



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:44 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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

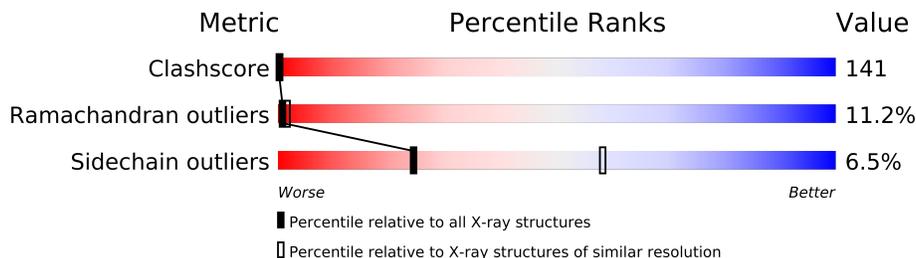
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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
			Total	C	N	O	S			
1	A	287	Total 2136	C 1351	N 360	O 420	S 5	0	3	1
1	B	287	Total 2130	C 1348	N 359	O 418	S 5	0	2	1
1	C	321	Total 2376	C 1502	N 406	O 462	S 6	0	3	0

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 1	Ca 1	0	0
2	A	3	Total 3	Ca 3	0	0
2	C	2	Total 2	Ca 2	0	0

T361	T362	T363	T364	T365	V366	S367	A368	V369	A370	A371	G372	L373	L374	L375	L376	L377	L378	L379	R380	L381	A382	N383	V384	N385	L386	L387																																		
D181	K182	D183	S184	D185	D186	P187	E188	P189	A190	D191	R192	G193	E194	L195	L196	N197	F198	G199	V200	L201	K202	E203	T204	F205	P206	W207	A208	E209	A210	M211	L212	R213	V214	R215	T216	D217	K218	V219	K220	R221	G222	C223	D224	D225	D226	S227	A228	T229	G230	Q231	K232	L233	T234	D235	L236	G237	Q238	L239	P240	
L241	A242	T243	Y244	G245	G246	A247	G248	A249	D250	A251	V252	G253	E254	L255	F256	L257	A258	R259	S260	V261	T262	L263	Y264	F265	P266	Q267	A268	T269	N270	A271	T272	L273	L274	S275	D276	K277	R278	D279	L280	T281	G282	S283	L284	A285	D286	A287	T288	G289	F290	G291	Y292	L293	V294	L295	V296	T297	T298	P299	L299	T300
V301	L302	T303	H304	T305	F306	R307	A308	V309	G310	T311	F312	N313	L314	S315	L316	G317	L318	R319	C320	L321	T322	S323	L324	L325	L326	G327	A328	T329	G330	A331	V332	V333	L334	D335	N336	L337	L338	A339	L340	N341	N342	V343	G344	T345	A346	S347	D348	Y349	F350	L351	N352	C353	T354	V355	L356	S357	L358	P359	L360	A360

• Molecule 1: TOMATO BUSHY STUNT VIRUS

Chain C:

ALA	MET	THR	THR	ARG	ASN	ASN	ASN	ASN	VAL	LEU	VAL	VAL	SER	LYS	LYS	GLN	LEU	LEU	GLY	VAL	LEU	ALA	SER	ALA	ALA	VAL	GLY	LEU	LEU	ARG	ASN	TYR	ILE	GLU	GLU	SER	SER	PRO	ALA	LEU	LEU	LEU	GLN	SER	ALA	VAL	GLY	GLY	LEU	GLY	LYS	ALA	LEU	ASN	ASN	LYS	VAL	ARG	ASN	ARG	ASN	ARG	ARG	ARG	ARG	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L361	V362	F363	F364	T365	V366	S367	A368	V369	A370	A371	G372	L373	L374	L375	L376	L377	L378	L379	R380	L381	A382	N383	V384	N385	L386	L387	L388	L389	R390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	G401	G402	V403	T404	V405	L406	S407	H408	R409	E410	Y411	L412	L413	L414	V415	L416	L417	L418	L419	L420	F421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	F436	S437	M438	L439	M440	L441	T442	F443	S444	W445	L446	L447	L448	A449	S450	N451	F452	R453	P454	Q455	Q456	L457	L458	F459	T460	D461	L462	L463	N464	S465	A466	T467	C468	D469	T470	T471	E472	L473	L474	R475	V476	A477	L478	L479	F480	D481	K482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	F498	G499	V500	T501	T502	P503	W504	K505	E506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000

4 Data and refinement statistics

Xtrriage (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, 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.	Xtrriage
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

Continued on next page...

Continued from previous page...

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 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 141.

The worst 5 of 1878 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	1 2
1	B	287/387 (74%)	212 (74%)	43 (15%)	32 (11%)	1 2
1	C	322/387 (83%)	240 (74%)	45 (14%)	37 (12%)	1 1
All	All	897/1161 (77%)	660 (74%)	137 (15%)	100 (11%)	1 2

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	130	ASN
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%)	24 58
1	B	233/309 (75%)	217 (93%)	16 (7%)	22 54
1	C	258/309 (84%)	242 (94%)	16 (6%)	26 61
All	All	723/927 (78%)	676 (94%)	47 (6%)	24 58

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 chains 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

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.

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 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.