

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID : 1BS9

Title : ACETYLXYLAN ESTERASE FROM P. PURPUROGENUM REFINED AT

1.10 ANGSTROMS

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Deposited on : 1998-09-01

Resolution : 1.10 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 $\frac{\text{https://www.wwpdb.org/validation/2017/XrayValidationReportHelp}}{\text{with specific help available everywhere you see the (i) symbol.}$

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

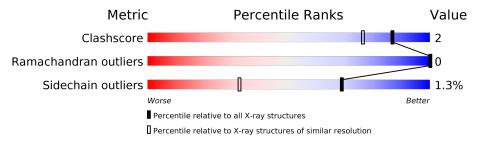
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.10 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)

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 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 <=5%

Note EDS was not executed.

Quality of chain					
5%					
•					



2 Entry composition (i)

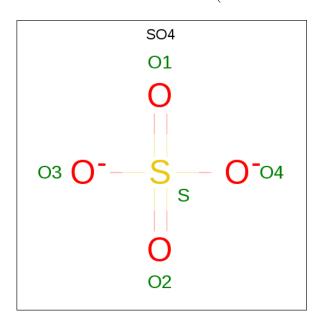
There are 3 unique types of molecules in this entry. The entry contains 1598 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL XYLAN ESTERASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	207	Total	С	N	О	S	0	4	0
1	A	207	1450	890	244	302	14	0	4	0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 5	O 4	S 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	143	Total O 143 143	0	0

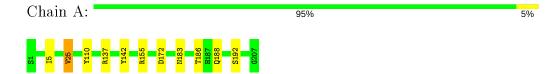


3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ACETYL XYLAN ESTERASE





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	$34.89 \text{\AA} 60.98 \text{Å} 72.42 \text{Å}$	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	99.00 - 1.10	Depositor	
% Data completeness	69.2 (99.00-1.10)	Depositor	
(in resolution range)	03.2 (33.00 1.10)		
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	SHELX	Depositor	
R, R_{free}	0.123 , 0.182	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1598	wwPDB-VP	
Average B, all atoms (Å ²)	14.0	wwPDB-VP	



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: SO4

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		
IVIOI	Mol Chain		# Z >5	RMSZ	# Z > 5	
1	A	0.68	0/1495	1.12	$6/2027 \ (0.3\%)$	

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	Α	25	VAL	CG1-CB-CG2	7.57	123.01	110.90
1	A	172	ASP	C-N-CA	6.25	137.32	121.70
1	A	142	TYR	CB-CG-CD2	5.72	124.43	121.00
1	A	110	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	A	172	ASP	O-C-N	-5.25	114.30	122.70
1	A	25	VAL	N-CA-CB	5.08	122.67	111.50

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	1450	0	1356	6	0
2	A	5	0	0	0	0
3	A	143	0	0	3	0
All	All	1598	0	1356	6	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 2.

All (6) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	Clash overlap (Å)
1:A:137:ARG:HD2	1:A:155:ARG:O	2.00	0.61
1:A:188:GLN:OE1	1:A:188:GLN:HA	2.06	0.55
1:A:5:ILE:HB	3:A:441:HOH:O	2.13	0.47
1:A:183:ASN:ND2	3:A:315:HOH:O	2.48	0.46
1:A:5:ILE:N	3:A:441:HOH:O	2.40	0.43
1:A:183:ASN:OD1	1:A:186:THR:N	2.49	0.40

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	209/207 (101%)	206 (99%)	3 (1%)	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 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.

\mathbf{N}	Iol	Chain	ain Analysed Rotameric Outliers		Percentiles	
	1	A	$154/150 \; (103\%)$	152 (99%)	2 (1%)	69 32



All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	192	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	116	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand 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	SO4	A	208	-	4,4,4	1.46	1 (25%)	6,6,6	2.18	2 (33%)

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
2	A	208	SO4	O1-S	2.35	1.58	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	A	208	SO4	O4-S-O3	3.22	122.81	109.06
2	A	208	SO4	O3-S-O1	-3.01	93.61	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

