wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 03:25 AM UTC

PDB ID	:	1GTM / pdb_00001gtm
Title	:	STRUCTURE OF GLUTAMATE DEHYDROGENASE
Authors	:	Yip, K.S.P.; Stillman, T.J.; Britton, K.L.; Pasquo, A.; Rice, D.W.
Deposited on	:	1996-08-22
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

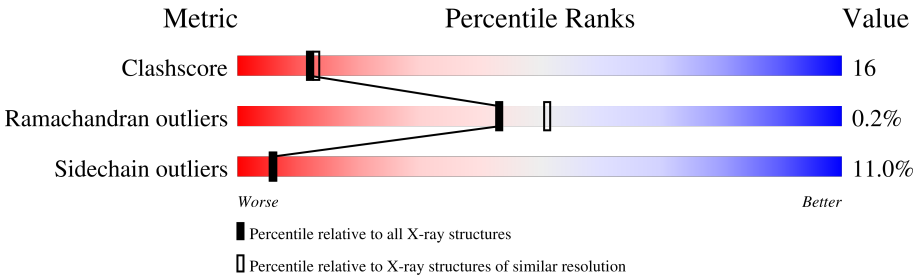
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	419	58% 30% 9%
1	B	419	70% 21% 8%
1	C	419	64% 27% 7%

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	SO4	A	421	-	-	X	-
2	SO4	C	420	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10224 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.

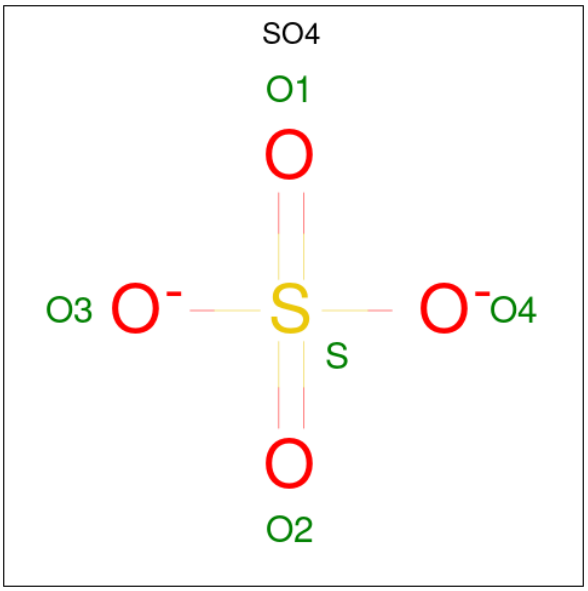
- Molecule 1 is a protein called GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			
1	B	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			
1	C	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	GLN	conflict	UNP P80319
B	3	ALA	GLN	conflict	UNP P80319
C	3	ALA	GLN	conflict	UNP P80319

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	112	Total O 112 112	0	0
3	C	99	Total O 99 99	0	0

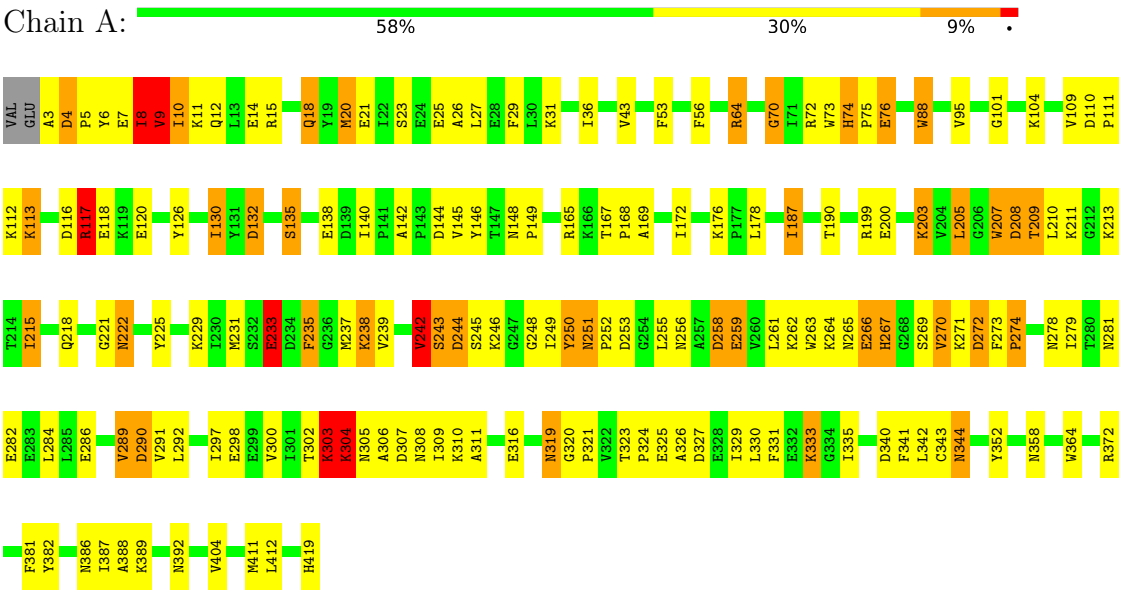
3 Residue-property plots (i)

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.

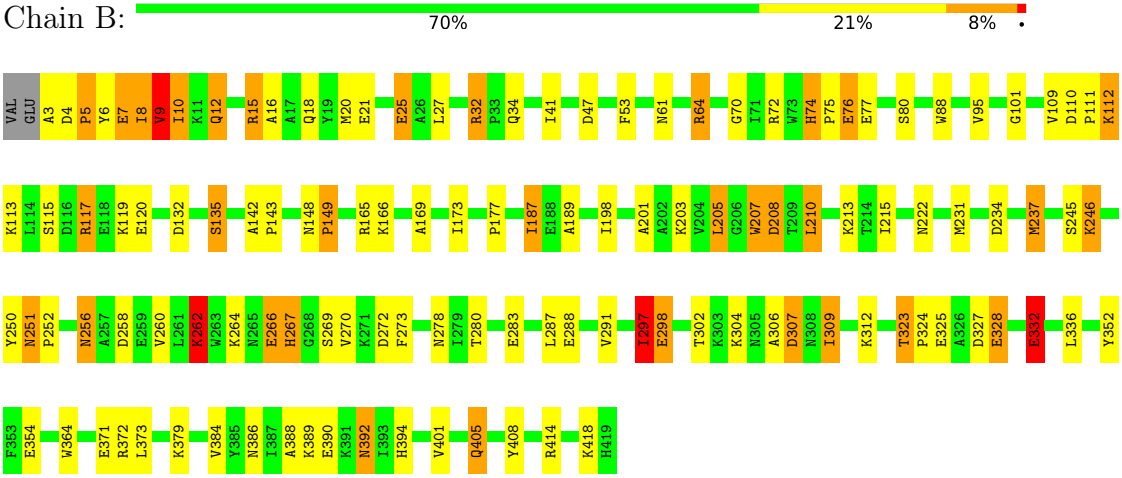
• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain A:



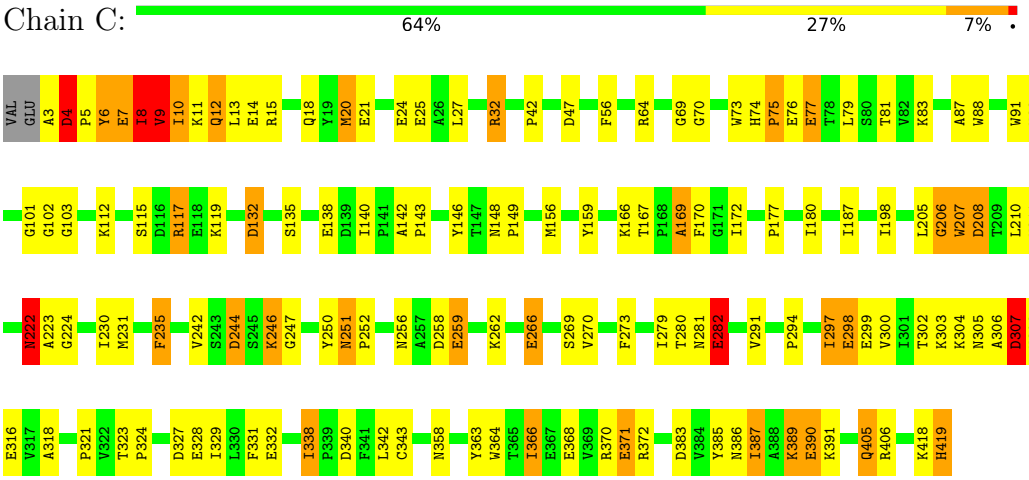
• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain B:



• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain C:


64%
27%
7%
VAL GLU A3 D4 P5 Y6 E7 I8 V9 I10 K11 Q12 L13 E14 R15 Q18 Y19 M20 E21 E24 E25 A26 L27 R32 P42 D47 F56 R64 G69 G70 W73 H74 P75 E76 E77 T78 L79 S80 T81 V82 K83 A87 W88 W91 K92 V95 M96 D97
G101 G102 G103 K112 S115 D116 R117 E118 K119 D132 S135 E138 D139 I140 P141 A142 P143 Y146 T147 N148 P149 M156 Y159 K166 T167 P168 A169 F170 G171 I172 P177 I180 I187 I198 L205 G206 W207 D208 T209 L210 K211 I215 A216 I217
W222 A223 G224 I230 M231 F235 V242 S243 D244 S245 K246 G247 Y250 N251 P252 N256 A257 D258 E259 K262 E266 S269 V270 F273 I279 T280 N281 E282 V291 P294 I297 E298 E299 V300 I301 T302 K303 K304 N305 A306 D307 N308 I309 K310 A315
E316 V317 A318 P321 V322 T323 P324 D327 E328 I329 L330 F331 E332 I338 P339 D340 F341 L342 C343 N358 Y363 W364 T365 I366 E367 E368 V369 R370 E371 R372 D383 V384 Y385 N386 I387 A388 K389 E390 K391 Q405 R406 K418 H419

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.20Å 167.20Å 172.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.2 (10.00-2.20)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10224	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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: SO4

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	1.08	0/3365	1.94	85/4560 (1.9%)
1	B	1.07	0/3365	1.92	75/4560 (1.6%)
1	C	1.07	1/3365 (0.0%)	1.93	82/4560 (1.8%)
All	All	1.07	1/10095 (0.0%)	1.93	242/13680 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	282	GLU	CD-OE2	5.16	1.35	1.25

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	267	HIS	CA-CB-CG	-12.76	101.04	113.80
1	A	251	ASN	CA-C-N	10.83	130.43	119.82
1	A	251	ASN	C-N-CA	10.83	130.43	119.82
1	B	386	ASN	CA-CB-CG	-10.11	102.49	112.60
1	B	208	ASP	CA-CB-CG	9.39	121.99	112.60

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	3292	0	3290	115	0
1	B	3292	0	3290	95	0
1	C	3292	0	3290	102	0
2	A	10	0	0	3	0
2	B	10	0	0	0	0
2	C	10	0	0	3	0
3	A	107	0	0	0	0
3	B	112	0	0	0	0
3	C	99	0	0	0	0
All	All	10224	0	9870	310	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 16.

The worst 5 of 310 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:8:ILE:CD1	1:B:8:ILE:C	2.03	1.31
1:B:8:ILE:CD1	1:B:9:VAL:N	1.99	1.25
1:B:8:ILE:C	1:B:8:ILE:HD13	1.55	1.24
1:B:8:ILE:HD12	1:B:9:VAL:N	1.52	1.23
1:A:25:GLU:OE1	1:A:419:HIS:HD2	1.28	1.16

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	415/419 (99%)	393 (95%)	20 (5%)	2 (0%)	24 27
1	B	415/419 (99%)	401 (97%)	14 (3%)	0	100 100
1	C	415/419 (99%)	396 (95%)	18 (4%)	1 (0%)	43 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1245/1257 (99%)	1190 (96%)	52 (4%)	3 (0%)	43 51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	C	4	ASP
1	A	304	LYS

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	343/345 (99%)	303 (88%)	40 (12%)	5 5
1	B	343/345 (99%)	307 (90%)	36 (10%)	6 6
1	C	343/345 (99%)	306 (89%)	37 (11%)	6 6
All	All	1029/1035 (99%)	916 (89%)	113 (11%)	6 6

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	205	LEU
1	C	387	ILE
1	B	328	GLU
1	C	371	GLU
1	C	266	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	18	GLN
1	C	308	ASN
1	C	392	ASN

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Mol	Chain	Res	Type
1	C	386	ASN
1	A	386	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	SO4	A	420	-	4,4,4	0.71	0	6,6,6	0.26	0
2	SO4	C	421	-	4,4,4	0.87	0	6,6,6	0.24	0
2	SO4	A	421	-	4,4,4	1.13	0	6,6,6	0.15	0
2	SO4	C	420	-	4,4,4	0.64	0	6,6,6	0.33	0
2	SO4	B	420	-	4,4,4	0.62	0	6,6,6	0.55	0
2	SO4	B	421	-	4,4,4	0.55	0	6,6,6	0.44	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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	421	SO4	3	0
2	C	420	SO4	3	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.