



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PW2
Title : Ternary complex of Aflatoxin B1 Adduct modified DNA (AFB1-FAPY) with DNA Polymerase IV and incoming dTTP
Authors : Banerjee, S.
Deposited on : 2010-12-07
Resolution : 2.74 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

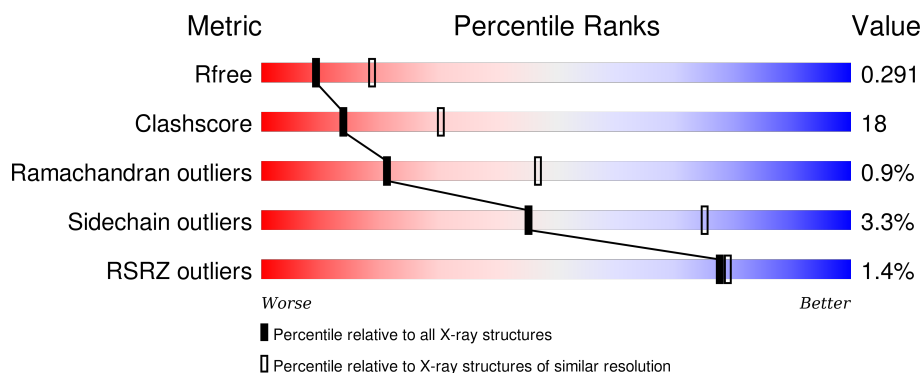
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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))
R_{free}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div></div> <div>65%</div> <div>31%</div> <div>..</div> </div>
2	B	15	<div> <div>47%</div> <div>53%</div> </div>
3	C	13	<div> <div>69%</div> <div>31%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3486 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 DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2754	1766	475	506	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
A	0	HIS	-	EXPRESSION TAG	UNP Q97W02
A	1	HIS	-	EXPRESSION TAG	UNP Q97W02

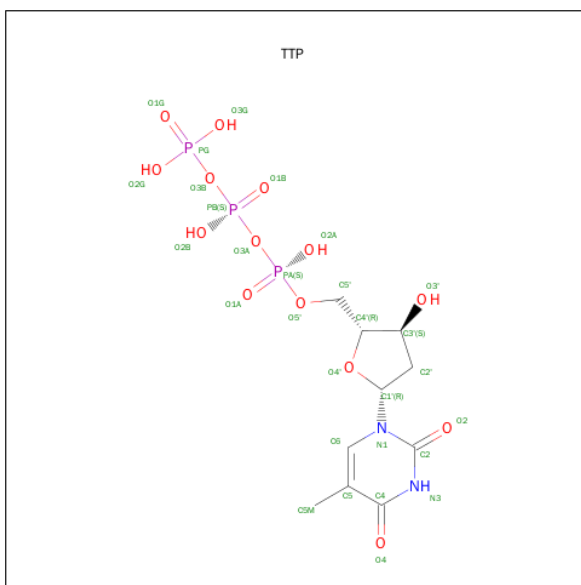
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*(PVX)P*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			319	160	46	99	14			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	
			29	10	2	14	3	

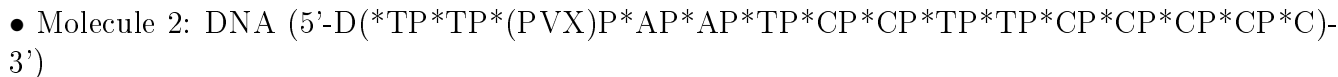
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca		
			3	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O		
			77	77	0	0
6	B	21	Total	O		
			21	21	0	0
6	C	10	Total	O		
			10	10	0	0

- Molecule 1: DNA polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.25Å 104.41Å 52.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 2.74 45.77 – 2.74	Depositor EDS
% Data completeness (in resolution range)	93.3 (29.09-2.74) 93.3 (45.77-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.294 0.218 , 0.291	Depositor DCC
R_{free} test set	1337 reflections (10.14%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 13582 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3486	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: PVX, CA, TTP

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	0.36	0/2794	0.59	0/3751
2	B	0.43	0/300	0.76	0/456
3	C	0.42	0/308	0.78	0/476
All	All	0.38	0/3402	0.63	0/4683

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 [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	A	2754	0	2896	102	0
2	B	319	0	183	16	0
3	C	273	0	147	4	0
4	A	29	0	12	4	0
5	A	3	0	0	0	0
6	A	77	0	0	6	2
6	B	21	0	0	3	0
6	C	10	0	0	0	0
All	All	3486	0	3238	122	2

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 18.

The worst 5 of 122 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)
4:A:400:TTP:H6	4:A:400:TTP:H5'1	1.02	1.13
2:B:381:DT:H2''	2:B:382:DC:H5'	1.32	1.11
4:A:400:TTP:C6	4:A:400:TTP:H5'1	1.89	1.07
1:A:15:GLN:HE22	1:A:140:THR:N	1.66	0.93
1:A:174:ARG:HH11	1:A:174:ARG:HB2	1.34	0.91

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
6:A:2100:HOH:O	6:A:2100:HOH:O[2_435]	2.08	0.12
6:A:2090:HOH:O	6:A:2095:HOH:O[1_556]	2.17	0.03

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	A	340/347 (98%)	309 (91%)	28 (8%)	3 (1%)	21 47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ASP
1	A	11	TYR
1	A	25	LYS

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	301/306 (98%)	291 (97%)	10 (3%)	45 75

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	118	ASP
1	A	178	GLU
1	A	64	GLU
1	A	174	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	305	HIS
1	A	189	ASN
1	A	15	GLN
1	A	255	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PVX	B	374	2	44,53,54	3.09	17 (38%)	50,81,84	2.13	19 (38%)

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	PVX	B	374	2	-	0/11/66/67	0/7/7/7

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	374	PVX	CB1-C1	-5.54	1.41	1.49
2	B	374	PVX	O4-C4	-2.40	1.19	1.24
2	B	374	PVX	C3A-CB1	-2.02	1.39	1.41
2	B	374	PVX	O6A-C5M	2.01	1.40	1.37
2	B	374	PVX	C4-N3	2.28	1.37	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	374	PVX	C5-C6-N6	-4.88	119.43	123.57
2	B	374	PVX	C3A-C3-C2A	-4.58	103.21	109.07
2	B	374	PVX	N3-C2-N1	-2.93	120.73	125.53
2	B	374	PVX	C5B-C5M-C9B	-2.82	121.70	124.26
2	B	374	PVX	C5B-C4B-C4A	-2.12	117.44	120.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	374	PVX	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 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	$\# Z > 2$
4	TTP	A	400	5	21,30,30	3.15	6 (28%)	31,47,47	3.89	8 (25%)

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
4	TTP	A	400	5	-	0/18/34/34	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	TTP	O3'-C3'	-8.81	1.23	1.43
4	A	400	TTP	O5'-C5'	-5.63	1.21	1.44
4	A	400	TTP	C6-C5	-2.11	1.34	1.40
4	A	400	TTP	PA-O2A	-2.09	1.46	1.54
4	A	400	TTP	C6-N1	3.74	1.40	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	TTP	C5-C4-N3	-10.78	113.13	125.14
4	A	400	TTP	O4'-C4'-C5'	-5.57	89.39	109.32
4	A	400	TTP	C2'-C1'-N1	-4.36	103.55	114.16
4	A	400	TTP	O4'-C4'-C3'	2.54	112.05	105.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	TTP	O2A-PA-O5'	3.47	125.97	108.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	400	TTP	4	0

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/347 (98%)	0.10	5 (1%) 76 78	8, 33, 58, 77	1 (0%)
2	B	14/15 (93%)	-0.11	0 100 100	25, 44, 60, 70	0
3	C	13/13 (100%)	-0.38	0 100 100	20, 31, 62, 70	0
All	All	369/375 (98%)	0.07	5 (1%) 78 79	8, 33, 59, 77	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	ASP	2.9
1	A	217	MET	2.5
1	A	193	GLU	2.3
1	A	114	ASP	2.2
1	A	117	ARG	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PVX	B	374	47/48	0.95	0.16	-	9,21,30,34	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	TTP	A	400	29/29	0.93	0.19	0.91	20,28,33,36	0
5	CA	A	1002	1/1	0.91	0.11	-3.65	15,15,15,15	0
5	CA	A	1003	1/1	0.94	0.09	-	39,39,39,39	0
5	CA	A	1001	1/1	0.93	0.19	-	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.