

Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 11:18 pm BST

PDB ID : 1E46

> Title : L-Fuculose 1-Phosphate Aldolase from Escherichia coli Mutant E73S

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2000-06-30 Deposited on

2.55 Å(reported) Resolution

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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

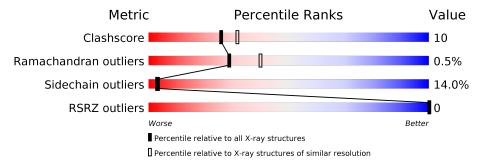
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries}, ext{resolution range}(ext{Å})) \end{aligned}$
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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.

Mo	l Chain	Length	Quality of chain		
1	Р	215	63%	26%	6% • •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1715 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.

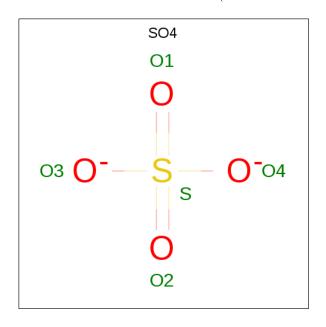
• Molecule 1 is a protein called L-FUCULOSE 1-PHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	D	206	Total	С	N	О	S	0		0
1	Γ	_ ∠00	1605	1018	281	295	11	0)	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
Р	73	SER	GLU	engineered mutation	UNP P11550

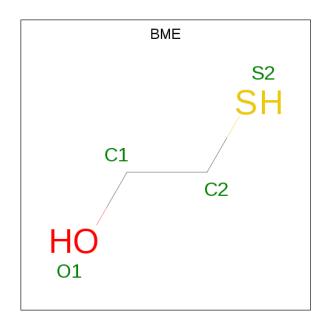
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Р	1	Total O 5 4	S 1	0	0

• Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Р	1	Total 4	C 2	O 1	S 1	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

\mathbf{N}	Iol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
	4	Р	1	Total Zn 1 1	0	0

• Molecule 5 is water.

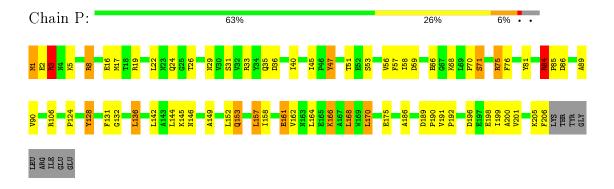
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	Р	100	Total O 100 100	0	0



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	94.10Å 94.10Å 43.50Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 2.55	Depositor
Resolution (A)	9.97 - 2.55	EDS
% Data completeness	$95.0 \ (10.00 - 2.55)$	Depositor
(in resolution range)	95.8 (9.97-2.55)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$4.39 \; ({\rm at} \; 2.56 {\rm \AA})$	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.229	Depositor
10, 10 free	0.143 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 91.5	EDS
L-test for twinning ²	$ < L > = 0.45, < L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1715	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ 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, 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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Р	0.71	0/1658	1.97	37/2255~(1.6%)	

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	106	ARG	NE-CZ-NH2	-18.87	110.86	120.30
1	Р	86	ASP	CB-CG-OD1	13.92	130.83	118.30
1	Р	84	ARG	NE-CZ-NH1	13.87	127.23	120.30
1	Р	84	ARG	CD-NE-CZ	12.28	140.79	123.60
1	Р	8	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	Р	128	TYR	CB-CG-CD1	-11.88	113.87	121.00
1	Р	75	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	Р	106	ARG	NE-CZ-NH1	11.45	126.03	120.30
1	Р	36	ASP	CB-CG-OD1	9.37	126.73	118.30
1	Р	128	TYR	CB-CG-CD2	9.19	126.51	121.00
1	Р	84	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	Р	149	ALA	N-CA-CB	7.72	120.91	110.10
1	Р	75	ARG	NH1-CZ-NH2	7.46	127.60	119.40
1	Р	33	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	Р	136	LEU	CB-CA-C	6.80	123.11	110.20
1	Р	86	ASP	OD1-CG-OD2	-6.40	111.14	123.30
1	Р	157	LEU	CB-CG-CD2	6.38	121.84	111.00
1	Р	124	PRO	O-C-N	-6.34	112.56	122.70
1	Р	56	VAL	CA-C-N	6.12	130.66	117.20
1	Р	47	TYR	CB-CG-CD2	6.08	124.65	121.00
1	Р	170	LEU	CB-CG-CD2	6.07	121.31	111.00
1	Р	8	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	Р	196	ASP	CB-CG-OD1	5.93	123.64	118.30
1	Р	175	GLU	OE1-CD-OE2	-5.86	116.26	123.30

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Mol	Chain	Res	Type	Atoms	${f Z}$	$Observed(^o)$	$Ideal(^{o})$
1	Р	200	ALA	N-CA-CB	5.72	118.11	110.10
1	Р	106	ARG	CD-NE-CZ	5.68	131.55	123.60
1	Р	36	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	Р	33	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	Р	196	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	Р	33	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	Р	75	ARG	CG-CD-NE	-5.41	100.44	111.80
1	Р	136	LEU	CA-CB-CG	5.38	127.67	115.30
1	Р	75	ARG	CD-NE-CZ	5.35	131.09	123.60
1	Р	3	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	Р	136	LEU	CB-CG-CD2	5.31	120.02	111.00
1	Р	186	ALA	N-CA-CB	5.19	117.37	110.10
1	Р	1	MET	CA-CB-CG	5.08	121.94	113.30

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	Р	1605	0	1617	34	0
2	Р	5	0	0	1	0
3	Р	4	0	5	0	0
4	Р	1	0	0	0	0
5	Р	100	0	0	11	0
All	All	1715	0	1622	34	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 10.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:P:2:GLU:HG3	5:P:496:HOH:O	1.90	0.71
1:P:31:SER:HB3	1:P:40:ILE:HG13	1.71	0.71

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Continued from pred		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:P:128:TYR:HB2	1:P:153:GLN:HG2	1.80	0.64
1:P:71:SER:HB2	2:P:301:SO4:O2	1.98	0.64
1:P:205:LYS:HB3	5:P:439:HOH:O	2.00	0.62
1:P:152:LEU:HD11	1:P:158[A]:ILE:HD12	1.80	0.60
1:P:89:ALA:HB1	1:P:164:LEU:HD23	1.83	0.60
1:P:131:PHE:HB2	5:P:405:HOH:O	2.03	0.59
1:P:85:PRO:HG2	5:P:497:HOH:O	2.03	0.59
1:P:75:ARG:HB2	5:P:434:HOH:O	2.04	0.58
1:P:84:ARG:HD2	1:P:144:LEU:O	2.03	0.57
1:P:2:GLU:OE1	1:P:5:LYS:NZ	2.33	0.55
1:P:166:LYS:HZ2	1:P:166:LYS:HB3	1.70	0.55
1:P:189:ASP:OD1	1:P:190:PRO:HA	2.07	0.55
1:P:24:GLN:HB2	5:P:410:HOH:O	2.09	0.52
1:P:131:PHE:HD2	5:P:476:HOH:O	1.93	0.51
1:P:17:MET:HG3	1:P:22:LEU:HB2	1.93	0.50
1:P:132:GLY:N	5:P:405:HOH:O	2.45	0.48
1:P:201:VAL:O	1:P:205:LYS:HB2	2.13	0.48
1:P:166:LYS:NZ	1:P:166:LYS:HB3	2.29	0.47
1:P:146:ASN:N	1:P:146:ASN:OD1	2.48	0.47
1:P:2:GLU:HG2	1:P:3:ARG:H	1.79	0.46
1:P:75:ARG:NH1	5:P:407:HOH:O	2.47	0.46
1:P:16:GLU:OE1	1:P:16:GLU:HA	2.15	0.46
1:P:198:GLU:HB2	5:P:483:HOH:O	2.16	0.46
1:P:191:VAL:HG12	1:P:192:PRO:HD2	1.98	0.45
1:P:161:GLU:OE1	1:P:162:VAL:HG13	2.18	0.44
1:P:81:TYR:CZ	1:P:90:VAL:HG23	2.53	0.43
1:P:1:MET:SD	1:P:1:MET:O	2.77	0.43
1:P:16:GLU:HG3	1:P:168:LEU:HD11	2.02	0.42
1:P:58:ILE:HD11	1:P:70:PRO:CB	2.50	0.42
1:P:161:GLU:HA	5:P:467:HOH:O	2.20	0.42
1:P:57:PHE:CZ	1:P:59:ASP:HA	2.56	0.41
1:P:199:ILE:HD13	1:P:199:ILE:HA	1.83	0.40

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	Percentiles
1	Р	209/215 (97%)	195 (93%)	13 (6%)	1 (0%)	29 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Р	26	THR

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	Percentiles		
1	Р	176/179 (98%)	152 (86%)	24 (14%)	3 3		

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Р	3	ARG
1	Р	8	ARG
1	Р	19	ARG
1	Р	29	ASN
1	Р	35	GLN
1	Р	45	ILE
1	Р	47	TYR
1	Р	51	THR
1	Р	53	SER
1	Р	66	GLU
1	Р	68	LYS
1	Р	71	SER
1	Р	76	PHE
1	Р	84	ARG
1	Р	136	LEU
1	Р	142	LEU

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Mol	Chain	Res	Type
1	Р	145	LYS
1	Р	153	GLN
1	Р	157	LEU
1	Р	161	GLU
1	Р	166	LYS
1	Р	168	LEU
1	Р	170	LEU
1	Р	206	PHE

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

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	T	Chain	Dog	T in le	B	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	BME	Р	302	1	3,3,3	0.51	0	1,2,2	1.03	0
2	SO4	Р	301	-	4,4,4	0.71	0	6,6,6	0.42	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
3	BME	Р	302	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	302	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Р	301	SO4	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 (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	$\langle { m RSRZ} \rangle$	# RSRZ > 2		$OWAB(\AA^2)$	Q < 0.9
1	Р	$206/215 \; (95\%)$	-0.90	0 100	100	10, 26, 52, 72	0

There are no RSRZ outliers to report.

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\text{-}factors}(\mathbf{A}^2) $	Q<0.9
2	SO4	Р	301	5/5	0.95	0.17	77,77,78,78	0
3	BME	Р	302	4/4	0.99	0.04	25,27,29,33	0
4	ZN	Р	303	1/1	1.00	0.04	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.

