



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:38 AM UTC

PDB ID : 1WYE / pdb_00001wye
Title : Crystal structure of 2-keto-3-deoxygluconate kinase (form 1) from Sulfolobus Tokodaii
Authors : Toyoda, T.; Suzuki, K.; Hossain, M.T.; Koike, I.; Sekiguchi, T.; Takenaka, A.
Deposited on : 2005-02-12
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

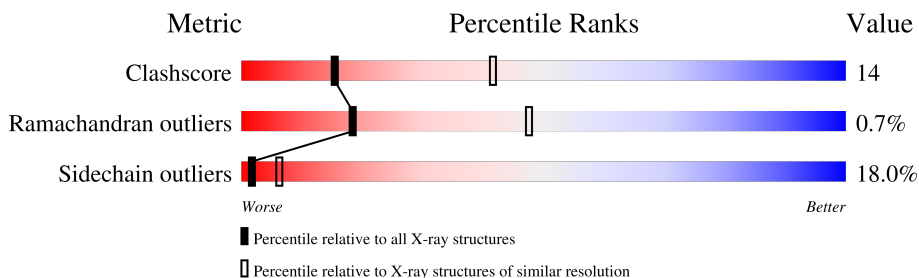
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	
1	C	311	
1	D	311	
1	E	311	
1	F	311	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14836 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 2-keto-3-deoxygluconate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	B	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	C	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	D	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	E	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	F	309	Total	C	N	O	S	0	0	0
			2406	1545	388	466	7			

- Molecule 2 is water.

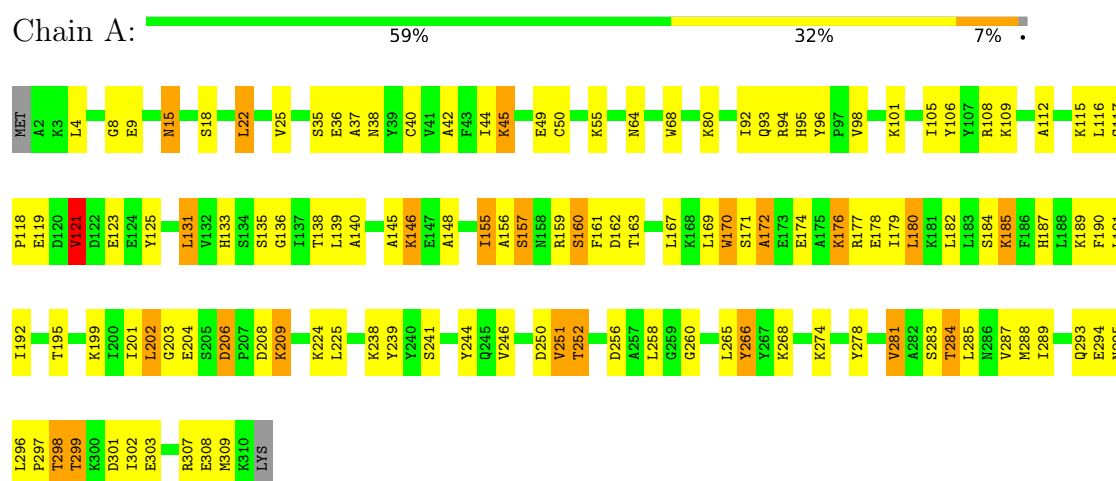
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	45	Total	O	0	0
			45	45		
2	C	71	Total	O	0	0
			71	71		
2	D	79	Total	O	0	0
			79	79		
2	E	76	Total	O	0	0
			76	76		
2	F	54	Total	O	0	0
			54	54		

3 Residue-property plots

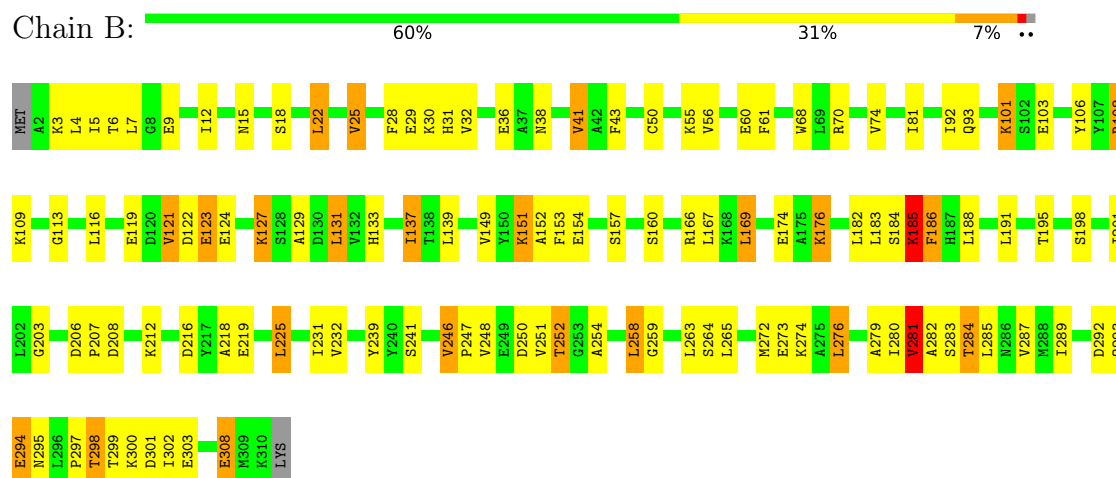
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 2-keto-3-deoxygluconate kinase

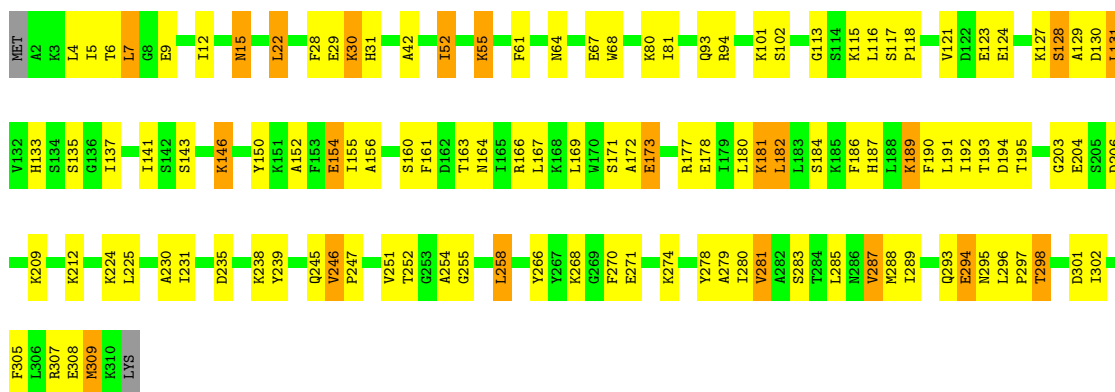


• Molecule 1: 2-keto-3-deoxygluconate kinase



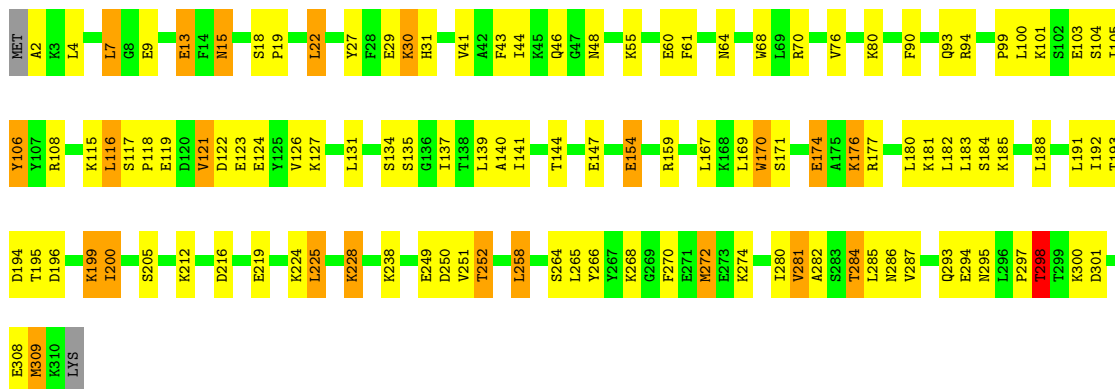
• Molecule 1: 2-keto-3-deoxygluconate kinase





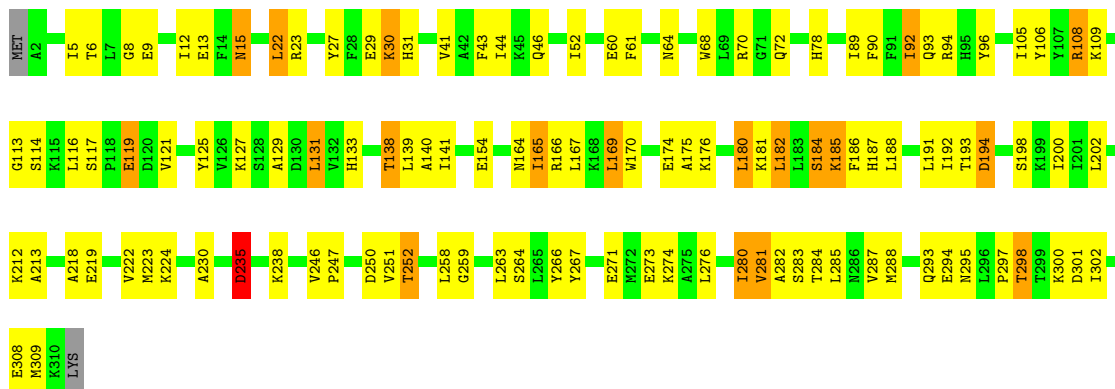
• Molecule 1: 2-keto-3-deoxygluconate kinase

Chain D: 62% 30% 7%



• Molecule 1: 2-keto-3-deoxygluconate kinase

Chain E: 61% 32% 6%



• Molecule 1: 2-keto-3-deoxygluconate kinase

Chain F: 65% 27% 6%



S117	P118	E119	D120	V121	D122	E123	E124	L131	V132	H133	A140	I141	S142	S143	T144	A145	K146	E147	A148	K151	N158	R159	S160	L167	K168	L169	W170	E173	R177	E178	I179	L180	K181	L182	L183	S184	K185	F186	H187	L188	L191	T195	D196	I201	L202	G203	E204	S205	D206
P207	D208	K212	A213	F214	S215	A218	E219	M223	K224	L225	K228	Y234	D235	G236	K237	K238	Y239	V246	D250	V251	T252	D256	A257	L258	S264	E273	I280	V281	T284	V287	Q293	E294	T299	K300	E308	M309	K310	LYS											

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.67Å 149.10Å 161.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.8 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14836	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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	0.94	2/2461 (0.1%)	1.17	6/3324 (0.2%)
1	B	0.93	2/2461 (0.1%)	1.16	8/3324 (0.2%)
1	C	0.96	1/2461 (0.0%)	1.17	5/3324 (0.2%)
1	D	0.97	0/2461	1.20	8/3324 (0.2%)
1	E	0.94	2/2461 (0.1%)	1.18	5/3324 (0.2%)
1	F	0.88	0/2457	1.17	8/3320 (0.2%)
All	All	0.94	7/14762 (0.0%)	1.18	40/19940 (0.2%)

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	1
1	F	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	281	VAL	CA-CB	8.68	1.64	1.54
1	B	272	MET	SD-CE	6.36	1.95	1.79
1	E	281	VAL	CA-CB	5.96	1.62	1.54
1	B	281	VAL	CA-CB	5.75	1.61	1.54
1	E	222	VAL	CA-CB	5.63	1.61	1.54

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	122	ASP	N-CA-C	9.59	124.15	108.52
1	F	185	LYS	N-CA-C	-8.06	100.19	110.19
1	C	155	ILE	N-CA-C	-7.79	106.31	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLY	N-CA-C	-7.35	104.68	115.63
1	F	218	ALA	N-CA-C	7.01	120.10	109.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ILE	Peptide
1	F	234	TYR	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	2410	0	2392	66	0
1	B	2410	0	2392	68	0
1	C	2410	0	2392	70	0
1	D	2410	0	2392	73	0
1	E	2410	0	2392	70	0
1	F	2406	0	2381	57	0
2	A	55	0	0	3	0
2	B	45	0	0	3	0
2	C	71	0	0	3	0
2	D	79	0	0	5	0
2	E	76	0	0	3	0
2	F	54	0	0	2	0
All	All	14836	0	14341	390	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.

The worst 5 of 390 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:C:30:LYS:HE2	1:C:64:ASN:OD1	1.44	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:SER:O	1:E:185:LYS:HG2	1.56	1.05
1:A:146:LYS:HE2	1:A:178:GLU:OE1	1.56	1.04
1:A:15:ASN:HD21	1:A:94:ARG:HD3	1.23	1.00
1:D:258:LEU:HD11	1:D:280:ILE:HD13	1.42	1.00

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	307/311 (99%)	283 (92%)	22 (7%)	2 (1%)	18	47
1	B	307/311 (99%)	292 (95%)	12 (4%)	3 (1%)	12	38
1	C	307/311 (99%)	295 (96%)	11 (4%)	1 (0%)	36	66
1	D	307/311 (99%)	291 (95%)	16 (5%)	0	100	100
1	E	307/311 (99%)	293 (95%)	11 (4%)	3 (1%)	12	38
1	F	307/311 (99%)	284 (92%)	19 (6%)	4 (1%)	9	31
All	All	1842/1866 (99%)	1738 (94%)	91 (5%)	13 (1%)	18	47

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	PHE
1	C	128	SER
1	E	185	LYS
1	F	142	SER
1	F	186	PHE

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	257/260 (99%)	207 (80%)	50 (20%)	1	5
1	B	257/260 (99%)	206 (80%)	51 (20%)	1	5
1	C	257/260 (99%)	216 (84%)	41 (16%)	2	9
1	D	257/260 (99%)	208 (81%)	49 (19%)	1	5
1	E	257/260 (99%)	217 (84%)	40 (16%)	2	9
1	F	256/260 (98%)	210 (82%)	46 (18%)	2	6
All	All	1541/1560 (99%)	1264 (82%)	277 (18%)	2	6

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	7	LEU
1	F	119	GLU
1	F	208	ASP
1	B	295	ASN
1	B	284	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	48	ASN
1	F	46	GLN
1	E	72	GLN
1	E	293	GLN
1	F	93	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 oligosaccharides 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.