



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 14, 2016 – 12:01 PM EDT

PDB ID : 5ET7  
Title : Human muscle fructose-1,6-bisphosphatase in inactive T-state  
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Deposited on : 2015-11-17  
Resolution : 2.99 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027790

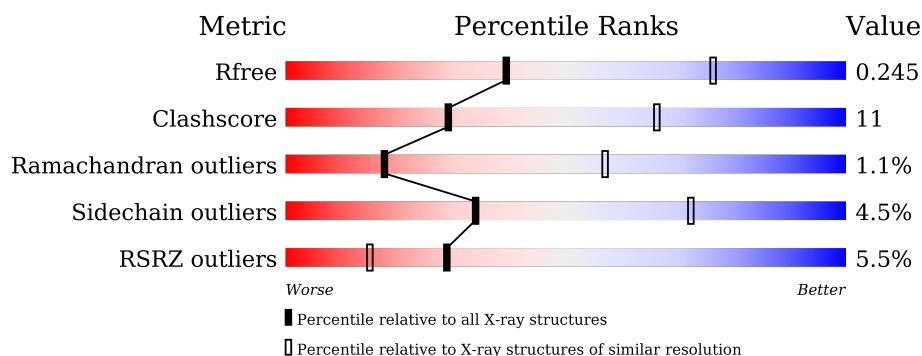
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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))
$R_{free}$	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	338	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>21%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	338	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>21%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	338	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>19%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	338	<div> <div>7%</div> <div> <div></div> <div>58%</div> <div>20%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8589 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-1,6-bisphosphatase isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2205	1410	363	423	9			
1	C	278	Total	C	N	O	S	0	0	0
			2132	1369	350	404	9			
1	B	280	Total	C	N	O	S	0	0	0
			2152	1381	355	407	9			
1	D	273	Total	C	N	O	S	0	0	0
			2100	1349	346	396	9			

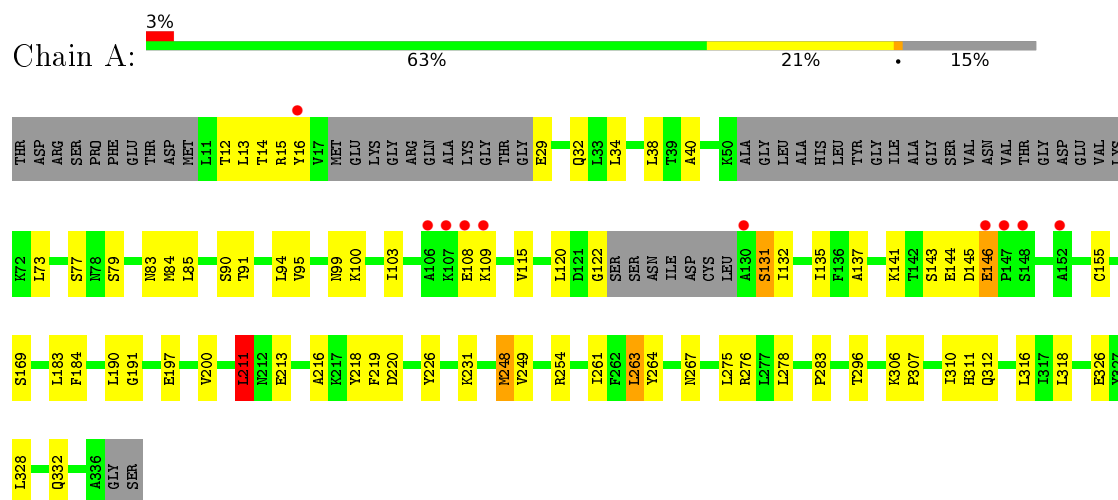
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	VAL	variant	UNP O00757
C	85	LEU	VAL	variant	UNP O00757
B	85	LEU	VAL	variant	UNP O00757
D	85	LEU	VAL	variant	UNP O00757

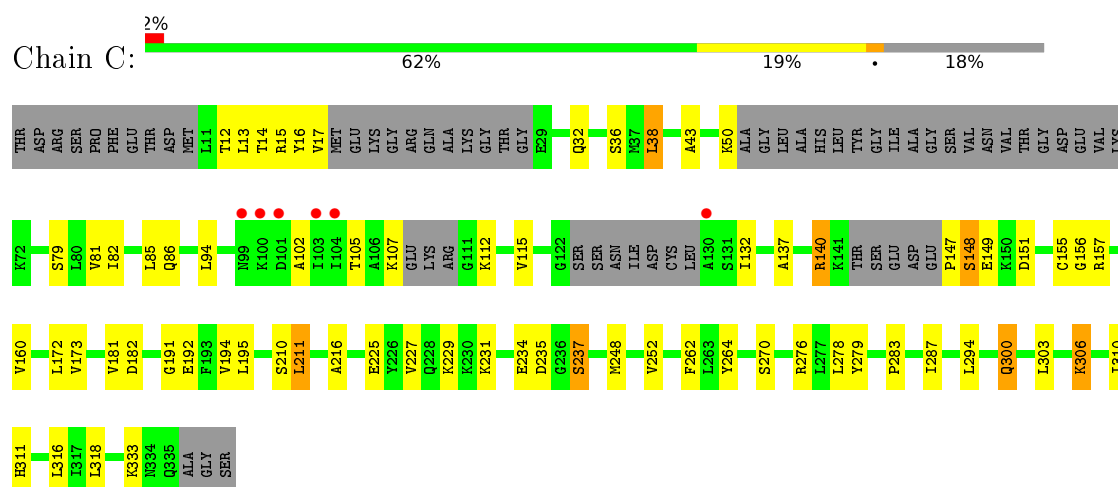
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

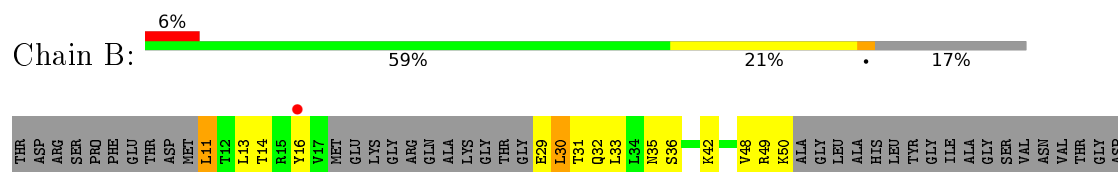
#### • Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

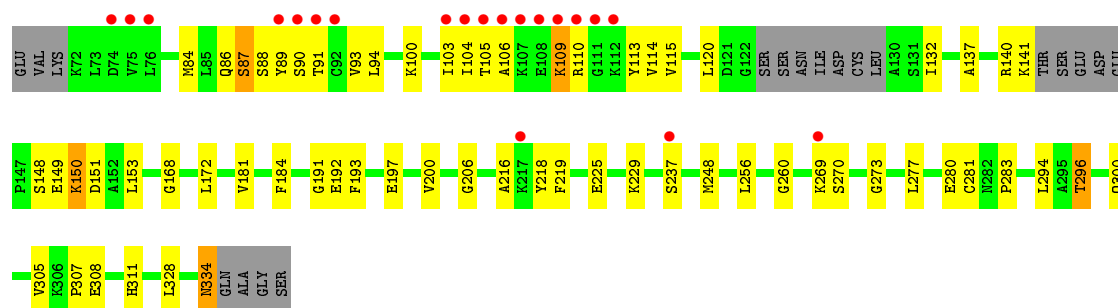


#### • Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

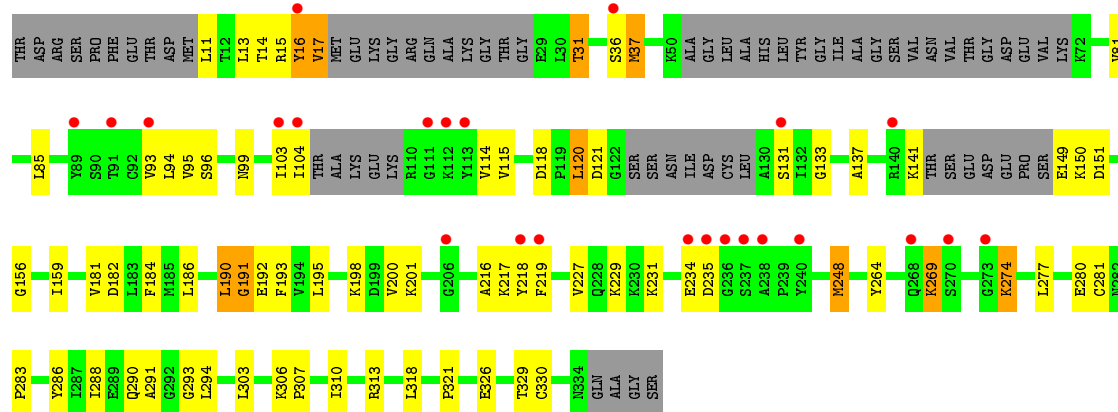


#### • Molecule 1: Fructose-1,6-bisphosphatase isozyme 2





- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.51Å 234.80Å 71.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.46 – 2.99 45.91 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.46-2.99) 99.5 (45.91-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.177 , 0.244 0.179 , 0.245	Depositor DCC
$R_{free}$ test set	999 reflections (2.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 71.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

### 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	0.77	0/2239	0.88	4/3027 (0.1%)
1	B	0.63	0/2185	0.77	0/2951
1	C	0.85	1/2164 (0.0%)	0.90	4/2923 (0.1%)
1	D	0.64	0/2131	0.82	0/2878
All	All	0.73	1/8719 (0.0%)	0.85	8/11779 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	CYS	CB-SG	-14.46	1.57	1.82

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	C	211	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	C	211	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	131	SER	N-CA-C	5.39	125.55	111.00
1	C	300	GLN	CA-CB-CG	5.21	124.85	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	GLU	Peptide
1	A	16	TYR	Peptide
1	B	300	GLN	Peptide
1	C	147	PRO	Peptide

## 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	2205	0	2257	45	0
1	B	2152	0	2216	64	0
1	C	2132	0	2191	50	0
1	D	2100	0	2158	52	0
All	All	8589	0	8822	199	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 11.

The worst 5 of 199 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:148:SER:OG	1:C:149:GLU:N	2.10	0.84
1:D:293:GLY:HA2	1:D:321:PRO:HD3	1.61	0.83
1:B:29:GLU:HB3	1:B:31:THR:HG22	1.61	0.82
1:B:137:ALA:HB2	1:B:283:PRO:HG3	1.64	0.78
1:D:274:LYS:O	1:D:313:ARG:HD3	1.87	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	279/338 (82%)	266 (95%)	11 (4%)	2 (1%)	26	68
1	B	270/338 (80%)	246 (91%)	21 (8%)	3 (1%)	17	57
1	C	266/338 (79%)	247 (93%)	18 (7%)	1 (0%)	39	79
1	D	261/338 (77%)	234 (90%)	21 (8%)	6 (2%)	8	35
All	All	1076/1352 (80%)	993 (92%)	71 (7%)	12 (1%)	17	57

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	D	150	LYS
1	D	190	LEU
1	D	235	ASP
1	B	87	SER

### 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	240/279 (86%)	231 (96%)	9 (4%)	40	77
1	B	234/279 (84%)	227 (97%)	7 (3%)	48	82
1	C	232/279 (83%)	217 (94%)	15 (6%)	21	57
1	D	228/279 (82%)	217 (95%)	11 (5%)	31	70
All	All	934/1116 (84%)	892 (96%)	42 (4%)	34	72

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	234	GLU
1	C	306	LYS

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Mol	Chain	Res	Type
1	D	234	GLU
1	C	237	SER
1	C	270	SER

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

Mol	Chain	Res	Type
1	C	32	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 carbohydrates 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 [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	287/338 (84%)	-0.08	10 (3%) 48 27	35, 58, 105, 171	0
1	B	280/338 (82%)	0.14	21 (7%) 17 8	52, 81, 120, 169	0
1	C	278/338 (82%)	-0.13	6 (2%) 65 42	31, 57, 105, 132	0
1	D	273/338 (80%)	0.20	24 (8%) 12 6	58, 86, 123, 149	0
All	All	1118/1352 (82%)	0.03	61 (5%) 29 15	31, 72, 116, 171	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	4.8
1	B	108	GLU	3.9
1	D	270	SER	3.9
1	A	16	TYR	3.8
1	B	105	THR	3.8

### 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.