



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:30 am GMT

PDB ID : 1FWF  
Title : KLEBSIELLA AEROGENES UREASE, C319D VARIANT  
Authors : Pearson, M.A.; Karplus, P.A.  
Deposited on : 1997-04-23  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

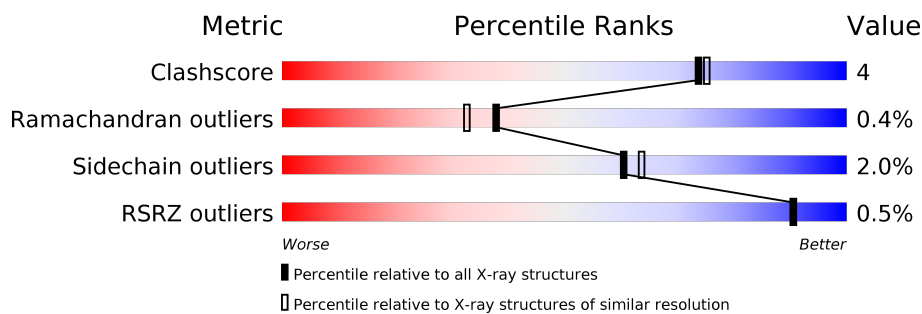
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	A	100	<div> <div></div> <div>93%7%</div> </div>
2	B	106	<div> <div>%</div> <div>84%11%5%</div> </div>
3	C	567	<div> <div>%</div> <div>87%9%..</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5962 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 UREASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			776	491	134	146	5			

- Molecule 2 is a protein called UREASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			784	496	150	135	3			

- Molecule 3 is a protein called UREASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	551	Total	C	N	O	S	0	0	0
			4115	2582	722	790	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	217	KCX	LYS	MODIFIED RESIDUE	UNP P18314
C	319	ASP	CYS	CONFLICT	UNP P18314

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Ni	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	23	Total 23	O 23	0	0
5	C	234	Total 234	O 234	0	0



- Molecule 1: UREASE

Category	Count
M1	100
K10	100
R22	100
I43	100
M44	100
V53	100
M57	100
V95	100
I100	100

- Molecule 2: UREASE

Position	Amino Acid	Count
M1	Met	1
G4	Gly	1
H7	His	1
K50	Lys	1
R53	Arg	1
E72	Asp	1
Q75	Gln	1
A83	Ala	1
R88	Arg	1
A89	Ala	1
V97	Val	1
P100	Pro	1
L101	Leu	1

Legend: GLU, VAL, ASN, ASP, GLU

- Molecule 3: UREASE

Category	Item	Value
Top 10	R518	100
	V545	95
	E548	90
	F567	85
	R336	80
	I337	75
	R338	70
	B349	65
	L356	60
	S359	55
Next 10	D360	50
	A363	45
	K364	40
	G365	35
	L372	30
	N396	25
	D396	20
	N397	15
	K406	10
	A418	5
Bottom 10	H419	0
	K428	-5
	K449	-10
	D460	-15
	A463	-20
	G481	-25
	L489	-30
	L507	-35
	R508	-40
	S509	-45

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.80Å 170.80Å 170.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 15.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (10.00-2.00) 93.7 (15.22-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.171 , (Not available) 0.165 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, KCX

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	0.36	0/787	0.58	0/1061
2	B	0.37	0/804	0.66	0/1087
3	C	0.37	0/4183	0.70	2/5696 (0.0%)
All	All	0.37	0/5774	0.68	2/7844 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	299	ASN	N-CA-C	5.93	127.02	111.00
3	C	372	LEU	CA-CB-CG	5.29	127.48	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	A	776	0	807	4	0
2	B	784	0	775	8	0
3	C	4115	0	4071	33	0
4	C	2	0	0	0	0
5	A	28	0	0	1	0
5	B	23	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	234	0	0	1	0
All	All	5962	0	5653	43	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.

The worst 5 of 43 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)
3:C:545:VAL:O	3:C:548:GLU:HG2	1.90	0.71
3:C:316:LEU:HD23	3:C:337:ILE:HD11	1.73	0.71
3:C:460:ASP:HB3	3:C:463:ALA:HB2	1.82	0.61
3:C:300:PRO:HD3	3:C:365:GLY:HA2	1.83	0.61
3:C:188:PRO:O	3:C:449:LYS:HD2	2.03	0.59

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	A	98/100 (98%)	98 (100%)	0	0	100	100
2	B	99/106 (93%)	94 (95%)	5 (5%)	0	100	100
3	C	546/567 (96%)	515 (94%)	28 (5%)	3 (0%)	32	26
All	All	743/773 (96%)	707 (95%)	33 (4%)	3 (0%)	38	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	360	ASP
3	C	364	MET

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Mol	Chain	Res	Type
3	C	481	GLY

### 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	85/85 (100%)	85 (100%)	0	100	100
2	B	78/83 (94%)	77 (99%)	1 (1%)	73	78
3	C	429/443 (97%)	418 (97%)	11 (3%)	51	52
All	All	592/611 (97%)	580 (98%)	12 (2%)	60	64

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	316	LEU
3	C	336	ARG
3	C	449	LYS
3	C	282	PRO
3	C	395	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	166	HIS
3	C	201	GLN
3	C	395	ASN
3	C	142	GLN
3	C	362	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	KCX	C	217	3,4	8,11,12	0.76	0	6,12,14	1.07	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	KCX	C	217	3,4	-	0/6/10/12	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	217	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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<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	100/100 (100%)	-0.84	0 100 100	7, 15, 32, 42	0
2	B	101/106 (95%)	-0.45	1 (0%) 82 82	12, 22, 39, 54	0
3	C	550/567 (97%)	-0.83	3 (0%) 90 90	6, 14, 33, 76	0
All	All	751/773 (97%)	-0.78	4 (0%) 90 90	6, 15, 35, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	101	LEU	4.0
3	C	313	LEU	3.0
3	C	316	LEU	3.0
3	C	333	ALA	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	KCX	C	217	12/13	0.97	0.08	-	8,12,23,24	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NI	C	575	1/1	1.00	0.03	-4.09	17,17,17,17	1
4	NI	C	574	1/1	0.99	0.02	-4.53	17,17,17,17	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.