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 ($R_{FFM} < R_{FSM}$, $R_{FFM} \geq 0.5$) 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.

Code Name	R_{FFM}	R_{FSM}
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	0.406	0.407
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	0.246	0.251
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	0.426	0.428
ZOPI	0.39	0.41
FLUO2	0.40	0.46