

wwPDB EM Validation Summary Report (i)

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PDB ID : 8KGY EMDB ID EMD-37235 : Title : Human glutamate dehydrogenase I Authors Su, M.-Y. : Deposited on 2023-08-20 : 2.59 Å(reported) Resolution : Based on initial model 1L1F:

This is a wwPDB EM 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/EMValidationReportHelp 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 (1)) were used in the production of this report:

EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 2.59 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain				
1	А	558	78%	9%	13%		
1	В	558	75%	12%	12%		
1	С	558	76%	12%	12%		
1	D	558	73%	14%	13%		
1	Е	558	77%	10%	13%		
1	F	558	73%	14%	13%		



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21846 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.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	Δ	188	Total	С	Ν	0	S	0	0
1	Π	400	3552	2271	630	634	17	0	0
1	В	489	Total	С	Ν	0	\mathbf{S}	0	0
1	D		3670	2332	651	669	18	0	0
1	C	480	Total	С	Ν	0	S	0	0
	409	3658	2323	647	670	18	0	0	
1	П	195	Total	С	Ν	0	S	0	0
1	D	400	3641	2309	639	675	18	0	0
1	F	195	Total	С	Ν	0	S	0	0
	480	3648	2316	644	670	18	0	U	
1	1 E	485	Total	С	Ν	0	S	0	0
	Ľ	400	3677	2329	650	680	18	0	0

• Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.



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.

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial





P489 1284 F493 1284 S503 S517 S517 S28 A518 M290 A518 T303 V555 T303 THR T303 THR T303 M522 F304 V555 T303 F557 T303 T1303 T333 M364 M385 M364 M385 M364 M385 M364 M385 M364 M383 M364 M385 M364 M385 M364 M385 M364 M385 M364 M385 M365 M365 M366 M366

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D:	73%	14%	13%
MET TYR TYR ARG TYR LEU GLU GLU CLEU LEU LEU LEU SER ARG	GLY ALA ALA ALA ALA CLEU CLEU CLEU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ALA ALA ALA ALA ALA GLN GLN GLV GLV LEU ALA ALA ALA	ANG ARG HIS TYR SER GLU GLU VAL ALA ALA ASP ASP
GLU ASP ASP P64 ASP V81 V81 V81 AR9 AR9 CLU	SSR 595 595 596 697 709 709 709 1005 1106 1106 1106 1106 1106 1106 1123 1123 1123 1123 1123 1123 1123 1123 1123 1123 1123 1123 1123 1123 1136 11	1150 1150 1152 1152 1152 1152 1153 1153 1153 1153	AL24 K187 1188 1188 1188 1198 1198 1198 1201
D220 P224 M233 E286 E286 M200 C293 C293	T296 PR0 GLY CLY CLY CLY CL CL CL CL CL CL CL CL CL CL CL CL CL	A364 8384 8385 8385 8385 8385 8387 8387 8387 8387	F411 E412 A413 F417 F417 1425 1425 F426
0433 6437 6437 6437 6475 6475 6483 6483 6483	1484 1486 1486 1487 1487 1486 1486 1486 1488 1488 1488 1488 1508 1508 1532 1532 1532 1532 1532 1532 1535 17555 1532 1532 1535 1535 1535 1535 1535 1	THR THR	
• Molecule 1: Gluta	amate dehydrogenase 1, mitoch	ondrial	
Chain E:	77%	10%	13%
MET TYR TYR ARG CLY GLY GLV GLU LEU LEU LEU SER ARG ALA	CLY ALA ALA ALA ALA ALA SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ALA ALA ALA ALA PRO GLN PRO GLV LEU ALA ALA	ARG HIS TYR SER SER GLU ALA ALA ALA ASP ARG
GLU ASP ASP ASP A64 M65 A65 A78 A78 A78 A78 R90 R90	T91 ARG GLU SER SER E95 H102 R107 R107 R107 R107 H139 T144 T144 T144 T144 T144 T146 L164	T169 V175 K183 A183 A183 T188 T188 Y193	E149 R203 P220 P224 R224 R223 R223 R223 R223 R223 R223 R
R274 L293 F206 F20 F20 F20 F20 F20 F20 F20 F20 F20 F20	H315 1337 1337 1337 1338 1335 1335 1335 1335 1335 1335 1335	0427 0427 6433 6457 1467 1467 0479	LTS H1S G483 C483 1485 1485 1485 1486 V488 V488 P489
7493 1510 1510 1510 1517 1557 1657			
• Molecule 1: Gluta	amate dehydrogenase 1, mitoch	ondrial	
Chain F:	73%	14%	13%
MET TYR TYR ARG TYR LEU GLU GLU CLEU LEU LEU LEU SER SER ARG	GLY PRO ALA ALA ALA ALA GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ALA ALA ALA ALA ALA PRO GLN CLN CLU LEU ALA ALA ALA	ARG HRS TYR SER SER GLU VAL ALA ALA ASP ASP
GLU ASP ASP P64 N65 P66 N69 R69 R96 R90 T91 T91 ARC	GLU SER 896 896 896 896 898 899 8103 8104 8106 8104 8106 8106 8106 8107 81106 81106 81106 81106 81106 81106 81106 81107 81106 81108 811008 81108 8108 8108 8108 81008 81008 81008 81008 81008 81008 81008 81	1150 8153 8153 8154 1154 1154 1155 1164 1164 1164 1164 1	V186 V186 K187 1188 E199 R203 D220
1239 1243 1243 1243 1243 1243 1243 1274 1274 1274	M290 1293 1296 1296 1296 1296 1296 1296 1293 111 1337 1337 1337 1337 1337 1337 1336 1366 1336 1	E403 E403 E403 E412 F417 F417 F417 F417	6433 Y461 L467 L467 6471 8472 8472 S474



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	79181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	1.072	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	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 > 5	RMSZ	# Z > 5	
1	А	0.26	0/3633	0.46	0/4939	
1	В	0.26	0/3751	0.47	0/5083	
1	С	0.26	0/3738	0.47	0/5068	
1	D	0.26	0/3718	0.46	0/5038	
1	Е	0.26	0/3725	0.46	0/5043	
1	F	0.25	0/3754	0.47	0/5080	
All	All	0.26	0/22319	0.46	0/30251	

There are no bond length outliers.

There are no bond angle outliers.

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	А	3552	0	3342	36	0
1	В	3670	0	3537	46	0
1	С	3658	0	3511	41	0
1	D	3641	0	3505	46	0
1	Е	3648	0	3531	36	0
1	F	3677	0	3567	51	0
All	All	21846	0	20993	235	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 5.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ILE:HG22	1:C:400:ILE:HB	1.71	0.71
1:E:66:PHE:HA	1:E:69:MET:HG3	1.74	0.69
1:F:90:ARG:HH21	1:F:99:ARG:HB3	1.57	0.69
1:F:64:PRO:O	1:F:386:LYS:NZ	2.26	0.67
1:A:338:TRP:HB2	1:A:367:TYR:HB2	1.78	0.65

The worst 5 of 235 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Perce	ntiles
1	А	482/558~(86%)	468 (97%)	13 (3%)	1 (0%)	47	71
1	В	483/558~(87%)	467 (97%)	15 (3%)	1 (0%)	47	71
1	С	483/558~(87%)	464 (96%)	18 (4%)	1 (0%)	47	71
1	D	477/558~(86%)	463 (97%)	12 (2%)	2(0%)	34	57
1	Е	477/558~(86%)	461 (97%)	16 (3%)	0	100	100
1	F	477/558~(86%)	458 (96%)	18 (4%)	1 (0%)	47	71
All	All	2879/3348~(86%)	2781 (97%)	92 (3%)	6 (0%)	50	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	555	VAL
1	А	555	VAL
1	D	124	ARG
1	С	555	VAL
1	D	555	VAL



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	334/452~(74%)	334 (100%)	0	100	100
1	В	367/452~(81%)	367~(100%)	0	100	100
1	С	364/452~(80%)	364 (100%)	0	100	100
1	D	368/452~(81%)	368 (100%)	0	100	100
1	Ε	368/452~(81%)	368 (100%)	0	100	100
1	F	375/452~(83%)	375 (100%)	0	100	100
All	All	2176/2712 (80%)	2176 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	285	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 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.

