



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:32 AM EDT

PDB ID : 6VP4
Title : Ethylene forming enzyme (EFE) 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 : 1.83 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 ⓘ 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 ⓘ](#)) 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 1.83 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 11760 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	333	Total 2618	C 1670	N 447	O 485	S 16	0	4	0
1	B	340	Total 2685	C 1706	N 458	O 503	S 18	0	4	0
1	C	339	Total 2651	C 1690	N 453	O 492	S 16	0	2	0
1	D	331	Total 2588	C 1652	N 443	O 478	S 15	0	3	0

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

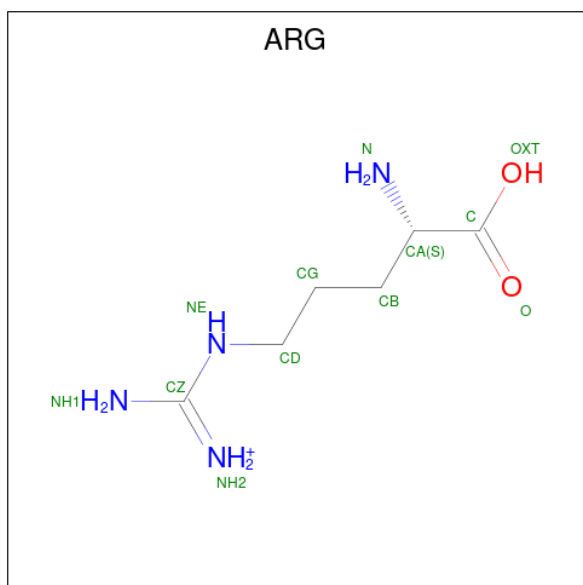
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



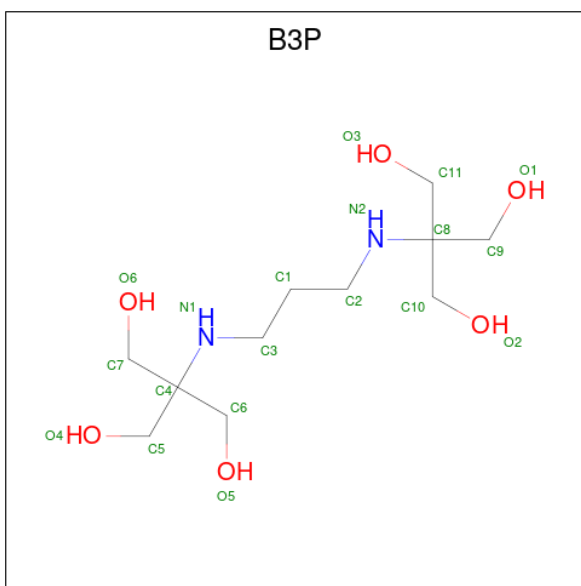
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- 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	266	Total	O	0	0
			266	266		
6	B	319	Total	O	0	0
			319	319		
6	C	269	Total	O	0	0
			269	269		
6	D	253	Total	O	0	0
			253	253		

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, α , β , γ	49.73Å 78.81Å 195.91Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	40.77 – 1.83	Depositor
% Data completeness (in resolution range)	98.8 (40.77-1.83)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.174 , 0.197	Depositor
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.402	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
Total number of atoms	11760	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 20.36 % 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 8.8331e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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.

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](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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
4	ARG	B	403	-	10,11,11	0.72	0	11,13,13	1.08	2 (18%)
5	B3P	D	404	-	18,18,18	0.11	0	21,23,23	0.33	0
3	AKG	D	402	2	9,9,9	5.66	2 (22%)	11,11,11	1.86	2 (18%)
4	ARG	A	403	-	10,11,11	0.75	1 (10%)	11,13,13	1.17	2 (18%)
4	ARG	C	403	-	10,11,11	0.75	1 (10%)	11,13,13	1.14	2 (18%)
4	ARG	D	403	-	10,11,11	0.72	1 (10%)	11,13,13	1.07	2 (18%)
3	AKG	A	402	2	9,9,9	5.70	2 (22%)	11,11,11	1.93	3 (27%)
3	AKG	B	402	2	9,9,9	5.68	2 (22%)	11,11,11	1.78	1 (9%)
3	AKG	C	402	2	9,9,9	5.76	2 (22%)	11,11,11	1.75	1 (9%)

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
4	ARG	B	403	-	-	0/11/11/11	-
5	B3P	D	404	-	-	0/28/28/28	-
3	AKG	D	402	2	-	4/9/9/9	-
4	ARG	A	403	-	-	0/11/11/11	-
4	ARG	C	403	-	-	1/11/11/11	-
4	ARG	D	403	-	-	0/11/11/11	-
3	AKG	A	402	2	-	4/9/9/9	-
3	AKG	B	402	2	-	2/9/9/9	-
3	AKG	C	402	2	-	2/9/9/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	AKG	C2-C1	-17.00	1.30	1.53
3	A	402	AKG	C2-C1	-16.79	1.30	1.53
3	B	402	AKG	C2-C1	-16.72	1.31	1.53
3	D	402	AKG	C2-C1	-16.65	1.31	1.53
3	D	402	AKG	O2-C1	-2.46	1.23	1.30
3	A	402	AKG	O2-C1	-2.37	1.23	1.30
3	B	402	AKG	O2-C1	-2.36	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	AKG	O2-C1	-2.30	1.23	1.30
4	C	403	ARG	OXT-C	-2.14	1.23	1.30
4	A	403	ARG	OXT-C	-2.10	1.23	1.30
4	D	403	ARG	OXT-C	-2.07	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	AKG	C3-C2-C1	4.54	124.39	115.97
3	B	402	AKG	C3-C2-C1	4.53	124.38	115.97
3	A	402	AKG	C3-C2-C1	4.46	124.25	115.97
3	D	402	AKG	C3-C2-C1	4.40	124.13	115.97
4	A	403	ARG	OXT-C-O	-3.12	117.02	124.09
3	A	402	AKG	O1-C1-C2	-3.07	117.62	121.72
4	C	403	ARG	OXT-C-O	-2.81	117.70	124.09
4	D	403	ARG	OXT-C-O	-2.64	118.10	124.09
4	B	403	ARG	OXT-C-CA	2.44	121.71	113.38
3	D	402	AKG	O1-C1-C2	-2.41	118.50	121.72
4	B	403	ARG	OXT-C-O	-2.41	118.61	124.09
4	C	403	ARG	OXT-C-CA	2.37	121.47	113.38
4	D	403	ARG	OXT-C-CA	2.26	121.07	113.38
4	A	403	ARG	OXT-C-CA	2.20	120.87	113.38
3	A	402	AKG	O2-C1-C2	2.13	119.79	113.97

There are no chirality outliers.

All (13) 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	C	402	AKG	C1-C2-C3-C4
3	D	402	AKG	C1-C2-C3-C4
3	C	402	AKG	O5-C2-C3-C4
3	B	402	AKG	O5-C2-C3-C4
3	A	402	AKG	C3-C4-C5-O4
4	C	403	ARG	NE-CD-CG-CB
3	D	402	AKG	C3-C4-C5-O4
3	A	402	AKG	C3-C4-C5-O3
3	D	402	AKG	C3-C4-C5-O3
3	A	402	AKG	O5-C2-C3-C4
3	D	402	AKG	O5-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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