



Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 01:59 AM GMT

PDB ID : 2AFB
Title : Crystal structure of 2-dehydro-3- deoxygluconokinase (EC 2.7.1.45) (tm0067)
from THERMOTOGA MARITIMA at 2.05 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-07-25
Resolution : 2.05 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

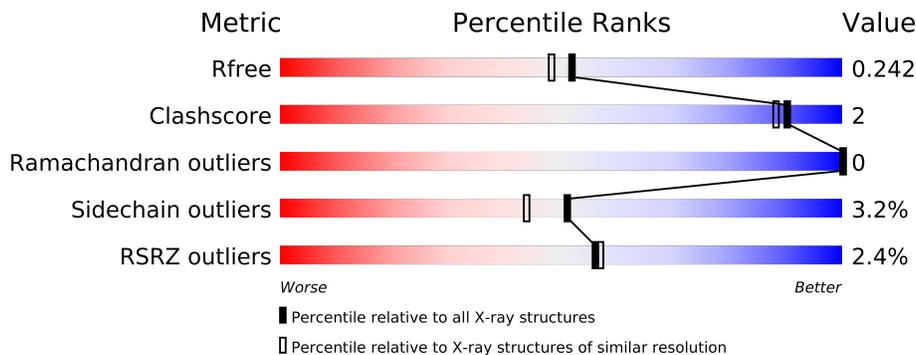
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.05 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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	B	344	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5444 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 2-keto-3-deoxygluconatekinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	329	2543	1633	434	467	2	7	0	0	0
1	B	326	2497	1604	423	461	2	7	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	MODIFIED RESIDUE	GB 15642842
A	-10	GLY	-	LEADER SEQUENCE	GB 15642842
A	-9	SER	-	LEADER SEQUENCE	GB 15642842
A	-8	ASP	-	LEADER SEQUENCE	GB 15642842
A	-7	LYS	-	LEADER SEQUENCE	GB 15642842
A	-6	ILE	-	LEADER SEQUENCE	GB 15642842
A	-5	HIS	-	LEADER SEQUENCE	GB 15642842
A	-4	HIS	-	LEADER SEQUENCE	GB 15642842
A	-3	HIS	-	LEADER SEQUENCE	GB 15642842
A	-2	HIS	-	LEADER SEQUENCE	GB 15642842
A	-1	HIS	-	LEADER SEQUENCE	GB 15642842
A	0	HIS	-	LEADER SEQUENCE	GB 15642842
A	1	MSE	MET	MODIFIED RESIDUE	GB 15642842
A	10	MSE	MET	MODIFIED RESIDUE	GB 15642842
A	45	MSE	MET	MODIFIED RESIDUE	GB 15642842
A	181	MSE	MET	MODIFIED RESIDUE	GB 15642842
A	185	MSE	MET	MODIFIED RESIDUE	GB 15642842
A	255	MSE	MET	MODIFIED RESIDUE	GB 15642842
A	292	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	-11	MSE	-	MODIFIED RESIDUE	GB 15642842
B	-10	GLY	-	LEADER SEQUENCE	GB 15642842
B	-9	SER	-	LEADER SEQUENCE	GB 15642842
B	-8	ASP	-	LEADER SEQUENCE	GB 15642842
B	-7	LYS	-	LEADER SEQUENCE	GB 15642842
B	-6	ILE	-	LEADER SEQUENCE	GB 15642842

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	LEADER SEQUENCE	GB 15642842
B	-4	HIS	-	LEADER SEQUENCE	GB 15642842
B	-3	HIS	-	LEADER SEQUENCE	GB 15642842
B	-2	HIS	-	LEADER SEQUENCE	GB 15642842
B	-1	HIS	-	LEADER SEQUENCE	GB 15642842
B	0	HIS	-	LEADER SEQUENCE	GB 15642842
B	1	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	10	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	45	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	181	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	185	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	255	MSE	MET	MODIFIED RESIDUE	GB 15642842
B	292	MSE	MET	MODIFIED RESIDUE	GB 15642842

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Ni 3 3	0	0
2	A	3	Total Ni 3 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is water.

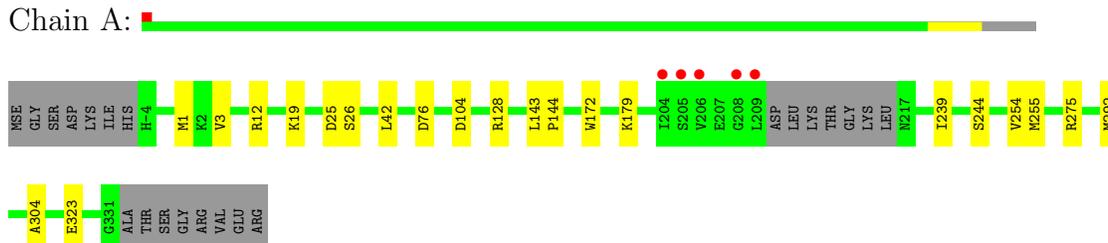
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	217	Total O 217 217	0	0
4	B	177	Total O 177 177	0	0

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.

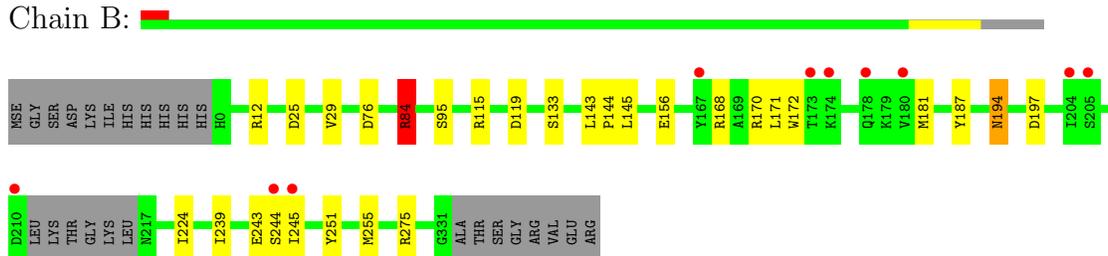
- Molecule 1: 2-keto-3-deoxygluconatekinase

Chain A:



- Molecule 1: 2-keto-3-deoxygluconatekinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	120.99Å 120.99Å 260.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.63 – 2.05 49.63 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.63-2.05) 98.1 (49.63-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.176 , 0.230 0.190 , 0.242	Depositor DCC
R_{free} test set	1069 reflections (2.41%)	DCC
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.311	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 45506 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5444	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3766e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: NI, CA

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	0.82	3/2595 (0.1%)	0.84	3/3502 (0.1%)
1	B	0.76	0/2544	0.84	6/3437 (0.2%)
All	All	0.79	3/5139 (0.1%)	0.84	9/6939 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	LYS	CE-NZ	5.35	1.62	1.49
1	A	25	ASP	CB-CG	5.07	1.62	1.51
1	A	323	GLU	CG-CD	5.04	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	B	84	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	A	25	ASP	CB-CG-OD1	10.65	127.88	118.30
1	A	128	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	119	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	25	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	12	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	12	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	25	ASP	CB-CG-OD2	-5.05	113.76	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2543	0	2476	8	0
1	B	2497	0	2426	15	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	217	0	0	0	0
4	B	177	0	0	1	0
All	All	5444	0	4902	21	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 2.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:ASN:ND2	1:B:197:ASP:H	1.95	0.64
1:B:194:ASN:C	1:B:194:ASN:HD22	2.04	0.61
1:A:104:ASP:OD1	1:B:84:ARG:HD2	2.01	0.61
1:A:3:VAL:HG11	1:A:42:LEU:HD13	1.82	0.60
1:B:275:ARG:HD3	4:B:398:HOH:O	2.01	0.60
1:B:181:MSE:HA	1:B:181:MSE:HE2	1.86	0.58
1:A:239:ILE:HD12	1:A:255:MSE:CE	2.38	0.53
1:B:239:ILE:HD12	1:B:255:MSE:CE	2.38	0.53
1:A:239:ILE:HD12	1:A:255:MSE:HE1	1.91	0.53
1:B:239:ILE:HD12	1:B:255:MSE:HE1	1.91	0.52
1:A:26:SER:HA	1:B:29:VAL:HG23	1.92	0.51
1:A:254:VAL:HG22	1:A:304:ALA:HB2	1.93	0.49
1:B:194:ASN:HD22	1:B:197:ASP:H	1.60	0.45
1:B:115:ARG:HD3	1:B:145:LEU:HB3	1.99	0.44
1:B:243:GLU:HB2	1:B:251:TYR:HB2	1.99	0.44
1:A:1:MSE:SE	1:A:292:MSE:HE1	2.68	0.43
1:B:115:ARG:HD3	1:B:145:LEU:CB	2.50	0.42
1:B:245:ILE:HD13	1:B:245:ILE:N	2.35	0.42
1:B:143:LEU:N	1:B:144:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:LEU:N	1:A:144:PRO:CD	2.85	0.41
1:B:168:ARG:HB2	1:B:171:LEU:HD12	2.03	0.41

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	325/351 (93%)	323 (99%)	2 (1%)	0	100	100
1	B	322/351 (92%)	316 (98%)	6 (2%)	0	100	100
All	All	647/702 (92%)	639 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	257/280 (92%)	252 (98%)	5 (2%)	69	66
1	B	250/280 (89%)	239 (96%)	11 (4%)	39	29
All	All	507/560 (90%)	491 (97%)	16 (3%)	51	44

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	A	172	TRP

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Mol	Chain	Res	Type
1	A	179	LYS
1	A	244	SER
1	A	275	ARG
1	B	76	ASP
1	B	84	ARG
1	B	95	SER
1	B	133	SER
1	B	156	GLU
1	B	170	ARG
1	B	172	TRP
1	B	187	TYR
1	B	194	ASN
1	B	224	ILE
1	B	244	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	107	HIS
1	B	194	ASN
1	B	261	GLN
1	B	297	GLN

5.3.3 RNA [i](#)

There are no RNA chains 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](#)

Of 10 ligands modelled in this entry, 10 are 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.

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 (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, 95th 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	329/351 (93%)	-0.31	5 (1%) 70 72	22, 29, 44, 75	0
1	B	326/351 (92%)	-0.11	10 (3%) 47 46	21, 29, 45, 68	0
All	All	655/702 (93%)	-0.21	15 (2%) 56 58	21, 29, 45, 75	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ILE	4.4
1	A	208	GLY	4.3
1	A	206	VAL	3.5
1	A	205	SER	3.2
1	A	209	LEU	2.8
1	B	204	ILE	2.6
1	B	167	TYR	2.5
1	B	174	LYS	2.5
1	B	205	SER	2.5
1	B	173	THR	2.3
1	B	244	SER	2.2
1	A	204	ILE	2.2
1	B	210	ASP	2.1
1	B	180	VAL	2.1
1	B	178	GLN	2.0

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

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	B	344	1/1	0.26	10.78	12,12,12,12	1
3	CA	A	344	1/1	0.08	-1.47	47,47,47,47	0
2	NI	A	342	1/1	0.06	-2.44	42,42,42,42	0
2	NI	A	340	1/1	0.04	-4.22	32,32,32,32	0
2	NI	B	340	1/1	0.02	-8.56	33,33,33,33	0
2	NI	A	341	1/1	0.01	-10.20	17,17,17,17	1
2	NI	B	342	1/1	0.04	-10.99	50,50,50,50	0
2	NI	B	341	1/1	0.03	-11.00	14,14,14,14	1
3	CA	B	343	1/1	0.05	-	56,56,56,56	1
3	CA	A	343	1/1	0.06	-	52,52,52,52	1

6.5 Other polymers

There are no such residues in this entry.