



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:21 am BST

PDB ID : 2TBV
Title : STRUCTURE OF TOMATO BUSHY STUNT VIRUS. V. COAT PROTEIN SEQUENCE DETERMINATION AND ITS STRUCTURAL IMPLICATIONS
Authors : Harrison, S.C.
Deposited on : 1984-06-22
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

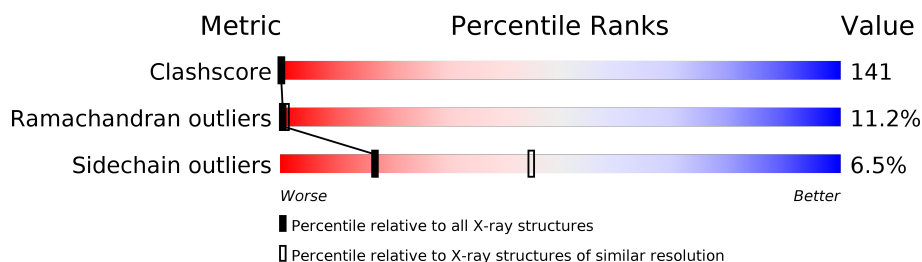
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	387	
1	B	387	
1	C	387	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6648 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TOMATO BUSHY STUNT VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	3	1
			2136	1351	360	420	5			
1	B	287	Total	C	N	O	S	0	2	1
			2130	1348	359	418	5			
1	C	321	Total	C	N	O	S	0	3	0
			2376	1502	406	462	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	GLY	SER	CONFLICT	UNP P11795
A	107	SER	GLY	CONFLICT	UNP P11795
B	102	GLY	SER	CONFLICT	UNP P11795
B	107	SER	GLY	CONFLICT	UNP P11795
C	102	GLY	SER	CONFLICT	UNP P11795
C	107	SER	GLY	CONFLICT	UNP P11795

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	3	Total	Ca	0	0
			3	3		
2	C	2	Total	Ca	0	0
			2	2		

T241	T301	V301	T361
A242	L302	L302	V362
Y244	T303	T303	V363
G245	H304	H304	F364
G246	T305	T305	T365
A247	F306	F306	V366
G248	R307	R307	S367
A249	A308	A308	G368
D250	T309	T309	V369
A251	G310	G310	A370
V252	T311	T311	A371
G253	F312	F312	G372
E254	N313	N313	I373
L255	L314	L314	L374
F256	S315	S315	L375
L257	G316	G316	V376
A258	G317	G317	G377
R259	L318	L318	R378
S260	R319	R319	A379
V261	G320	G320	R380
T262	L321	L321	A381
L263	S322	S322	N382
Y264	S323	S323	V383
F265	L324	L324	R384
P266	T325	T325	N385
Q267	L326	L326	L386
P268	G327	G327	L387
T269	A328	A328	
N270	T269	T269	
T271	G330	G330	
L272	A331	A331	
L273	V332	V332	
S274	V333	V333	
S275	I334	I334	
K276	N335	N335	
R277	D336	D336	
L278	I337	I337	
D279	L338	L338	
L280	A339	A339	
T281	L340	L340	
G282	D341	D341	
S283	N342	N342	
L284	V343	V343	
A285	G344	G344	
D286	T345	T345	
A287	A346	A346	
T288	S347	S347	
G289	D348	D348	
P290	Y349	Y349	
L291	F350	F350	
Y292	L351	L351	
L293	N352	N352	
V294	C353	C353	
L295	T354	T354	
T296	V355	V355	
R297	S356	S356	
T298	S357	S357	
P299	L358	L358	
T300	P359	P359	

• Molecule 1: TOMATO BUSHY STUNT VIRUS

Chain C: 

ALA	LYS	V123	S184	Y244	T305	T365
MET	GLN	M124	Q185	G245	F306	V366
THR	GLY	G125	D186	G246	R307	S367
ARG	ASN	G126	P187	A249	A308	G368
ASN	GLN	I127	E188	D250	G310	V369
ASN	GLN	V128	P189	A251	T311	A371
ASN	GLN	G129	A190	V252	F312	G372
ASN	GLN	M130	D191	G253	N313	I373
ASN	GLN	S131	R192	E254	L314	L374
VAL	T69	L132	V193	L255	S315	L375
LEU	H70	Q133	E194	F256	G316	V376
ALA	V74	L134	L195	L257	F317	G377
ALA	G75	M135	A196	A258	L318	R378
SER	G76	N136	N197	R259	R319	A379
LYS	S77	F136	F198	S260	C320	R380
LYS	S78	M138	G199	V261	L321	A381
GLN	M79	T139	V200	T262	T322	N382
LEU	A80	G140	L201	L263	S323	V383
GLY	P81	L141	K202	L264	G324	V384
VAL	V82	F142	E203	Y265	T325	N385
LEU	A83	S143	T204	P266	L326	L386
ALA	H84	M144	A205	Q267	G327	L387
ALA	S85	L145	P206	P268	A328	
SER	R86	P146	N207	T269	T329	
ALA	G87	A147	A208	N270	G330	
ALA	L88	L148	E209	T271	A331	
VAL	H89	A149	A210	L272	V332	
GLY	G90	S150	K211	L273	V333	
ALA	S91	M151	L212	S274	N335	
LEU	R92	F152	K213	S275	D336	
ARG	P93	D153	T214	K276	I337	
ASN	K94	Q154	P215	R277	A339	
TTR	F95	Y155	T216	L278	L340	
ILE	T96	S156	D217	D279	D341	
GLY	G97	F157	K218	L280	R342	
GLU	R98	M158	V219	G282	V343	
SER	T99	S159	K220	S283	G344	
SER	S100	V160	R221	L284	T345	
PRO	G101	V161	Y222	A285	A346	
ALA	L162	L162	C223	D286	S347	
LEU	V103	D163	N224	A287	D348	
LEU	T104	Y164	D225	T288	V349	
GLN	V105	V165	S226	G289	F350	
SER	T106	P166	A227	T296	S357	
ALA	S107	L167	T228	R297	L358	
VAL	H108	G168	V229	G298	P359	
GLY	R109	G169	D230	P299	A360	
LEU	E110	Q231	Q231	V301	T362	
LEU	Y111	T171	K232	L302	T363	
GLY	L112	E172	L233	H304	F364	
LYS	T113	R175	T234			
LYS	Q114	V176	D235			
ALA	V115	A177	L236			
ASN	N116	L178	G237			
LYS	N117	L179	Q238			
VAL	S118	Y179	L239			
ARG	S119	F180	G240			
ASN	G120	D181	T241			
ARG	F121	K182	L242			
ARG	V122	D183	T243			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	383.20Å 383.20Å 383.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.53	29/2165 (1.3%)	2.19	119/2956 (4.0%)
1	B	1.52	29/2171 (1.3%)	2.16	123/2964 (4.1%)
1	C	1.47	32/2409 (1.3%)	2.12	125/3286 (3.8%)
All	All	1.50	90/6745 (1.3%)	2.16	367/9206 (4.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	35
1	B	3	28
1	C	3	32
All	All	8	95

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	ASN	N-CA	-24.59	0.97	1.46
1	C	138	ASN	N-CA	-24.56	0.97	1.46
1	A	138	ASN	N-CA	-24.55	0.97	1.46
1	B	137	SER	N-CA	-17.72	1.10	1.46
1	A	137	SER	N-CA	-17.70	1.10	1.46

The worst 5 of 367 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLN	C-N-CD	-22.78	70.48	120.60
1	B	165	VAL	C-N-CD	-19.72	77.22	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	C-N-CD	-18.03	80.94	120.60
1	A	135	ASN	CA-C-O	-15.93	86.65	120.10
1	C	135	ASN	CA-C-O	-15.91	86.70	120.10

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	146	PRO	CA
1	A	189	PRO	CA
1	B	146	PRO	CA
1	B	166	PRO	CA
1	B	189	PRO	CA

5 of 95 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	SER	Peptide
1	A	123	VAL	Mainchain
1	A	124	ASN	Peptide
1	A	126	GLY	Mainchain,Peptide
1	A	127	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2136	0	2111	647	0
1	B	2130	0	2111	596	2
1	C	2376	0	2374	695	19
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
All	All	6648	0	6596	1878	19

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 141.

The worst 5 of 1878 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:HG3	1:A:268:PRO:CD	1.18	1.59
1:B:122:VAL:CA	1:B:122:VAL:N	1.68	1.56
1:B:107:SER:N	1:B:107:SER:CA	1.70	1.53
1:C:223:CYS:C	1:C:223:CYS:CA	1.75	1.52
1:A:172:GLU:CA	1:A:172:GLU:N	1.70	1.51

The worst 5 of 19 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ILE:CD1	1:C:348:ASP:CG[2_555]	1.00	1.20
1:C:340:ILE:CD1	1:C:348:ASP:OD2[2_555]	1.13	1.07
1:C:340:ILE:CG1	1:C:348:ASP:OD2[2_555]	1.24	0.96
1:C:340:ILE:CD1	1:C:348:ASP:OD1[2_555]	1.60	0.60
1:C:373:ILE:CD1	1:C:386:LEU:N[2_555]	1.67	0.53

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/387 (74%)	208 (72%)	49 (17%)	31 (11%)	0	1
1	B	287/387 (74%)	212 (74%)	43 (15%)	32 (11%)	0	1
1	C	322/387 (83%)	240 (74%)	45 (14%)	37 (12%)	0	1
All	All	897/1161 (77%)	660 (74%)	137 (15%)	100 (11%)	0	1

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	130	ASN

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Mol	Chain	Res	Type
1	A	139	GLY
1	A	166	PRO
1	A	170	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/309 (75%)	217 (94%)	15 (6%)	17	45
1	B	233/309 (75%)	217 (93%)	16 (7%)	15	41
1	C	258/309 (84%)	242 (94%)	16 (6%)	18	47
All	All	723/927 (78%)	676 (94%)	47 (6%)	17	45

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	201	LEU
1	B	321	LEU
1	C	326	LEU
1	B	257	LEU
1	B	326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	GLN
1	B	335	ASN
1	C	304	HIS
1	B	238	GLN
1	A	158	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.