wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:04 PM GMT

PDB ID	:	1GYL
Title	:	INVOLVEMENT OF TYR24 AND TRP108 IN SUBSTRATE BINDING AND SUBSTRATE SPECIFICITY OF GLYCOLATE OXIDASE
Authors	:	Lindqvist, Y.; Stenberg, K.
Deposited on	:	1995-01-30
Resolution	:	3.00 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 (i) symbol.

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

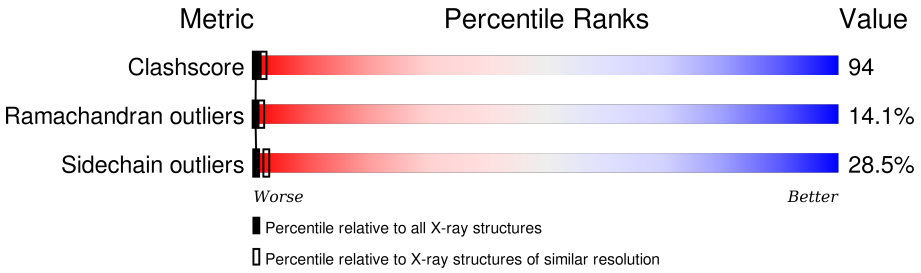
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 <=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	369	17% 54% 22% • 5%
1	B	369	11% 51% 26% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5436 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.

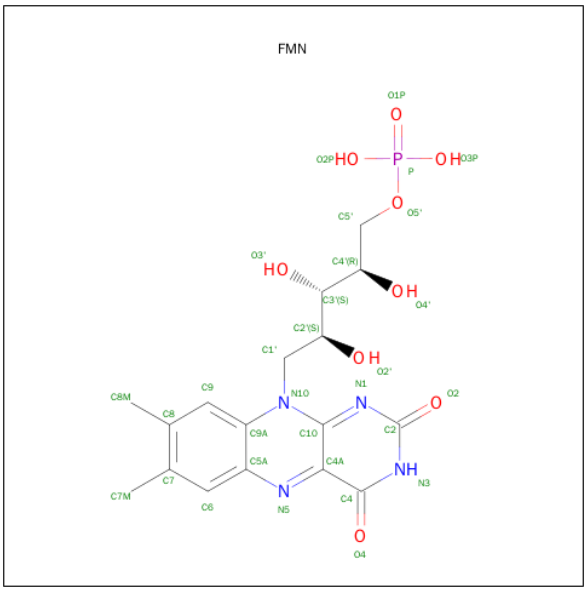
- Molecule 1 is a protein called GLYCOLATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2708	1726	474	495	13			
1	B	350	Total	C	N	O	S	0	0	0
			2695	1718	471	493	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	PHE	TYR	CONFLICT	UNP P05414
B	24	PHE	TYR	CONFLICT	UNP P05414

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0

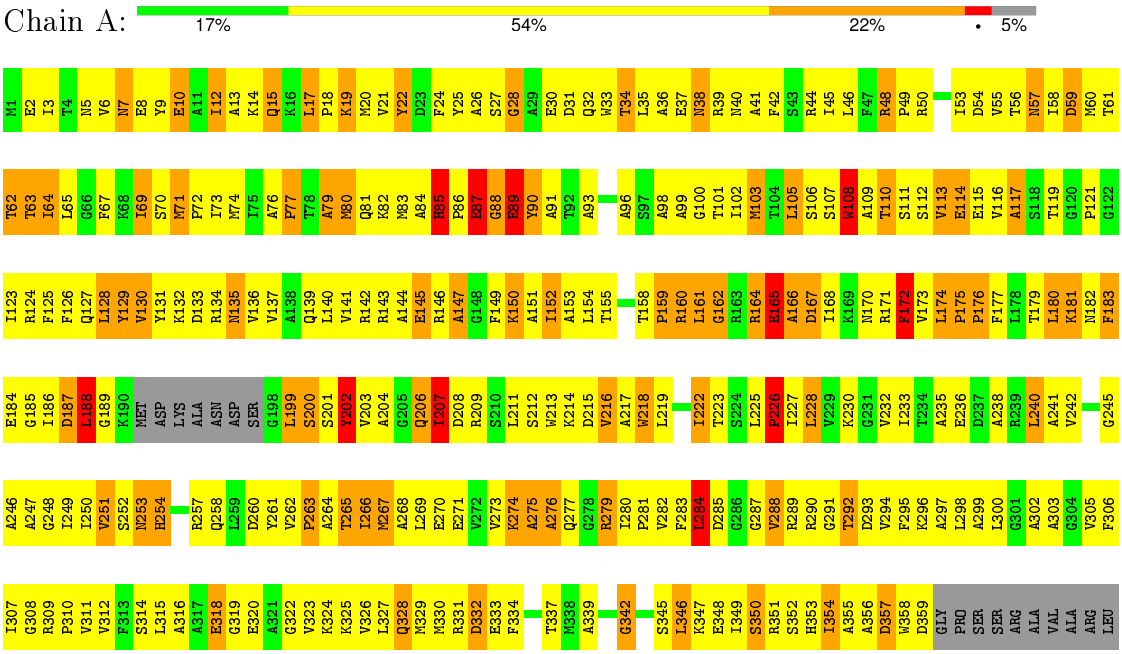
3 Residue-property plots (i)

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.

Note EDS was not executed.

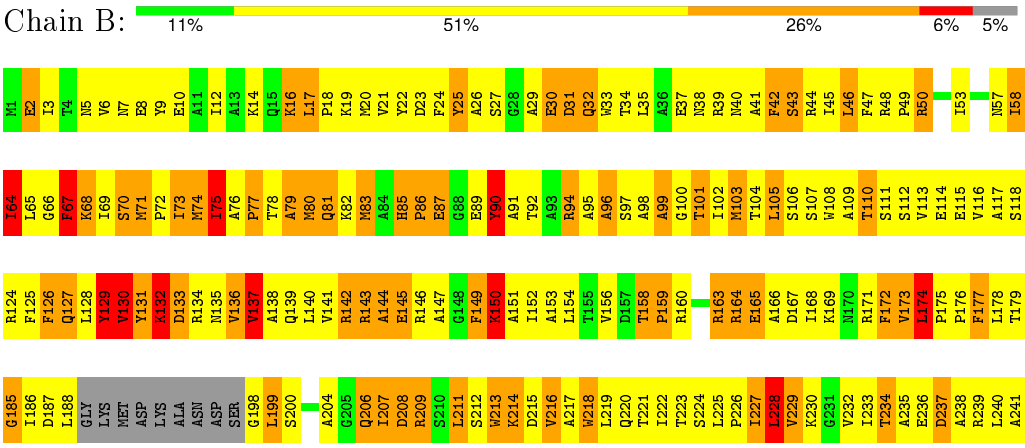
- Molecule 1: GLYCOLATE OXIDASE

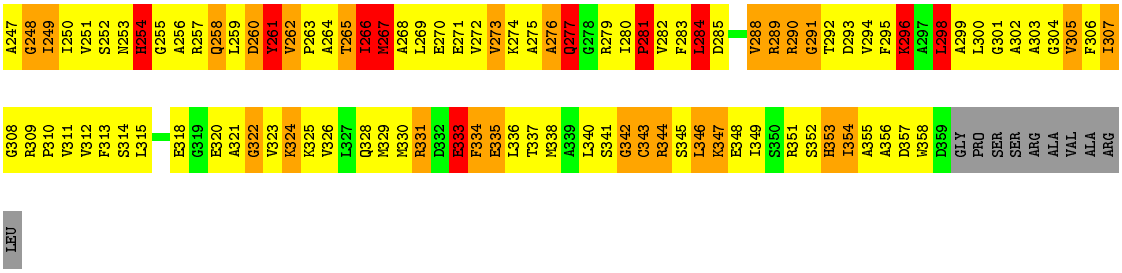
Chain A:



- Molecule 1: GLYCOLATE OXIDASE

Chain B:




A247 G248 I249 I250 V251 S252 N253 H254 G255 A256 R257 Q258 L259 D260 Y261 V262 P263 A264 T265 I266 M267 A268 L269 E270 E271 Y272 V273 K274 A275 A276 Q277 G278 R279 I280 P281 V282 F283 I284 D285 V288 R289 R290 G291 T292 D293 Y294 F295 K296 A297 L298 A299 L300 G301 A302 A303 G304 Y305 F306 I307
G308 R309 P310 V311 V312 F313 S314 L315 E318 G319 E320 A321 G322 V323 K324 K325 V326 L327 Q328 M329 M330 R331 D332 E333 F334 E335 L336 T337 M338 A339 L340 S341 G342 C343 R344 S345 L346 K347 E348 I349 S350 R351 S352 H353 I354 A355 A356 D357 W358 D359 GLY PRO SER SER ARG ALA VAL ALA ARG
LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	145.50Å 145.50Å 100.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: FMN

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	0.75	1/2756 (0.0%)	1.09	13/3729 (0.3%)
1	B	0.78	0/2743	1.15	11/3713 (0.3%)
All	All	0.77	1/5499 (0.0%)	1.12	24/7442 (0.3%)

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	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CG-CD	5.40	1.60	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	LEU	CA-CB-CG	7.61	132.80	115.30
1	B	228	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	160	ARG	N-CA-C	-6.48	93.51	111.00
1	A	147	ALA	N-CA-C	-6.45	93.57	111.00
1	B	298	LEU	CA-CB-CG	6.25	129.68	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	TYR	Sidechain
1	B	90	TYR	Sidechain

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	2708	0	2771	408	0
1	B	2695	0	2755	681	0
2	A	31	0	19	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5436	0	5545	1032	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 94.

The worst 5 of 1032 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:B:235:ALA:HA	1:B:238:ALA:HB3	1.18	1.14
1:A:80:MET:HG2	1:A:110:THR:HG23	1.27	1.14
1:B:82:LYS:HB2	1:B:178:LEU:HD11	1.22	1.13
1:B:227:ILE:HB	1:B:246:ALA:HB1	1.17	1.09
1:B:165:GLU:HA	1:B:168:ILE:HB	1.16	1.09

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	348/369 (94%)	238 (68%)	64 (18%)	46 (13%)	0 1
1	B	346/369 (94%)	203 (59%)	91 (26%)	52 (15%)	0 1
All	All	694/738 (94%)	441 (64%)	155 (22%)	98 (14%)	0 1

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	19	LYS
1	A	89	GLU
1	A	150	LYS
1	A	165	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	A	281/294 (96%)	216 (77%)	65 (23%)	1 5
1	B	280/294 (95%)	185 (66%)	95 (34%)	0 1
All	All	561/588 (95%)	401 (72%)	160 (28%)	0 2

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	LEU
1	B	85	HIS
1	B	305	VAL
1	B	57	ASN
1	B	68	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	ASN
1	B	38	ASN
1	B	206	GLN
1	A	254	HIS
1	B	81	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	FMN	A	370	-	32,33,33	3.42	13 (40%)	34,50,50	2.99	14 (41%)

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	FMN	A	370	-	-	0/18/18/18	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370	FMN	C1'-N10	-8.92	1.38	1.48
2	A	370	FMN	C6-C5A	-3.26	1.36	1.41
2	A	370	FMN	C6-C7	2.05	1.43	1.37
2	A	370	FMN	O4'-C4'	2.38	1.48	1.43
2	A	370	FMN	C9A-N10	2.42	1.42	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	370	FMN	N3-C2-N1	-8.04	114.16	127.69
2	A	370	FMN	C4A-C4-N3	-4.44	117.72	123.52
2	A	370	FMN	O2P-P-O5'	-2.51	99.39	106.72
2	A	370	FMN	C7M-C7-C8	-2.20	115.99	120.73
2	A	370	FMN	O3P-P-O2P	2.16	115.38	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	370	FMN	6	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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.