

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 11:17 PM EDT

:	3CQK
:	Crystal Structure of L-xylulose-5-phosphate 3-epimerase UlaE (form B)
	complex with $Zn2+$ and sulfate
:	Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Ge-
	nomics Initiative (BSGI)
:	2008-04-03
:	2.33 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

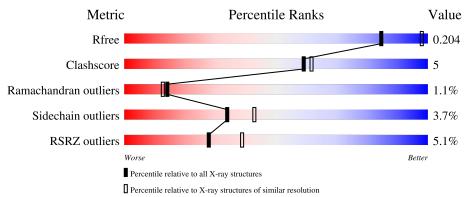
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.33 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$2096 \ (2.36-2.32)$
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 of 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	А	295	86%	6% • 6%
1	В	295	9%	13% •• 6%



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4480 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	276	Total	С	Ν	0	\mathbf{S}	0	0	0
		270	2192	1387	381	409	15	0		
1	В	276	Total	С	Ν	0	S	0	0	0
	ГБ	270	2192	1387	381	409	15	0	0	0

• Molecule 1 is a protein called L-ribulose-5-phosphate 3-epimerase ulaE.

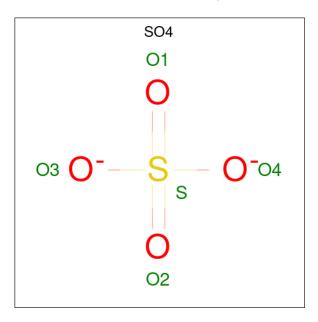
Chain	Residue	Modelled	Actual	Comment	Reference
А	-10	MET	-	expression tag	UNP Q8XDI5
А	-9	GLY	-	expression tag	UNP Q8XDI5
А	-8	SER	-	expression tag	UNP Q8XDI5
А	-7	SER	-	expression tag	UNP Q8XDI5
А	-6	HIS	-	expression tag	UNP Q8XDI5
А	-5	HIS	-	expression tag	UNP Q8XDI5
А	-4	HIS	-	expression tag	UNP Q8XDI5
А	-3	HIS	-	expression tag	UNP Q8XDI5
А	-2	HIS	-	expression tag	UNP Q8XDI5
А	-1	HIS	-	expression tag	UNP Q8XDI5
A	0	GLY	-	expression tag	UNP Q8XDI5
А	1	SER	-	expression tag	UNP Q8XDI5
В	-10	MET	-	expression tag	UNP Q8XDI5
В	-9	GLY	-	expression tag	UNP Q8XDI5
В	-8	SER	-	expression tag	UNP Q8XDI5
В	-7	SER	-	expression tag	UNP Q8XDI5
В	-6	HIS	-	expression tag	UNP Q8XDI5
В	-5	HIS	-	expression tag	UNP Q8XDI5
В	-4	HIS	-	expression tag	UNP Q8XDI5
В	-3	HIS	-	expression tag	UNP Q8XDI5
В	-2	HIS	-	expression tag	UNP Q8XDI5
В	-1	HIS	-	expression tag	UNP Q8XDI5
В	0	GLY	-	expression tag	UNP Q8XDI5
В	1	SER	_	expression tag	UNP Q8XDI5

There are 24 discrepancies between the modelled and reference sequences:



• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0
2	В	2	Total Zn 2 2	0	0



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

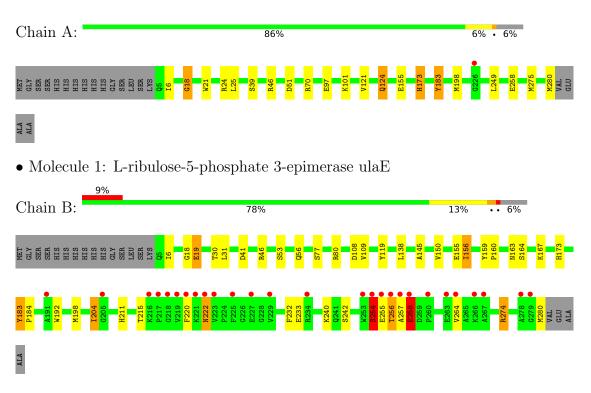
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	43	Total O 43 43	0	0
4	В	39	Total O 39 39	0	0



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 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-ribulose-5-phosphate 3-epimerase ulaE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	105.03Å 132.55Å 82.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.24 – 2.33	Depositor
Resolution (A)	44.24 - 2.33	EDS
% Data completeness	93.7 (44.24-2.33)	Depositor
(in resolution range)	93.6(44.24-2.33)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.24 (at 2.32 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.187 , 0.211	Depositor
R, R_{free}	0.181 , 0.204	DCC
R_{free} test set	1151 reflections (4.92%)	wwPDB-VP
Wilson B-factor $(Å^2)$	31.8	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 39.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4480	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.10% 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: SO4, ZN $\,$

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.59	0/2238	0.65	1/3027~(0.0%)	
1	В	0.57	0/2238	0.68	0/3027	
All	All	0.58	0/4476	0.67	1/6054~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	A	249	LEU	CA-CB-CG	5.66	128.31	115.30

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	А	2192	0	2153	13	0
1	В	2192	0	2153	29	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
4	А	43	0	0	2	0
4	В	39	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4480	0	4306	41	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 5.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:18:GLY:HA3	4:B:331:HOH:O	1.82	0.78
1:B:19:GLU:OE2	1:B:19:GLU:HA	1.88	0.74
1:B:173:HIS:CE1	4:B:349:HOH:O	2.51	0.63
1:B:80:ARG:HD2	1:B:119:TYR:CE2	2.36	0.61
1:B:53:SER:H	1:B:56:GLN:HE21	1.49	0.61
1:B:233:GLU:HG3	1:B:274:ARG:HG3	1.85	0.58
1:B:258:GLU:HA	1:B:258:GLU:OE1	2.08	0.54
1:A:18:GLY:O	1:A:24:ARG:NH2	2.37	0.53
1:A:21:TRP:O	1:A:25:LEU:HG	2.08	0.53
1:A:275:MET:HB3	1:A:280:MET:HG3	1.90	0.52
1:B:109:VAL:CG1	1:B:109:VAL:O	2.58	0.51
1:B:109:VAL:O	1:B:109:VAL:HG12	2.10	0.51
1:B:80:ARG:HD2	1:B:119:TYR:HE2	1.75	0.51
1:B:240:LYS:HB2	1:B:280:MET:HE3	1.93	0.50
1:A:173:HIS:CE1	4:A:328:HOH:O	2.64	0.50
1:B:164:SER:OG	1:B:167:LYS:HG2	2.13	0.49
1:A:51:ASP:OD1	1:A:101:LYS:NZ	2.44	0.48
1:A:70:ARG:NH2	1:B:108:ASP:OD1	2.41	0.48
1:B:155:GLU:HA	1:B:183:TYR:O	2.14	0.48
1:B:254:SER:C	1:B:256:THR:N	2.67	0.47
1:A:97:GLU:O	1:A:101:LYS:HG3	2.15	0.47
1:B:145:ALA:HB1	1:B:150:VAL:O	2.14	0.47
1:B:156:ILE:N	1:B:156:ILE:HD13	2.31	0.46
1:A:124:GLN:HG3	4:A:314:HOH:O	2.16	0.45
1:A:6:ILE:HG12	1:A:280:MET:HE2	1.98	0.45
1:B:204:ILE:HG13	1:B:242:SER:HB3	1.98	0.45
1:B:163:ASN:HB2	1:B:192:TRP:CE2	2.51	0.45
1:B:41:ASP:OD1	1:B:46:ARG:HB2	2.17	0.44
1:B:215:THR:HG22	1:B:220:PHE:O	2.17	0.44
1:B:183:TYR:CE2	1:B:211:HIS:CD2	3.06	0.43
1:B:232:PHE:HB2	1:B:274:ARG:HG2	2.00	0.43
1:B:156:ILE:HG12	1:B:184:PRO:HA	2.00	0.43
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:HA	1:A:183:TYR:O	2.20	0.42
1:B:41:ASP:HA	1:B:77:SER:OG	2.21	0.41
1:A:6:ILE:N	1:A:6:ILE:HD12	2.35	0.41
1:A:39:SER:O	1:A:46:ARG:HD3	2.20	0.41
1:B:159:TYR:HA	1:B:160:PRO:HD3	1.96	0.40
1:B:6:ILE:HD11	1:B:280:MET:HB3	2.04	0.40
1:A:275:MET:O	1:A:280:MET:HG2	2.21	0.40
1:B:31:LEU:HD13	1:B:264:VAL:HG21	2.03	0.40

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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	А	274/295~(93%)	262 (96%)	11 (4%)	1 (0%)	34 38
1	В	274/295~(93%)	261 (95%)	8 (3%)	5(2%)	8 5
All	All	548/590~(93%)	523 (95%)	19 (4%)	6 (1%)	14 13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	254	SER
1	В	257	ALA
1	В	255	GLU
1	А	18	GLY
1	В	222	ASN
1	В	258	GLU



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	229/244~(94%)	223~(97%)	6 (3%)	46 56		
1	В	229/244~(94%)	218 (95%)	11 (5%)	25 32		
All	All	458/488 (94%)	441 (96%)	17 (4%)	34 43		

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

Mol	Chain	Res	Type
1	А	121	VAL
1	А	124	GLN
1	А	173	HIS
1	А	183	TYR
1	А	198	MET
1	А	258	GLU
1	В	19	GLU
1	В	30	THR
1	В	156	ILE
1	В	183	TYR
1	В	198	MET
1	В	204	ILE
1	В	222	ASN
1	В	254	SER
1	В	256	THR
1	В	258	GLU
1	В	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	94	GLN
1	В	56	GLN
1	В	115	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are 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	Type	Chain	Res Link		B	ond leng	gths	В	ond ang	gles
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	SO4	А	287	-	4,4,4	0.16	0	$6,\!6,\!6$	0.10	0
3	SO4	В	287	-	4,4,4	0.11	0	$6,\!6,\!6$	0.20	0

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.

No monomer is involved in short contacts.

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	276/295~(93%)	-0.00	1 (0%) 92 96	17, 29, 43, 49	0
1	В	276/295~(93%)	0.45	27 (9%) 7 12	17, 33, 61, 76	0
All	All	552/590~(93%)	0.23	28 (5%) 28 39	17, 30, 55, 76	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	217	PRO	6.3
1	В	229	VAL	5.6
1	В	254	SER	5.1
1	В	257	ALA	5.0
1	В	253	TRP	4.4
1	В	219	VAL	3.8
1	В	222	ASN	3.6
1	В	260	PRO	3.4
1	В	227	GLU	3.1
1	В	256	THR	3.1
1	В	221	LYS	3.0
1	В	255	GLU	2.9
1	В	279	GLY	2.9
1	В	223	VAL	2.9
1	В	216	LYS	2.8
1	В	220	PHE	2.8
1	В	264	VAL	2.8
1	В	191	ALA	2.7
1	В	218	GLY	2.6
1	В	266	LYS	2.5
1	В	225	PHE	2.4
1	А	226	GLY	2.4
1	В	267	ALA	2.3
1	В	205	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	В	278	ALA	2.1
1	В	263	GLU	2.1
1	В	234	ARG	2.1
1	В	258	GLU	2.0

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 monosaccharides 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	ZN	В	286	1/1	0.87	0.15	76,76,76,76	0
2	ZN	А	286	1/1	0.89	0.07	74,74,74,74	0
3	SO4	В	287	5/5	0.93	0.20	87,87,87,88	0
3	SO4	А	287	5/5	0.94	0.12	97,97,97,97	0
2	ZN	В	285	1/1	0.98	0.03	$55,\!55,\!55,\!55$	0
2	ZN	А	285	1/1	0.99	0.06	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.

