

Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 - 12:41 am BST

PDB ID	:	1E47
Title	:	L-Fuculose 1-Phosphate Aldolase from Escherichia coli Mutant $E73Q$
Authors	:	Joerger, A.C.; Schulz, G.E.
Deposited on		
Resolution	:	2.15 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 (i) symbol.

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

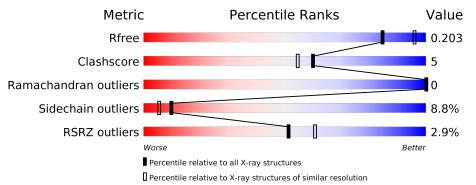
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585(2.16-2.16)
Ramachandran outliers	138981	$1560 \ (2.16-2.16)$
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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% 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	Р	215	3% 80%	14%	•••



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1750 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.

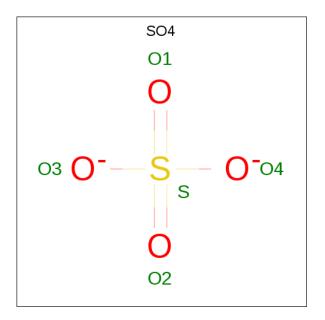
• Molecule 1 is a protein called L-FUCULOSE 1-PHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Р	206	Total 1608	C 1020	N 282	O 295	S 11	0	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Р	73	GLN	GLU	engineered mutation	UNP P11550

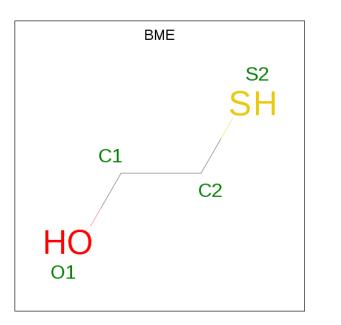
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Р	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	1
2	Р	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

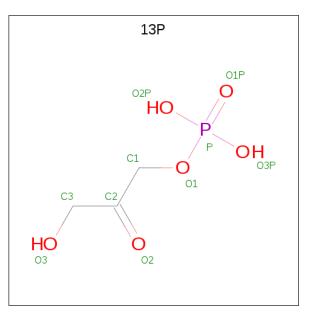
• Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Р	1	Total 4	$\begin{array}{c} \mathrm{C} \\ 2 \end{array}$	0 1	${ m S}$ 1	0	0

• Molecule 4 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).



[Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
	4	Р	1	Total 10	С 3	O 6	Р 1	0	1

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Р	1	Total 1	Zn 1	0	0

• Molecule 6 is water.

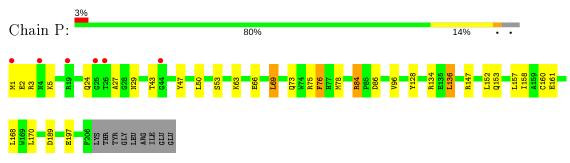
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Р	117	Total O 117 117	0	0



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 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: L-FUCULOSE 1-PHOSPHATE ALDOLASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants	93.90Å 93.90Å 43.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 2.15	Depositor
Resolution (A)	9.95 - 2.15	EDS
% Data completeness	95.0 (10.00-2.15)	Depositor
(in resolution range)	$95.6 \ (9.95 - 2.15)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	5.49 (at 2.15\AA)	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.150 , 0.205	Depositor
R, R_{free}	0.151 , 0.203	DCC
R_{free} test set	602 reflections $(5.83%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 65.4	EDS
L-test for twinning ²	$ \langle L \rangle = 0.47, \langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1750	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: ZN, 13P, SO4, BME

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	Bo	nd angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Р	0.48	0/1661	1.23	9/2259~(0.4%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Р	84	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	Р	147	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	Р	147	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	Р	75	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	Р	84	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	Р	157	LEU	CA-CB-CG	6.01	129.13	115.30
1	Р	189	ASP	CB-CG-OD1	5.99	123.69	118.30
1	Р	66	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	Р	86	ASP	CB-CG-OD1	5.47	123.22	118.30

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	Р	1608	0	1620	15	0
2	Р	10	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Р	4	0	5	0	0
4	Р	10	0	4	2	0
5	Р	1	0	0	0	0
6	Р	117	0	0	1	0
All	All	1750	0	1629	15	0

Continued from previous page...

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 5.

All (15) 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:P:76:PHE:CD1	1:P:158[B]:ILE:HD11	2.28	0.69
1:P:128:TYR:H	1:P:153:GLN:HE21	1.41	0.68
1:P:152:LEU:HD11	1:P:158[A]:ILE:HG13	1.83	0.60
1:P:76:PHE:CE1	1:P:158[B]:ILE:HD11	2.37	0.59
1:P:76:PHE:HD2	1:P:136:LEU:HD13	1.67	0.59
1:P:128:TYR:H	1:P:153:GLN:NE2	2.02	0.57
1:P:43:THR:HG22	1:P:69:LEU:HB3	1.87	0.55
1:P:84:ARG:HD3	1:P:160[B]:CYS:SG	2.47	0.55
1:P:47:TYR:O	1:P:50:LEU:HB2	2.10	0.52
1:P:76:PHE:CD2	1:P:136:LEU:HD13	2.47	0.49
1:P:73:GLN:HG2	4:P:304[B]:13P:H32	2.02	0.42
1:P:2:GLU:HG2	1:P:3:ARG:N	2.35	0.42
1:P:27:ALA:O	4:P:304[B]:13P:O2	2.38	0.41
1:P:197:GLU:HG3	6:P:419:HOH:O	2.19	0.41
1:P:152:LEU:HD11	1:P:158[A]:ILE:CG1	2.48	0.41

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	Percentil	es
1	Р	209/215~(97%)	203~(97%)	6 (3%)	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.

Mol	Chain	Analysed	Rotameric	Outliers			
1	Р	176/179~(98%)	159~(90%)	17 (10%)	8 4		

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Р	1	MET
1	Р	5	LYS
1	Р	24	GLN
1	Р	29	ASN
1	Р	53	SER
1	Р	63	LYS
1	Р	69	LEU
1	Р	76	PHE
1	Р	78[A]	MET
1	Р	78[B]	MET
1	Р	96[A]	VAL
1	Р	96[B]	VAL
1	Р	134	ARG
1	Р	136	LEU
1	Р	161	GLU
1	Р	168	LEU
1	Р	170	LEU

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

Mol	Chain	\mathbf{Res}	\mathbf{Type}
1	Р	35	GLN



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
1	Р	153	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)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	Tune	Chain	Res	Link	B	ond leng	gths	В	ond ang	jles
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	Р	302	-	$4,\!4,\!4$	0.61	0	$6,\!6,\!6$	0.14	0
2	SO4	Р	301[A]	-	$4,\!4,\!4$	0.68	0	$6,\!6,\!6$	0.07	0
4	13P	Р	304[B]	5	$9,\!9,\!9$	3.40	4 (44%)	$10,\!12,\!12$	1.57	2 (20%)
3	BME	Р	303	1	3,3,3	0.31	0	1,2,2	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	\mathbf{Link}	Chirals	Torsions	Rings
4	13P	Р	304[B]	5	-	2/7/8/8	-



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	Р	303	1	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	Р	304[B]	13P	O2-C2	6.68	1.33	1.21
4	Р	304[B]	13P	C3-C2	-6.23	1.34	1.50
4	Р	304[B]	13P	P-O1P	3.25	1.61	1.50
4	Р	304[B]	13P	O3-C3	-2.31	1.33	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Р	304[B]	13P	C3-C2-C1	3.23	124.67	117.25
4	Р	304[B]	13P	O2-C2-C3	-2.14	117.51	120.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Р	304[B]	13P	C1-O1-P-O2P
4	Р	304[B]	13P	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Р	304[B]	13P	2	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 (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, 95^{th} 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	Р	206/215~(95%)	-0.35	6 (2%) 51 61	10, 20, 56, 76	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Р	25	GLY	5.2
1	Р	44	GLY	3.4
1	Р	26	THR	3.3
1	Р	1	MET	3.0
1	Р	4	ASN	2.4
1	Р	19	ARG	2.3

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	Р	302	5/5	0.95	0.16	44,45,45,46	5



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	$Q{<}0.9$
4	13P	Р	304[B]	10/10	0.95	0.16	$34,\!35,\!36,\!36$	10
2	SO4	Р	301[A]	5/5	0.96	0.12	$59,\!60,\!60,\!60$	5
3	BME	Р	303	4/4	0.97	0.09	$23,\!28,\!30,\!33$	0
5	ZN	Р	305	1/1	1.00	0.01	14,14,14,14	0

Continued from previous page...

6.5 Other polymers (i)

There are no such residues in this entry.

