



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:07 PM BST

PDB ID : 5UYY
Title : Crystal structure of prephenate dehydrogenase tyrA from Bacillus anthracis in complex with L-tyrosine
Authors : Shabalin, I.G.; Hou, J.; Cymborowski, M.T.; Kwon, K.; Christendat, D.; Gritsunov, A.O.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-02-24
Resolution : 2.60 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

<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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.14.4.dev1

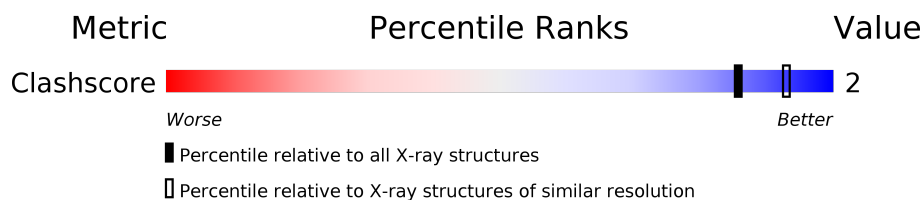
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

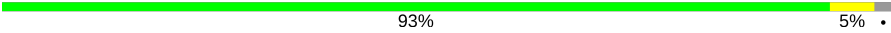



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	381	 93% 5% .
1	B	381	 90% 6% .
1	C	381	 90% 8% .
1	D	381	 92% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11890 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.

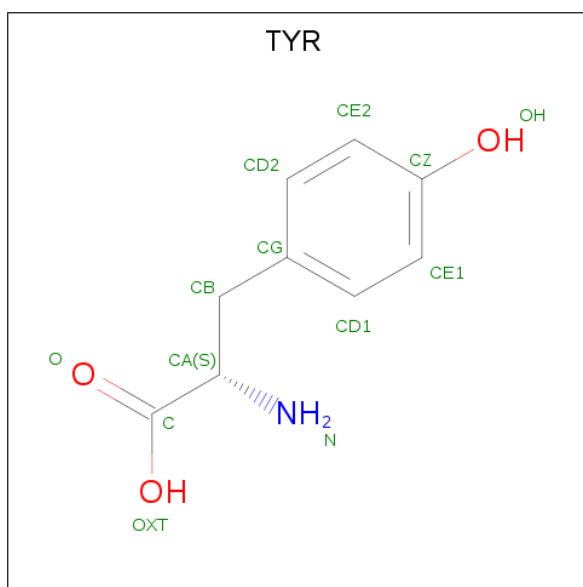
- Molecule 1 is a protein called Prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2881	1831	490	550	10			
1	B	365	Total	C	N	O	S	0	0	0
			2792	1777	484	523	8			
1	C	373	Total	C	N	O	S	0	0	0
			2876	1829	493	544	10			
1	D	365	Total	C	N	O	S	0	0	0
			2783	1773	478	524	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81P63
A	-1	ASN	-	expression tag	UNP Q81P63
A	0	ALA	-	expression tag	UNP Q81P63
B	-2	SER	-	expression tag	UNP Q81P63
B	-1	ASN	-	expression tag	UNP Q81P63
B	0	ALA	-	expression tag	UNP Q81P63
C	-2	SER	-	expression tag	UNP Q81P63
C	-1	ASN	-	expression tag	UNP Q81P63
C	0	ALA	-	expression tag	UNP Q81P63
D	-2	SER	-	expression tag	UNP Q81P63
D	-1	ASN	-	expression tag	UNP Q81P63
D	0	ALA	-	expression tag	UNP Q81P63

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: C₉H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		
2	C	1	Total	C	N	O	0	0
			13	9	1	3		
2	D	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	113	Total	O	0	0
			113	113		
3	C	178	Total	O	0	0
			178	178		
3	D	98	Total	O	0	0
			98	98		

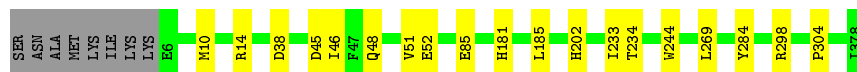
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 failed to run properly.

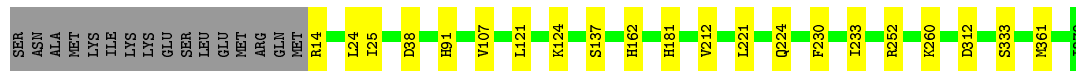
- Molecule 1: Prephenate dehydrogenase

Chain A: 




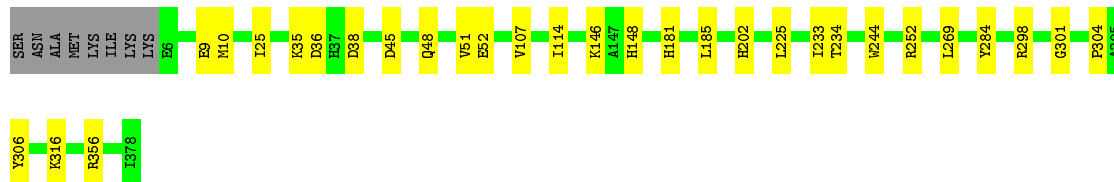
- Molecule 1: Prephenate dehydrogenase

Chain B: 



- Molecule 1: Prephenate dehydrogenase

Chain C: 



- Molecule 1: Prephenate dehydrogenase

Chain D: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.68Å 105.59Å 179.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.9 (50.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.189 , 0.246	Depositor
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.368	Xtriage
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
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5304e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.77	0/2937	0.89	1/3976 (0.0%)
1	B	0.79	0/2848	0.85	3/3860 (0.1%)
1	C	0.85	1/2933 (0.0%)	0.90	4/3970 (0.1%)
1	D	0.80	0/2839	0.88	1/3848 (0.0%)
All	All	0.80	1/11557 (0.0%)	0.88	9/15654 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	GLU	CD-OE2	6.76	1.33	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	C	252	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	312	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	252	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	181	HIS	N-CA-CB	5.42	120.36	110.60
1	C	10	MET	CB-CG-SD	-5.35	96.35	112.40
1	A	10	MET	CB-CG-SD	-5.17	96.90	112.40
1	D	181	HIS	N-CA-CB	5.12	119.82	110.60
1	C	356	ARG	NE-CZ-NH2	5.01	122.80	120.30

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	2881	0	2808	14	0
1	B	2792	0	2726	14	0
1	C	2876	0	2808	19	0
1	D	2783	0	2692	13	0
2	A	13	0	8	1	0
2	B	13	0	8	0	0
2	C	13	0	8	1	0
2	D	13	0	8	0	0
3	A	117	0	0	0	0
3	B	113	0	0	0	0
3	C	178	0	0	3	0
3	D	98	0	0	2	0
All	All	11890	0	11066	50	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 (50) 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:C:185:LEU:HD21	1:D:221:LEU:HD11	1.66	0.77
1:A:185:LEU:HD21	1:B:221:LEU:HD11	1.70	0.73
1:D:24:LEU:HD21	1:D:137:SER:HB3	1.81	0.61
1:B:25:ILE:HG21	1:B:107:VAL:HG11	1.83	0.60
1:B:24:LEU:HD21	1:B:137:SER:HB3	1.83	0.60
1:C:38:ASP:OD2	3:C:501:HOH:O	2.17	0.59
1:A:45:ASP:HB2	1:A:51:VAL:HG13	1.84	0.59
3:C:602:HOH:O	1:D:260:LYS:HE2	2.02	0.58
1:C:45:ASP:HB2	1:C:51:VAL:HG13	1.87	0.56
1:A:185:LEU:CD2	1:B:221:LEU:HD11	2.40	0.52
1:A:298:ARG:HH12	1:B:224:GLN:HA	1.75	0.52
2:A:401:TYR:N	1:B:333:SER:HG	2.10	0.50
1:C:185:LEU:HD21	1:D:221:LEU:CD1	2.39	0.50
1:A:202:HIS:CE1	1:A:244:TRP:CE2	3.01	0.48
1:C:202:HIS:CE1	1:C:244:TRP:CE2	3.03	0.47
1:C:316:LYS:HE3	3:C:659:HOH:O	2.14	0.46
1:C:35:LYS:HG2	1:C:36:ASP:OD1	2.16	0.46
1:C:225:LEU:HD12	1:D:193:VAL:HG11	1.98	0.45
1:D:260:LYS:HD2	1:D:260:LYS:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:GLN:O	1:C:52:GLU:HG3	2.17	0.45
1:C:225:LEU:HD12	1:D:193:VAL:CG1	2.47	0.45
1:B:260:LYS:HD2	1:B:260:LYS:HA	1.82	0.44
1:C:25:ILE:HG21	1:C:107:VAL:HG11	1.98	0.44
1:B:212:VAL:HG21	1:B:230:PHE:CE1	2.53	0.44
2:C:401:TYR:N	1:D:333:SER:HG	2.16	0.44
1:A:48:GLN:O	1:A:52:GLU:HG3	2.18	0.43
1:C:233:ILE:HG22	1:C:234:THR:HG23	2.00	0.43
1:B:124:LYS:HA	1:B:162:HIS:CD2	2.54	0.43
1:D:187:THR:HG22	3:D:589:HOH:O	2.17	0.43
1:C:298:ARG:HG3	1:C:306:TYR:CE2	2.54	0.43
1:D:235:ARG:HG2	1:D:306:TYR:CZ	2.53	0.43
1:D:212:VAL:HG21	1:D:230:PHE:CE1	2.54	0.43
1:A:181:HIS:ND1	1:A:304:PRO:HG3	2.34	0.43
1:A:14:ARG:NH1	1:A:38:ASP:OD1	2.48	0.42
1:A:298:ARG:NH1	1:B:224:GLN:HA	2.34	0.42
1:A:46:ILE:HG23	1:A:85:GLU:OE2	2.20	0.42
1:A:233:ILE:HG23	1:B:233:ILE:HG13	2.01	0.42
1:B:91:HIS:CE1	1:B:121:LEU:HD21	2.55	0.42
1:A:181:HIS:CG	1:A:304:PRO:HG3	2.55	0.41
1:C:114:ILE:HA	1:C:114:ILE:HD12	1.89	0.41
1:B:361:MET:CE	1:C:301:GLY:HA3	2.50	0.41
1:A:269:LEU:HD13	1:A:284:TYR:CZ	2.56	0.41
1:C:181:HIS:ND1	1:C:304:PRO:HG3	2.35	0.41
1:D:338:GLN:HG2	3:D:534:HOH:O	2.21	0.41
1:C:181:HIS:CG	1:C:304:PRO:HG3	2.56	0.41
1:B:14:ARG:HD3	1:B:38:ASP:OD1	2.21	0.40
1:A:233:ILE:HG22	1:A:234:THR:HG23	2.03	0.40
1:C:269:LEU:HD13	1:C:284:TYR:CZ	2.57	0.40
1:C:146:LYS:HD2	1:C:148:HIS:CE1	2.56	0.40
1:D:111:LYS:HA	1:D:111:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	TYR	B	401	-	10,13,13	0.80	0	12,17,17	0.67	0
2	TYR	D	401	-	10,13,13	0.75	0	12,17,17	0.62	0
2	TYR	A	401	-	10,13,13	0.57	0	12,17,17	0.32	0
2	TYR	C	401	-	10,13,13	0.58	0	12,17,17	0.29	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	TYR	B	401	-	-	0/4/8/8	0/1/1/1
2	TYR	D	401	-	-	0/4/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYR	A	401	-	-	0/4/8/8	0/1/1/1
2	TYR	C	401	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TYR	1	0
2	C	401	TYR	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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.