



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:42 pm GMT

PDB ID : 5K12
EMDB ID: : EMD-8194
Title : Cryo-EM structure of glutamate dehydrogenase at 1.8 Å resolution
Authors : Merk, A.; Bartesaghi, A.; Banerjee, S.; Falconieri, V.; Rao, P.; Earl, L.; Milne, J.; Subramaniam, S.
Deposited on : 2016-05-17
Resolution : 1.80 Å (reported)
Based on PDB ID : 1NR7

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

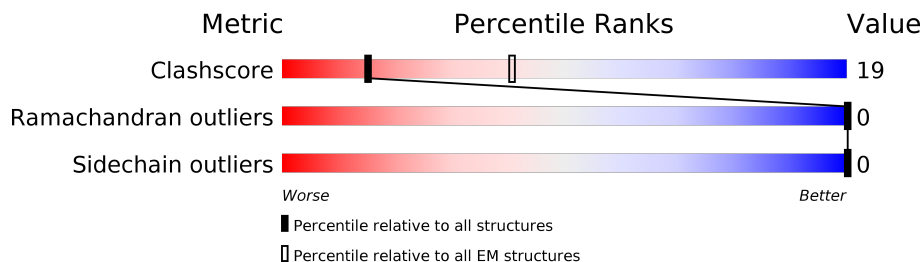
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.80 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	558	36% 16% 47%
1	B	558	36% 16% 47%
1	C	558	36% 16% 47%
1	D	558	36% 16% 47%
1	E	558	37% 16% 47%
1	F	558	36% 16% 47%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	B	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	C	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	D	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	E	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	F	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	LYS	ASN	conflict	UNP P00366
B	387	LYS	ASN	conflict	UNP P00366
C	387	LYS	ASN	conflict	UNP P00366
D	387	LYS	ASN	conflict	UNP P00366
E	387	LYS	ASN	conflict	UNP P00366
F	387	LYS	ASN	conflict	UNP P00366

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	A	181	Total	O	0
			181	181	
2	B	182	Total	O	0
			182	182	
2	C	180	Total	O	0
			180	180	
2	D	181	Total	O	0
			181	181	

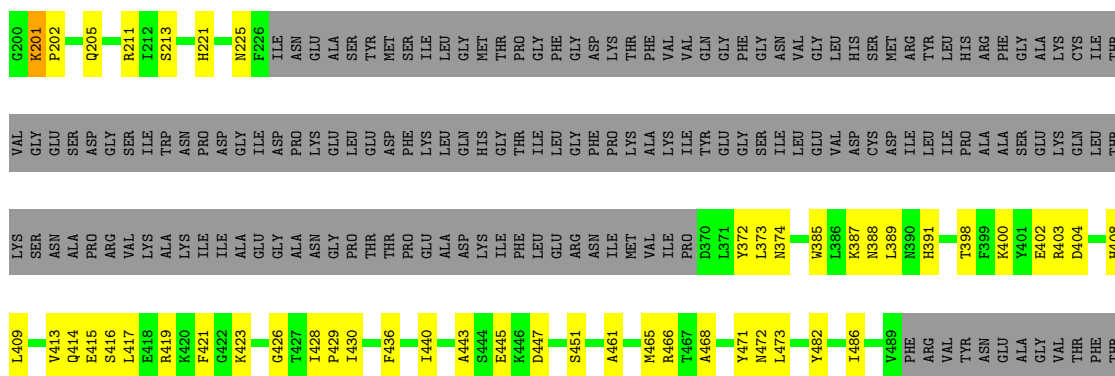
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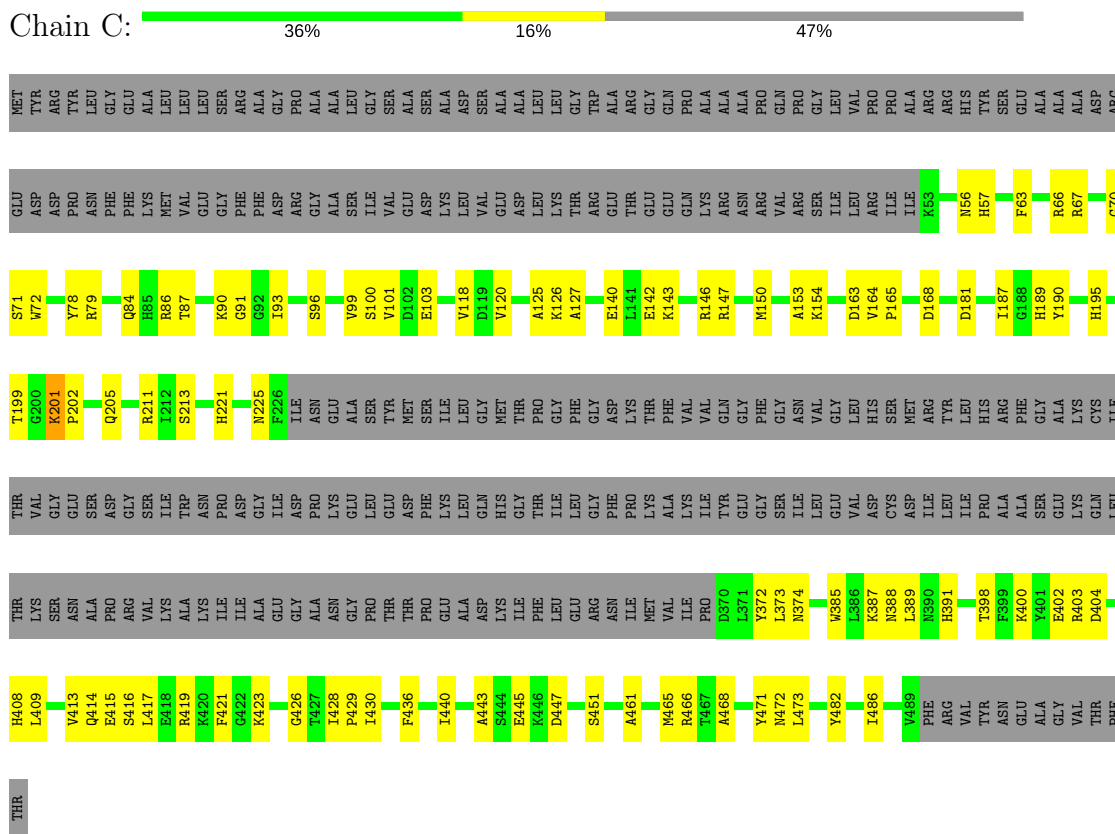
Mol	Chain	Residues	Atoms		AltConf
2	E	181	Total 181	O 181	0
2	F	181	Total 181	O 181	0

- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

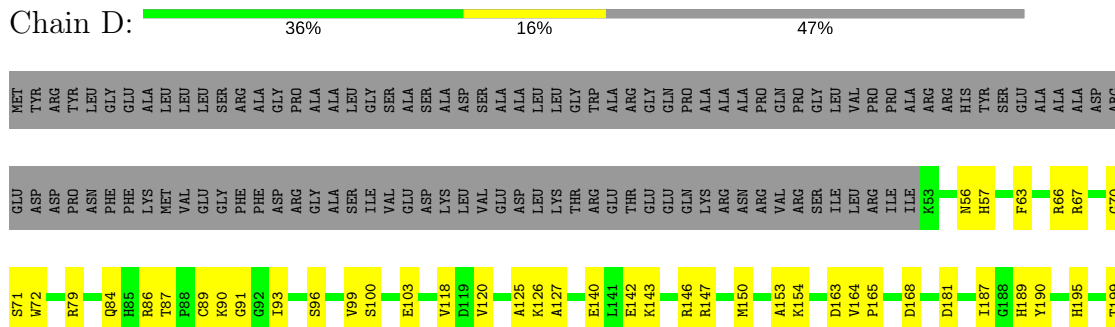




- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial





V413	Q414	E415	S416	L417	E418	R419	K420	F421	K422	K423	H424	G425	G426	I427	I428	P429	I430	F436	I440	A443	S444	E445	K446	D447	S451	A461	M465	R466	T467	A468	Y471	N472	L473	Y482	I486	V489	PHE	ARG	VAL	TYR	ASN	GLU	ALA	GLY	VAL	THR	THR																																												
																																SER	ASN	ALA	PRO	ARG	VAL	LYS	ALA	LYS	ILE	ILE	ALA	GLU	GLY	PRO	THR	THR	PRO	GLU	ALA	ASP	LYS	ILE	PHE	LEU	GLY	ASN	ILE	MET	VAL	ILE	PRO	D370	L371	Y372	L373			W385	L386	K387	N388	L389	N390	H391			T398	F399	K400	Y401	E402	R403	D404			H408	L409		
GLY	GLU	SER	ASP	GLY	SER	ILE	TRP	ASN	PRO	ASP	GLY	ILE	ASP	PRO	LYS	GLU	LEU	GLU	ASP	PHE	LYS	GLN	HIS	GLY	THR	ILE	LEU	GLY	PHE	PRO	LYS	ALA	LYS	ILE	TYR	GLU	GLY	SER	ILE	LEU	GLU	VAL	ASP	CYS	ASP	ILE	LEU	ILE	PRO	ALA	ALA	SER	GLU	LYS	GLN	LEU	THR	LYS																																	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	21818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	78000	Depositor
Image detector	Not provided	Depositor

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	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.43	0/2345	0.55	1/3166 (0.0%)
1	B	0.43	0/2345	0.55	1/3166 (0.0%)
1	C	0.43	0/2345	0.55	1/3166 (0.0%)
1	D	0.43	0/2345	0.55	0/3166
1	E	0.43	0/2345	0.55	1/3166 (0.0%)
1	F	0.43	0/2345	0.55	1/3166 (0.0%)
All	All	0.43	0/14070	0.55	5/18996 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	LYS	C-N-CD	5.02	138.94	128.40
1	A	201	LYS	C-N-CD	5.01	138.93	128.40
1	F	201	LYS	C-N-CD	5.01	138.92	128.40
1	E	201	LYS	C-N-CD	5.00	138.91	128.40
1	C	201	LYS	C-N-CD	5.00	138.90	128.40

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	2295	0	2261	94	0
1	B	2295	0	2261	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2295	0	2261	93	0
1	D	2295	0	2261	92	0
1	E	2295	0	2261	89	0
1	F	2295	0	2261	92	0
2	A	181	0	0	18	0
2	B	182	0	0	20	0
2	C	180	0	0	18	0
2	D	181	0	0	20	0
2	E	181	0	0	16	0
2	F	181	0	0	16	0
All	All	14856	0	13566	512	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 19.

The worst 5 of 512 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:142:GLU:O	1:B:146:ARG:HG3	1.62	0.99
1:D:142:GLU:O	1:D:146:ARG:HG3	1.62	0.99
1:A:142:GLU:O	1:A:146:ARG:HG3	1.62	0.99
1:C:142:GLU:O	1:C:146:ARG:HG3	1.62	0.99
1:E:142:GLU:O	1:E:146:ARG:HG3	1.62	0.98

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 PDB entries followed by that with respect to all EM entries.

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	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	B	290/558 (52%)	279 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	D	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	E	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	F	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
All	All	1740/3348 (52%)	1674 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	244/456 (54%)	244 (100%)	0	100	100
1	B	244/456 (54%)	244 (100%)	0	100	100
1	C	244/456 (54%)	244 (100%)	0	100	100
1	D	244/456 (54%)	244 (100%)	0	100	100
1	E	244/456 (54%)	244 (100%)	0	100	100
1	F	244/456 (54%)	244 (100%)	0	100	100
All	All	1464/2736 (54%)	1464 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	388	ASN
1	D	195	HIS
1	F	209	HIS
1	D	189	HIS
1	D	209	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.