



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2018 – 03:12 PM EDT

PDB ID : 1A5C
Title : FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE FROM PLASMODIUM FALCIPARUM
Authors : Kim, H.; Certa, U.; Dobeli, H.; Jakob, P.; Hol, W.G.J.
Deposited on : 1998-02-13
Resolution : 3.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

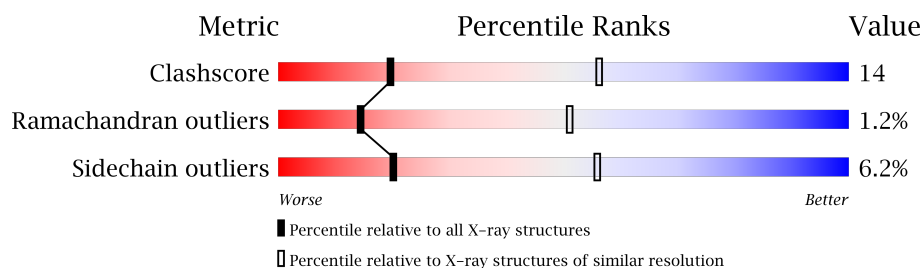
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5204 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2602	1647	452	495	8			
1	B	342	Total	C	N	O	S	0	0	0
			2602	1647	452	495	8			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.20 Å 119.20 Å 132.30 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.0 (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.239 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5204	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	0.39	0/2645	0.65	0/3585
1	B	0.37	0/2645	0.63	0/3585
All	All	0.38	0/5290	0.64	0/7170

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	2602	0	2655	73	0
1	B	2602	0	2655	74	0
All	All	5204	0	5310	144	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 14.

All (144) 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:14:PRO:HB2	1:A:17:VAL:HG12	1.61	0.82
1:B:14:PRO:HB2	1:B:17:VAL:HG12	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:H	1:A:58:ILE:HD12	1.47	0.80
1:A:341:SER:O	1:A:344:THR:HB	1.82	0.79
1:A:205:ILE:HG12	1:A:258:LEU:HD23	1.70	0.74
1:B:215:VAL:O	1:B:219:VAL:HG23	1.90	0.71
1:A:117:LEU:HD13	1:A:127:LYS:HG2	1.72	0.70
1:A:323:LYS:HA	1:A:326:VAL:HG23	1.74	0.68
1:A:87:THR:HA	1:A:90:GLN:HG2	1.76	0.68
1:B:54:LEU:HD22	1:B:60:ASN:ND2	2.09	0.66
1:B:211:VAL:O	1:B:215:VAL:HG23	1.96	0.65
1:B:341:SER:O	1:B:344:THR:HB	1.97	0.65
1:A:138:ARG:HB3	1:A:142:TYR:CE2	2.33	0.63
1:A:64:TYR:CZ	1:A:316:LEU:HD13	2.33	0.63
1:B:275:VAL:HB	1:B:306:SER:HB2	1.79	0.62
1:B:58:ILE:H	1:B:58:ILE:HD12	1.64	0.62
1:A:260:VAL:O	1:A:264:ARG:HG3	2.00	0.62
1:A:275:VAL:HB	1:A:306:SER:HB2	1.80	0.62
1:A:43:GLN:O	1:A:46:LYS:HB3	2.00	0.62
1:A:27:LYS:HE3	1:A:108:ILE:HD11	1.83	0.60
1:A:54:LEU:HD22	1:A:60:ASN:ND2	2.15	0.60
1:A:186:GLN:HG3	1:B:121:PRO:HB3	1.83	0.60
1:B:64:TYR:CZ	1:B:316:LEU:HD13	2.38	0.58
1:B:332:VAL:O	1:B:335:GLN:HB3	2.05	0.57
1:B:275:VAL:O	1:B:275:VAL:HG23	2.05	0.57
1:A:121:PRO:O	1:A:122:CYS:HB2	2.04	0.57
1:A:200:ASP:HA	1:A:244:TYR:HD2	1.68	0.56
1:B:260:VAL:O	1:B:264:ARG:HG3	2.07	0.55
1:A:52:ILE:HG21	1:A:316:LEU:O	2.06	0.55
1:B:118:VAL:HG23	1:B:128:SER:HB3	1.86	0.55
1:B:118:VAL:HG22	1:B:128:SER:O	2.07	0.55
1:B:87:THR:HA	1:B:90:GLN:HG2	1.87	0.55
1:B:205:ILE:HG12	1:B:258:LEU:HD23	1.90	0.54
1:B:181:ALA:O	1:B:185:GLN:HG3	2.07	0.54
1:B:29:VAL:HG12	1:B:304:THR:HG21	1.88	0.54
1:B:134:GLY:O	1:B:136:ALA:N	2.41	0.54
1:A:219:VAL:O	1:A:223:LEU:HD13	2.09	0.53
1:A:274:VAL:HB	1:A:303:LEU:HD12	1.91	0.53
1:A:180:TYR:CE1	1:A:184:CYS:SG	3.02	0.52
1:A:305:PHE:HB2	1:A:307:TYR:CD1	2.43	0.52
1:A:256:GLY:HA2	1:A:293:ILE:HG12	1.90	0.52
1:A:151:LYS:HE2	1:A:194:GLU:OE1	2.09	0.52
1:B:293:ILE:CG2	1:B:303:LEU:HD23	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:O	1:A:275:VAL:HG23	2.10	0.52
1:B:24:THR:O	1:B:28:LEU:HB2	2.09	0.52
1:A:307:TYR:O	1:A:311:LEU:HD12	2.10	0.52
1:A:288:VAL:O	1:A:291:ASN:HB3	2.11	0.51
1:A:286:ALA:HB1	1:A:307:TYR:CE2	2.44	0.51
1:B:314:SER:HB3	1:B:332:VAL:HG11	1.93	0.51
1:A:17:VAL:HG23	1:A:188:ARG:HD2	1.93	0.50
1:B:290:LEU:HD22	1:B:305:PHE:HB3	1.93	0.50
1:A:154:THR:OG1	1:A:195:PRO:HA	2.11	0.50
1:A:207:VAL:O	1:A:211:VAL:HG23	2.12	0.50
1:B:240:VAL:HG11	1:B:258:LEU:HB3	1.94	0.50
1:B:43:GLN:O	1:B:46:LYS:HB3	2.12	0.50
1:B:121:PRO:O	1:B:122:CYS:HB2	2.12	0.49
1:A:58:ILE:H	1:A:58:ILE:CD1	2.20	0.49
1:A:82:ILE:HG12	1:A:149:PHE:HE2	1.76	0.49
1:B:119:ASN:OD1	1:B:127:LYS:HE2	2.12	0.49
1:B:34:GLY:HA3	1:B:305:PHE:CZ	2.47	0.49
1:A:336:ARG:HA	1:A:336:ARG:HE	1.78	0.49
1:A:92:ASN:HD21	1:A:96:VAL:HB	1.77	0.49
1:B:36:LEU:O	1:B:81:ALA:HA	2.12	0.49
1:B:109:PRO:HB2	1:B:146:GLY:O	2.12	0.49
1:A:282:SER:OG	1:A:285:GLU:HB2	2.13	0.49
1:A:58:ILE:N	1:A:58:ILE:HD12	2.22	0.49
1:B:64:TYR:CE1	1:B:316:LEU:HD13	2.48	0.48
1:A:39:ASP:HB3	1:A:82:ILE:HG22	1.96	0.48
1:A:47:LYS:HE3	1:A:48:ARG:HH12	1.78	0.48
1:A:179:ARG:HH12	1:B:121:PRO:HD3	1.79	0.48
1:A:41:SER:O	1:A:45:ILE:HG22	2.14	0.47
1:B:52:ILE:HG13	1:B:54:LEU:HB2	1.96	0.47
1:B:82:ILE:HD13	1:B:151:LYS:HD2	1.96	0.47
1:B:58:ILE:N	1:B:58:ILE:HD12	2.28	0.47
1:A:300:PRO:HG2	1:A:301:TRP:CE2	2.50	0.47
1:A:69:PHE:N	1:A:69:PHE:CD1	2.82	0.47
1:A:166:THR:O	1:A:170:ILE:HG13	2.15	0.47
1:A:230:LEU:HD22	1:A:271:LEU:HD23	1.96	0.47
1:A:156:LEU:HD11	1:A:173:THR:HG21	1.97	0.46
1:A:83:LEU:O	1:A:111:ILE:HD12	2.15	0.46
1:A:92:ASN:ND2	1:A:96:VAL:HB	2.30	0.46
1:B:64:TYR:OH	1:B:312:GLN:HB3	2.15	0.46
1:B:69:PHE:CD1	1:B:69:PHE:N	2.83	0.46
1:A:239:MET:HE2	1:A:293:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HD13	1:B:108:ILE:HD12	1.98	0.45
1:A:215:VAL:O	1:A:219:VAL:HG23	2.16	0.45
1:A:91:LYS:HA	1:A:97:PRO:HA	1.97	0.45
1:A:28:LEU:HG	1:A:35:ILE:HD11	1.99	0.45
1:B:148:ARG:HD3	1:B:148:ARG:HA	1.73	0.45
1:B:58:ILE:HG13	1:B:61:ARG:HH22	1.81	0.45
1:B:117:LEU:HB3	1:B:127:LYS:HG2	1.98	0.45
1:B:323:LYS:HB2	1:B:323:LYS:HE2	1.74	0.45
1:B:14:PRO:HD2	1:B:17:VAL:HG11	2.00	0.44
1:B:323:LYS:HA	1:B:326:VAL:HG23	1.98	0.44
1:A:194:GLU:HG2	1:A:194:GLU:O	2.16	0.44
1:B:283:GLU:HG2	1:B:310:ALA:HA	1.98	0.44
1:A:82:ILE:HG12	1:A:149:PHE:CE2	2.52	0.44
1:A:118:VAL:O	1:A:127:LYS:HA	2.17	0.44
1:B:82:ILE:HG21	1:B:151:LYS:HD3	1.99	0.44
1:A:284:GLU:OE1	1:A:284:GLU:HA	2.18	0.43
1:B:220:PHE:CE2	1:B:267:VAL:HG22	2.53	0.43
1:A:291:ASN:ND2	1:A:348:TYR:H	2.16	0.43
1:A:35:ILE:HG23	1:A:80:GLY:O	2.17	0.43
1:B:256:GLY:O	1:B:260:VAL:HG23	2.18	0.43
1:B:249:LYS:HA	1:B:249:LYS:NZ	2.34	0.43
1:B:156:LEU:HD11	1:B:173:THR:HG21	1.99	0.43
1:A:115:LYS:HE3	1:A:131:GLY:HA2	2.00	0.43
1:B:339:ALA:HB1	1:B:348:TYR:CE1	2.54	0.43
1:B:184:CYS:HB3	1:B:189:LEU:O	2.18	0.43
1:A:83:LEU:HD11	1:A:102:LEU:HD11	2.01	0.42
1:B:92:ASN:ND2	1:B:96:VAL:HB	2.34	0.42
1:B:197:ILE:HD11	1:B:215:VAL:HG21	1.99	0.42
1:A:17:VAL:O	1:A:21:LEU:HG	2.19	0.42
1:A:55:GLU:O	1:A:60:ASN:ND2	2.52	0.42
1:B:46:LYS:HB2	1:B:56:ASN:ND2	2.34	0.42
1:B:198:LEU:HB3	1:B:200:ASP:OD2	2.19	0.42
1:B:300:PRO:HG2	1:B:301:TRP:CD2	2.54	0.42
1:B:92:ASN:HD21	1:B:96:VAL:HB	1.84	0.42
1:A:33:LYS:HG2	1:A:76:LYS:O	2.20	0.42
1:B:118:VAL:HG21	1:B:130:GLN:NE2	2.35	0.42
1:A:260:VAL:HG21	1:A:296:LEU:HD12	2.03	0.41
1:B:151:LYS:HE2	1:B:194:GLU:OE1	2.20	0.41
1:A:75:GLY:HA3	1:A:105:GLU:O	2.21	0.41
1:A:211:VAL:O	1:A:215:VAL:HG23	2.20	0.41
1:B:41:SER:HA	1:B:84:PHE:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:O	1:B:281:GLN:HG3	2.21	0.41
1:B:99:VAL:HA	1:B:102:LEU:HD12	2.02	0.41
1:B:336:ARG:HE	1:B:336:ARG:HA	1.86	0.41
1:B:44:THR:HA	1:B:47:LYS:HE2	2.01	0.41
1:A:332:VAL:O	1:A:335:GLN:HB3	2.21	0.41
1:A:35:ILE:O	1:A:306:SER:HA	2.21	0.41
1:B:54:LEU:HD22	1:B:60:ASN:HD21	1.81	0.41
1:A:133:ASP:HB2	1:B:133:ASP:OD2	2.21	0.40
1:A:138:ARG:O	1:A:141:GLU:HB3	2.21	0.40
1:A:291:ASN:HD22	1:A:343:ALA:HA	1.85	0.40
1:B:108:ILE:HA	1:B:109:PRO:HD3	1.82	0.40
1:B:244:TYR:OH	1:B:280:GLY:HA3	2.20	0.40
1:B:322:LYS:NZ	1:B:322:LYS:HB3	2.35	0.40
1:B:246:CYS:SG	1:B:248:ALA:HB3	2.61	0.40
1:B:300:PRO:HG2	1:B:301:TRP:CE2	2.56	0.40
1:A:108:ILE:HA	1:A:109:PRO:HD3	1.94	0.40
1:A:47:LYS:HE3	1:A:48:ARG:NH1	2.36	0.40
1:B:127:LYS:HD2	1:B:127:LYS:N	2.36	0.40
1:B:249:LYS:HZ2	1:B:249:LYS:HA	1.86	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	340/368 (92%)	303 (89%)	34 (10%)	3 (1%)	19	59
1	B	340/368 (92%)	296 (87%)	39 (12%)	5 (2%)	11	45
All	All	680/736 (92%)	599 (88%)	73 (11%)	8 (1%)	14	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	LEU
1	A	297	GLY
1	B	71	THR
1	B	351	GLY
1	A	351	GLY
1	B	188	ARG
1	A	195	PRO
1	B	308	GLY

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	276/297 (93%)	257 (93%)	19 (7%)	17	51
1	B	276/297 (93%)	261 (95%)	15 (5%)	24	62
All	All	552/594 (93%)	518 (94%)	34 (6%)	20	56

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	42	THR
1	A	54	LEU
1	A	114	ASP
1	A	127	LYS
1	A	160	THR
1	A	168	LEU
1	A	180	TYR
1	A	206	GLU
1	A	218	CYS
1	A	224	GLN
1	A	252	THR
1	A	258	LEU
1	A	265	ARG
1	A	271	LEU
1	A	301	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	303	LEU
1	A	323	LYS
1	A	336	ARG
1	B	19	GLU
1	B	54	LEU
1	B	127	LYS
1	B	137	GLU
1	B	168	LEU
1	B	180	TYR
1	B	188	ARG
1	B	206	GLU
1	B	224	GLN
1	B	237	PRO
1	B	258	LEU
1	B	265	ARG
1	B	301	TRP
1	B	323	LYS
1	B	336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	103	HIS
1	A	203	HIS
1	A	213	GLN
1	A	253	GLN
1	A	291	ASN
1	A	320	GLN
1	B	60	ASN
1	B	203	HIS
1	B	213	GLN
1	B	224	GLN
1	B	253	GLN
1	B	291	ASN
1	B	320	GLN

5.3.3 RNA ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.