



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:55 am GMT

PDB ID : 1IWP  
Title : Glycerol Dehydratase-cyanocobalamin Complex of *Klebsiella pneumoniae*  
Authors : Yamanishi, M.; Yunoki, M.; Tobimatsu, T.; Toraya, T.  
Deposited on : 2002-05-28  
Resolution : 2.10 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](mailto: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.

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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

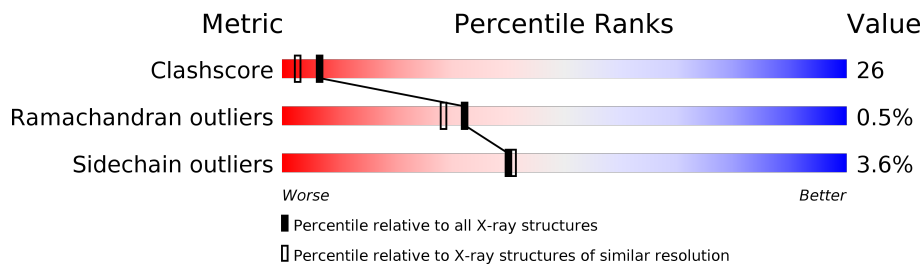
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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  $\geq 3$ , 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	A	555	
1	L	555	
2	B	194	
2	E	194	
3	G	141	
3	M	141	

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
5	PGO	A	1602	X	-	-	-
5	PGO	L	2602	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14631 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 Dehydratase Alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4244	2639	737	838	30			
1	L	555	Total	C	N	O	S	0	0	0
			4244	2639	737	838	30			

- Molecule 2 is a protein called Glycerol Dehydratase Beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1424	899	257	264	4			
2	E	184	Total	C	N	O	S	0	0	0
			1424	899	257	264	4			

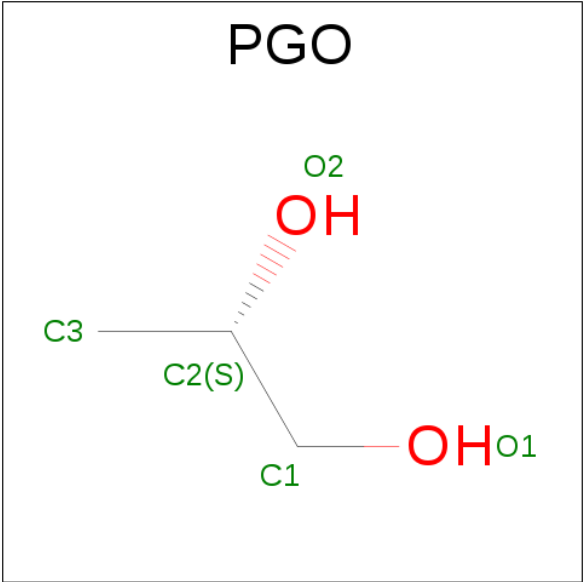
- Molecule 3 is a protein called Glycerol Dehydratase Gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	138	Total	C	N	O	S	0	0	0
			1110	693	209	205	3			
3	M	138	Total	C	N	O	S	0	0	0
			1110	693	209	205	3			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

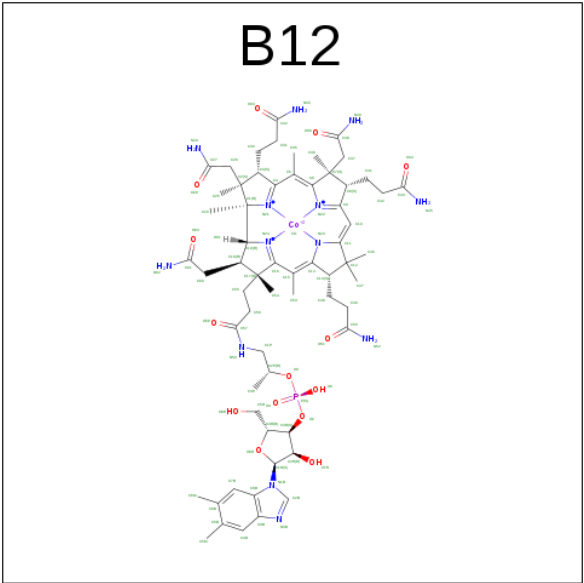
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total	0	0
			1 K		
4	L	1	Total	0	0
			1 K		

- Molecule 5 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	3	2		
5	L	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 7 is water.

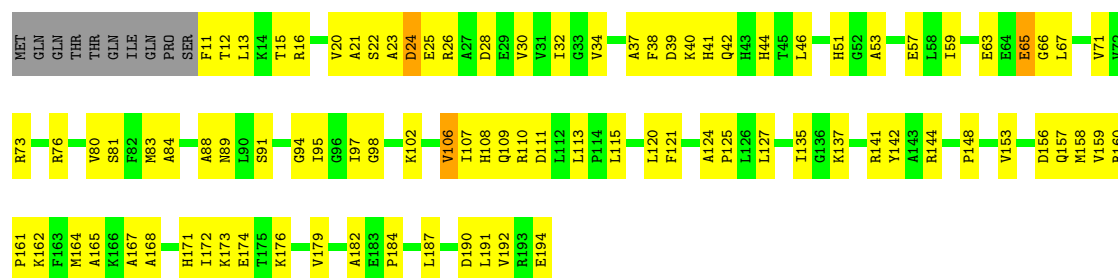
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	267	Total 267	O 267	0	0
7	B	98	Total 98	O 98	0	0
7	G	85	Total 85	O 85	0	0
7	L	254	Total 254	O 254	0	0
7	E	94	Total 94	O 94	0	0
7	M	83	Total 83	O 83	0	0





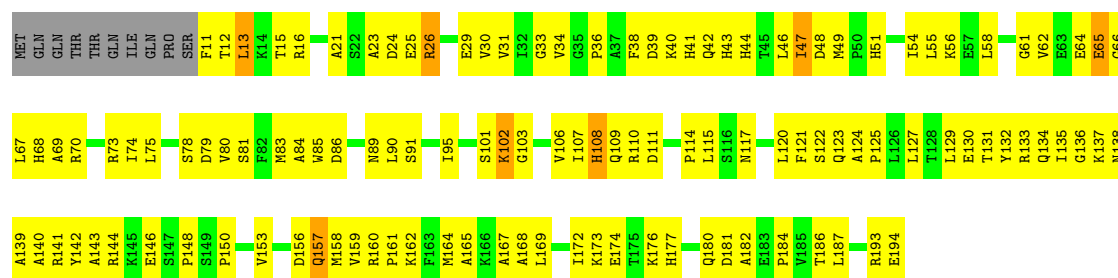
• Molecule 2: Glycerol Dehydratase Beta subunit

Chain B: 48% 45% 5%



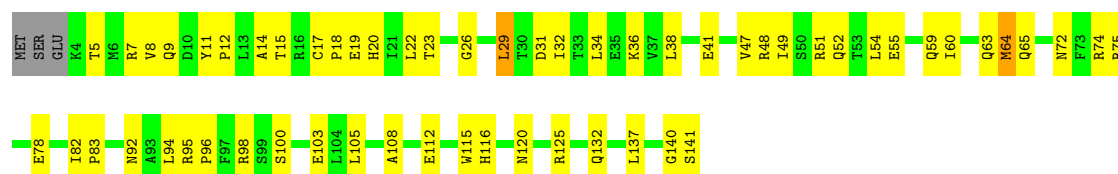
• Molecule 2: Glycerol Dehydratase Beta subunit

Chain E: 33% 58% 5%



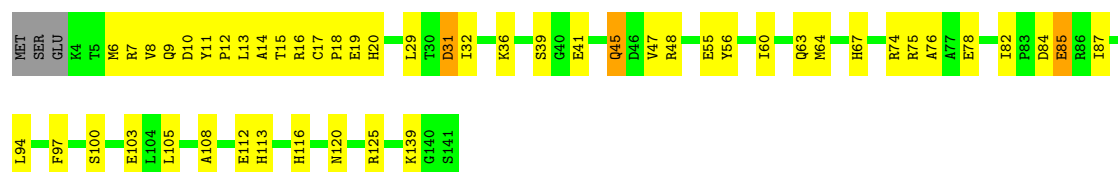
• Molecule 3: Glycerol Dehydratase Gamma subunit

Chain G: 57% 40% ..



• Molecule 3: Glycerol Dehydratase Gamma subunit

Chain M: 62% 33% ..



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.38Å 108.22Å 113.14Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	45.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.9 (45.00-2.10)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.209 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: PGO, K, B12

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	0.33	0/4307	0.63	1/5831 (0.0%)
1	L	0.33	0/4307	0.63	0/5831
2	B	0.31	0/1451	0.61	0/1964
2	E	0.29	0/1451	0.59	0/1964
3	G	0.30	0/1130	0.56	0/1529
3	M	0.30	0/1130	0.57	0/1529
All	All	0.32	0/13776	0.61	1/18648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ALA	N-CA-C	-5.43	96.32	111.00

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	A	4244	0	4195	207	0
1	L	4244	0	4195	182	0
2	B	1424	0	1446	87	0
2	E	1424	0	1446	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1110	0	1120	63	0
3	M	1110	0	1120	56	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	A	5	0	6	1	0
5	L	5	0	6	0	0
6	B	91	0	88	7	0
6	E	91	0	88	9	0
7	A	267	0	0	46	0
7	B	98	0	0	23	0
7	E	94	0	0	58	0
7	G	85	0	0	7	0
7	L	254	0	0	37	0
7	M	83	0	0	8	0
All	All	14631	0	13710	720	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 26.

The worst 5 of 720 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:A:522:ILE:HD12	1:A:522:ILE:H	1.22	1.01
1:A:137:ARG:HH11	1:A:524:ASP:H	1.06	0.97
3:M:11:TYR:HB2	3:M:60:ILE:HD13	1.45	0.97
1:L:141:ASN:HD21	1:L:362:PHE:HB2	1.31	0.95
1:L:306:MET:HE2	2:E:164:MET:HG2	1.48	0.94

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	553/555 (100%)	527 (95%)	23 (4%)	3 (0%)	32	28
1	L	553/555 (100%)	520 (94%)	30 (5%)	3 (0%)	32	28
2	B	182/194 (94%)	171 (94%)	10 (6%)	1 (0%)	32	28
2	E	182/194 (94%)	153 (84%)	27 (15%)	2 (1%)	17	11
3	G	136/141 (96%)	133 (98%)	3 (2%)	0	100	100
3	M	136/141 (96%)	133 (98%)	3 (2%)	0	100	100
All	All	1742/1780 (98%)	1637 (94%)	96 (6%)	9 (0%)	32	28

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	24	ASP
1	A	2	LYS
2	B	24	ASP
1	A	364	GLY
1	L	544	ASN

### 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	453/453 (100%)	444 (98%)	9 (2%)	60	66
1	L	453/453 (100%)	438 (97%)	15 (3%)	43	45
2	B	153/163 (94%)	147 (96%)	6 (4%)	37	37
2	E	153/163 (94%)	145 (95%)	8 (5%)	27	24
3	G	117/120 (98%)	111 (95%)	6 (5%)	28	25
3	M	117/120 (98%)	109 (93%)	8 (7%)	18	15
All	All	1446/1472 (98%)	1394 (96%)	52 (4%)	40	41

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	46	ASN

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Mol	Chain	Res	Type
1	L	255	LEU
3	M	64	MET
1	L	51	GLU
1	L	141	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	133	GLN
1	L	170	GLN
3	M	63	GLN
1	L	46	ASN
1	L	120	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
5	PGO	A	1602	4	4,4,4	0.35	0	2,4,4	0.93	0
6	B12	B	1601	-	73,101,101	1.47	8 (10%)	111,166,166	1.80	27 (24%)
6	B12	E	2601	-	73,101,101	1.55	11 (15%)	111,166,166	1.85	27 (24%)
5	PGO	L	2602	4	4,4,4	0.36	0	2,4,4	0.74	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
5	PGO	A	1602	4	1/1/1/1	0/2/2/2	0/0/0/0
6	B12	B	1601	-	-	0/51/223/223	0/3/11/11
6	B12	E	2601	-	-	0/51/223/223	0/3/11/11
5	PGO	L	2602	4	1/1/1/1	0/2/2/2	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1601	B12	C11-C10	-3.67	1.34	1.41
6	E	2601	B12	C11-C10	-3.61	1.34	1.41
6	B	1601	B12	C8B-N1B	-2.70	1.35	1.38
6	E	2601	B12	C8B-N1B	-2.54	1.35	1.38
6	E	2601	B12	P-O5	-2.05	1.44	1.55

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2601	B12	O58-C57-C56	-6.11	110.53	122.01
6	B	1601	B12	O58-C57-C56	-5.96	110.80	122.01
6	E	2601	B12	C4R-O6R-C1R	-4.38	105.11	109.77
6	B	1601	B12	C7B-C8B-C9B	-4.16	116.43	120.54
6	E	2601	B12	C7B-C8B-C9B	-4.15	116.44	120.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	2602	PGO	C2
5	A	1602	PGO	C2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1602	PGO	1	0
6	B	1601	B12	7	0
6	E	2601	B12	9	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.