



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 05:35 AM EDT

PDB ID : 6VP5  
Title : Ethylene forming enzyme (EFE) D191E variant in complex with Fe(II), L-arginine, and 2OG  
Authors : Davis, K.M.; Copeland, R.A.; Boal, A.K.  
Deposited on : 2020-02-01  
Resolution : 1.97 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

## 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 1.97 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11986 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 2-oxoglutarate-dependent ethylene/succinate-forming enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2651	1689	455	492	15	0	3	0
1	B	342	2708	1722	460	509	17	0	5	0
1	C	337	2664	1699	456	493	16	0	3	0
1	D	331	2601	1661	444	481	15	0	3	0

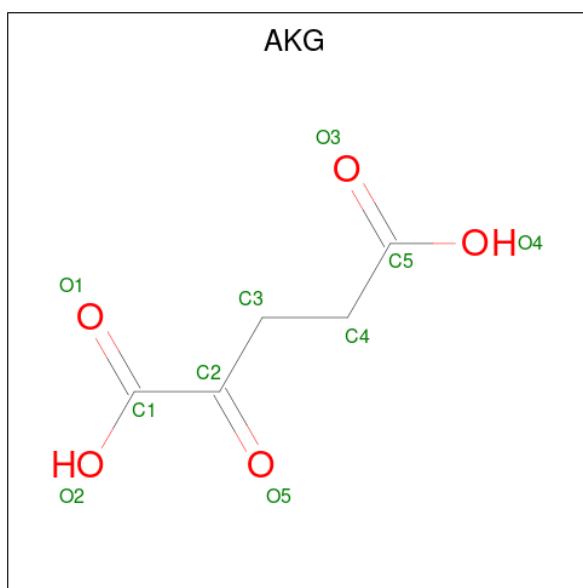
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P32021
A	191	GLU	ASP	engineered mutation	UNP P32021
B	0	SER	-	expression tag	UNP P32021
B	191	GLU	ASP	engineered mutation	UNP P32021
C	0	SER	-	expression tag	UNP P32021
C	191	GLU	ASP	engineered mutation	UNP P32021
D	0	SER	-	expression tag	UNP P32021
D	191	GLU	ASP	engineered mutation	UNP P32021

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

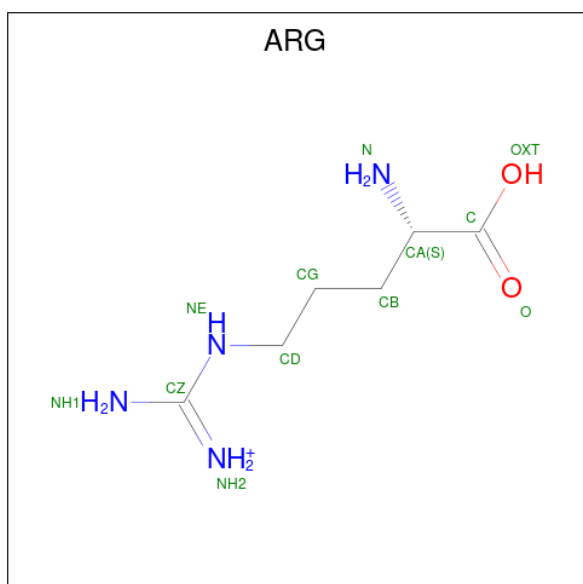
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



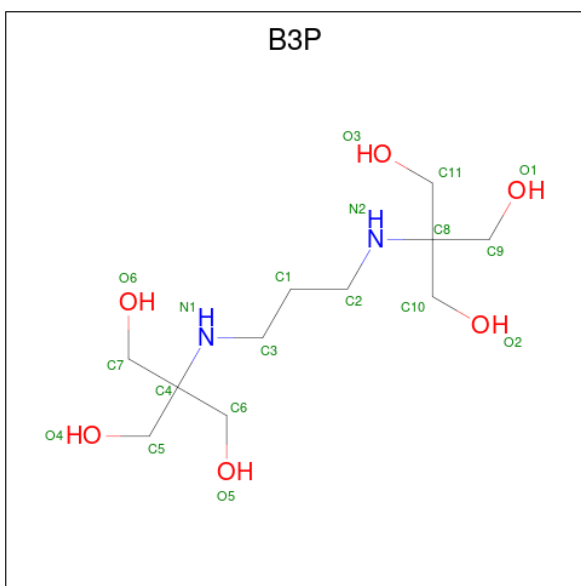
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0

- Molecule 4 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		
4	B	1	Total	C	N	O	0	0
			12	6	4	2		
4	C	1	Total	C	N	O	0	0
			12	6	4	2		
4	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	294	Total	O	0	0
			294	294		
6	B	338	Total	O	0	0
			338	338		
6	C	310	Total	O	0	0
			310	310		
6	D	309	Total	O	0	0
			309	309		

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.54Å 78.50Å 195.49Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	49.52 – 1.97	Depositor
% Data completeness (in resolution range)	99.2 (49.52-1.97)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.97Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.173 , 0.207	Depositor
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtrriage
Anisotropy	0.043	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtrriage
Total number of atoms	11986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AKG	C	402	2	9,9,9	5.84	2 (22%)	11,11,11	1.72	2 (18%)
3	AKG	B	402	2	9,9,9	5.87	2 (22%)	11,11,11	1.72	1 (9%)
3	AKG	A	402	2	9,9,9	5.83	2 (22%)	11,11,11	1.91	2 (18%)
3	AKG	D	402	2	9,9,9	5.80	2 (22%)	11,11,11	1.82	2 (18%)
4	ARG	B	403	-	10,11,11	0.76	1 (10%)	11,13,13	1.10	2 (18%)
4	ARG	C	403	-	10,11,11	0.74	1 (10%)	11,13,13	1.10	2 (18%)
4	ARG	A	403	-	10,11,11	0.74	1 (10%)	11,13,13	1.02	2 (18%)
4	ARG	D	403	-	10,11,11	0.74	1 (10%)	11,13,13	1.04	2 (18%)
5	B3P	D	404	-	18,18,18	0.08	0	21,23,23	0.50	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	AKG	C	402	2	-	1/9/9/9	-
3	AKG	B	402	2	-	2/9/9/9	-
3	AKG	A	402	2	-	3/9/9/9	-
3	AKG	D	402	2	-	2/9/9/9	-
4	ARG	B	403	-	-	0/11/11/11	-
4	ARG	C	403	-	-	0/11/11/11	-
4	ARG	A	403	-	-	0/11/11/11	-
4	ARG	D	403	-	-	0/11/11/11	-
5	B3P	D	404	-	-	0/28/28/28	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	AKG	C2-C1	-17.31	1.30	1.53
3	C	402	AKG	C2-C1	-17.22	1.30	1.53
3	A	402	AKG	C2-C1	-17.19	1.30	1.53
3	D	402	AKG	C2-C1	-17.10	1.30	1.53
3	B	402	AKG	O2-C1	-2.51	1.23	1.30
3	A	402	AKG	O2-C1	-2.49	1.23	1.30
3	D	402	AKG	O2-C1	-2.46	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	AKG	O2-C1	-2.44	1.23	1.30
4	C	403	ARG	OXT-C	-2.13	1.23	1.30
4	A	403	ARG	OXT-C	-2.11	1.23	1.30
4	D	403	ARG	OXT-C	-2.11	1.23	1.30
4	B	403	ARG	OXT-C	-2.09	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	AKG	C3-C2-C1	4.47	124.27	115.97
3	B	402	AKG	C3-C2-C1	4.36	124.07	115.97
3	C	402	AKG	C3-C2-C1	4.30	123.95	115.97
3	D	402	AKG	C3-C2-C1	4.23	123.83	115.97
3	A	402	AKG	O1-C1-C2	-2.82	117.96	121.72
4	C	403	ARG	OXT-C-O	-2.75	117.85	124.09
3	D	402	AKG	O1-C1-C2	-2.72	118.09	121.72
4	B	403	ARG	OXT-C-O	-2.71	117.93	124.09
4	D	403	ARG	OXT-C-O	-2.69	117.98	124.09
4	A	403	ARG	OXT-C-O	-2.58	118.23	124.09
4	B	403	ARG	OXT-C-CA	2.31	121.24	113.38
4	C	403	ARG	OXT-C-CA	2.28	121.14	113.38
4	A	403	ARG	OXT-C-CA	2.08	120.48	113.38
4	D	403	ARG	OXT-C-CA	2.05	120.38	113.38
3	C	402	AKG	O1-C1-C2	-2.00	119.04	121.72

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	AKG	C1-C2-C3-C4
3	B	402	AKG	C1-C2-C3-C4
3	A	402	AKG	C3-C4-C5-O4
3	D	402	AKG	C3-C4-C5-O4
3	B	402	AKG	O5-C2-C3-C4
3	C	402	AKG	C1-C2-C3-C4
3	A	402	AKG	C3-C4-C5-O3
3	D	402	AKG	C3-C4-C5-O3

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.