



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:54 am GMT

PDB ID : 1XUP
Title : ENTEROCOCCUS CASSELI FLAVUS GLYCEROL KINASE COMPLEXED WITH GLYCEROL
Authors : Yeh, J.I.; Charrier, V.; Paulo, J.; Hou, L.; Darbon, E.; Hol, W.G.J.; Deutscher, J.
Deposited on : 2004-10-26
Resolution : 2.75 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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
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

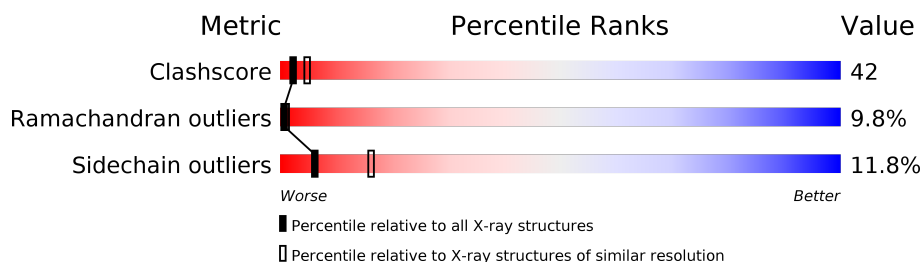
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)

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	487	
1	X	487	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	O	500	-	-	X	-
2	GOL	X	501	-	-	X	-

2 Entry composition [i](#)

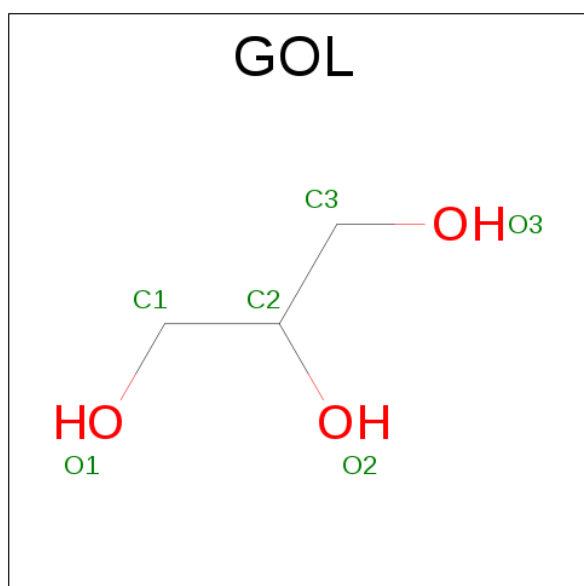
There are 2 unique types of molecules in this entry. The entry contains 7557 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	487	Total	C	N	O	S	0	0	0
			3776	2392	629	741	14			
1	X	487	Total	C	N	O	S	0	0	0
			3769	2387	627	741	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



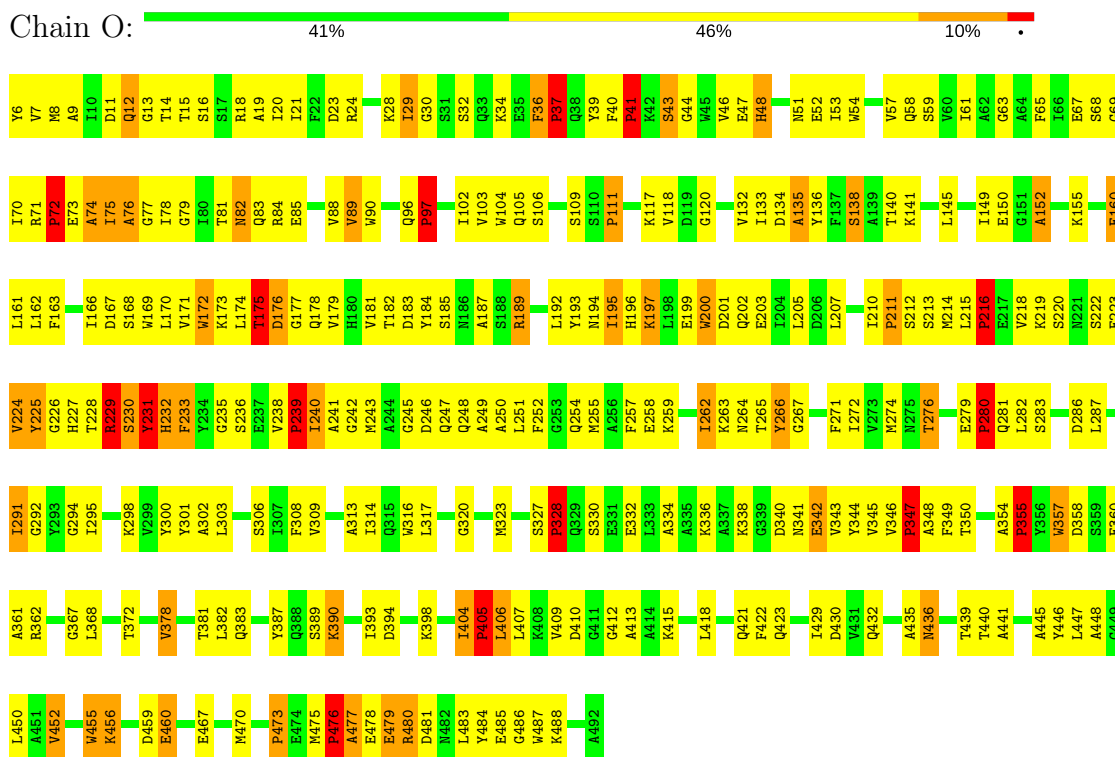
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

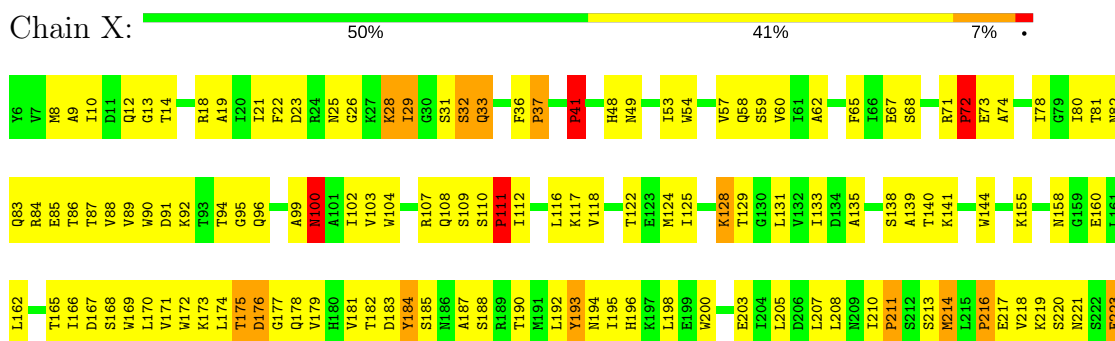
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



V224	V225	G226	H227	T228	R229	F233	Y234	G235	S236	E237	V238	P239	I240	A241	M243	A244	G245	D246	Q247	Q248	M255	G260	M261	T262	K263	Y266	G267	T268	G269	F270	F271	T272	V273	M274	E278	E279	P280	Q281	S282	D283	D284	N285	D286	L287	L288	T289	T290	T291	G292	N296	G297	K298
V299	Y300	Y301	A302	L303	E304	F308	G311	S312	A313	I314	E325	T326	S327	P328	Q329	S330	E331	E332	L333	A334	A335	K336	A337	D340	V343	P347	A348	G269	A354	P355	G357	T373	K374	E375	D376	F377	V378	R379	A380	Q383	A386	K390	I393	P405	L406	L407						
K408	V409	A414	D417	L418	L419	A424	D425	T426	L427	D430	T439	G443	A444	A445	Y446	L447	A448	G449	V452	G453	F454	N455	K456	D457	L458	D459	E460	L461	F471	T472	P473	E474	N475	P476	A477	R480	Q489	A492														

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	68.01Å 107.67Å 201.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.75	Depositor
% Data completeness (in resolution range)	87.0 (6.00-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7557	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.48	0/3855	1.08	23/5229 (0.4%)
1	X	0.43	0/3847	0.96	19/5218 (0.4%)
All	All	0.45	0/7702	1.02	42/10447 (0.4%)

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	355	PRO	CA-N-CD	-18.62	85.44	111.50
1	O	405	PRO	CA-N-CD	-17.28	87.30	111.50
1	O	347	PRO	CA-N-CD	-16.64	88.20	111.50
1	O	111	PRO	CA-N-CD	-15.73	89.48	111.50
1	X	405	PRO	CA-N-CD	-14.63	91.01	111.50

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	O	3776	0	3673	323	0
1	X	3769	0	3661	326	0
2	O	6	0	8	9	0
2	X	6	0	8	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7557	0	7350	626	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 42.

The worst 5 of 626 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:175:THR:HG21	1:X:179:VAL:CG1	1.41	1.50
1:X:175:THR:HB	1:X:227:HIS:CB	1.46	1.43
1:X:84:ARG:CG	2:X:501:GOL:H12	1.58	1.33
1:X:167:ASP:HA	1:X:243:MET:CE	1.60	1.31
1:X:32:SER:O	1:X:33:GLN:NE2	1.61	1.31

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	485/487 (100%)	330 (68%)	103 (21%)	52 (11%)	0	1
1	X	485/487 (100%)	330 (68%)	112 (23%)	43 (9%)	1	1
All	All	970/974 (100%)	660 (68%)	215 (22%)	95 (10%)	1	1

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	24	ARG
1	O	117	LYS
1	O	135	ALA
1	O	138	SER

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Mol	Chain	Res	Type
1	O	203	GLU

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	O	395/395 (100%)	345 (87%)	50 (13%)	5	13
1	X	393/395 (100%)	350 (89%)	43 (11%)	7	20
All	All	788/790 (100%)	695 (88%)	93 (12%)	6	16

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	406	LEU
1	X	37	PRO
1	X	406	LEU
1	O	422	PHE
1	O	467	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	254	GLN
1	O	421	GLN
1	X	108	GLN
1	O	247	GLN
1	X	202	GLN

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](#)

2 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	GOL	O	500	-	5,5,5	0.91	0	5,5,5	0.84	0
2	GOL	X	501	-	5,5,5	0.90	0	5,5,5	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	O	500	-	-	0/4/4/4	0/0/0/0
2	GOL	X	501	-	-	0/4/4/4	0/0/0/0

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.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	500	GOL	9	0
2	X	501	GOL	14	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

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.