



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2022 – 06:04 PM JST

PDB ID : 7EFS
Title : Fructose-bisphosphate aldolase in Artemisia sieversiana pollen
Authors : Li, Z.; Wei, C.; Ji Fu, W.; Zhi Qiang, X.
Deposited on : 2021-03-23
Resolution : 2.50 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 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	:	2.27
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)	:	2.27

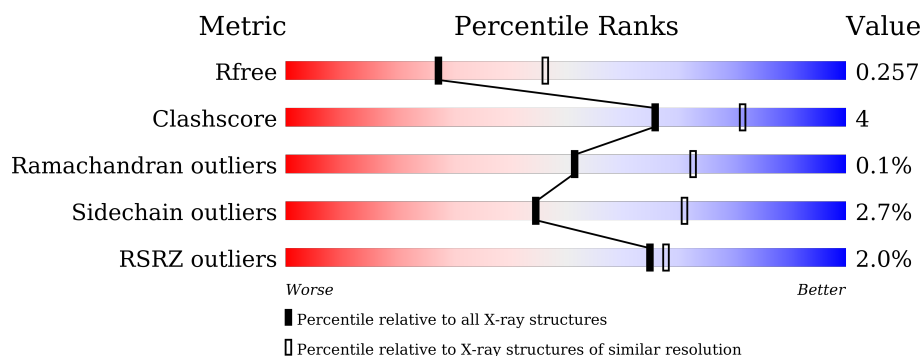
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	365	<div> <div>85%</div> <div>8% • 7%</div> </div>
1	B	365	<div> <div>6%</div> <div>84%</div> <div>8% • 7%</div> </div>
1	C	365	<div> <div>%</div> <div>82%</div> <div>11% • 7%</div> </div>
1	D	365	<div> <div>%</div> <div>83%</div> <div>9% • 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10397 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 Fructose-bisphosphate aldolase.

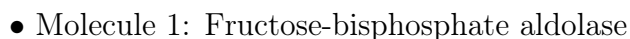
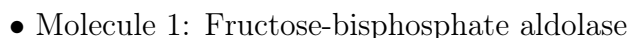
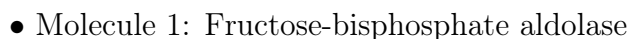
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2565	1620	442	490	13			
1	B	339	Total	C	N	O	S	0	0	0
			2565	1620	442	490	13			
1	C	339	Total	C	N	O	S	0	0	0
			2565	1620	442	490	13			
1	D	340	Total	C	N	O	S	0	0	0
			2569	1622	443	491	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	49	Total	O	0	0
			49	49		
2	B	30	Total	O	0	0
			30	30		
2	C	33	Total	O	0	0
			33	33		
2	D	21	Total	O	0	0
			21	21		

i

- Molecule 1: Fructose-bisphosphate aldolase



T324	R325	N329	S330	T333	L334	G340	ALA	ALA	VAL	GLU	GLY	GLY	ALA	THR	GLU	SER	LEU	HIS	VAL	LYS	ASP	TYR	LYS	TYR	LEU	GLU	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.01Å 129.69Å 157.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.49 – 2.50 48.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.49-2.50) 100.0 (48.80-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.209 , 0.259 0.210 , 0.257	Depositor DCC
R_{free} test set	3795 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10397	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

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	0.54	0/2609	0.67	0/3535
1	B	0.54	0/2609	0.68	0/3535
1	C	0.54	0/2609	0.68	0/3535
1	D	0.52	0/2613	0.66	0/3540
All	All	0.54	0/10440	0.67	0/14145

There are no bond length outliers.

There are no bond angle outliers.

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	2565	0	2595	27	0
1	B	2565	0	2595	16	0
1	C	2565	0	2595	24	0
1	D	2569	0	2598	23	0
2	A	49	0	0	2	0
2	B	30	0	0	1	0
2	C	33	0	0	2	0
2	D	21	0	0	2	0
All	All	10397	0	10383	82	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 (82) 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:C:311:LYS:HD2	1:C:313:GLU:OE2	1.65	0.95
1:A:280:ALA:O	1:A:284:LEU:HD12	1.74	0.85
1:A:281:MET:HA	1:A:284:LEU:HD13	1.68	0.76
1:D:272:GLU:O	1:D:276:VAL:HG23	1.97	0.65
1:A:280:ALA:O	1:A:284:LEU:CD1	2.45	0.64
1:B:285:GLN:NE2	2:B:401:HOH:O	2.32	0.62
1:D:330:SER:O	1:D:334:LEU:HD23	2.01	0.60
1:A:255:MET:O	1:A:290:TRP:HZ3	1.85	0.59
1:A:290:TRP:HD1	1:A:290:TRP:O	1.86	0.59
1:D:23:GLY:HA2	1:D:334:LEU:HD21	1.86	0.57
1:A:194:ILE:HB	1:A:231:PRO:HD3	1.85	0.56
1:D:317:LYS:O	1:D:321:VAL:HG23	2.08	0.54
1:B:275:THR:OG1	1:B:325:ARG:NH2	2.42	0.53
1:A:290:TRP:O	1:A:290:TRP:CD1	2.62	0.52
1:D:132:GLN:NE2	2:D:401:HOH:O	2.34	0.52
1:A:30:ASP:OD2	1:A:103:LYS:HE3	2.09	0.52
1:D:1:MET:HG3	1:D:216:HIS:NE2	2.25	0.52
1:C:123:LEU:HD13	1:C:168:ARG:HG2	1.93	0.51
1:C:68:TYR:CZ	1:C:327:LYS:HG2	2.46	0.51
1:D:255:MET:O	1:D:290:TRP:HZ3	1.93	0.51
1:D:330:SER:O	1:D:334:LEU:CD2	2.59	0.51
1:D:329:ASN:O	1:D:333:THR:HG23	2.12	0.50
1:C:311:LYS:HB3	1:C:313:GLU:OE1	2.12	0.50
1:A:334:LEU:HB2	1:A:336:LYS:HE2	1.93	0.50
1:C:210:LYS:HG2	1:D:210:LYS:HG2	1.94	0.50
1:C:216:HIS:HE1	2:C:431:HOH:O	1.95	0.49
1:D:35:THR:HG22	1:D:39:ARG:NH1	2.28	0.49
1:A:255:MET:O	1:A:290:TRP:CZ3	2.66	0.49
1:D:255:MET:O	1:D:290:TRP:CZ3	2.66	0.49
1:B:194:ILE:HB	1:B:231:PRO:HD3	1.95	0.48
1:A:298:ARG:HD2	2:A:446:HOH:O	2.13	0.48
1:C:30:ASP:OD2	1:C:103:LYS:HE3	2.14	0.48
1:D:271:GLU:HB3	1:D:325:ARG:HD2	1.95	0.47
1:C:272:GLU:O	1:C:276:VAL:HG23	2.14	0.47
1:D:104:VAL:CG2	1:D:169:TYR:HE1	2.27	0.47
1:C:68:TYR:CE2	1:C:327:LYS:HG2	2.50	0.47
1:C:46:GLU:HB3	1:C:48:VAL:HG23	1.97	0.47
1:B:45:VAL:HG21	1:B:310:GLY:HA3	1.98	0.45
1:A:244:ALA:HB1	1:A:284:LEU:CD1	2.47	0.45
1:C:62:THR:OG1	1:C:319:GLN:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:HD2	1:C:336:LYS:HA	1.76	0.45
1:B:104:VAL:CG2	1:B:169:TYR:HE1	2.30	0.45
1:B:250:ALA:O	1:B:254:THR:OG1	2.33	0.44
1:A:287:LYS:HE3	1:B:257:PRO:O	2.17	0.44
1:A:252:GLN:HA	1:B:257:PRO:HG2	1.98	0.44
1:C:329:ASN:O	1:C:333:THR:HG23	2.16	0.44
1:C:263:VAL:HG12	1:C:293:THR:HG23	2.00	0.44
1:D:320:GLU:O	1:D:324:ILE:HG12	2.17	0.44
1:C:224:LEU:HG	1:C:226:PRO:HD3	1.99	0.44
1:A:25:GLY:HA3	1:A:294:PHE:CZ	2.53	0.43
1:A:209:TYR:CD1	1:A:212:LEU:HD12	2.53	0.43
1:A:104:VAL:HG21	1:A:169:TYR:HE1	1.82	0.43
1:A:257:PRO:HG2	1:B:252:GLN:HA	1.99	0.43
1:B:263:VAL:HG12	1:B:293:THR:HG23	1.99	0.43
1:C:43:ILE:HD13	1:C:305:LEU:HG	2.01	0.43
1:B:209:TYR:CD1	1:B:212:LEU:HD12	2.54	0.43
1:C:255:MET:O	1:C:290:TRP:CZ3	2.71	0.43
1:B:262:VAL:HB	1:B:292:LEU:HD23	2.01	0.42
1:C:255:MET:O	1:C:290:TRP:HZ3	2.01	0.42
1:D:125:GLY:O	1:D:129:ARG:HG3	2.19	0.42
1:D:333:THR:OG1	1:D:334:LEU:HD22	2.19	0.42
1:B:255:MET:O	1:B:290:TRP:HZ3	2.03	0.42
1:C:203:ARG:HD2	2:D:420:HOH:O	2.19	0.42
1:A:257:PRO:HD3	1:B:257:PRO:HD3	2.00	0.42
1:B:263:VAL:HG23	1:B:263:VAL:O	2.19	0.41
1:C:25:GLY:HA3	1:C:294:PHE:CE1	2.56	0.41
1:D:104:VAL:O	1:D:129:ARG:NH2	2.53	0.41
1:D:228:MET:HE2	1:D:269:GLN:HE22	1.83	0.41
1:A:244:ALA:HB1	1:A:284:LEU:HD11	2.02	0.41
1:C:215:HIS:HD2	2:C:419:HOH:O	2.02	0.41
1:A:25:GLY:HA3	1:A:294:PHE:CE1	2.55	0.41
1:C:236:LYS:HA	1:C:236:LYS:HD3	1.93	0.41
1:C:66:LEU:HD23	1:C:96:ALA:HB3	2.01	0.41
1:D:38:LYS:HA	1:D:41:ASP:OD1	2.21	0.41
1:A:244:ALA:CB	1:A:284:LEU:HD11	2.50	0.41
1:A:103:LYS:HE2	2:A:404:HOH:O	2.20	0.40
1:A:168:ARG:HD3	1:D:161:GLU:OE1	2.22	0.40
1:A:289:PRO:O	1:B:287:LYS:HD3	2.22	0.40
1:C:252:GLN:HA	1:D:257:PRO:HG2	2.03	0.40
1:A:329:ASN:O	1:A:333:THR:HG23	2.22	0.40
1:D:180:PRO:HD2	1:D:221:GLY:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:O	1:A:129:ARG:NH2	2.55	0.40

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	337/365 (92%)	327 (97%)	10 (3%)	0	100	100
1	B	337/365 (92%)	328 (97%)	8 (2%)	1 (0%)	41	61
1	C	337/365 (92%)	327 (97%)	10 (3%)	0	100	100
1	D	338/365 (93%)	333 (98%)	5 (2%)	0	100	100
All	All	1349/1460 (92%)	1315 (98%)	33 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	PRO

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/289 (93%)	263 (98%)	5 (2%)	57 80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	268/289 (93%)	258 (96%)	10 (4%)	34	60
1	C	268/289 (93%)	260 (97%)	8 (3%)	41	68
1	D	268/289 (93%)	262 (98%)	6 (2%)	52	77
All	All	1072/1156 (93%)	1043 (97%)	29 (3%)	44	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	153	GLU
1	A	169	TYR
1	A	290	TRP
1	A	325	ARG
1	B	2	SER
1	B	38	LYS
1	B	39	ARG
1	B	42	SER
1	B	46	GLU
1	B	48	VAL
1	B	56	ARG
1	B	57	GLU
1	B	169	TYR
1	B	290	TRP
1	C	56	ARG
1	C	169	TYR
1	C	266	SER
1	C	284	LEU
1	C	287	LYS
1	C	290	TRP
1	C	316	GLN
1	C	336	LYS
1	D	56	ARG
1	D	169	TYR
1	D	233	SER
1	D	290	TRP
1	D	306	LYS
1	D	317	LYS

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

Mol	Chain	Res	Type
1	C	316	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](#)

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, 95th 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 ²)	Q<0.9
1	A	339/365 (92%)	-0.25	1 (0%) 94 94	30, 43, 58, 76	0
1	B	339/365 (92%)	0.14	21 (6%) 20 21	32, 48, 84, 117	0
1	C	339/365 (92%)	-0.15	2 (0%) 89 90	32, 53, 72, 83	0
1	D	340/365 (93%)	-0.01	3 (0%) 84 86	34, 53, 78, 90	0
All	All	1357/1460 (92%)	-0.07	27 (1%) 65 68	30, 48, 74, 117	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	ILE	7.4
1	B	40	PHE	4.9
1	B	39	ARG	4.9
1	B	37	GLY	4.7
1	B	46	GLU	4.4
1	B	36	ILE	4.1
1	B	45	VAL	3.9
1	B	41	ASP	3.8
1	B	32	SER	3.4
1	B	42	SER	3.4
1	B	33	THR	3.2
1	B	47	ASN	3.2
1	B	236	LYS	3.2
1	D	268	GLY	3.1
1	D	1	MET	3.1
1	B	34	GLY	3.0
1	C	320	GLU	2.8
1	B	44	LYS	2.8
1	C	310	GLY	2.7
1	A	211	ALA	2.7
1	B	75	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	2.4
1	D	242	VAL	2.3
1	B	300	LEU	2.3
1	B	59	LEU	2.2
1	B	56	ARG	2.2
1	B	35	THR	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.