Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 06:07 AM EDT

PDB ID	:	6MPS
Title	:	TagT bound to LIIa-WTA
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Deposited on	:	2018-10-08
Resolution	:	1.86 Å(reported)

This is a Full wwPDB X-ray Structure 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 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:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
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)	:	2.35.1

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 1.86 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4270 atoms, of which 2049 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.

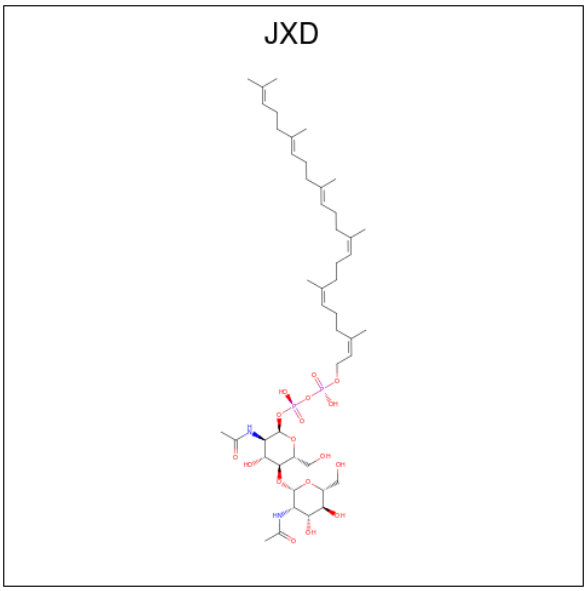
- Molecule 1 is a protein called Polyisoprenyl-teichoic acid–peptidoglycan teichoic acid transferase TagT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	255	3945	1246	1973	336	386	4	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MET	-	initiating methionine	UNP Q7WY78
A	323	LEU	-	expression tag	UNP Q7WY78
A	324	GLU	-	expression tag	UNP Q7WY78
A	325	HIS	-	expression tag	UNP Q7WY78
A	326	HIS	-	expression tag	UNP Q7WY78
A	327	HIS	-	expression tag	UNP Q7WY78
A	328	HIS	-	expression tag	UNP Q7WY78
A	329	HIS	-	expression tag	UNP Q7WY78
A	330	HIS	-	expression tag	UNP Q7WY78

- Molecule 2 is 2-(acetylamino)-4-O-[2-(acetylamino)-2-deoxy-beta-D-mannopyranosyl]-2-deoxy-1-O-[(S)-{[(R)-{[(2Z,6Z,10Z,14E,18E)-3,7,11,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaen-1-yl]oxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]-alpha-D-glucopyranose (three-letter code: JXD) (formula: $C_{46}H_{78}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			143	46	76	2	17	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total	O	0	0
			180	180		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	66.37Å 66.37Å 145.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.35 – 1.86	Depositor
% Data completeness (in resolution range)	99.0 (60.35-1.86)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.216 , 0.235	Depositor
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.068	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4270	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	JXD	A	401	3	65,68,68	1.99	12 (18%)	87,93,93	2.20	30 (34%)

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	JXD	A	401	3	-	13/63/104/104	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	JXD	P25-O24	8.21	1.82	1.60
2	A	401	JXD	P28-O30	5.04	1.79	1.59
2	A	401	JXD	C05-C14	4.86	1.61	1.53
2	A	401	JXD	O30-C31	-4.79	1.36	1.43
2	A	401	JXD	C23-C63	4.29	1.60	1.53
2	A	401	JXD	C12-C14	3.21	1.59	1.53
2	A	401	JXD	C48-C49	2.72	1.39	1.33
2	A	401	JXD	C44-C45	2.56	1.39	1.33
2	A	401	JXD	C02-C63	2.43	1.57	1.53
2	A	401	JXD	C03-C19	2.22	1.58	1.52
2	A	401	JXD	C52-C53	2.20	1.38	1.32
2	A	401	JXD	O22-C19	-2.10	1.39	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	JXD	O27-P25-O24	6.11	114.81	102.48
2	A	401	JXD	C47-C46-C45	5.38	130.67	112.98
2	A	401	JXD	C50-C49-C48	5.26	131.77	121.12
2	A	401	JXD	C46-C45-C44	5.12	131.48	121.12
2	A	401	JXD	C17-C16-N15	4.13	123.09	116.10
2	A	401	JXD	C51-C50-C49	3.70	125.16	112.98
2	A	401	JXD	C66-C65-N64	3.70	122.36	116.10
2	A	401	JXD	C47-C48-C49	-3.62	118.95	127.66
2	A	401	JXD	O22-C23-O24	-3.51	106.78	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	JXD	C43-C44-C45	-3.47	119.31	127.66
2	A	401	JXD	C51-C52-C53	-3.45	115.95	127.75
2	A	401	JXD	C57-C45-C46	-3.34	109.66	115.27
2	A	401	JXD	C54-C53-C52	3.15	131.76	122.65
2	A	401	JXD	O67-C65-C66	-3.09	116.32	122.06
2	A	401	JXD	C23-C63-N64	3.01	116.19	111.00
2	A	401	JXD	C05-C14-N15	2.99	116.15	111.00
2	A	401	JXD	O22-C19-C20	2.92	113.70	106.44
2	A	401	JXD	C34-C35-C36	2.73	120.86	111.88
2	A	401	JXD	C56-C49-C50	-2.70	110.73	115.27
2	A	401	JXD	O18-C16-C17	-2.69	117.06	122.06
2	A	401	JXD	O22-C23-C63	-2.69	105.33	110.58
2	A	401	JXD	O62-P25-O24	-2.65	96.30	106.78
2	A	401	JXD	O04-C03-C19	2.53	116.39	109.45
2	A	401	JXD	O24-C23-C63	2.49	112.91	108.40
2	A	401	JXD	C38-C39-C40	2.43	119.86	111.88
2	A	401	JXD	C56-C49-C48	-2.41	117.50	123.68
2	A	401	JXD	C43-C42-C41	2.32	120.61	112.98
2	A	401	JXD	C55-C53-C54	-2.30	109.53	114.60
2	A	401	JXD	O62-P25-O26	2.17	122.98	112.24
2	A	401	JXD	C39-C38-C37	2.15	120.06	112.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

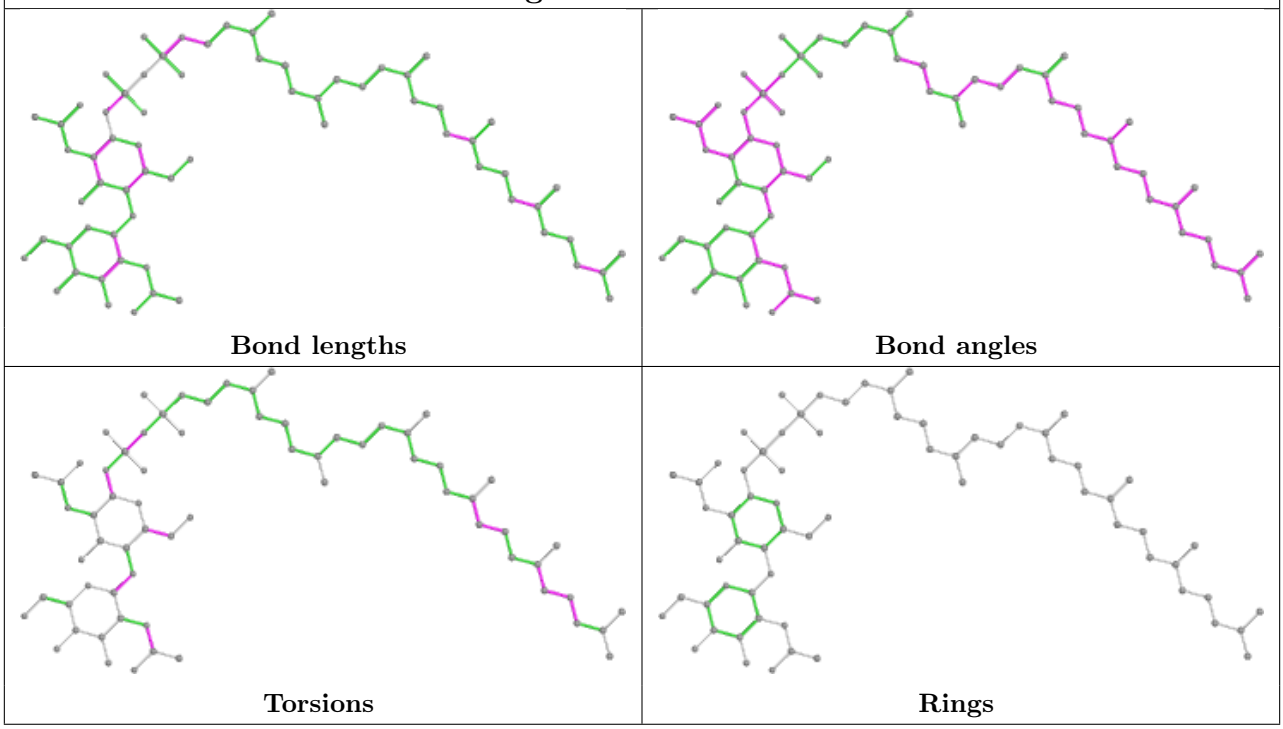
Mol	Chain	Res	Type	Atoms
2	A	401	JXD	O22-C23-O24-P25
2	A	401	JXD	C49-C50-C51-C52
2	A	401	JXD	C17-C16-N15-C14
2	A	401	JXD	O18-C16-N15-C14
2	A	401	JXD	C57-C45-C46-C47
2	A	401	JXD	C45-C46-C47-C48
2	A	401	JXD	C44-C45-C46-C47
2	A	401	JXD	C14-C05-O04-C03
2	A	401	JXD	P28-O27-P25-O24
2	A	401	JXD	C56-C49-C50-C51
2	A	401	JXD	C48-C49-C50-C51
2	A	401	JXD	C50-C51-C52-C53
2	A	401	JXD	C03-C19-C20-O21

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand JXD A 401



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.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.