Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:09 PM GMT

PDB ID	:	3T2F
Title	:	Fructose-1,6-bisphosphate aldolase/phosphatase from Thermoproteus neutrophilus, soaked with EDTA and DHAP
Authors	:	Du, J.; Say, R.; Lue, W.; Fuchs, G.; Einsle, O.
Deposited on	:	2011-07-22
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

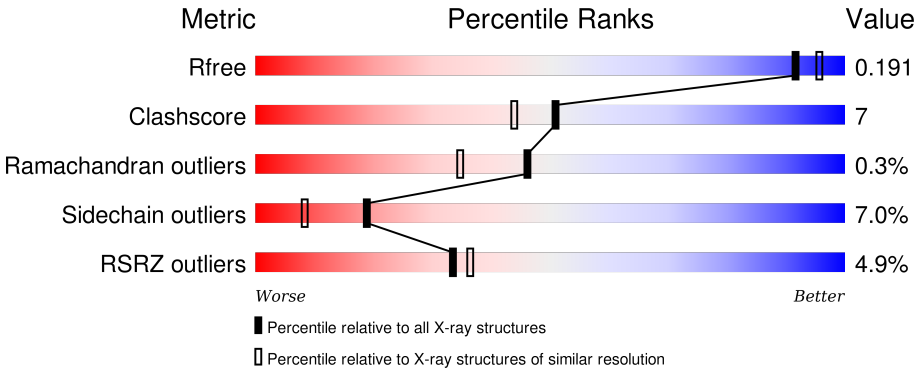
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	407	5% 77% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3223 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-bisphosphate aldolase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			3061	1973	525	550	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LEU	-	EXPRESSION TAG	UNP B1YAL1
A	401	GLU	-	EXPRESSION TAG	UNP B1YAL1
A	402	HIS	-	EXPRESSION TAG	UNP B1YAL1
A	403	HIS	-	EXPRESSION TAG	UNP B1YAL1
A	404	HIS	-	EXPRESSION TAG	UNP B1YAL1
A	405	HIS	-	EXPRESSION TAG	UNP B1YAL1
A	406	HIS	-	EXPRESSION TAG	UNP B1YAL1
A	407	HIS	-	EXPRESSION TAG	UNP B1YAL1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

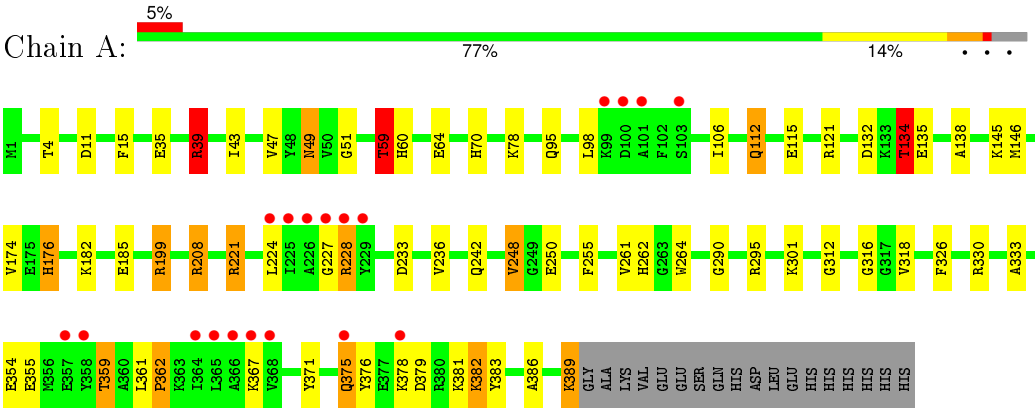
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		

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 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-bisphosphate aldolase/phosphatase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	112.30Å 112.30Å 151.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 1.90 47.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.66-1.90) 100.0 (47.66-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.151 , 0.191 0.151 , 0.191	Depositor DCC
R_{free} test set	1917 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.3	EDS
Estimated twinning fraction	0.016 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.025 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 38337 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3223	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.47	19/3141 (0.6%)	1.23	15/4252 (0.4%)

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	1	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	GLU	CB-CG	-8.58	1.35	1.52
1	A	295	ARG	CG-CD	6.80	1.69	1.51
1	A	248	VAL	CB-CG2	6.21	1.65	1.52
1	A	145	LYS	CE-NZ	6.18	1.64	1.49
1	A	47	VAL	CB-CG2	6.13	1.65	1.52
1	A	318	VAL	CB-CG2	5.96	1.65	1.52
1	A	236	VAL	CB-CG2	5.92	1.65	1.52
1	A	326	PHE	CD2-CE2	5.70	1.50	1.39
1	A	59	THR	CB-CG2	-5.68	1.33	1.52
1	A	255	PHE	CD2-CE2	5.58	1.50	1.39
1	A	333	ALA	CA-CB	5.58	1.64	1.52
1	A	326	PHE	CE2-CZ	5.54	1.47	1.37
1	A	35	GLU	CG-CD	5.49	1.60	1.51
1	A	316	GLY	N-CA	5.40	1.54	1.46
1	A	172	ASP	C-O	5.31	1.33	1.23
1	A	376	TYR	CD1-CE1	5.27	1.47	1.39
1	A	301	LYS	CD-CE	5.19	1.64	1.51
1	A	15	PHE	CE2-CZ	5.16	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	TRP	CE3-CZ3	5.12	1.47	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	A	199	ARG	NE-CZ-NH1	-13.45	113.57	120.30
1	A	341	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	208	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	A	11	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	A	233	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	121	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	A	330	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	199	ARG	CD-NE-CZ	5.73	131.62	123.60
1	A	134	THR	CB-CA-C	-5.53	96.68	111.60
1	A	59	THR	OG1-CB-CG2	5.49	122.61	110.00
1	A	208	ARG	CG-CD-NE	-5.40	100.47	111.80
1	A	39	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	185	GLU	CB-CA-C	-5.08	100.24	110.40
1	A	59	THR	CA-CB-CG2	5.01	119.41	112.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	59	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	GLY	Peptide

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	3061	0	3064	42	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	161	0	0	2	0
All	All	3223	0	3064	42	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 7.

All (42) 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:A:389:LYS:HD3	1:A:389:LYS:O	1.45	1.16
1:A:59:THR:HG21	1:A:312:GLY:O	1.60	1.00
1:A:389:LYS:O	1:A:389:LYS:CD	2.26	0.82
1:A:386:ALA:O	1:A:389:LYS:HD2	1.82	0.79
1:A:146:MET:O	1:A:153:THR:HG21	1.85	0.75
1:A:379:ASP:HA	1:A:382:LYS:HE2	1.69	0.74
1:A:59:THR:CG2	1:A:312:GLY:O	2.37	0.68
1:A:70:HIS:HD2	1:A:106:ILE:H	1.42	0.66
1:A:153:THR:HB	1:A:250:GLU:HB3	1.80	0.64
1:A:112:GLN:HE21	1:A:112:GLN:HA	1.62	0.64
1:A:172:ASP:OD1	1:A:199:ARG:HD2	1.98	0.62
1:A:134:THR:HG21	1:A:138:ALA:HB2	1.83	0.60
1:A:242:GLN:NE2	1:A:248:VAL:H	2.00	0.58
1:A:134:THR:HG22	1:A:135:GLU:H	1.70	0.55
1:A:70:HIS:CD2	1:A:106:ILE:H	2.23	0.55
1:A:379:ASP:HA	1:A:382:LYS:CE	2.36	0.54
1:A:64:GLU:OE1	3:A:541:HOH:O	2.18	0.53
1:A:221:ARG:HH21	1:A:221:ARG:HB3	1.73	0.53
1:A:49:ASN:ND2	1:A:290:GLY:H	2.06	0.52
1:A:367:LYS:O	1:A:367:LYS:HG2	2.09	0.51
1:A:134:THR:HG22	1:A:262:HIS:O	2.11	0.50
1:A:379:ASP:HB2	1:A:383:TYR:CE2	2.46	0.50
1:A:98:LEU:HD21	1:A:228:ARG:NH2	2.27	0.50
1:A:221:ARG:HD2	3:A:519:HOH:O	2.13	0.48
1:A:221:ARG:NH2	1:A:221:ARG:HB3	2.30	0.47
1:A:174:VAL:CG2	1:A:199:ARG:HD3	2.46	0.46
1:A:352:PRO:HB2	1:A:355:GLU:HG3	1.97	0.46
1:A:389:LYS:O	1:A:389:LYS:CG	2.64	0.46
1:A:371:TYR:CE1	1:A:383:TYR:CE1	3.04	0.45
1:A:49:ASN:O	1:A:290:GLY:HA3	2.16	0.45
1:A:134:THR:HG21	1:A:261:VAL:HB	2.00	0.43
1:A:51:GLY:HA3	1:A:132:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:CG2	1:A:262:HIS:O	2.66	0.43
1:A:361:LEU:HB3	1:A:362:PRO:CD	2.49	0.43
1:A:359:THR:HG23	1:A:362:PRO:HD2	2.00	0.43
1:A:176:HIS:NE2	1:A:221:ARG:HG3	2.35	0.42
1:A:39:ARG:HD3	1:A:39:ARG:N	2.34	0.42
1:A:382:LYS:HZ3	1:A:382:LYS:H	1.67	0.42
1:A:4:THR:HB	1:A:60:HIS:CE1	2.55	0.41
1:A:43:ILE:HB	1:A:59:THR:HG23	2.01	0.41
1:A:375:GLN:HB2	1:A:375:GLN:HE21	1.69	0.41
1:A:146:MET:O	1:A:153:THR:CG2	2.63	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	388/407 (95%)	373 (96%)	14 (4%)	1 (0%)	46 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	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	316/331 (96%)	294 (93%)	22 (7%)	19 8

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	49	ASN
1	A	59	THR
1	A	78	LYS
1	A	95	GLN
1	A	112	GLN
1	A	115	GLU
1	A	134	THR
1	A	153	THR
1	A	176	HIS
1	A	182	LYS
1	A	208	ARG
1	A	221	ARG
1	A	224	LEU
1	A	228	ARG
1	A	354	GLU
1	A	359	THR
1	A	375	GLN
1	A	378	LYS
1	A	381	LYS
1	A	382	LYS
1	A	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	70	HIS
1	A	112	GLN
1	A	242	GLN

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	389/407 (95%)	-0.18	19 (4%) 33 36	13, 23, 56, 75	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ASP	5.5
1	A	224	LEU	4.8
1	A	225	ILE	4.7
1	A	229	TYR	4.7
1	A	227	GLY	4.6
1	A	101	ALA	4.6
1	A	226	ALA	4.0
1	A	358	TYR	3.2
1	A	103	SER	3.2
1	A	366	ALA	3.2
1	A	228	ARG	2.7
1	A	375	GLN	2.6
1	A	99	LYS	2.5
1	A	365	LEU	2.4
1	A	378	LYS	2.4
1	A	364	ILE	2.3
1	A	368	VAL	2.3
1	A	367	LYS	2.2
1	A	357	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	408	1/1	0.99	0.04	-2.52	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.