

Supplementary Information

(1)

Most relevant T-shaped (Upper part) and π -stacking (lower part) non covalent interactions:

- Alpha = Dihedral Angle between Planes I and J (°)
- Beta = Angle Cg(I) $\rightarrow$ Cg(J) or Cg(I) $\rightarrow$ Me vector and normal to plane I (°)
- Gamma = Angle Cg(I) $\rightarrow$ Cg(J) vector and normal to plane J (°)
- Cg-Cg = Distance between ring Centroids (Å)

Cg (I)	$\rightarrow$	Cg (J)	Cg-Cg	Alpha	Beta	Gamma	
Cg2	$\rightarrow$	Cg7	4.4178	2.491	38.98	38.73	(π -stacking)
Cg3	$\rightarrow$	Cg5	4.6976	2.781	42.26	39.92	(π -stacking)
Cg4	$\rightarrow$	Cg7	4.9375	89.606	12.75	85.73	(T-shaped)

Analysis of Potential Hydrogen Bonds

Nr	Type	Donor	--- H...	Acceptor	D - H (Å)	H...A (Å)	D...A (Å)	D - H...A (°)
1	Inter	O143	--H1431	..O22	0.82	1.78	2.5928	176
2	Inter	O43	--H431	..O103	0.82	1.81	2.6181	171
3	Inter	C441	--H4411	..O102	0.97	2.45	3.2302	138
4	Inter	C106	--H1061	..O46	0.93	2.56	3.4717	167
5	Intra	C138	--H1381	..N115	0.93	2.50	2.8384	101
6	Intra	C136	--H1361	..N115	0.92	2.60	3.1723	121
7	Inter	C26	--H261	..O146	0.93	2.59	3.5105	173
8	Intra	C38	--H381	..O2	0.93	2.43	3.3339	165

Analysis of the Coordination Geometry

Distances are calculated from atom I of Unique Molecule Coordinate List to atom J in Asymmetric Residue Unit.

Phi = Azimuth angle(counter clockwise from XO in XO,YO-Plane), Mu = Angle between D and XO,YO-plane.

'--' = Bonded atoms, '<<' = lower than. sum vdW-radii - 0.2, '<' = lower than. sum vdW-radii, '..' = greater than sum vdW-radii.

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3.6 Angstrom Coordination Sphere Around Atom I = U1												

Nr	d(I,J)	To	Atom J	Type	Phi	Mu	X	Y	Z	XO	YO	ZO

1	1.7754	--	O46	Intra	-105.14	-36.76	0.70900	0.42880	1.02100	4.7132	8.5567	13.6638
2	1.7871	--	O2	Intra	79.36	34.43	0.81120	0.57020	1.17590	5.3567	11.3783	15.7368
3	2.2333	--	O3	Intra	-172.81	24.99	0.63840	0.48490	1.17090	3.0763	9.6762	15.6698
4	2.2784	--	O22	Intra	27.58	-33.07	0.85910	0.54190	1.00750	6.7769	10.8136	13.4831
5	2.4170	--	O43	Intra	132.73	-40.46	0.63010	0.56530	0.98320	3.8368	11.2806	13.1579
6	2.5722	--	N15	Intra	-75.46	63.90	0.84590	0.44270	1.27300	5.3686	8.8341	17.0362
7	2.5925	--	N18	Intra	-32.17	6.76	0.93590	0.42890	1.12320	7.2637	8.5587	15.0315
8	3.2359	<<	C4	Intra	177.24	40.83	0.63610	0.50350	1.25850	2.6390	10.0473	16.8422
9	3.3936	<	C21	Intra	9.19	-36.60	0.91360	0.51940	0.94920	7.7740	10.3646	12.7029
10	3.4640	<	C17	Intra	-49.41	22.61	0.95520	0.37590	1.19990	7.1650	7.5011	16.0579
11	3.4720	<	C14	Intra	-119.04	73.23	0.81450	0.45370	1.34880	4.5982	9.0536	18.0506
12	3.4745	<	<C440	Intra	158.06	-36.66	0.51660	0.54980	0.94540	2.4991	10.9713	12.6520
13	3.4822	<	>C441	Intra	146.88	-58.52	0.57300	0.54740	0.87850	3.5615	10.9234	11.7567
14	3.5578	<	C16	Intra	-49.71	47.88	0.94890	0.40640	1.29760	6.6276	8.1097	17.3654
15	3.5580	<	C19	Intra	-24.05	-7.20	0.99470	0.42550	1.06710	8.3080	8.4909	14.2807
16	2.87	<	H431	Intra	119.69	-30.04	0.63490	0.60570	0.99310	3.8548	12.0867	13.2904
17	3.33	..	H381	Intra	20.59	46.60	0.98800	0.53790	1.28110	7.2254	10.7338	17.1446
18	3.34	..	H1431	Inter	57.76	-19.72	0.86090	0.63070	1.01630	6.7600	12.5856	13.6009
19	3.39	..	<H4402	Intra	171.44	-25.18	0.49910	0.52050	0.99250	2.0472	10.3866	13.2824
20	3.40	..	>H4412	Intra	178.59	-64.54	0.57520	0.49940	0.87120	3.6247	9.9655	11.6590

Polyhedral Volume 15.955 Å³

3.6 Angstrom Coordination Sphere Around Atom I = U101												
Nr	d(I,J)	To	Atom J	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	1.7780	--	O102	Intra	-101.48	-40.40	0.68170	0.67820	0.81870	5.2882	13.5335	10.9564
2	1.7827	--	O146	Intra	77.40	40.49	0.78420	0.81100	0.99130	5.8535	16.1835	13.2663
3	2.2378	--	O122	Intra	5.48	-20.92	0.86720	0.75470	0.84510	7.6386	15.0600	11.3097
4	2.2941	--	O103	Intra	-150.46	31.36	0.63510	0.69630	0.99400	3.8533	13.8947	13.3024
5	2.4185	--	O143	Intra	-49.94	38.10	0.86260	0.67170	1.01630	6.7827	13.4038	13.6009
6	2.5341	--	N118	Intra	89.54	-52.39	0.68060	0.82220	0.75480	5.5701	16.4070	10.1013
7	2.5873	--	N115	Intra	151.01	-9.89	0.55310	0.80660	0.87160	3.3282	16.0957	11.6644
8	3.2272	<<	C121	Intra	-1.78	-38.92	0.86740	0.74080	0.75330	8.0673	14.7827	10.0812
9	3.3541	<<	C104	Intra	-169.80	36.59	0.58510	0.72080	1.05420	2.9073	14.3836	14.1081
10	3.4233	<	C119	Intra	61.76	-63.39	0.70670	0.81240	0.67610	6.2833	16.2114	9.0481
11	3.4742	<	C144	Intra	-24.27	39.15	0.97320	0.68920	1.06870	8.0139	13.7530	14.3021
12	3.4777	<	C117	Intra	110.79	-36.07	0.60380	0.87640	0.75180	4.5601	17.4886	10.0611
13	3.5087	<	C114	Intra	157.02	6.46	0.50140	0.81290	0.93430	2.3480	16.2214	12.5035
14	3.5296	<	<C1450	Intra	5.99	42.95	0.98720	0.75820	1.08450	8.1272	15.1299	14.5136
15	3.5449	<	C116	Intra	139.40	-28.28	0.51040	0.84650	0.77930	3.1874	16.8919	10.4292
16	2.97	<	H1431	Intra	-62.14	30.11	0.86090	0.63070	1.01630	6.7600	12.5856	13.6009
17	3.17	..	<H1452	Intra	20.57	29.94	0.96570	0.79300	1.02290	8.1265	15.8243	13.6892
18	3.37	..	>H1443	Intra	-6.18	32.13	0.99130	0.72930	1.03870	8.3945	14.5532	13.9006
19	3.42	..	<H1453	Intra	10.91	60.47	0.93360	0.76070	1.12730	7.2140	15.1798	15.0864
20	3.45	..	H1381	Intra	-166.43	-35.36	0.47460	0.71160	0.75550	2.8206	14.2000	10.1107
21	3.46	..	H431	Inter	-121.55	19.95	0.63490	0.60570	0.99310	3.8548	12.0867	13.2904

Polyhedral Volume 16.241 Å³

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Å, Probe Radius = 1.20 Å

van der Waals (or ion) Radii used in the Analysis

C	H	N	O	U
1.70	1.20	1.55	1.52	1.86

Total Potential Solvent Area Vol 14.5 Å³
per Unit Cell Vol 3560.2 Å³ [0.4%]

Area	VolPerc.	Vol (Å ³)	X (av)	Y (av)	Z (av)	Eigenvector (frac)	Sig (Å)
1	0	7	0.153	0.823	0.292	1 -0.040-0.021 1.000	0.54
						2 -0.088 1.000 0.011	0.54
						3 -1.000-0.034-0.341	0.53
2	0	7	0.847	0.323	0.708	1 -0.051-0.012 1.000	0.54
						2 -0.050 1.000 0.006	0.54
						3 -1.000-0.020-0.348	0.53

(2)

Most relevant T-shaped (Upper part) and π -stacking (lower part) non covalent interactions:

- Alpha = Dihedral Angle between Planes I and J (°)
- Beta = Angle Cg(I) $\rightarrow$ Cg(J) or Cg(I) $\rightarrow$ Me vector and normal to plane I (°)
- Gamma = Angle Cg(I) $\rightarrow$ Cg(J) vector and normal to plane J (°)
- Cg-Cg = Distance between ring Centroids (Å)

Cg(I)	$\rightarrow$	Cg(J)	Cg-Cg	Alpha	Beta	Gamma	
Cg1	$\rightarrow$	Cg5	5.4429	9.042	38.78	30.11	(π -stacking)
Cg3	$\rightarrow$	Cg6	3.8059	13.353	13.90	27.02	(π -stacking)
Cg4	$\rightarrow$	Cg5	4.5571	18.561	34.21	44.84	(π -stacking)
Cg4	$\rightarrow$	Cg7	3.8989	17.747	32.53	14.98	(π -stacking)
Cg2	$\rightarrow$	Cg3	5.2736	83.146	14.59	84.12	(T-shaped)
Cg2	$\rightarrow$	Cg5	5.6314	80.912	49.25	67.55	(T-shaped)
Cg2	$\rightarrow$	Cg6	5.3673	87.899	24.03	76.16	(T-shaped)
Cg7	$\rightarrow$	Cg2	5.3212	79.804	12.94	79.17	(T-shaped)

Analysis of Potential Hydrogen Bonds

Nr	Type	Donor	---	H....Acceptor	D - H (Å)	H...A (Å)	D...A (Å)	D - H...A (°)	Sum(XY,YZ)
1	Inter	O136	--	H1361 ..O23	0.83	1.75	2.5835	176	
2	Inter	O36	--	H361 ..O123	0.82	1.77	2.5676	164	
3	Inter	C127	--	H1271 ..O2	0.93	2.49	3.3576	155	
4	Inter	C127	--	H1271 ..O35	0.93	2.57	3.1673	123'	346.00 3-Centre (bifurcated)
5	Intra	C129	--	H1291 ..N119	0.93	2.54	2.8575	100	
6	Intra	C13	--	H131 ..O34	0.93	2.52	3.4275	164	
7	Inter	C27	--	H271 ..O102	0.92	2.36	3.2670	166	
8	Intra	C29	--	H291 ..N19	0.93	2.60	2.9236	101	
9	Inter	C37	--	H372 ..O134	0.98	2.60	3.1548	116	

Analysis of the Coordination Geometry

Distances are calculated from atom I of Unique Molecule Coordinate List to atom J in Asymmetric Residue Unit.

Phi = Azimuth angle(counter clockwise from XO in XO,YO-Plane), Mu = Angle between D and XO,YO-plane.

'--' = Bonded atoms, '<<' = lower than. sum vdW-radii - 0.2, '<' = lower than. sum vdW-radii, '...' = greater than sum vdW-radii.

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3.6 Angstrom Coordination Sphere Around Atom I = U1												
Nr	d(I,J)	To	Atom J	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	1.7747	--	O34	Intra	122.90	21.58	0.05650	0.28800	0.27880	-0.3320	5.5118	3.4995
2	1.7943	--	O35	Intra	-50.87	-25.22	0.19340	0.14980	0.16590	1.5887	2.8669	2.0824
3	2.2272	--	O2	Intra	-171.23	-50.04	-0.04790	0.20420	0.09080	-0.8494	3.9080	1.1397
4	2.2853	--	O23	Intra	23.64	39.58	0.30080	0.25250	0.34280	2.1779	4.8324	4.3029
5	2.4129	--	O36	Intra	55.34	-36.74	0.18340	0.29870	0.11180	1.6639	5.7166	1.4033
6	2.5749	--	N19	Intra	-82.80	46.78	0.18660	0.12420	0.37630	0.7854	2.3770	4.7234
7	2.5945	--	N10	Intra	-153.64	18.74	-0.05580	0.15860	0.29320	-1.6373	3.0353	3.6803

Polyhedral Volume 15.669 Å³

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3.6 Angstrom Coordination Sphere Around Atom I = U101												
Nr	d(I,J)	To	Atom J	Type	Phi	Mu	X	Y	Z	XO	YO	ZO

1	1.7691	--	O135	Intra	129.10	22.66	0.28930	0.53500	0.32270	2.1188	10.2390	4.0506
2	1.7835	--	O134	Intra	-53.38	-21.90	0.43650	0.39940	0.21540	4.1353	7.6438	2.7037
3	2.2341	--	O102	Intra	3.06	54.67	0.52490	0.47240	0.41360	4.4385	9.0409	5.1916
4	2.2961	--	O123	Intra	-155.44	-37.44	0.18190	0.42920	0.15720	1.4902	8.2142	1.9732
5	2.4306	--	O136	Intra	-124.92	36.14	0.29940	0.38470	0.38260	2.0247	7.3625	4.8025
6	2.5422	--	N110	Intra	33.18	-10.81	0.53980	0.54020	0.23040	5.2383	10.3385	2.8920
7	2.5658	--	N119	Intra	94.56	-53.87	0.30280	0.54760	0.10330	3.0281	10.4801	1.2966

Polyhedral Volume 16.097 Å³

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Å, Probe Radius = 1.20 Å

van der Waals (or ion) Radii used in the Analysis

C	H	N	O	U

1.70	1.20	1.55	1.52	1.86

Unit cell Contains NO Residual Solvent Accessible Void.

Complete comparison among U_iso and U_aniso: X-ray experimental vs. MD calculated ones. Table A contains the data of (1) while Table B the data of (2).

(A) bis(p-tert-butyl-salicylidene)-1,2-diphenylethylenediamine (1)

	X-ray	MD		X-ray						MD						
	U_ISO	U_ISO		U_11	U_22	U_33	U_12	U_13	U_23		U_11	U_22	U_33	U_12	U_13	U_23
U1	0.0172	0.0199		0.0207	0.0145	0.0177	0.0013	0.0081	-0.0003		0.0268	0.0139	0.0248	-0.0005	0.0164	-0.0010
O2	0.0229	0.0267		0.0247	0.0234	0.0225	0.0020	0.0105	-0.0029		0.0288	0.0199	0.0359	-0.0023	0.0168	-0.0080
O3	0.0220	0.0311		0.0181	0.0294	0.0184	-0.0059	0.0060	-0.0027		0.0385	0.0320	0.0327	-0.0110	0.0249	-0.0054
C4	0.0196	0.0242		0.0191	0.0137	0.0280	-0.0031	0.0103	-0.0001		0.0315	0.0179	0.0324	-0.0075	0.0227	-0.0040
C5	0.0208	0.0230		0.0186	0.0240	0.0233	0.0011	0.0115	-0.0006		0.0305	0.0211	0.0256	-0.0015	0.0200	-0.0050
C6	0.0274	0.0302		0.0268	0.0382	0.0230	-0.0022	0.0160	-0.0035		0.0319	0.0383	0.0279	-0.0002	0.0200	-0.0103
C7	0.0265	0.0302		0.0279	0.0316	0.0227	-0.0025	0.0118	-0.0003		0.0323	0.0295	0.0396	-0.0068	0.0262	-0.0135
C8	0.0246	0.0376		0.0206	0.0232	0.0304	-0.0035	0.0088	-0.0084		0.0329	0.0360	0.0538	-0.0043	0.0277	-0.0133
C9	0.0246	0.0345		0.0184	0.0215	0.0357	0.0014	0.0114	0.0053		0.0337	0.0295	0.0482	-0.0052	0.0243	-0.0068
C10	0.0383	0.0447		0.0252	0.0667	0.0268	-0.0040	0.0139	-0.0122		0.0438	0.0586	0.0446	-0.0035	0.0316	-0.0191
C11	0.0563	0.6824		0.0557	0.0793	0.0481	-0.0134	0.0363	-0.0053		0.7886	1.1422	0.2232	0.2542	0.3114	-0.1524
C12	0.0590	0.6750		0.0747	0.0590	0.0529	0.0060	0.0340	-0.0273		0.7989	1.0908	0.3220	-0.2108	0.4334	-0.3534
C13	0.0586	0.6768		0.0339	0.1102	0.0319	0.0101	0.0109	-0.0225		1.2641	0.6736	0.3440	0.0720	0.6015	-0.0951
C14	0.0245	0.0269		0.0244	0.0300	0.0206	0.0038	0.0093	0.0006		0.0337	0.0312	0.0217	0.0080	0.0170	-0.0016
N15	0.0218	0.0220		0.0218	0.0218	0.0253	0.0003	0.0127	-0.0040		0.0335	0.0169	0.0216	0.0079	0.0171	0.0005
C16	0.0225	0.0231		0.0270	0.0256	0.0165	0.0076	0.0092	0.0027		0.0332	0.0191	0.0196	0.0112	0.0122	0.0017
C17	0.0214	0.0211		0.0282	0.0198	0.0184	0.0066	0.0107	0.0040		0.0314	0.0133	0.0220	0.0095	0.0135	0.0018
N18	0.0197	0.0203		0.0243	0.0154	0.0221	0.0010	0.0112	-0.0017		0.0288	0.0147	0.0216	0.0085	0.0138	0.0017
C19	0.0210	0.0252		0.0235	0.0174	0.0216	0.0022	0.0066	0.0029		0.0330	0.0221	0.0256	0.0143	0.0166	0.0051
C20	0.0213	0.0242		0.0258	0.0200	0.0217	-0.0043	0.0129	-0.0002		0.0314	0.0216	0.0243	0.0132	0.0153	0.0035
C21	0.0239	0.0267		0.0271	0.0263	0.0199	0.0017	0.0100	0.0050		0.0342	0.0164	0.0400	0.0094	0.0263	0.0064
O22	0.0262	0.0422		0.0357	0.0214	0.0300	0.0106	0.0224	0.0069		0.0642	0.0190	0.0701	0.0189	0.0575	0.0170
C23	0.0305	0.0390		0.0497	0.0203	0.0276	0.0075	0.0211	0.0035		0.0522	0.0278	0.0517	0.0207	0.0371	0.0168
C24	0.0249	0.0426		0.0265	0.0244	0.0212	0.0058	0.0042	0.0093		0.0584	0.0397	0.0407	0.0276	0.0311	0.0173

C25	0.0264	0.0411		0.0314	0.0269	0.0250	-0.0043	0.0147	-0.0047		0.0591	0.0440	0.0270	0.0317	0.0236	0.0113
C26	0.0229	0.0396		0.0253	0.0186	0.0290	0.0012	0.0147	0.0004		0.0578	0.0410	0.0279	0.0343	0.0250	0.0123
C27	0.0340	0.0756		0.0438	0.0368	0.0288	0.0098	0.0219	0.0032		0.1214	0.0840	0.0382	0.0718	0.0492	0.0260
C28	0.0480	0.7118		0.0573	0.0424	0.0585	0.0064	0.0382	0.0087		1.0216	1.0058	0.3173	0.9141	0.5030	0.3981
C29	0.0559	0.5392		0.0653	0.0713	0.0355	0.0099	0.0225	-0.0138		1.0036	0.2891	0.6846	-0.1409	0.7564	-0.2471
C30	0.0510	0.5443		0.0628	0.0606	0.0473	0.0305	0.0422	0.0126		0.3045	1.0822	0.3851	-0.2209	0.2978	-0.4552
C31	0.0243	0.0254		0.0313	0.0166	0.0266	0.0104	0.0118	0.0047		0.0375	0.0129	0.0314	0.0066	0.0188	0.0028
C32	0.0290	0.0382		0.0378	0.0188	0.0313	0.0026	0.0125	0.0003		0.0597	0.0237	0.0347	-0.0067	0.0205	-0.0037
C33	0.0382	0.0515		0.0524	0.0240	0.0373	-0.0008	0.0135	-0.0014		0.0701	0.0317	0.0550	-0.0141	0.0243	-0.0097
C34	0.0462	0.0558		0.0361	0.0296	0.0755	-0.0048	0.0219	-0.0096		0.0626	0.0302	0.0855	-0.0124	0.0394	-0.0095
C35	0.0461	0.0550		0.0477	0.0231	0.0846	-0.0042	0.0450	-0.0055		0.0695	0.0314	0.0865	-0.0116	0.0558	-0.0056
C36	0.0349	0.0416		0.0393	0.0313	0.0446	0.0014	0.0281	-0.0009		0.0606	0.0256	0.0566	-0.0041	0.0432	-0.0025
C37	0.0267	0.0284		0.0261	0.0332	0.0209	0.0063	0.0078	-0.0092		0.0283	0.0297	0.0244	0.0121	0.0053	-0.0060
C38	0.0395	0.0392		0.0309	0.0365	0.0442	0.0056	0.0028	-0.0070		0.0309	0.0301	0.0485	0.0044	0.0027	-0.0097
C39	0.0504	0.0637		0.0266	0.0400	0.0655	-0.0005	-0.0110	-0.0241		0.0396	0.0433	0.0916	-0.0006	0.0005	-0.0308
C40	0.0542	0.0793		0.0325	0.0621	0.0619	-0.0022	0.0071	-0.0343		0.0395	0.0682	0.1037	0.0036	-0.0105	-0.0467
C41	0.0481	0.0656		0.0227	0.0840	0.0302	0.0062	-0.0014	-0.0098		0.0354	0.0772	0.0645	0.0162	-0.0089	-0.0263
C42	0.0337	0.0442		0.0331	0.0437	0.0236	0.0123	0.0085	-0.0010		0.0344	0.0519	0.0374	0.0193	0.0004	-0.0053
O43	0.0271	0.0509		0.0293	0.0195	0.0290	0.0028	0.0049	0.0045		0.0629	0.0252	0.0505	0.0051	0.0005	0.0012
O46	0.0268	0.0382		0.0280	0.0241	0.0265	0.0003	0.0065	-0.0018		0.0445	0.0240	0.0470	-0.0031	0.0166	-0.0155
C440	0.0400	0.1632		0.0285	0.0420	0.0417	0.0095	0.0011	-0.0031		0.1364	0.0814	0.1769	-0.0324	-0.0719	-0.0034
C441	0.0373			0.0345	0.0323	0.0342	-0.0051	-0.0034	-0.0005							
C450	0.0628	0.2247		0.0474	0.0550	0.0588	0.0075	-0.0197	-0.0204		0.1423	0.3874	0.1280	-0.1570	0.0239	-0.0585
C451	0.0731			0.0524	0.0695	0.0679	-0.0016	-0.0204	-0.0020							
U101	0.0170	0.0201		0.0207	0.0152	0.0172	0.0010	0.0091	0.0002		0.0275	0.0142	0.0225	-0.0026	0.0137	-0.0017
O146	0.0254	0.0379		0.0331	0.0218	0.0256	-0.0001	0.0156	-0.0044		0.0536	0.0250	0.0366	-0.0088	0.0169	-0.0132
O102	0.0220	0.0296		0.0249	0.0205	0.0237	-0.0024	0.0123	0.0019		0.0333	0.0242	0.0363	-0.0058	0.0181	-0.0127
O103	0.0228	0.0372		0.0295	0.0181	0.0283	0.0049	0.0198	0.0037		0.0517	0.0179	0.0605	0.0153	0.0435	0.0122
C104	0.0199	0.0270		0.0299	0.0143	0.0214	0.0016	0.0164	-0.0015		0.0311	0.0172	0.0386	0.0092	0.0198	0.0046
C105	0.0215	0.0298		0.0245	0.0196	0.0245	0.0067	0.0135	0.0030		0.0389	0.0262	0.0244	0.0189	0.0111	0.0014
C106	0.0256	0.0517		0.0331	0.0250	0.0237	0.0132	0.0162	0.0034		0.0804	0.0499	0.0292	0.0467	0.0245	0.0110
C107	0.0251	0.0502		0.0330	0.0284	0.0186	0.0116	0.0147	0.0056		0.0730	0.0522	0.0284	0.0386	0.0210	0.0092

C110	0.0344	0.0927		0.0478	0.0415	0.0237	0.0155	0.0252	0.0050		0.1497	0.1009	0.0387	0.0871	0.0468	0.0221
C111	0.0467	0.7446		0.0593	0.0576	0.0375	0.0061	0.0354	0.0044		0.8859	1.1047	0.4867	0.3124	0.5516	-0.0984
C113	0.0591	0.7190		0.0896	0.0623	0.0442	0.0476	0.0476	0.0210		0.9360	0.9231	0.5893	0.0611	0.6398	-0.2591
C112	0.0505	0.7451		0.0610	0.0672	0.0298	0.0116	0.0239	-0.0107		1.0861	0.8688	0.5723	0.2967	0.6635	-0.0876
C108	0.0316	0.0445		0.0500	0.0313	0.0233	0.0084	0.0254	0.0063		0.0549	0.0438	0.0406	0.0248	0.0239	0.0145
C109	0.0251	0.0408		0.0228	0.0287	0.0289	0.0104	0.0154	0.0077		0.0512	0.0304	0.0522	0.0211	0.0325	0.0168
C114	0.0236	0.0330		0.0265	0.0236	0.0262	0.0044	0.0160	-0.0011		0.0443	0.0320	0.0228	0.0248	0.0114	0.0028
N115	0.0203	0.0246		0.0268	0.0225	0.0137	0.0012	0.0096	0.0042		0.0331	0.0187	0.0209	0.0123	0.0079	-0.0007
C116	0.0216	0.0266		0.0297	0.0203	0.0168	0.0105	0.0102	0.0074		0.0367	0.0205	0.0194	0.0151	0.0053	-0.0020
C137	0.0245	0.0306		0.0234	0.0327	0.0194	0.0042	0.0098	-0.0088		0.0281	0.0336	0.0260	0.0155	0.0036	-0.0095
C138	0.0295	0.0371		0.0281	0.0356	0.0243	0.0030	0.0080	-0.0012		0.0306	0.0369	0.0393	0.0067	0.0058	-0.0161
C139	0.0444	0.0543		0.0488	0.0407	0.0487	-0.0067	0.0229	-0.0119		0.0408	0.0601	0.0569	-0.0026	0.0098	-0.0329
C140	0.0472	0.0654		0.0321	0.0766	0.0293	0.0044	0.0050	-0.0172		0.0393	0.0883	0.0582	0.0016	0.0028	-0.0414
C141	0.0457	0.0637		0.0353	0.0735	0.0231	0.0164	0.0025	-0.0022		0.0431	0.0847	0.0462	0.0223	-0.0073	-0.0271
C142	0.0367	0.0480		0.0415	0.0454	0.0233	0.0160	0.0107	0.0020		0.0451	0.0526	0.0329	0.0266	-0.0045	-0.0126
C117	0.0224	0.0273		0.0273	0.0219	0.0196	0.0089	0.0100	0.0031		0.0461	0.0155	0.0180	0.0096	0.0078	0.0030
N118	0.0210	0.0250		0.0270	0.0147	0.0266	0.0024	0.0162	-0.0007		0.0450	0.0157	0.0177	0.0065	0.0152	0.0021
C119	0.0253	0.0294		0.0254	0.0296	0.0240	0.0025	0.0125	0.0064		0.0475	0.0264	0.0177	0.0039	0.0155	-0.0015
C120	0.0234	0.0252		0.0275	0.0262	0.0205	0.0026	0.0134	0.0025		0.0410	0.0198	0.0225	-0.0073	0.0207	-0.0062
C121	0.0218	0.0248		0.0219	0.0244	0.0228	-0.0099	0.0122	-0.0028		0.0359	0.0178	0.0301	-0.0120	0.0235	-0.0070
O122	0.0223	0.0294		0.0237	0.0259	0.0217	0.0009	0.0135	0.0005		0.0361	0.0310	0.0293	-0.0101	0.0217	-0.0056
C123	0.0224	0.0341		0.0237	0.0226	0.0232	-0.0048	0.0110	-0.0049		0.0400	0.0273	0.0462	-0.0093	0.0293	-0.0102
C124	0.0275	0.0398		0.0188	0.0267	0.0402	0.0024	0.0142	-0.0012		0.0486	0.0338	0.0527	-0.0089	0.0378	-0.0145
C125	0.0257	0.0338		0.0192	0.0356	0.0286	-0.0099	0.0164	-0.0111		0.0500	0.0282	0.0379	-0.0160	0.0340	-0.0150
C126	0.0273	0.0329		0.0223	0.0364	0.0232	-0.0022	0.0075	0.0016		0.0493	0.0333	0.0247	-0.0068	0.0239	-0.0087
C127	0.0365	0.0484		0.0307	0.0549	0.0287	-0.0080	0.0161	-0.0147		0.0673	0.0521	0.0445	-0.0179	0.0434	-0.0208
C128	0.0618	0.7209		0.0695	0.0825	0.0539	-0.0265	0.0481	-0.0122		1.0541	1.0350	0.2696	0.0043	0.4807	-0.1511
C130	0.0871	0.7376		0.1773	0.0505	0.0657	-0.0390	0.0835	-0.0353		1.0478	1.0909	0.2728	-0.0108	0.4834	-0.1579
C129	0.0725	0.7310		0.0603	0.1363	0.0232	0.0226	0.0170	-0.0119		1.0872	1.0316	0.2731	0.0415	0.4906	-0.1341
C131	0.0270	0.0331		0.0362	0.0194	0.0267	0.0056	0.0120	0.0024		0.0533	0.0144	0.0266	0.0089	0.0071	0.0017
C136	0.0313	0.0583		0.0410	0.0220	0.0313	-0.0008	0.0125	0.0010		0.1236	0.0234	0.0262	-0.0109	0.0231	-0.0043
C135	0.0360	0.0689		0.0430	0.0231	0.0382	0.0010	0.0082	-0.0051		0.1340	0.0302	0.0357	-0.0136	0.0198	-0.0095

C134	0.0444	0.0624		0.0391	0.0297	0.0638	-0.0026	0.0160	-0.0145		0.0833	0.0301	0.0668	-0.0061	0.0160	-0.0147
C133	0.0590	0.0706		0.0588	0.0382	0.0980	-0.0117	0.0501	-0.0048		0.0820	0.0414	0.1031	-0.0204	0.0505	-0.0285
C132	0.0450	0.0552		0.0529	0.0367	0.0630	-0.0060	0.0428	0.0002		0.0693	0.0338	0.0753	-0.0104	0.0412	-0.0188
O143	0.0261	0.0447		0.0229	0.0223	0.0317	0.0042	0.0071	0.0042		0.0523	0.0267	0.0480	-0.0003	0.0078	0.0090
C144	0.0462	0.1736		0.0369	0.0520	0.0477	-0.0045	0.0110	0.0019		0.1556	0.0869	0.1692	-0.0578	-0.0882	0.0371
C1450	0.0532	0.1891		0.0467	0.0542	0.0547	-0.0071	0.0111	-0.0021		0.0984	0.3070	0.1278	-0.0919	-0.0066	0.0046
C1451	0.0674			0.0728	0.0646	0.0586	-0.0140	0.0130	-0.0070							

(B) bis(salicylidene)-1,2-diphenylethylenediamine (2)

	Xray	MD		Xray							MD					
	iso	iso		U_11	U_22	U_33	U_12	U_13	U_23		U_11	U_22	U_33	U_12	U_13	U_23
U1	0.0209	0.0236		0.0213	0.0166	0.0248	0.0003	0.0063	0.0004		0.0271	0.0213	0.0198	0.0004	-0.0015	-0.0002
O2	0.0272	0.0296		0.0235	0.0285	0.0295	0.0033	0.0068	-0.0016		0.0278	0.0327	0.0252	0.0006	-0.0022	-0.0006
C3	0.0235	0.0270		0.0236	0.0129	0.0322	-0.0027	0.0043	-0.0013		0.0285	0.0249	0.0223	0.0004	-0.0074	-0.0007
C4	0.0288	0.0304		0.0179	0.0365	0.0308	0.0028	0.0045	0.0049		0.0249	0.0367	0.0250	0.0001	-0.0060	-0.0007
C5	0.0414	0.0499		0.0219	0.0650	0.0411	0.0179	0.0149	0.0151		0.0366	0.0726	0.0352	0.0000	-0.0055	-0.0007
C6	0.0472	0.0554		0.0314	0.0502	0.0600	0.0155	0.0119	0.0089		0.0503	0.0650	0.0406	0.0003	-0.0158	-0.0005
C7	0.0414	0.0498		0.0303	0.0467	0.0451	0.0123	0.0063	0.0134		0.0596	0.0445	0.0340	0.0008	-0.0182	-0.0008
C8	0.0310	0.0391		0.0280	0.0384	0.0248	-0.0002	0.0041	0.0090		0.0474	0.0357	0.0270	0.0005	-0.0099	-0.0009
C9	0.0283	0.0305		0.0277	0.0287	0.0279	0.0003	0.0064	0.0009		0.0208	0.0420	0.0263	0.0001	-0.0009	-0.0007
N10	0.0244	0.0239		0.0221	0.0248	0.0260	0.0007	0.0059	0.0002		0.0189	0.0264	0.0239	0.0001	-0.0017	0.0000
C11	0.0250	0.0230		0.0211	0.0202	0.0340	0.0031	0.0080	0.0023		0.0179	0.0271	0.0232	0.0003	0.0019	0.0000
C12	0.0333	0.0252		0.0213	0.0346	0.0422	0.0042	0.0051	0.0036		0.0182	0.0350	0.0219	0.0004	0.0029	0.0001
C13	0.0361	0.0323		0.0369	0.0363	0.0365	0.0120	0.0122	0.0000		0.0360	0.0343	0.0261	0.0005	0.0045	0.0000
C14	0.0435	0.0405		0.0471	0.0470	0.0361	0.0103	0.0107	-0.0086		0.0392	0.0478	0.0316	0.0004	-0.0002	0.0000
C15	0.0513	0.0497		0.0420	0.0759	0.0334	0.0013	0.0056	-0.0104		0.0478	0.0711	0.0269	0.0001	-0.0004	0.0001
C16	0.0535	0.0488		0.0491	0.0811	0.0283	0.0063	0.0066	0.0142		0.0483	0.0737	0.0234	-0.0001	0.0047	0.0002
C17	0.0373	0.0356		0.0393	0.0454	0.0270	-0.0057	0.0085	0.0101		0.0308	0.0516	0.0241	0.0002	0.0047	0.0002
C18	0.0248	0.0207		0.0283	0.0149	0.0296	0.0014	0.0048	0.0023		0.0192	0.0201	0.0220	0.0002	0.0020	-0.0001
N19	0.0261	0.0192		0.0246	0.0220	0.0336	-0.0032	0.0113	0.0033		0.0180	0.0190	0.0196	0.0001	0.0011	-0.0001
C20	0.0255	0.0230		0.0288	0.0181	0.0283	0.0055	0.0054	0.0083		0.0187	0.0227	0.0255	-0.0001	-0.0005	0.0001

C21	0.0240	0.0194		0.0249	0.0220	0.0230	0.0050	0.0027	0.0029		0.0179	0.0190	0.0202	0.0000	0.0010	0.0000
C22	0.0260	0.0212		0.0210	0.0295	0.0264	0.0015	0.0046	0.0016		0.0237	0.0168	0.0206	0.0000	-0.0014	-0.0001
O23	0.0253	0.0357		0.0198	0.0147	0.0374	0.0014	0.0006	0.0039		0.0323	0.0181	0.0468	0.0000	-0.0164	-0.0003
C24	0.0268	0.0291		0.0269	0.0216	0.0308	-0.0038	0.0055	0.0061		0.0297	0.0242	0.0327	-0.0001	0.0044	0.0000
C25	0.0300	0.0334		0.0241	0.0273	0.0407	-0.0004	0.0122	0.0051		0.0238	0.0324	0.0448	-0.0003	0.0090	0.0000
C26	0.0338	0.0322		0.0228	0.0246	0.0523	0.0076	0.0068	0.0043		0.0183	0.0342	0.0430	-0.0003	0.0037	0.0001
C27	0.0316	0.0290		0.0290	0.0282	0.0357	0.0003	0.0051	0.0117		0.0191	0.0281	0.0373	-0.0002	-0.0007	0.0001
C28	0.0298	0.0235		0.0320	0.0216	0.0344	0.0006	0.0063	0.0071		0.0237	0.0203	0.0253	0.0002	0.0022	0.0000
C29	0.0375	0.0311		0.0385	0.0295	0.0486	-0.0048	0.0188	-0.0042		0.0292	0.0268	0.0366	0.0000	0.0049	-0.0001
C30	0.0430	0.0391		0.0503	0.0324	0.0529	0.0041	0.0254	-0.0037		0.0426	0.0327	0.0418	-0.0001	0.0081	-0.0002
C31	0.0441	0.0407		0.0551	0.0356	0.0416	-0.0019	0.0128	-0.0107		0.0502	0.0334	0.0371	0.0003	0.0056	0.0000
C32	0.0536	0.0405		0.0475	0.0488	0.0608	-0.0092	0.0079	-0.0238		0.0400	0.0396	0.0390	0.0007	0.0007	0.0001
C33	0.0466	0.0335		0.0469	0.0346	0.0592	-0.0068	0.0157	-0.0091		0.0275	0.0338	0.0366	0.0005	0.0004	0.0001
O34	0.0257	0.0279		0.0284	0.0192	0.0282	-0.0021	0.0055	-0.0001		0.0302	0.0246	0.0258	0.0005	-0.0022	-0.0002
O35	0.0278	0.0350		0.0297	0.0191	0.0330	0.0008	0.0053	0.0052		0.0442	0.0289	0.0328	0.0003	0.0099	0.0001
O36	0.0288	0.0534		0.0311	0.0208	0.0345	-0.0033	0.0088	-0.0006		0.0985	0.0251	0.0448	0.0005	0.0345	0.0002
C37	0.0436	0.0672		0.0431	0.0405	0.0503	-0.0089	0.0178	-0.0069		0.1038	0.0573	0.0504	0.0003	0.0390	0.0006
C38	0.0645	0.1155		0.0967	0.0514	0.0505	-0.0233	0.0286	-0.0151		0.1711	0.1129	0.0842	0.0012	0.0777	0.0014
U101	0.0211	0.0228		0.0212	0.0164	0.0259	0.0005	0.0065	-0.0003		0.0244	0.0210	0.0198	0.0003	-0.0030	0.0003
O102	0.0243	0.0299		0.0220	0.0236	0.0261	0.0007	0.0042	-0.0002		0.0276	0.0319	0.0257	-0.0001	-0.0052	0.0005
C103	0.0250	0.0288		0.0149	0.0299	0.0284	-0.0014	0.0024	-0.0058		0.0266	0.0218	0.0302	-0.0001	-0.0127	0.0006
C104	0.0253	0.0308		0.0231	0.0191	0.0328	0.0005	0.0060	-0.0050		0.0207	0.0352	0.0310	0.0001	-0.0079	0.0006
C105	0.0335	0.0485		0.0263	0.0396	0.0352	-0.0048	0.0094	0.0021		0.0247	0.0674	0.0467	0.0001	-0.0096	0.0005
C106	0.0404	0.0592		0.0234	0.0461	0.0480	0.0094	0.0030	0.0072		0.0337	0.0584	0.0714	0.0002	-0.0232	0.0006
C107	0.0387	0.0572		0.0265	0.0369	0.0502	-0.0022	0.0058	0.0120		0.0447	0.0359	0.0728	-0.0001	-0.0321	0.0005
C108	0.0322	0.0434		0.0316	0.0232	0.0407	0.0004	0.0079	-0.0061		0.0418	0.0269	0.0482	-0.0003	-0.0231	0.0005
C109	0.0258	0.0296		0.0237	0.0263	0.0283	-0.0012	0.0087	-0.0002		0.0187	0.0403	0.0281	0.0001	0.0003	0.0006
N110	0.0256	0.0223		0.0254	0.0209	0.0296	0.0005	0.0057	0.0038		0.0179	0.0244	0.0224	0.0001	-0.0009	0.0005
C111	0.0259	0.0218		0.0325	0.0137	0.0339	-0.0019	0.0132	0.0041		0.0216	0.0234	0.0202	0.0001	0.0031	0.0005
C112	0.0271	0.0248		0.0370	0.0175	0.0277	-0.0012	0.0104	0.0013		0.0330	0.0204	0.0214	0.0001	0.0065	0.0003
C113	0.0409	0.0353		0.0337	0.0355	0.0561	-0.0137	0.0167	-0.0195		0.0437	0.0322	0.0300	-0.0001	0.0073	0.0004
C114	0.0487	0.0447		0.0551	0.0368	0.0567	-0.0230	0.0193	-0.0197		0.0692	0.0313	0.0341	-0.0002	0.0112	0.0002

C115	0.0463	0.0452		0.0635	0.0299	0.0494	-0.0108	0.0220	-0.0147		0.0824	0.0225	0.0330	-0.0001	0.0169	-0.0001
C116	0.0422	0.0404		0.0452	0.0393	0.0465	0.0036	0.0200	-0.0056		0.0636	0.0240	0.0360	0.0000	0.0154	-0.0002
C117	0.0367	0.0311		0.0386	0.0255	0.0481	0.0000	0.0150	-0.0071		0.0399	0.0218	0.0326	0.0001	0.0096	-0.0001
C118	0.0270	0.0200		0.0295	0.0242	0.0278	-0.0030	0.0083	0.0032		0.0198	0.0207	0.0187	0.0002	0.0019	0.0002
N119	0.0236	0.0193		0.0242	0.0131	0.0337	-0.0001	0.0083	0.0000		0.0184	0.0189	0.0193	0.0003	0.0005	0.0001
C120	0.0244	0.0282		0.0278	0.0184	0.0286	-0.0026	0.0102	-0.0002		0.0189	0.0270	0.0361	0.0003	-0.0003	0.0001
C121	0.0266	0.0237		0.0257	0.0246	0.0294	0.0042	0.0070	-0.0001		0.0185	0.0232	0.0273	0.0004	-0.0003	0.0001
C122	0.0224	0.0214		0.0284	0.0203	0.0174	0.0114	0.0040	0.0012		0.0215	0.0188	0.0212	0.0004	-0.0021	0.0000
O123	0.0255	0.0292		0.0219	0.0185	0.0323	0.0013	0.0006	-0.0016		0.0252	0.0188	0.0378	0.0004	-0.0077	0.0000
C124	0.0290	0.0301		0.0356	0.0146	0.0346	0.0004	0.0055	-0.0007		0.0264	0.0277	0.0343	0.0004	0.0015	0.0000
C125	0.0402	0.0346		0.0231	0.0447	0.0521	-0.0045	0.0089	-0.0036		0.0233	0.0384	0.0409	0.0005	0.0034	0.0004
C126	0.0355	0.0357		0.0242	0.0357	0.0438	0.0045	0.0042	0.0091		0.0198	0.0433	0.0420	0.0005	0.0015	0.0003
C127	0.0311	0.0363		0.0250	0.0291	0.0376	0.0022	0.0057	0.0074		0.0199	0.0379	0.0487	0.0004	0.0012	0.0000
C128	0.0286	0.0227		0.0246	0.0329	0.0313	-0.0011	0.0126	0.0010		0.0200	0.0286	0.0181	0.0002	0.0006	0.0003
C129	0.0394	0.0320		0.0547	0.0323	0.0348	0.0065	0.0180	0.0023		0.0371	0.0302	0.0283	0.0001	0.0058	0.0005
C130	0.0507	0.0414		0.0527	0.0500	0.0509	0.0020	0.0165	-0.0105		0.0417	0.0450	0.0360	0.0004	0.0039	0.0007
C131	0.0484	0.0456		0.0429	0.0644	0.0381	0.0101	0.0113	-0.0138		0.0398	0.0667	0.0293	0.0006	0.0043	0.0007
C132	0.0570	0.0461		0.0587	0.0738	0.0442	-0.0140	0.0235	-0.0034		0.0493	0.0657	0.0256	0.0007	0.0129	0.0004
C133	0.0454	0.0354		0.0481	0.0497	0.0444	-0.0081	0.0226	-0.0077		0.0415	0.0426	0.0236	0.0004	0.0103	0.0002
O134	0.0272	0.0338		0.0245	0.0266	0.0293	-0.0006	0.0049	-0.0012		0.0345	0.0315	0.0311	0.0000	-0.0040	0.0001
O135	0.0288	0.0303		0.0348	0.0209	0.0318	0.0007	0.0106	-0.0028		0.0345	0.0244	0.0307	0.0003	0.0033	0.0002
O136	0.0229	0.0424		0.0253	0.0175	0.0281	-0.0022	0.0110	-0.0004		0.0649	0.0242	0.0374	-0.0003	0.0085	0.0001
C137	0.0285	0.0468		0.0368	0.0236	0.0286	-0.0058	0.0149	-0.0011		0.0542	0.0458	0.0416	-0.0003	0.0127	-0.0001
C138	0.0450	0.0580		0.0622	0.0339	0.0407	-0.0035	0.0169	-0.0034		0.0610	0.0689	0.0442	-0.0003	0.0108	-0.0003

Detailed Molecular Orbitals, electron density and electrostatic potential description of (2).

All ab-initio calculation were carried out as described in the Experimental Section of the manuscript.
The corresponding description for (1) is almost identical but for the para-butyl groups.

