



wwPDB EM Validation Summary Report ⓘ

Mar 3, 2025 – 12:32 pm GMT

PDB ID : 9HBX
EMDB ID : EMD-52033
Title : TiLV-NP hexamer (pseudo-C6) (local refinement around 2 TiLV-NPs)
Authors : Arragain, B.; Cusack, S.
Deposited on : 2024-11-08
Resolution : 3.04 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

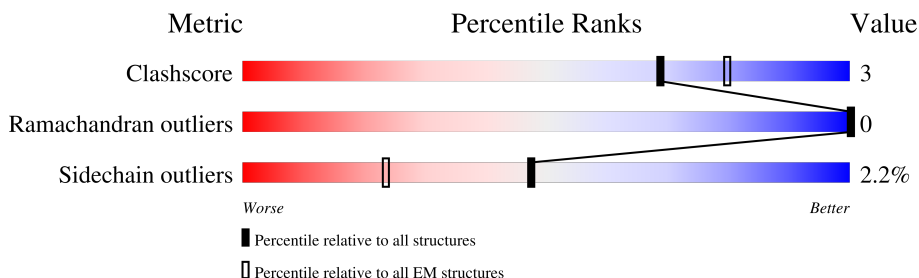
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	C	354	76% 6% . 18%
1	D	354	81% 8% 10%
1	E	354	5% .. 94%
2	N	52	10% 8% . 81%
2	O	52	6% 12% 6% 77%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5261 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tilapia Lake Virus nucleoprotein (segment 4).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	292	Total	C	N	O	S	0	0
			2251	1417	408	410	16		
1	D	317	Total	C	N	O	S	0	0
			2422	1521	439	445	17		
1	E	21	Total	C	N	O	S	0	0
			147	92	26	28	1		

- Molecule 2 is a DNA chain called 40-mer vRNA loop.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	10	Total	C	N	O	P	0	0
			201	97	34	60	10		
2	O	12	Total	C	N	O	P	0	0
			240	116	40	72	12		

- [illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156453	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5P, Y5P

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	C	0.26	0/2290	0.48	0/3083
1	D	0.26	0/2464	0.48	0/3320
1	E	0.26	0/148	0.45	0/199
All	All	0.26	0/4902	0.48	0/6602

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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	C	2251	0	2290	14	0
1	D	2422	0	2457	19	0
1	E	147	0	143	5	0
2	N	201	0	107	2	0
2	O	240	0	129	7	0
All	All	5261	0	5126	36	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 3.

The worst 5 of 36 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:D:321:GLU:OE2	1:E:303:SER:OG	2.04	0.75
1:D:340:SER:OG	1:E:295:LEU:O	2.06	0.73
1:C:327:LYS:HG3	1:C:328:GLN:H	1.58	0.66
1:D:338:GLY:O	1:E:308:SER:OG	2.19	0.60
1:C:113:SER:OG	1:C:113:SER:O	2.20	0.59

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 PDB entries followed by that with respect to all EM entries.

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	C	288/354 (81%)	282 (98%)	6 (2%)	0	100	100
1	D	315/354 (89%)	303 (96%)	12 (4%)	0	100	100
1	E	19/354 (5%)	17 (90%)	2 (10%)	0	100	100
All	All	622/1062 (59%)	602 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	C	238/285 (84%)	234 (98%)	4 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	256/285 (90%)	251 (98%)	5 (2%)	50 75
1	E	15/285 (5%)	13 (87%)	2 (13%)	3 13
All	All	509/855 (60%)	498 (98%)	11 (2%)	47 73

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	246	ASP
1	D	303	SER
1	E	308	SER
1	E	293	CYS
1	D	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	P5P	N	5	2	16,23,24	0.78	0	14,33,36	0.73	0
2	P5P	N	11	2	16,23,24	0.76	0	14,33,36	0.73	0
2	Y5P	O	2	2	14,19,20	3.66	1 (7%)	18,26,29	0.79	1 (5%)
2	P5P	O	3	2	16,23,24	0.77	0	14,33,36	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P5P	N	3	2	16,23,24	0.78	0	14,33,36	0.74	0
2	P5P	N	4	2	16,23,24	0.77	0	14,33,36	0.74	0
2	P5P	O	10	2	16,23,24	0.77	0	14,33,36	0.75	0
2	P5P	O	6	2	16,23,24	0.77	0	14,33,36	0.75	0
2	P5P	N	10	2	16,23,24	0.79	0	14,33,36	0.79	0
2	Y5P	N	9	2	14,19,20	2.34	1 (7%)	18,26,29	1.02	1 (5%)
2	P5P	N	6	2	16,23,24	0.78	0	14,33,36	0.76	0
2	P5P	O	4	2	16,23,24	0.78	0	14,33,36	0.74	0
2	P5P	N	7	2	16,23,24	0.78	0	14,33,36	0.72	1 (7%)
2	P5P	O	1	2	16,23,24	1.31	3 (18%)	14,33,36	1.92	2 (14%)
2	Y5P	O	8	2	14,19,20	2.33	1 (7%)	18,26,29	0.98	1 (5%)
2	Y5P	O	12	2	14,19,20	2.33	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	O	7	2	16,23,24	0.78	0	14,33,36	0.75	0
2	Y5P	N	8	2	14,19,20	2.31	1 (7%)	18,26,29	0.98	1 (5%)
2	Y5P	O	9	2	14,19,20	2.34	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	O	11	2	16,23,24	0.78	0	14,33,36	0.72	0
2	P5P	O	5	2	16,23,24	0.78	0	14,33,36	0.74	0
2	Y5P	N	12	2	14,19,20	2.35	1 (7%)	18,26,29	1.00	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P5P	N	5	2	-	0/3/25/26	0/3/3/3
2	P5P	N	11	2	-	0/3/25/26	0/3/3/3
2	Y5P	O	2	2	-	4/7/33/34	0/2/2/2
2	P5P	O	3	2	-	3/3/25/26	0/3/3/3
2	P5P	N	3	2	-	0/3/25/26	0/3/3/3
2	P5P	N	4	2	-	0/3/25/26	0/3/3/3
2	P5P	O	10	2	-	1/3/25/26	0/3/3/3
2	P5P	O	6	2	-	1/3/25/26	0/3/3/3
2	P5P	N	10	2	-	1/3/25/26	0/3/3/3
2	Y5P	N	9	2	-	1/7/33/34	0/2/2/2
2	P5P	N	6	2	-	0/3/25/26	0/3/3/3
2	P5P	O	4	2	-	0/3/25/26	0/3/3/3
2	P5P	N	7	2	-	0/3/25/26	0/3/3/3
2	P5P	O	1	2	-	2/3/25/26	0/3/3/3
2	Y5P	O	8	2	-	3/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y5P	O	12	2	-	1/7/33/34	0/2/2/2
2	P5P	O	7	2	-	0/3/25/26	0/3/3/3
2	Y5P	N	8	2	-	3/7/33/34	0/2/2/2
2	Y5P	O	9	2	-	1/7/33/34	0/2/2/2
2	P5P	O	11	2	-	1/3/25/26	0/3/3/3
2	P5P	O	5	2	-	0/3/25/26	0/3/3/3
2	Y5P	N	12	2	-	1/7/33/34	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	Y5P	C4-N3	-13.53	1.33	1.46
2	N	12	Y5P	C4-N3	-8.64	1.38	1.46
2	N	9	Y5P	C4-N3	-8.63	1.38	1.46
2	O	9	Y5P	C4-N3	-8.60	1.38	1.46
2	O	12	Y5P	C4-N3	-8.55	1.38	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	P5P	C6-N1-C2	6.40	125.01	115.84
2	N	12	Y5P	N1-C2-N3	-3.59	114.81	125.33
2	O	8	Y5P	N1-C2-N3	-3.59	114.81	125.33
2	O	12	Y5P	N1-C2-N3	-3.59	114.81	125.33
2	O	9	Y5P	N1-C2-N3	-3.58	114.84	125.33

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	2	Y5P	C3'-C4'-C5'-O5'
2	O	3	P5P	O4'-C4'-C5'-O5'
2	N	8	Y5P	C3'-C4'-C5'-O5'
2	N	8	Y5P	O4'-C1'-N1-C2
2	O	8	Y5P	O4'-C1'-N1-C2

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	3	P5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	6	P5P	2	0
2	N	6	P5P	1	0
2	O	4	P5P	1	0
2	N	7	P5P	2	0
2	O	1	P5P	1	0
2	O	8	Y5P	2	0
2	O	7	P5P	1	0
2	O	9	Y5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

There are no chain breaks in this entry.