



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:34 am BST

PDB ID : 3NUI
Title : Crystal structure of omega-transferase from Vibrio Fluvialis JS17
Authors : Park, H.H.; Jang, T.
Deposited on : 2010-07-07
Resolution : 2.00 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

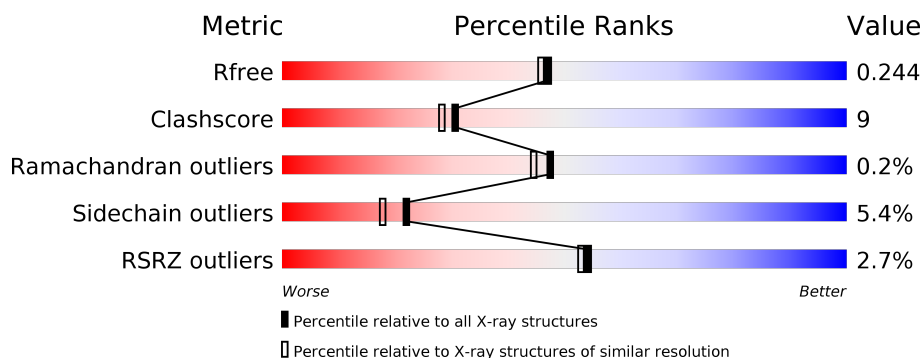
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	478	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	478	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7096 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 Pyruvate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3297	2111	559	608	19			
1	B	419	Total	C	N	O	S	0	0	0
			3256	2086	551	600	19			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP F2XBU9
A	-12	ALA	-	EXPRESSION TAG	UNP F2XBU9
A	-11	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-10	MET	-	EXPRESSION TAG	UNP F2XBU9
A	-9	THR	-	EXPRESSION TAG	UNP F2XBU9
A	-8	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-6	GLN	-	EXPRESSION TAG	UNP F2XBU9
A	-5	GLN	-	EXPRESSION TAG	UNP F2XBU9
A	-4	MET	-	EXPRESSION TAG	UNP F2XBU9
A	-3	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-2	ARG	-	EXPRESSION TAG	UNP F2XBU9
A	-1	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	0	SER	-	EXPRESSION TAG	UNP F2XBU9
A	454	ALA	-	EXPRESSION TAG	UNP F2XBU9
A	455	ALA	-	EXPRESSION TAG	UNP F2XBU9
A	456	ALA	-	EXPRESSION TAG	UNP F2XBU9
A	457	LEU	-	EXPRESSION TAG	UNP F2XBU9
A	458	GLU	-	EXPRESSION TAG	UNP F2XBU9
A	459	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	460	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	461	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	462	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	463	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	464	HIS	-	EXPRESSION TAG	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	EXPRESSION TAG	UNP F2XBU9
B	-12	ALA	-	EXPRESSION TAG	UNP F2XBU9
B	-11	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-10	MET	-	EXPRESSION TAG	UNP F2XBU9
B	-9	THR	-	EXPRESSION TAG	UNP F2XBU9
B	-8	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-6	GLN	-	EXPRESSION TAG	UNP F2XBU9
B	-5	GLN	-	EXPRESSION TAG	UNP F2XBU9
B	-4	MET	-	EXPRESSION TAG	UNP F2XBU9
B	-3	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-2	ARG	-	EXPRESSION TAG	UNP F2XBU9
B	-1	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	0	SER	-	EXPRESSION TAG	UNP F2XBU9
B	454	ALA	-	EXPRESSION TAG	UNP F2XBU9
B	455	ALA	-	EXPRESSION TAG	UNP F2XBU9
B	456	ALA	-	EXPRESSION TAG	UNP F2XBU9
B	457	LEU	-	EXPRESSION TAG	UNP F2XBU9
B	458	GLU	-	EXPRESSION TAG	UNP F2XBU9
B	459	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	460	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	461	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	462	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	463	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	464	HIS	-	EXPRESSION TAG	UNP F2XBU9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	282	Total O 282 282	0	0
2	B	261	Total O 261 261	0	0

- Molecule 1: Pyruvate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.08Å 95.03Å 123.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.00 48.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.33-2.00) 99.8 (48.33-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.191 , 0.242 0.194 , 0.244	Depositor DCC
R_{free} test set	3150 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7096	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.18	5/3380 (0.1%)	1.14	15/4583 (0.3%)
1	B	1.06	2/3337 (0.1%)	0.97	5/4522 (0.1%)
All	All	1.12	7/6717 (0.1%)	1.06	20/9105 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
All	All	1	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	CYS	CB-SG	-8.12	1.68	1.82
1	A	273	THR	CB-CG2	-5.92	1.32	1.52
1	B	431	GLU	CG-CD	5.71	1.60	1.51
1	A	207	GLU	CB-CG	5.58	1.62	1.52
1	A	101	VAL	CB-CG1	5.22	1.63	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ARG	NE-CZ-NH2	26.98	133.79	120.30
1	A	373	ARG	NE-CZ-NH1	-26.84	106.88	120.30
1	A	373	ARG	CD-NE-CZ	11.56	139.78	123.60
1	A	359	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	A	359	ARG	NE-CZ-NH2	9.16	124.88	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	273	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	284	SER	Peptide

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	3297	0	3241	49	0
1	B	3256	0	3200	72	1
2	A	282	0	0	11	1
2	B	261	0	0	14	0
All	All	7096	0	6441	119	1

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 119 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:258:VAL:HG13	1:B:284:SER:OG	1.28	1.31
1:A:267:ASN:HD22	1:A:273:THR:HG22	1.30	0.96
1:B:424:CYS:HB3	2:B:726:HOH:O	0.76	0.94
1:A:180:THR:HG23	1:A:204:GLU:OE2	1.71	0.91
1:B:127:MET:HE1	1:B:299:LEU:HD21	1.53	0.90

All (1) 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)
1:B:78:ARG:NH2	2:A:582:HOH:O[4_445]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	423/478 (88%)	405 (96%)	17 (4%)	1 (0%)	47	44
1	B	415/478 (87%)	399 (96%)	15 (4%)	1 (0%)	47	44
All	All	838/956 (88%)	804 (96%)	32 (4%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	B	231	VAL

5.3.2 Protein sidechains

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	344/386 (89%)	333 (97%)	11 (3%)	39	38
1	B	339/386 (88%)	313 (92%)	26 (8%)	13	8
All	All	683/772 (88%)	646 (95%)	37 (5%)	22	18

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	160	MET
1	B	247	ARG
1	B	415	ARG
1	B	163	LYS

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Mol	Chain	Res	Type
1	B	166	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	342	ASN
1	B	75	GLN
1	A	65	HIS
1	B	65	HIS

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](#)

There are no ligands in this entry.

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	425/478 (88%)	-0.32	8 (1%) 66 65	9, 16, 31, 49	0
1	B	419/478 (87%)	-0.06	15 (3%) 42 42	12, 21, 46, 76	0
All	All	844/956 (88%)	-0.19	23 (2%) 54 53	9, 19, 40, 76	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	TYR	6.7
1	B	160	MET	6.1
1	B	317	PHE	4.7
1	B	313	ALA	4.2
1	B	158	ALA	3.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.