



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 10:05 PM GMT

PDB ID : 2YFK
Title : Crystal structure of a putative transcarbamoylase from *Enterococcus faecalis*
Authors : Polo, L.M.; Fita, I.; Rubio, V.
Deposited on : 2011-04-06
Resolution : 2.55 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

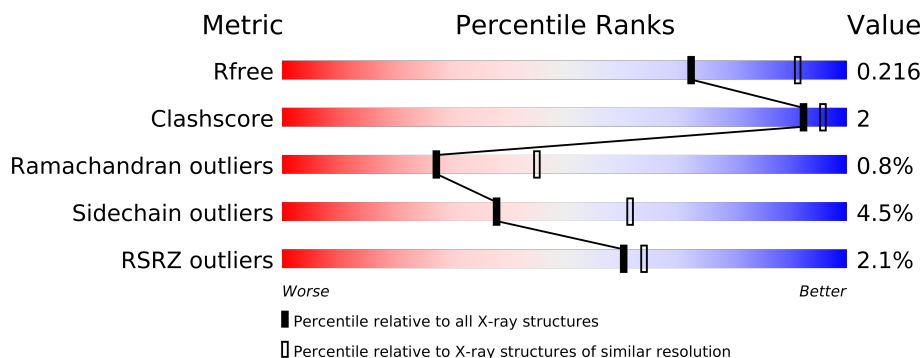
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.55 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	418	
1	B	418	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6056 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ASPARTATE/ORNITHINE CARBAMOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2994	1897	488	590	19			
1	B	386	Total	C	N	O	S	0	0	0
			2999	1901	488	591	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ASP	-	EXPRESSION TAG	UNP C7YCV8
A	399	PRO	-	EXPRESSION TAG	UNP C7YCV8
A	400	ASN	-	EXPRESSION TAG	UNP C7YCV8
A	401	SER	-	EXPRESSION TAG	UNP C7YCV8
A	402	SER	-	EXPRESSION TAG	UNP C7YCV8
A	403	SER	-	EXPRESSION TAG	UNP C7YCV8
A	404	VAL	-	EXPRESSION TAG	UNP C7YCV8
A	405	ASP	-	EXPRESSION TAG	UNP C7YCV8
A	406	LYS	-	EXPRESSION TAG	UNP C7YCV8
A	407	LEU	-	EXPRESSION TAG	UNP C7YCV8
A	408	ALA	-	EXPRESSION TAG	UNP C7YCV8
A	409	ALA	-	EXPRESSION TAG	UNP C7YCV8
A	410	ALA	-	EXPRESSION TAG	UNP C7YCV8
A	411	LEU	-	EXPRESSION TAG	UNP C7YCV8
A	412	GLU	-	EXPRESSION TAG	UNP C7YCV8
A	413	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	414	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	415	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	416	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	417	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	418	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	398	ASP	-	EXPRESSION TAG	UNP C7YCV8
B	399	PRO	-	EXPRESSION TAG	UNP C7YCV8
B	400	ASN	-	EXPRESSION TAG	UNP C7YCV8
B	401	SER	-	EXPRESSION TAG	UNP C7YCV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	402	SER	-	EXPRESSION TAG	UNP C7YCV8
B	403	SER	-	EXPRESSION TAG	UNP C7YCV8
B	404	VAL	-	EXPRESSION TAG	UNP C7YCV8
B	405	ASP	-	EXPRESSION TAG	UNP C7YCV8
B	406	LYS	-	EXPRESSION TAG	UNP C7YCV8
B	407	LEU	-	EXPRESSION TAG	UNP C7YCV8
B	408	ALA	-	EXPRESSION TAG	UNP C7YCV8
B	409	ALA	-	EXPRESSION TAG	UNP C7YCV8
B	410	ALA	-	EXPRESSION TAG	UNP C7YCV8
B	411	LEU	-	EXPRESSION TAG	UNP C7YCV8
B	412	GLU	-	EXPRESSION TAG	UNP C7YCV8
B	413	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	414	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	415	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	416	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	417	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	418	HIS	-	EXPRESSION TAG	UNP C7YCV8

- Molecule 2 is water.

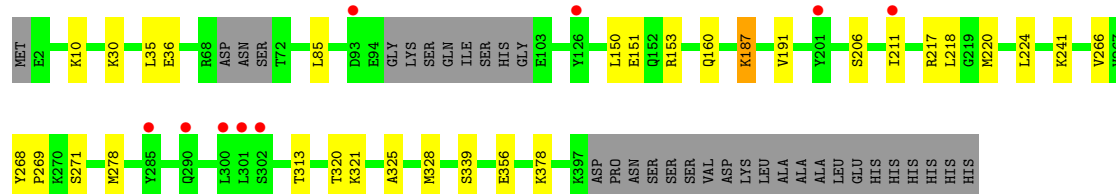
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	28	Total O 28 28	0	0
2	B	35	Total O 35 35	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

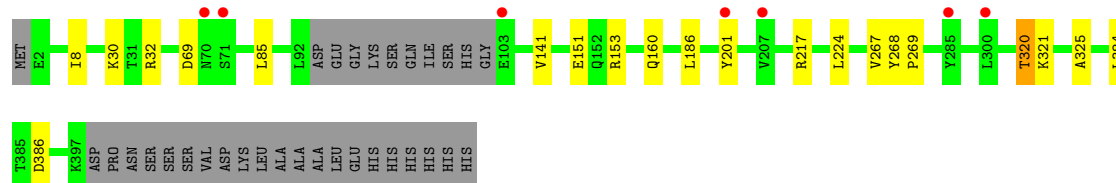
• Molecule 1: ASPARTATE/ORNITHINE CARBAMOYLTRANSFERASE

Chain A: 



• Molecule 1: ASPARTATE/ORNITHINE CARBAMOYLTRANSFERASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	117.37Å 117.37Å 120.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.55 29.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.55) 99.8 (29.52-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0112	Depositor
R, R_{free}	0.169 , 0.202 0.187 , 0.216	Depositor DCC
R_{free} test set	1541 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.2	EDS
Estimated twinning fraction	0.551 for H, K, L 0.449 for K, H, -L 0.115 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.551 for H, K, L 0.449 for K, H, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30624 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6056	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 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.38	1/3050 (0.0%)	0.49	0/4121
1	B	0.38	1/3057 (0.0%)	0.49	0/4136
All	All	0.38	2/6107 (0.0%)	0.49	0/8257

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	GLU	CD-OE2	6.80	1.33	1.25
1	A	151	GLU	CD-OE2	6.53	1.32	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2994	0	0	8	0
1	B	2999	0	0	3	0
2	A	28	0	0	2	0
2	B	35	0	0	0	0
All	All	6056	0	0	11	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 2.

All (11) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:320:THR:CG2	1:A:325:ALA:CB	2.61	0.78
1:A:356:GLU:OE1	2:A:2026:HOH:O	2.16	0.62
1:A:266:VAL:CG1	1:A:328:MET:CE	2.79	0.61
1:A:10:LYS:NZ	1:A:36:GLU:OE2	2.33	0.60
1:A:30:LYS:O	1:A:217:ARG:NH2	2.40	0.55
1:B:30:LYS:O	1:B:217:ARG:NH2	2.40	0.54
1:A:320:THR:CG2	1:A:321:LYS:N	2.70	0.53
1:A:191:VAL:CG2	1:A:220:MET:CE	2.86	0.52
1:B:320:THR:CG2	1:B:321:LYS:N	2.73	0.52
1:B:320:THR:CG2	1:B:325:ALA:CB	2.90	0.49
1:A:187:LYS:NZ	2:A:2017:HOH:O	2.53	0.41

There are no symmetry-related clashes.

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	379/418 (91%)	363 (96%)	14 (4%)	2 (0%)	38	60
1	B	382/418 (91%)	367 (96%)	11 (3%)	4 (1%)	22	37
All	All	761/836 (91%)	730 (96%)	25 (3%)	6 (1%)	27	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	B	160	GLN
1	A	269	PRO
1	B	201	TYR
1	B	69	ASP
1	B	269	PRO

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	314/358 (88%)	298 (95%)	16 (5%)	33	55
1	B	315/358 (88%)	303 (96%)	12 (4%)	44	70
All	All	629/716 (88%)	601 (96%)	28 (4%)	38	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	85	LEU
1	A	150	LEU
1	A	153	ARG
1	A	187	LYS
1	A	206	SER
1	A	211	ILE
1	A	218	LEU
1	A	224	LEU
1	A	241	LYS
1	A	268	TYR
1	A	271	SER
1	A	278	MET
1	A	313	THR
1	A	339	SER
1	A	378	LYS
1	B	8	ILE
1	B	32	ARG
1	B	85	LEU
1	B	141	VAL
1	B	153	ARG
1	B	186	LEU
1	B	224	LEU
1	B	267	VAL
1	B	268	TYR
1	B	320	THR
1	B	384	LEU
1	B	386	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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, 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	385/418 (92%)	0.05	9 (2%) 57 61	21, 34, 60, 72	0
1	B	386/418 (92%)	0.02	7 (1%) 65 69	19, 33, 54, 72	0
All	All	771/836 (92%)	0.03	16 (2%) 60 64	19, 33, 55, 72	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ASN	4.3
1	B	201	TYR	4.2
1	A	301	LEU	3.1
1	A	126	TYR	3.0
1	B	103	GLU	2.9
1	A	201	TYR	2.9
1	A	300	LEU	2.8
1	B	71	SER	2.7
1	B	285	TYR	2.6
1	A	285	TYR	2.5
1	A	93	ASP	2.5
1	A	211	ILE	2.3
1	A	302	SER	2.2
1	B	300	LEU	2.1
1	A	290	GLN	2.1
1	B	207	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.