



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 17, 2018 – 05:13 pm GMT

PDB ID : 1V6V
Title : Crystal Structure Of Xylanase From Streptomyces Olivaceoviridis E-86 Complexed With 3(2)-alpha-L-arabinofuranosyl-xylotriose
Authors : Fujimoto, Z.; Kaneko, S.; Kuno, A.; Kobayashi, H.; Kusakabe, I.; Mizuno, H.
Deposited on : 2003-12-04
Resolution : 2.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

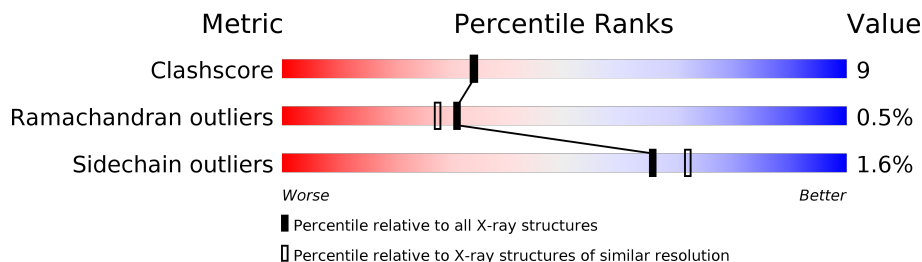
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	122078	5107 (2.10-2.10)
Ramachandran outliers	120005	5057 (2.10-2.10)
Sidechain outliers	119972	5058 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	 85% 14% .
1	B	436	 83% 16% .

2 Entry composition [i](#)

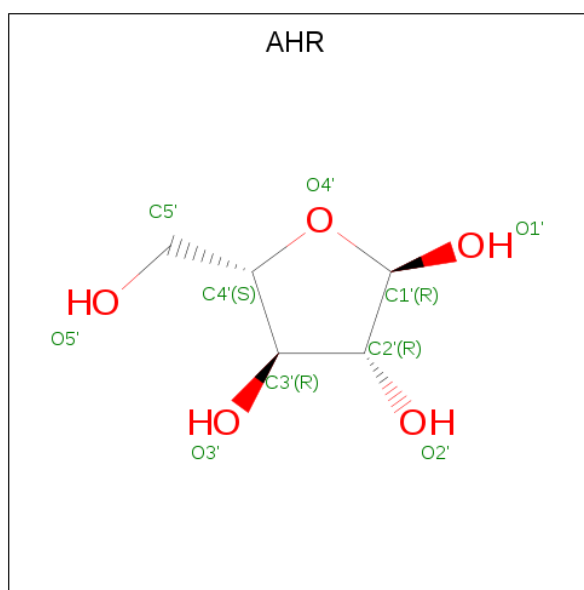
There are 4 unique types of molecules in this entry. The entry contains 7722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDO-1,4-BETA-D-XYLANASE.

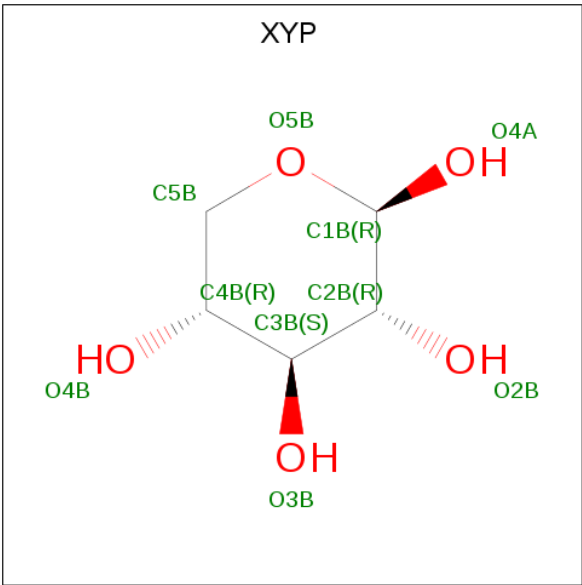
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3288	2020	596	656	16			
1	B	436	Total	C	N	O	S	0	0	0
			3288	2020	596	656	16			

- Molecule 2 is ALPHA-L-ARABINOFURANOSE (three-letter code: AHR) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	5	4		
2	A	1	Total	C	O	0	0
			9	5	4		
2	B	1	Total	C	O	0	0
			9	5	4		

- Molecule 3 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	5	4		
3	A	1	Total	C	O	0	0
			9	5	4		
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			9	5	4		
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			9	5	4		
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			9	5	4		
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			9	5	4		
3	B	1	Total	C	O	0	0
			9	5	4		
3	B	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			9	5	4		
3	B	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			9	5	4		
3	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	420	Total	O	0	0
			420	420		
4	B	520	Total	O	0	0
			520	520		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.56Å 93.99Å 139.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.10	Depositor
% Data completeness (in resolution range)	98.7 (29.97-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7722	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.29	0/3356	0.60	0/4556
1	B	0.31	0/3356	0.60	0/4556
All	All	0.30	0/6712	0.60	0/9112

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	A	3288	0	3093	56	0
1	B	3288	0	3090	63	0
2	A	18	0	16	1	0
2	B	9	0	8	0	0
3	A	103	0	87	12	0
3	B	76	0	67	11	0
4	A	420	0	0	7	0
4	B	520	0	0	5	0
All	All	7722	0	6361	120	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 9.

The worst 5 of 120 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:B:774:TRP:HH2	3:B:956:XYP:H4B	1.43	0.83
2:A:470:AHR:O2'	2:A:470:AHR:H5'1	1.78	0.83
1:A:274:TRP:HH2	3:A:456:XYP:H4B	1.46	0.81
1:B:927:ASN:HA	1:B:932:ARG:CZ	2.13	0.78
1:A:144:GLN:HE22	1:A:148:ASN:HA	1.55	0.71

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	A	434/436 (100%)	419 (96%)	13 (3%)	2 (0%)	31	27
1	B	434/436 (100%)	417 (96%)	15 (4%)	2 (0%)	31	27
All	All	868/872 (100%)	836 (96%)	28 (3%)	4 (0%)	31	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	GLY
1	B	844	SER
1	A	2	GLU
1	B	809	PRO

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	341/341 (100%)	336 (98%)	5 (2%)	67	73
1	B	341/341 (100%)	335 (98%)	6 (2%)	62	67
All	All	682/682 (100%)	671 (98%)	11 (2%)	65	72

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

Mol	Chain	Res	Type
1	A	423	TYR
1	B	555	GLN
1	B	747	TYR
1	A	280	PRO
1	B	701	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	B	511	GLN
1	B	814	GLN
1	A	205	GLN
1	B	694	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

22 ligands 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	AHR	A	449	3	9,9,10	0.68	0	9,12,14	1.54	1 (11%)
3	XYP	A	450	3	9,9,10	0.63	0	10,12,14	0.84	1 (10%)
3	XYP	A	451	3,2	9,9,10	0.61	0	10,12,14	1.06	1 (10%)
3	XYP	A	452	3	10,10,10	0.47	0	14,14,14	0.67	0
3	XYP	A	456	3	9,9,10	0.61	0	10,12,14	0.83	1 (10%)
3	XYP	A	457	3	10,10,10	0.54	0	14,14,14	0.62	0
3	XYP	A	461	3	9,9,10	0.63	0	10,12,14	0.85	1 (10%)
3	XYP	A	462	3	9,9,10	0.63	0	10,12,14	0.81	0
3	XYP	A	463	3	10,10,10	0.58	0	14,14,14	0.60	0
2	AHR	A	470	3	9,9,10	0.67	0	9,12,14	1.56	1 (11%)
3	XYP	A	471	3	9,9,10	0.61	0	10,12,14	0.92	1 (10%)
3	XYP	A	472	3,2	9,9,10	0.65	0	10,12,14	0.95	0
3	XYP	A	473	3	10,10,10	0.53	0	14,14,14	0.59	0
2	AHR	B	949	3	9,9,10	0.74	0	9,12,14	1.56	1 (11%)
3	XYP	B	950	3	9,9,10	0.61	0	10,12,14	0.87	1 (10%)
3	XYP	B	951	3,2	9,9,10	0.62	0	10,12,14	0.99	1 (10%)
3	XYP	B	952	3	10,10,10	0.46	0	14,14,14	0.64	0
3	XYP	B	956	3	9,9,10	0.64	0	10,12,14	0.84	1 (10%)
3	XYP	B	957	3	10,10,10	0.56	0	14,14,14	0.60	0
3	XYP	B	961	-	10,10,10	0.56	0	14,14,14	0.61	0
3	XYP	B	970	3	9,9,10	0.63	0	10,12,14	0.85	1 (10%)
3	XYP	B	971	3	10,10,10	0.55	0	14,14,14	0.62	0

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	AHR	A	449	3	-	0/2/15/18	0/1/1/1
3	XYP	A	450	3	-	0/0/14/17	0/1/1/1
3	XYP	A	451	3,2	-	0/0/14/17	0/1/1/1
3	XYP	A	452	3	-	0/0/17/17	0/1/1/1
3	XYP	A	456	3	-	0/0/14/17	0/1/1/1
3	XYP	A	457	3	-	0/0/17/17	0/1/1/1
3	XYP	A	461	3	-	0/0/14/17	0/1/1/1
3	XYP	A	462	3	-	0/0/14/17	0/1/1/1
3	XYP	A	463	3	-	0/0/17/17	0/1/1/1
2	AHR	A	470	3	-	0/2/15/18	0/1/1/1
3	XYP	A	471	3	-	0/0/14/17	0/1/1/1
3	XYP	A	472	3,2	-	0/0/14/17	0/1/1/1
3	XYP	A	473	3	-	0/0/17/17	0/1/1/1
2	AHR	B	949	3	-	0/2/15/18	0/1/1/1
3	XYP	B	950	3	-	0/0/14/17	0/1/1/1
3	XYP	B	951	3,2	-	0/0/14/17	0/1/1/1
3	XYP	B	952	3	-	0/0/17/17	0/1/1/1
3	XYP	B	956	3	-	0/0/14/17	0/1/1/1
3	XYP	B	957	3	-	0/0/17/17	0/1/1/1
3	XYP	B	961	-	-	0/0/17/17	0/1/1/1
3	XYP	B	970	3	-	0/0/14/17	0/1/1/1
3	XYP	B	971	3	-	0/0/17/17	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	470	AHR	C1'-C2'-C3'	-4.13	95.32	101.67
2	A	449	AHR	C1'-O4'-C4'	-3.93	98.79	108.15
2	B	949	AHR	C1'-O4'-C4'	-3.86	98.94	108.15
3	B	951	XYP	C4B-C3B-C2B	-2.54	107.91	110.86
3	A	451	XYP	C4B-C3B-C2B	-2.51	107.94	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	452	XYP	3	0
3	A	456	XYP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	461	XYP	2	0
3	A	462	XYP	3	0
2	A	470	AHR	1	0
3	B	952	XYP	3	0
3	B	956	XYP	4	0
3	B	961	XYP	3	0
3	B	971	XYP	1	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.