



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2017 – 05:34 PM EDT

PDB ID : 5KY6
Title : Human muscle fructose-1,6-bisphosphate aldolase
Authors : Wisniewski, J.; Barciszewski, J.; Jaskolski, M.; Rakus, D.
Deposited on : 2016-07-21
Resolution : 1.94 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : rb-20029077
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) : rb-20029077

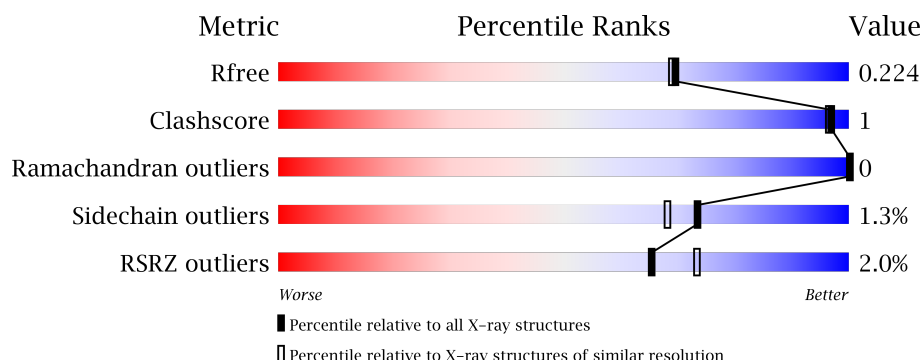
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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}	100719	3233 (1.96-1.92)
Clashscore	112137	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

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 ≥ 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	363	<div> <div>2%</div> <div>85%</div> <div>11%</div> </div>
1	B	363	<div> <div>2%</div> <div>88%</div> <div>5%</div> <div>8%</div> </div>
1	C	363	<div> <div>%</div> <div>89%</div> <div>8%</div> </div>
1	D	363	<div> <div>2%</div> <div>85%</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20854 atoms, of which 10190 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 A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	H	N	O	S	0	1	0
			4987	1566	2507	433	469	12			
1	B	335	Total	C	H	N	O	S	0	1	0
			5156	1623	2587	448	486	12			
1	C	334	Total	C	H	N	O	S	0	1	0
			5142	1619	2580	447	484	12			
1	D	325	Total	C	H	N	O	S	0	2	0
			5007	1571	2516	436	472	12			

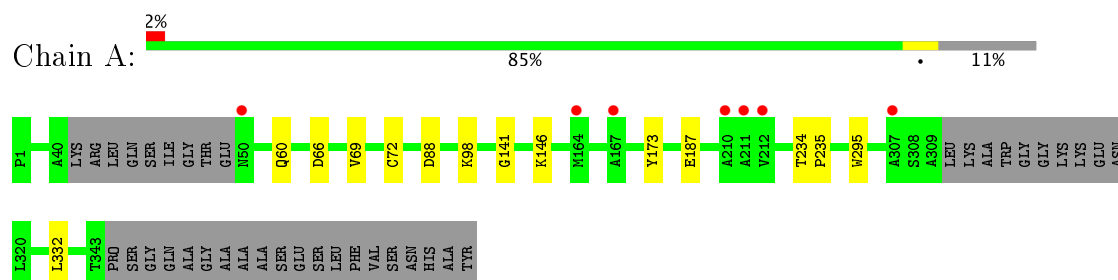
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	147	Total	O	0	0
			147	147		
2	C	127	Total	O	0	0
			127	127		
2	D	146	Total	O	0	0
			146	146		

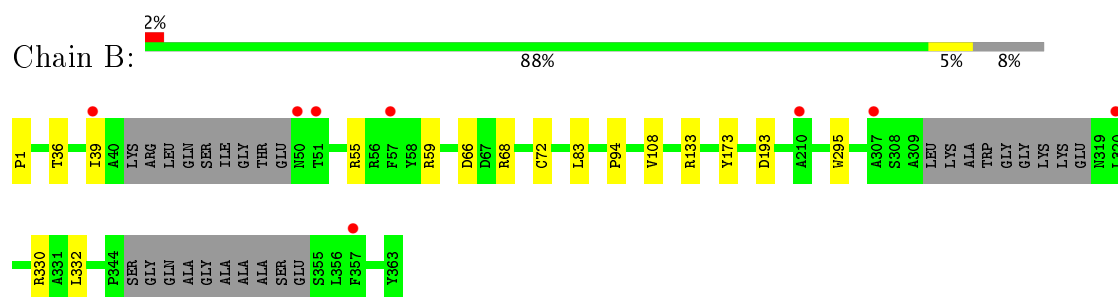
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

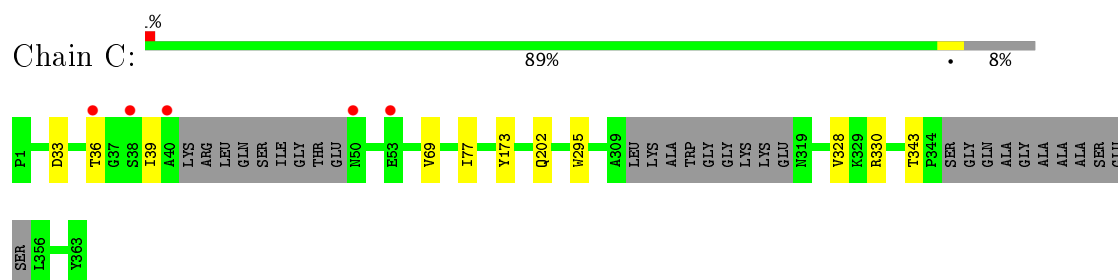
- Molecule 1: Fructose-bisphosphate aldolase A



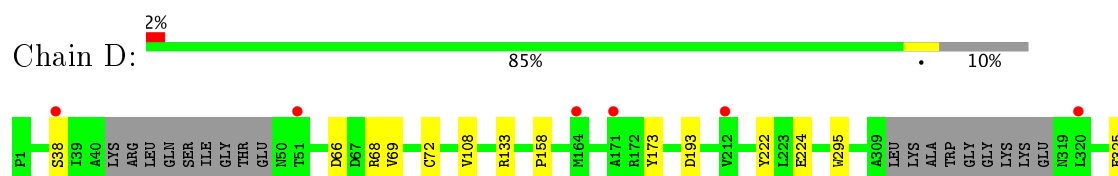
- Molecule 1: Fructose-bisphosphate aldolase A



- Molecule 1: Fructose-bisphosphate aldolase A



- Molecule 1: Fructose-bisphosphate aldolase A



1332	PRO
1343	SER
	GLY
	GLN
	ALA
	GLY
	ALA
	ALA
	SER
	GLU
	SER
	LEU
	PHE
	VAL
	SER
	ASN
	HIS
	ALA
	TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.51Å 57.25Å 164.02Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	46.72 – 1.94 46.72 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.72-1.94) 99.0 (46.72-1.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.186 , 0.223 0.186 , 0.224	Depositor DCC
R_{free} test set	1002 reflections (0.89%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20854	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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

5.1 Standard geometry

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	0.49	0/2529	0.60	0/3427
1	B	0.49	0/2621	0.63	0/3551
1	C	0.44	0/2615	0.60	0/3543
1	D	0.50	0/2546	0.61	0/3450
All	All	0.48	0/10311	0.61	0/13971

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

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	2480	2507	2507	6	0
1	B	2569	2587	2585	7	0
1	C	2562	2580	2576	4	0
1	D	2491	2516	2507	6	0
2	A	142	0	0	0	0
2	B	147	0	0	0	0
2	C	127	0	0	1	0
2	D	146	0	0	0	0
All	All	10664	10190	10175	22	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 1.

All (22) 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:B:66:ASP:OD2	1:B:68:ARG:NH1	2.27	0.67
1:D:68:ARG:NH2	1:D:325:GLU:OE1	2.32	0.58
1:D:108:VAL:O	1:D:133:ARG:NH2	2.39	0.54
1:A:98:LYS:NZ	1:A:141:GLY:O	2.42	0.52
1:B:1:PRO:HD3	1:D:158:PRO:O	2.12	0.49
1:C:69:VAL:HG13	1:C:328:VAL:HG22	1.96	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.47
1:A:72:CYS:SG	1:A:332:LEU:HD23	2.55	0.47
1:C:202:GLN:OE1	2:C:401:HOH:O	2.20	0.47
1:C:36:THR:O	1:C:39:ILE:HG22	2.15	0.47
1:A:60:GLN:OE1	1:A:88:ASP:N	2.44	0.46
1:B:108:VAL:O	1:B:133:ARG:NH2	2.48	0.45
1:B:72:CYS:SG	1:B:332:LEU:HD23	2.56	0.45
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.97	0.45
1:D:72:CYS:SG	1:D:332:LEU:HD23	2.56	0.45
1:C:33:ASP:HB3	1:C:77:ILE:HG22	2.02	0.42
1:A:146:LYS:HE2	1:A:187:GLU:OE1	2.19	0.41
1:B:36:THR:O	1:B:39:ILE:HG22	2.19	0.41
1:D:222:TYR:CZ	1:D:224:GLU:HB2	2.56	0.41
1:A:234:THR:HB	1:A:235:PRO:HD2	2.01	0.41
1:B:55:ARG:O	1:B:59:ARG:HG2	2.21	0.40
1:A:66:ASP:O	1:A:69:VAL:HG12	2.22	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	319/363 (88%)	309 (97%)	10 (3%)	0	100	100
1	B	328/363 (90%)	321 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	327/363 (90%)	318 (97%)	9 (3%)	0	100	100
1	D	321/363 (88%)	311 (97%)	10 (3%)	0	100	100
All	All	1295/1452 (89%)	1259 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	264/291 (91%)	262 (99%)	2 (1%)	85	82
1	B	274/291 (94%)	270 (98%)	4 (2%)	70	63
1	C	273/291 (94%)	269 (98%)	4 (2%)	70	63
1	D	266/291 (91%)	262 (98%)	4 (2%)	70	63
All	All	1077/1164 (92%)	1063 (99%)	14 (1%)	73	68

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	TYR
1	A	295	TRP
1	B	173	TYR
1	B	193	ASP
1	B	295	TRP
1	B	330	ARG
1	C	173	TYR
1	C	295	TRP
1	C	330	ARG
1	C	343	THR
1	D	38	SER
1	D	173	TYR
1	D	193	ASP
1	D	295	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	324/363 (89%)	0.03	7 (2%) 62 71	7, 18, 49, 68	0
1	B	335/363 (92%)	0.05	8 (2%) 59 68	7, 20, 47, 74	0
1	C	334/363 (92%)	-0.04	5 (1%) 74 80	9, 22, 50, 76	0
1	D	325/363 (89%)	0.00	6 (1%) 69 76	7, 17, 43, 72	0
All	All	1318/1452 (90%)	0.01	26 (1%) 65 73	7, 20, 48, 76	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	ILE	4.2
1	D	164[A]	MET	3.2
1	C	38	SER	3.1
1	B	307	ALA	2.9
1	B	57	PHE	2.8
1	D	38	SER	2.7
1	A	211	ALA	2.5
1	B	51	THR	2.5
1	A	164[A]	MET	2.4
1	D	212	VAL	2.4
1	A	50	ASN	2.4
1	B	50	ASN	2.4
1	A	210	ALA	2.3
1	C	53	GLU	2.3
1	A	167	ALA	2.3
1	D	51	THR	2.3
1	A	307	ALA	2.3
1	B	357	PHE	2.2
1	B	320	LEU	2.2
1	B	210	ALA	2.2
1	C	50	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	36	THR	2.2
1	A	212	VAL	2.2
1	D	320	LEU	2.2
1	C	40	ALA	2.2
1	D	171	ALA	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 carbohydrates 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.