Supplementary material for:

RAMM: a new RAndom Model based Method for solving *ab initio* crystal structure by EXPO package

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In Table S1, for each one of the 31 test structures, we give the following information: R_{FFM} is the R_F value corresponding to the final model (FM) obtained by *EXPORAMM*; R_{FSM} is the R_F value calculated by using the corresponding refined random starting model (SM); the character '*' indicates that the stopping condition [see (1) in the paper] is never attained in all the *ntrial* attempts (*ntrial*=15) and the trial corresponding to the smallest R_{FFM} value has been selected as the most reliable.

The analysis of the R_{FFM} and R_{FSM} values (see Table S1) points out that:

- 1) for AGPZ, AMODIAQ and DFQP ($R_{FFM} > R_{FSM}$) the selection of the model corresponding to the smallest R_{FFM} value among the *ntrial* attempts guarantees the correct solution even if the R_{FFM} value is quite large (e.g., see AGPZ);
- 2) for PPH3D8 and TARTRATE ($R_{FFM} < R_{FSM}$, $R_{FFM} \ge 0.5$) all the *ntrial* attempts are explored because the criterion (1) is not fully verified. If we omitted the condition $R_{FFM} < 0.5$ in (1) we could not obtain the solution. *E.g.*, for PPH3D8, the model corresponding to the first attempt ($R_{FFM} = 0.58$, $R_{FSM} = 0.59$) is completely wrong;
- 3) for the remaining 26 cases the stopping criterion (1) is successfully attained. The reader should notice that the R_{FFM} value corresponding to the correct solution varies in a quite wide range (from 0.24 to 0.47). Moreover the efficiency of (1) doesn't depend on how much R_{FFM} improves with respect to R_{FSM} (for PIPERAZINE, BUPIA and ETHYLB the differences are very small).
- **Table S1.** For each test structure: R_{FFM} is the R_F value corresponding to the final model (FM) obtained by *EXPORAMM*; R_{FSM} is the R_F value calculated by the corresponding refined random starting model (SM); the character '*' indicates that all the *ntrial* attempts (*ntrial*=15) have been executed and the trial corresponding to the smallest R_{FFM} value has been selected.

METYL 0.33 0.36 AGPZ 0.56 0.52 * * MERCA 0.29 0.30 ALPHA 0.25 0.26 CAMPHOR 0.40 0.48 BENZOS1 0.45 0.46 CAPTO 0.26 0.28 LAMO 0.41 0.45 CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.56 BUPIA 0.24 0.251 6 0.00 0.47 AMODIAQ 0.37 0.31 * * 0.42 </th <th>Code Name</th> <th>R_{FFM}</th> <th>R_{FSM}</th>	Code Name	R _{FFM}	R _{FSM}
AGPZ 0.56 0.52 ** ** MERCA 0.29 0.30 ALPHA 0.25 0.26 CAMPHOR 0.40 0.48 BENZOS1 0.45 0.46 CAPTO 0.26 0.28 LAMO 0.41 0.45 CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 DAPSONE 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * * TARTRATE 0.50 0.52 <tr< td=""><td></td><td></td><td></td></tr<>			
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ALPHA 0.25 0.26 CAMPHOR 0.40 0.48 BENZOS1 0.45 0.46 CAPTO 0.26 0.28 LAMO 0.41 0.45 CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 <t< td=""><td></td><td>*</td><td></td></t<>		*	
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BENZOS1 0.45 0.46 CAPTO 0.26 0.28 LAMO 0.41 0.45 CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47	ALPHA	0.25	0.26
CAPTO 0.26 0.28 LAMO 0.41 0.45 CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB	CAMPHOR	0.40	0.48
LAMO 0.41 0.45 CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41	BENZOS1	0.45	0.46
CROX 0.43 0.54 DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41	CAPTO	0.26	0.28
DADA 0.33 0.35 PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41	LAMO	0.41	0.45
PIPERAZINE 0.40 0.407 6 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 50DIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * * TARTRATE 0.50 0.52 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 EOPI 0.39 0.41	CROX	0.43	0.54
DAPSONE 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41	DADA	0.33	0.35
DAPSONE 0.24 0.26 CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41	PIPERAZINE	0.40	0.407
CARBAMA 0.33 0.40 PPH3D8 0.52 0.60 * BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 0.42 0.428 ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41		6	
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* BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41	CARBAMA	0.33	0.40
BENZOS2 0.43 0.44 CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41	PPH3D8	0.52	0.60
CAINE 0.38 0.40 ARABINITOL 0.33 0.35 NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 0.39 0.47 AMODIAQ 0.37 0.31 * * 0.50 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * * ETHYLB 0.42 0.428 ZOPI 0.39 0.41		*	
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NICKEL 0.41 0.47 SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 0.39 0.47 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 2OPI 0.39 0.41	CAINE	0.38	0.40
SAPO 0.47 0.54 NBPO 0.47 0.56 BUPIA 0.24 0.251 6 0.24 0.251 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * 1BUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41	ARABINITOL	0.33	0.35
NBPO 0.47 0.56 BUPIA 0.24 0.251 6 0.39 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * 1BUPS 0.50 0.52 * 1BUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 2OPI 0.39 0.41	NICKEL	0.41	0.47
BUPIA 0.24 0.251 6 SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41	SAPO	0.47	0.54
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SODIUM 0.36 0.39 CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 0.33 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41	BUPIA	0.24	0.251
CLOMIPRA 0.39 0.47 AMODIAQ 0.37 0.31 * TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 ZOPI 0.39 0.41		6	
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* TARTRATE 0.50 0.52 * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41	CLOMIPRA	0.39	0.47
TARTRATE 0.50 0.52 * * IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * * ETHYLB 0.42 0.428 6 0.39 0.41	AMODIAQ	0.37	0.31
* IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41		*	
IBUPS 0.37 0.39 CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * * ETHYLB 0.42 0.428 6 0.39 0.41	TARTRATE	0.50	0.52
CHLORIDO 0.44 0.45 DFQP 0.47 0.33 * * ETHYLB 0.42 0.428 6 0.39 0.41			
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ETHYLB 0.42 0.428 6 ZOPI 0.39 0.41	DFQP	0.47	0.33
6 ZOPI 0.39 0.41		*	
ZOPI 0.39 0.41	ETHYLB	0.42	0.428
		6	
FLUO2 0.40 0.46	ZOPI	0.39	0.41
	FLUO2	0.40	0.46