0.382   0.107   0.1210   0.00000   # H   - HC
 2 18  2   0.500   0.382  -0.102   0.1775   0.00000   # H   - CC
 2 19  2   0.500   0.382   0.104   0.1210   0.00000   # H   - HC
 2 20  2   0.500   0.382   0.073   0.1775   0.00000   # H   - CC
 2 21  2   0.500   0.382  -0.395   0.1535   0.00000   # H   - OH
 2 22  2   0.500   0.382   0.341   0.0000   0.00000   # H   - HH
 2 23  2   0.500   0.382  -0.107   0.1775   0.00000   # H   - CC
 2 24  2   0.500   0.382   0.112   0.1210   0.00000   # H   - HC
 2 25  2   0.500   0.382   0.072   0.1775   0.00000   # H   - CZ
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2  26   2    0.500    0.382   -0.382    0.1535    0.00000    # H    - OH
2  27   2    0.500    0.382    0.364    0.0000    0.00000    # H    - HH
3  12   2    0.500    0.364    0.117    0.1250    0.00000    # H    - HA
3  13   2    0.500    0.364   -0.423    0.1535    0.00000    # H    - OH
3  14   2    0.500    0.364    0.347    0.0000    0.00000    # H    - HO
3  15   2    0.500    0.364   -0.030    0.1775    0.00000    # H    - CC
3  16   2    0.500    0.364   -0.105    0.1775    0.00000    # H    - CC
3  17   2    0.500    0.364    0.107    0.1210    0.00000    # H    - HC
3  18   2    0.500    0.364   -0.102    0.1775    0.00000    # H    - CC
3  19   2    0.500    0.364    0.104    0.1210    0.00000    # H    - HC
3  20   2    0.500    0.364    0.073    0.1775    0.00000    # H    - CC
3  21   2    0.500    0.364   -0.395    0.1535    0.00000    # H    - OH
3  22   2    0.500    0.364    0.341    0.0000    0.00000    # H    - HH
3  23   2    0.500    0.364   -0.107    0.1775    0.00000    # H    - CC
3  24   2    0.500    0.364    0.112    0.1210    0.00000    # H    - HC
3  25   2    0.500    0.364    0.072    0.1775    0.00000    # H    - CZ
3  26   2    0.500    0.364   -0.382    0.1535    0.00000    # H    - OH
3  27   2    0.500    0.364    0.364    0.0000    0.00000    # H    - HH
4  12   2    0.500   -0.077    0.117    0.3125    0.23483    # C    - HA
4  13   2    0.500   -0.077   -0.423    0.3410    0.55900    # C    - OH
4  14   2    0.500   -0.077    0.347    0.1875    0.00000    # C    - HO
4  15   2    0.500   -0.077   -0.030    0.3650    0.35870    # C    - CC
4  16   2    0.500   -0.077   -0.105    0.3650    0.35870    # C    - CC
4  17   2    0.500   -0.077    0.107    0.3085    0.23483    # C    - HC
4  18   2    0.500   -0.077   -0.102    0.3650    0.35870    # C    - CC
4  19   2    0.500   -0.077    0.104    0.3085    0.23483    # C    - HC
4  20   2    0.500   -0.077    0.073    0.3650    0.35870    # C    - CC
4  21   2    0.500   -0.077   -0.395    0.3410    0.55900    # C    - OH
4  22   2    0.500   -0.077    0.341    0.1875    0.00000    # C    - HH
4  23   2    0.500   -0.077   -0.107    0.3650    0.35870    # C    - CC
4  24   2    0.500   -0.077    0.112    0.3085    0.23483    # C    - HC
4  25   2    0.500   -0.077    0.072    0.3650    0.35870    # C    - CZ
4  26   2    0.500   -0.077   -0.382    0.3410    0.55900    # C    - OH
4  27   2    0.500   -0.077    0.364    0.1875    0.00000    # C    - HH
5   9   2    0.500    0.137    0.138    0.2500    0.12552    # HA   - HA
5  10   2    0.500    0.137    0.133    0.2500    0.12552    # HA   - HA
5  11   2    0.500    0.137    0.028    0.3000    0.18618    # HA   - CB
5  12   2    0.500    0.137    0.117    0.2500    0.12552    # HA   - HA
5  13   2    0.500    0.137   -0.423    0.2785    0.29880    # HA   - OH
5  14   2    0.500    0.137    0.347    0.1250    0.00000    # HA   - HO
5  15   2    0.500    0.137   -0.030    0.3025    0.19173    # HA   - CC
5  16   2    0.500    0.137   -0.105    0.3025    0.19173    # HA   - CC
5  17   2    0.500    0.137    0.107    0.2460    0.12552    # HA   - HC
5  18   2    0.500    0.137   -0.102    0.3025    0.19173    # HA   - CC
5  19   2    0.500    0.137    0.104    0.2460    0.12552    # HA   - HC
5  20   2    0.500    0.137    0.073    0.3025    0.19173    # HA   - CC
5  21   2    0.500    0.137   -0.395    0.2785    0.29880    # HA   - OH
5  22   2    0.500    0.137    0.341    0.1250    0.00000    # HA   - HH
5  23   2    0.500    0.137   -0.107    0.3025    0.19173    # HA   - CC
5  24   2    0.500    0.137    0.112    0.2460    0.12552    # HA   - HC
5  25   2    0.500    0.137    0.072    0.3025    0.19173    # HA   - CZ
5  26   2    0.500    0.137   -0.382    0.2785    0.29880    # HA   - OH
5  27   2    0.500    0.137    0.364    0.1250    0.00000    # HA   - HH
6   9   2    0.500    0.135    0.138    0.2500    0.12552    # HA   - HA
6  10   2    0.500    0.135    0.133    0.2500    0.12552    # HA   - HA
6  11   2    0.500    0.135    0.028    0.3000    0.18618    # HA   - CB
6  12   2    0.500    0.135    0.117    0.2500    0.12552    # HA   - HA
6  13   2    0.500    0.135   -0.423    0.2785    0.29880    # HA   - OH
6  14   2    0.500    0.135    0.347    0.1250    0.00000    # HA   - HO
6  15   2    0.500    0.135   -0.030    0.3025    0.19173    # HA   - CC
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 6  16   2    0.500    0.135   -0.105    0.3025    0.19173    # HA   - CC
 6  17   2    0.500    0.135    0.107    0.2460    0.12552    # HA   - HC
 6  18   2    0.500    0.135   -0.102    0.3025    0.19173    # HA   - CC
 6  19   2    0.500    0.135    0.104    0.2460    0.12552    # HA   - HC
 6  20   2    0.500    0.135    0.073    0.3025    0.19173    # HA   - CC
 6  21   2    0.500    0.135   -0.395    0.2785    0.29880    # HA   - OH
 6  22   2    0.500    0.135    0.341    0.1250    0.00000    # HA   - HH
 6  23   2    0.500    0.135   -0.107    0.3025    0.19173    # HA   - CC
 6  24   2    0.500    0.135    0.112    0.2460    0.12552    # HA   - HC
 6  25   2    0.500    0.135    0.072    0.3025    0.19173    # HA   - CZ
 6  26   2    0.500    0.135   -0.382    0.2785    0.29880    # HA   - OH
 6  27   2    0.500    0.135    0.364    0.1250    0.00000    # HA   - HH
 7   9   2    0.500    0.135    0.138    0.2500    0.12552    # HA   - HA
 7  10   2    0.500    0.135    0.133    0.2500    0.12552    # HA   - HA
 7  11   2    0.500    0.135    0.028    0.3000    0.18618    # HA   - CB
 7  12   2    0.500    0.135    0.117    0.2500    0.12552    # HA   - HA
 7  13   2    0.500    0.135   -0.423    0.2785    0.29880    # HA   - OH
 7  14   2    0.500    0.135    0.347    0.1250    0.00000    # HA   - HO
 7  15   2    0.500    0.135   -0.030    0.3025    0.19173    # HA   - CC
 7  16   2    0.500    0.135   -0.105    0.3025    0.19173    # HA   - CC
 7  17   2    0.500    0.135    0.107    0.2460    0.12552    # HA   - HC
 7  18   2    0.500    0.135   -0.102    0.3025    0.19173    # HA   - CC
 7  19   2    0.500    0.135    0.104    0.2460    0.12552    # HA   - HC
 7  20   2    0.500    0.135    0.073    0.3025    0.19173    # HA   - CC
 7  21   2    0.500    0.135   -0.395    0.2785    0.29880    # HA   - OH
 7  22   2    0.500    0.135    0.341    0.1250    0.00000    # HA   - HH
 7  23   2    0.500    0.135   -0.107    0.3025    0.19173    # HA   - CC
 7  24   2    0.500    0.135    0.112    0.2460    0.12552    # HA   - HC
 7  25   2    0.500    0.135    0.072    0.3025    0.19173    # HA   - CZ
 7  26   2    0.500    0.135   -0.382    0.2785    0.29880    # HA   - OH
 7  27   2    0.500    0.135    0.364    0.1250    0.00000    # HA   - HH
 8  17   2    0.500   -0.024    0.107    0.2960    0.18618    # CA   - HC
 8  19   2    0.500   -0.024    0.104    0.2960    0.18618    # CA   - HC
 8  20   2    0.500   -0.024    0.073    0.3525    0.28439    # CA   - CC
 8  21   2    0.500   -0.024   -0.395    0.3285    0.44319    # CA   - OH
 8  22   2    0.500   -0.024    0.341    0.1750    0.00000    # CA   - HH
 8  23   2    0.500   -0.024   -0.107    0.3525    0.28439    # CA   - CC
 8  24   2    0.500   -0.024    0.112    0.2960    0.18618    # CA   - HC
 8  25   2    0.500   -0.024    0.072    0.3525    0.28439    # CA   - CZ
 8  26   2    0.500   -0.024   -0.382    0.3285    0.44319    # CA   - OH
 8  27   2    0.500   -0.024    0.364    0.1750    0.00000    # CA   - HH
 9  14   2    0.500    0.138    0.347    0.1250    0.00000    # HA   - HO
 9  16   2    0.500    0.138   -0.105    0.3025    0.19173    # HA   - CC
 9  17   2    0.500    0.138    0.107    0.2460    0.12552    # HA   - HC
 9  18   2    0.500    0.138   -0.102    0.3025    0.19173    # HA   - CC
 9  19   2    0.500    0.138    0.104    0.2460    0.12552    # HA   - HC
 9  20   2    0.500    0.138    0.073    0.3025    0.19173    # HA   - CC
 9  21   2    0.500    0.138   -0.395    0.2785    0.29880    # HA   - OH
 9  22   2    0.500    0.138    0.341    0.1250    0.00000    # HA   - HH
 9  23   2    0.500    0.138   -0.107    0.3025    0.19173    # HA   - CC
 9  24   2    0.500    0.138    0.112    0.2460    0.12552    # HA   - HC
 9  25   2    0.500    0.138    0.072    0.3025    0.19173    # HA   - CZ
 9  26   2    0.500    0.138   -0.382    0.2785    0.29880    # HA   - OH
 9  27   2    0.500    0.138    0.364    0.1250    0.00000    # HA   - HH
10  14   2    0.500    0.133    0.347    0.1250    0.00000    # HA   - HO
10  16   2    0.500    0.133   -0.105    0.3025    0.19173    # HA   - CC
10  17   2    0.500    0.133    0.107    0.2460    0.12552    # HA   - HC
10  18   2    0.500    0.133   -0.102    0.3025    0.19173    # HA   - CC
10  19   2    0.500    0.133    0.104    0.2460    0.12552    # HA   - HC
10  20   2    0.500    0.133    0.073    0.3025    0.19173    # HA   - CC
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10 21 2 0.500 0.133 -0.395 0.2785 0.29880 # HA - OH
10 22 2 0.500 0.133 0.341 0.1250 0.00000 # HA - HH
10 23 2 0.500 0.133 -0.107 0.3025 0.19173 # HA - CC
10 24 2 0.500 0.133 0.112 0.2460 0.12552 # HA - HC
10 25 2 0.500 0.133 0.072 0.3025 0.19173 # HA - CZ
10 26 2 0.500 0.133 -0.382 0.2785 0.29880 # HA - OH
10 27 2 0.500 0.133 0.364 0.1250 0.00000 # HA - HH
11 21 2 0.500 0.028 -0.395 0.3285 0.44319 # CB - OH
11 22 2 0.500 0.028 0.341 0.1750 0.00000 # CB - HH
11 24 2 0.500 0.028 0.112 0.2960 0.18618 # CB - HC
11 25 2 0.500 0.028 0.072 0.3525 0.28439 # CB - CZ
11 26 2 0.500 0.028 -0.382 0.3285 0.44319 # CB - OH
11 27 2 0.500 0.028 0.364 0.1750 0.00000 # CB - HH
12 17 2 0.500 0.117 0.107 0.2460 0.12552 # HA - HC
12 19 2 0.500 0.117 0.104 0.2460 0.12552 # HA - HC
12 20 2 0.500 0.117 0.073 0.3025 0.19173 # HA - CC
12 21 2 0.500 0.117 -0.395 0.2785 0.29880 # HA - OH
12 22 2 0.500 0.117 0.341 0.1250 0.00000 # HA - HH
12 23 2 0.500 0.117 -0.107 0.3025 0.19173 # HA - CC
12 24 2 0.500 0.117 0.112 0.2460 0.12552 # HA - HC
12 25 2 0.500 0.117 0.072 0.3025 0.19173 # HA - CZ
12 26 2 0.500 0.117 -0.382 0.2785 0.29880 # HA - OH
12 27 2 0.500 0.117 0.364 0.1250 0.00000 # HA - HH
13 17 2 0.500 -0.423 0.107 0.2745 0.29880 # OH - HC
13 19 2 0.500 -0.423 0.104 0.2745 0.29880 # OH - HC
13 20 2 0.500 -0.423 0.073 0.3310 0.45642 # OH - CC
13 21 2 0.500 -0.423 -0.395 0.3070 0.71128 # OH - OH
13 22 2 0.500 -0.423 0.341 0.1535 0.00000 # OH - HH
13 23 2 0.500 -0.423 -0.107 0.3310 0.45642 # OH - CC
13 24 2 0.500 -0.423 0.112 0.2745 0.29880 # OH - HC
13 25 2 0.500 -0.423 0.072 0.3310 0.45642 # OH - CZ
13 26 2 0.500 -0.423 -0.382 0.3070 0.71128 # OH - OH
13 27 2 0.500 -0.423 0.364 0.1535 0.00000 # OH - HH
14 16 2 0.500 0.347 -0.105 0.1775 0.00000 # HO - CC
14 17 2 0.500 0.347 0.107 0.1210 0.00000 # HO - HC
14 18 2 0.500 0.347 -0.102 0.1775 0.00000 # HO - CC
14 19 2 0.500 0.347 0.104 0.1210 0.00000 # HO - HC
14 20 2 0.500 0.347 0.073 0.1775 0.00000 # HO - CC
14 21 2 0.500 0.347 -0.395 0.1535 0.00000 # HO - OH
14 22 2 0.500 0.347 0.341 0.0000 0.00000 # HO - HH
14 23 2 0.500 0.347 -0.107 0.1775 0.00000 # HO - CC
14 24 2 0.500 0.347 0.112 0.1210 0.00000 # HO - HC
14 25 2 0.500 0.347 0.072 0.1775 0.00000 # HO - CZ
14 26 2 0.500 0.347 -0.382 0.1535 0.00000 # HO - OH
14 27 2 0.500 0.347 0.364 0.0000 0.00000 # HO - HH
15 22 2 0.500 -0.030 0.341 0.1775 0.00000 # CC - HH
15 26 2 0.500 -0.030 -0.382 0.3310 0.45642 # CC - OH
15 27 2 0.500 -0.030 0.364 0.1775 0.00000 # CC - HH
16 24 2 0.500 -0.105 0.112 0.2985 0.19173 # CC - HC
16 27 2 0.500 -0.105 0.364 0.1775 0.00000 # CC - HH
17 19 2 0.500 0.107 0.104 0.2420 0.12552 # HC - HC
17 22 2 0.500 0.107 0.341 0.1210 0.00000 # HC - HH
17 23 2 0.500 0.107 -0.107 0.2985 0.19173 # HC - CC
17 24 2 0.500 0.107 0.112 0.2420 0.12552 # HC - HC
17 26 2 0.500 0.107 -0.382 0.2745 0.29880 # HC - OH
17 27 2 0.500 0.107 0.364 0.1210 0.00000 # HC - HH
18 21 2 0.500 -0.102 -0.395 0.3310 0.45642 # CC - OH
18 22 2 0.500 -0.102 0.341 0.1775 0.00000 # CC - HH
18 27 2 0.500 -0.102 0.364 0.1775 0.00000 # CC - HH
19 20 2 0.500 0.104 0.073 0.2985 0.19173 # HC - CC
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    19  21   2    0.500    0.104   -0.395    0.2745    0.29880    #  HC   - OH
    19  22   2    0.500    0.104    0.341    0.1210    0.00000    #  HC   - HH
    19  26   2    0.500    0.104   -0.382    0.2745    0.29880    #  HC   - OH
    19  27   2    0.500    0.104    0.364    0.1210    0.00000    #  HC   - HH
    21  24   2    0.500   -0.395    0.112    0.2745    0.29880    #  OH   - HC
    21  27   2    0.500   -0.395    0.364    0.1535    0.00000    #  OH   - HH
    22  23   2    0.500    0.341   -0.107    0.1775    0.00000    #  HH   - CC
    22  24   2    0.500    0.341    0.112    0.1210    0.00000    #  HH   - HC
    22  26   2    0.500    0.341   -0.382    0.1535    0.00000    #  HH   - OH
    22  27   2    0.500    0.341    0.364    0.0000    0.00000    #  HH   - HH
    24  27   2    0.500    0.112    0.364    0.1210    0.00000    #  HC   - HH

; Exclusions from default nonbonded
[ exclusions ]
; ai        aj
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dopa.itp

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; OPLS AA force field parameters of L-DOPA generated with JOYCE

[ moleculetype ]
; Name            nrexcl
DAH     3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
; residue   1 DAH rtp DAH  q +0.0
     1   oplsm_287      1    DAH     N      1   -0.570913    14.0027
     2   oplsm_290      1    DAH    H1      1    0.344381      1.008
     3   oplsm_290      1    DAH    H2      1    0.325205      1.008
     4   oplsm_290      1    DAH    H3      1    0.377593      1.008
     5   oplsm_293      1    DAH    CA      1    0.028407     12.011
     6   oplsm_140      1    DAH    HA      1    0.132597      1.008
     7   oplsm_149      1    DAH    CB      2   -0.140334     12.011
     8   oplsm_140      1    DAH   HB1      2    0.102677      1.008
     9   oplsm_140      1    DAH   HB2      2    0.101894      1.008
    10   oplsm_145      1    DAH    CG      2   -0.026831     12.011
    11   oplsm_145      1    DAH   CD1      3   -0.110132     12.011
    12   oplsm_146      1    DAH   HD1      3    0.100316      1.008
    13   oplsm_145      1    DAH   CD2      4   -0.108542     12.011
    14   oplsm_146      1    DAH   HD2      4    0.102219      1.008
    15   oplsm_166      1    DAH   CE1      5    0.072835     12.011
    16   oplsm_167      1    DAH   OE1      5   -0.394908     15.9994
    17   oplsm_168      1    DAH   HE1      5    0.339949      1.008
    18   oplsm_145      1    DAH   CE2      6   -0.108072     12.011
    19   oplsm_146      1    DAH   HE2      6    0.111219      1.008
    20   oplsm_166      1    DAH    CZ      7    0.068134     12.011
    21   oplsm_167      1    DAH    OH      7   -0.384411     15.9994
    22   oplsm_168      1    DAH    HH      7    0.362376      1.008
    23   oplsm_271      1    DAH     C      8    0.188364     12.011
    24   oplsm_272      1    DAH    O1      8   -0.450134     15.9994
    25   oplsm_272      1    DAH    O2      8   -0.463910     15.9994   ; qtot 0.000021

; Stretchings
[ bonds ]
     1    2   1    0.1026    368489.034
     1    3   1    0.1054    368489.034
     1    4   1    0.1020    368489.034
     1    5   1    0.1506    180341.536
     5    6   1    0.1095    318058.259
     5    7   1    0.1536    180195.043
     7    8   1    0.1098    314597.457
     7    9   1    0.1096    314597.457
     7   10   1    0.1512    214106.063
    10   11   1    0.1405    332239.630
    11   12   1    0.1090    331723.534
    10   13   1    0.1401    332239.630
    13   14   1    0.1091    331723.534
    11   15   1    0.1391    332239.630
    15   16   1    0.1368    305030.302
    16   17   1    0.0969    480979.109
    13   18   1    0.1402    332239.630
    18   19   1    0.1091    331723.534
    15   20   1    0.1408    309763.805
    18   20   1    0.1391    309763.805
    20   21   1    0.1374    305476.385
```

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    21    22   1     0.0966     480979.109
     5    23   1     0.1560     136630.345
    23    24   1     0.1269     478155.015
    23    25   1     0.1247     478155.015

; Bendings
[ angles ]
     2    1    3   1    108.76     338.0992
     2    1    4   1    108.90     338.0992
     2    1    5   1    111.79     354.8638
     3    1    4   1    111.69     338.0992
     3    1    5   1    101.35     354.8638
     4    1    5   1    114.10     354.8638
     1    5    6   1    107.34     467.6459
     1    5    7   1    111.77     482.7422
     1    5   23   1    105.54     528.7628
     6    5    7   1    109.70     396.4863
     6    5   23   1    107.64     316.9483
     5    7    8   1    109.02     342.6356
     5    7    9   1    106.28     342.6356
     5    7   10   1    112.82     622.4218
     7    5   23   1    114.51     523.3779
     8    7    9   1    107.62     295.6076
     8    7   10   1    109.80     348.8275
     9    7   10   1    111.11     348.8275
     7   10   11   1    120.42     495.9408
     7   10   13   1    120.67     495.9408
    10   11   12   1    120.47     295.1435
    11   10   13   1    118.84     539.0730
    10   11   15   1    120.58     539.0730
    12   11   15   1    118.94     295.1435
    10   13   14   1    119.99     295.1435
    10   13   18   1    120.86     539.0730
    14   13   18   1    119.14     295.1435
    11   15   16   1    119.53     574.6185
    11   15   20   1    120.05     379.8506
    15   16   17   1    108.53     518.3672
    16   15   20   1    120.42     796.0599
    13   18   19   1    120.37     295.1435
    13   18   20   1    119.76     379.8506
    19   18   20   1    119.86     327.6687
    15   20   18   1    119.90      99.2215
    15   20   21   1    115.28     699.1805
    18   20   21   1    124.82     699.1805
    20   21   22   1    110.60     449.2292
     5   23   24   1    114.70     372.9536
     5   23   25   1    116.62     372.9536
    24   23   25   1    128.67     683.7864

; Torsions
[ dihedrals ]
     6   5  23  24   1    320.79      9.731   2
     6   5  23  25   1    318.43      9.731   2
     2   1   5   6   1    127.76      2.482   3
     3   1   5   6   1    140.68      2.482   3
    18  20  21  22   1      0.00      3.251   1
    18  20  21  22   1    179.99      8.441   2
     6   5   7   8   1   -193.73      5.697   1
     6   5   7   8   1    -94.39      1.592   2
     6   5   7   8   1    -14.05      6.757   3
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     6   5   7   8   1     8.32      0.158   4
     8   7  10  13   1   242.40      0.135   1
     8   7  10  13   1   199.06      8.060   2
     8   7  10  13   1   252.02      0.038   3
     8   7  10  13   1   -62.10      2.030   4
     8   7  10  11   1   242.40      0.135   1
     8   7  10  11   1   199.06      8.060   2
     8   7  10  11   1   252.02      0.038   3
     8   7  10  11   1   -62.10      2.030   4
    11  15  16  17   1   359.82      3.153   1
    11  15  16  17   1   179.64      9.114   2

; Nonbonded terms
[ pairs ]
; 1-4 interactions
     1   8   2   0.500   -0.571    0.103    0.2875    0.14940    # N    - HA
     1   9   2   0.500   -0.571    0.102    0.2875    0.14940    # N    - HA
     1  10   2   0.500   -0.571   -0.027    0.3400    0.22821    # N    - CC
     1  24   2   0.500   -0.571   -0.450    0.3105    0.39527    # N    - O
     1  25   2   0.500   -0.571   -0.464    0.3105    0.39527    # N    - O
     2   6   2   0.500    0.344    0.133    0.1250    0.00000    # H    - HA
     2   7   2   0.500    0.344   -0.140    0.1750    0.00000    # H    - CB
     2  23   2   0.500    0.344    0.188    0.1875    0.00000    # H    - C
     3   6   2   0.500    0.325    0.133    0.1250    0.00000    # H    - HA
     3   7   2   0.500    0.325   -0.140    0.1750    0.00000    # H    - CB
     3  23   2   0.500    0.325    0.188    0.1875    0.00000    # H    - C
     4   6   2   0.500    0.378    0.133    0.1250    0.00000    # H    - HA
     4   7   2   0.500    0.378   -0.140    0.1750    0.00000    # H    - CB
     4  23   2   0.500    0.378    0.188    0.1875    0.00000    # H    - C
     5  11   2   0.500    0.028   -0.110    0.3525    0.14219    # CA   - CC
     5  13   2   0.500    0.028   -0.109    0.3525    0.14219    # CA   - CC
     6   8   2   0.500    0.133    0.103    0.2500    0.06276    # HA   - HA
     6   9   2   0.500    0.133    0.102    0.2500    0.06276    # HA   - HA
     6  10   2   0.500    0.133   -0.027    0.3025    0.09587    # HA   - CC
     6  24   2   0.500    0.133   -0.450    0.2730    0.16605    # HA   - O
     6  25   2   0.500    0.133   -0.464    0.2730    0.16605    # HA   - O
     7  12   2   0.500   -0.140    0.100    0.2960    0.09309    # CB   - HC
     7  14   2   0.500   -0.140    0.102    0.2960    0.09309    # CB   - HC
     7  15   2   0.500   -0.140    0.073    0.3525    0.14219    # CB   - CC
     7  18   2   0.500   -0.140   -0.108    0.3525    0.14219    # CB   - CC
     7  24   2   0.500   -0.140   -0.450    0.3230    0.24629    # CB   - O
     7  25   2   0.500   -0.140   -0.464    0.3230    0.24629    # CB   - O
     8  11   2   0.500    0.103   -0.110    0.3025    0.09587    # HA   - CC
     8  13   2   0.500    0.103   -0.109    0.3025    0.09587    # HA   - CC
     8  23   2   0.500    0.103    0.188    0.3125    0.11741    # HA   - C
     9  11   2   0.500    0.102   -0.110    0.3025    0.09587    # HA   - CC
     9  13   2   0.500    0.102   -0.109    0.3025    0.09587    # HA   - CC
     9  23   2   0.500    0.102    0.188    0.3125    0.11741    # HA   - C
    10  16   2   0.500   -0.027   -0.395    0.3310    0.22821    # CC   - OH
    10  19   2   0.500   -0.027    0.111    0.2985    0.09587    # CC   - HC
    10  20   2   0.500   -0.027    0.068    0.3550    0.14644    # CC   - CZ
    10  23   2   0.500   -0.027    0.188    0.3650    0.17935    # CC   - C
    11  14   2   0.500   -0.110    0.102    0.2985    0.09587    # CC   - HC
    11  17   2   0.500   -0.110    0.340    0.1775    0.00000    # CC   - HH
    11  18   2   0.500   -0.110   -0.108    0.3550    0.14644    # CC   - CC
    11  21   2   0.500   -0.110   -0.384    0.3310    0.22821    # CC   - OH
    12  13   2   0.500    0.100   -0.109    0.2985    0.09587    # HC   - CC
    12  16   2   0.500    0.100   -0.395    0.2745    0.14940    # HC   - OH
    12  20   2   0.500    0.100    0.068    0.2985    0.09587    # HC   - CZ
    13  15   2   0.500   -0.109    0.073    0.3550    0.14644    # CC   - CC
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13  21   2    0.500   -0.109   -0.384    0.3310    0.22821    #  CC   - OH
14  19   2    0.500    0.102    0.111    0.2420    0.06276    #  HC   - HC
14  20   2    0.500    0.102    0.068    0.2985    0.09587    #  HC   - CZ
15  19   2    0.500    0.073    0.111    0.2985    0.09587    #  CC   - HC
15  22   2    0.500    0.073    0.362    0.1775    0.00000    #  CC   - HH
16  18   2    0.500   -0.395   -0.108    0.3310    0.22821    #  OH   - CC
16  21   2    0.500   -0.395   -0.384    0.3070    0.35564    #  OH   - OH
17  20   2    0.500    0.340    0.068    0.1775    0.00000    #  HH   - CZ
18  22   2    0.500   -0.108    0.362    0.1775    0.00000    #  CC   - HH
19  21   2    0.500    0.111   -0.384    0.2745    0.14940    #  HC   - OH
 1  11   2    0.500   -0.571   -0.110    0.3400    0.45642    #  N    - CC
 1  12   2    0.500   -0.571    0.100    0.2835    0.29880    #  N    - HC
 1  13   2    0.500   -0.571   -0.109    0.3400    0.45642    #  N    - CC
 1  14   2    0.500   -0.571    0.102    0.2835    0.29880    #  N    - HC
 1  15   2    0.500   -0.571    0.073    0.3400    0.45642    #  N    - CC
 1  16   2    0.500   -0.571   -0.395    0.3160    0.71128    #  N    - OH
 1  17   2    0.500   -0.571    0.340    0.1625    0.00000    #  N    - HH
 1  18   2    0.500   -0.571   -0.108    0.3400    0.45642    #  N    - CC
 1  19   2    0.500   -0.571    0.111    0.2835    0.29880    #  N    - HC
 1  20   2    0.500   -0.571    0.068    0.3400    0.45642    #  N    - CZ
 1  21   2    0.500   -0.571   -0.384    0.3160    0.71128    #  N    - OH
 1  22   2    0.500   -0.571    0.362    0.1625    0.00000    #  N    - HH
 2   8   2    0.500    0.344    0.103    0.1250    0.00000    #  H    - HA
 2   9   2    0.500    0.344    0.102    0.1250    0.00000    #  H    - HA
 2  10   2    0.500    0.344   -0.027    0.1775    0.00000    #  H    - CC
 2  11   2    0.500    0.344   -0.110    0.1775    0.00000    #  H    - CC
 2  12   2    0.500    0.344    0.100    0.1210    0.00000    #  H    - HC
 2  13   2    0.500    0.344   -0.109    0.1775    0.00000    #  H    - CC
 2  14   2    0.500    0.344    0.102    0.1210    0.00000    #  H    - HC
 2  15   2    0.500    0.344    0.073    0.1775    0.00000    #  H    - CC
 2  16   2    0.500    0.344   -0.395    0.1535    0.00000    #  H    - OH
 2  17   2    0.500    0.344    0.340    0.0000    0.00000    #  H    - HH
 2  18   2    0.500    0.344   -0.108    0.1775    0.00000    #  H    - CC
 2  19   2    0.500    0.344    0.111    0.1210    0.00000    #  H    - HC
 2  20   2    0.500    0.344    0.068    0.1775    0.00000    #  H    - CZ
 2  21   2    0.500    0.344   -0.384    0.1535    0.00000    #  H    - OH
 2  22   2    0.500    0.344    0.362    0.0000    0.00000    #  H    - HH
 2  24   2    0.500    0.344   -0.450    0.1480    0.00000    #  H    - O
 2  25   2    0.500    0.344   -0.464    0.1480    0.00000    #  H    - O
 3   8   2    0.500    0.325    0.103    0.1250    0.00000    #  H    - HA
 3   9   2    0.500    0.325    0.102    0.1250    0.00000    #  H    - HA
 3  10   2    0.500    0.325   -0.027    0.1775    0.00000    #  H    - CC
 3  11   2    0.500    0.325   -0.110    0.1775    0.00000    #  H    - CC
 3  12   2    0.500    0.325    0.100    0.1210    0.00000    #  H    - HC
 3  13   2    0.500    0.325   -0.109    0.1775    0.00000    #  H    - CC
 3  14   2    0.500    0.325    0.102    0.1210    0.00000    #  H    - HC
 3  15   2    0.500    0.325    0.073    0.1775    0.00000    #  H    - CC
 3  16   2    0.500    0.325   -0.395    0.1535    0.00000    #  H    - OH
 3  17   2    0.500    0.325    0.340    0.0000    0.00000    #  H    - HH
 3  18   2    0.500    0.325   -0.108    0.1775    0.00000    #  H    - CC
 3  19   2    0.500    0.325    0.111    0.1210    0.00000    #  H    - HC
 3  20   2    0.500    0.325    0.068    0.1775    0.00000    #  H    - CZ
 3  21   2    0.500    0.325   -0.384    0.1535    0.00000    #  H    - OH
 3  22   2    0.500    0.325    0.362    0.0000    0.00000    #  H    - HH
 3  24   2    0.500    0.325   -0.450    0.1480    0.00000    #  H    - O
 3  25   2    0.500    0.325   -0.464    0.1480    0.00000    #  H    - O
 4   8   2    0.500    0.378    0.103    0.1250    0.00000    #  H    - HA
 4   9   2    0.500    0.378    0.102    0.1250    0.00000    #  H    - HA
 4  10   2    0.500    0.378   -0.027    0.1775    0.00000    #  H    - CC
 4  11   2    0.500    0.378   -0.110    0.1775    0.00000    #  H    - CC
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4  12  2   0.500   0.378   0.100   0.1210   0.00000   # H   - HC
4  13  2   0.500   0.378  -0.109   0.1775   0.00000   # H   - CC
4  14  2   0.500   0.378   0.102   0.1210   0.00000   # H   - HC
4  15  2   0.500   0.378   0.073   0.1775   0.00000   # H   - CC
4  16  2   0.500   0.378  -0.395   0.1535   0.00000   # H   - OH
4  17  2   0.500   0.378   0.340   0.0000   0.00000   # H   - HH
4  18  2   0.500   0.378  -0.108   0.1775   0.00000   # H   - CC
4  19  2   0.500   0.378   0.111   0.1210   0.00000   # H   - HC
4  20  2   0.500   0.378   0.068   0.1775   0.00000   # H   - CZ
4  21  2   0.500   0.378  -0.384   0.1535   0.00000   # H   - OH
4  22  2   0.500   0.378   0.362   0.0000   0.00000   # H   - HH
4  24  2   0.500   0.378  -0.450   0.1480   0.00000   # H   - O
4  25  2   0.500   0.378  -0.464   0.1480   0.00000   # H   - O
5  12  2   0.500   0.028   0.100   0.2960   0.18618   # CA  - HC
5  14  2   0.500   0.028   0.102   0.2960   0.18618   # CA  - HC
5  15  2   0.500   0.028   0.073   0.3525   0.28439   # CA  - CC
5  16  2   0.500   0.028  -0.395   0.3285   0.44319   # CA  - OH
5  17  2   0.500   0.028   0.340   0.1750   0.00000   # CA  - HH
5  18  2   0.500   0.028  -0.108   0.3525   0.28439   # CA  - CC
5  19  2   0.500   0.028   0.111   0.2960   0.18618   # CA  - HC
5  20  2   0.500   0.028   0.068   0.3525   0.28439   # CA  - CZ
5  21  2   0.500   0.028  -0.384   0.3285   0.44319   # CA  - OH
5  22  2   0.500   0.028   0.362   0.1750   0.00000   # CA  - HH
6  11  2   0.500   0.133  -0.110   0.3025   0.19173   # HA  - CC
6  12  2   0.500   0.133   0.100   0.2460   0.12552   # HA  - HC
6  13  2   0.500   0.133  -0.109   0.3025   0.19173   # HA  - CC
6  14  2   0.500   0.133   0.102   0.2460   0.12552   # HA  - HC
6  15  2   0.500   0.133   0.073   0.3025   0.19173   # HA  - CC
6  16  2   0.500   0.133  -0.395   0.2785   0.29880   # HA  - OH
6  17  2   0.500   0.133   0.340   0.1250   0.00000   # HA  - HH
6  18  2   0.500   0.133  -0.108   0.3025   0.19173   # HA  - CC
6  19  2   0.500   0.133   0.111   0.2460   0.12552   # HA  - HC
6  20  2   0.500   0.133   0.068   0.3025   0.19173   # HA  - CZ
6  21  2   0.500   0.133  -0.384   0.2785   0.29880   # HA  - OH
6  22  2   0.500   0.133   0.362   0.1250   0.00000   # HA  - HH
7  16  2   0.500  -0.140  -0.395   0.3285   0.44319   # CB  - OH
7  17  2   0.500  -0.140   0.340   0.1750   0.00000   # CB  - HH
7  19  2   0.500  -0.140   0.111   0.2960   0.18618   # CB  - HC
7  20  2   0.500  -0.140   0.068   0.3525   0.28439   # CB  - CZ
7  21  2   0.500  -0.140  -0.384   0.3285   0.44319   # CB  - OH
7  22  2   0.500  -0.140   0.362   0.1750   0.00000   # CB  - HH
8  12  2   0.500   0.103   0.100   0.2460   0.12552   # HA  - HC
8  14  2   0.500   0.103   0.102   0.2460   0.12552   # HA  - HC
8  15  2   0.500   0.103   0.073   0.3025   0.19173   # HA  - CC
8  16  2   0.500   0.103  -0.395   0.2785   0.29880   # HA  - OH
8  17  2   0.500   0.103   0.340   0.1250   0.00000   # HA  - HH
8  18  2   0.500   0.103  -0.108   0.3025   0.19173   # HA  - CC
8  19  2   0.500   0.103   0.111   0.2460   0.12552   # HA  - HC
8  20  2   0.500   0.103   0.068   0.3025   0.19173   # HA  - CZ
8  21  2   0.500   0.103  -0.384   0.2785   0.29880   # HA  - OH
8  22  2   0.500   0.103   0.362   0.1250   0.00000   # HA  - HH
8  24  2   0.500   0.103  -0.450   0.2730   0.33209   # HA  - O
8  25  2   0.500   0.103  -0.464   0.2730   0.33209   # HA  - O
9  12  2   0.500   0.102   0.100   0.2460   0.12552   # HA  - HC
9  14  2   0.500   0.102   0.102   0.2460   0.12552   # HA  - HC
9  15  2   0.500   0.102   0.073   0.3025   0.19173   # HA  - CC
9  16  2   0.500   0.102  -0.395   0.2785   0.29880   # HA  - OH
9  17  2   0.500   0.102   0.340   0.1250   0.00000   # HA  - HH
9  18  2   0.500   0.102  -0.108   0.3025   0.19173   # HA  - CC
9  19  2   0.500   0.102   0.111   0.2460   0.12552   # HA  - HC
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 9  20   2    0.500    0.102    0.068    0.3025    0.19173    #  HA   - CZ
 9  21   2    0.500    0.102   -0.384    0.2785    0.29880    #  HA   - OH
 9  22   2    0.500    0.102    0.362    0.1250    0.00000    #  HA   - HH
 9  24   2    0.500    0.102   -0.450    0.2730    0.33209    #  HA   - O
 9  25   2    0.500    0.102   -0.464    0.2730    0.33209    #  HA   - O
10  17   2    0.500   -0.027    0.340    0.1775    0.00000    #  CC   - HH
10  21   2    0.500   -0.027   -0.384    0.3310    0.45642    #  CC   - OH
10  22   2    0.500   -0.027    0.362    0.1775    0.00000    #  CC   - HH
10  24   2    0.500   -0.027   -0.450    0.3255    0.50728    #  CC   - O
10  25   2    0.500   -0.027   -0.464    0.3255    0.50728    #  CC   - O
11  19   2    0.500   -0.110    0.111    0.2985    0.19173    #  CC   - HC
11  22   2    0.500   -0.110    0.362    0.1775    0.00000    #  CC   - HH
11  23   2    0.500   -0.110    0.188    0.3650    0.35870    #  CC   - C
11  24   2    0.500   -0.110   -0.450    0.3255    0.50728    #  CC   - O
11  25   2    0.500   -0.110   -0.464    0.3255    0.50728    #  CC   - O
12  14   2    0.500    0.100    0.102    0.2420    0.12552    #  HC   - HC
12  17   2    0.500    0.100    0.340    0.1210    0.00000    #  HC   - HH
12  18   2    0.500    0.100   -0.108    0.2985    0.19173    #  HC   - CC
12  19   2    0.500    0.100    0.111    0.2420    0.12552    #  HC   - HC
12  21   2    0.500    0.100   -0.384    0.2745    0.29880    #  HC   - OH
12  22   2    0.500    0.100    0.362    0.1210    0.00000    #  HC   - HH
12  23   2    0.500    0.100    0.188    0.3085    0.23483    #  HC   - C
12  24   2    0.500    0.100   -0.450    0.2690    0.33209    #  HC   - O
12  25   2    0.500    0.100   -0.464    0.2690    0.33209    #  HC   - O
13  16   2    0.500   -0.109   -0.395    0.3310    0.45642    #  CC   - OH
13  17   2    0.500   -0.109    0.340    0.1775    0.00000    #  CC   - HH
13  22   2    0.500   -0.109    0.362    0.1775    0.00000    #  CC   - HH
13  23   2    0.500   -0.109    0.188    0.3650    0.35870    #  CC   - C
13  24   2    0.500   -0.109   -0.450    0.3255    0.50728    #  CC   - O
13  25   2    0.500   -0.109   -0.464    0.3255    0.50728    #  CC   - O
14  15   2    0.500    0.102    0.073    0.2985    0.19173    #  HC   - CC
14  16   2    0.500    0.102   -0.395    0.2745    0.29880    #  HC   - OH
14  17   2    0.500    0.102    0.340    0.1210    0.00000    #  HC   - HH
14  21   2    0.500    0.102   -0.384    0.2745    0.29880    #  HC   - OH
14  22   2    0.500    0.102    0.362    0.1210    0.00000    #  HC   - HH
14  23   2    0.500    0.102    0.188    0.3085    0.23483    #  HC   - C
14  24   2    0.500    0.102   -0.450    0.2690    0.33209    #  HC   - O
14  25   2    0.500    0.102   -0.464    0.2690    0.33209    #  HC   - O
15  23   2    0.500    0.073    0.188    0.3650    0.35870    #  CC   - C
15  24   2    0.500    0.073   -0.450    0.3255    0.50728    #  CC   - O
15  25   2    0.500    0.073   -0.464    0.3255    0.50728    #  CC   - O
16  19   2    0.500   -0.395    0.111    0.2745    0.29880    #  OH   - HC
16  22   2    0.500   -0.395    0.362    0.1535    0.00000    #  OH   - HH
16  23   2    0.500   -0.395    0.188    0.3410    0.55900    #  OH   - C
16  24   2    0.500   -0.395   -0.450    0.3015    0.79054    #  OH   - O
16  25   2    0.500   -0.395   -0.464    0.3015    0.79054    #  OH   - O
17  18   2    0.500    0.340   -0.108    0.1775    0.00000    #  HH   - CC
17  19   2    0.500    0.340    0.111    0.1210    0.00000    #  HH   - HC
17  21   2    0.500    0.340   -0.384    0.1535    0.00000    #  HH   - OH
17  22   2    0.500    0.340    0.362    0.0000    0.00000    #  HH   - HH
17  23   2    0.500    0.340    0.188    0.1875    0.00000    #  HH   - C
17  24   2    0.500    0.340   -0.450    0.1480    0.00000    #  HH   - O
17  25   2    0.500    0.340   -0.464    0.1480    0.00000    #  HH   - O
18  23   2    0.500   -0.108    0.188    0.3650    0.35870    #  CC   - C
18  24   2    0.500   -0.108   -0.450    0.3255    0.50728    #  CC   - O
18  25   2    0.500   -0.108   -0.464    0.3255    0.50728    #  CC   - O
19  22   2    0.500    0.111    0.362    0.1210    0.00000    #  HC   - HH
19  23   2    0.500    0.111    0.188    0.3085    0.23483    #  HC   - C
19  24   2    0.500    0.111   -0.450    0.2690    0.33209    #  HC   - O
19  25   2    0.500    0.111   -0.464    0.2690    0.33209    #  HC   - O
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    20  23   2    0.500    0.068    0.188    0.3650     0.35870    #  CZ   - C
    20  24   2    0.500    0.068   -0.450    0.3255     0.50728    #  CZ   - O
    20  25   2    0.500    0.068   -0.464    0.3255     0.50728    #  CZ   - O
    21  23   2    0.500   -0.384    0.188    0.3410     0.55900    #  OH   - C
    21  24   2    0.500   -0.384   -0.450    0.3015     0.79054    #  OH   - O
    21  25   2    0.500   -0.384   -0.464    0.3015     0.79054    #  OH   - O
    22  23   2    0.500    0.362    0.188    0.1875     0.00000    #  HH   - C
    22  24   2    0.500    0.362   -0.450    0.1480     0.00000    #  HH   - O
    22  25   2    0.500    0.362   -0.464    0.1480     0.00000    #  HH   - O

; Exclusions from default nonbonded
[ exclusions ]
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droxidopa.itp

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; OPLS AA force field parameters of Droxidopa generated with JOYCE

[ moleculetype ]
; Name            nrexcl
DRO     3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
; residue   1 DRO rtp DRO  q +0.0
     1   oplsm_287      1    DRO     N      1   -0.563874    14.0027
     2   oplsm_290      1    DRO    H1      1    0.334884     1.008
     3   oplsm_290      1    DRO    H2      1    0.383193     1.008
     4   oplsm_290      1    DRO    H3      1    0.347978     1.008
     5   oplsm_293      1    DRO    CA      1    0.025501    12.011
     6   oplsm_140      1    DRO    HA      1    0.138072     1.008
     7   oplsm_149      1    DRO    CB      2    0.018493    12.011
     8   oplsm_140      1    DRO   HB1      2    0.112580     1.008
     9   oplsm_154      1    DRO    OG      3   -0.469561    15.9994
    10   oplsm_155      1    DRO    HG      3    0.286741     1.008
    11   oplsm_145      1    DRO    CG      3   -0.037767    12.011
    12   oplsm_145      1    DRO   CD1      4   -0.106979    12.011
    13   oplsm_146      1    DRO   HD1      4    0.113467     1.008
    14   oplsm_145      1    DRO   CD2      5   -0.106878    12.011
    15   oplsm_146      1    DRO   HD2      5    0.096655     1.008
    16   oplsm_166      1    DRO   CE1      6    0.071455    12.011
    17   oplsm_167      1    DRO   OE1      6   -0.382444    15.9994
    18   oplsm_168      1    DRO   HE1      6    0.363284     1.008
    19   oplsm_145      1    DRO   CE2      7   -0.103248    12.011
    20   oplsm_146      1    DRO   HE2      7    0.108686     1.008
    21   oplsm_166      1    DRO    CZ      8    0.073032    12.011
    22   oplsm_167      1    DRO    OH      8   -0.393531    15.9994
    23   oplsm_168      1    DRO    HH      8    0.341308     1.008
    24   oplsm_271      1    DRO     C      9    0.201167    12.011
    25   oplsm_272      1    DRO    O1      9   -0.421581    15.9994
    26   oplsm_272      1    DRO    O2      9   -0.430621    15.9994   ; qtot 0.000013

; Stretchings
[ bonds ]
     1    2   1    0.1048    373470.846
     1    3   1    0.1021    373470.846
     1    4   1    0.1027    373470.846
     1    5   1    0.1499    207081.212
     5    6   1    0.1096    317299.775
     5    7   1    0.1551    154162.502
     7    8   1    0.1099    305252.010
     7    9   1    0.1420    225968.096
     9   10   1    0.0987    383776.997
     7   11   1    0.1520    208485.422
    11   12   1    0.1404    316021.400
    12   13   1    0.1093    332268.673
    11   14   1    0.1401    316021.400
    14   15   1    0.1089    332268.673
    12   16   1    0.1395    316021.400
    16   17   1    0.1372    289583.572
    17   18   1    0.0966    481033.117
    14   19   1    0.1396    316021.400
    19   20   1    0.1090    332268.673
    16   21   1    0.1404    321359.557
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    19    21   1    0.1395    321359.557
    21    22   1    0.1367    309471.243
    22    23   1    0.0969    481033.117
     5    24   1    0.1558    132339.541
    24    25   1    0.1259    479501.584
    24    26   1    0.1257    479501.584

; Bendings
[ angles ]
     2    1    3   1    111.49    343.4745
     2    1    4   1    108.24    343.4745
     2    1    5   1    102.59    361.7045
     3    1    4   1    108.69    343.4745
     3    1    5   1    114.05    361.7045
     4    1    5   1    111.56    361.7045
     1    5    6   1    107.66    519.9423
     1    5    7   1    111.87    553.7967
     1    5   24   1    105.89    484.0496
     6    5    7   1    108.85    417.8032
     6    5   24   1    107.90    291.6417
     5    7    8   1    107.60    419.7621
     5    7    9   1    108.48    744.6744
     5    7   11   1    111.66    365.0700
     7    5   24   1    114.39    468.9387
     8    7    9   1    106.95    492.3242
     8    7   11   1    107.98    276.5572
     7    9   10   1    105.60    632.6532
     9    7   11   1    113.89    449.8951
     7   11   12   1    119.34    687.2295
     7   11   14   1    121.60    687.2295
    11   12   13   1    120.26    298.4541
    12   11   14   1    119.01    496.0446
    11   12   16   1    120.54    496.0446
    13   12   16   1    119.19    298.4541
    11   14   15   1    120.01    298.4541
    11   14   19   1    120.51    496.0446
    15   14   19   1    119.48    298.4541
    12   16   17   1    124.40    731.9646
    12   16   21   1    120.09    377.2683
    16   17   18   1    110.69    453.9904
    17   16   21   1    115.50    634.4644
    14   19   20   1    120.87    298.4541
    14   19   21   1    120.33    377.2683
    20   19   21   1    118.80    323.2446
    16   21   19   1    119.52    209.4400
    16   21   22   1    120.77    671.0560
    19   21   22   1    119.71    671.0560
    21   22   23   1    108.62    481.9262
     5   24   25   1    116.12    324.2452
     5   24   26   1    115.50    324.2452
    25   24   26   1    128.37    813.2475

; Torsions
[ dihedrals ]
     6   5  24  25   1    328.39     10.451   2
     6   5  24  26   1    330.59     10.451   2
     2   1   5   6   1    125.59      2.547   3
     3   1   5   6   1    123.45      2.547   3
    19  21  22  23   1    359.86      3.272   1
    19  21  22  23   1    179.73      8.853   2
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     6   5   7   8   1   -218.42      3.367   1
     6   5   7   8   1    -87.74      9.305   2
     6   5   7   8   1    -25.06      9.134   3
     6   5   7   8   1   -144.67      0.009   4
     8   7  11  14   1   -120.90      0.702   1
     8   7  11  14   1    185.55     10.437   2
     8   7  11  14   1     41.83      0.182   3
     8   7  11  14   1      0.00      0.042   4
     8   7  11  12   1   -120.90      0.702   1
     8   7  11  12   1    185.55     10.437   2
     8   7  11  12   1     41.83      0.182   3
     8   7  11  12   1      0.00      0.042   4
    12  16  17  18   1      0.00      3.272   1
    12  16  17  18   1    179.99      8.853   2
     5   7   9  10   1   -215.05     12.202   1
     5   7   9  10   1    128.96      6.720   2
     5   7   9  10   1    777.43      2.465   3
     5   7   9  10   1     43.77      0.432   4

; Nonbonded terms
[ pairs ]
; 1-4 interactions
     1   8   2    0.500   -0.564    0.113    0.2875    0.14940    # N    - HA
     1   9   2    0.500   -0.564   -0.470    0.3160    0.35564    # N    - OH
     1  11   2    0.500   -0.564   -0.038    0.3400    0.22821    # N    - CC
     1  25   2    0.500   -0.564   -0.422    0.3105    0.39527    # N    - O
     1  26   2    0.500   -0.564   -0.431    0.3105    0.39527    # N    - O
     2   6   2    0.500    0.335    0.138    0.1250    0.00000    # H    - HA
     2   7   2    0.500    0.335    0.018    0.1750    0.00000    # H    - CB
     2  24   2    0.500    0.335    0.201    0.1875    0.00000    # H    - C
     3   6   2    0.500    0.383    0.138    0.1250    0.00000    # H    - HA
     3   7   2    0.500    0.383    0.018    0.1750    0.00000    # H    - CB
     3  24   2    0.500    0.383    0.201    0.1875    0.00000    # H    - C
     4   6   2    0.500    0.348    0.138    0.1250    0.00000    # H    - HA
     4   7   2    0.500    0.348    0.018    0.1750    0.00000    # H    - CB
     4  24   2    0.500    0.348    0.201    0.1875    0.00000    # H    - C
     5  10   2    0.500    0.026    0.287    0.1750    0.00000    # CA   - HO
     5  12   2    0.500    0.026   -0.107    0.3525    0.14219    # CA   - CC
     5  14   2    0.500    0.026   -0.107    0.3525    0.14219    # CA   - CC
     6   8   2    0.500    0.138    0.113    0.2500    0.06276    # HA   - HA
     6   9   2    0.500    0.138   -0.470    0.2785    0.14940    # HA   - OH
     6  11   2    0.500    0.138   -0.038    0.3025    0.09587    # HA   - CC
     6  25   2    0.500    0.138   -0.422    0.2730    0.16605    # HA   - O
     6  26   2    0.500    0.138   -0.431    0.2730    0.16605    # HA   - O
     7  13   2    0.500    0.018    0.113    0.2960    0.09309    # CB   - HC
     7  15   2    0.500    0.018    0.097    0.2960    0.09309    # CB   - HC
     7  16   2    0.500    0.018    0.071    0.3525    0.14219    # CB   - CC
     7  19   2    0.500    0.018   -0.103    0.3525    0.14219    # CB   - CC
     7  25   2    0.500    0.018   -0.422    0.3230    0.24629    # CB   - O
     7  26   2    0.500    0.018   -0.431    0.3230    0.24629    # CB   - O
     8  10   2    0.500    0.113    0.287    0.1250    0.00000    # HA   - HO
     8  12   2    0.500    0.113   -0.107    0.3025    0.09587    # HA   - CC
     8  14   2    0.500    0.113   -0.107    0.3025    0.09587    # HA   - CC
     8  24   2    0.500    0.113    0.201    0.3125    0.11741    # HA   - C
     9  12   2    0.500   -0.470   -0.107    0.3310    0.22821    # OH   - CC
     9  14   2    0.500   -0.470   -0.107    0.3310    0.22821    # OH   - CC
     9  24   2    0.500   -0.470    0.201    0.3410    0.27950    # OH   - C
    10  11   2    0.500    0.287   -0.038    0.1775    0.00000    # HO   - CC
    11  17   2    0.500   -0.038   -0.382    0.3310    0.22821    # CC   - OH
    11  20   2    0.500   -0.038    0.109    0.2985    0.09587    # CC   - HC
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11  21   2    0.500   -0.038    0.073    0.3550    0.14644    # CC   - CZ
11  24   2    0.500   -0.038    0.201    0.3650    0.17935    # CC   - C
12  15   2    0.500   -0.107    0.097    0.2985    0.09587    # CC   - HC
12  18   2    0.500   -0.107    0.363    0.1775    0.00000    # CC   - HH
12  19   2    0.500   -0.107   -0.103    0.3550    0.14644    # CC   - CC
12  22   2    0.500   -0.107   -0.394    0.3310    0.22821    # CC   - OH
13  14   2    0.500    0.113   -0.107    0.2985    0.09587    # HC   - CC
13  17   2    0.500    0.113   -0.382    0.2745    0.14940    # HC   - OH
13  21   2    0.500    0.113    0.073    0.2985    0.09587    # HC   - CZ
14  16   2    0.500   -0.107    0.071    0.3550    0.14644    # CC   - CC
14  22   2    0.500   -0.107   -0.394    0.3310    0.22821    # CC   - OH
15  20   2    0.500    0.097    0.109    0.2420    0.06276    # HC   - HC
15  21   2    0.500    0.097    0.073    0.2985    0.09587    # HC   - CZ
16  20   2    0.500    0.071    0.109    0.2985    0.09587    # CC   - HC
16  23   2    0.500    0.071    0.341    0.1775    0.00000    # CC   - HH
17  19   2    0.500   -0.382   -0.103    0.3310    0.22821    # OH   - CC
17  22   2    0.500   -0.382   -0.394    0.3070    0.35564    # OH   - OH
18  21   2    0.500    0.363    0.073    0.1775    0.00000    # HH   - CZ
19  23   2    0.500   -0.103    0.341    0.1775    0.00000    # CC   - HH
20  22   2    0.500    0.109   -0.394    0.2745    0.14940    # HC   - OH
 1  10   2    0.500   -0.564    0.287    0.1625    0.00000    # N    - HO
 1  12   2    0.500   -0.564   -0.107    0.3400    0.45642    # N    - CC
 1  13   2    0.500   -0.564    0.113    0.2835    0.29880    # N    - HC
 1  14   2    0.500   -0.564   -0.107    0.3400    0.45642    # N    - CC
 1  15   2    0.500   -0.564    0.097    0.2835    0.29880    # N    - HC
 1  16   2    0.500   -0.564    0.071    0.3400    0.45642    # N    - CC
 1  17   2    0.500   -0.564   -0.382    0.3160    0.71128    # N    - OH
 1  18   2    0.500   -0.564    0.363    0.1625    0.00000    # N    - HH
 1  19   2    0.500   -0.564   -0.103    0.3400    0.45642    # N    - CC
 1  20   2    0.500   -0.564    0.109    0.2835    0.29880    # N    - HC
 1  21   2    0.500   -0.564    0.073    0.3400    0.45642    # N    - CZ
 1  22   2    0.500   -0.564   -0.394    0.3160    0.71128    # N    - OH
 1  23   2    0.500   -0.564    0.341    0.1625    0.00000    # N    - HH
 2   8   2    0.500    0.335    0.113    0.1250    0.00000    # H    - HA
 2   9   2    0.500    0.335   -0.470    0.1535    0.00000    # H    - OH
 2  10   2    0.500    0.335    0.287    0.0000    0.00000    # H    - HO
 2  11   2    0.500    0.335   -0.038    0.1775    0.00000    # H    - CC
 2  12   2    0.500    0.335   -0.107    0.1775    0.00000    # H    - CC
 2  13   2    0.500    0.335    0.113    0.1210    0.00000    # H    - HC
 2  14   2    0.500    0.335   -0.107    0.1775    0.00000    # H    - CC
 2  15   2    0.500    0.335    0.097    0.1210    0.00000    # H    - HC
 2  16   2    0.500    0.335    0.071    0.1775    0.00000    # H    - CC
 2  17   2    0.500    0.335   -0.382    0.1535    0.00000    # H    - OH
 2  18   2    0.500    0.335    0.363    0.0000    0.00000    # H    - HH
 2  19   2    0.500    0.335   -0.103    0.1775    0.00000    # H    - CC
 2  20   2    0.500    0.335    0.109    0.1210    0.00000    # H    - HC
 2  21   2    0.500    0.335    0.073    0.1775    0.00000    # H    - CZ
 2  22   2    0.500    0.335   -0.394    0.1535    0.00000    # H    - OH
 2  23   2    0.500    0.335    0.341    0.0000    0.00000    # H    - HH
 2  25   2    0.500    0.335   -0.422    0.1480    0.00000    # H    - O
 2  26   2    0.500    0.335   -0.431    0.1480    0.00000    # H    - O
 3   8   2    0.500    0.383    0.113    0.1250    0.00000    # H    - HA
 3   9   2    0.500    0.383   -0.470    0.1535    0.00000    # H    - OH
 3  10   2    0.500    0.383    0.287    0.0000    0.00000    # H    - HO
 3  11   2    0.500    0.383   -0.038    0.1775    0.00000    # H    - CC
 3  12   2    0.500    0.383   -0.107    0.1775    0.00000    # H    - CC
 3  13   2    0.500    0.383    0.113    0.1210    0.00000    # H    - HC
 3  14   2    0.500    0.383   -0.107    0.1775    0.00000    # H    - CC
 3  15   2    0.500    0.383    0.097    0.1210    0.00000    # H    - HC
 3  16   2    0.500    0.383    0.071    0.1775    0.00000    # H    - CC
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3  17   2    0.500    0.383   -0.382    0.1535     0.00000    # H    - OH
3  18   2    0.500    0.383    0.363    0.0000     0.00000    # H    - HH
3  19   2    0.500    0.383   -0.103    0.1775     0.00000    # H    - CC
3  20   2    0.500    0.383    0.109    0.1210     0.00000    # H    - HC
3  21   2    0.500    0.383    0.073    0.1775     0.00000    # H    - CZ
3  22   2    0.500    0.383   -0.394    0.1535     0.00000    # H    - OH
3  23   2    0.500    0.383    0.341    0.0000     0.00000    # H    - HH
3  25   2    0.500    0.383   -0.422    0.1480     0.00000    # H    - O
3  26   2    0.500    0.383   -0.431    0.1480     0.00000    # H    - O
4   8   2    0.500    0.348    0.113    0.1250     0.00000    # H    - HA
4   9   2    0.500    0.348   -0.470    0.1535     0.00000    # H    - OH
4  10   2    0.500    0.348    0.287    0.0000     0.00000    # H    - HO
4  11   2    0.500    0.348   -0.038    0.1775     0.00000    # H    - CC
4  12   2    0.500    0.348   -0.107    0.1775     0.00000    # H    - CC
4  13   2    0.500    0.348    0.113    0.1210     0.00000    # H    - HC
4  14   2    0.500    0.348   -0.107    0.1775     0.00000    # H    - CC
4  15   2    0.500    0.348    0.097    0.1210     0.00000    # H    - HC
4  16   2    0.500    0.348    0.071    0.1775     0.00000    # H    - CC
4  17   2    0.500    0.348   -0.382    0.1535     0.00000    # H    - OH
4  18   2    0.500    0.348    0.363    0.0000     0.00000    # H    - HH
4  19   2    0.500    0.348   -0.103    0.1775     0.00000    # H    - CC
4  20   2    0.500    0.348    0.109    0.1210     0.00000    # H    - HC
4  21   2    0.500    0.348    0.073    0.1775     0.00000    # H    - CZ
4  22   2    0.500    0.348   -0.394    0.1535     0.00000    # H    - OH
4  23   2    0.500    0.348    0.341    0.0000     0.00000    # H    - HH
4  25   2    0.500    0.348   -0.422    0.1480     0.00000    # H    - O
4  26   2    0.500    0.348   -0.431    0.1480     0.00000    # H    - O
5  13   2    0.500    0.026    0.113    0.2960     0.18618    # CA   - HC
5  15   2    0.500    0.026    0.097    0.2960     0.18618    # CA   - HC
5  16   2    0.500    0.026    0.071    0.3525     0.28439    # CA   - CC
5  17   2    0.500    0.026   -0.382    0.3285     0.44319    # CA   - OH
5  18   2    0.500    0.026    0.363    0.1750     0.00000    # CA   - HH
5  19   2    0.500    0.026   -0.103    0.3525     0.28439    # CA   - CC
5  20   2    0.500    0.026    0.109    0.2960     0.18618    # CA   - HC
5  21   2    0.500    0.026    0.073    0.3525     0.28439    # CA   - CZ
5  22   2    0.500    0.026   -0.394    0.3285     0.44319    # CA   - OH
5  23   2    0.500    0.026    0.341    0.1750     0.00000    # CA   - HH
6  10   2    0.500    0.138    0.287    0.1250     0.00000    # HA   - HO
6  12   2    0.500    0.138   -0.107    0.3025     0.19173    # HA   - CC
6  13   2    0.500    0.138    0.113    0.2460     0.12552    # HA   - HC
6  14   2    0.500    0.138   -0.107    0.3025     0.19173    # HA   - CC
6  15   2    0.500    0.138    0.097    0.2460     0.12552    # HA   - HC
6  16   2    0.500    0.138    0.071    0.3025     0.19173    # HA   - CC
6  17   2    0.500    0.138   -0.382    0.2785     0.29880    # HA   - OH
6  18   2    0.500    0.138    0.363    0.1250     0.00000    # HA   - HH
6  19   2    0.500    0.138   -0.103    0.3025     0.19173    # HA   - CC
6  20   2    0.500    0.138    0.109    0.2460     0.12552    # HA   - HC
6  21   2    0.500    0.138    0.073    0.3025     0.19173    # HA   - CZ
6  22   2    0.500    0.138   -0.394    0.2785     0.29880    # HA   - OH
6  23   2    0.500    0.138    0.341    0.1250     0.00000    # HA   - HH
7  17   2    0.500    0.018   -0.382    0.3285     0.44319    # CB   - OH
7  18   2    0.500    0.018    0.363    0.1750     0.00000    # CB   - HH
7  20   2    0.500    0.018    0.109    0.2960     0.18618    # CB   - HC
7  21   2    0.500    0.018    0.073    0.3525     0.28439    # CB   - CZ
7  22   2    0.500    0.018   -0.394    0.3285     0.44319    # CB   - OH
7  23   2    0.500    0.018    0.341    0.1750     0.00000    # CB   - HH
8  13   2    0.500    0.113    0.113    0.2460     0.12552    # HA   - HC
8  15   2    0.500    0.113    0.097    0.2460     0.12552    # HA   - HC
8  16   2    0.500    0.113    0.071    0.3025     0.19173    # HA   - CC
8  17   2    0.500    0.113   -0.382    0.2785     0.29880    # HA   - OH
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 8  18   2    0.500    0.113    0.363    0.1250    0.00000    # HA   - HH
 8  19   2    0.500    0.113   -0.103    0.3025    0.19173    # HA   - CC
 8  20   2    0.500    0.113    0.109    0.2460    0.12552    # HA   - HC
 8  21   2    0.500    0.113    0.073    0.3025    0.19173    # HA   - CZ
 8  22   2    0.500    0.113   -0.394    0.2785    0.29880    # HA   - OH
 8  23   2    0.500    0.113    0.341    0.1250    0.00000    # HA   - HH
 8  25   2    0.500    0.113   -0.422    0.2730    0.33209    # HA   - O
 8  26   2    0.500    0.113   -0.431    0.2730    0.33209    # HA   - O
 9  13   2    0.500   -0.470    0.113    0.2745    0.29880    # OH   - HC
 9  15   2    0.500   -0.470    0.097    0.2745    0.29880    # OH   - HC
 9  16   2    0.500   -0.470    0.071    0.3310    0.45642    # OH   - CC
 9  17   2    0.500   -0.470   -0.382    0.3070    0.71128    # OH   - OH
 9  18   2    0.500   -0.470    0.363    0.1535    0.00000    # OH   - HH
 9  19   2    0.500   -0.470   -0.103    0.3310    0.45642    # OH   - CC
 9  20   2    0.500   -0.470    0.109    0.2745    0.29880    # OH   - HC
 9  21   2    0.500   -0.470    0.073    0.3310    0.45642    # OH   - CZ
 9  22   2    0.500   -0.470   -0.394    0.3070    0.71128    # OH   - OH
 9  23   2    0.500   -0.470    0.341    0.1535    0.00000    # OH   - HH
 9  25   2    0.500   -0.470   -0.422    0.3015    0.79054    # OH   - O
 9  26   2    0.500   -0.470   -0.431    0.3015    0.79054    # OH   - O
10  12   2    0.500    0.287   -0.107    0.1775    0.00000    # HO   - CC
10  13   2    0.500    0.287    0.113    0.1210    0.00000    # HO   - HC
10  14   2    0.500    0.287   -0.107    0.1775    0.00000    # HO   - CC
10  15   2    0.500    0.287    0.097    0.1210    0.00000    # HO   - HC
10  16   2    0.500    0.287    0.071    0.1775    0.00000    # HO   - CC
10  17   2    0.500    0.287   -0.382    0.1535    0.00000    # HO   - OH
10  18   2    0.500    0.287    0.363    0.0000    0.00000    # HO   - HH
10  19   2    0.500    0.287   -0.103    0.1775    0.00000    # HO   - CC
10  20   2    0.500    0.287    0.109    0.1210    0.00000    # HO   - HC
10  21   2    0.500    0.287    0.073    0.1775    0.00000    # HO   - CZ
10  22   2    0.500    0.287   -0.394    0.1535    0.00000    # HO   - OH
10  23   2    0.500    0.287    0.341    0.0000    0.00000    # HO   - HH
10  24   2    0.500    0.287    0.201    0.1875    0.00000    # HO   - C
10  25   2    0.500    0.287   -0.422    0.1480    0.00000    # HO   - O
10  26   2    0.500    0.287   -0.431    0.1480    0.00000    # HO   - O
11  18   2    0.500   -0.038    0.363    0.1775    0.00000    # CC   - HH
11  22   2    0.500   -0.038   -0.394    0.3310    0.45642    # CC   - OH
11  23   2    0.500   -0.038    0.341    0.1775    0.00000    # CC   - HH
11  25   2    0.500   -0.038   -0.422    0.3255    0.50728    # CC   - O
11  26   2    0.500   -0.038   -0.431    0.3255    0.50728    # CC   - O
12  20   2    0.500   -0.107    0.109    0.2985    0.19173    # CC   - HC
12  23   2    0.500   -0.107    0.341    0.1775    0.00000    # CC   - HH
12  24   2    0.500   -0.107    0.201    0.3650    0.35870    # CC   - C
12  25   2    0.500   -0.107   -0.422    0.3255    0.50728    # CC   - O
12  26   2    0.500   -0.107   -0.431    0.3255    0.50728    # CC   - O
13  15   2    0.500    0.113    0.097    0.2420    0.12552    # HC   - HC
13  18   2    0.500    0.113    0.363    0.1210    0.00000    # HC   - HH
13  19   2    0.500    0.113   -0.103    0.2985    0.19173    # HC   - CC
13  20   2    0.500    0.113    0.109    0.2420    0.12552    # HC   - HC
13  22   2    0.500    0.113   -0.394    0.2745    0.29880    # HC   - OH
13  23   2    0.500    0.113    0.341    0.1210    0.00000    # HC   - HH
13  24   2    0.500    0.113    0.201    0.3085    0.23483    # HC   - C
13  25   2    0.500    0.113   -0.422    0.2690    0.33209    # HC   - O
13  26   2    0.500    0.113   -0.431    0.2690    0.33209    # HC   - O
14  17   2    0.500   -0.107   -0.382    0.3310    0.45642    # CC   - OH
14  18   2    0.500   -0.107    0.363    0.1775    0.00000    # CC   - HH
14  23   2    0.500   -0.107    0.341    0.1775    0.00000    # CC   - HH
14  24   2    0.500   -0.107    0.201    0.3650    0.35870    # CC   - C
14  25   2    0.500   -0.107   -0.422    0.3255    0.50728    # CC   - O
14  26   2    0.500   -0.107   -0.431    0.3255    0.50728    # CC   - O
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    15  16   2    0.500    0.097    0.071    0.2985    0.19173    #  HC   - CC
    15  17   2    0.500    0.097   -0.382    0.2745    0.29880    #  HC   - OH
    15  18   2    0.500    0.097    0.363    0.1210    0.00000    #  HC   - HH
    15  22   2    0.500    0.097   -0.394    0.2745    0.29880    #  HC   - OH
    15  23   2    0.500    0.097    0.341    0.1210    0.00000    #  HC   - HH
    15  24   2    0.500    0.097    0.201    0.3085    0.23483    #  HC   - C
    15  25   2    0.500    0.097   -0.422    0.2690    0.33209    #  HC   - O
    15  26   2    0.500    0.097   -0.431    0.2690    0.33209    #  HC   - O
    16  24   2    0.500    0.071    0.201    0.3650    0.35870    #  CC   - C
    16  25   2    0.500    0.071   -0.422    0.3255    0.50728    #  CC   - O
    16  26   2    0.500    0.071   -0.431    0.3255    0.50728    #  CC   - O
    17  20   2    0.500   -0.382    0.109    0.2745    0.29880    #  OH   - HC
    17  23   2    0.500   -0.382    0.341    0.1535    0.00000    #  OH   - HH
    17  24   2    0.500   -0.382    0.201    0.3410    0.55900    #  OH   - C
    17  25   2    0.500   -0.382   -0.422    0.3015    0.79054    #  OH   - O
    17  26   2    0.500   -0.382   -0.431    0.3015    0.79054    #  OH   - O
    18  19   2    0.500    0.363   -0.103    0.1775    0.00000    #  HH   - CC
    18  20   2    0.500    0.363    0.109    0.1210    0.00000    #  HH   - HC
    18  22   2    0.500    0.363   -0.394    0.1535    0.00000    #  HH   - OH
    18  23   2    0.500    0.363    0.341    0.0000    0.00000    #  HH   - HH
    18  24   2    0.500    0.363    0.201    0.1875    0.00000    #  HH   - C
    18  25   2    0.500    0.363   -0.422    0.1480    0.00000    #  HH   - O
    18  26   2    0.500    0.363   -0.431    0.1480    0.00000    #  HH   - O
    19  24   2    0.500   -0.103    0.201    0.3650    0.35870    #  CC   - C
    19  25   2    0.500   -0.103   -0.422    0.3255    0.50728    #  CC   - O
    19  26   2    0.500   -0.103   -0.431    0.3255    0.50728    #  CC   - O
    20  23   2    0.500    0.109    0.341    0.1210    0.00000    #  HC   - HH
    20  24   2    0.500    0.109    0.201    0.3085    0.23483    #  HC   - C
    20  25   2    0.500    0.109   -0.422    0.2690    0.33209    #  HC   - O
    20  26   2    0.500    0.109   -0.431    0.2690    0.33209    #  HC   - O
    21  24   2    0.500    0.073    0.201    0.3650    0.35870    #  CZ   - C
    21  25   2    0.500    0.073   -0.422    0.3255    0.50728    #  CZ   - O
    21  26   2    0.500    0.073   -0.431    0.3255    0.50728    #  CZ   - O
    22  24   2    0.500   -0.394    0.201    0.3410    0.55900    #  OH   - C
    22  25   2    0.500   -0.394   -0.422    0.3015    0.79054    #  OH   - O
    22  26   2    0.500   -0.394   -0.431    0.3015    0.79054    #  OH   - O
    23  24   2    0.500    0.341    0.201    0.1875    0.00000    #  HH   - C
    23  25   2    0.500    0.341   -0.422    0.1480    0.00000    #  HH   - O
    23  26   2    0.500    0.341   -0.431    0.1480    0.00000    #  HH   - O

; Exclusions from default nonbonded
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