wwPDB X-ray Structure Validation Summary Report (i)

Apr 10, 2023 – 04:10 PM EDT

PDB ID	:	1TMF
Title	:	THREE-DIMENSIONAL STRUCTURE OF THEILER MURINE ENCEPHALOMYELITIS VIRUS (BEAN STRAIN)
Authors	:	Luo, M.; Toth, K.S.
Deposited on	:	1992-02-20
Resolution	:	3.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

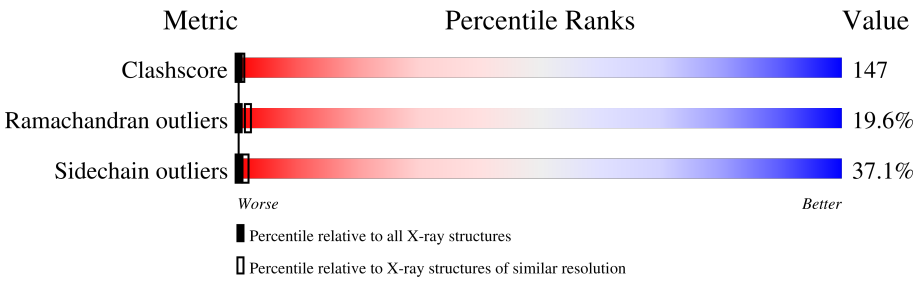
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY 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)

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	276	8% 28% 36% 29%
2	2	267	18% 40% 27% 15%
3	3	232	17% 33% 34% 16%
4	4	45	9% 24% 16% 20% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6260 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 THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	276	2156	1385	361	400	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	138	THR	MET	conflict	UNP P08544
1	139	ASP	THR	conflict	UNP P08544
1	140	THR	ARG	conflict	UNP P08544

- Molecule 2 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	267	2078	1299	367	404	8	0	0	0

- Molecule 3 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	232	1785	1148	288	338	11	0	0	0

- Molecule 4 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	4	31	241	148	40	53	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	12	ASN	GLN	conflict	UNP P13899
4	13	GLU	SER	conflict	UNP P13899
4	55	LEU	ILE	conflict	UNP P13899

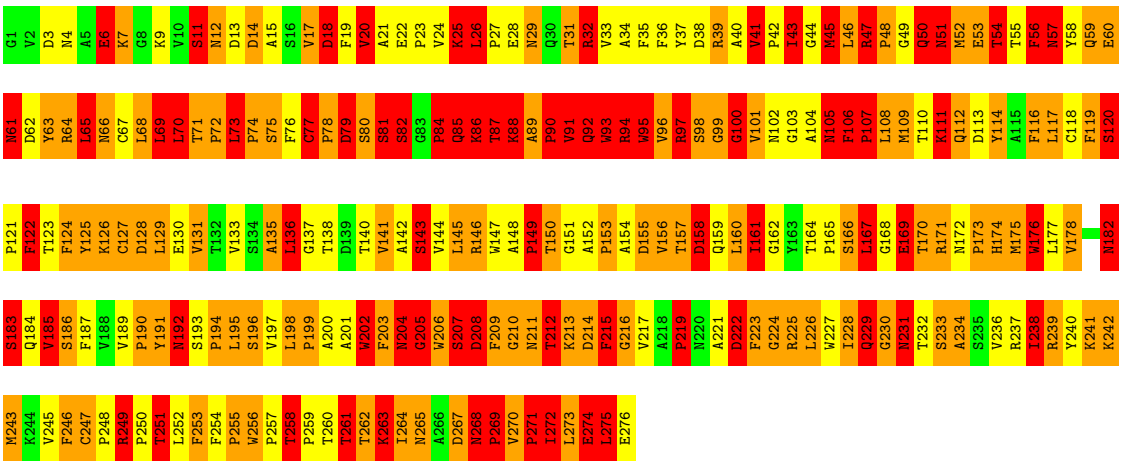
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

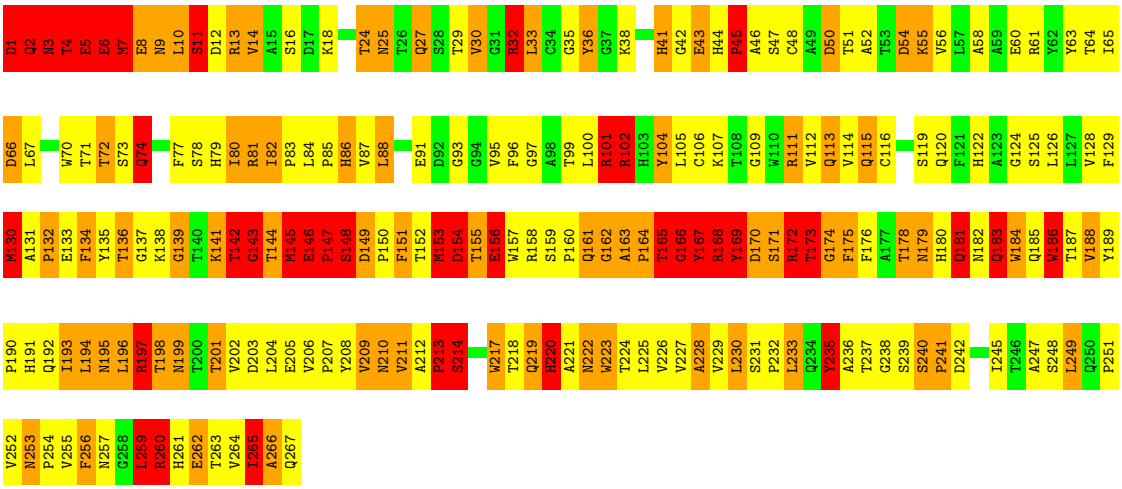
• Molecule 1: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1)

Chain 1: 8% 28% 36% 29%



• Molecule 2: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2)

Chain 2: 18% 40% 27% 15%



• Molecule 3: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3)

Chain 3: 17% 33% 34% 16%

S1 V7 R8 E9 H10 K11 G12 C13 F14 Y15 S16 T17 N18 P19 D20 T21 T22 V23 P24 T25 Y26 T29 P33 S34 D35 Y36 M37 L44 L45 E46 L47 C48 K49 L50 P51 T52 F53 L54 G55 N56 P57 N58 T59 N60 N61 K62 R63 Y64 P65 Y66 F67 S68 A69 T70 N71 S72

V73 P74 A75 T76 S77 M78 V79 D80 Y81 Q82 V83 A84 L85 S86 C87 S88 C89 M90 A91 N92 S93 M94 L95 A96 A97 V98 A99 R100 N101 F102 N103 Q104 Y105 R106 G107 S108 L109 N110 F111 L112 F113 V114 F115 T116 G117 A118 A119 M120 V121 K122 G123 K124 F125 L126 I127 A128 Y129 T130 P131 P132

G133 K136 P137 T138 T139 R140 D141 Q142 A143 M144 Q145 S146 T147 Y148 A149 I150 W151 D152 L153 G154 L155 N156 S157 S158 F159 N160 F161 T162 A163 P164 F165 I166 S167 P168 T169 H170 Y171 R172 Q173 T174 S175 Y176 T177 S178 P179 T180 I181 T182 S183 V184 D185 G186 W187 V188 T189 V190 W191 Q192 L193

T194 P195 L196 T197 Y198 T202 P203 T204 N205 S206 D207 I208 L209 T210 L211 V212 S213 A214 G215 D216 D217 F218 T219 L220 R221 M222 P223 I224 S225 P226 T227 K228 W229 V230 P231 Q232

- Molecule 4: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4)

Chain 4: 9% 24% 16% 20% 31%

N12 E13 S14 G15 N16 E17 G18 V19 I20 I21 N22 N23 F24 Y25 S26 N27 Q28 Y29 Q30 N31 S32 I33 D34 L35 S36 A37 SER GLY GLY ASN ALA GLY ASP ALA PRO GLN THR ASN GLY GLN L52 S53 N54 L55 L56

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	331.86Å 331.86Å 796.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	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	6260	wwPDB-VP
Average B, all atoms ($Å^2$)	0.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1	2.15	60/2222 (2.7%)	2.83	192/3039 (6.3%)
2	2	1.78	34/2136 (1.6%)	2.48	107/2922 (3.7%)
3	3	1.48	20/1840 (1.1%)	2.19	97/2525 (3.8%)
4	4	1.92	2/242 (0.8%)	3.39	16/326 (4.9%)
All	All	1.84	116/6440 (1.8%)	2.57	412/8812 (4.7%)

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	1	0	41
2	2	0	15
3	3	0	8
4	4	0	3
All	All	0	67

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	105	ASN	C-N	26.88	1.95	1.34
2	2	260	ARG	C-N	23.70	1.88	1.34
4	4	34	ASP	C-N	-22.21	0.82	1.34
1	1	272	ILE	CB-CG1	21.32	2.13	1.54
2	2	143	GLY	C-N	19.07	1.77	1.34

The worst 5 of 412 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	34	ASP	O-C-N	-39.99	58.72	122.70
2	2	5	GLU	O-C-N	-31.94	71.59	122.70
2	2	8	GLU	O-C-N	-31.39	72.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3	ASN	O-C-N	-29.43	75.61	122.70
1	1	271	PRO	O-C-N	25.77	163.93	122.70

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	12	ASN	Mainchain
1	1	25	LYS	Mainchain
1	1	32	ARG	Peptide,Mainchain
1	1	56	PHE	Mainchain
1	1	57	ASN	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	1	2156	0	2050	880	0
2	2	2078	0	1953	564	0
3	3	1785	0	1711	472	0
4	4	241	0	220	36	0
All	All	6260	0	5934	1795	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 147.

The worst 5 of 1795 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)
2:2:183:GLN:HB2	2:2:186:TRP:CZ3	1.31	1.64
3:3:7:VAL:CG2	3:3:11:LYS:HE2	1.18	1.62
1:1:192:ASN:HB3	3:3:222:MET:CE	1.17	1.61
1:1:192:ASN:CB	3:3:222:MET:HE1	1.14	1.61
1:1:108:LEU:CD1	1:1:112:GLN:HE22	0.98	1.59

There are no symmetry-related clashes.

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	1	270/276 (98%)	157 (58%)	48 (18%)	65 (24%)	0 0
2	2	265/267 (99%)	175 (66%)	43 (16%)	47 (18%)	0 2
3	3	230/232 (99%)	149 (65%)	46 (20%)	35 (15%)	0 3
4	4	27/45 (60%)	9 (33%)	10 (37%)	8 (30%)	0 0
All	All	792/820 (97%)	490 (62%)	147 (19%)	155 (20%)	0 2

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	18	ASP
1	1	51	ASN
1	1	57	ASN
1	1	70	LEU
1	1	81	SER

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	1	236/237 (100%)	141 (60%)	95 (40%)	0 1
2	2	225/225 (100%)	155 (69%)	70 (31%)	0 2
3	3	198/204 (97%)	120 (61%)	78 (39%)	0 1
4	4	28/36 (78%)	16 (57%)	12 (43%)	0 0
All	All	687/702 (98%)	432 (63%)	255 (37%)	0 1

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	88	LEU
3	3	173	GLN
2	2	186	TRP
3	3	161	PHE
3	3	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	92	ASN
4	4	22	ASN
3	3	103	ASN
3	3	156	ASN
4	4	28	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	19
2	2	8
3	3	8
4	4	1

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	265:ASN	C	266:ALA	N	23.91
1	1	259:PRO	C	260:THR	N	2.69
1	1	105:ASN	C	106:PHE	N	1.95
1	2	260:ARG	C	261:HIS	N	1.88
1	2	143:GLY	C	144:THR	N	1.77

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.