



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 08:36 PM GMT

PDB ID : 2PC4
Title : Crystal structure of fructose-bisphosphatealdolase from Plasmodium falciparum in complex with TRAP-tail determined at 2.4 angstrom resolution
Authors : Bosch, J.; Buscaglia, C.A.; Krumm, B.; Cardozo, T.; Nussenzweig, V.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2007-03-29
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

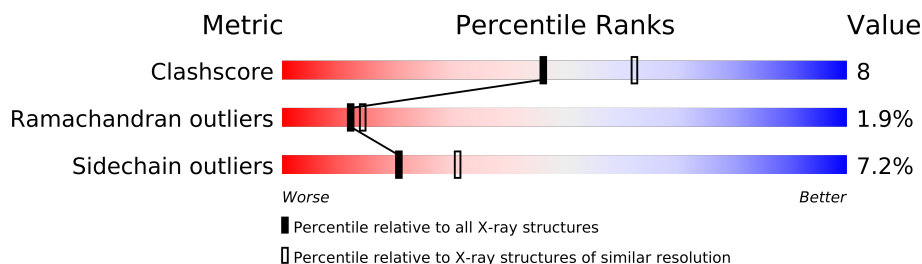
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	369	
1	B	369	
1	C	369	
1	D	369	
2	H	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11457 atoms, of which 0 are hydrogen and 0 are deuterium.

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-bisphosphatealdolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2749	1741	476	522	10			
1	B	351	Total	C	N	O	S	0	2	0
			2688	1702	466	510	10			
1	C	365	Total	C	N	O	S	0	1	0
			2781	1757	484	530	10			
1	D	351	Total	C	N	O	S	0	2	0
			2689	1702	467	510	10			

- Molecule 2 is a protein called PbTRAP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	3	Total	C	N	O	0	0	0
			31	19	5	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	131	Total	O	0	0
			131	131		
3	C	134	Total	O	0	0
			134	134		
3	D	125	Total	O	0	0
			125	125		
3	H	2	Total	O	0	0
			2	2		

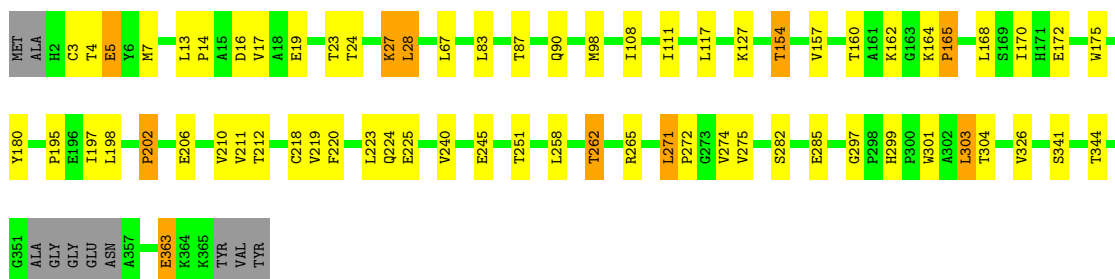
3 Residue-property plots

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.

Note EDS failed to run properly.

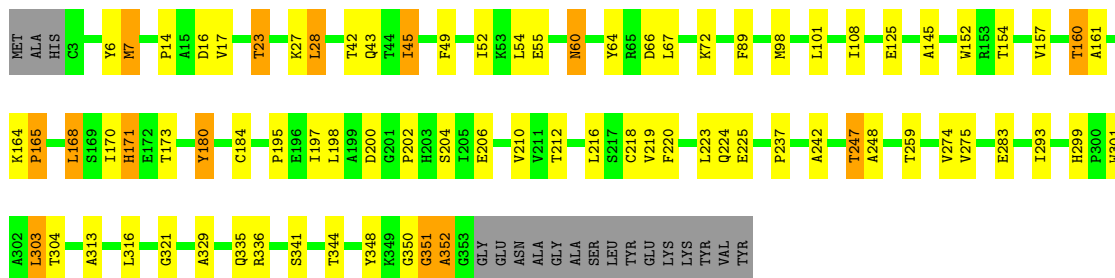
- Molecule 1: Fructose-bisphosphatealdolase

Chain A:



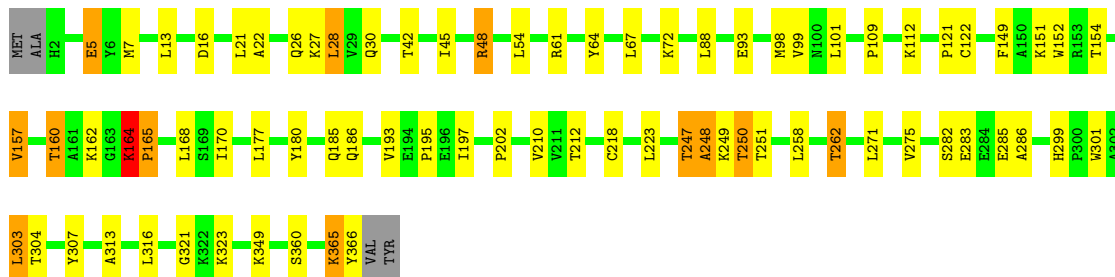
- Molecule 1: Fructose-bisphosphatealdolase

Chain B:



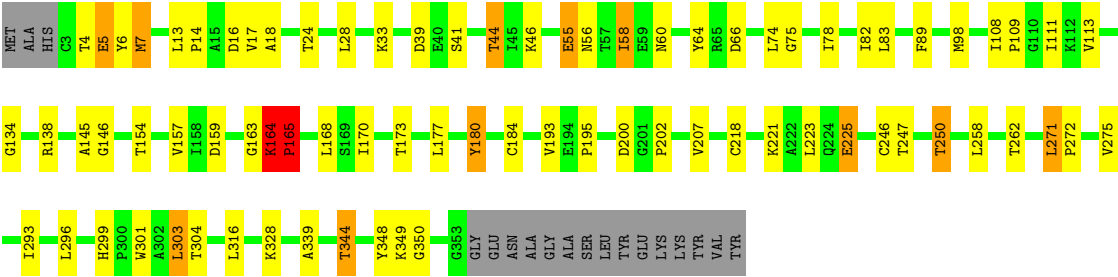
- Molecule 1: Fructose-bisphosphatealdolase

Chain C:



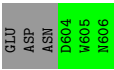
- Molecule 1: Fructose-bisphosphatealdolase

Chain D: 



- Molecule 2: PbTRAP

Chain H: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.39Å 145.52Å 148.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.40	Depositor
% Data completeness (in resolution range)	94.7 (19.97-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.250	Depositor
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.750	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 62422 reflections (0.005%)	Xtriage
Total number of atoms	11457	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.43	0/2798	0.55	0/3788
1	B	0.42	0/2740	0.58	0/3713
1	C	0.42	0/2831	0.57	0/3837
1	D	0.42	0/2740	0.56	0/3712
2	H	0.45	0/32	0.45	0/42
All	All	0.42	0/11141	0.56	0/15092

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	3
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	LYS	Peptide
1	A	297	GLY	Peptide
1	A	363	GLU	Peptide
1	B	164	LYS	Peptide
1	C	164	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2749	0	2805	43	0
1	B	2688	0	2744	56	0
1	C	2781	0	2811	42	0
1	D	2689	0	2750	52	0
2	H	31	0	19	0	0
3	A	127	0	0	3	0
3	B	131	0	0	6	0
3	C	134	0	0	6	0
3	D	125	0	0	3	0
3	H	2	0	0	0	0
All	All	11457	0	11129	180	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 180 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:SER:HA	1:B:247:THR:HG21	1.26	1.10
1:D:157:VAL:O	1:D:165:PRO:HD3	1.51	1.10
1:C:258:LEU:O	1:C:262:THR:HG23	1.54	1.08
1:A:258:LEU:O	1:A:262:THR:HG23	1.66	0.95
1:B:157:VAL:O	1:B:165:PRO:CD	2.17	0.92

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	356/369 (96%)	334 (94%)	18 (5%)	4 (1%)	21	29
1	B	351/369 (95%)	326 (93%)	17 (5%)	8 (2%)	10	10
1	C	364/369 (99%)	336 (92%)	22 (6%)	6 (2%)	14	18
1	D	351/369 (95%)	326 (93%)	16 (5%)	9 (3%)	8	8
2	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1423/1482 (96%)	1323 (93%)	73 (5%)	27 (2%)	12	14

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	B	165	PRO
1	B	247	THR
1	B	352	ALA
1	C	247	THR

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	293/298 (98%)	273 (93%)	20 (7%)	22	34
1	B	287/298 (96%)	267 (93%)	20 (7%)	21	33
1	C	293/298 (98%)	268 (92%)	25 (8%)	15	23
1	D	287/298 (96%)	268 (93%)	19 (7%)	24	35
2	H	3/6 (50%)	3 (100%)	0	100	100
All	All	1163/1198 (97%)	1079 (93%)	84 (7%)	21	31

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	303	LEU
1	C	109	PRO
1	D	225	GLU
1	B	336	ARG
1	C	16	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	312	GLN
1	D	56	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.