Satellite Tobacco Mosaic Virus Refined to 1.4 Å Resolution

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SUPPORTING INFORMATION

Table S1. B factor comparison between the various refinements at 1.8 A. RT and LT refer to data sets collected at 290 K and 100 K, respectively. The maximum B factor in *SHELX-97* is 157.91 Å^2. The average, minimum and maximum B factors are listed for all atoms, protein atoms, RNA atoms, ions and water oxygen atoms.

	RT	LT	RT	LT	RT	LT
Programs	<B>all	<B>all	Bmin	Bmin	Bmax	Bmax
CNS cons	22.33	32.68	5.74	11.53	109.47	122.17
CNS rest	22.34	32.38	2.00	2.00	115.77	124.35
REFMAC5	23.41	46.37	3.19	18.76	109.89	143.32
SHELX-97	25.03	38.63	0.00	0.00	157.91	157.91
	<B>prot	<B>prot	Bmin	Bmin	Bmax	Bmax
CNS cons	14.10	23.70	5.74	15.00	75.49	85.47
CNS rest	13.73	22.90	2.91	7.01	75.49	81.52
REFMAC5	15.81	36.56	6.56	28.52	64.32	82.63
SHELX-97	15.61	26.26	0.00	0.00	157.91	157.91
	<B>rna	<B>rna	Bmin	Bmin	Bmax	Bmax
CNS cons	46.63	63.10	8.45	22.16	109.47	122.17
CNS rest	48.11	64.01	2.00	10.42	112.93	124.35
REFMAC5	44.77	80.81	7.14	28.57	97.78	143.32
SHELX-97	53.24	78.34	0.00	11.43	157.91	157.91
	<B>ions	<B>ions	Bmin	Bmin	Bmax	Bmax
CNS cons	51.02	55.69	6.41	11.53	95.38	83.22
CNS rest	60.73	56.56	2.00	2.00	115.77	91.16
REFMAC5	57.90	73.72	3.19	18.76	109.89	115.79
SHELX-97	59.44	63.12	0.00	5.07	157.91	124.30
	<B>wat	<B>wat	Bmin	Bmin	Bmax	Bmax
CNS cons	37.53	43.61	7.31	18.29	74.33	81.49
CNS rest	37.01	42.84	6.04	15.45	93.02	100.16
REFMAC5	38.08	55.36	8.33	28.91	87.73	118.50
SHELX-97	41.47	54.12	6.24	17.31	157.91	157.91

Table S2. R.m.s. deviations between models from refinements using the programs *CNS*, *REFMAC5* and *SHELX-97*. The upper triangle contains the deviations between protein models and the lower triangle contains the deviations between RNA models. RT and LT refer to data collected at 290 K and 100 K, respectively.

		RT				LT (1.45 Å)				
		CNS-cons	*CNS*-rest	*REF-MAC5*	*SHELX-97*	*CNS*-cons	*CNS*-rest	*REF-MAC5*	*SHELX-97*	
RT	*CNS*-cons		0.108	0.113	0.147	0.415	0.444	0.443	0.451	P
	CNS-rest	0.573		0.041	0.103	0.429	0.431	0.430	0.439	R
	REFMAC5	0.146	0.118		0.090	0.431	0.434	0.430	0.439	O
	SHELX-97	0.149	0.166	0.575		0.439	0.442	0.437	0.441	T
LT	*CNS*-cons	0.814	0.946	0.280	0.313		0.159	0.161	0.176	E
	CNS-rest	0.902	1.147	0.345	0.363	0.632		0.039	0.080	I
	REFMAC5	0.335	0.297	0.817	1.070	0.273	0.070		0.066	N
	SHELX-97	0.814	0.946	0.292	0.323	0.225	0.174	0.157		

RNA

Table S3. R factor comparisons for the various refinements at 1.8Å. RT and LT refer to data sets collected at 290 K and 100 K, respectively.

	RT	LT	
Programs	Rfree	Rfree	ΔRfree(LT-RT)
CNS cons	0.1735	0.2549	0.0814
CNS rest	0.1715	0.2407	0.0692
REFMAC5	0.1629	0.2162	0.0533
SHELX-97	0.1811	0.2372	0.0561

	R	R	ΔR(LT-RT)
CNS cons	0.1719	0.2527	0.0808
CNS rest	0.1445	0.2076	0.0631
REFMAC5	0.1355	0.1802	0.0447
SHELX-97	0.1484	0.2072	0.0588

	Rfree-R	Rfree-R
CNS cons	0.0016	0.0022
CNS rest	0.0270	0.0331
REFMAC5	0.0274	0.0302
SHELX-97	0.0327	0.0300

Table S4. Differences between the expanded constrained and the restrained low temperature 1.4 Å models expressed as r.m.s. deviations and centroid differences between corresponding subunits. The maximum deviation for any atom used in the r.m.s. deviation calculations and the residue containing that atom are identified in the last two columns. Maximum values for the r.m.s. deviation, centroid difference and difference between them are in bold. The four highlighted subunits (D, F, K and N) are the principal contact points between particles in the crystal lattice.

A. Differences in monomer subunits based on CA positions

chain ID	Rms dev aa 17-159	centroid difference aa 17-159	difference	aa #	Max dev
A	0.140	0.088	0.052	S105	0.404
B	0.080	0.058	0.022	M22	0.174
C	0.090	0.065	0.025	M22	0.175
D	0.195	0.170	0.025	T71	0.602
E	0.102	0.087	0.015	R148	0.190
F	0.187	0.161	0.026	T71	0.537
G	0.086	0.062	0.024	S46	0.192
H	0.101	0.081	0.020	D18	0.203
I	0.194	0.155	0.039	S105	0.417
J	0.139	0.119	0.020	F109	0.219
K	0.177	0.130	0.047	I51	0.516
L	0.157	0.145	0.012	R24	0.258
M	**0.208**	**0.199**	0.009	G50	0.314
N	0.173	0.119	**0.054**	I51	0.498
O	0.124	0.102	0.022	G50	0.203

B. Differences in monomer subunits based on all highest occupied atomic positions

chain ID	Rms dev aa 17-159	centroid difference aa 17-159	difference	aa #	Max dev
A	0.189	0.092	**0.097**	K97	1.957
B	0.110	0.061	0.049	R24	0.673
C	0.115	0.069	0.046	R24	0.801
D	0.225	0.173	0.052	K54	2.813
E	0.120	0.085	0.035	R24	0.798
F	0.211	0.163	0.048	K54	2.280
G	0.106	0.060	0.046	R24	0.697
H	0.119	0.078	0.041	R24	0.831
I	**0.228**	0.154	0.074	K97	2.423
J	0.166	0.125	0.041	K97	1.216
K	0.203	0.127	0.076	F53	1.294
L	0.172	0.147	0.025	R24	0.513
M	0.220	**0.201**	0.019	R24	0.620
N	0.199	0.117	0.082	F53	1.309
O	0.151	0.098	0.053	M22	1.175