

Table 1

Details of ACORN, ARP/wARP and REFMAC results for ab initio case

In put	<i>ab initio</i>		
PROGRAM	Resolution Limit	20-0.9	
<i>ACORN</i> [Random atom trial]	Total no. of reflections	431701	
	The strong reflections with $E > 1.2$	101079	
	The medium reflections with $0.1 < E < 1.2$	327165	
	The weak reflections with $0.0 < E < 0.1$	3457	
	<i>Initial</i>	R= 79.4	CC= 0.0285
	<i>Final</i>	R= 36.5	CC= 0.5246
	5000 random atom trials		
<i>ARP/wARP</i>	No. of DDM cycles	78	
	<i>Initial</i>	Rw= 31.8	Rf=31.6
	No. of auto building cycles	10	
	No. of Refmac cycles in each auto building cycle	5	
	<i>Final</i>	Rw= 14.6	Rf= 18.4
	Connectivity Index	0.97	
	No. Chains	8	
	No. Res. Built	482	
No. of Dummy atoms	1265		
Final model with solvent atoms [solvent building carried out using 20 cycles of ARP/wARP: building solvent atoms script]		Rw = 14.0	Rf = 16.2
		r.m.s deviation of backbone atoms: 0.143 Å	

Table 2

Details of ACORN, ARP/wARP and REFMAC results for fragments of helices/sheets (SET No. 4)

In put	SET No. 4(76 a.a)		
PROGRAM	Resolution Limit	20-1.5	
ACORN [Phasing with known starting coordinates]	Total no. of reflections	94138	
	The strong reflections with $E > 1.2$	22015	
	The medium reflections with $0.1 < E < 1.2$	69788	
	The weak reflections with $0.0 < E < 0.1$	2335	
	<i>Initial</i>	R= 54.2	CC= 0.0469
	<i>Final</i>	R= 53.9	CC= 0.0711
	5000 random atom trials		
	No. of DDM cycles	56	
ARP/wARP	<i>Initial</i>	Rw= 44.8	Rf=44.4
	No. of auto building cycles	10	
	No. of Refmac cycles in each auto building cycle	5	
	<i>Final</i>	Rw= 28.9	Rf= 36.3
	Connectivity Index	0.79	
	No. Chains	22	
	No. Res. Built	212	
ARP/wARP	<i>Initial</i>	Rw= 28.9	Rf= 36.3
	No. of auto building cycles	10	
	No. of Refmac cycles in each auto building cycle	5	
	<i>Final</i>	Rw= 14.0	Rf= 17.6
	Connectivity Index	0.97	
	No. Chains	7	
	No. Res. Built	481	
No. of Dummy atoms	1287		
Final model with solvent atoms [solvent building carried out using 20 cycles of ARP/wARP: building solvent atoms script]		Rw = 13.6	Rf = 15.6
		r.m.s deviation of backbone atoms: 0.176 Å	

Table 3

**Results of ACORN and ARP/wARP using Ncap, Ccap and Middle portions of helices/sheets (1gwe)
Resolution 20-1.5 Å**

PROGRAM		Ncap region of helices/sheets		Ccap region of helices/sheets		Middle region of helices/sheets	
		R-factor (%)	CC	R-factor (%)	CC	R-factor (%)	CC
ACORN	STARTING						
Input	Large E (L)	0.435	0.1118	0.437	0.1076	0.434	0.1319
	Medium E (M)	0.539	0.0569	0.542	0.0553	0.538	0.0623
	76 a.a		76 a.a		76 a.a		
	After 51 cycles of DDM			After 53 cycles of DDM		After 52 cycles of DDM	
	FINAL	L	0.275	0.6270	0.271	0.6307	0.272
		M	0.534	0.0901	0.533	0.0946	0.533
ARP/wARP		R-factor (%)	Rfree	R-factor (%)	Rfree	R-factor (%)	Rfree
AUTOBUILDING : 10 Cycles REFMAC : 5 Cycles for each auto building; Side dock after 6 cycles of auto building	INITIAL	44.5	44.8	44.4	44.9	44.7	44.5
	FINAL	14.9	18.6	14.5	18.2	15.2	19.1
<i>Details of ARP/wARP result</i>	10 chains, 470 residues, missing residues 1-7, 39, 40, 59, 60, 113, 114, 142, 143, 174, 175, 176, 195-202, 331, 332, 388, 389, 401, 402, 503, dummy atoms 1308, connectivity index 0.95		9 chains, 474 residues, missing residues 1-7, 39-40, 59, 60, 142, 143, 174, 175, 186, 187, 201, 202, 331, 332, 388, 389, 503, dummy atoms 1277, connectivity index 0.96		8 chains, 479 residues, missing residues 1-7, 60, 110-114, 142, 143, 175, 176, 186, 187, 388, 389, 503, dummy atoms 1230, connectivity index 0.97		
		R-factor (%)	Rfree	R-factor (%)	Rfree	R-factor (%)	Rfree
Without dummy atoms made by ARP/wARP		28.9	29.3	28.3	29.3	27.8	28.7
After manual model building for missing residues and solvent building		13.3	16.2	14.6	17.4	13.0	15.8
r.m.s deviation of the model with backbone atoms superposed with that of 1gwe		0.218		0.183		0.151	

Table 4

**Results of ACORN and ARP/wARP using only C α atoms (1gwe)
Resolution 20-1.3 Å**

PROGRAM		C α atoms alone		Mean Positional Error (MPE) of C α atoms			
				0.1 Å		0.2 Å	
ACORN	STARTING	R-factor (%)	CC	R-factor (%)	CC	R-factor (%)	CC
Input (1 atom /a.a - ~13% of the total structure)	Large E (L)	0.446	0.0607	0.445	0.0640	0.446	0.0543
	Medium E (M)	0.551	0.0368	0.551	0.0348	0.552	0.0303
	503 atoms		503 atoms		503 atoms		
	After 123 cycles of DDM			After 121 cycles of DDM		After 165 cycles of DDM	
	FINAL L	0.254	0.6542	0.255	0.6520	0.257	0.6452
	M	0.503	0.1944	0.505	0.1904	0.508	0.1826
ARP/wARP		R-factor (%)	Rfree	R-factor (%)	Rfree	R-factor (%)	Rfree
AUTOBUILDING : 10 Cycles REFMAC : 5 Cycles for each auto building; Side dock after 6 cycles of auto building	<i>INITIAL</i>	39.9	40.6	40.5	40.6	40.7	40.4
	FINAL	13.3	16.8	14.7	18.4	14.5	18.2
<i>Details of ARP/wARP result</i>	9 chains, 474 residues, missing residues 1-7, 34-40,59,60,113,114,142,143,174,175,186,187,388,389,401, 402,503, dummy atoms 1389, connectivity index 0.96			7 chains, 483 residues, missing residues 1-7, 59, 60, 113, 114, 142, 143, 186, 187, 331, 332, 388, 389, 503, dummy atoms 1225, connectivity index 0.97		8 chains, 481 residues, missing residues 1-7, 59, 60, 113, 114, 142, 143, 175, 176, 201, 202, 331, 332, 388, 389, 503, dummy atoms 1247, connectivity index 0.97	
		R-factor (%)	Rfree	R-factor (%)	Rfree	R-factor (%)	Rfree
Without dummy atoms made by ARP/wARP		28.2	28.9	26.9	28.1	27.5	28.5
After manual model building for missing residues and solvent building		15.1	17.1	14.2	16.0	14.4	16.1
r.m.s. deviations of the model with backbone atoms superposed with that of 1gwe		0.132		0.169		0.163	

Table 5

Results of ACORN and ARP/wARP using polyala model (5atoms/a.a) (1gwe) Resolution 20 – 1.5 Å

PROGRAM		First 120 residues of polyala		First 120 residues of polyala with a mean positional error (MPE) of 0.1 Å	
		R-factor (%)	CC	R-factor (%)	CC
ACORN	STARTING				
	Large E (L)	0.439	0.0915	0.442	0.0853
	Medium E (M)	0.541	0.0525	0.541	0.0499
		After 56 cycles of DDM		After 55 cycles of DDM	
	FINAL L	0.276	0.6196	0.274	0.6195
	M	0.537	0.0807	0.540	0.0775
ARP/wARP		R-factor (%)	Rfree	R-factor (%)	Rfree
AUTOBUILDING : 10 Cycles REFMAC : 5 Cycles for each auto building; Side dock after 6 cycles of auto building	INITIAL	45.1	44.4	45.1	44.9
	FINAL	32.3	42.7	24.5	45.1
DETAILS OF ARP/wARP result		15 chains, 111 residues, connectivity index 0.88, dummy atoms 4437		0 chains, 0 residues, connectivity index 0.00, dummy atoms 6948	
ARP/wARP		R-factor (%)	Rfree	R-factor (%)	Rfree
AUTOBUILDING : 10 Cycles REFMAC : 10 Cycles for each auto building; Side dock after 6 cycles of auto building	INITIAL	32.3	42.8	24.5	45.2
	FINAL	13.1	16.6	26.8	35.8
Details of ARP/wARP result		6 chains, 480 residues, missing residues 1-9, 59, 60, 110-114, 142, 143, 174, 175, 388, 389, 503, dummy atoms 1354, connectivity index 0.98		20 chains, 282 residues, dummy atoms 3271, connectivity index 0.85	
ARP/wARP				R-factor (%)	Rfree
AUTOBUILDING : 10 Cycles REFMAC : 10 Cycles for each auto building; Side dock after 6 cycles of auto building	INITIAL			26.9	35.8
	FINAL			13.6	17.5
Details of ARP/wARP result				8 chains, 481 residues, missing residues 1-7, 39, 40, 59, 60, 142, 143, 174, 175, 186, 187, 388, 389, 401, 402, 503, dummy atoms 1201, connectivity index 0.97	
		R-factor (%)	Rfree	R-factor (%)	Rfree
Without dummy atoms made by ARP/wARP		27.3	28.0	27.1	28.0
After manual model building for missing residues and solvent building		14.0	15.7	14.0	15.5
r.m.s. deviations of the model with backbone atoms superposed with that of 1gwe		0.176		0.173	

