Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Fenamic acid crystal with two asymmetric units (Z′ = 2): why Z′ =2 rather than Z′ =1?

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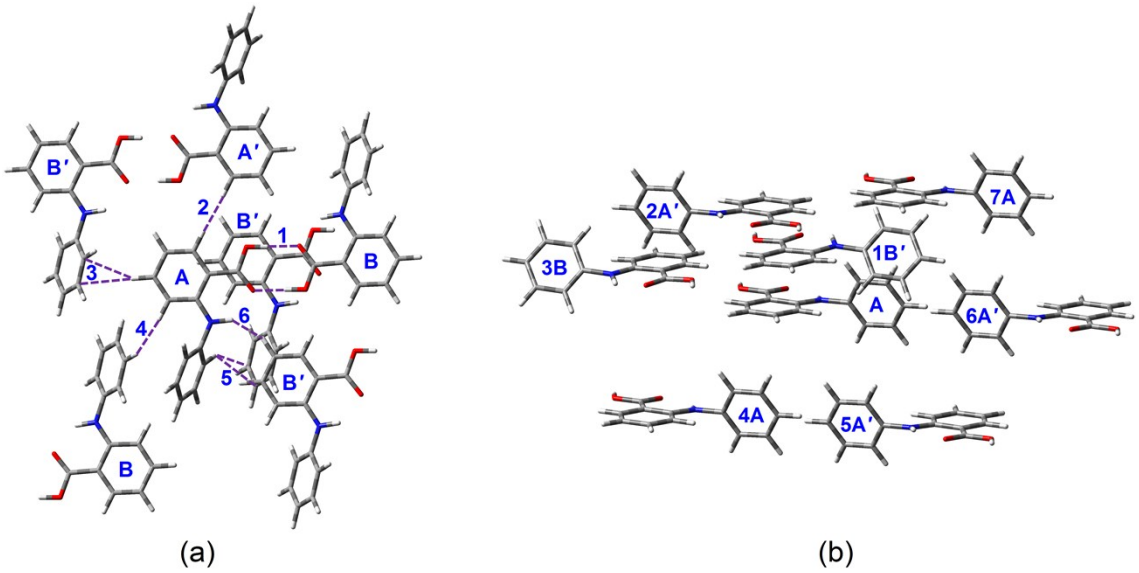

Fig. S1 Six FA molecules interacting with conformer **A** through close contacts (a); seven FA molecules interacting with conformer **A** through π-π interactions (b). The number represents the different complex formed between molecules.

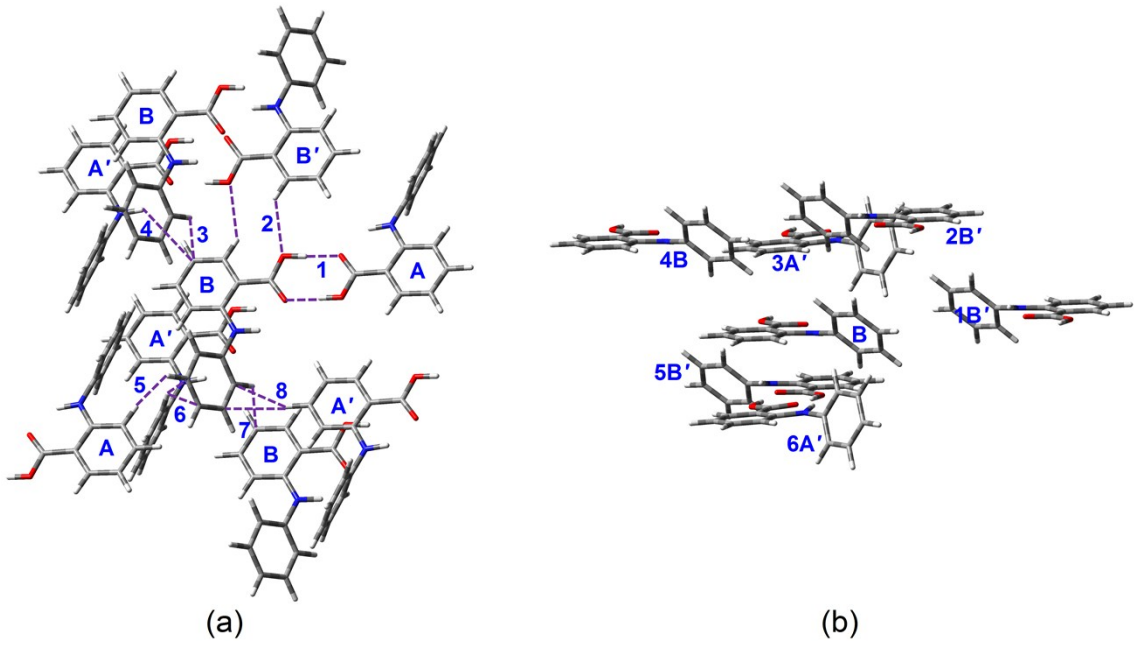

Fig. S2 Eight FA molecules interacting with conformer **B** through close contacts (a); six FA molecules interacting with conformer **B** through π-π interactions (b). The number represents the different complex formed between molecules.

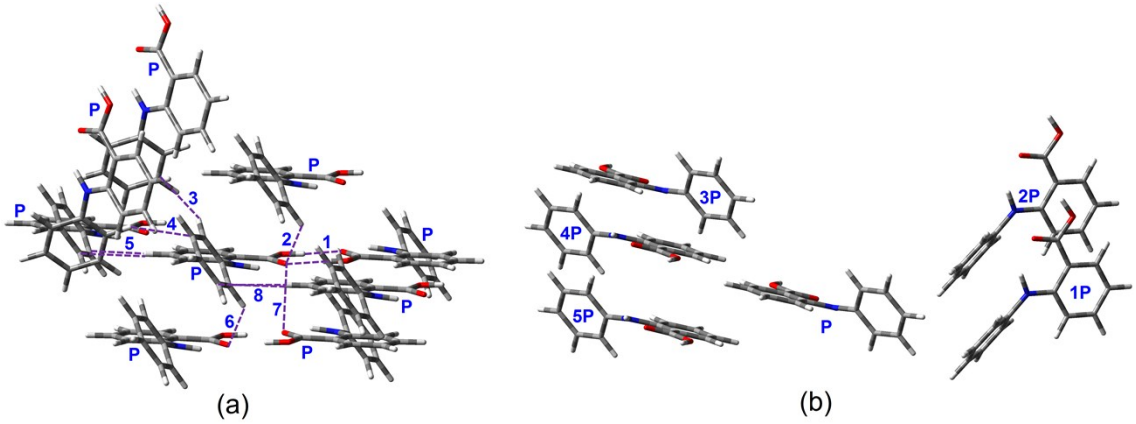

Fig. S3 Eight FA molecules interacting with conformer **P** through close contacts (a); five FA molecules interacting with conformer **P** through π-π interactions (b). The number represents the different complex formed between molecules.

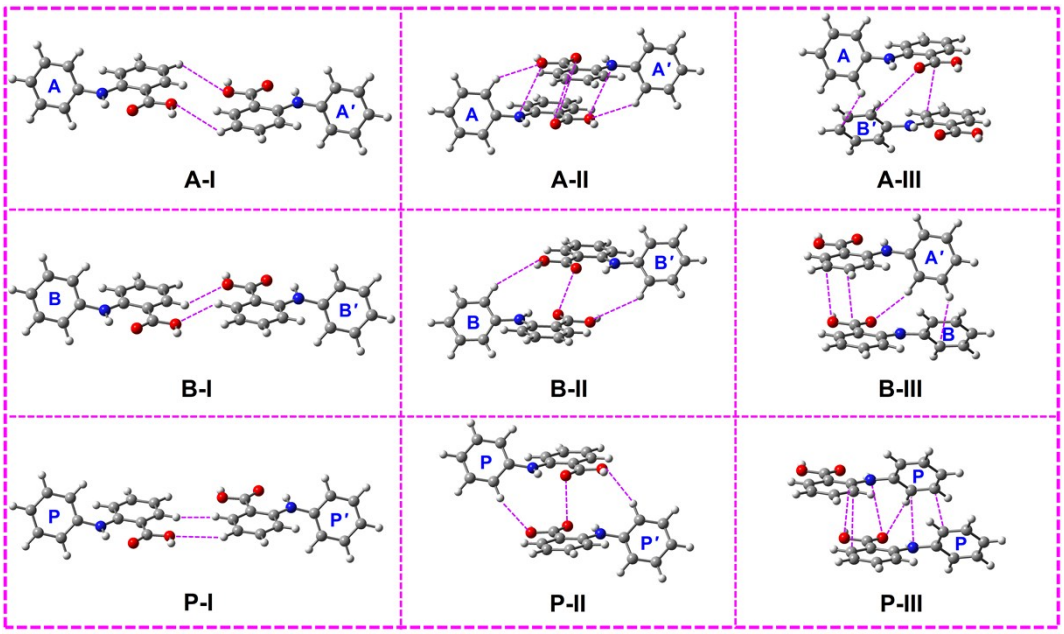

Fig. S4 The molecular pairs (type 1) of the adjacent molecules directly interacting with the carboxyl groups of **A**, **B** and **P** in the partly optimized (Z′=2) and predicted (Z′=1) FA crystals and the interacting atoms at BCPs listed in Table S2.

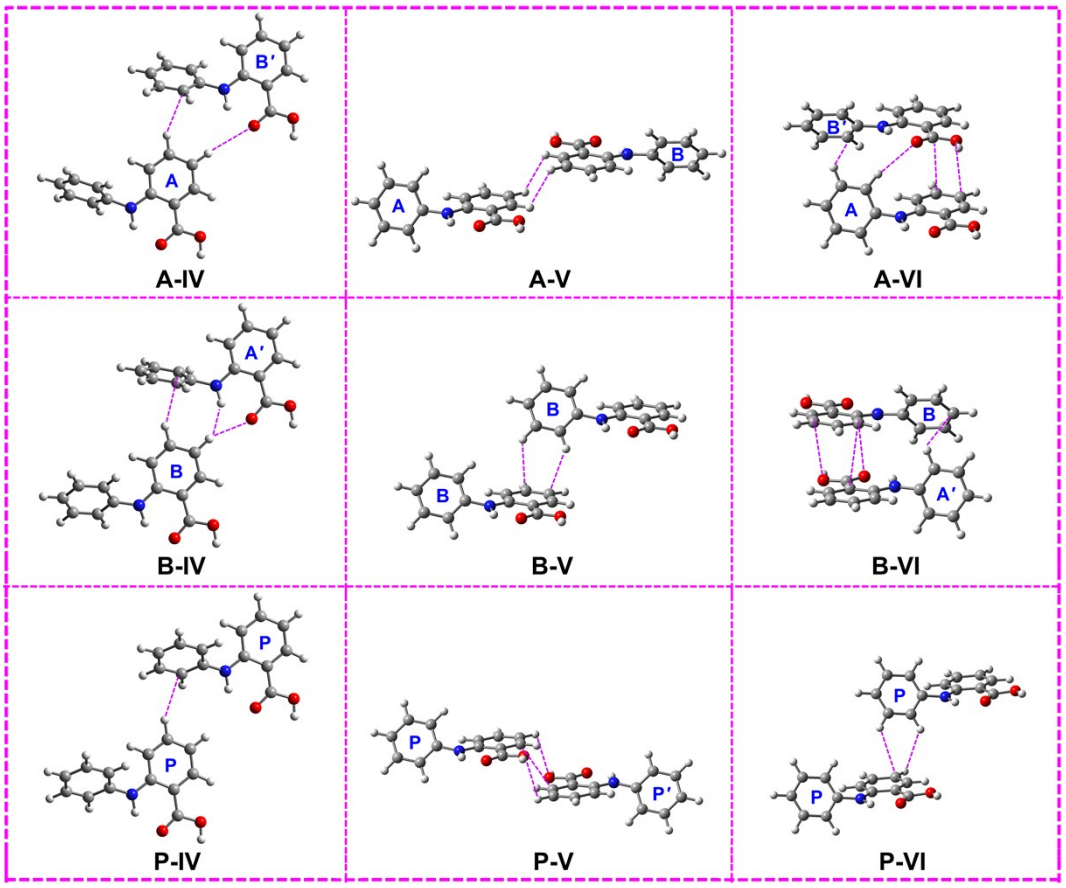

Fig. S5 The molecular pairs (type 2) of the adjacent molecules directly interacting with the carboxyl groups of **A**, **B** and **P** in the partly optimized (Z′=2) and predicted (Z′=1) FA crystals and the interacting atoms at BCPs listed in Table S3.

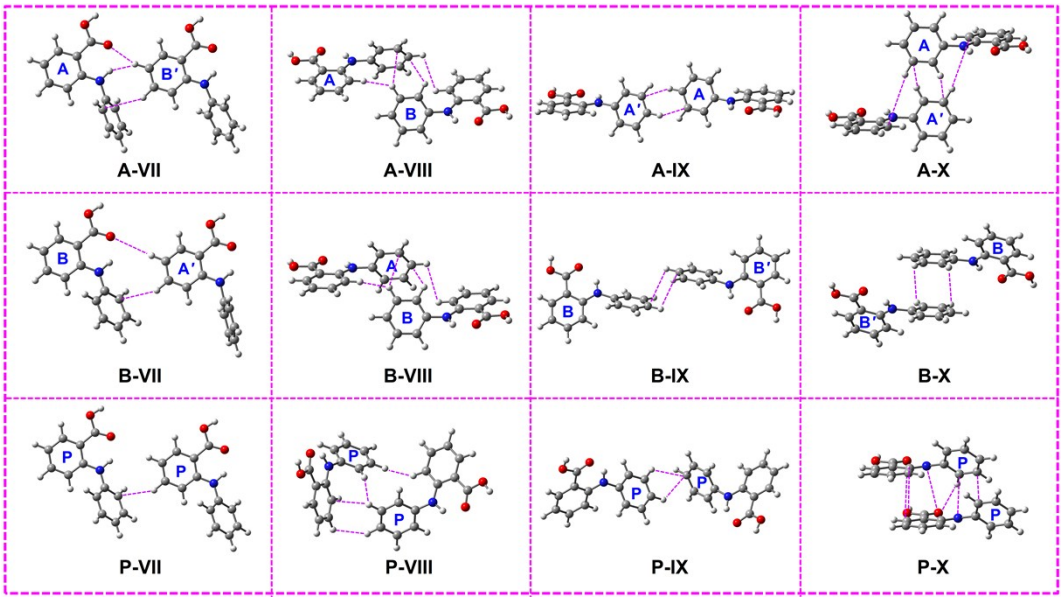

Fig. S6 The molecular pairs (type 3) of the adjacent molecules directly interacting with the carboxyl groups of **A**, **B** and **P** in the partly optimized (Z′=2) and predicted (Z′=1) FA crystals and the interacting atoms at BCPs listed in Table S4.

Table S1 Crystallographic data for the experimental observed, partly optimized and predicted FA crystals.

	Exp FA crystal	Partly optimized crystal	#1FA_22
Formula	$C_{13}H_{11}NO_2$	$C_{13}H_{11}NO_2$	$C_{13}H_{11}NO_2$
Molecular weight/gmol^{-1}	213.23	213.23	213.23
Space group	$P\ \bar{1}$	$P\ 1$	$P\ 2_1/c$
a/Å	8.0995(5)	8.09950	8.7
b/Å	9.8268(6)	9.82680	4.7
c/Å	14.0593(11)	14.05929	27.2
α/º	85.96(6)	85.96	90
β/º	88.62(7)	88.62	73.9
γ/º	73.39(4)	73.39	90
Z, Z'	4, 2	4, 2	4, 1
V/Å^3	1069.64	1069.64	1058.84

Table S2 Intermolecular bond critical points (BCPs), electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic potential energy density (V, in a.u.), the electronic kinetic energy density (G, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of the complexes involving conformer **A**.[a]

	BCP	ρ	$\nabla^2\rho$	V	G	H
A···B	$H15^{A}\cdots O16^{B}$	0.04601	0.12909	-0.04218	0.03723	-0.00495
	$O16^{A}\cdots H15^{B}$	0.04666	0.12822	-0.04273	0.03739	-0.00534
A-I	$H3^{A}\cdots O15^{A'}$	0.00208	0.00889	-0.00121	0.00171	0.00051
	$O15^{A}\cdots H3^{A'}$	0.00208	0.00889	-0.00121	0.00171	0.00051
A-II	$O15^{A}\cdots H9^{A'}$	0.00149	0.00674	-0.00076	0.00122	0.00046
	$O15^{A}\cdots N7^{A'}$	0.00239	0.00895	-0.00132	0.00178	0.00046
	$N7^{A}\cdots O15^{A'}$	0.00239	0.00895	-0.00132	0.00178	0.00046
	$H9^{A}\cdots O15^{A'}$	0.00149	0.00674	-0.00076	0.00122	0.00046
	$O16^{A}\cdots C1^{A'}$	0.00339	0.01089	-0.00157	0.00215	0.00058
	$C1^{A}\cdots O16^{A'}$	0.00339	0.01089	-0.00157	0.00215	0.00058
A-III	$H13^{A}\cdots C11^{B'}$	0.00644	0.02004	-0.00331	0.00416	0.00085
	$O16^{A}\cdots C9^{B'}$	0.00351	0.01187	-0.00184	0.00241	0.00057
	$C1^{A}\cdots C5^{B'}$	0.00542	0.01417	-0.00214	0.00284	0.00070
A-IV	$H3^{A}\cdots O16^{B'}$	0.00148	0.00663	-0.00078	0.00122	0.00044
	$H4^{A}\cdots C13^{B'}$	0.00729	0.02369	-0.00371	0.00482	0.00111
A-V	$H2^{A}\cdots H3^{B}$	0.00456	0.01421	-0.00214	0.00285	0.00071
	$H3^{A}\cdots H2^{B}$	0.00474	0.01473	-0.00226	0.00297	0.00071
A-VI	$H9^{A}\cdots O16^{B'}$	0.00471	0.01616	-0.00278	0.00341	0.00062
	$C4^{A}\cdots C14^{B'}$	0.00394	0.01090	-0.00160	0.00216	0.00056
	$C3^{A}\cdots O15^{B'}$	0.00440	0.01380	-0.00226	0.00286	0.00060
	$H10^{A}\cdots C13^{B'}$	0.00478	0.01413	-0.00233	0.00293	0.00060
A-VII	$O16^{A}\cdots H3^{B'}$	0.00471	0.01655	-0.00285	0.00349	0.00064
	$H7^{A}\cdots H3^{B'}$	0.00411	0.01484	-0.00233	0.00302	0.00069
	$C9^{A}\cdots H4^{B'}$	0.00430	0.01248	-0.00202	0.00257	0.00055
A-VIII	$H5^{A}\cdots H10^{B}$	0.00686	0.02116	-0.00370	0.00449	0.00079
	$C12^{A}\cdots H10^{B}$	0.00459	0.01309	-0.00216	0.00271	0.00055
	$C11^{A}\cdots H9^{B}$	0.00496	0.01484	-0.00219	0.00295	0.00076
	$H11^{A}\cdots H5^{B}$	0.00312	0.01012	-0.00146	0.00199	0.00053
A-IX	$C12^{A}\cdots H11^{A'}$	0.00445	0.01385	-0.00190	0.00268	0.00078
	$H11^{A}\cdots C12^{A'}$	0.00445	0.01384	-0.00190	0.00268	0.00078
A-X	$H12^{A}\cdots C9^{A'}$	0.00077	0.00254	-0.00026	0.00045	0.00019
	$C12^{A}\cdots H13^{A'}$	0.00267	0.00796	-0.00108	0.00153	0.00045
	$H13^{A}\cdots C12^{A'}$	0.00267	0.00796	-0.00108	0.00153	0.00045
	$C5^{A}\cdots H12^{A'}$	0.00078	0.00254	-0.00026	0.00045	0.00019

[a] The atom numbering of the conformer in Fig. 1 is used here.

Table S3 Intermolecular bond critical points (BCPs), electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic potential energy density (V, in a.u.), the electronic kinetic energy density (G, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of the complexes involving conformer **B**. [a]

	BCP	ρ	$\nabla^2\rho$	V	G	H
B-I	$O15^{B}\cdots H2^{B'}$	0.00610	0.02064	-0.00385	0.00451	0.00065
	$H2^{B}\cdots O15^{B'}$	0.00610	0.02064	-0.00385	0.00451	0.00065
B-II	$O15^{B}\cdots H13^{B'}$	0.00132	0.00581	-0.00062	0.00104	0.00042
	$O16^{B}\cdots O16^{B'}$	0.00508	0.01936	-0.00295	0.00389	0.00095
	$H13^{B}\cdots O15^{B'}$	0.00131	0.00580	-0.00062	0.00104	0.00042
B-III	$O15^{B}\cdots C3^{A'}$	0.00440	0.01380	-0.00226	0.00286	0.00059
	$C14^{B}\cdots C4^{A'}$	0.00394	0.01090	-0.00160	0.00216	0.00057
	$O16^{B}\cdots H9^{A'}$	0.00471	0.01615	-0.00278	0.00341	0.00063
	$C13^{B}\cdots H10^{A'}$	0.00479	0.01414	-0.00233	0.00293	0.00060
B-IV	$H3^{B}\cdots O16^{A'}$	0.00471	0.01656	-0.00285	0.00350	0.00064
	$H3^{B}\cdots H7^{A'}$	0.00411	0.01484	-0.00233	0.00302	0.00069
	$H4^{B}\cdots C9^{A'}$	0.00430	0.01248	-0.00202	0.00257	0.00055
B-V	$C4^{B}\cdots H12^{B}$	0.00396	0.01108	-0.00172	0.00225	0.00052
	$C3^{B}\cdots H13^{B}$	0.00582	0.01635	-0.00259	0.00334	0.00075
B-VI	$C2^{B}\cdots O15^{A'}$	0.00351	0.01187	-0.00184	0.00241	0.00056
	$C5^{B}\cdots C1^{A'}$	0.00542	0.01417	-0.00214	0.00284	0.00070
	$C6^{B}\cdots O16^{A'}$	0.00500	0.01679	-0.00259	0.00340	0.00080
	$C11^{B}\cdots H13^{A'}$	0.00644	0.02004	-0.00331	0.00416	0.00085
B-VII	$O16^{B}\cdots H3^{A'}$	0.00148	0.00663	-0.00079	0.00122	0.00044
	$C13^{B}\cdots H4^{A'}$	0.00729	0.02370	-0.00371	0.00482	0.00111
B-VIII	$H5^{B}\cdots H11^{A}$	0.00312	0.01011	-0.00145	0.00199	0.00054
	$H9^{B}\cdots C11^{A}$	0.00496	0.01485	-0.00219	0.00295	0.00076
	$H10^{B}\cdots C10^{A}$	0.00459	0.01309	-0.00216	0.00271	0.00056
	$H10^{B}\cdots H5^{A}$	0.00685	0.02115	-0.00370	0.00450	0.00079
B-IX	$H11^{B}\cdots C11^{B'}$	0.00385	0.01094	-0.00157	0.00215	0.00058
	$C11^{B}\cdots H11^{B'}$	0.00385	0.01094	-0.00157	0.00215	0.00058
B-X	$H10^{B}\cdots H9^{B'}$	0.00447	0.01402	-0.00205	0.00278	0.00073
	$H9^{B}\cdots H10^{B'}$	0.00447	0.01402	-0.00205	0.00278	0.00073

[a] The atom numbering of the conformer in Fig. 1 is used here.

Table S4 Intermolecular bond critical points (BCPs), electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic potential energy density (V, in a.u.), the electronic kinetic energy density (G, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of the complexes involving conformer **P**. [a]

	BCP	$\rho(r)$	$\nabla^2\rho(r)$	V	G	H
P-I	O15^{P}···H3$^{P'}$	0.00140	0.00657	-0.00080	0.00122	0.00042
	H18^{P}···H2$^{P'}$	0.00340	0.01139	-0.00172	0.00228	0.00057
P-II	H13^{P}···O15$^{P'}$	0.00331	0.01235	-0.00187	0.00248	0.00061
	O16^{P}···O16$^{P'}$	0.00761	0.02707	-0.00538	0.00608	0.00069
	O15^{P}···H13$^{P'}$	0.00331	0.01235	-0.00187	0.00248	0.00061
P-III	C9^{P}···C12^{P}	0.00504	0.01328	-0.00197	0.00265	0.00067
	N7^{P}···C13^{P}	0.00475	0.01360	-0.00216	0.00278	0.00062
	O16^{P}···H13^{P}	0.00937	0.03217	-0.00598	0.00701	0.00103
	O16^{P}…N7^{P}	0.00437	0.01407	-0.00244	0.00298	0.00054
	C2^{P}···C5^{P}	0.00557	0.01507	-0.00223	0.00300	0.00077
	O15^{P}···C6^{P}	0.00511	0.01697	-0.00276	0.00350	0.00074
P-IV	C13^{P}···H4^{P}	0.00602	0.01780	-0.00273	0.00359	0.00086
P-V	H3^{P}···O15$^{P'}$	0.00291	0.01050	-0.00150	0.00206	0.00056
	C2^{P}···C$^{2P'}$	0.00532	0.01588	-0.00224	0.00311	0.00086
	O15^{P}···H3$^{P'}$	0.00291	0.01050	-0.00150	0.00206	0.00056
P-VI	H3^{P}···H13^{P}	0.00229	0.00810	-0.00109	0.00156	0.00047
	C3^{P}···H12^{P}	0.00277	0.00829	-0.00117	0.00162	0.00045
P-VII	C13^{P}···H4^{P}	0.00602	0.01779	-0.00273	0.00359	0.00086
P-VIII	H11^{P}···H4^{P}	0.00433	0.01364	-0.00212	0.00277	0.00064
	H10^{P}···C5^{P}	0.00518	0.01389	-0.00225	0.00286	0.00061
	H10^{P}···H9^{P}	0.00559	0.01736	-0.00272	0.00353	0.00081
	H5^{P}···H10^{P}	0.00220	0.00787	-0.00105	0.00151	0.00046
P-IX	C11^{P}···H12^{P}	0.00495	0.01570	-0.00236	0.00314	0.00078
	C11^{P}···H11^{P}	0.00545	0.01515	-0.00243	0.00311	0.00068
P-X	C9^{P}···C12^{P}	0.00504	0.01328	-0.00197	0.00265	0.00067
	N7^{P}···C13^{P}	0.00475	0.01360	-0.00216	0.00278	0.00062
	O16^{P}···H13^{P}	0.00937	0.03217	-0.00598	0.00701	0.00103
	O16^{P}···N7^{P}	0.00437	0.01407	-0.00244	0.00298	0.00054
	C2^{P}···C5^{P}	0.00557	0.01506	-0.00222	0.00300	0.00077
	O15^{P}···C6^{P}	0.00512	0.01697	-0.00276	0.00350	0.00074

[a] The atom numbering of the conformer in Fig. 1 is used here.