SUPPLEMENTARY INFORMATION

Section 1: Graphical examples on the use of the C-map in Patterson deconvolution procedures.

Figure S1. a) A three-atom two-dimensional target structure, plane group *p2* (it simulates a centric distribution of the peaks); b) the corresponding Patterson map, plane group *p2;* c) the *C*-map, plane group *p2*, when the S atom is the only atom in the model structure; d) the corresponding *C*' map.

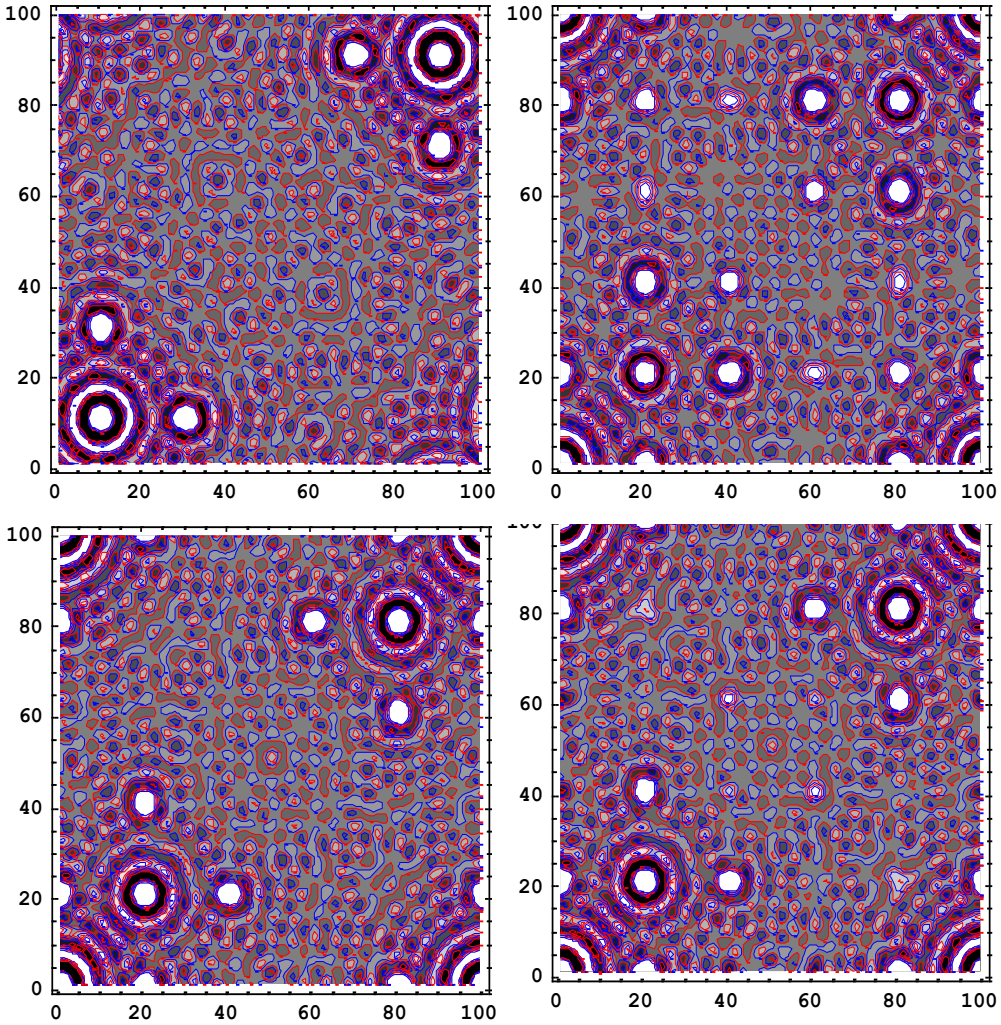


Figure S2. a) *SMF* map corresponding to the structure illustrated in Fig.2a); b) Patterson map shifted by $\mathbf{r}_S$ ($\mathbf{r}_S$ is the sulphur position highlighted by the yellow arrow); c),d) symmetry minimum function obtained according to eq. (12) and (21).

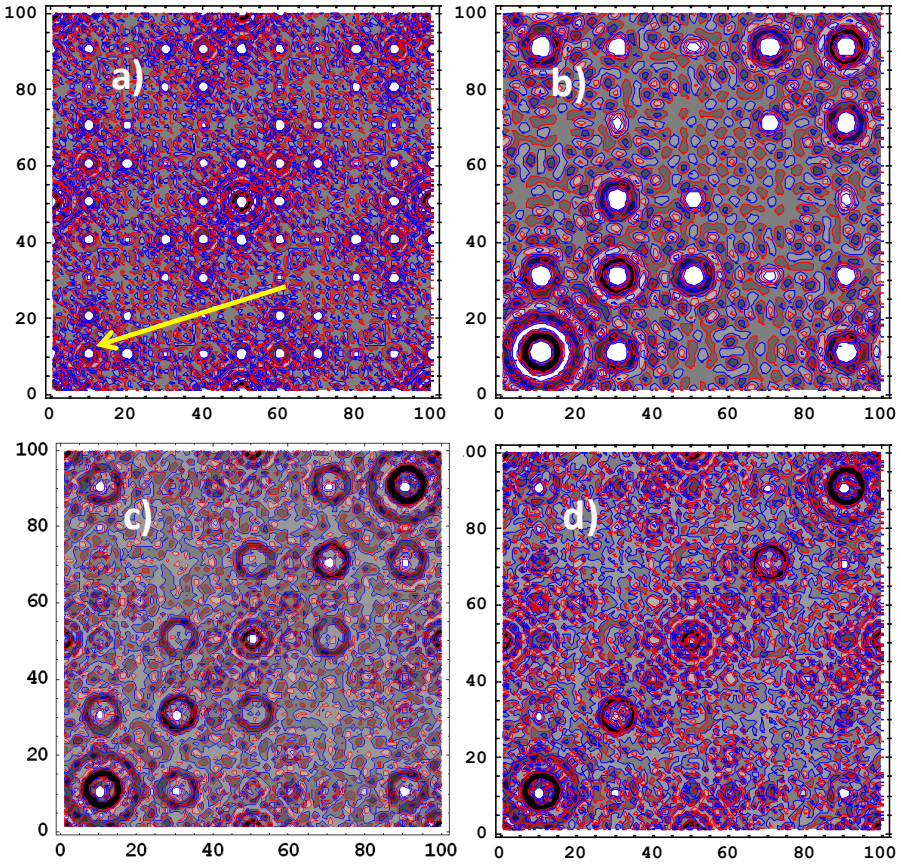
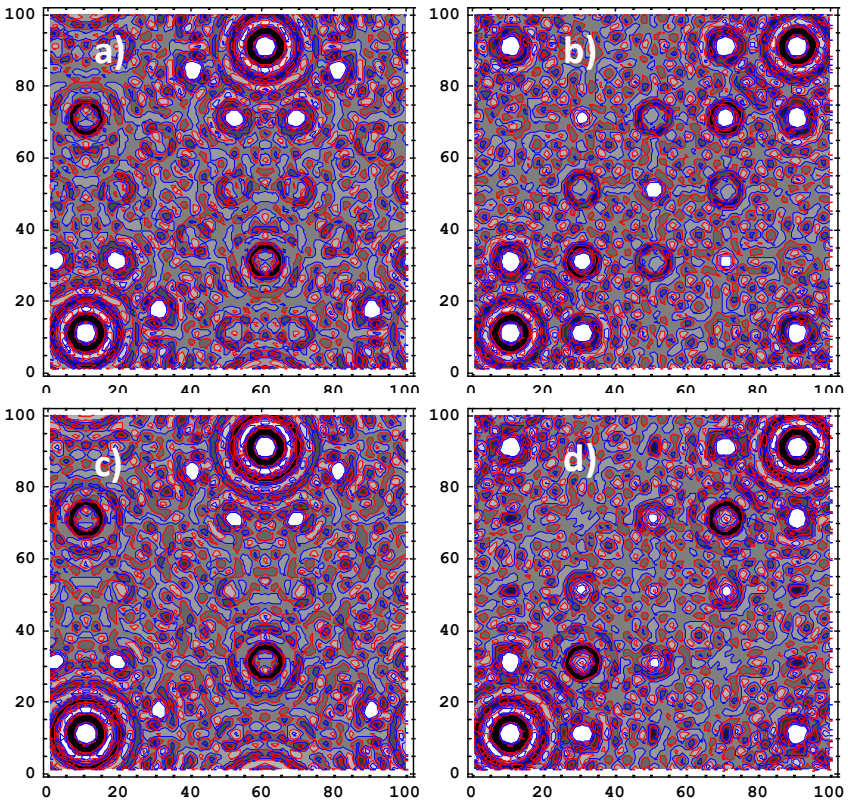


Figure S3. a) *S* map obtained by eq. (22) for the target structure illustrated in Fig.1a; b) *S* map obtained by eq. (22) for the target structure illustrated in Fig. 2a; c) *S* map obtained by eq. (23) for the target structure illustrated in Fig. 1a ; d) *S* map obtained by eq. (23) for the target structure illustrated in Fig. 2a .



Section 2: Crystallographic data of the test structures.

Table S1. Crystallographic data of the test structure with a number of non-hydrogen atom in the asymmetric unit (N_{asym}) ranging from 81 to 400 (medium-size molecules). ID is the identification number in Crystallography Open Database, the Protein Data Bank code or the reference number.

Name	ID	Space group	N_{asym}	Cell content	Pivot peak	R (%)	Time (min)
alley2	2104681	P bca	158	C_{960} H_{688} Na_{80} O_{184} Fe_{40}	5	15.8	5.4
amphisin	2012193	P $2_12_12_1$	102	C_{264} H_{464} N_{48} O_{96}	62	11.3	14.0
at119	2228715	P $2_12_12_1$	259	C_{764} H_{892} N_{48} O_{208} S_{16}	1	12.6	2.0
babu	2222265	C c	204	C_{528} H_{576} N_{96} O_{192}	1	13.1	0.8
bcdimp	(1)	P 2_1	96	C_{110} H_{152} N_8 O_{74}	12	14.6	2.1
bk53m	2228724	P -1	156	C_{216} H_{169} N_{56} O_{33} S_8	1	11.4	0.5
brock	2104241	B 2_1	208	C_{320} H_{768} N_{64} O_{416} Fe_{32}	1	10.4	1.2
budka	2229223	P 2_1/c	153	C_{564} H_{808} O_{40} Cl_8	1	15.5	1.2
bulged	1P79	P 42_12	138	C_{456} N_{168} O_{488} P_{48} K_{24}	4	20	3.0
c8new	(2)	P 2_1	130	C_{196} H_{272} N_{32} O_{32}	9	17.4	3.5
cah	(3)	P 2_1	155	C_{210} H_{260} N_{20} O_{30} F_{50}	5	17.4	2.0
carbru_1	2016443	P $2_12_12_1$	121	C_{428} H_{432} N_{16} O_{20} Cl_{16} Ru_4	1	8.2	0.4
carbru_2	2016444	P $2_12_12_1$	121	C_{428} H_{432} N_{16} O_{20} Cl_{16} Ru_4	1	7.8	0.4
cb3_pap	(4)	P 2_1/n	92	C_{304} H_{288} O_{64}	66	22.9	10.5
ceho1z	(5)	P 2_1	116	C_{128} H_{160} N_{16} O_{88}	1	16.1	0.3
ceho2z	(5)	P 2_1	232	C_{264} H_{304} $N_{32}O_{168}$			
cemc1z	(6)	P 2_1	228	C_{248} H_{296} N_{32} O_{168} Cl_8	18	13.8	21.2
cemc2z	(6)	P 2_1	207	C_{210} H_{444} N_4 O_{200}			
cephaibol_a	1OB4	P 2_12_12	113	C_{308} N_{72} O_{72}	9	19.1	6.2
cephaibol_c	1OB7	P $2_12_12_1$	112	C_{300} N_{72} O_{72}	4	16.2	2.4
cofi5a	2218002	P 2_1/c	107	C_{388} H_{520} O_{32} Cl_8	1	17.1	0.9
cyclo_bnz	2103881	P 2_1	206	C_{216} H_{224} N_8 O_{189}	18	13.8	27.5
cyclo_dba	2103880	P $2_12_12_1$	219	C_{508} H_{448} N_{16} O_{352}	43	13.8	39.5
dasco6	2200556	P 2_1	124	C_{162} H_{270} N_{38} O_{40} S_8	1	15.8	0.2
dext	(3)	P 2_1	94	C_{110} H_{152} O_{74} N_4	2	13	0.5
dextxtal2	(3)	P 2_1	94	C_{110} H_{152} O_{74} N_4	3	7.7	0.5
diene	2226177	P $2_12_12_1$	90	C_{264} H_{480} B_{12} F_{48} P_{24} Rh_{12}	1	10.6	0.5
dioxolan	2011222	P 2_1	141	C_{220} H_{252} N_{12} O_{48} Ru_2	1	7.4	0.3
dodeca	(7)	P $2_12_12_1$	200	C_{568} H_{912} N_{96} O_{136}	4	17.5	1.4
echino	2101407	p 65	89	C_{363} H_{486} N_{60} O_{102} S_{12}	1	11.6	0.5
ergop21	(8)	P 2_1	116	C224 H352 O8	4	14.3	1.0
gago	2227102	P 2_1/n	129	C_{240} H_{288} N_{48} O_{156} S_{24} Cl_{24} Mo_{24}	1	16.6	0.8
giorgi	(9)	P 2_1	88	C_{148} H_{220} N_4 O_{24}	1	13.8	0.3
glici2	(10)	C 2	139	C_{480} H_{760} O_{76}	3	12.9	2.1
gna	2WNA	C 222_1	146	C_{456} O_{384} N_{192} P_{96} Co_{16} Mg_{16} Br_8	1	20.1	0.6
guest	2202059	P $2_12_12_1$	105	C_{224} H_{440} O_{188} S_8	1	17	0.4
h104	(11)	P 2_1/c	84	C_{252} H_{384} $N_{12}O_{60}$ Cl_{12}	1	20.9	0.4
hao	2226460	A ba2	84	C_{416} H_{496} N_{88} O_{144} S_{16} Gd_8	6	11.4	1.4
helix	1VRZ	C 2	164	C_{472} H_{736} N_{92} O_{92}	45	19.6	19.2
hepta	2103676	P $2_12_12_1$	109	C_{288} H_{550} O_{150}	6	14.9	6.2
hexa	2103675	P $2_12_12_1$	100	C_{252} H_{599} O_{149}	1	12.9	2.0
hsy115	2225069	P $na2_1$	120	C_{384} H_{480} N_{32} O_{64}	1	10.8	0.4

iak48bm	2225123	P $2_1/c$	140	C_{416} H_{296} O_{96} P_8 As_{16} Ru_{24}	6	17.8	8.9
iled	(12)	P $2_12_12_1$	84	C_{240} H_{408} N_{24} O_{72}	1	13.7	0.4
inclu_rt	(13)	P 1	194	C_{97} H_{157} O_{97}	1	13.1	0.6
jamilas	(14)	P 1	100	C_{64} H_{68} O_{20} N_8 S_4 K_4	1	14.2	0.1
jebas	2220423	P 21/c	121.5	C_{342} H_{456} N_{32} O_{80} S_{32}	1	18.1	1.1
kemer	2015969	C 2/c	126	C_{648} H_{1056} N_{168} O_{96} S_{72} Cr_{12} Er_{12}	5	9.4	3.9
kfb44	2103879	P -1	368	C_{656} H_{576} N_{16} O_{32} Si_{32}	5	17.9	8.5
lasso	2NJW	P $2_12_12_1$	146	C_{608} N_{92} O_{104} S_8	1	15.3	1.6
macro	(15)	P $2_12_12_1$	123	C_{420} H_{432} O_{72}	46	9.9	20.4
mghex	(16)	P 3_1	95	C_{168} H_{240} N_{48} O_{60} Cl_6 Mg_3	1	13.8	0.3
mor59	(17)	P2_1	126	C_{192} H_{328} N_{24} O_{36}	5	18.5	1.6
oe410	2204692	P $2_1/n$	135	C_{432} H_{320} N_{48} O_{12} P_{16} Te_{16} Re_{16}	1	11.5	1.8
ohba	2202173	P 2_1	92	$C_{162}H_{174}$ N_2 O_{20}	5	11.8	0.9
ohba_p1	2203226	P 1	188	C_{166} H_{158} N_2 O_{20}	1	13.5	0.6
pnib	1AKG	P $2_12_12_1$	114	C_{280} N_{72} O_{88} S_{16}	1	20.2	0.4
quail_a	2012678	P $2_12_12_1$	81	C_{220} H_{396} N_{36} O_{68}	6	9.3	1.7
quail_b	2012679	P $2_12_12_1$	83	C_{228} H_{412} N_{36} O_{68}	1	11.2	0.2
rac	2211608	P -1	93	C_{140} H_{138} N_{22} O_{16} Cl_4 Cu_4	5	9.1	1.1
rauf20	2220764	P $2_1/n$	104	C_{232} H_{104} N_{32} O_{16} S_{16} Cl_{120}	1	14.1	0.7
shen	2230103	P c	90	C_{128} H_{184} N_8 O_{40} Co_4	1	8.7	0.1
so99	2016923	P -1	144	C_{224} H_{232} N_{32} O_{32}	6	15.3	1.2
sr166	(18)	P2_1	112	C_{192} H_{192} O_{16} N_{16}	3	15.8	1.4
s6	(14)	P -1	89	C_{132} H_{141} N_{10} O_{24} S_{12}	37	14.1	6.0
ta	(19)	P2_1	142	C_{170} H_{224} O_{114}	16	7.8	5.5
tato	(20)	P $2_12_12_1$	109	C_{224} H_{368} N_8 O_{204}	6	13.5	2.1
tb	(19)	P $2_12_12_1$	186	C_{520} H_{784} O_{224}	22	11.2	52.5
tb02rlm	(21)	P 1	197	C_{96} H_{224} O_{101}	1	12	0.3
tensin	2010528	P $2_12_12_1$	107	C_{284} H_{508} N_{48} O_{96}	5	14	1.8
theo	2227537	P $2_12_12_1$	110.8	C_{280} H_{500} N_{52} O_{111}	37	19.5	15.5
thebo	2008512	P $2_1/c$	112	C_{360} H_{368} N_{48} O_{40}	1	15.3	0.7
thio2	2104680	P $2_1/c$	144	C_{444} H_{288} N_{12} F_{72} P_{24} S_{12} Ag_{12}	1	7.5	0.5
tp	(19)	P 2_1	161	C_{210} H_{308} O_{112}	17	9.1	12.2
triazole	2221962	P -1	243	C_{378} H_{414} N_{72} S_{18} Cl_{18}	15	12	9.6
trip04e	2100208	P 2_1	223.5	C_{283} H_{295} O_{160} Cl_4	31	15.2	22.1
triostin_a	2101409	P $2_12_12_1$	94	C_{256} H_{360} N_{48} O_{64} S_8	17	22.8	7.9
triostin_c	2101408	P $2_12_12_1$	83.5	C_{219} H_{283} N_{48} O_{51} S_8 Cl_8	15	12.4	2.0
tval	(16)	P 1	156	C_{108} H_{180} N_{12} O_{36}	1	11.9	0.3
winter	(16)	P 2_1	88	C_{110} H_{178} N_{22} O_{32} Cl_{12}	1	20.6	0.3
x124	(22)	P 1	120	C_{92} H_{76} N_4 O_{12} S_4 Cl_8	1	11.2	0.2
y54	(23)	P $2_12_12_1$	100	C_{264} H_{344} N_{56} O_{80}	2	14.9	2.0
zaib	(24)	P -1	141	C_{193} H_{316} N_{36} O_{53}	35	21.9	13.7
zippercl	2WQ0	I 2_13	275	C_{4008} N_{1272} O_{1224} S_{24} Cl_{72}	1	23.5	6.1
zipperbr	2WQ1	I 2_13	275	C_{4008} N_{1272} O_{1224} S_{24} Br_{72}	1	22.8	6.5

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The following structures have resolution lower than 1.0Å:

Name	**Resolution (Å)**
bulged	1.01
echino	1.01
ergop21	1.02
helix	1.01
pnib	1.10
triostin_a	1.14
zippercl	1.08
zipperbr	1.08

Table S2. Crystallographic data of the test structure with a number of non-hydrogen atom in the asymmetric unit (N_{asym}) lower than 80 (small-size molecules). ID is the identification number in Crystallography Open Database or the reference number.

Name	ID	Space group	N_{asym}	Cell content	Pivot peak	R (%)	Time (sec)
alley1	2104682	P -1	66	C_{112} H_{104} O_{16} Fe_4	3	10.2	16
alley	2225745	R 3c	54	C_{828} H_{720} N_{72} O_{36} Fe_{36}	1	8.3	48
allof	2230280	P 6_1	22	C_{78} H_{126} N_6 O_{48}	1	12.2	4
amide	(1)	P $bc2_1$	24	C_{56} H_{72} N_{24} O_{16}	1	12.3	2
apapa	(2)	P 4_12_12	69	C_{240} H_{296} N_{168} O_{128} P_{16}	6	14	61
av2pr	2103455	P 6_1	56	C_{205} H_{374} N_{48} O_{83}	3	15.9	151
ax118	(3)	P ccn	25	C_{152} H_{168} N_{16} O_{24} Cl_8	1	18.4	6
azet	(2)	P $ca2_1$	48	C_{168} H_{128} N_8 O_8 Cl_8	3	10.4	20
azi	(4)	P 2_1	77	C_{84} H_{144} N_4 O_{66}	21	16.9	251
bao	2230161	P bcm	24	C_{112} H_{88} N_{40} F_{24} P_8 Co_8	1	14	2
bats	2226585	P -42_1c	16	C_{120} H_{104} I_8	1	12.6	3
becker	2017537	P $6_3/m$	40	$C_{354}H_{432}N_{18}$ O_{60} P_{12} Cl_{30} C_6	4	18.8	143
bed	(2)	I 4	34	C_{208} H_{208} N_{32} O_{32}	3	19.8	34
blake	2016921	C 2/c	72	C_{300} H_{220} N_{60} O_{160} Cl_{40} Pb_{20}	1	12.2	9
bobby	(2)	P 2_13	5	$C_{24}H_{24}N_4$ O_{24} Na_4 Ca_4	1	7.4	1
butyl	2222707	R -3	22	C_{342} H_{342} N_{18} O_{36}	1	17.3	10
carbamato	2226134	I 2/a	59	C_{344} H_{320} N_{32} O_{48} P_{16} S_{16} Au_{16}	1	9.3	9
carbamide	2219630	P n	15	C_{24} H_{20} N_4 O_2	1	11.2	1
cephal	(3)	C 2	46	C_{144} $H_{168}N_8$ O_{32}	5	12.3	20
choror	2104300	P 3_221	54	C_{264} H_{180} N_{12} O_{48}	143	9.9	1625
cime	(5)	Cc	18	C_{40} H_{72} N_{24} O_4 S_4	1	8.8	1
cubane	2222097	I -42d	27.5	$C_{316}H_{288}N_{32}$ O_{76} Zn_{16}	1	7.1	8
cuimid	(2)	P 3_221	12	C_{36} H_{48} N_{24} Cl_6 Cu_6	1	15.9	1
diam	(2)	P $4_2/n$	15	C_{112} H_{160} O_8	1	16.3	3
diben	2228788	F dd2	32	C_{448} H_{448} O_{32} S_{32}	2	12.8	95
diole	(2)	I -42d	12.25	C_{160} H_{288} O_{36}	15	15.4	58
eg1scrat	(6)	C 12/c1	12	O_{60} Cs_8Si_{24} Ti_4	2	16.8	9
ergo	(7)	P $2_12_12_1$	58	C_{224} H_{352} O_8	11	17.2	62
erica	(8)	P 2_1	43	C_{74} H_{86} O_8 P_2 Fe_2	1	15.7	304
euclor	(9)	C 2/c	21	O_{104} Na_8 S_{24} K_8 Cu_{24}	2	17.7	12
ewa	2017580	I mmm	6	Mg_{14} Zn_{50} Ce_{32}	1	20.6	1
fegas	(10)	P $6_3/mmc$	0.75	S_{10} Fe_4 Ga_4	1	8.9	1
fisk	2017323	P $6_3/mmc$	0.42	P_4Ca_2 In_4	1	8.5	1
flubo	2017493	P -31c	2.17	B_4 O_{12} F_2 K_2 Zn_4 Cd_2	6	7.4	3
fnltk	(11)	I 2/c	44	C_{304} H_{192} N_{40} As_8	1	14.6	6
freies	(12)	P $2_1/a$	6	S_{12} Ag_4 Sb_4 Pb_4	2	4.9	2
furan	2222612	P nma	4	C_{16} H_{12} O_{12} Cl_4	1	13.3	1
giac	(13)	P $2_1/c$	21	C_{68} H_{32} N_4 O_8 S_4	1	12.1	1
gold	(2)	Cc	56	C_{224} H_{128}	1	11.1	6
golen	2230759	I $4_1/a$	44	C_{640} H_{704} N_{32} Cl_{32}	1	19.2	34
gra4	(3)	P -1	36	C_{60} H_{44} N_4 O_8	18	21.3	64
haddon	2103727	P 3c1	66	C_{234} Cl_{162}	2	23.3	74
hexakis	2226269	C mca	28.5	$C_{96}H_{400}N_{48}$ O_{232} V_{80}	1	11.2	7
hfac	2103750	I 4_1cd	33	$C_{224}H_{96}$ N_{32} O_{64} F_{192} Cu_{16}	1	15.5	13
hkw0m	2016712	P $n2_1m$	7	$C_4H_{24}N_8$ O_8 Na_4 Cl_4	2	7.4	4
hov1	(2)	C 2/m	15.5	Si_{36} Pr_{56} Ni_{32}	13	14.4	29
hwk3	2016711	I 2	7	C_4 H_{24} N_8 O_8 Na_4 Cl_4	1	8.9	1

indide	2225931	I 4/mcm	4.38	Ru_{41} In_{15} La_{84}	5	10.8	15
inos	(14)	P 2_1/n	26	C_{48} H_{112} O_{56}	1	13.2	3
jing	2230031	I 4	33.5	C_{192} H_{176} N_{24} O_{44} Cu_8	1	11.1	6
kirillov	2218097	F d-3m	2	C_{384} H_{768} N_{192} O_{192} P_{192} Cl_{192} Cu_{192}	5	8.9	119
kumar	2227526	P -42$_1$c	38.38	C_{268} H_{246} N_{16} O_{23}	19	15.4	763
lei	2225988	P bca	52	C_{304} H_{432} N_{48} O_{48} S_{16}	1	10.1	10
litho	(15)	P $2_12_12_1$	27	C_{96} H_{120} O_{12}	5	14.5	11
loganin	(2)	P $2_12_12_1$	27	C_{68} H_{104} O_{40}	1	13	4
lough	(16)	F mm2	9	C_{112} H_{120} N_8 O_{16} Fe_8	1	13.7	3
mag255	(17)	P $2_12_12_1$	68	C_{224} H_{248} O_{24} N_{24}	15	13.7	2
mbh2	(2)	P 1	54	C_{45} H_{72} O_9	1	12.9	10
mema	2223241	R 3c	14.11	$C_{216}H_{400}N_{18}$ O_2 Cl_{18}	1	15.5	8
mlx12b	2017265	I 4/m	2.38	$O_{28}H_{16}P_4$ V_4 Co_2	1	2.9	1
munic	(2)	C 2	40	C_{160} H_{128}	3	11.4	18
nabei_1	2016619	Cc	67	B_8 $C_{180}H_{124}N_{36}$ O_8 F_{32} Co_4	1	12.3	8
nabei_2	2016620	C 2/c	74	B_{24} C_{364} H_{260} N_{76} O_{24} F_{96} Co_8	1	17.1	20
newqb	(2)	P -1	62	C_{96} H_{80} N_8 O_{20}	1	9.9	3
no55	(2)	F dd2	24	C_{320} H_{384} N_{64}	4	16	65
pge2	(2)	P 1	25	C_{20} H_{32} O_5	1	21.1	8
photo	(18)	P $2_12_12_1$	17	C_{48} H_{52} N_4 O_{16}	10	15.8	15
picol	2217894	P 6_522	41.5	$C_{288}H_{276}N_{48}$ O_{138} K_{12} Tb_{12}	1	9.3	12
pocro	(19)	B 112/m	3.5	K_2 Se_{16} Cr_{10}	1	10.3	1
pyrid	2219167	I 4_1/acd	10.5	$C_{208}H_{144}N_{80}$ O_{32} Mn_{16}	3	9.3	23
quinol	(2)	R -3	24	C_{324} H_{324} O_{108}	2	10.8	36
quinone	2103571	P ccn	8	C_{40} H_{32} O_8 S_{16}	1	24.9	2
ramesh	2219800	R -3	40	C_{558} H_{612} N_{36} O_{126}	1	14.1	33
rauf4n	2229326	P 4_32_12	33	C_{240} H_{368} O_{24}	32	18.8	403
rc62	(3)	P 2_1	80	C_{136} O_{24}	1	12.6	8
rifolo	(20)	P 2_1	53	C_{78} H_{98} N_2 O_{26}	1	17.9	7
ringe	2016743	P 4/nmm	0.44	Cu_1 Sb_4 U_2	1	6.9	1
sahlberg	2016995	P 4/mbm	0.62	Mg_2 Sc_4 Ga_4	1	4.7	1
salex	(21)	P -3	15.83	H_{60} O_{69} Na_4 S_{12} K_4 Fe_6	1	16.8	2
schwarz	(22)	P 1	73	C_{46} H_{70} O_{27}	1	16.4	10
seidel	2228989	P 4_2/n	49	C_{320} H_{192} N_{64} Zn_8	2	16.3	46
selenid	(2)	P 2_1	25	C_{44} H_{56} O_4 Se_2	1	11.3	1
skn1	(23)	P 3_1	13	C_{21} H_{48} N_3 O_{12} Cl_3	2	9.2	11
sliva	2225554	P -43n	24.5	$C_{336}H_{504}N_{72}$ O_{120} Na_6 P_{24} S_{24} Nd_6	1	17	21
solokha	2016696	F -43m	5	Mg_{76} Zn_{324} Ce_{80}	1	14.2	8
suoa	(2)	P $2_12_12_1$	47	C_{112} H_{152} O_{76}	45	11	182
sutovi	2016784	P 6_3/m	7	H_3 O_{41} Cl_7 As_{12} Cd_{24}	1	9.1	1
teoh	2226240	I -4	50	C_{336} H_{320} O_{48} Sn_{16}	4	9.1	58
tetrakis	2219750	I -43d	19.58	$C_{672}H_{480}N_{192}$ O_{48} P_8 S_4 Ni_{16}	6	9.6	114
thiourea	2230193	I bca	18	C_{224} H_{304} N_{48} S_{16}	1	15.7	8
tiny3	(24)	P $2_12_12_1$	33	C_{88} H_{100} Cl_4 N_8 O_{32}	1	8.4	3
togr44	2017713	C 2/c	59	C_{392} H_{496} O_{32} Cl_{48}	1	14.9	20
totc	(2)	P 6_1	42.5	C_{219} H_{260} O_{36}	1	13.5	10
tpala	(2)	P 2_1	39	C_{56} H_{84} N_8 O_{14}	5	19.2	8
tph	(2)	B 22_12	39	C_{288} H_{240} N_{24}	3	11.9	207
triosic	2101410	C 222_1	43.5	C_{224} H_{308} N_{56} O_{56} S_8 Cl_4	3	14.9	25
tungsto	2218160	R 3	61.33	$C_{324}H_{216}N_{54}$ O_{126} Fe_{12} W_{36}	3	15.7	101
tur10	(2)	P 6_322	17.33	C_{180} H_{288} O_{28}	5	14.6	25
wall26	2218446	P -43n	8	$C_{128}H_{288}O_{32}$ Tl_{32}	1	6.1	12
xanthene	2220578	P na2_1	67	C_{220} H_{320} N_4 O_{44}	1	11.2	12

y75	(25)	P 21/n	34	$C_{100}\ H_{136}\ N_{12}\ O_{24}$	1	10.9	3
yah140	2230578	P 4/n	19.5	$C_{96}H_{80}N_{32}\ O_{24}\ Mo_2\ Tb_2$	1	5.9	2
zhang	2222739	C 2/c	64.5	$C_{304}H_{408}N_{48}\ O_{148}\ S_8\ Mn_8$	1	13.4	10

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The following structures have resolution lower than 1.0Å:

Name	**Resolution (Å)**
azet	1.01
ergo	1.01
newqb	1.04