wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 03:47 am GMT

PDB ID	:	2VJV
Title	:	Crystal structure of the IS608 transposase in complex with left end 26-mer DNA hairpin and a 6-mer DNA representing the left end cleavage site
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Deposited on	:	2007-12-13
Resolution	:	1.90 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3622 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 TRANSPOSASE ORFA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1023	659	181	177	6			
1	B	125	Total	C	N	O	S	0	0	0
			1023	659	181	177	6			

- Molecule 2 is a DNA chain called 5'-D(*DA*DA*DA*DG*DC*DC*DC*DC*DT*DA*DG*DC*DTP*DT *DT*DT*DA*DG*DC*DT*DA*DT*DG*DG*DG*DGP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	26	Total	C	N	O	P	0	0	0
			531	254	97	155	25			
2	D	26	Total	C	N	O	P	0	0	0
			531	254	97	155	25			

- Molecule 3 is a DNA chain called 5'-D(*DT*DA*DT*DT*DA*DCP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	P	0	0	0
			118	59	19	35	5			
3	F	6	Total	C	N	O	P	0	0	0
			118	59	19	35	5			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	B	70	Total O 70 70	0	0
5	C	53	Total O 53 53	0	0
5	D	59	Total O 59 59	0	0
5	E	20	Total O 20 20	0	0
5	F	10	Total O 10 10	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.29Å 72.41Å 110.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.61 – 1.90 24.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.8 (24.61-1.90) 87.9 (24.61-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.227 0.193 , 0.218	Depositor DCC
R_{free} test set	1131 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3622	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.55% 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.

3 Model quality

3.1 Standard geometry

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

3.2 Too-close contacts

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

3.3 Torsion angles

3.3.1 Protein backbone

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

3.3.2 Protein sidechains

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

3.3.3 RNA

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

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

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

3.5 Carbohydrates

There are no monosaccharides in this entry.

3.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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, 95^{th} 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	125/159 (78%)	0.17	5 (4%) 38 41	16, 24, 52, 63	0
1	B	125/159 (78%)	0.27	8 (6%) 19 22	13, 23, 55, 71	0
2	C	26/26 (100%)	-0.19	0 100 100	18, 28, 44, 64	0
2	D	26/26 (100%)	-0.27	0 100 100	18, 27, 44, 56	0
3	E	6/6 (100%)	0.04	1 (16%) 1 1	24, 26, 33, 80	0
3	F	6/6 (100%)	-0.07	1 (16%) 1 1	23, 24, 32, 81	0
All	All	314/382 (82%)	0.13	15 (4%) 30 33	13, 25, 55, 81	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	ASN	6.0
1	A	6	LEU	4.4
1	A	122	ASN	3.9
3	E	-6	DT	3.1
1	A	98	HIS	3.0

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

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

4.3 Carbohydrates

There are no monosaccharides in this entry.

4.4 Ligands

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
4	MG	E	1042	1/1	0.97	0.15	41,41,41,41	0
4	MG	D	1042	1/1	0.99	0.03	16,16,16,16	0
4	MG	C	1042	1/1	0.99	0.06	20,20,20,20	0

4.5 Other polymers

There are no such residues in this entry.