

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 08:39 AM EDT

PDB ID : 1B3B

Title : THERMOTOGA MARITIMA GLUTAMATE DEHYDROGENASE MU-

TANT N97D, G376K

Authors: Knapp, S.; Lebbink, J.H.G.; Van Der Oost, J.; Devos, W.M.; Rice, D.; Laden-

stein, R.

Deposited on : 1998-12-07

Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

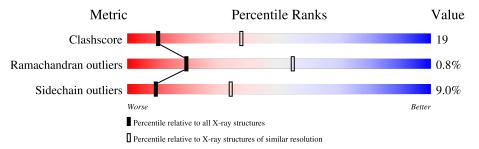
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 3.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 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 o	chain	
1	A	415	56%	39%	• •
1	В	415	57%	39%	
1	С	415	55%	40%	
1	D	415	57%	39%	
1	E	415	51%	44%	
1	F	415	55%	40%	



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19008 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 PROTEIN (GLUTAMATE DEHYDROGENASE).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	A 409	Total	С	N	О	S	0	0	0
1	Λ		3168	2011	552	592	13	0	U	
1	В	409	Total	С	N	О	S	0	0	0
1	Б	409	3168	2011	552	592	13	0	U	
1	С	409	Total	С	N	О	S	0	0	0
1		409	3168	2011	552	592	13	0	U	0
1	D	409	Total	С	N	О	S	0	0	0
1	D	409	3168	2011	552	592	13	0	U	
1	Е	409	Total	С	N	О	S	0	0	0
1	l L	409	3168	2011	552	592	13	0	U	
1	F	409	Total	С	N	О	S	0	0	0
1	I'	409	3168	2011	552	592	13	U	U	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASP	ASN	engineered mutation	UNP P96110
A	376	LYS	GLY	engineered mutation	UNP P96110
В	97	ASP	ASN	engineered mutation	UNP P96110
В	376	LYS	GLY	engineered mutation	UNP P96110
С	97	ASP	ASN	engineered mutation	UNP P96110
С	376	LYS	GLY	engineered mutation	UNP P96110
D	97	ASP	ASN	engineered mutation	UNP P96110
D	376	LYS	GLY	engineered mutation	UNP P96110
Е	97	ASP	ASN	engineered mutation	UNP P96110
Е	376	LYS	GLY	engineered mutation	UNP P96110
F	97	ASP	ASN	engineered mutation	UNP P96110
F	376	LYS	GLY	engineered mutation	UNP P96110

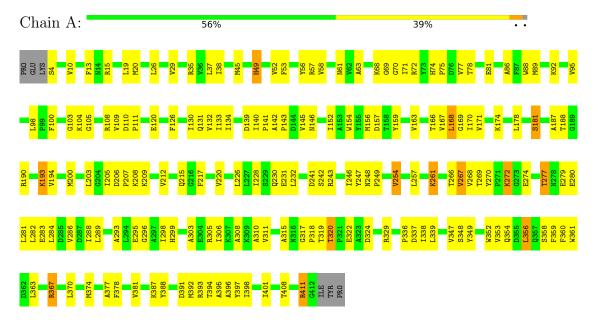


3 Residue-property plots (i)

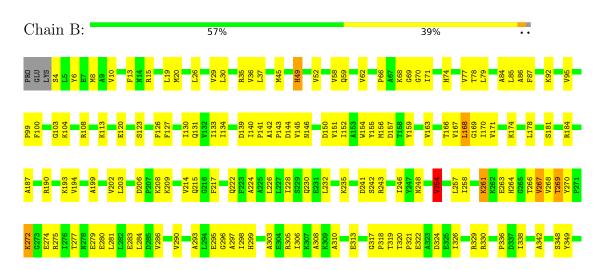
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PROTEIN (GLUTAMATE DEHYDROGENASE)



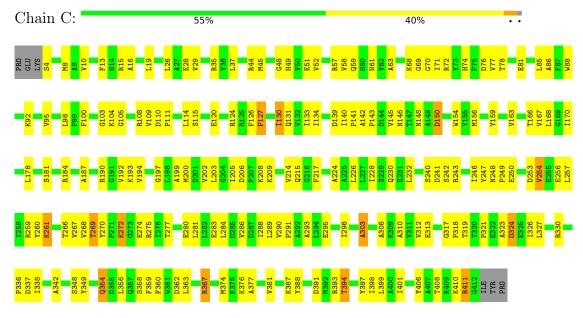
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)



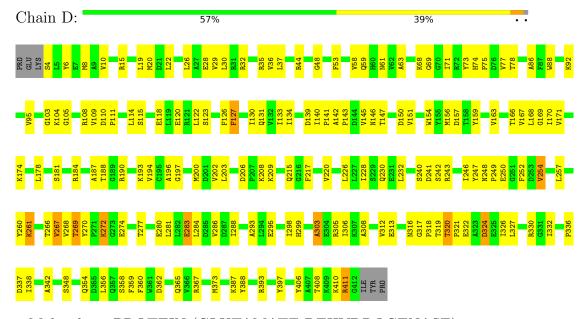




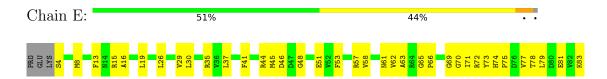
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)



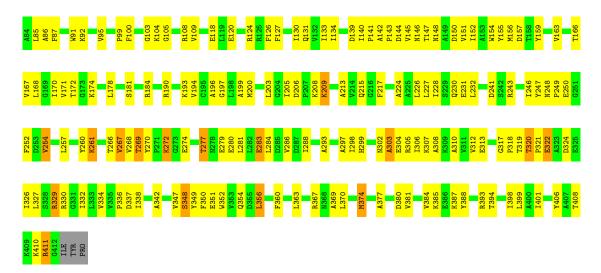
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)



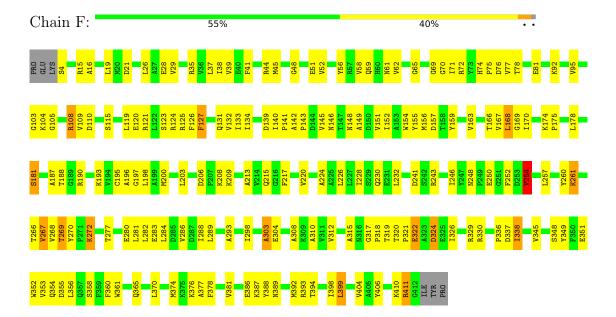
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)







• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	145.10Å 145.10Å 272.50Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	8.00 - 3.10	Depositor	
% Data completeness	94.0 (8.00-3.10)	Depositor	
(in resolution range)	34.0 (0.00 9.10)	Берозног	
R_{merge}	0.10	Depositor	
R_{sym}	0.05	Depositor	
Refinement program	X-PLOR 3.8	Depositor	
R, R_{free}	0.225 , 0.298	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	19008	wwPDB-VP	
Average B, all atoms (Å ²)	51.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

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		
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.34	0/3227	0.53	0/4367	
1	В	0.33	0/3227	0.52	0/4367	
1	С	0.33	0/3227	0.51	0/4367	
1	D	0.31	0/3227	0.51	0/4367	
1	Е	0.35	0/3227	0.53	0/4367	
1	F	0.33	0/3227	0.51	1/4367 (0.0%)	
All	All	0.33	0/19362	0.52	$1/26202 \ (0.0\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	F	168	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	3168	0	3192	118	18
1	В	3168	0	3192	117	20
1	С	3168	0	3192	114	2
1	D	3168	0	3192	124	2
1	Е	3168	0	3192	139	18
1	F	3168	0	3192	123	20

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19008	0	19152	722	40

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 19.

The worst 5 of 722 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{aligned}$
1:E:248:ASN:HD21	1:E:272:LYS:HE2	1.22	1.03
1:F:248:ASN:HD21	1:F:272:LYS:HE2	1.32	0.95
1:A:248:ASN:HD21	1:A:272:LYS:HE2	1.38	0.88
1:E:224:ALA:O	1:E:228:ILE:HG13	1.74	0.88
1:C:354:GLN:HG2	1:C:360:PHE:HA	1.55	0.87

The worst 5 of 40 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:CG	1:E:304:GLU:OE1[6_655]	0.79	1.41
1:B:279:GLU:CG	1:F:330:ARG:O[6_665]	1.00	1.20
1:A:279:GLU:OE1	1:E:330:ARG:NE[6_655]	1.11	1.09
1:B:296:GLY:O	1:F:329:ARG:NH2[6_665]	1.20	1.00
1:A:299:HIS:ND1	1:E:304:GLU:OE1[6_655]	1.28	0.92

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	Perce	entiles
1	A	407/415~(98%)	365 (90%)	39 (10%)	3 (1%)	22	57
1	В	407/415~(98%)	366 (90%)	37 (9%)	4 (1%)	15	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	С	407/415 (98%)	369 (91%)	35 (9%)	3 (1%)	22	57
1	D	407/415 (98%)	370 (91%)	33 (8%)	4 (1%)	15	49
1	E	407/415 (98%)	373 (92%)	32 (8%)	2 (0%)	29	64
1	F	407/415 (98%)	366 (90%)	37 (9%)	4 (1%)	15	49
All	All	2442/2490 (98%)	2209 (90%)	213 (9%)	20 (1%)	19	54

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	178	LEU
1	A	178	LEU
1	A	303	ALA
1	В	178	LEU
1	В	303	ALA

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	Perce	entiles
1	A	333/339 (98%)	303 (91%)	30 (9%)	9	34
1	В	333/339 (98%)	303 (91%)	30 (9%)	9	34
1	С	333/339 (98%)	301 (90%)	32 (10%)	8	31
1	D	333/339 (98%)	303 (91%)	30 (9%)	9	34
1	E	333/339 (98%)	305 (92%)	28 (8%)	11	38
1	F	333/339 (98%)	304 (91%)	29 (9%)	10	36
All	All	1998/2034 (98%)	1819 (91%)	179 (9%)	9	34

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	348	SER
1	Ε	348	SER

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Mol	Chain	Res	Type
1	D	373	MET
1	Е	217	PHE
1	F	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	357	GLN
1	F	357	GLN
1	С	365	GLN
1	D	61	ASN
1	D	230	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

