



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 06:59 PM BST

PDB ID : 6L2R  
Title : IlvC, a ketol-acid reductoisomerase, from Streptococcus pneumoniae\_E195S  
Authors : Gyuhee, K.; Donghyuk, S.; Sumin, L.; Jaesook, Y.; Sangho, L.  
Deposited on : 2019-10-06  
Resolution : 2.02 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](mailto: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.

---

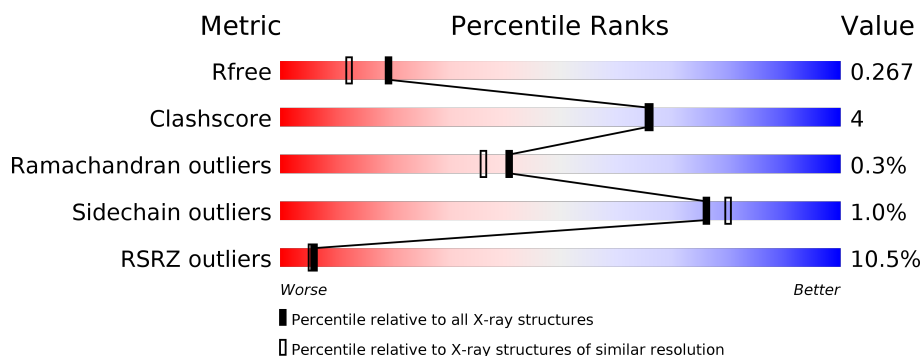
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

**i**

## X-RAY DIFFRACTION

A.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
$R_{free}$	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

Mol	Chain	Length	Quality of chain
1	A	340	<div> <div style="width: 8%; background-color: red;"></div> <div style="width: 85%; background-color: green;"></div> <div style="width: 10%; background-color: yellow;"></div> <div style="width: 5%; background-color: gray;"></div> </div>
1	B	340	<div> <div style="width: 12%; background-color: red;"></div> <div style="width: 87%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 5%; background-color: gray;"></div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4990 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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2495	1586	416	482	11			
1	B	324	Total	C	N	O	S	0	0	0
			2495	1586	416	482	11			

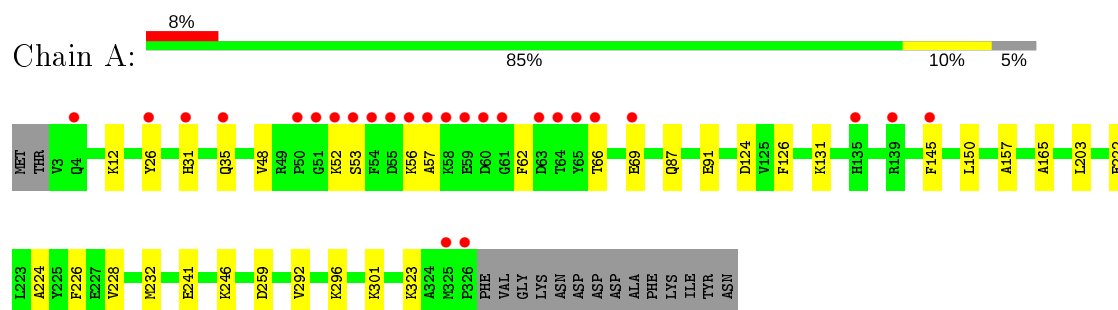
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	SER	GLU	engineered mutation	UNP Q04M32
B	195	SER	GLU	engineered mutation	UNP Q04M32

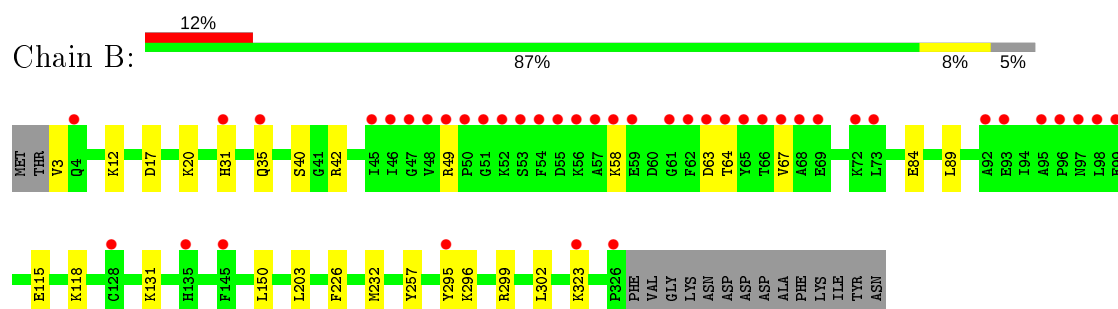
### 3 Residue-property plots [i](#)

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: Ketol-acid reductoisomerase (NADP(+))



- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.13Å 104.44Å 111.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.42 – 2.02 43.42 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.42-2.02) 99.6 (43.42-2.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.77 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.16 _3549	Depositor
R, $R_{free}$	0.230 , 0.267 0.230 , 0.267	Depositor DCC
$R_{free}$ test set	2696 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 42.40 % 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 2.0511e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.41	0/2542	0.57	1/3434 (0.0%)
1	B	0.41	0/2542	0.54	0/3434
All	All	0.41	0/5084	0.56	1/6868 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CG-OD1	6.71	124.34	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	A	2495	0	2453	28	0
1	B	2495	0	2451	19	0
All	All	4990	0	4904	40	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 4.

All (40) 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:A:26:TYR:HB3	1:A:53:SER:HB3	1.59	0.83
1:A:226:PHE:CB	1:B:131:LYS:HE3	2.19	0.73
1:B:17:ASP:OD1	1:B:42:ARG:NH1	2.22	0.64
1:B:84:GLU:HG3	1:B:295:TYR:CZ	2.38	0.59
1:B:295:TYR:OH	1:B:299:ARG:NH2	2.36	0.59
1:A:226:PHE:HB3	1:B:131:LYS:HE3	1.86	0.57
1:B:299:ARG:HD3	1:B:302:LEU:HD23	1.87	0.56
1:A:57:ALA:HB1	1:A:62:PHE:HB2	1.88	0.56
1:A:66:THR:HG22	1:A:69:GLU:HB2	1.86	0.56
1:A:26:TYR:HH	1:A:62:PHE:HE2	1.54	0.56
1:B:131:LYS:HE2	1:B:150:LEU:HD21	1.89	0.54
1:A:292:VAL:O	1:A:296:LYS:HG2	2.10	0.52
1:A:226:PHE:CD1	1:B:131:LYS:HD3	2.46	0.51
1:A:48:VAL:HG11	1:A:53:SER:HB2	1.93	0.50
1:B:203:LEU:HD11	1:B:232:MET:SD	2.52	0.50
1:A:31:HIS:NE2	1:A:35:GLN:HG3	2.27	0.49
1:B:115:GLU:HB3	1:B:118:LYS:HD3	1.94	0.49
1:A:131:LYS:HD3	1:B:226:PHE:CD1	2.49	0.48
1:A:226:PHE:CG	1:B:131:LYS:HE3	2.48	0.47
1:A:26:TYR:OH	1:A:31:HIS:HD2	1.98	0.46
1:A:126:PHE:HB2	1:A:165:ALA:HB2	1.98	0.46
1:A:203:LEU:HD11	1:A:232:MET:SD	2.56	0.46
1:A:131:LYS:HE2	1:A:150:LEU:HD21	1.98	0.46
1:A:56:LYS:HB3	1:A:56:LYS:NZ	2.31	0.45
1:A:224:ALA:O	1:A:228:VAL:HG22	2.16	0.45
1:A:31:HIS:CE1	1:A:35:GLN:HG3	2.52	0.44
1:A:57:ALA:HA	1:A:62:PHE:HD2	1.83	0.44
1:A:241:GLU:OE2	1:A:246:LYS:NZ	2.49	0.43
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.86	0.43
1:A:87:GLN:O	1:A:91:GLU:HG3	2.19	0.42
1:B:31:HIS:CE1	1:B:35:GLN:HG3	2.54	0.42
1:A:222:GLU:OE1	1:B:3:VAL:HG12	2.20	0.42
1:B:58:LYS:HG3	1:B:64:THR:HB	2.00	0.42
1:B:12:LYS:HD3	1:B:12:LYS:HA	1.81	0.42
1:A:301:LYS:HD3	1:B:257:TYR:OH	2.19	0.42
1:B:67:VAL:HG11	1:B:89:LEU:HD11	2.02	0.41
1:A:124:ASP:OD1	1:A:157:ALA:N	2.53	0.41
1:A:323:LYS:HB3	1:A:323:LYS:HE2	1.79	0.41
1:A:66:THR:HG23	1:A:69:GLU:H	1.86	0.40
1:B:323:LYS:HB3	1:B:323:LYS:HE3	1.92	0.40

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	322/340 (95%)	308 (96%)	13 (4%)	1 (0%)	41	36
1	B	322/340 (95%)	311 (97%)	10 (3%)	1 (0%)	41	36
All	All	644/680 (95%)	619 (96%)	23 (4%)	2 (0%)	41	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	ASP
1	A	52	LYS

### 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	253/267 (95%)	252 (100%)	1 (0%)	91	93
1	B	253/267 (95%)	249 (98%)	4 (2%)	62	66
All	All	506/534 (95%)	501 (99%)	5 (1%)	76	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	B	20	LYS
1	B	40	SER
1	B	49	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	296	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS

### 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](#)

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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/340 (95%)	0.53	26 (8%) 12 11	17, 27, 57, 104	0
1	B	324/340 (95%)	0.64	42 (12%) 3 3	17, 29, 57, 68	0
All	All	648/680 (95%)	0.59	68 (10%) 6 5	17, 28, 57, 104	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	ASP	8.5
1	B	54	PHE	7.9
1	A	57	ALA	7.7
1	A	54	PHE	6.9
1	A	326	PRO	6.3
1	A	58	LYS	6.2
1	A	61	GLY	6.0
1	B	48	VAL	6.0
1	A	51	GLY	5.9
1	B	326	PRO	5.6
1	A	50	PRO	5.3
1	B	50	PRO	4.8
1	B	55	ASP	4.2
1	B	145	PHE	3.9
1	B	64	THR	3.9
1	B	52	LYS	3.8
1	B	68	ALA	3.7
1	B	49	ARG	3.6
1	B	66	THR	3.6
1	A	53	SER	3.5
1	A	59	GLU	3.4
1	B	63	ASP	3.4
1	A	66	THR	3.3
1	A	64	THR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	61	GLY	3.3
1	A	63	ASP	3.3
1	A	31	HIS	3.2
1	A	65	TYR	3.1
1	B	69	GLU	3.1
1	A	56	LYS	3.1
1	B	65	TYR	3.1
1	B	92	ALA	3.1
1	B	67	VAL	3.0
1	B	53	SER	3.0
1	A	139	ARG	2.9
1	B	56	LYS	2.9
1	B	31	HIS	2.8
1	B	57	ALA	2.8
1	A	135	HIS	2.8
1	B	35	GLN	2.7
1	B	72	LYS	2.7
1	A	52	LYS	2.6
1	B	58	LYS	2.6
1	A	69	GLU	2.5
1	B	323	LYS	2.4
1	B	97	ASN	2.4
1	B	62	PHE	2.4
1	A	60	ASP	2.4
1	A	325	MET	2.4
1	B	295	TYR	2.4
1	B	93	GLU	2.3
1	B	128	CYS	2.3
1	B	96	PRO	2.3
1	B	99	GLU	2.3
1	B	4	GLN	2.2
1	B	51	GLY	2.2
1	B	59	GLU	2.2
1	B	45	ILE	2.2
1	B	95	ALA	2.2
1	A	35	GLN	2.2
1	A	26	TYR	2.2
1	A	145	PHE	2.1
1	B	135	HIS	2.1
1	B	46	ILE	2.1
1	B	73	LEU	2.1
1	A	4	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	98	LEU	2.0
1	B	47	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.