Molecular complexes of 4-halophenylboronic acids: A systematic exploration of isostructurality and structural landscape

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Supporting Information

Experimental

All the boronic acids and *N*-donor compounds were obtained commercially and the crystallization experiments were carried out by dissolving them in spectroscopic grade solvents, as the case may be. Single crystals suitable for x-ray diffraction were obtained, over a period of one week time, by slow-evaporation of the respective solution at room temperature.

A general procedure for the synthesis of complexes

In a typical co-crystallization experiment, 4-halophenylboronic acid (–Cl, –Br or –I) (0.100 mmol) and the *N*-donor ligand (**bpy**, **bpye**, **phen**, **phenz** or **acr**) (0.100 mmol), as the case may be, were dissolved in solvents (10 mL) in a 25 mL conical flask by warming on a water bath. The resultant solution was allowed to evaporate under ambient conditions and colorless single crystals were obtained over a period of one week to ten days.

Different solvents (methanol, ethanol, tetrahydrofuran, 1,4-dioxane, acetone and acetonitrile) and 1:1 solvent mixtures (methanol-water, ethanol-water, ethanol-acetonitrile and acetonitrile-dichloromethane) were used for crystallization.

In the case of complexes **13** and **14**, the reaction components were dissolved in acetonitrile and kept for slow evaporation at a temperature of 22 ^{o}C. Yellowish-green crystals appeared over a period of 3-4 days. The crystals were harvested and were dispersed in NVH immersion oil to stabilize the crystals. Over a period of time the crystals redissolve and emerge as stable crystals. Both the crystal types were structurally characterized.

Crystal Structure Determination

Single crystals of suitable for X-ray diffraction studies were carefully chosen after they were viewed through a Leica microscope supported by a rotating polarizing stage and a CCD camera.

The diffraction data for crystals **1**-**9** were collected using a Bruker diffractometer equipped with a SMART APEX CCD area detector.[1a] The intensity data were processed using Bruker's suite of data processing programs (SAINT), and absorption corrections were applied using SADABS.[1b] The structure solution was carried out by direct methods, and the refinements were performed by full-matrix least-squares on F^2 using the SHELXTL suite of programs.[1c] All the structures converged to good *R*-factors. All the non-hydrogen atoms were

refined anisotropically, and the hydrogen atoms obtained from Fourier maps were refined isotropically.

The diffraction data of single crystals of **10**-**17** were collected on a Rigaku Saturn 724+ diffractometer using graphite monochromated Mo-Kα radiation. In these cases, data were processed with the Rigaku CrystalClear software.[2] The structure solution was carried out by direct methods, and the refinements were performed by full-matrix least-squares on F^2 using the SHELXTL[1c] suite of programs.

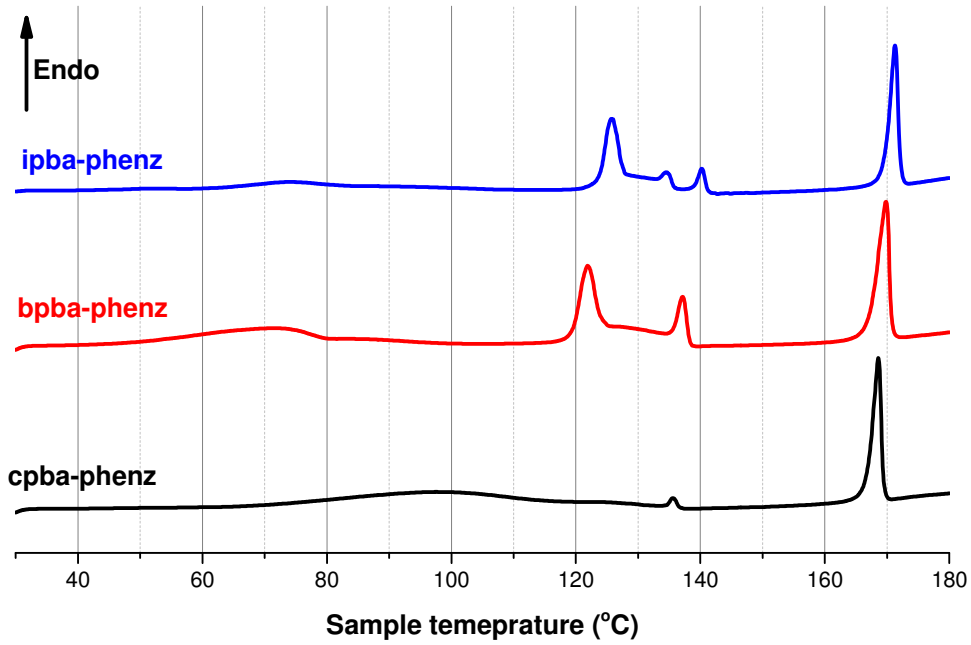
All calculations of intermolecular interactions were done with the HBOND NORM option of PLATON.[3]

References:

(1) a) Siemens, SMART System, Siemens Analytical X-ray Instruments Inc., Madison, WI, USA, **1995**; b) Sheldrick, G. M. SADABS Siemens Area Detector Absorption Correction Program, University of Gottingen, Gottingen, Germany, **1994**; c) Sheldrick, G. M. SHELXTL-PLUS Program for Crystal Structure Solution and Refinement, University of Gottingen, Gottingen, Germany.

(2) a) CrystalClear 2.1; Rigaku Corporation: Tokyo, Japan; b) Pflugrath, J. W. *Acta Crystallogr., Sect. D* **1999**, *55*, 1718–1725.

(3) Spek, A. L. PLATON, Molecular Geometry Program, University of Utrecht, The Netherlands, **1995**.



DSC plots of the complexes **10-12**

All the DSC curves exhibit small and broad humps with an onset temperature of ~60 °C. Interestingly, all the compounds have approximately same melting point (~170 °C).

Table 1: Crystallographic information of the structures **1-17.**

	1	***2***	***3***	***4***	***5***	***6***	***7***	***8***	***9***
Formula	($ClC_6H_6BO_2$): ($C_{10}H_8N_2$):(H_2O)	($BrC_6H_6BO_2$): ($C_{10}H_8N_2$): (H_2O)	($IC_6H_6BO_2$): ($C_{10}H_8N_2$): (H_2O)	($ClC_6H_6BO_2$): ($C_{12}H_8N_2$)	($BrC_6H_6BO_2$) ($C_{12}H_8N_2$)	2($IC_6H_6BO_2$): (C_{12} H_8 N_2)	($ClC_6H_6BO_2$): ($C_{12}H_{10}N_2$): (H_2O)	($BrC_6H_6BO_2$): ($C_{12}H_{10}N_2$): (H_2O)	2($IC_6H_6BO_2$): 3($C_{12}H_{10}N_2$)
CCDC Nos.	CCDC 603971	CCDC 603968	CCDC 603974	CCDC 603969	CCDC 603965	CCDC 603972	CCDC 603970	CCDC 603967	CCDC 603973
Formula Wt.	330.57	375.03	422.02	336.57	381.03	675.84	356.60	401.06	1042.30
Crystal habit	Block	Block	Block	Block	Block	Block	Block	Block	Plate
Crystal color	Colorless	Colorless	Colorless	Yellow	Yellow	Yellow	Colorless	Colorless	Colorless
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	12.606(5)	12.805(3)	13.251(5)	7.506(2)	7.621(4)	7.202(2)	12.259(5)	12.301(3)	10.129(4)
b (Å)	6.878(3)	6.834(1)	6.858(3)	9.118(2)	9.054(5)	34.347(8)	12.938(2)	12.969(2)	10.900(4)
c (Å)	18.873(8)	18.647(4)	18.594(8)	11.635(4)	11.668(6)	21.339(5)	13.211(3)	13.309(1)	12.521(4)
α (º)	90	90	90	79.24(3)	80.58(2)	90	96.91(1)	96.25(1)	69.96(8)
β (º)	102.79(7)	102.74(3)	103.50(7)	88.39(2)	88.21(2)	105.660(8)	116.79(2)	116.94(1)	66.85(8)
γ (º)	90	90	90	84.33(2)	84.07(2)	90	99.83(2)	100.13(1)	70.21(7)
V (Å^3)	1595.8(1)	1591.6(6)	1643.1(1)	778.4(4)	789.9(7)	5083(2)	1796.1(1)	1819.8(2)	1160.4(7)
Z	4	4	4	2	2	**8**	4	4	1
D_{calc} (g cm^{-3})	1.376	1.565	1.706	1.436	1.602	1.766	1.319	1.464	1.492
T(K)	133(2)	120(2)	133(2)	120(2)	120(2)	298(2)	120(2)	120(2)	298(2)
(λ)Mo K_α	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
μ(mm^{-1})	0.254	2.598	1.964	0.258	2.615	**2.508**	0.232	2.278	1.405
2θ range (º)	50.14	66.34	56.64	46.50	66.28	50.08	56.54	66.32	50.14
Total Reflns.	7645	25462	13672	6062	11774	25538	21875	35702	8478
Unique Reflns.	2806	6089	3837	2234	5648	8980	8872	13851	3961
Reflns. Used	2389	4546	3301	1960	4517	5605	6490	9042	1841
No. Parameters	272	216	272	225	273	625	507	495	284
GOF on F^2	1.161	1.005	1.085	1.135	0.936	1.000	1.029	0.896	0.830
Final R_1, wR_2	0.0566, 0.1430	0.0332, 0.0748	0.0395, 0.0886	0.0275, 0.0744	0.0289, 0.0650	0.0420, 0.1002	0.0465, 0.1246	0.0385, 0.0876	0.0549, 0.1271

	10	***11***	***12***	***13***	***14***	***15***	***16***	***17***
Formula	($ClC_6H_6BO_2$): ($C_{12}H_8N_2$),	($BrC_6H_6BO_2$): 2($C_{12}H_8N_2$): (H_2O)	($IC_6H_6BO_2$): 2($C_{12}H_8N_2$): (H_2O)	($IC_6H_6BO_2$): ($C_{12}H_8N_2$)	($BrC_6H_5BO_2$): ($C_{12}H_8N_2$): (H_2O)	($ClC_6H_6BO_2$): ($C_{13}H_9N$)	($BrC_6H_6BO_2$): ($C_{13}H_9N$)	($IC_6H_6BO_2$): ($C_{13}H_9N$)
CCDC Nos.	CCDC 958561	CCDC 958562	CCDC 958563	CCDC 958564	CCDC 958565	CCDC 958566	CCDC 958567	CCDC 958568
Formula Wt.	336.57	579.25	626.24	428.02	396.02	335.58	380.04	427.03
Crystal habit	Block	Block	Block	Acicular	Block	Block	Block	Block
Crystal color	Pale yellow	Pale green	Pale green	Pale green	Pale green	Pale yellow	Pale green	Pale green
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
a (Å)	6.939(4)	8.982(6)	8.996(5)	19.700(8)	7.095(4)	11.092(6)	7.218(4)	7.384(8)
b (Å)	9.959(5)	12.482(8)	12.502(6)	7.072(3)	10.015(6)	7.246(4)	11.132(6)	11.183(9)
c (Å)	12.125(7)	13.945(8)	14.051(7)	25.731(10)	13.341(8)	21.061(13)	11.861(7)	12.070(2)
α (°)	80.167(14)	109.230(5)	109.397(4)	90	90.954(13)	90	109.402(10)	110.2970(10)
β (°)	87.694(15)	95.719(5)	94.074(6)	107.705(6)	95.037(11)	99.211(11)	104.453(4)	103.060(2)
γ (°)	83.066(15)	110.223(7)	110.188(6)	90	93.988(14)	90	94.515(5)	94.720(2)
V (Å^3)	819.5(8)	1344.4(15)	1367.9(12)	3415(2)	941.8(10)	1671.0(17)	856.7(8)	896.4(12)
Z	2	2	2	8	2	4	2	2
D_{calc} (g cm^{-3})	1.364	1.431	1.520	1.665	1.397	1.334	1.473	1.582
T(K)	301(2)	301(2)	300(2)	300(2)	301(2)	301(2)	301(2)	301(2)
(λ)Mo K_α	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
μ(mm^{-1})	0.245	1.568	1.210	1.887	2.200	0.239	2.409	1.887
2θ range (°)	53.00	53.00	53.00	53.00	53.00	53.00	53.00	53.00
Total Reflns.	6674	11097	10922	26597	8124	10588	6963	6732
Unique Reflns.	3286	5387	5467	7044	4163	3809	3421	3555
Reflns. Used	1916	2449	3934	5504	1531	2274	1824	1869
No. Parameters	225	368	363	449	226	229	225	218
GOF on F^2	0.840	0.826	0.930	1.090	0.882	1.073	0.834	1.021
Final R_1, wR_2	0.0405, 0.0813	0.0519, 0.0944	0.0376, 0.0896	0.0540; 0.1271	0.0732; 0.2001	0.0665; 0.1341	0.0481; 0.1114	0.0920; 0.2804

Table 2: Characteristics of various intermolecular interactions (distances/Å and angles/º) [#]

Compound	Interaction type							
	O–H···O	**O–H···N**	**C–H···O**	**C–H···N**	**C–H···Cl**	**C–H···Br**	**C–H···I**	**X···X/X···N**
1	1.86 2.79 158 2.05 2.96 154	1.74 2.71 172 1.92 2.86 159	2.66 3.71 163 2.84 3.65 131		2.95 3.74 130			
2	1.91 2.78 147 1.98 2.95 171	1.78 2.70 154 1.89 2.86 169	2.60 3.64 161 2.75 3.83 175			3.00 3.84 134		
3	1.85 2.79 160 2.03 3.02 177	1.74 2.71 166 1.89 2.86 167	2.55 3.60 158 2.62 3.52 140				3.28 4.12 136	
4	1.76 2.66 155 1.79 2.67 151 1.93 2.80 146	1.81 2.78 169 1.82 2.77 162 1.83 2.77 161	2.47 3.47 152 2.56 3.62 166 2.58 3.59 154	2.69 3.79 179 2.97 3.81 135	2.66 3.71 161 2.77 3.73 148			
5	1.75 2.70 157 1.79 2.69 152 1.92 2.81 147	1.81 2.76 161 1.82 2.79 167 1.83 2.77 159	2.48 3.45 149 2.51 3.51 154 2.55 3.63 169	2.66 3.76 177 2.76 3.65 139		2.79 3.84 161 2.85 3.78 145		**(Br···Br)** 3.42
6		1.81 2.74 157 1.95 2.84 151						**(I···N)** 3.09
7	1.78 2.76 177	1.74 2.70 164	2.36 3.30 142 2.57 3.36 129	2.80 3.80 152				
8	1.78 2.76 171	1.76 2.70 159	2.44 3.35 141 2.54 3.37 132	2.74 3.77 159				
9	1.73 2.71 171 1.78 2.76 173 1.80 2.78 173 1.86 2.84 175	1.78 2.75 168 1.81 2.77 165 1.82 2.76 159	2.28 3.22 144					**(I···I)** 3.78

[#]The three numbers in each column indicate H···A, D···A distances and D–H···A angles, respectively.

Compound	Interaction type				
	O–H···O	**O–H···N**	**C–H···O**	**C–H···N**	**C–H···Cl**
10	1.82 2.81 179	1.91 2.86 164	2.70 3.48 129 2.81 3.80 153	2.57 3.40 133 2.63 3.63 154	2.76 3.74 150
11	1.72 2.70 173 1.96 2.92 165	1.87 2.84 169 1.87 2.82 163	2.78 3.39 127 2.61 3.57 146 2.66 3.59 144 2.68 3.56 138 2.69 3.69 154 2.90 3.55 126 2.83 3.54 123 2.90 3.65 126	2.50 3.53 159 2.78 3.55 128 2.82 3.68 136	
12	1.76 2.71 161 1.92 2.88 165	1.87 2.84 172 1.89 2.86 166	2.62 3.58 147 2.58 3.55 148 2.69 3.45 127 2.71 3.72 155 2.74 3.63 140 2.91 3.66 126 2.89 3.54 119	2.49 3.53 160 2.77 3.64 137 2.80 3.56 128	
13	1.79 2.77 174 1.91 2.85 159	1.86 2.82 163 1.89 2.83 161	2.52 3.35 132 2.65 3.63 149 2.77 3.54 128	2.92 3.96 161 2.63 3.45 131 2.66 3.41 126 2.72 3.45 124 2.96 3.71 127	
14	– 1.78 –	1.97 2.85 148	2.91 3.72 132	2.59 3.62 159 2.70 3.56 136	
15	1.81 2.76 162	1.76 2.71 162	2.38 3.43 162 2.91 3.80 140 2.92 3.59 121		2.86 3.76 141 2.94 3.79 136
16	1.79 2.76 171	1.78 2.74 164	2.36 3.42 164 2.90 3.60 123 2.90 3.61 124	2.72 3.58 137	
17	1. 82 2.79 169	1.86 2.75 149	2.37 3.42 163 2.93 3.81 139 2.94 3.66 124 2.95 3.65 123	2.70 3.60 140	

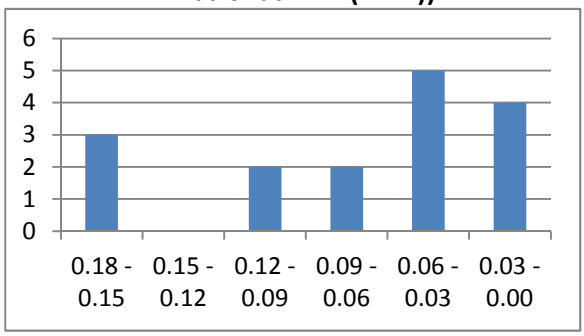
[#]The three numbers in each column indicate H···A, D···A distances and D–H···A angles, respectively.

CSD Analysis Compilation

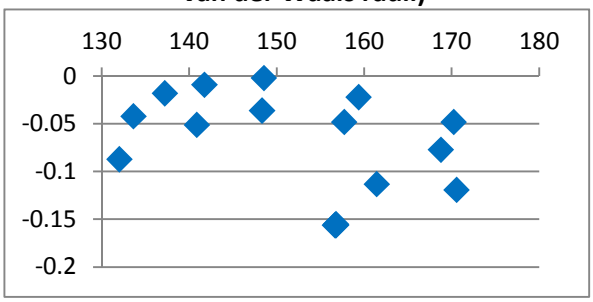
Cl···N$_{(alicyclic)}$ interactions

No.	REFCODE	C–X–N angle (°)	X···N distance (Å)
1	BELYUN	141.716	3.291
2	BELYUN01	137.191	3.282
3	DAPLUC	159.337	3.278
4	ELEYEZ	133.607	3.258
5	GALDON	157.692	3.252
6	HAZPHZ	156.627	3.144
7	HAZPHZ	156.749	3.144
8	HAZPHZ	156.746	3.145
9	KIKCUD	168.736	3.223
10	MELFIT	161.412	3.187
11	OCAKOT	170.203	3.252
12	OGEWIG	148.297	3.264
13	UPIQAM	170.53	3.181
14	UXIYOQ01	131.996	3.213
15	WUBWOF	148.503	3.298
16	CEFRIQ	140.847	3.249

No. of Hits plotted against (sum of van der Waals radii – D(X···N))



C–X–N angle plotted against (D(X···N) – sum of van der Waals radii)



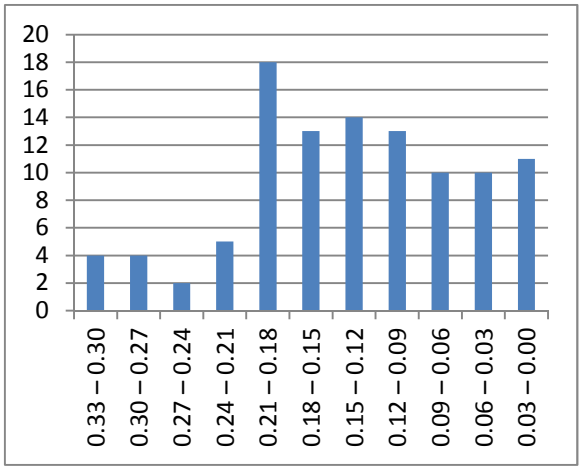
Mean angle: 152.51°; Mean distance: 3.22 Å

Cl···N$_{(aromatic)}$ interactions

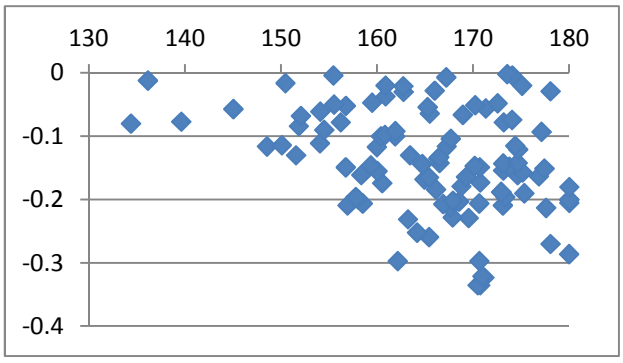
No.	REFCODE	C–X–N angle (°)	X···N distance (Å)
1	NEHBAF	166.34	3.165
2	ADILUV	158.495	3.094
3	AJIGOP	139.616	3.223
4	ANORUR	173.538	3.298
5	AYEFIT	172.535	3.252
6	BAGWAI	161.881	3.2

7	BIHNEL	173.084	3.091
8	BIZFEW	157.772	3.104
9	CAVYIH	160.818	3.202
10	CEHXIW	149.157	2.553
11	CEXOXP	156.735	3.151
12	DCMPHN10	174.675	3.179
13	DEPFUZ	154.048	3.189
14	DICYIY	174.073	3.296
15	DUNSUB	170.617	3.094
16	DUNSUB	157.972	3.101
17	DUWKAI	160.033	3.145
18	ECACIU	148.53	3.184
19	ECIWIX	167.853	3.072
20	ECIWIX	170.682	3.151
21	ETOZOC	167.893	3.098
22	FARQAR	175.317	3.11
23	FARQAR	165.386	3.135
24	FOHGAL	175.086	3.28
25	GUKBUJ	163.428	3.17
26	GUKJEC	171.302	3.244
27	GUZLIX	168.777	3.121
28	HCPYIN	174.624	3.158
29	HCTDPY	150.082	3.186
30	HUFXUB	154.08	3.239
31	HUFXUB	166.881	3.093
32	HUGDAP	162.143	3.003
33	HURSUI	178.04	3.03
34	IFULUQ04	158.356	3.139
35	ILEKEP	169.518	3.071
36	ILEKEP01	169.266	3.136
37	IPCLTZ10	177.407	3.149
38	JAKWIC	162.752	3.27
39	JEHYIF	155.517	3.25
40	JODLOE	170.203	3.249
41	KADPAG	160.522	3.126
42	KEMZIM	174.046	3.226
43	KEYWER	164.165	3.048
44	LAPLAR	176.839	3.137
45	LIQPUW	168.921	3.234
46	MAGZIE	165.4	3.041
47	MAGZIE	167.597	3.088
48	MCPYZF	174.368	3.185
49	MEDPEQ	162.719	3.279
50	MOLFUP	165.994	3.272
51	MOSRUI	167.67	3.196
52	MOSRUI	156.746	3.248

No. of Hits plotted against (sum of van der Waals radii – D(X···N))



C–X–N angle plotted against (D(X···N) – sum of van der Waals radii)



53	MUSZIK	180	3.095
54	MUSZOQ	177.587	3.087
55	NAMTOM	156.922	3.091
56	OLALUI	166.129	3.116
57	PACMEN	167.195	3.293
58	PCLPYR	179.98	3.014
59	PIJBIT	177.108	3.207
60	PIJBOO	168.52	3.097
61	PIJBOZ	150.456	3.284
62	PUKRAP	160.403	3.2
63	PUKRAP	156.216	3.222
64	REJMAU	173.178	3.222
65	REMDIW	134.373	3.22
66	REMDIW	178.042	3.271
67	RETMOT	170.638	3.003
68	RIYXIH	159.975	3.183
69	ROZTOQ	159.482	3.253
70	RUJJIQ	159.349	3.154
71	RUPYIK	160.874	3.28
72	RUPYOQ	167.24	3.184
73	SEQJED	165.251	3.246
74	TEGYAF	170.73	3.127
75	TIKVAL	145.037	3.243
76	TITVIC	161.888	3.208
77	UHAPIC	175.132	3.143
78	UHAPIC	173.341	3.104
79	UHOBID	163.211	3.069
80	UMUYUX	136.149	3.288
81	VACFEM	151.851	3.216
82	VOCHOL	154.49	3.21
83	VOJYEZ	166.495	3.158
84	VUGSIZ	180	3.1
85	VUGSIZ	172.912	3.112
86	VUGSIZ02	173.13	3.146
87	VUGSIZ02	180	3.12
88	VUGSIZ10	180	3.1
89	VUGSIZ10	172.912	3.112
90	WARYAQ	173.118	3.157
91	WARYAQ	170.157	3.153
92	WASBAV	155.451	3.296
93	WIBYUB	174.618	3.139
94	WUVLIJ	164.925	3.132
95	WUVLIJ01	164.694	3.156
96	WUVLOP	166.459	3.167
97	XAJRIL	173.767	3.152
98	XUDRAQ	165.479	3.236

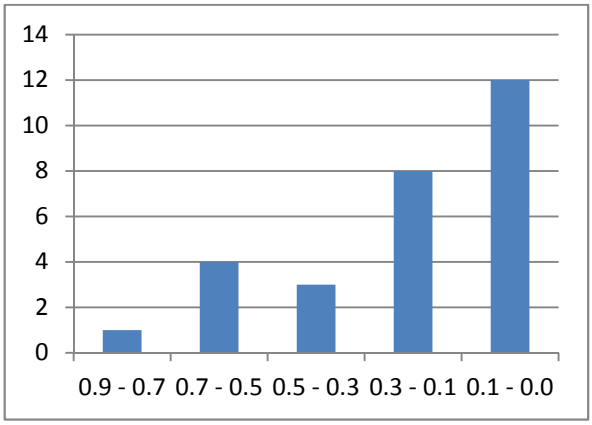
99	YICPOQ	152.072	3.232
100	YUZGUV	160.878	3.263
101	MEBGOR	170.739	2.965
102	MEBGOR	170.943	2.979
103	MEBGUX	171.157	2.977
104	MEBGUX	170.466	2.965
105	FEQHIU	151.558	3.17

Mean angle: 164.03°; Mean distance: 3.13 Å

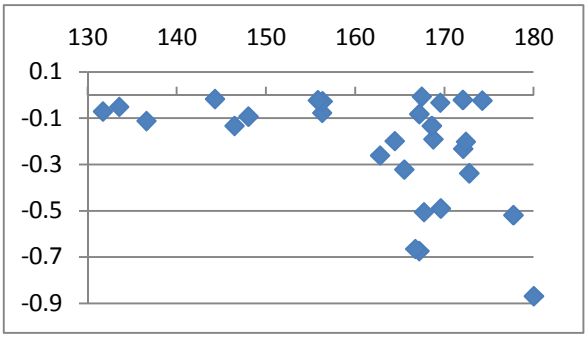
Br···N$_{(alicyclic)}$ interactions

No.	REFCODE	C–X–N angle (°)	X···N distance (Å)
1	BFHMTA	172.759	3.062
2	BPMBPA	167.44	3.393
3	BPZCHX10	168.74	3.209
4	CAHZIW	174.225	3.376
5	DIVDOC	177.722	2.881
6	DIVDUI	169.573	2.91
7	DIVDUI	167.689	2.894
8	EDEWAM	172.388	3.198
9	EDEWAM	146.457	3.267
10	EXEJOH	164.417	3.201
11	EXEKAU	167.171	3.318
12	EXEKAU	168.575	3.267
13	FEGYAR01	166.715	2.735
14	FEGYAR01	167.158	2.726
15	FEGYEV	180	2.531
16	GOTQEL	162.77	3.139
17	HILYAD	156.327	3.373
18	HIRJAU	172.05	3.379
19	HOPDAS	155.805	3.377
20	LUQMIT	144.268	3.383
21	NUHGIH	133.538	3.349
22	OGEWOM	148.01	3.307
23	QUYFUM	169.515	3.367
24	TAPZEP	156.279	3.323
25	USOJOC	165.476	3.078
26	UXIZAD	136.592	3.288
27	UXUHUR	131.71	3.329
28	VORGOZ	172.085	3.168

No. of Hits plotted against (sum of van der Waals radii – D(X···N))



C–X–N angle plotted against D(X···N) – sum of van der Waals radii)

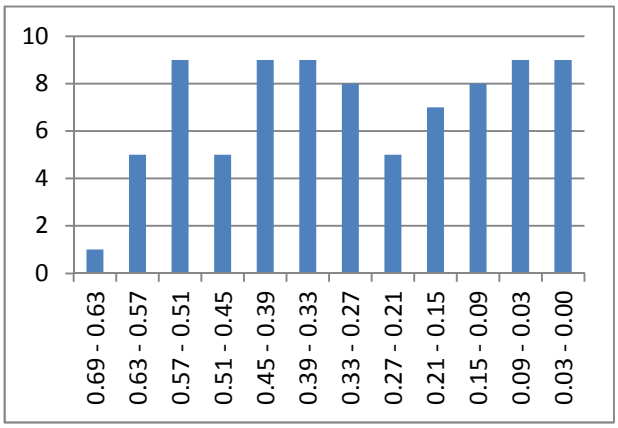


Mean angle: 161.98°; Mean distance: 3.17 Å

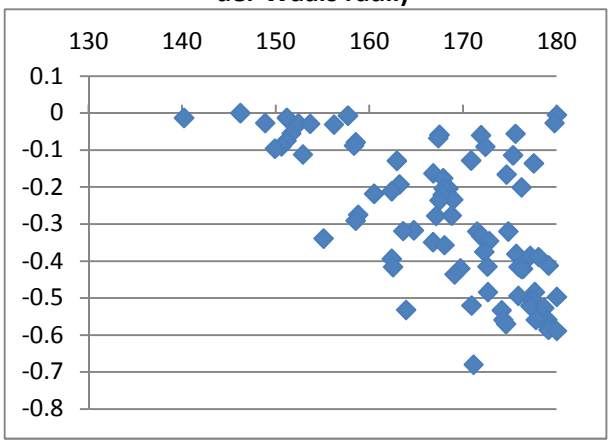
Br···N$_{(aromatic)}$ interactions

No.	REFCODE	C–X–N angle (°)	X···N distance (Å)
1	LEFMIU	169.703	2.98
2	AJEQAH	174.809	3.08
3	BEPYRZ10	175.666	3.019
4	BRADOS	178.05	3.011
5	BRADOS01	177.157	3.014
6	DAMNAI	171.913	3.34
7	EMEJIP	146.207	3.4
8	ENUCIA	167.459	3.341
9	EPIWAC	177.333	2.896
10	EQOVUC	175.588	3.344
11	EQOVUC	160.484	3.182
12	FIHSOF	172.783	3.054
13	FOKSIH	168.947	3.166
14	GUZLET	162.369	3.006
15	GUZLIX	152.883	3.288
16	GUZMAQ	175.331	3.286
17	HUFWAH	168.004	3.043
18	HUFWAH	169.08	2.964
19	HUKPIM	172.369	3.309
20	IKAVEW	150.594	3.31
21	IKUHUR	179.111	2.814
22	IKUHUR01	178.653	2.873
23	IKUHUR02	179.005	2.841
24	IKUHUR03	179.075	2.829
25	IKUHUR05	179.185	2.822
26	IKUJAZ	174.288	2.841
27	IKUJIH	179.121	2.988
28	IKUJIH	175.918	2.984
29	IKUJIH	172.641	2.916
30	IKUJIH	163.897	2.868
31	IKUJON	170.894	2.88
32	IKUJON	162.51	2.984
33	IKUJUT	177.211	2.878
34	IKUJUT	176.402	2.979
35	IKUJUT01	177.215	2.88
36	IKUJUT01	176.248	2.978
37	ILISIF	177.537	3.264
38	ISAFUE	158.526	3.321
39	IVETOS	157.682	3.393
40	JICWIB10	171.109	2.72
41	JICWIB10	174.577	2.83

No. of Hits plotted against (sum of van der Waals radii – D(X···N))



C–X–N angle plotted against D(X···N) – sum of van der Waals radii)



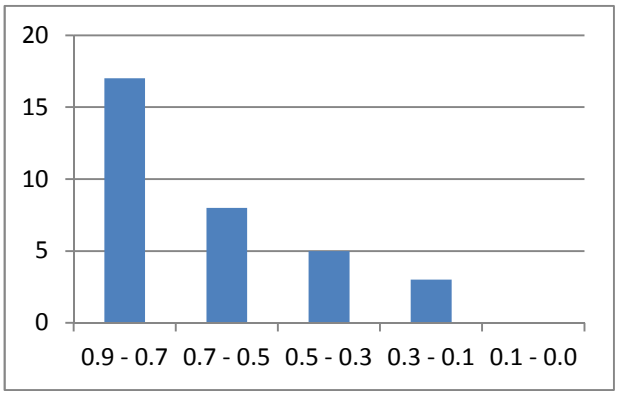
42	KAVFIX	177.764	2.841
43	KELGEO	151.125	3.325
44	KETWIQ	152.397	3.372
45	KEZNEJ	166.783	3.051
46	KOTMIP	151.163	3.387
47	KUSPIY	149.896	3.304
48	MIHQOK	151.651	3.345
49	MOSJUA	171.487	3.08
50	MOSJUA	140.18	3.387
51	OCILAP	180	2.811
52	PAMLOG	148.854	3.373
53	QIHDAM	172.256	3.025
54	RAQJIE	158.789	3.125
55	RIRFOO	167.463	3.164
56	SIBTAZ	180	3.395
57	SIBTAZ01	180	2.903
58	SITNOZ	167.785	3.179
59	SUGTIY	174.632	3.234
60	SULWEC	155.088	3.061
61	TAQVIR	176.234	3.199
62	TEKWAH	158.332	3.312
63	TIWNIX	174.109	2.867
64	TORDOU	167.103	3.122
65	UBEZAC	170.855	3.272
66	UCURIV	171.906	3.067
67	USOJIW	156.199	3.369
68	VESVEV	168.764	3.123
69	VOMGUA	172.585	2.985
70	VUZJOQ	163.19	3.207
71	WASHEE	158.52	3.109
72	XAZLOA	153.659	3.371
73	XEBSIH	179.753	3.373
74	XEHLAY	166.801	3.237
75	XESQOB	167.862	3.224
76	XOHWUN	177.653	2.916
77	XOKGEK	164.723	3.083
78	YEDTIL	162.364	3.189
79	YIQFEK	162.923	3.271
80	YOFWUM	163.59	3.081
81	YOFWUM	175.888	2.906
82	YULYOU	167.336	3.332
83	ZEBZAH	167.914	3.196
84	ZEBZAH01	168.429	3.196

Mean angle: 168.11°; Mean distance: 3.11 Å

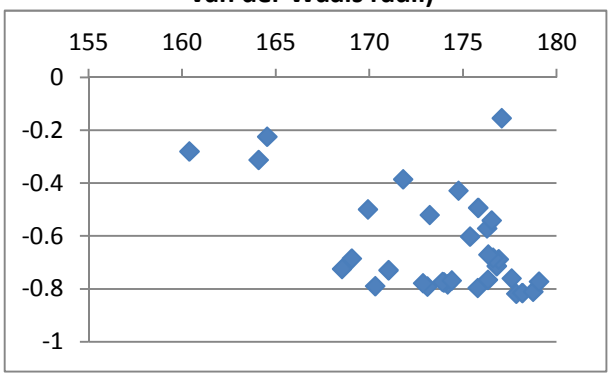
I···N$_{(alicyclic)}$ interactions

No.	REFCODE	C–X–N angle (°)	X···N distance (Å)
1	DATCEI	170.302	2.741
2	DATCEI	171.013	2.801
3	DATCIM	173.89	2.757
4	AHEVIT	176.337	2.86
5	AHEVOZ	176.598	2.848
6	DIVCUH	176.893	2.842
7	HEXAIF10	176.52	2.989
8	HEXAIF10	175.799	3.037
9	IPUDED	171.792	3.145
10	ISIHUN	174.169	2.748
11	ISIHUN	173.089	2.739
12	ISIHUN01	172.853	2.752
13	ISIHUN01	173.969	2.755
14	MASWEK	178.735	2.72
15	MASWEK	178.162	2.715
16	MIDKOA	174.75	3.102
17	MORIPA01	177.834	2.712
18	NUHGUT	164.533	3.306
19	NUHHAA	160.379	3.25
20	PEHTOM	177.058	3.376
21	QIHCIT	173.212	3.01
22	QIHCOZ	169.051	2.845
23	QIHCOZ01	168.529	2.806
24	QIHCUF	169.913	3.031
25	RUWVOV	179.049	2.758
26	RUWVOV	177.586	2.77
27	ULOKEL	176.791	2.817
28	VOHHOQ	164.074	3.218
29	VOMHOV	175.367	2.928
30	VOMHOV	176.273	2.959
31	VUJSOJ	176.319	2.765
32	VUJSOJ	175.772	2.734
33	VUJSOJ01	174.389	2.762

No. of hits plotted against (sum of van der Waals radii – D(X···N))



(C–X–N angle plotted against D(X···N) – sum of van der Waals radii)

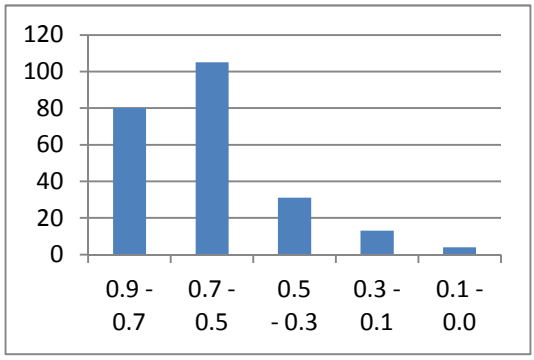


Mean angle: 173.67°; Mean distance: 2.90 Å

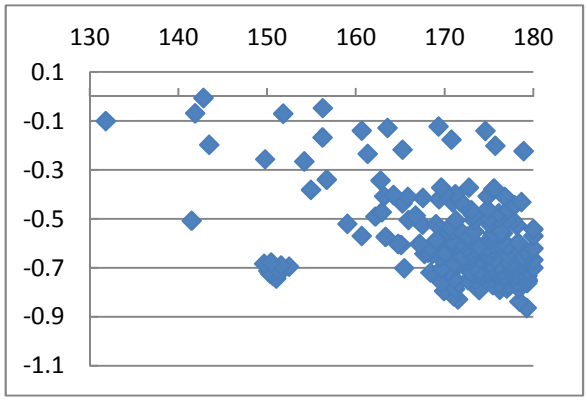
I···N$_{(aromatic)}$ interactions

No.	REFCODE	C–X–N angle (°)	X···N distance (Å)
1	ADOLIP	172.861	2.86
2	ANUPUV	174.826	3.123
3	ANUPUV	169.012	3.009
4	BAGCET	170.907	2.983
5	BAGCET	170.373	2.977
6	BAGCIX	180	2.91
7	BAGCOD	174.813	3.07
8	BAGCUJ	175.027	3.011
9	BAGDEU	177.697	3.024
10	BERQUK	171.787	3.101
11	BUFWAB	172.736	3.158
12	CAHZOC	169.645	2.772
13	CAHZUI	173.38	3.023
14	CAHZUI	177.071	3.028
15	CAJBAS	131.807	3.43
16	COKNOG	176.973	2.794
17	COKNUM	176.7	2.802
18	COWHUS	170.736	2.941
19	COWJAA	178.132	3.004
20	CUPJAZ	174.21	2.909
21	CUPJED	175.475	2.926
22	CUPJIH	174.7	2.88
23	CUPJON	177.83	2.848
24	CUPJUT	175.546	2.817
25	CUPKAA	172.052	2.872
26	CUPKEE	171.494	2.702
27	CUPKII	178.428	2.693
28	DARZOM	171.541	2.989
29	DARZOM	170.893	3.098
30	DENMIT	176.997	2.746
31	DIXXEO	175.994	2.931
32	DIXXEO	169.309	3.408
33	DOKZUZ	156.26	3.483
34	DUJSAD	175.701	3.329
35	EPIVUV	167.502	3.006
36	EPIWEG	170.036	3.133
37	EQOWEN	178.899	3.307
38	EQOWEN	162.777	3.187
39	ETOZOC	177.886	3.086
40	EVANUL	178.656	3.099
41	EXIFAT	165.098	2.924

No. of hits plotted against (sum of van der Waals radii – D(X···N))



(C–X–N angle plotted against D(X···N) – sum of van der Waals radii)



42	EXIFEX	154.928	3.149
43	EXIFIB	156.239	3.363
44	GIDMAI	173.81	2.919
45	GIDMEM	175.025	2.882
46	HETMAV	178.271	2.934
47	HETMAV	173.388	2.907
48	HETMAV	176.204	2.741
49	HETMAV	176.161	2.84
50	HETMAV	171.358	2.926
51	HETMAV	173.333	2.979
52	HETMEZ	175.637	2.867
53	HETMEZ	178.875	2.842
54	HETMEZ	177.314	2.819
55	HETMEZ	173.926	2.869
56	HETMEZ	178.583	2.813
57	HETMEZ	175.224	2.849
58	HIZBEY	178.389	2.801
59	HOFGEO	180	2.988
60	IETPYA10	176.452	2.974
61	IHUMON	174.743	2.885
62	IHUMUT	168.359	2.915
63	IHUNEE	175.361	2.949
64	IHUNUU	174.393	2.895
65	IHUNUU	172.413	2.913
66	IMEZOP	165.24	3.094
67	IQEWIK	168.401	2.811
68	ISIJEZ	169.369	3.111
69	ISIJEZ01	169.611	3.158
70	ISOFAY	176.755	2.798
71	ISOFEC	176.274	2.967
72	ITUJEN	151.804	3.46
73	JAQMAQ	177.147	3.067
74	JAQMEU	174.881	2.821
75	JAQMIY	159.03	3.01
76	JAQMIY	149.759	3.274
77	KABLAC	177.926	2.838
78	LACWOD	175.035	3.032
79	LACWOD	172.141	3.087
80	LEZPIQ	180	2.863
81	LEZPOW	180	2.961
82	LEZPUC	180	2.831
83	LEZPUC01	178.691	2.841
84	LEZQAJ	173.888	2.806
85	LOCJIX	171.202	3.131
86	LUKMIN	170.572	2.998
87	MASWAG	175.333	2.832

88	MAVVEM	156.7	3.191
89	MAVVIQ	162.912	3.058
90	MEKWOO	175.839	2.793
91	MIYKOU	172.074	2.928
92	MIYKOU	172.452	2.909
93	MIYKOU	176.158	2.964
94	MIYKOU	175.364	2.958
95	MIYKOU01	172.964	2.871
96	MIYKOU01	174.821	2.915
97	MIYKOU01	171.764	2.936
98	MIYKOU01	170.093	2.889
99	MIYKOU01	173.115	2.88
100	MIYKOU01	175.064	2.945
101	MIYKOU01	178.026	2.917
102	MIYKOU01	173.102	2.892
103	PAMLIA	176.782	2.822
104	PAMLOG	171.26	3.025
105	PAMLUM	173.213	3.046
106	PAPRIJ	175.538	2.808
107	PELLUO	167.535	3.116
108	PIFVIK	175.156	2.817
109	PIFWAD	177.298	2.756
110	PIFWAD	170.995	2.715
111	PIFWAD	178.381	2.746
112	PIFWAD	169.919	2.736
113	PUKHUZ	174.586	3.39
114	PUXLOJ	164.232	3.128
115	QABZUQ	177.661	2.794
116	QABZUQ	162.188	3.04
117	QABZUQ	173.289	2.837
118	QABZUQ	174.038	2.913
119	QACBAZ	177.85	2.819
120	QACBAZ	178.767	2.816
121	QACBAZ	177.616	2.791
122	QACBAZ	175.33	2.785
123	QIHBAK	176.047	3.032
124	QIHBEO	177.271	2.851
125	QIHBEO01	176.949	2.864
126	QIHBEO02	177.129	2.822
127	QIHBEO03	177.039	2.829
128	QIHBIS	169.065	2.944
129	QIHCAL	179.288	2.811
130	QIHCAL01	179.32	2.78
131	QIHCAL02	179.321	2.784
132	QIHCAL03	179.312	2.82
133	QIHCAL04	179.329	2.798

134	QIHCAL05	179.347	2.776
135	QIHCAL06	179.282	2.768
136	QIHCEP	178.704	2.843
137	REWGIJ	165.923	3.026
138	RIWZIH	172.712	2.943
139	RIWZIH	177.125	2.838
140	RUYHID	179.245	2.667
141	RUYHOJ	174.304	2.8
142	RUYHOJ	174.596	2.781
143	RUYHOJ	171.085	2.783
144	RUYHOJ	171.176	2.744
145	RUYHUP	178.519	2.768
146	RUYHUP	168.107	2.892
147	RUYJAX	168.581	2.886
148	RUYJAX	176.149	2.766
149	SAMYAH	160.655	3.391
150	SAMYAH	154.181	3.265
151	SIMHAY	175.631	2.901
152	SUWYIT	178.813	2.798
153	SUWYOZ	176.867	2.784
154	SUWYOZ	176.597	2.8
155	TIWNET	175.086	2.812
156	TOJBAW	174.766	2.808
157	TOJBAW	178.046	2.804
158	TOJBEA	173.814	2.81
159	TOJBOK	176.103	2.843
160	TOJBUQ	173.47	2.779
161	TOJBUQ	172.627	2.78
162	TOJCAX	174.65	2.879
163	TOJCAX	178.828	2.875
164	TOJCAX	174.811	2.819
165	TOJCAX	175.275	2.829
166	TOJCEB	165.85	3.121
167	TONMAL	169.501	2.872
168	ULOKUB	170.766	2.928
169	UYOVIO	175.495	3.152
170	UYOVIO	175.564	3.155
171	UYOVOU	176.784	3.12
172	VABNUJ	172.649	2.959
173	VEBQEZ	176.085	3.054
174	VEBQEZ	166.72	3.044
175	VITKOZ	167.716	2.888
176	VOMHAH	175.446	2.97
177	VOMHIP	176.548	2.971
178	VUJTAW	172.015	2.874
179	WANNOP	169.668	2.828

180	WANNUV	172.942	2.812
181	WANNUV	173.883	2.74
182	WANNUV01	174.821	2.805
183	WANPAD	175.424	2.76
184	WANPAD	171.511	2.769
185	WANPAD	175.616	2.803
186	WANPAD	178.425	2.798
187	WANPEH	177.588	2.789
188	WANPIL	169.728	2.827
189	WANPOR	170.474	2.817
190	WEXVUR	165.443	2.829
191	WEXVUR	173.192	2.799
192	WEXVUR	160.655	2.961
193	WEXVUR	167.165	2.928
194	WEXWAY	171.135	2.846
195	WEXWAY	173.953	2.821
196	WEXWEC	164.745	2.928
197	WEXWEC	171.525	2.842
198	WOJQAN	173.01	3.066
199	WOJQOB	163.185	3.123
200	WUZMUZ	176.617	2.823
201	WUZMUZ	177.076	2.92
202	XOHWIB	178.103	2.915
203	XOHWOH	179.067	2.9
204	XUHNUJ	178.063	2.771
205	YIPCIK	177.741	2.858
206	YIPCIK	179.037	2.859
207	YUHLAP	151.151	2.825
208	YUHLAP	152.47	2.835
209	YUHLAP	150.442	2.853
210	YUHLAP	151.557	2.84
211	YUHLAP	150.317	2.808
212	YUHLAP	149.656	2.847
213	YUHLAP	151.551	2.817
214	YUHLAP	150.133	2.818
215	YUHLET	150.658	2.797
216	YUHLET	151.018	2.787
217	YUHLIX	176.472	2.937
218	YUHLOD	163.336	2.957
219	YUHLOD	141.479	3.023
220	TEGGET	170.439	2.818
221	TEGGET	173.472	2.807
222	IFOQUI01	176.357	2.98
223	NEJVIJ	172.399	2.859
224	NEJVOP	176.311	2.819
225	TEPKEG	169.239	2.944

226	TEPKEG	175.383	2.908
227	TEPKIK	161.318	3.296
228	TEPKIK	177.033	2.886
229	TEPKOQ	178.893	2.863
230	TEPLAD	143.457	3.333
231	TEPLAD	165.251	3.313
232	TEPLAD	170.761	3.354
233	TEPLAD	141.877	3.462
234	VEMTIS	163.557	3.402
235	YANHOM	142.822	3.524

Mean angle: 171.49°; Mean distance: 2.93 Å