wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 03:28 AM EDT

PDB ID	:	2YW3
Title	:	Crystal Structure Analysis of the 4-hydroxy-2-oxoglutarate aldolase/2-deydro -3-deoxyphosphogluconate aldolase from TTHB1
Authors	:	Kawano, Y.; Hashimoto, K.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-04-19
Resolution	:	1.67 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

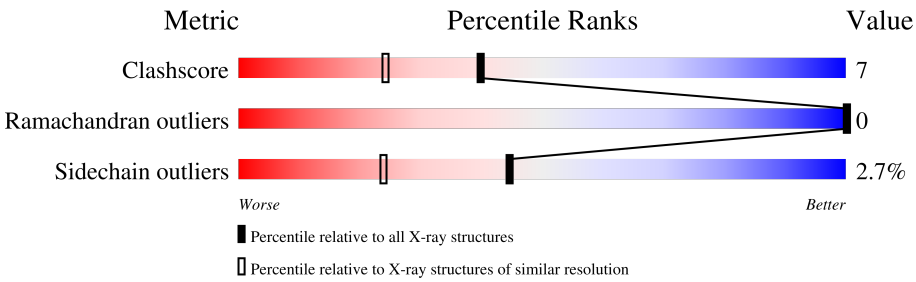
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.67 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	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	207	84% 10% 6%
1	B	207	86% 8% 5%
1	C	207	88% 6% • 5%
1	D	207	82% 12% • •
1	E	207	82% 14% • •
1	F	207	83% 12% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	2006	-	-	X	-
2	PO4	D	2012	-	-	X	-
2	PO4	E	2014	-	-	X	-
2	PO4	F	2008	-	X	-	-

2 Entry composition (i)

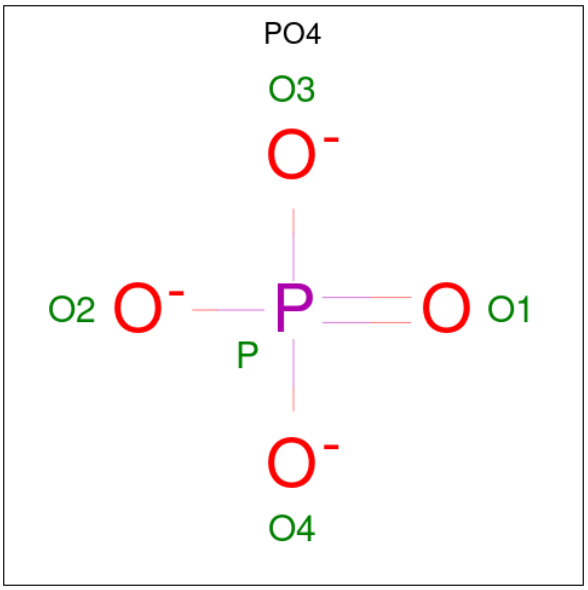
There are 3 unique types of molecules in this entry. The entry contains 10084 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphog luconate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O				
1	A	195	1465	948	256	261		0	3	0
			Total	C	N	O				
1	B	197	1480	958	258	264		0	3	0
			Total	C	N	O				
1	C	197	1488	964	257	267		0	4	0
			Total	C	N	O	S			
1	D	199	1529	996	259	273	1	0	10	0
			Total	C	N	O	S			
1	E	200	1509	980	260	268	1	0	5	0
			Total	C	N	O	S			
1	F	199	1506	978	259	268	1	0	5	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	4	3	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	132	132	132	0	0
3	B	132	132	132	0	0
3	C	130	130	130	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	220	220	220	0	0
			Total	O		
3	E	198	198	198	0	0
			Total	O		
3	F	211	211	211	0	0

3 Residue-property plots (i)

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

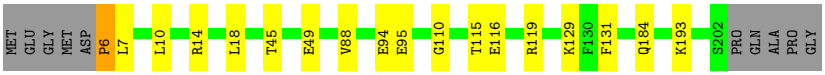
Note EDS was not executed.

• Molecule 1: 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphogluconate aldolase

Chain A:

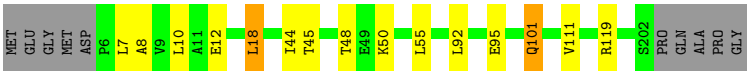
• Molecule 1: 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphogluconate aldolase

Chain B:



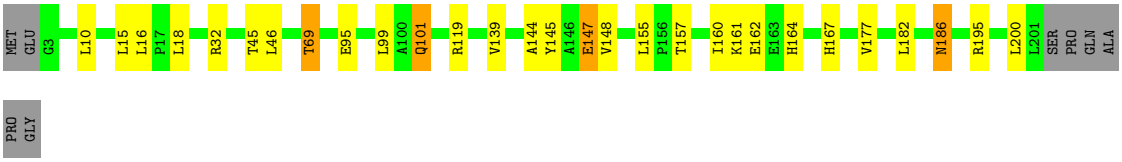
• Molecule 1: 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphogluconate aldolase

Chain C:



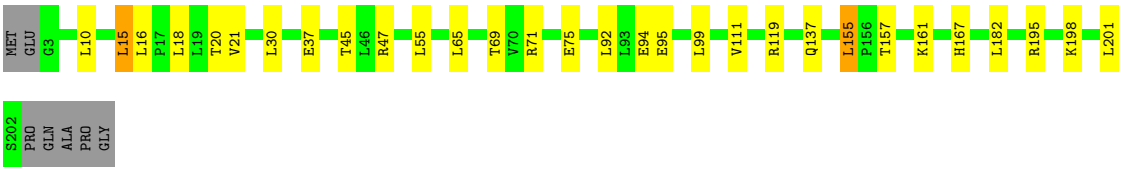
• Molecule 1: 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphogluconate aldolase

Chain D:



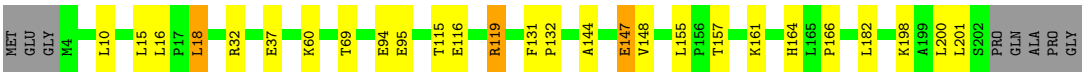
• Molecule 1: 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphogluconate aldolase

Chain E:



• Molecule 1: 4-hydroxy-2-oxoglutarate aldolase/2-deydro-3-deoxyphosphogluconate aldolase

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.92Å 72.69Å 161.31Å 90.00° 91.07° 90.00°	Depositor
Resolution (Å)	35.58 – 1.67	Depositor
% Data completeness (in resolution range)	100.0 (35.58-1.67)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10084	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.60	0/1498	0.65	0/2033
1	B	0.60	0/1513	0.65	1/2053 (0.0%)
1	C	0.62	0/1525	0.64	0/2070
1	D	0.74	0/1584	0.80	1/2153 (0.0%)
1	E	0.73	0/1549	0.78	2/2104 (0.1%)
1	F	0.72	0/1546	0.75	0/2100
All	All	0.67	0/9215	0.72	4/12513 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	6	PRO	N-CA-CB	5.67	110.10	103.30
1	D	32	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	15[A]	LEU	CA-CB-CG	5.28	127.45	115.30
1	E	15[B]	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1465	0	1560	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1480	0	1572	18	0
1	C	1488	0	1585	13	0
1	D	1529	0	1646	38	0
1	E	1509	0	1614	34	0
1	F	1506	0	1613	23	0
2	A	5	0	0	0	0
2	B	15	0	0	2	0
2	C	5	0	0	0	0
2	D	20	0	0	3	0
2	E	20	0	0	4	0
2	F	19	0	0	1	0
3	A	132	0	0	4	0
3	B	132	0	0	8	0
3	C	130	0	0	2	0
3	D	220	0	0	10	1
3	E	198	0	0	4	1
3	F	211	0	0	8	0
All	All	10084	0	9590	136	1

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.

The worst 5 of 136 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:E:15[B]:LEU:HD21	1:E:201:LEU:CD1	1.41	1.46
1:E:15[B]:LEU:CD2	1:E:201:LEU:CD1	2.15	1.25
1:F:18[B]:LEU:HD21	3:F:2098:HOH:O	1.06	1.21
1:D:46:LEU:H	1:D:69:THR:CG2	1.66	1.06
1:A:118:GLU:HG3	3:B:2088:HOH:O	1.57	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2230:HOH:O	3:E:2209:HOH:O[3_555]	1.83	0.37

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	196/207 (95%)	192 (98%)	4 (2%)	0	100	100
1	B	198/207 (96%)	193 (98%)	5 (2%)	0	100	100
1	C	199/207 (96%)	194 (98%)	5 (2%)	0	100	100
1	D	207/207 (100%)	205 (99%)	2 (1%)	0	100	100
1	E	203/207 (98%)	199 (98%)	4 (2%)	0	100	100
1	F	202/207 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	1205/1242 (97%)	1182 (98%)	23 (2%)	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	146/153 (95%)	144 (99%)	2 (1%)	67	51
1	B	147/153 (96%)	144 (98%)	3 (2%)	55	36
1	C	150/153 (98%)	148 (99%)	2 (1%)	69	54
1	D	157/153 (103%)	151 (96%)	6 (4%)	33	12
1	E	152/153 (99%)	147 (97%)	5 (3%)	38	16
1	F	153/153 (100%)	144 (94%)	9 (6%)	19	5
All	All	905/918 (99%)	878 (97%)	27 (3%)	44	20

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	69	THR
1	E	155	LEU
1	F	147	GLU
1	E	137	GLN
1	F	18[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	137	GLN
1	E	184	GLN
1	F	184	GLN
1	F	164	HIS
1	D	164	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	D	2002	-	4,4,4	0.76	0	6,6,6	0.60	0
2	PO4	F	1169	1	0,3,4	-	-	0,3,6	-	-
2	PO4	F	2009	-	4,4,4	0.93	0	6,6,6	1.40	1 (16%)
2	PO4	F	2007	-	4,4,4	0.73	0	6,6,6	0.46	0
2	PO4	E	2014	-	4,4,4	0.78	0	6,6,6	0.88	0
2	PO4	B	2015	-	4,4,4	1.02	0	6,6,6	0.47	0
2	PO4	C	2016	-	4,4,4	0.88	0	6,6,6	0.97	1 (16%)
2	PO4	B	2003	-	4,4,4	1.12	0	6,6,6	1.00	1 (16%)
2	PO4	D	2001	-	4,4,4	0.93	0	6,6,6	0.91	0
2	PO4	F	2008	-	4,4,4	0.34	0	6,6,6	2.27	4 (66%)
2	PO4	D	2011	-	4,4,4	1.13	0	6,6,6	0.35	0
2	PO4	E	2010	-	4,4,4	0.95	0	6,6,6	1.20	0
2	PO4	A	2005	-	4,4,4	1.50	0	6,6,6	1.18	0
2	PO4	E	2004	-	4,4,4	0.75	0	6,6,6	0.64	0
2	PO4	E	2013	-	4,4,4	0.93	0	6,6,6	0.77	0
2	PO4	B	2006	-	4,4,4	1.05	0	6,6,6	1.73	1 (16%)
2	PO4	D	2012	-	4,4,4	0.93	0	6,6,6	0.93	0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2008	PO4	O4-P-O3	3.03	117.69	107.97
2	F	2008	PO4	O4-P-O2	-2.89	98.69	107.97
2	F	2009	PO4	O4-P-O3	2.56	116.18	107.97
2	F	2008	PO4	O2-P-O1	-2.25	102.67	110.89
2	B	2003	PO4	O4-P-O2	2.17	114.94	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1169	PO4	1	0
2	E	2014	PO4	3	0
2	E	2010	PO4	1	0
2	E	2004	PO4	1	0
2	B	2006	PO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2012	PO4	3	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.