



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

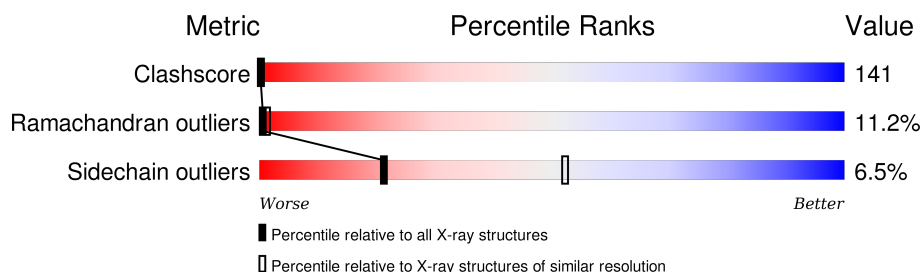
# 1 Overall quality at a glance

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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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		



Note EDS was not executed.

- Molecule 1: TOMATO BUSHY STUNT VIRUS

T365	H304	Y244	K182	F121	LVS	ALA
G366	T305	G245	D183	F122	GLN	MET
S367		G246	S184	V123	GLY	THR
G368	A308	A247	Q185	N124	ASN	THR
G369	T309	G248	D186	G125	GLN	ARG
A370	G310	A249	P187	G126	GLN	ASN
A371	T311	D250	E188	I127	ILE	ASN
L373	F312	A251	P189	V128	ILE	ASN
L374	G313	V252	A190	G129	THR	THR
L375	L314	G253	D191	N130	HIS	VAL
G376	S315	E254	R192	S131	VAL	LEU
G377	G316	L255	V193	L132	GLY	LEU
R378	L318	F256	E194	Q133	GLY	VAL
A379	R319	A258	L195	L134	VAL	SER
R380	G320	R259	A196	N135	GLY	LYS
A381	L321	S260		P136	GLY	LYS
N382	T322	V261	V200	S137	SER	GLN
G383	S323	T262	L201	N138	ILE	LEU
N385	L324	L263	K202	G139	MET	GLY
L386	T325	Y264	E203	T140	ALA	VAL
L387	L326	G265	T204	L141	PRO	LEU
	G327	P266	A205	F142	VAL	ALA
	A328	Q267	P206	S143	ALA	ALA
	T329	P268	W207	W144	VAL	SER
	G330	T269	E209	L145	SER	ALA
	A331	N270	A146	P147	ARG	ALA
	G332	T271	A210	A147	GLN	VAL
	G333	L272	L211		LEU	GLY
	L334	L273	R213	S150	VAL	ALA
	N336	S274	T214	N151	GLY	LEU
	L337	G275	P215	F152	SER	ARG
	L338	T276	T216	D153	LVS	ASN
	A339	R277	T217	Q154	PRO	TYR
	L340	L278	K218	Y155	LVS	ILE
	D341	D279	V219	S156	PHE	GLY
	N342	T281	R220	F157	THR	GLY
	G343	G282	R221	N158	GLY	SER
	G344	S283	Y222	S159	ARG	SER
	T345	L284	G223	V161	THR	PRO
A346	G346	A285	G224	L162	SER	ALA
	S347	D286	D225	D163	GLN	LEU
	D348	A287	S226	Y164	SER	GLN
	G349	T288	A227	V165	THR	SER
	F350	G289	T228	P166	ALA	ALA
	L351	P290	V229	L167	VAL	VAL
	N352	G291	D230	C168	GLY	GLY
	G353	Y292	Q231	C169	LEU	LEU
	T354	L293	K232	T170	GLY	GLY
	G355	V294	L233	T171	LYS	LYS
	S356	L295	G235	F172	LYS	LYS
	G357	T296	D236	V173	ALA	LEU
	L358	R297	L236	G174	LEU	LEU
	G359	T298	G237	R175	ASN	ASN
	A360	P299	Q238	V176	LYS	LYS
	T361	T300	L239	A177	VAL	VAL
	G362	V301	G240	L178	ARG	ARG
	T363	L302	I241	Y179	ASN	ASN
	T364	T202	K242	F180	ARG	ARG

- Molecule 1: TOMATO BUSHY STUNT VIRUS

F121	F122	F123	F124	F125	F126	F127	F128	F129	F130	F131	F132	F133	F134	F135	F136	F137	F138	F139	F140	F141	F142	F143	F144	F145	F146	F147	F148	F149	F150	F151	F152	F153	F154	F155	F156	F157	F158	F159	F160	F161	F162	F163	F164	F165	F166	F167	F168	F169	F170	F171	F172	F173	F174	F175	F176	F177	F178	F179	F180	
LYS	GLN	GLY	ASN	GLN	GLN	ILE	ILE	THR	HIS	VAL	GLY	GLY	VAL	GLY	GLY	SER	ILE	MET	ALA	PRO	VAL	ALA	VAL	SER	SER	ARG	GLN	LEU	VAL	GLY	SER	LYS	PRO	TYR	ASN	GLN	PHE	THR	GLY	THR	ARG	SER	PRO	ALA	LEU	ALA	GLN	SER	VAL	GLY	LEU	HIS	LYS	TYR	ILE	VAL	ASN	ARG	ARG	ARG
ALA	MET	THR	THR	ARG	ASN	ASN	ASN	ASN	VAL	LEU	ALA	VAL	SER	LYS	LYS	GLN	LEU	GLY	VAL	LEU	ALA	ALA	SER	ALA	ALA	GLY	GLY	LEU	ALA	LEU	ASN	ASN	TYR	ASN	TYR	ILE	GLY	GLU	SER	SER	SER	PRO	ALA	LEU	LEU	GLN	GLN	VAL	ALA	VAL	GLY	LEU	LYS	LYS	ALA	VAL	ASN	ARG	ARG	



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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

### 5.3.1 Protein backbone

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%)	21	52
1	B	233/309 (75%)	217 (93%)	16 (7%)	19	48
1	C	258/309 (84%)	242 (94%)	16 (6%)	23	55
All	All	723/927 (78%)	676 (94%)	47 (6%)	21	52

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.