



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:22 pm GMT

PDB ID : 1R59
Title : Enterococcus casseliflavus glycerol kinase
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Deposited on : 2003-10-09
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

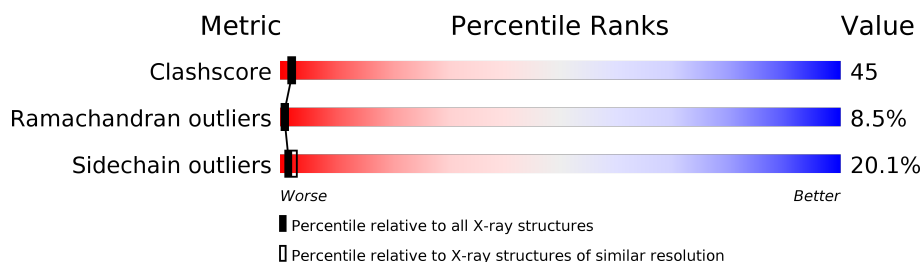
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	O	505	
1	X	505	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7532 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	480	Total	C	N	O	S	0	0	0
			3715	2350	621	730	14			
1	X	480	Total	C	N	O	S	0	0	0
			3715	2350	621	730	14			

- Molecule 2 is water.

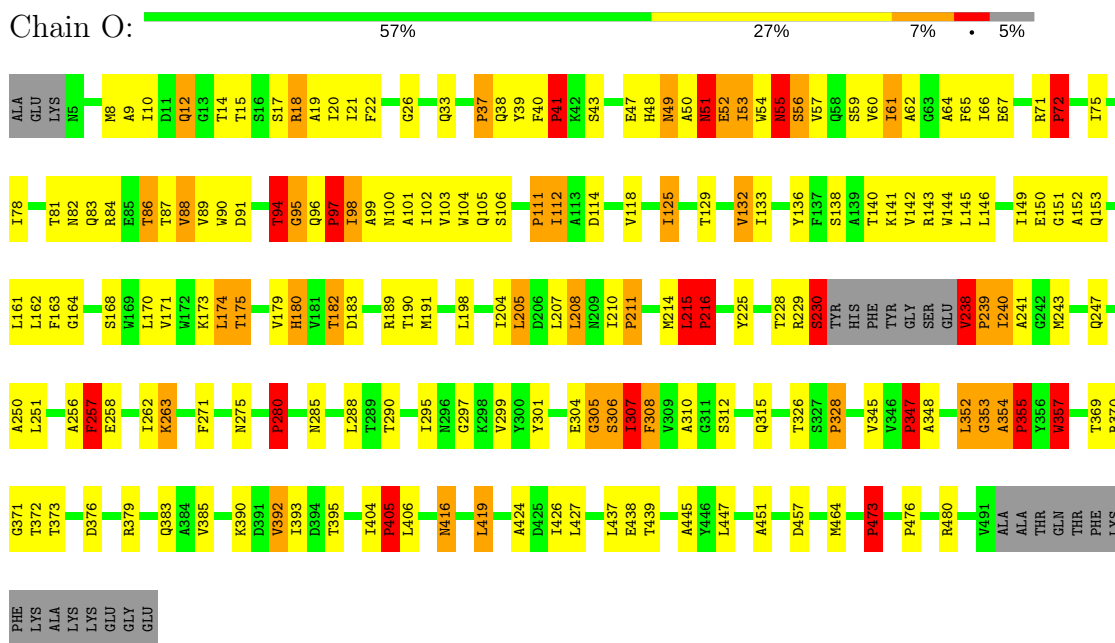
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	51	Total	O	0	0
			51	51		
2	X	51	Total	O	0	0
			51	51		

3 Residue-property plots

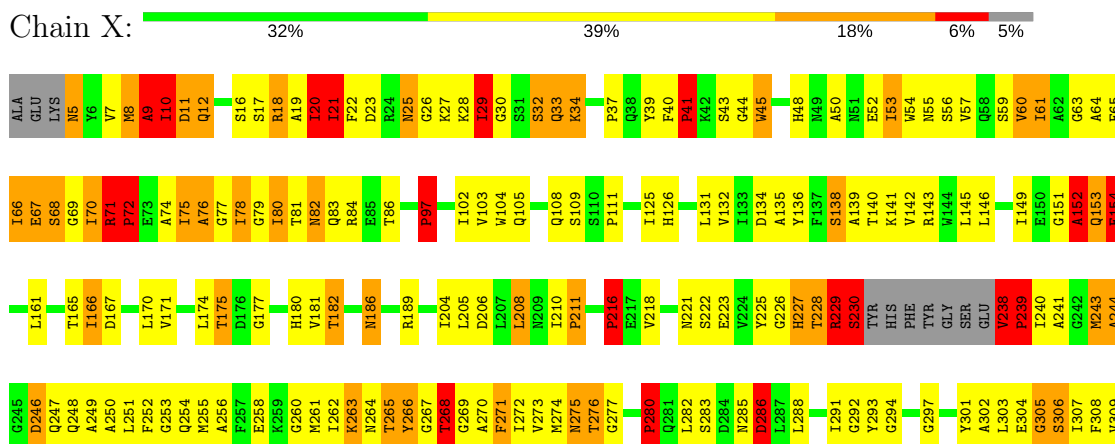
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 was not executed.

• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



LYS	L437	E375	A310
LYS	E438	D376	G311
GLU	T439	F377	S312
GLY	T440	V378	A313
GLU	A441	R379	I314
	L442	A380	Q315
	G443	T381	V316
	A444	L382	L317
	A445	Q383	R318
	Y446	A384	D319
	L447	V385	G320
	A448	A386	L321
	G449	Y387	R322
	L450	Q388	K323
		S389	T324
	F454	K390	
	N455	D391	S327
	K456	V392	P328
	D457	I393	Q329
	L458	D394	S330
	D459	T395	E331
	E460	M396	E332
	L461	K397	L333
	K462	K398	A334
	S463	D399	A335
	N464		K336
	A465	I402	A337
		D403	K338
	G468	I404	G339
		P405	D340
	F471	L406	N341
	T472	L407	E342
	P473	K408	V343
	E474	V409	Y344
	N475	D410	V345
	P476	G411	V346
		G412	P347
	E479	A413	
	R480	A414	T350
	D481	K415	G351
	N482	N416	L352
	L483	D417	G353
	Y484	L418	A354
	E485	L419	P355
	G486	M420	Y356
	W487	Q421	K357
	K488	F422	D358
	Q489	Q423	S359
	A490	A424	
	V491	D425	G363
	ALA	I426	A364
	ALA	L427	V365
	THR	D428	F366
	GLN	I429	G367
	THR	D430	
	PHE	V431	R370
	LYS	Q432	G371
	PHE	R433	T372
	LYS	Y434	T373
	ALA	K374	

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	67.83Å 107.11Å 201.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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	O	0.76	7/3790 (0.2%)	1.40	36/5141 (0.7%)
1	X	1.00	15/3790 (0.4%)	1.63	80/5141 (1.6%)
All	All	0.89	22/7580 (0.3%)	1.52	116/10282 (1.1%)

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	X	0	3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	238	VAL	N-CA	13.28	1.73	1.46
1	X	154	GLU	C-N	12.97	1.63	1.34
1	X	238	VAL	C-N	11.36	1.55	1.34
1	X	238	VAL	N-CA	10.89	1.68	1.46
1	O	230	SER	C-N	10.23	1.57	1.34

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	239	PRO	CA-N-CD	-22.07	80.60	111.50
1	O	239	PRO	CA-N-CD	-21.77	81.03	111.50
1	O	328	PRO	CA-N-CD	-20.94	82.18	111.50
1	O	355	PRO	CA-N-CD	-19.62	84.03	111.50
1	X	280	PRO	CA-N-CD	-19.20	84.62	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	154	GLU	Mainchain
1	X	266	TYR	Sidechain
1	X	446	TYR	Sidechain

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	O	3715	0	3626	217	0
1	X	3715	0	3624	454	0
2	O	51	0	0	8	0
2	X	51	0	0	11	0
All	All	7532	0	7250	664	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 45.

The worst 5 of 664 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:X:132:VAL:HG11	1:X:357:TRP:CZ2	1.32	1.60
1:X:238:VAL:CA	1:X:238:VAL:N	1.68	1.52
1:X:238:VAL:CA	1:X:238:VAL:C	1.76	1.51
1:O:230:SER:CA	1:O:230:SER:C	1.75	1.51
1:O:238:VAL:N	1:O:238:VAL:CA	1.72	1.50

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	O	478/505 (95%)	393 (82%)	63 (13%)	22 (5%)	3	3
1	X	478/505 (95%)	320 (67%)	99 (21%)	59 (12%)	0	0
All	All	956/1010 (95%)	713 (75%)	162 (17%)	81 (8%)	1	1

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	43	SER
1	O	238	VAL
1	O	257	PHE
1	O	258	GLU
1	O	308	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	O	390/409 (95%)	328 (84%)	62 (16%)	3	5
1	X	390/409 (95%)	295 (76%)	95 (24%)	1	1
All	All	780/818 (95%)	623 (80%)	157 (20%)	1	2

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	57	VAL
1	X	186	ASN
1	X	450	LEU
1	X	66	ILE
1	X	82	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	55	ASN
1	X	108	GLN
1	X	421	GLN
1	X	82	ASN
1	X	148	ASN

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 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.