wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:11 PM GMT

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
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:

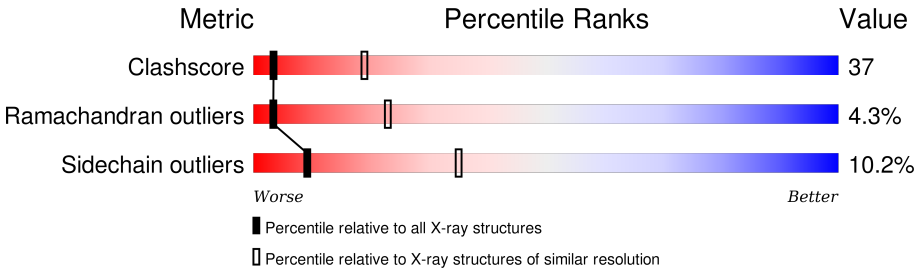
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.30 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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	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%

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Mol	Chain	Length	Quality of chain
1	H	496	46% 45% 8%
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 (i)

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			

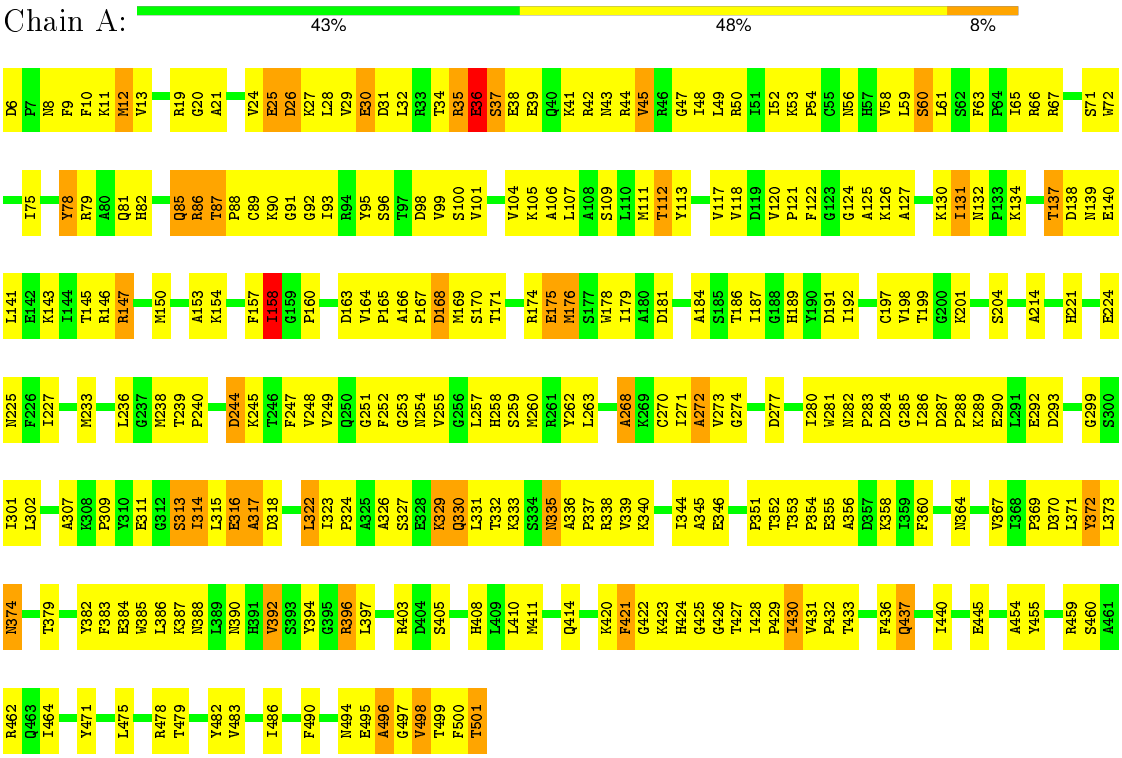
3 Residue-property plots (i)

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.

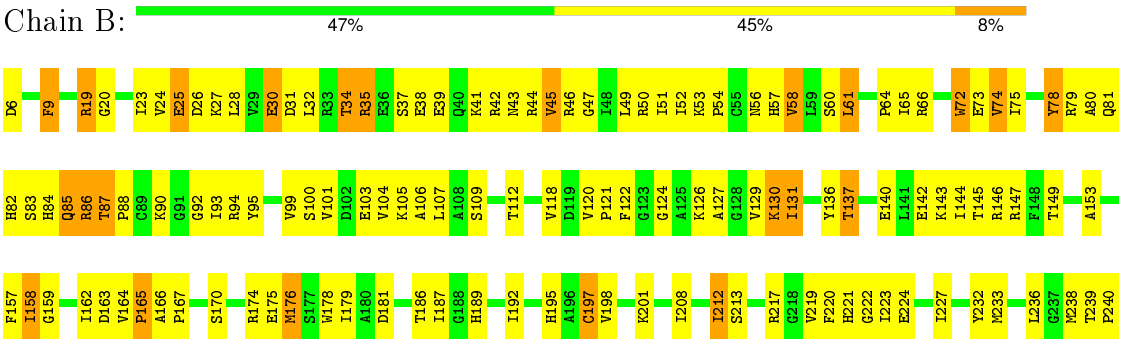
- Molecule 1: Glutamate dehydrogenase 1

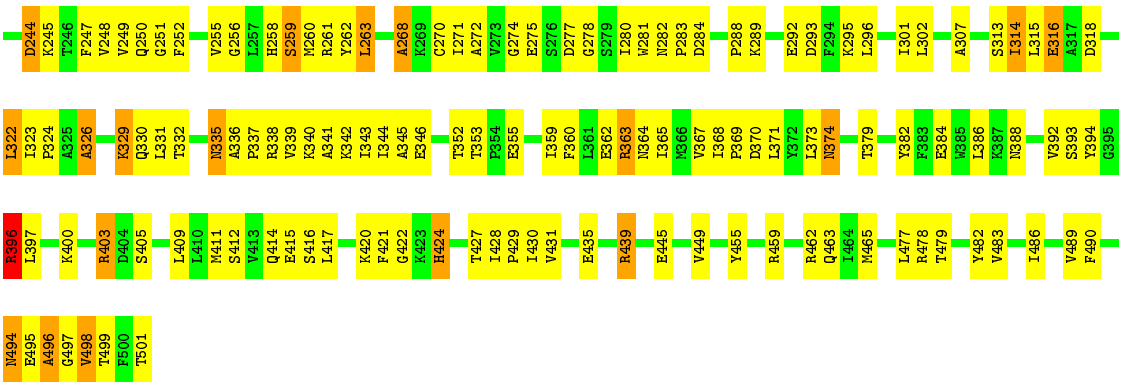
Chain A:



- Molecule 1: Glutamate dehydrogenase 1

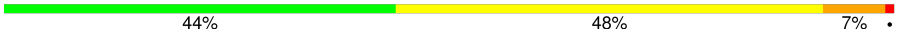
Chain B:

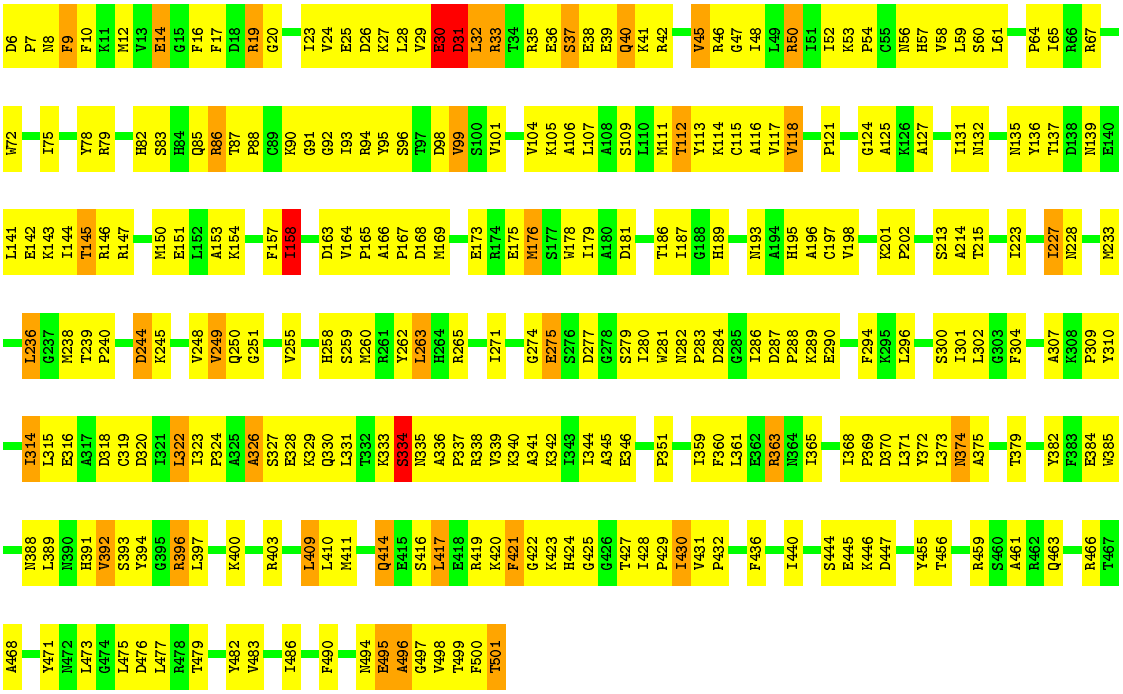




• Molecule 1: Glutamate dehydrogenase 1

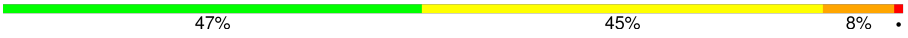
Chain C:

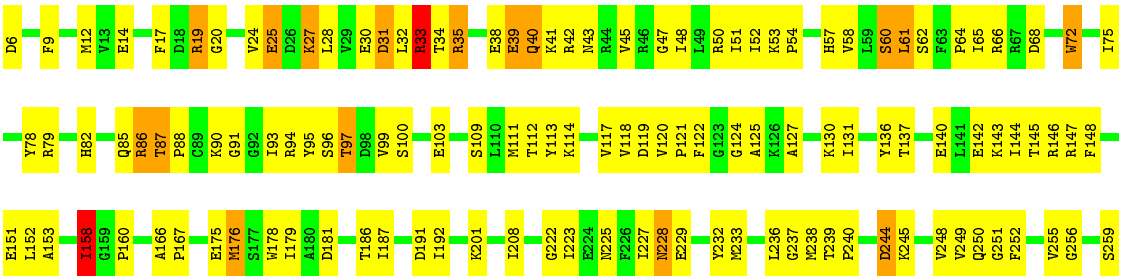


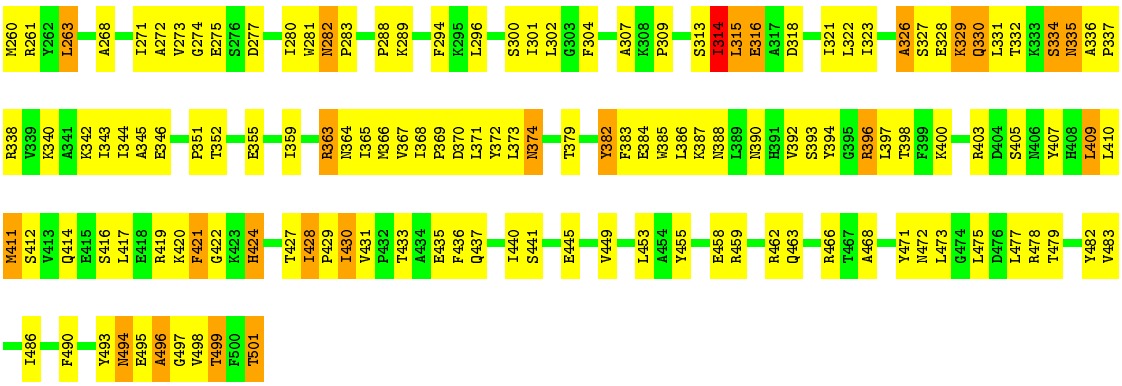


• Molecule 1: Glutamate dehydrogenase 1

Chain D:

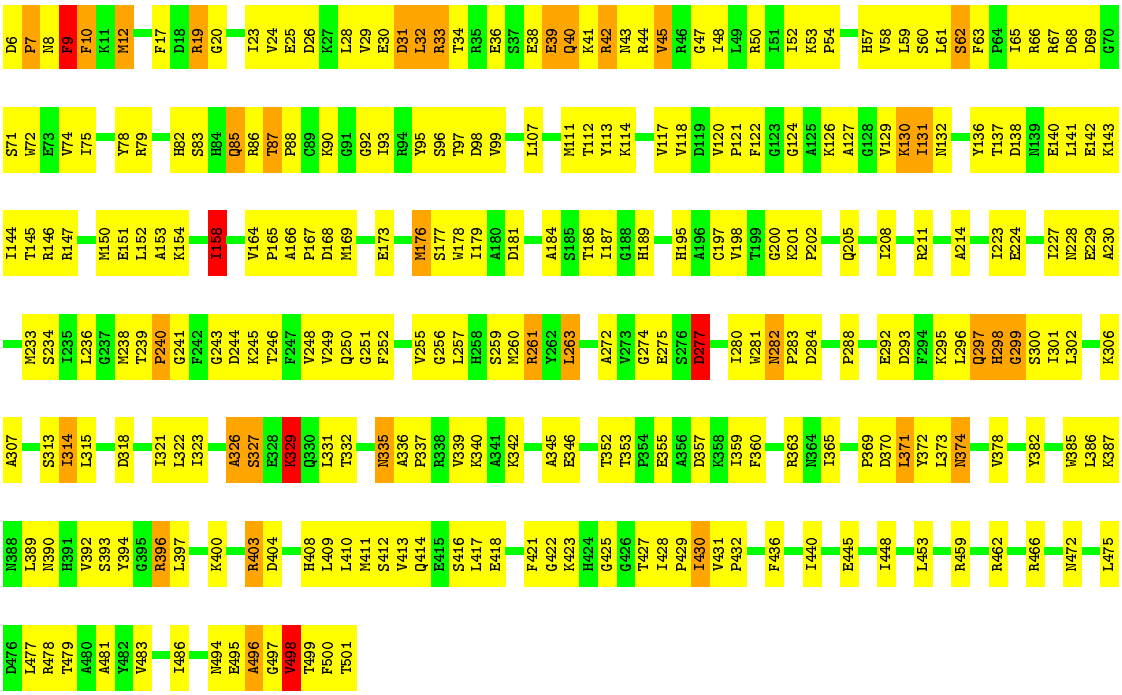






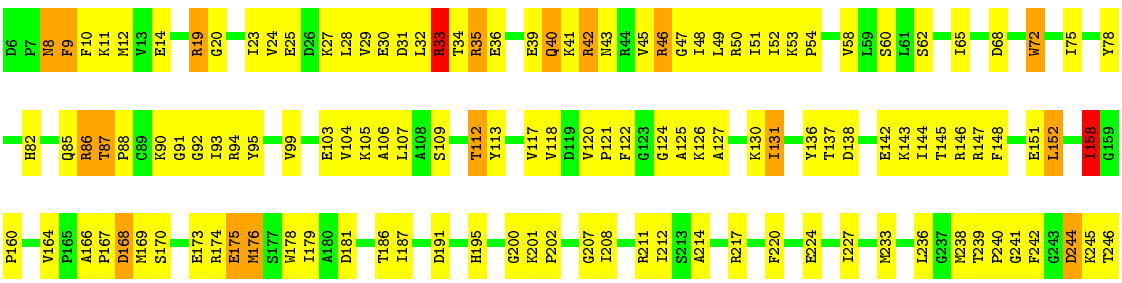
• Molecule 1: Glutamate dehydrogenase 1

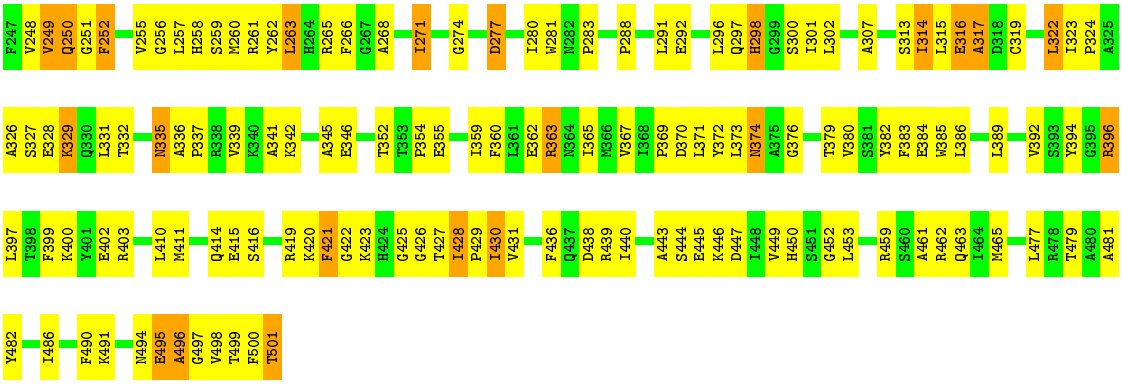
Chain E:



• Molecule 1: Glutamate dehydrogenase 1

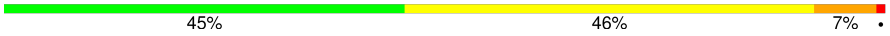
Chain F:

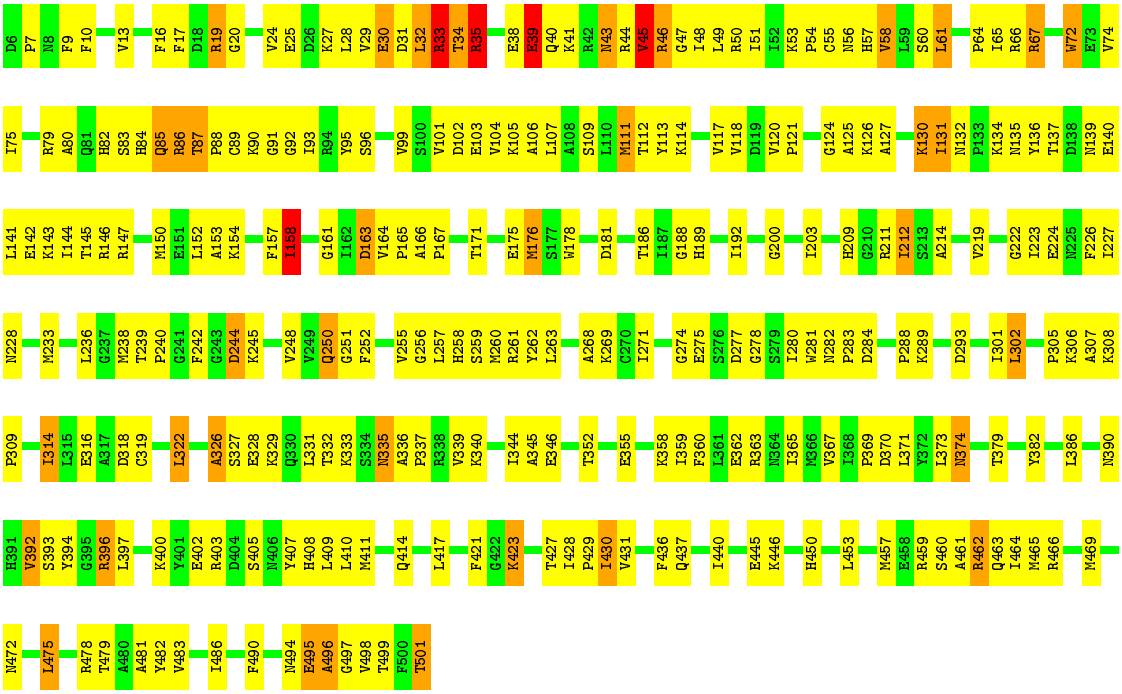




• Molecule 1: Glutamate dehydrogenase 1

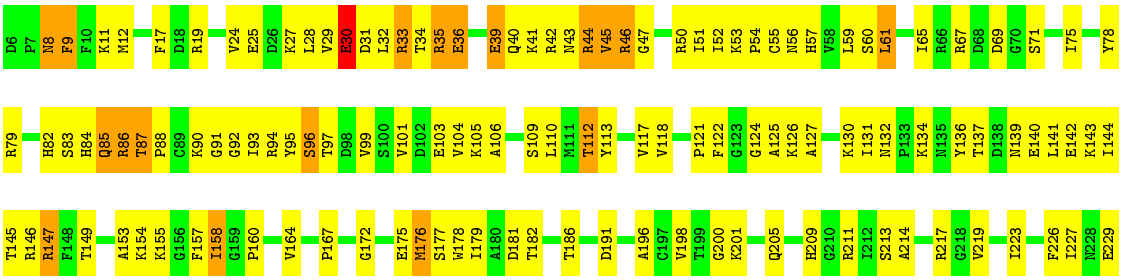
Chain G:

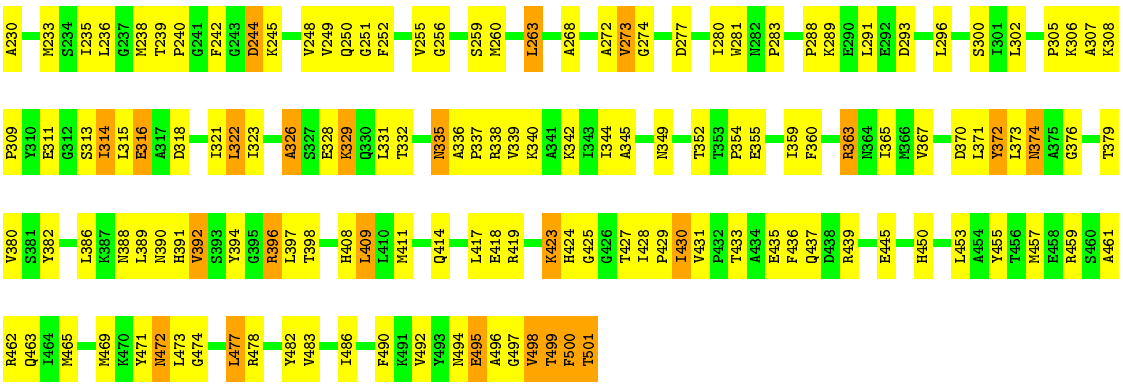




• Molecule 1: Glutamate dehydrogenase 1

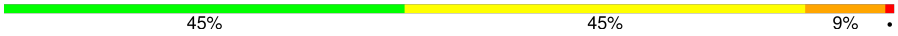
Chain H:

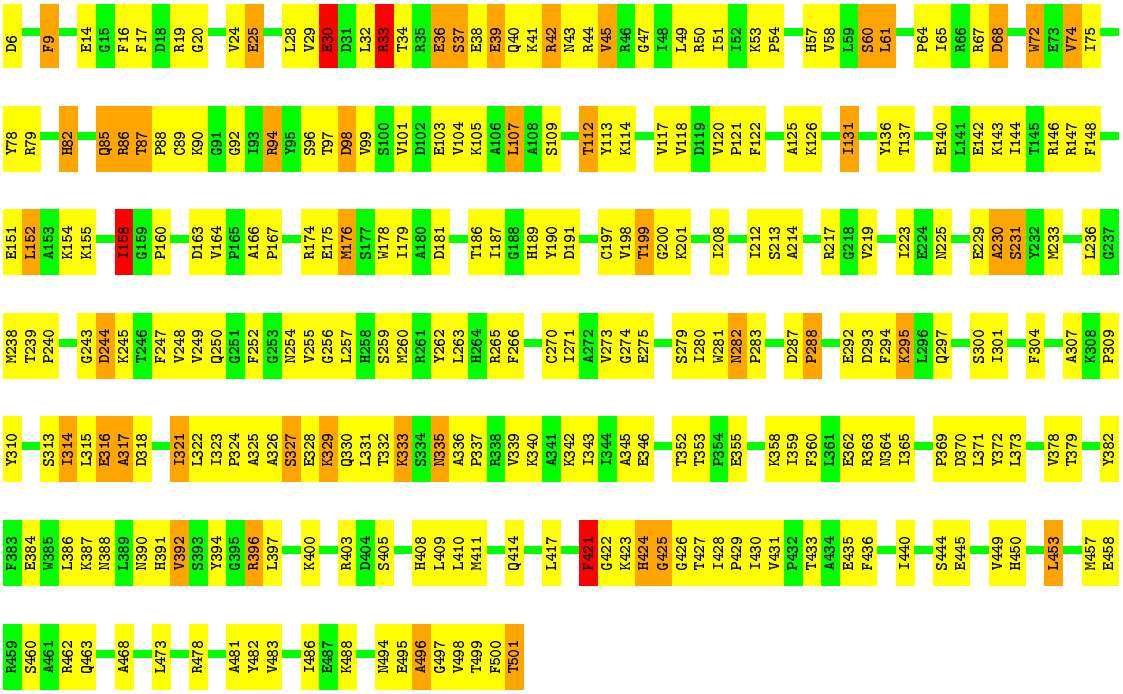




- Molecule 1: Glutamate dehydrogenase 1

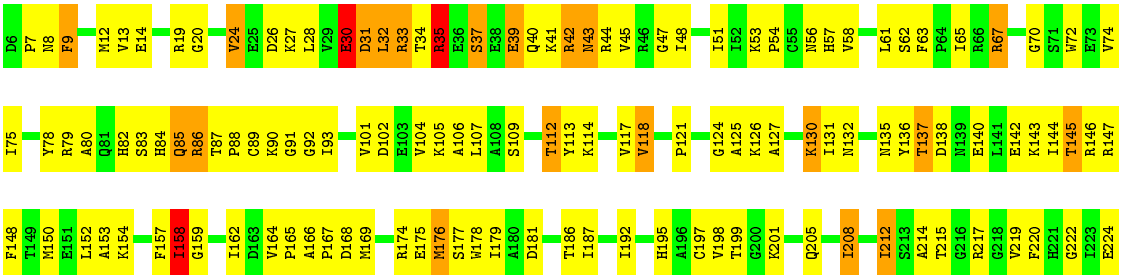
Chain I:

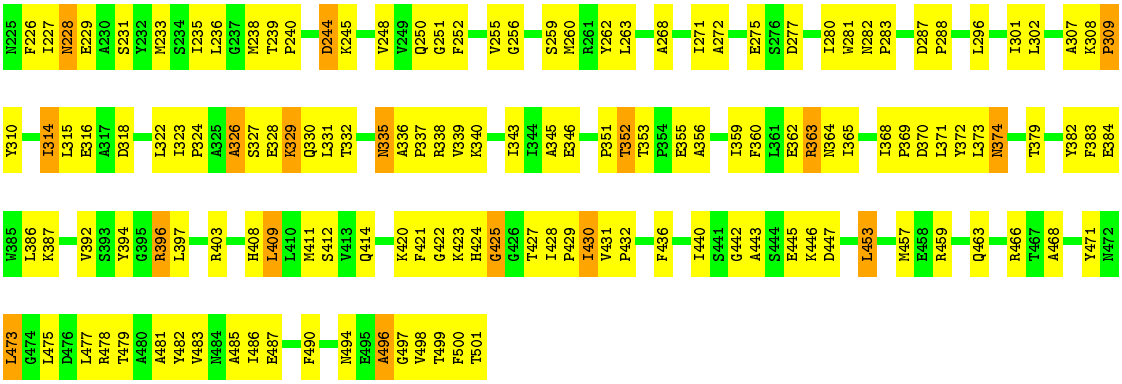




- Molecule 1: Glutamate dehydrogenase 1

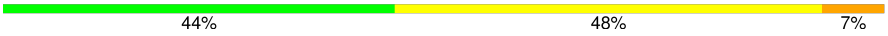
Chain J:

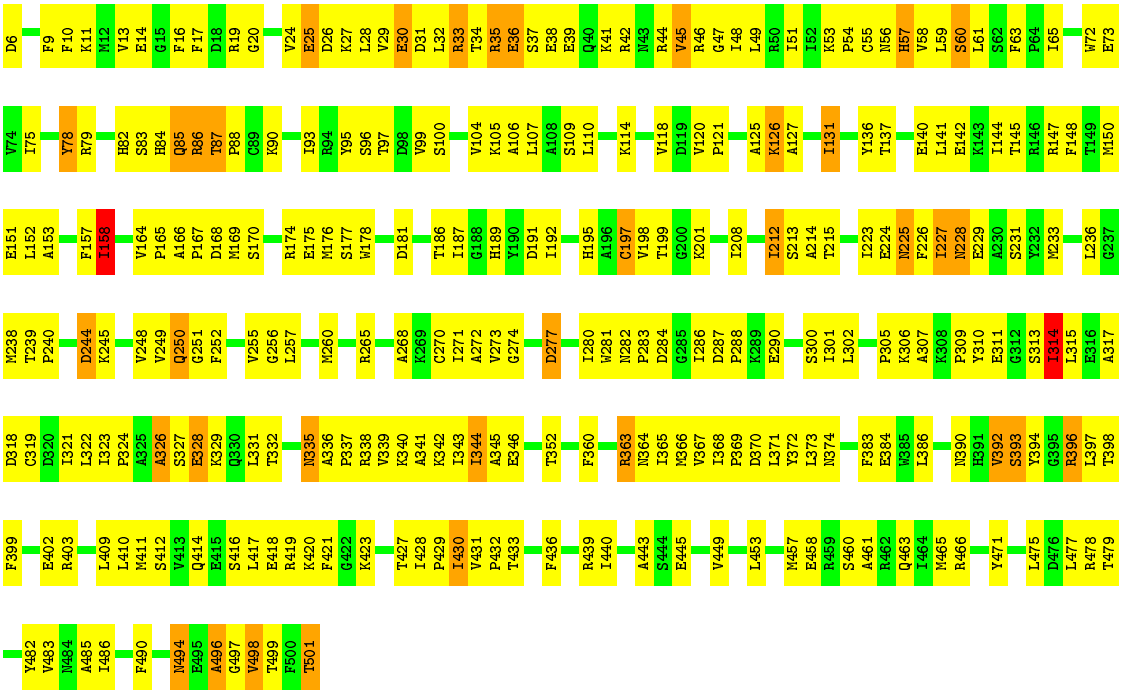




- Molecule 1: Glutamate dehydrogenase 1

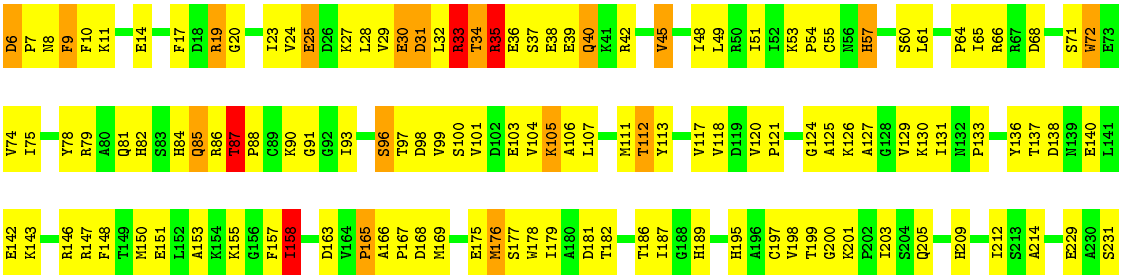
Chain K:

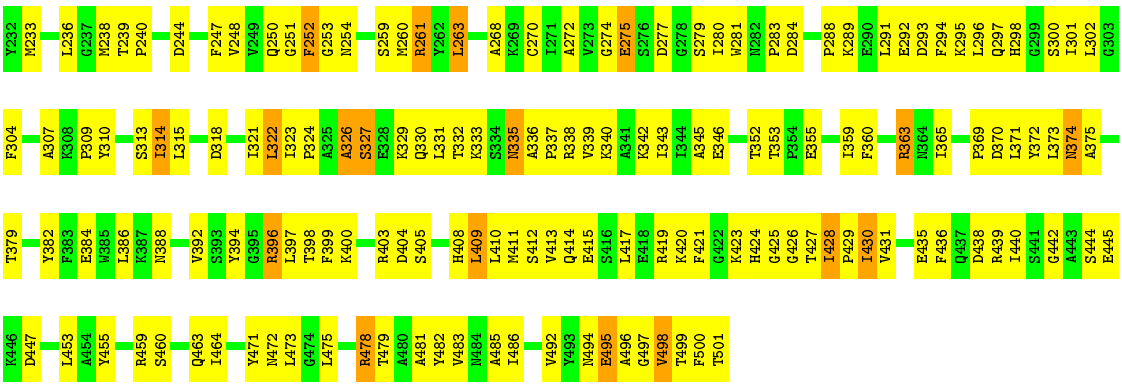




- Molecule 1: Glutamate dehydrogenase 1

Chain L:




Y232 M233 L236 G237 M238 T239 P240 D244 F247 V248 V249 Q250 G251 F252 G253 N254 S259 M260 R261 Y262 L263 A268 K269 C270 T271 A272 Y273 G274 E275 S276 D277 G278 S279 I280 W281 N282 P283 D284 P288 K289 E290 L291 E292 D293 F294 K295 L296 Q297 H298 G299 S300 I301 L302 G303
F304 A307 K308 P309 Y310 S313 I314 L315 D318 I321 L322 I323 P324 A325 A326 S327 E328 K329 Q330 L331 T332 K333 S334 N335 A336 P337 R338 V339 K340 A341 K342 I343 I344 A345 E346 T352 T353 P354 E355 I359 F360 R363 N364 I365 P369 D370 L371 Y372 L373 N374 A375
T379 Y382 F383 E384 W385 L386 K387 N388 V392 S393 Y394 G395 R396 L397 T398 F399 K400 R403 D404 S405 H408 L409 L410 M411 S412 V413 Q414 E415 S416 L417 E418 R419 K420 F421 G422 K423 H424 G425 G426 T427 I428 P429 I430 V431 E435 F436 Q437 D438 R439 I440 S441 G442 A443 S444 E445
K446 D447 L453 A454 Y455 R459 S460 Q463 I464 Y471 N472 L473 G474 L475 R478 T479 A480 A481 Y482 V483 N484 A485 I486 V492 Y493 N494 E495 A496 G497 V498 T499 P500 T501

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.46Å 172.06Å 440.75Å 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 1.1	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(^{o})	Ideal(^{o})
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 (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	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:HB2	1:G:33:ARG:HH11	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

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	494/496 (100%)	399 (81%)	70 (14%)	25 (5%)	2	19
1	B	494/496 (100%)	405 (82%)	71 (14%)	18 (4%)	4	28
1	C	494/496 (100%)	394 (80%)	80 (16%)	20 (4%)	4	24
1	D	494/496 (100%)	397 (80%)	75 (15%)	22 (4%)	3	21
1	E	494/496 (100%)	408 (83%)	61 (12%)	25 (5%)	2	19
1	F	494/496 (100%)	420 (85%)	56 (11%)	18 (4%)	4	28
1	G	494/496 (100%)	404 (82%)	69 (14%)	21 (4%)	3	23
1	H	494/496 (100%)	416 (84%)	63 (13%)	15 (3%)	5	33
1	I	494/496 (100%)	413 (84%)	57 (12%)	24 (5%)	3	19
1	J	494/496 (100%)	402 (81%)	73 (15%)	19 (4%)	4	26
1	K	494/496 (100%)	390 (79%)	82 (17%)	22 (4%)	3	21
1	L	494/496 (100%)	398 (81%)	73 (15%)	23 (5%)	3	20
All	All	5928/5952 (100%)	4846 (82%)	830 (14%)	252 (4%)	3	23

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

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%)	10 37
1	B	413/413 (100%)	376 (91%)	37 (9%)	12 42
1	C	413/413 (100%)	369 (89%)	44 (11%)	8 32
1	D	413/413 (100%)	372 (90%)	41 (10%)	10 37
1	E	413/413 (100%)	366 (89%)	47 (11%)	7 29
1	F	413/413 (100%)	372 (90%)	41 (10%)	10 37
1	G	413/413 (100%)	374 (91%)	39 (9%)	11 39
1	H	413/413 (100%)	364 (88%)	49 (12%)	6 27
1	I	413/413 (100%)	375 (91%)	38 (9%)	11 40
1	J	413/413 (100%)	370 (90%)	43 (10%)	9 34
1	K	413/413 (100%)	373 (90%)	40 (10%)	10 38
1	L	413/413 (100%)	368 (89%)	45 (11%)	8 32
All	All	4956/4956 (100%)	4451 (90%)	505 (10%)	9 35

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

Mol	Chain	Res	Type
1	F	175	GLU
1	G	417	LEU
1	L	40	GLN
1	F	271	ILE
1	G	39	GLU

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

Mol	Chain	Res	Type
1	F	228	ASN
1	G	388	ASN
1	L	250	GLN
1	F	258	HIS
1	G	57	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.