



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 02:56 AM EDT

PDB ID : 1NR7
Title : Crystal structure of apo bovine glutamate dehydrogenase
Authors : Banerjee, S.; Schmidt, T.; Fang, J.; Stanley, C.A.; Smith, T.J.
Deposited on : 2003-01-23
Resolution : 3.30 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 ⓘ 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 ⓘ](#)) 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) : 2.36.2

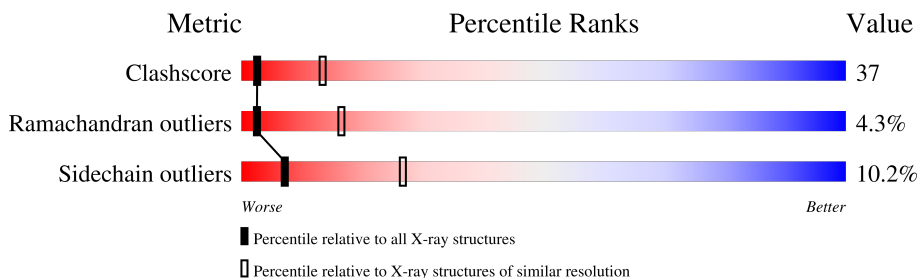
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)


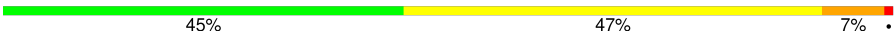


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	496	43% 48% 8%
1	B	496	47% 45% 8%
1	C	496	44% 48% 7% .
1	D	496	47% 45% 8% .
1	E	496	45% 47% 7% .
1	F	496	46% 45% 8%
1	G	496	45% 46% 7% .
1	H	496	46% 45% 8%

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Mol	Chain	Length	Quality of chain
1	I	496	 45% 45% 9% •
1	J	496	 45% 47% 7% •
1	K	496	 44% 48% 7%
1	L	496	 43% 49% 7% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 46488 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 1.

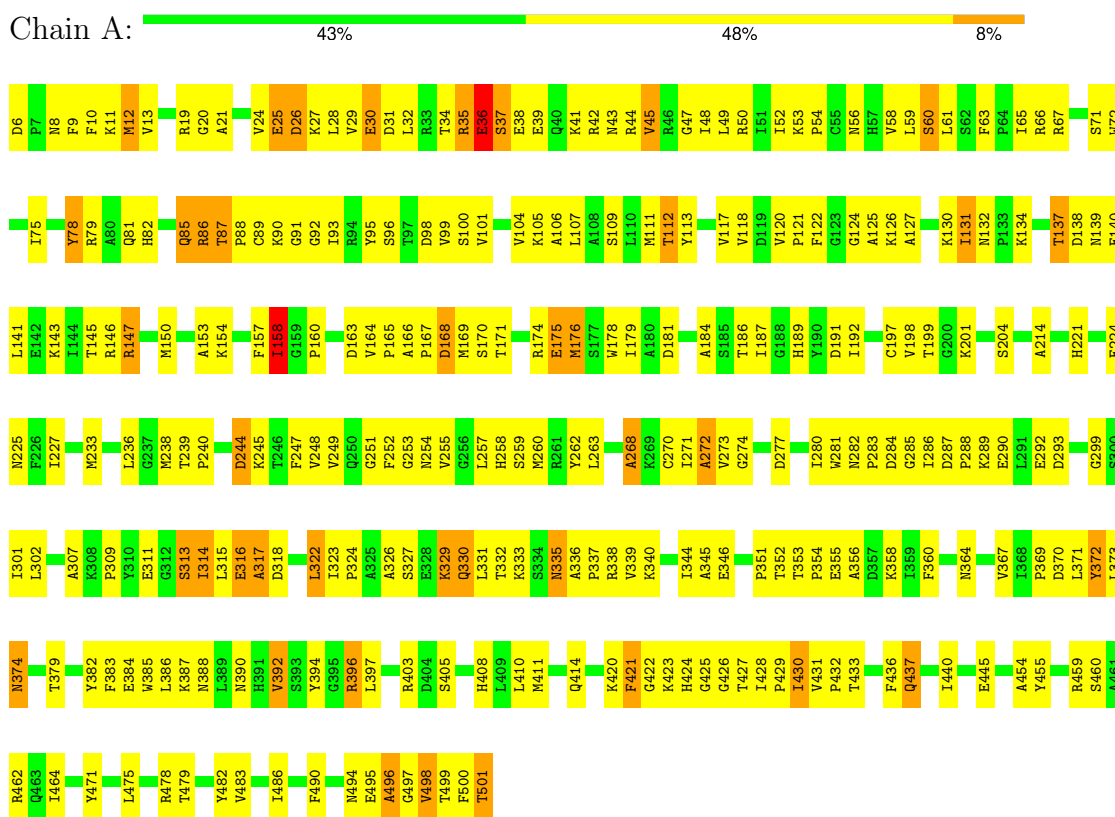
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	G	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	H	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	I	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	J	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	K	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	L	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			

3 Residue-property plots

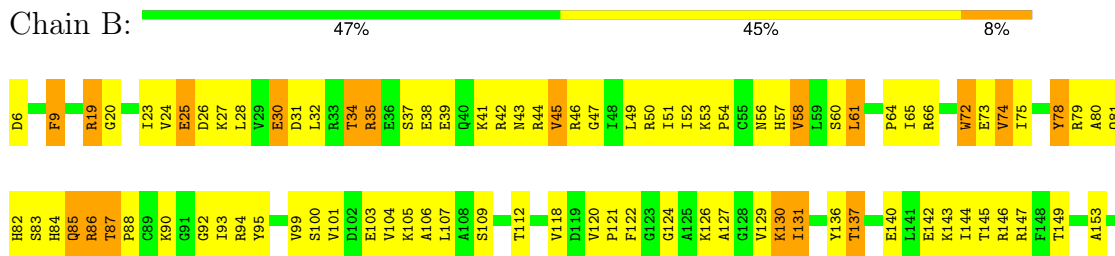
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

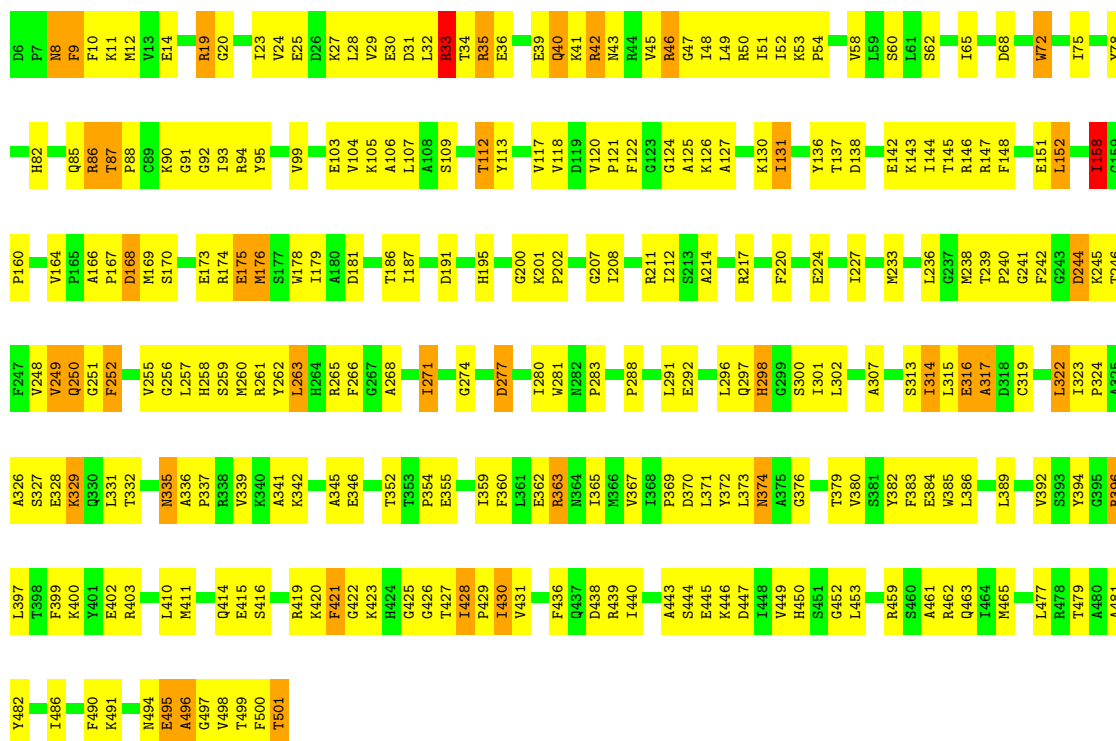
- Molecule 1: Glutamate dehydrogenase 1



- Molecule 1: Glutamate dehydrogenase 1

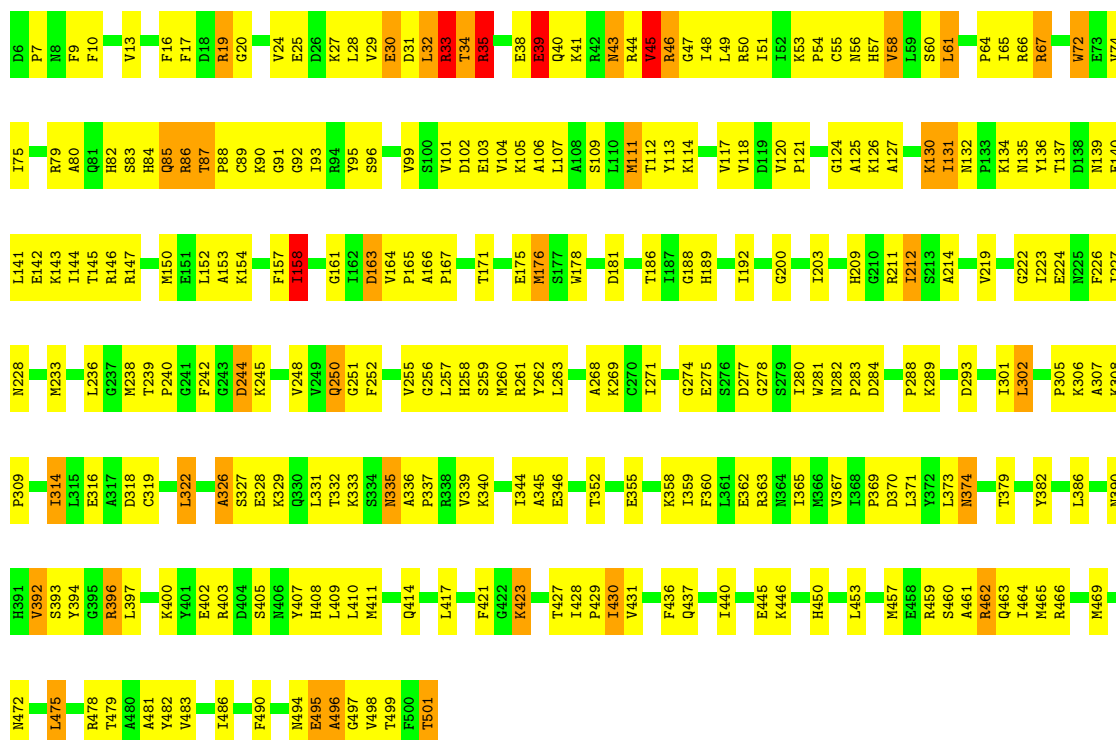






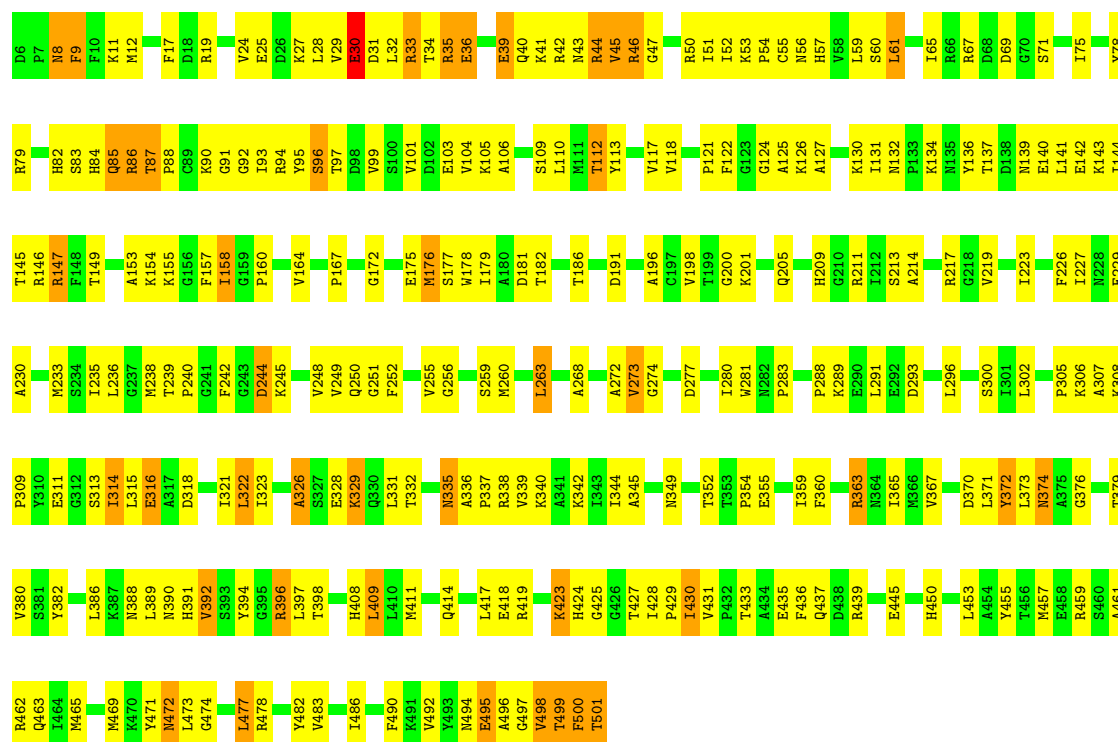
• Molecule 1: Glutamate dehydrogenase 1

Chain G: 45% 46% 7%



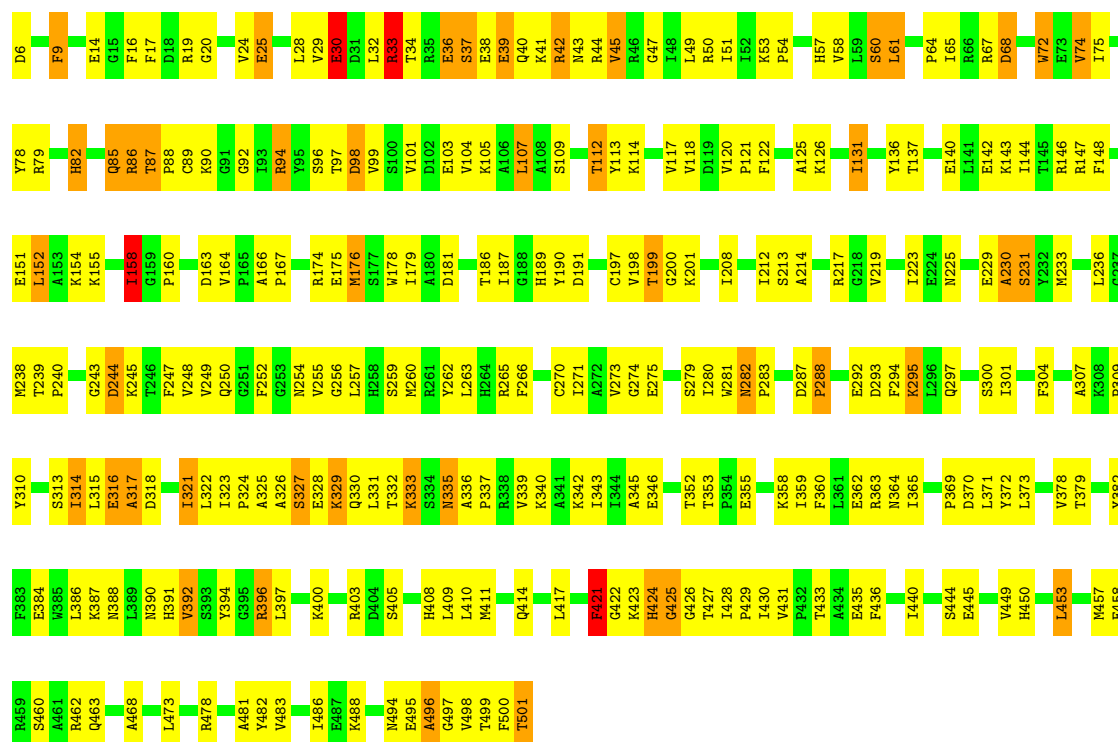
• Molecule 1: Glutamate dehydrogenase 1

Chain H:  46% 45% 8%



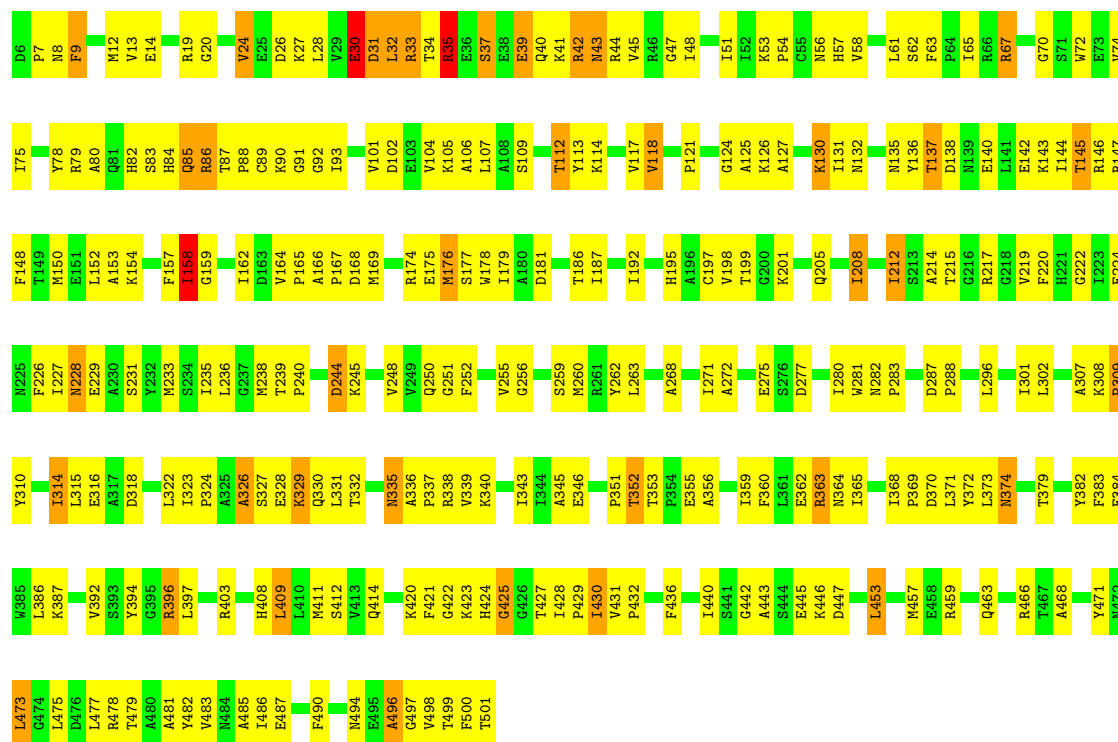
● Molecule 1: Glutamate dehydrogenase 1

Chain I:  45% 45% 9%



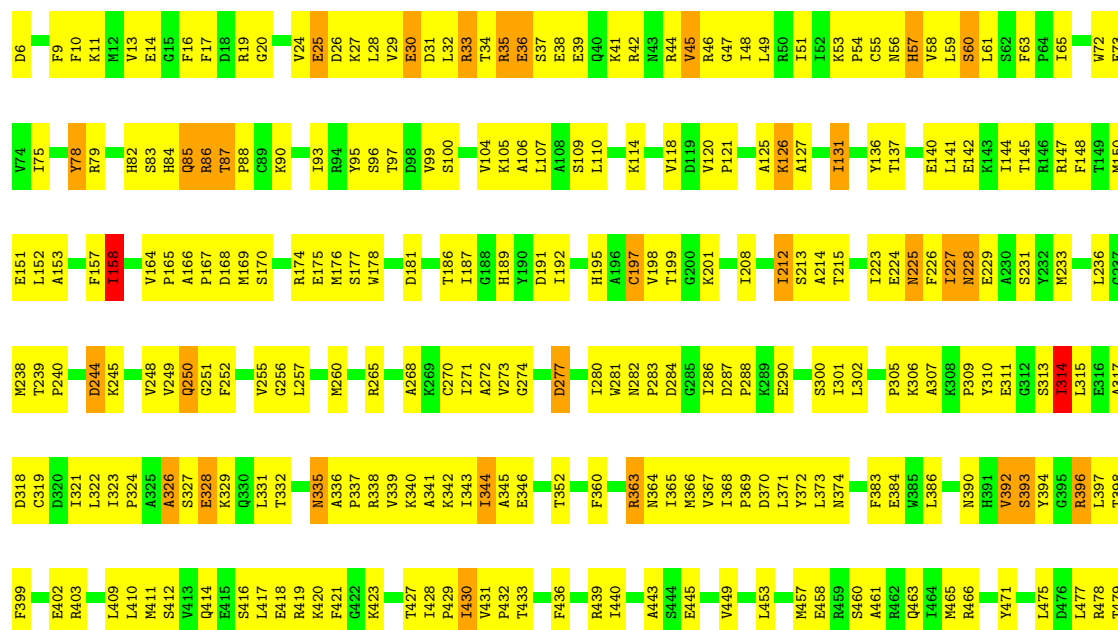
• Molecule 1: Glutamate dehydrogenase 1

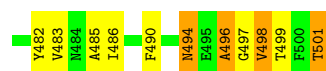
Chain J:  45% 47% 7%



• Molecule 1: Glutamate dehydrogenase 1

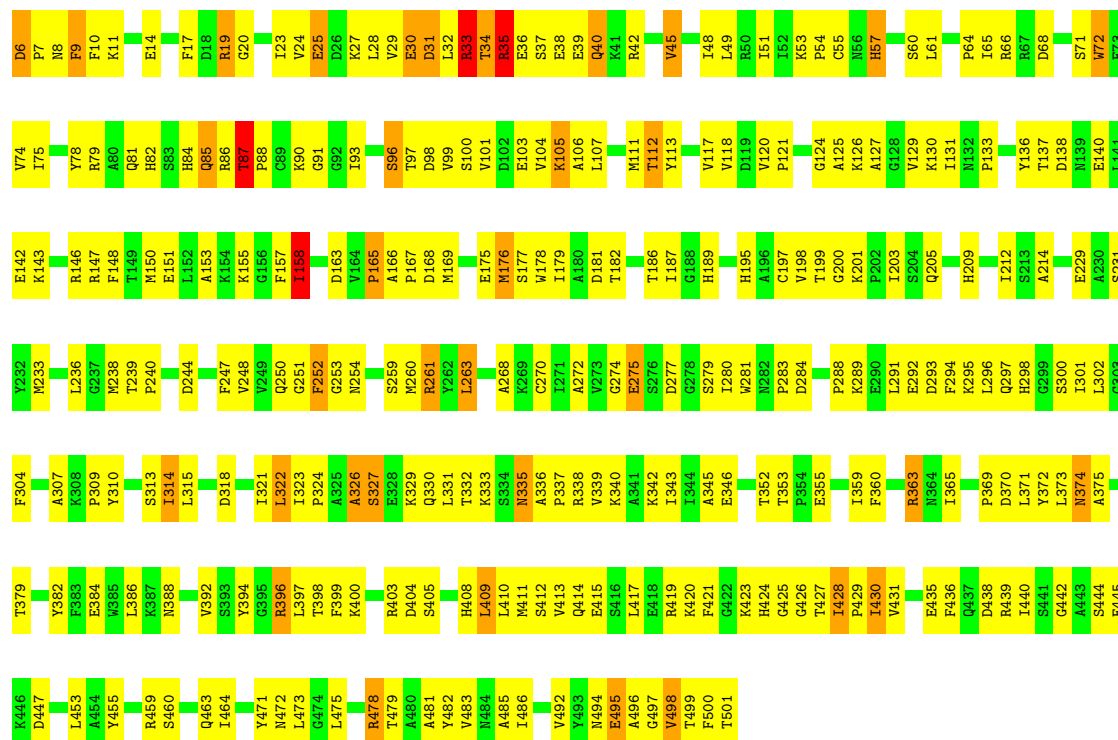
Chain K:  44% 48% 7%





● Molecule 1: Glutamate dehydrogenase 1

Chain L: 43% 49% 7%



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	96.46 Å 172.06 Å 440.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.30	Depositor
% Data completeness (in resolution range)	94.0 (19.99-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	46488	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.43	1/3958 (0.0%)	0.62	0/5340
1	B	0.48	1/3958 (0.0%)	0.64	0/5340
1	C	0.46	0/3958	0.65	0/5340
1	D	0.45	0/3958	0.63	1/5340 (0.0%)
1	E	0.48	0/3958	0.66	0/5340
1	F	0.48	0/3958	0.65	1/5340 (0.0%)
1	G	0.53	2/3958 (0.1%)	0.67	2/5340 (0.0%)
1	H	0.48	0/3958	0.66	1/5340 (0.0%)
1	I	0.43	0/3958	0.63	2/5340 (0.0%)
1	J	0.46	1/3958 (0.0%)	0.64	1/5340 (0.0%)
1	K	0.47	1/3958 (0.0%)	0.64	0/5340
1	L	0.46	0/3958	0.65	1/5340 (0.0%)
All	All	0.47	6/47496 (0.0%)	0.64	9/64080 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	CYS	CB-SG	-7.83	1.69	1.82
1	G	45	VAL	CB-CG1	6.31	1.66	1.52
1	J	89	CYS	CB-SG	-6.18	1.71	1.82
1	K	197	CYS	CB-SG	-5.46	1.73	1.81
1	A	89	CYS	CB-SG	-5.35	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	30	GLU	N-CA-C	7.50	131.25	111.00
1	I	30	GLU	N-CA-C	7.01	129.92	111.00
1	G	34	THR	N-CA-C	-6.43	93.65	111.00
1	L	34	THR	N-CA-C	-5.64	95.78	111.00
1	I	36	GLU	N-CA-C	-5.35	96.55	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	3874	0	3841	295	0
1	B	3874	0	3841	317	0
1	C	3874	0	3841	323	0
1	D	3874	0	3841	299	0
1	E	3874	0	3841	300	0
1	F	3874	0	3841	310	0
1	G	3874	0	3841	305	0
1	H	3874	0	3841	272	0
1	I	3874	0	3841	304	0
1	J	3874	0	3841	277	0
1	K	3874	0	3841	309	0
1	L	3874	0	3841	312	0
All	All	46488	0	46092	3398	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 37.

The worst 5 of 3398 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:G:33:ARG:HH11	1:G:33:ARG:HB2	1.04	1.14
1:L:33:ARG:HH11	1:L:33:ARG:HB2	1.06	1.11
1:C:28:LEU:HA	1:C:32:LEU:HD22	1.33	1.10
1:C:47:GLY:HA2	1:C:50:ARG:HD3	1.28	1.10
1:A:323:ILE:HG22	1:A:345:ALA:HB3	1.32	1.08

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	494/496 (100%)	399 (81%)	70 (14%)	25 (5%)	2	13
1	B	494/496 (100%)	405 (82%)	71 (14%)	18 (4%)	3	20
1	C	494/496 (100%)	394 (80%)	80 (16%)	20 (4%)	3	18
1	D	494/496 (100%)	397 (80%)	75 (15%)	22 (4%)	2	15
1	E	494/496 (100%)	408 (83%)	61 (12%)	25 (5%)	2	13
1	F	494/496 (100%)	420 (85%)	56 (11%)	18 (4%)	3	20
1	G	494/496 (100%)	404 (82%)	69 (14%)	21 (4%)	2	16
1	H	494/496 (100%)	416 (84%)	63 (13%)	15 (3%)	4	24
1	I	494/496 (100%)	413 (84%)	57 (12%)	24 (5%)	2	14
1	J	494/496 (100%)	402 (81%)	73 (15%)	19 (4%)	3	19
1	K	494/496 (100%)	390 (79%)	82 (17%)	22 (4%)	2	15
1	L	494/496 (100%)	398 (81%)	73 (15%)	23 (5%)	2	14
All	All	5928/5952 (100%)	4846 (82%)	830 (14%)	252 (4%)	2	16

5 of 252 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	36	GLU
1	A	254	ASN
1	A	496	ALA
1	B	30	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	413/413 (100%)	372 (90%)	41 (10%)	8	28
1	B	413/413 (100%)	376 (91%)	37 (9%)	9	32
1	C	413/413 (100%)	369 (89%)	44 (11%)	6	25
1	D	413/413 (100%)	372 (90%)	41 (10%)	8	28
1	E	413/413 (100%)	366 (89%)	47 (11%)	5	22
1	F	413/413 (100%)	372 (90%)	41 (10%)	8	28
1	G	413/413 (100%)	374 (91%)	39 (9%)	8	30
1	H	413/413 (100%)	364 (88%)	49 (12%)	5	21
1	I	413/413 (100%)	375 (91%)	38 (9%)	9	31
1	J	413/413 (100%)	370 (90%)	43 (10%)	7	25
1	K	413/413 (100%)	373 (90%)	40 (10%)	8	29
1	L	413/413 (100%)	368 (89%)	45 (11%)	6	24
All	All	4956/4956 (100%)	4451 (90%)	505 (10%)	7	27

5 of 505 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	250	GLN
1	K	311	GLU
1	G	472	ASN
1	K	215	THR
1	L	85	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	82	HIS
1	K	189	HIS
1	I	254	ASN
1	J	85	GLN
1	K	406	ASN

5.3.3 RNA ⓘ

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.