Supplementary Material for:

Direct space solution in the EXPO package: the combination of the *H*BB-BC algorithm with GRASP

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Table S1 For each test structure: code, compound name, molecular formula and reference.

Code	Compound Name	Molecular Formula	Reference
1	Hydrochlorothiazide	$C_7H_8ClN_3O_4S_2$	Florence *et al*. (2005)
2	RS-camphorquinone	$C_{10}H_{14}O_2$	by courtesy of Dr M. Brunelli
3	Decafluoroquarterphenyl	$C_{24}H_8F_{10}$	Smrčok *et al*. (2001)
4	*N*,*N'* -Bis[1-pyridin-4-yl-meth-(*E*)-ylidene]hydrazine	$C_{12}H_{10}N_4$	Florence *et al*. (2005)
5	2-Mercaptobenzoic acid	$C_7H_6O_2S$	Florence *et al*. (2005)
6	2,6-diamino-5-hydroxy-3-nitro-4*H*-pyrazolo[1,5-a]pyrimidin-7-one monohydrate	$C_6H_6N_6O_4 \cdot H_2O$	Chernyshev *et al*. (1999)
7	(2RS,3RS)-5-amino-3-(4-phenylpiperazin-1-yl)-1,2,3,4-tetrahydronaphthalen-2-ol	C20H25N3O	Assaad & Rukiah (2011)
8	Paracetamol (form I polymorph)	$C_8H_9NO_2$	Florence *et al*. (2005)
9	Phenylacetic acid	$C_8H_8O_2$	Florence *et al*. (2005)
10	Hydroflumethiazide	$C_8H_8F_3N_3O_4S_2$	Florence *et al*. (2005)
11	Aspirin	$C_9H_8O_4$	http://en.wikipedia.org/wiki/Aspirin
12	Triphenylphosphine	$P(C_6H_5)_3$	http://en.wikipedia.org/wiki/Triphenylphosphine
13	2,6-diamino-5-hydroxy-3-nitro-4H-pyrazolo[1,5-a]-pyrimidin-7-one monohydrate	$C_6H_6N_6O_4.H_2O$	Chernyshev *et al*. (1999)
14	Captopril	$C_9H_{15}NO_3S$	Fujinaga & James (1980)
15	Cu(II)-Schiff	$Cu(C_{15}H_{12}NO_2)_2$	Banerjee *et al*. (2002)
16	Ethyl 1' ,2' ,3' ,4' ,4a' ,5' ,6' ,7' -octahydrodispiro[cyclohexane-1,2' -quinazoline-4' ,1" -cyclohexane]-8' – carbodithioate	$C_{21}H_{34}N_2S_2$	Avila *et al*. (2009)
17	Fluorescein diacetate	$C_{24}H_{16}O_7$	Knudsen *et al*. (1998)
18	Ibuprofen	$C_{13}H_{18}O_2$	Shankland *et al*. (1998)

19	*l*-Glutamic acid	$C_5H_9NO_4$	Kariuki *et al*. (1998)
20	Tetracycline hydrochloride	$C_{22}H_{24}N_2O_8 \cdot HCl$	www.cristal.org/SDPDRR/samples.html (Sample2) (1998)
21	2-(4-Hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl)ethylammonium chloride	$C_9H_{11}N_2O_2S \cdot Cl$	Florence *et al*. (2005)
22	Citric acid	$C_6H_8O_7$	http://en.wikipedia.org/wiki/Citric_acid
23	Citric acid	$C_6H_8O_7$	http://en.wikipedia.org/wiki/Citric_acid
24	Salbutamol	$C_{13}H_{21}NO_3$	Florence *et al*. (2005)
25	2-[1-(2-aminoethyl)-2-imidazolidinylidene]-2-nitroacetonitrile	$C_7H_{11}N_5O_2$	Chernyshev *et al*. (1999)
26	2,5-dioxopyrrolidin-1-yl 2-(benzoylsulfanyl)acetate	$C_{13}H_{11}NO_5S$	Rukiah & Al-Ktaifani (2011)
27	Creatine monohydrate	$C_4H_9N_3O_2 \cdot H_2O$	Florence *et al*. (2005)
28	*m*-Toluidine	C_7H_9N	Rukiah *et al*. (2004)
29	α-Lactose monohydrate	$C_{12}H_{22}O_{11} \cdot H_2O$	Florence *et al*. (2005)
30	Tolbutamide	$C_{12}H_{18}N_2O_3S$	Florence *et al*. (2005)
31	Promazine hydrochloride	$C_{17}H_{21}N_2S \cdot Cl$	Florence *et al*. (2005)
32	Clomipramine hydrochloride	$C_{19}H_{24}ClN_2 \cdot Cl$	Florence *et al*. (2005)
33	Lithium benzilate hemihydrate	$C_{28}H_{22}O_6Li_2 \cdot H_2O$	Mora *et al*. (2003)
34	Potassium Vanadium Oxide	$K_2V_3O_8$	Liu and Greedan, (1995)
35	Benzene-Hexafluorobenzene	$C_6H_6:C_6F_6$	Williams *et al*. (1992)
36	Capecitabine	$C_{15}H_{22}FN_3O_6$	Rohlicek *et al*. (2009)
37	Carbamazepine dihydrate	$C_{15}H_{12}N_2O \cdot 2H_2O$	Florence *et al*. (2005)
38	*catena*-Poly[[dipyridinenickel(II)]-trans-di-μ-chlorido]	$[NiCl_2(C_5H_5N)_2]_n$	Alig *et al*. (2010)
39	Pigment Orange 36 (*β* phase)	$C_{17}H_{13}ClN_6O_5$	van de Streek *et al*. (2009)

40	Pigment Orange 62	$C_{17}H_{14}N_6O_5$	van de Streek *et al*. (2009)
41	Pigment Yellow 151	$C_{18}H_{15}N_5O_5$	van de Streek *et al*. (2009)
42	Pigment Yellow 154 (α phase)	$C_{18}H_{14}F_3N_5O_3$	van de Streek *et al*. (2009)
43	N-methyl-2,4-dinitro-N-phenyl-6-(phenylazo)benzamide	$C_{20}H_{15}N_5O_5$	Chernyshev *et al*. 2002
44	Barium sulfate	$BaSO_4$	Lee *et al*. (2005)
45	Bromotrifluoromethane	$CBrF_3$	Jouanneaux *et al.*, (1992)
46	Cimetidine	$C_{10}H_{16}N_6S$	diffraction data courtesy of Dr. Himeda, Rigaku, Japan
47	Famotidine	$C_8H_{15}N_7O_2S_3$	Florence *et al*. (2005)
48	Famotidine	$C_8H_{15}N_7O_2S_3$	Shankland *et al*. (2002)
49	[D_3]Methylsodium	$NaCD_3$	Weiss *et al*. (1990)
50	*trans*-Dichlorobis(triphenylphosphine)nickel(II)	$C_{36}H_{30}Cl_2NiP_2$	Florence *et al*. (2005)
51	(R)-1-phenylethylammonium (R)-2-phenylbutyrate (polymorph III)	$C_8H_{12}NC_{10}H_{11}O_2$	Fernandes *et al*. (2007a)
52	(R)-1-phenylethylammonium (R)-2-phenylbutyrate (polymorph II)	$C_8H_{12}NC_{10}H_{11}O_2$	Fernandes *et al*. (2007b)
53	meso-3,30 -[2,2-dimethylpropane-1,3-diylbis(azanediyl)]dibutan-2-one dioxime, commonly called meso-hexamethyl propylene amine oxime	$C_{13}H_{28}N_4O_2$	Al-Ktaifani and Rukiah (2010)
54	Diltiazem hydrochloride	$C_{22}H_{27}N_2O_4S{\cdot}Cl$	Florence *et al*. (2005)
55	Poly[(μ_2-2,2-dimethylpropane-1,3-diyl diisocyanide)-μ_2-iodido-silver(I)]	$[AgI(C_7H_{10}N_2)]_n$	Rukiah & Al-Ktaifani (2009)
56	Zopiclone dihydrate	$C_{17}H_{17}ClN_6O_3{\cdot}2H_2O$	Florence *et al*. (2005)

57	Capsaicin	$C_{18}H_{27}NO_3$	Florence *et al*. (2005)
58	S-Bupivacaine Hydrochloride (Form A)	$C_{18}H_{28}N_2O{\cdot}HCl$	Niederwanger *et al*. (2009)
59	N-formylurea	$C_2H_4N_2O_2$	Harris *et al*. (1998)
60	L-arabinitol	$C_5H_{12}O_5$	Derollez *et al*. (2012)
61	Tetracaine hydrochloride	$C_{15}H_{25}N_2O_2^+Cl^-$	Nowell *et al*. (2002)
62	Lanthanum disilicate	$La_2Si_2O_7$	Christensen (1994)
63	Nimustine hydrochloride	$C_9H_{14}ClN_6O_2^+{\cdot}Cl^-$	Beko *et al*. (2012)
64	Pigment Yellow 181 (polymorph β)	$C_{25}H_{21}N_7O_5$	van de Streek *et al*. (2009)
65	Sodium 4-[(*E*)-(4-hydroxyphenyl)diazenyl]benzene sulfonate dihydrate	$C_{12}H_9N_2O_4S{\cdot}Na{\cdot}2H_2O$	Florence *et al*. (2005)
66	*S*-Ibuprofen	$C_{13}H_{18}O_2$	Florence *et al*. (2005)
67	Verapamil hydrochloride	$C_{27}H_{39}N_2O_4{\cdot}Cl$	Florence *et al*. (2005)
68	Ampicillin trihydrate	$C_{16}H_{19}N_3O_4S{\cdot}3H_2O$	Burley *et al*. (2006)
69	Dapsone	$C_{12}H_{12}N_2O_2S$	Florence *et al*. (2005)
70	Amodiaquinium dichloride dihydrate	$C_{20}H_{24}ClN_3O^{2+}{\cdot}2Cl^-{\cdot}2H_2O$	Llinàs *et al*. (2006)
71	Deuterated potassium uranyl phospate trihydrate	$KUO_2PO_4{\cdot}3D_2O$	Fitch & Cole (1991)
72	barbituric acid:calcium iodide pentahydrate *co-crystal*	$C_4H_4N_2O_3{:}CaI_2{\cdot}5H_2O$	Braga *et al.* (2012)
73	Nifedipine (C polymorph)	$C_{17}H_{18}N_2O_6$	Bortolotti *et al*. (2011)
74	Antimony phosphate	$Sb_2(PO_4)_3$	Jouanneaux *et al*. (1991b)
75	Nickel zirconium phosphate	$Ni_{0.5}Zr_2(PO_4)_3$	Jouanneaux *et al*. (1991a)
76	Potassium titanium silicate monohydrate	$K_2TiSi_3O_9{\cdot}H_2O$	Dadachov & Le Bail (1997)

77	Carvedilol dihydrogen phosphate isopropanol solvate	$C_{27}H_{37}N_2O_9P$	Chernyshev *et al*. (2010)
78	Platinum (IV)	$C_{28}H_{32}N_4O_8Cl_4Pt_2$	Altomate *et al.*, (2009)
79	D-Sorbitol	$C_6H_{14}O_6$	Rukiah *et al*. (2004)
80	7-oxanorbornane	$C_6H_{10}O$	Palin *et al*. (2007)
81	Calcium tartrate tetrahydrate	$CaC_4H_4O_6{\cdot}4H_2O$	Le Bail *et al.* (2009)

Table S2 For each test structure: code, type of radiation (X for conventional X-ray, S for synchrotron data, N for neutron data); space group; content of non-H atoms in the asymmetric unit (NAT_{asym}); experimental data resolution (RES) and number of reflections (NREF) used in *H*BB-BC and G*H*BB-BC runs; total (internal and external) number of degrees of freedom (DOFs).

RES=$\lambda/2\sin(\theta_{max})$, where λ is the wavelength and θ_{max} is the maximum value of the Bragg angle in the experimental powder diffraction pattern used in the *H*BB-BC and G*H*BB-BC procedures. The value of RES is determined satisfying the condition that the number of reflections corresponding to RES must be larger than 7·DOFs, according to the following rule: it is usually set to 2 Å; if the condition is not satisfied it is reduced; RES larger than 2 Å corresponds to the experimentally available maximum value of RES.

NREF is the number of reflections corresponding to RES.

Code	**Type of radiation**	**Space Group**	**NAT_{asym}**	**RES**	**NREF**	**DOFs**
1	X	$P\,2_1$	17	2.0	90	6
2	S	$P2_1/n$	12	2.0	120	6
3	X	$I\,2_1/a$	17	2.0	116	7
4	X	$P\,2_1/c$	8	2.0	67	7
5	X	$P\,2_1/c$	10	2.0	85	7
6	S	$P\,2_1/n$	17	2.0	116	7
7	X	$P\,2_1/c$	24	2.0	234	8
8	X	$P\,2_1/n$	11	2.0	103	8

9	X	*P* 2_1/*a*	10	2.0	98	8
10	X	*P* 2_1	20	2.0	92	8
11	S	*P* 2_1/*c*	13	2.0	114	9
12	X	*P* 2_1/*c*	19	2.0	192	9
13	N	*P* 2_1/*n*	25	2.0	116	10
14	X	*P* 2_1 2_1 2_1	14	2.0	101	10
15	X	*P* -1	37	2.0	314	10
16	S	*P* 2_1/*n*	25	2.0	262	10
17	S	*P* -1	31	2.0	242	10
18	S	*P* 2_1/*c*	15	2.0	160	10
19	S	*P* 2_1 2_1 2_1	10	1.88	70	10
20	X	*P* 2_1 2_1 2_1	33	2.0	191	9
21	X	*P* 2_1/*a*	15	2.0	138	11
22	X	*P* 2_1/*c*	13	2.0	100	11
23	S	*P* 2_1/*c*	13	2.0	100	11
24	X	*P b c a*	17	2.0	184	11
25	N	*P* 2_1/*n*	25	2.0	118	12
26	X	*P* -1	20	2.0	175	12
27	X	*P* 2_1/*c*	10	2.0	96	12
28	X	*P* 2_1/*c*	16	2.0	162	12
29	X	*P* 2_1	25	2.0	106	12
30	X	*P n a* 2_1	18	2.0	106	12
31	X	*P* 2_1/*c*	21	2.0	221	13
32	X	*P* 2_1/*c*	23	2.0	241	13
33	S	*P* 2_1/*a*	37	2.0	314	13
34	S	*P 4 b m*	7	1.13	96	14

35	S	*P* $2_1/a$	9	1.78	98	14
36	S	*P* 2_1 2_1 2_1	30	2.0	164	14
37	X	*C m c a*	13	2.0	101	14
38	X	*P* 2/*c*	16	2.0	142	14
39	X	*P* -1	29	2.0	227	14
40	X	*P* -1	28	2.64	95	14
41	X	*P* -1	28	2.0	218	14
42	X	*P* $2_1/c$	29	2.0	226	14
43	X	*P* $2_1/c$	30	2.0	253	14
44	N	*P n a m*	5	1.26	105	15
45	N	*P* $2_1/a$	5	1.52	105	15
46	X	*P* $2_1/n$	17	2.0	167	15
47	X	*P* $2_1/c$	20	2.0	187	15
48	S	*P* $2_1/c$	20	2.0	187	15
49	S	*I* 2 2 2	5	1.44	105	15
50	X	*P* 2/*c*	21	2.0	208	15
51	X	*P* 2_1	21	2.0	135	15
52	X	*P* $2_12_12_1$	21	2.0	150	16
53	X	*P* $2_1/n$	19	2.0	209	16
54	X	*P* 2_1 2_1 2_1	30	2.16	164	16
55	X	*P b c a*	11	2.0	136	16
56	X	*P* $2_1/c$	29	2.0	257	16
57	X	*P* $2_1/c$	22	2.0	232	17
58	S	*P* 2_1	22	2.0	141	17
59	S	*P n* 2_1 *a*	6	1.22	119	17
60	X	*P* 1	20	1.82	119	17

61	S	*P* -1	20	2.0	213	18
62	N	*P* $2_1/c$	11	1.71	126	18
63	X	*P* $2_1/c$	19	2.0	188	18
64	X	*P* $2_1/c$	37	2.0	303	19
65	X	*P b c n*	22	2.0	180	19
66	X	*P* 2_1	30	2.0	193	19
67	X	*P* -1	34	2.0	363	19
68	S	*P* 2_1 2_1 2_1	27	2.0	176	20
69	X	*P* 2_1 2_1 2_1	17	1.82	147	21
70	X	*P* $2_1/c$	29	2.0	300	24
71	S	*P* 4/*n c c*	7	1.12	168	24
72	X	*P* $2_1/c$	22	2.0	185	24
73	S	*P* -1	50	2.39	258	24
74	S	*P* $2_1/n$	17	1.76	168	24
75	S	*P* $2_1/n$	18	1.75	189	27
76	X	*P* 2_1 2_1 2_1	16	1.49	189	27
77	X	*P* -1	39	2.0	373	28
78	S	*P* -1	23	2.0	239	30
79	S	*P* 2_1 2_1 2	36	1.99	231	33
80	S	*C* 2/*c*	21	1.91	252	36
81	X	*P* -1	15	1.56	266	38

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