



Full wwPDB Geometry-Only Validation Report ⓘ

May 18, 2020 – 06:27 am BST

PDB ID : 1VTM
Title : STRUCTURE OF THE U2 STRAIN OF TOBACCO MOSAIC VIRUS
REFINED AT 3.5 ANGSTROMS RESOLUTION USING X-RAY FIBER
DIFFRACTION
Authors : Stubbs, G.; Pattanayek, R.
Deposited on : 1992-03-30
Resolution : 3.50 Å(reported)

This is a Full wwPDB Geometry-Only Validation 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
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

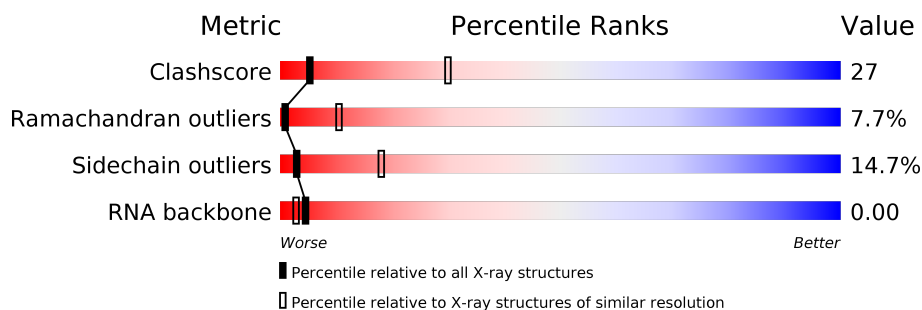
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

FIBER DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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	R	3	<div style="width: 100%; background-color: orange;"></div> 100%
2	P	158	<div style="display: flex; justify-content: space-between;"> <div style="width: 42%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 15%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> </div> 42% 40% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1307 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 RNA chain called RNA (5'-R(P*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	3	Total	C	N	O	P	0	0	0
			67	30	15	19	3			

- Molecule 2 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	158	Total	C	N	O	S	0	0	0
			1232	774	211	244	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	22	GLU	GLN	CONFLICT	UNP P03579
P	55	SER	VAL	CONFLICT	UNP P03579
P	57	VAL	SER	CONFLICT	UNP P03579
P	97	ASN	ASP	CONFLICT	UNP P03579

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	O	0	0
			1	1		
3	P	7	Total	O	0	0
			7	7		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: RNA (5'-R(P*GP*AP*A)-3')

Chain R: 

G1
A2
A3

- Molecule 2: Coat protein

Chain P: 

P1 Y2 T3 T4 N5 S6 P7 P8 S8 Q9 Y12 A16 A18 Y17 D19 P20 V21 E22 L23 L24 L26 L28 C27 T28 N29 Q34 F35 Q38 R41 T42 T43 V44 Q45 Q46 Q47 F48 A49 D50 A51 A52 E53 S55 S56 P56 V57 N58 T59 V60 R61 A64 Y68 Y69 Y70 R71

Y72 M73 S74 T75 L76 D77 P78 L79 T80 T81 A82 L83 L84 N85 S86 F87 D88 T89 R90 R91 R92 E95 V96 N97 N98 Q99 P100 A101 P102 N103 T104 T105 E106 I107 V108 N109 A110 T111 Q112 R113 V114 V119 V122 N126 N127 L128 A129 N130 E131 L132 T136 G137 M138 F139 N140

Q141 F144 S148 G149 L150 V151 W152 T153 T154 T158

4 Model quality

4.1 Standard geometry

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	R	2.66	2/75 (2.7%)	3.68	17/115 (14.8%)
2	P	0.87	0/1259	1.92	31/1726 (1.8%)
All	All	1.06	2/1334 (0.1%)	2.07	48/1841 (2.6%)

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
2	P	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	3	A	N9-C4	9.54	1.43	1.37
1	R	1	G	P-O5'	7.45	1.67	1.59

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	2	A	O4'-C1'-N9	14.47	119.77	108.20
1	R	1	G	P-O3'-C3'	10.98	132.88	119.70
2	P	106	GLU	CA-C-N	-10.36	94.42	117.20
1	R	2	A	C4'-C3'-C2'	10.27	112.86	102.60
1	R	2	A	C5'-C4'-C3'	-9.82	100.28	116.00
2	P	52	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	R	3	A	O4'-C1'-N9	8.71	115.17	108.20
2	P	52	TRP	CE2-CD2-CG	-8.59	100.43	107.30
2	P	17	TYR	CA-C-N	-8.28	98.98	117.20
2	P	152	TRP	CD1-CG-CD2	8.23	112.88	106.30
2	P	52	TRP	CG-CD2-CE3	8.05	141.14	133.90
2	P	52	TRP	CB-CG-CD1	-7.95	116.67	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	3	A	N9-C1'-C2'	7.82	124.17	114.00
2	P	44	VAL	CA-CB-CG2	-7.62	99.47	110.90
2	P	152	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	R	2	A	P-O5'-C5'	-7.52	108.86	120.90
1	R	1	G	C8-N9-C4	-7.46	103.42	106.40
2	P	106	GLU	O-C-N	7.10	134.06	122.70
2	P	96	VAL	N-CA-C	6.69	129.05	111.00
2	P	12	TYR	CB-CG-CD2	-6.66	117.00	121.00
1	R	3	A	C5-C6-N6	-6.62	118.40	123.70
2	P	61	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	P	72	TYR	CA-C-N	-6.56	102.76	117.20
2	P	27	CYS	CA-CB-SG	6.55	125.78	114.00
2	P	68	TYR	CA-C-N	-6.25	103.45	117.20
1	R	1	G	N7-C8-N9	6.19	116.19	113.10
1	R	3	A	C8-N9-C4	-6.13	103.35	105.80
1	R	3	A	C5-C6-N1	6.12	120.76	117.70
1	R	3	A	C3'-C2'-C1'	-6.12	96.60	101.50
2	P	79	LEU	CA-CB-CG	6.10	129.32	115.30
2	P	41	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	P	106	GLU	CA-CB-CG	-5.95	100.31	113.40
2	P	44	VAL	CA-CB-CG1	5.80	119.60	110.90
2	P	50	ASP	CA-CB-CG	5.75	126.06	113.40
2	P	17	TYR	CB-CG-CD1	-5.71	117.58	121.00
2	P	41	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	R	1	G	C5'-C4'-O4'	5.55	115.76	109.10
1	R	3	A	C5'-C4'-C3'	-5.54	107.14	116.00
1	R	2	A	N9-C1'-C2'	5.50	121.15	114.00
2	P	150	LEU	CA-CB-CG	5.38	127.68	115.30
2	P	91	ASN	CA-CB-CG	5.37	125.20	113.40
2	P	136	THR	N-CA-CB	-5.30	100.23	110.30
2	P	106	GLU	CA-C-O	5.27	131.17	120.10
1	R	1	G	C2'-C3'-O3'	5.23	122.06	113.70
2	P	152	TRP	CG-CD1-NE1	-5.21	104.89	110.10
2	P	88	ASP	CA-CB-CG	5.17	124.77	113.40
2	P	113	ARG	NE-CZ-NH1	5.05	122.82	120.30
2	P	52	TRP	CG-CD1-NE1	-5.03	105.08	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	99	GLN	Peptide

4.2 Too-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 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	R	67	0	34	4	0
2	P	1232	0	1194	67	0
3	P	7	0	0	0	0
3	R	1	0	0	0	0
All	All	1307	0	1228	67	0

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 27.

All (67) 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)
2:P:43:THR:HA	2:P:46:GLN:HB2	1.51	0.90
2:P:119:VAL:HG13	2:P:122:ARG:NH1	1.93	0.84
2:P:24:ILE:HD11	2:P:132:LEU:HD22	1.60	0.83
2:P:96:VAL:HG23	2:P:98:ASN:HB2	1.61	0.81
2:P:119:VAL:HG13	2:P:122:ARG:HH11	1.46	0.77
2:P:83:LEU:HG	2:P:87:PHE:CE1	2.30	0.67
2:P:55:SER:HB2	2:P:56:PRO:HD3	1.76	0.67
2:P:76:LEU:HA	2:P:79:LEU:HG	1.77	0.66
2:P:101:ALA:HB1	2:P:103:ASN:HD21	1.64	0.62
2:P:22:GLU:O	2:P:26:LEU:HB2	2.00	0.61
2:P:12:TYR:HB3	2:P:144:PHE:HE1	1.66	0.61
2:P:57:VAL:HG22	2:P:60:VAL:HG23	1.84	0.60
2:P:57:VAL:H	2:P:60:VAL:HB	1.67	0.60
2:P:70:TYR:HB3	2:P:139:PHE:CD1	2.38	0.58
2:P:113:ARG:HH11	2:P:113:ARG:HG3	1.69	0.58
2:P:38:GLN:O	2:P:42:THR:HG22	2.04	0.58
2:P:79:LEU:HD12	2:P:80:ILE:HG13	1.86	0.57
2:P:76:LEU:HD23	2:P:79:LEU:HD21	1.87	0.57
2:P:91:ASN:ND2	2:P:109:ASN:HD21	2.04	0.56
2:P:45:GLN:HA	2:P:48:PHE:CE1	2.40	0.56
2:P:44:VAL:HA	2:P:47:GLN:NE2	2.20	0.56
2:P:64:ALA:HA	2:P:141:GLN:HG3	1.87	0.55
2:P:83:LEU:HD23	2:P:84:LEU:HG	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:48:PHE:CE1	2:P:84:LEU:HD21	2.42	0.54
2:P:70:TYR:HB3	2:P:139:PHE:CE1	2.43	0.53
2:P:41:ARG:CZ	2:P:90:ARG:HE	2.21	0.53
1:R:1:G:C8	2:P:119:VAL:HG22	2.43	0.53
2:P:127:ASN:O	2:P:131:GLU:HG2	2.07	0.53
2:P:23:LEU:HD23	2:P:132:LEU:HD11	1.92	0.52
2:P:48:PHE:HE1	2:P:84:LEU:HD21	1.76	0.51
2:P:79:LEU:CD1	2:P:128:LEU:HD23	2.41	0.51
1:R:1:G:H2'	2:P:119:VAL:HG21	1.92	0.50
2:P:41:ARG:O	2:P:44:VAL:HB	2.10	0.50
2:P:95:GLU:HG2	2:P:96:VAL:HG22	1.93	0.49
2:P:38:GLN:HG2	2:P:92:ARG:HE	1.78	0.49
2:P:76:LEU:HD22	2:P:79:LEU:HD11	1.94	0.49
2:P:95:GLU:HB3	2:P:101:ALA:HA	1.94	0.49
2:P:41:ARG:NH2	2:P:90:ARG:HE	2.10	0.48
2:P:150:LEU:HD13	2:P:150:LEU:H	1.78	0.48
2:P:4:ILE:HA	2:P:9:GLN:HE22	1.78	0.48
2:P:139:PHE:HD2	2:P:144:PHE:HA	1.79	0.47
2:P:45:GLN:HA	2:P:48:PHE:CZ	2.50	0.47
2:P:101:ALA:HB1	2:P:103:ASN:ND2	2.30	0.47
2:P:17:TYR:HB2	2:P:53:LYS:O	2.15	0.47
2:P:75:THR:O	2:P:78:PRO:HD2	2.15	0.46
2:P:41:ARG:HH22	2:P:89:THR:C	2.19	0.46
2:P:44:VAL:HG12	2:P:87:PHE:CE2	2.51	0.45
2:P:2:TYR:HB2	2:P:58:MET:SD	2.57	0.45
2:P:104:THR:N	2:P:108:VAL:HG21	2.32	0.44
2:P:3:THR:OG1	2:P:151:VAL:HB	2.18	0.44
2:P:25:ASN:O	2:P:29:ASN:HB3	2.17	0.43
2:P:82:ALA:O	2:P:85:ASN:ND2	2.51	0.43
2:P:16:ALA:HB3	2:P:70:TYR:OH	2.18	0.43
2:P:6:SER:HA	2:P:7:PRO:HD2	1.85	0.43
2:P:48:PHE:HZ	2:P:87:PHE:CE2	2.36	0.43
2:P:22:GLU:O	2:P:26:LEU:HD12	2.18	0.43
2:P:83:LEU:CD2	2:P:84:LEU:HG	2.49	0.42
2:P:73:ASN:OD1	2:P:76:LEU:HB2	2.18	0.42
2:P:122:ARG:O	2:P:126:ASN:HB2	2.20	0.42
2:P:79:LEU:HD13	2:P:128:LEU:HD23	2.02	0.42
2:P:71:ARG:NH1	2:P:77:ASP:OD1	2.53	0.41
2:P:91:ASN:HD21	2:P:114:VAL:HG22	1.85	0.41
1:R:1:G:C8	2:P:119:VAL:CG2	3.04	0.40
2:P:119:VAL:O	2:P:122:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1:G:N7	2:P:122:ARG:NH1	2.59	0.40
2:P:144:PHE:O	2:P:148:SER:HB2	2.21	0.40
2:P:45:GLN:OE1	2:P:87:PHE:HB3	2.21	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	
2	P	156/158 (99%)	113 (72%)	31 (20%)	12 (8%)	1	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	55	SER
2	P	96	VAL
2	P	99	GLN
2	P	136	THR
2	P	20	PRO
2	P	34	GLN
2	P	35	PHE
2	P	4	ILE
2	P	42	THR
2	P	71	ARG
2	P	103	ASN
2	P	108	VAL

4.3.2 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
2	P	136/136 (100%)	116 (85%)	20 (15%)	3 18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	2	TYR
2	P	6	SER
2	P	19	ASP
2	P	26	LEU
2	P	29	ASN
2	P	52	TRP
2	P	57	VAL
2	P	71	ARG
2	P	83	LEU
2	P	91	ASN
2	P	95	GLU
2	P	109	ASN
2	P	111	THR
2	P	113	ARG
2	P	128	LEU
2	P	130	ASN
2	P	138	MET
2	P	141	GLN
2	P	150	LEU
2	P	154	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	33	ASN
2	P	47	GLN
2	P	91	ASN
2	P	103	ASN
2	P	130	ASN

4.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	2/3 (66%)	2 (100%)	1 (50%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	A
1	R	3	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	A

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.