



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 02:59 PM EDT

PDB ID : 3FKD
Title : The crystal structure of L-threonine-O-3-phosphate decarboxylase from *Porphyromonas gingivalis*
Authors : Zhang, Z.; Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

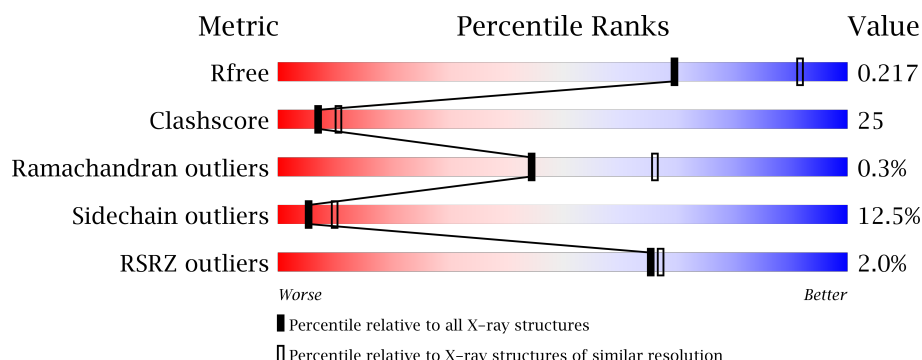
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	350	
1	B	350	
1	C	350	
1	D	350	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10610 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 L-threonine-O-3-phosphate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	Se	0	0	0
			2624	1677	454	481	5	7			
1	B	325	Total	C	N	O	S	Se	0	0	0
			2615	1672	453	478	5	7			
1	C	325	Total	C	N	O	S	Se	0	0	0
			2607	1666	451	478	5	7			
1	D	310	Total	C	N	O	S	Se	0	0	0
			2466	1571	432	452	5	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	GLU	-	expression tag	UNP Q7MXY2
A	344	GLY	-	expression tag	UNP Q7MXY2
A	345	HIS	-	expression tag	UNP Q7MXY2
A	346	HIS	-	expression tag	UNP Q7MXY2
A	347	HIS	-	expression tag	UNP Q7MXY2
A	348	HIS	-	expression tag	UNP Q7MXY2
A	349	HIS	-	expression tag	UNP Q7MXY2
A	350	HIS	-	expression tag	UNP Q7MXY2
B	343	GLU	-	expression tag	UNP Q7MXY2
B	344	GLY	-	expression tag	UNP Q7MXY2
B	345	HIS	-	expression tag	UNP Q7MXY2
B	346	HIS	-	expression tag	UNP Q7MXY2
B	347	HIS	-	expression tag	UNP Q7MXY2
B	348	HIS	-	expression tag	UNP Q7MXY2
B	349	HIS	-	expression tag	UNP Q7MXY2
B	350	HIS	-	expression tag	UNP Q7MXY2
C	343	GLU	-	expression tag	UNP Q7MXY2
C	344	GLY	-	expression tag	UNP Q7MXY2
C	345	HIS	-	expression tag	UNP Q7MXY2
C	346	HIS	-	expression tag	UNP Q7MXY2
C	347	HIS	-	expression tag	UNP Q7MXY2

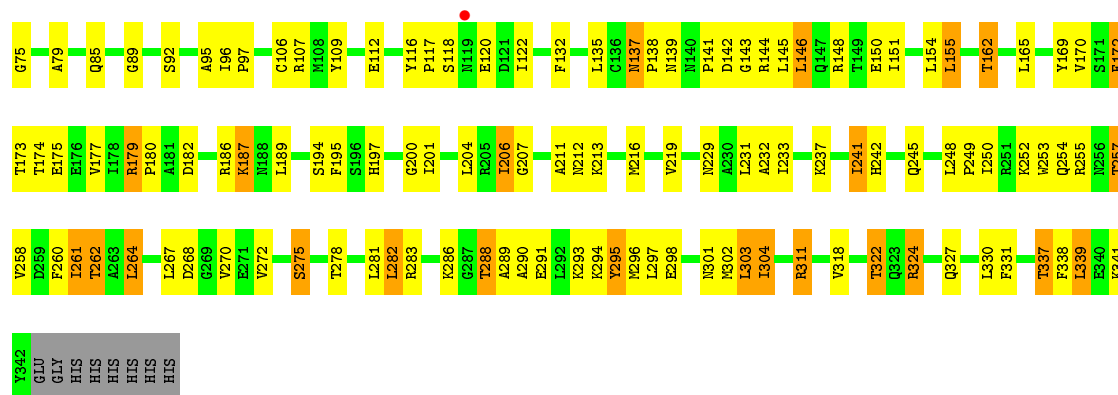
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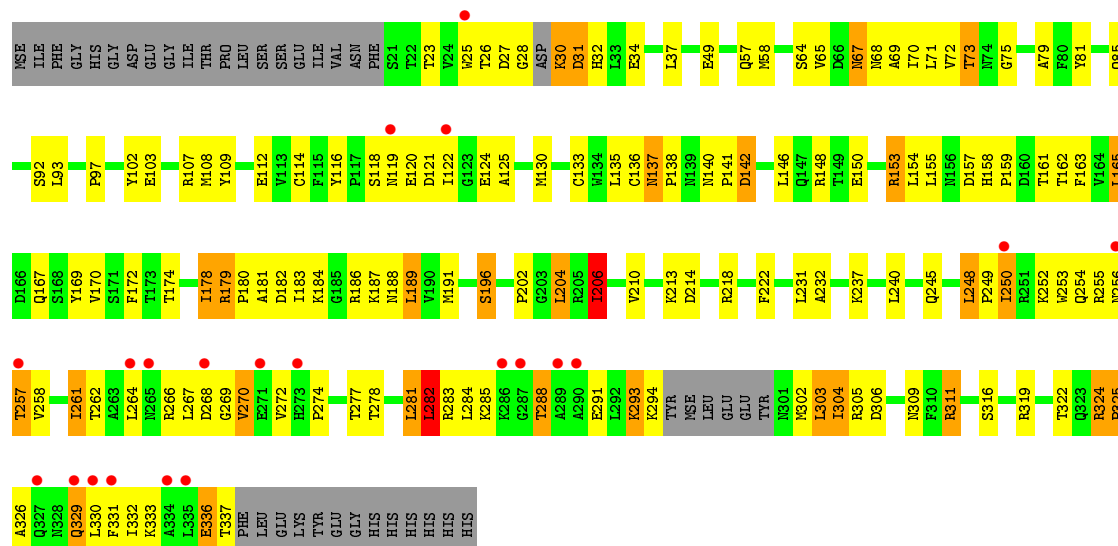
Chain	Residue	Modelled	Actual	Comment	Reference
C	348	HIS	-	expression tag	UNP Q7MXY2
C	349	HIS	-	expression tag	UNP Q7MXY2
C	350	HIS	-	expression tag	UNP Q7MXY2
D	343	GLU	-	expression tag	UNP Q7MXY2
D	344	GLY	-	expression tag	UNP Q7MXY2
D	345	HIS	-	expression tag	UNP Q7MXY2
D	346	HIS	-	expression tag	UNP Q7MXY2
D	347	HIS	-	expression tag	UNP Q7MXY2
D	348	HIS	-	expression tag	UNP Q7MXY2
D	349	HIS	-	expression tag	UNP Q7MXY2
D	350	HIS	-	expression tag	UNP Q7MXY2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0
2	B	75	Total O 75 75	0	0
2	C	96	Total O 96 96	0	0
2	D	63	Total O 63 63	0	0



• Molecule 1: L-threonine-O-3-phosphate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.44Å 101.51Å 93.71Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	46.86 – 2.50 93.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.86-2.50) 98.9 (93.71-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.224 , 0.275 0.188 , 0.217	Depositor DCC
R_{free} test set	2877 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.309 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10610	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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	0.66	0/2679	0.77	0/3624
1	B	0.67	0/2670	0.76	0/3612
1	C	0.67	1/2661 (0.0%)	0.78	2/3601 (0.1%)
1	D	0.65	0/2516	0.77	3/3405 (0.1%)
All	All	0.67	1/10526 (0.0%)	0.77	5/14242 (0.0%)

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	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	CYS	CB-SG	-5.07	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	LEU	CA-CB-CG	6.69	130.68	115.30
1	D	206	ILE	CB-CA-C	-5.87	99.86	111.60
1	C	282	LEU	CA-CB-CG	5.53	128.02	115.30
1	D	268	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	268	ASP	CB-CG-OD2	5.20	122.97	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	GLY	Peptide
1	B	89	GLY	Peptide
1	C	89	GLY	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	2624	0	2581	115	0
1	B	2615	0	2575	118	0
1	C	2607	0	2552	133	0
1	D	2466	0	2416	167	0
2	A	64	0	0	4	0
2	B	75	0	0	4	0
2	C	96	0	0	4	0
2	D	63	0	0	5	0
All	All	10610	0	10124	518	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 25.

The worst 5 of 518 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:218:ARG:HG2	1:B:218:ARG:HH11	0.99	1.16
1:C:288:THR:HG22	1:C:291:GLU:H	1.14	1.12
1:A:311:ARG:HH11	1:A:311:ARG:HG3	1.06	1.11
1:C:257:THR:HB	1:C:322:THR:HG21	1.28	1.08
1:A:54:THR:HG22	1:A:58:MSE:HE3	1.35	1.08

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	324/350 (93%)	307 (95%)	17 (5%)	0	100	100
1	B	323/350 (92%)	309 (96%)	12 (4%)	2 (1%)	28	48
1	C	321/350 (92%)	307 (96%)	14 (4%)	0	100	100
1	D	304/350 (87%)	282 (93%)	20 (7%)	2 (1%)	25	43
All	All	1272/1400 (91%)	1205 (95%)	63 (5%)	4 (0%)	44	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88	ARG
1	B	340	GLU
1	D	274	PRO
1	D	325	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	281/296 (95%)	263 (94%)	18 (6%)	20	38
1	B	280/296 (95%)	246 (88%)	34 (12%)	6	11
1	C	278/296 (94%)	237 (85%)	41 (15%)	3	6
1	D	262/296 (88%)	217 (83%)	45 (17%)	2	4
All	All	1101/1184 (93%)	963 (88%)	138 (12%)	5	10

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	162	THR
1	C	261	ILE
1	D	282	LEU
1	C	170	VAL
1	C	204	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	63	ASN
1	C	158	HIS
1	D	256	ASN
1	C	67	ASN
1	C	85	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](#)

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 ⓘ

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	319/350 (91%)	-0.18	0 100 100	16, 29, 45, 52	0
1	B	318/350 (90%)	-0.07	2 (0%) 89 89	17, 29, 47, 54	0
1	C	318/350 (90%)	-0.05	2 (0%) 89 89	18, 29, 50, 58	0
1	D	304/350 (86%)	0.34	21 (6%) 18 18	18, 34, 54, 71	0
All	All	1259/1400 (89%)	0.01	25 (1%) 65 67	16, 30, 50, 71	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	ILE	4.9
1	D	329	GLN	4.5
1	D	264	LEU	4.4
1	D	256	ASN	4.2
1	D	290	ALA	4.1

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.