wwPDB X-ray Structure Validation Summary Report (i)

Dec 13, 2023 – 09:07 pm GMT

PDB ID	:	2YFH
Title	:	Structure of a Chimeric Glutamate Dehydrogenase
Authors	:	Oliveira, T.; Panjikar, S.; Sharkey, M.A.; Carrigan, J.B.; Hamza, M.; Engel, P.C.; Khan, A.R.
Deposited on	:	2011-04-05
Resolution	:	2.69 Å(reported)

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 2.69 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		26
Ramachandran outliers		2.9%
Sidechain outliers		10.2%
RSRZ outliers		1.9%

Worse .... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
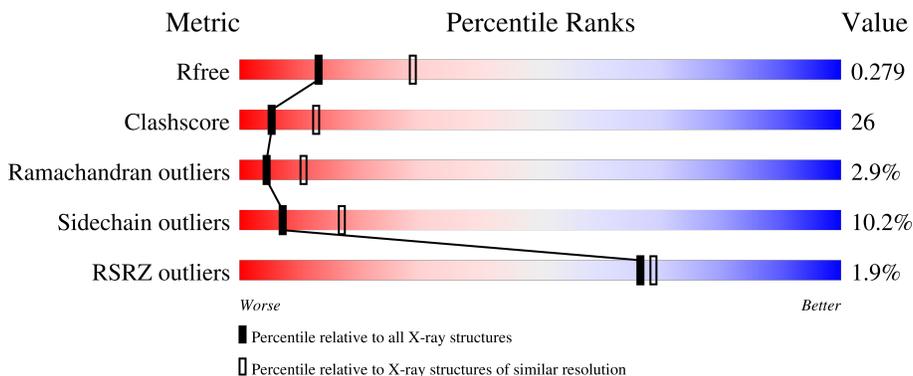
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	448	2% 57% 36% 5% ••
1	B	448	2% 62% 31% 6%
1	C	448	2% 56% 38% 6%
1	D	448	% 61% 31% 7% •
1	E	448	2% 54% 38% 6% •

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Mol	Chain	Length	Quality of chain
1	F	448	2% · 55% · 37% · 7% ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 20640 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, NAD-SPECIFIC GLU-TAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3371	2135	577	641	18			
1	B	447	Total	C	N	O	S	0	0	0
			3395	2149	584	645	17			
1	C	447	Total	C	N	O	S	0	0	0
			3395	2149	584	645	17			
1	D	444	Total	C	N	O	S	0	0	0
			3370	2136	578	639	17			
1	E	448	Total	C	N	O	S	0	0	0
			3403	2154	585	646	18			
1	F	447	Total	C	N	O	S	0	0	0
			3393	2148	583	645	17			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	55	Total	O	0	0
			55	55		
2	C	61	Total	O	0	0
			61	61		
2	D	60	Total	O	0	0
			60	60		
2	E	46	Total	O	0	0
			46	46		
2	F	46	Total	O	0	0
			46	46		

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 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.

• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDRO-GENASE, GLUTAMATE DEHYDROGENASE

• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDRO-GENASE, GLUTAMATE DEHYDROGENASE

W310 I316 P319 E325 V328 A331 L334 G338 G339 V342 A343 I352 E353 A354 T355 E356 L357 F358 Q359 L364 F365 A366 P367 G368 K369 A370 G374 G375 V376 A377 T378 S379 G380 L381 E382 M383 A384 Q385 N386 A387 A388 R389 K393 A394 E395 H402

R418 Y419 Y423 N424 L425 V426 A427 G428 A429 N430 I431 V432 G433 F434 I437 M441 Q444 G445 I446 A447 W448

● Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDRO-
GENASE, GLUTAMATE DEHYDROGENASE

Chain C:

2%
56%   38%   6%

MET S2 V5 V12 K15 Y16 E19 P20 E21 T25 V26 E27 V36 V46 A47 R51 V58 F61 R62 V63 P64 W65 E66 H73 G77 F82 G87 P88 Y89 K90 G91 G92 L93 R94 F95 V99 S102 I103 F106 F109 E110 Q111

A112 F113 K114 D115 S116 L117 T118 T119 L120 P121 M122 G123 G124 A125 K126 G127 F131 D132 P133 N134 M142 R143 F144 C145 Q146 L152 I156 D161 V162 P163 D166 V169 G170 A171 R172 E173 I174 G175 Y176 M177 Y181 V185 F188 L193 R198 I205 R206

P207 E208 Y212 G213 L214 V215 T218 E219 L222 K223 R224 H225 G226 M227 G228 F229 M232 R233 S237 G240 Q244 K249 A250 M251 F253 I258 T259 A260 S261 D262 S263 S264 G265 T266 V267 V268 D269 T274 K275 E276 K277 R280 L281 I282 E283 I284 K285 A286

S287 R288 D289 G290 R291 V292 A293 D294 Y295 A296 K297 F298 F299 G300 L301 E305 Q308 P309 W310 S311 L312 P313 A321 T322 E325 V328 L334 N337 G338 V339 K340 A341 V342 A343 E344 N347 M348 P349 T350 T351 I352 E353 A354 T355 E356 L357 F358 Q359 Q360 A361 G362 V363

L364 F365 A366 P367 G368 K369 N372 A373 G374 T378 S379 G380 L381 Q385 A388 R389 K393 K396 V397 L401 I404 M405 T406 D407 I408 S412 A413 A414 A415 A416 E417 R418 N424 L425 V426 A427 G428 A429 N430 I431 V432 G433 K436 M442 I446 A447 W448

● Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDRO-
GENASE, GLUTAMATE DEHYDROGENASE

Chain D:

%
61%   31%   7%   ·

MET S2 K3 Y4 V5 I9 K15 D18 E19 P20 E21 Q24 T25 V26 E27 E28 V29 L30 L33 V36 E44 V46 A47 L48 E56 R57 V58 I59 E60 F61 W65 K71 V72 H73 R79 V80 Q81 F82 I86 G87 K90 G91 R94 V99

N100 I103 M104 K105 F106 L107 G108 F109 E110 Q111 A112 F113 K114 D115 S116 L117 T118 G124 A125 S129 D130 F131 D132 P133 N134 R139 M142 Q146 E151 L152 V162 P163 L167 G168 V169 R172 E173 I174 Y178 G179 Q180 F188 L193 K196 A197 R198

S199 F200 G201 G202 I205 R206 P207 E208 L214 V215 T218 E219 A220 M221 L222 F229 E230 G231 V236 A243 Q244 Y245 A246 I247 E248 K249 E252 R256 V257 I258 T259 A260 S261 D262 S263 S264 V267 D268 D269 E270 F273 T274 K277 I282 E283 I284 K285 A286

SER ARG ASP G290 R291 V292 E298 F299 G300 L301 V302 Y303 L304 E305 G306 Q307 Q308 P309 W310 S311 L312 P313 A317 T322 Q323 N324 E325 D329 N337 V342 A343 P349 A354 T355 E356 L357 F358 Q359 Q360 A361 L364 F365 A366 G374 G375 V376 A377 T378 S379 G380

L381 Q385 N386 A387 A388 R389 L390 G391 W392 K396 A415 A416 E417 R418 Y419 G420 L421 G422 Y423 G428 V432 Q435 I446 A447 W448

• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDRO-GENASE, GLUTAMATE DEHYDROGENASE

Chain E:

• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDRO-GENASE, GLUTAMATE DEHYDROGENASE

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	100.10Å 113.86Å 109.58Å 116.54° 101.54° 104.09°	Depositor
Resolution (Å)	36.52 – 2.69 47.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (36.52-2.69) 93.6 (47.47-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.215 , 0.282 0.213 , 0.279	Depositor DCC
R_{free} test set	5046 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20640	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.47	1/3440 (0.0%)	0.66	1/4649 (0.0%)
1	B	0.45	0/3464	0.64	2/4681 (0.0%)
1	C	0.45	0/3464	0.65	0/4681
1	D	0.44	0/3438	0.62	0/4645
1	E	0.45	0/3472	0.64	0/4691
1	F	0.40	0/3462	0.61	1/4679 (0.0%)
All	All	0.44	1/20740 (0.0%)	0.64	4/28026 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	SER	CB-OG	8.11	1.52	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	ASN	N-CA-C	6.72	129.15	111.00
1	B	191	GLY	N-CA-C	-5.61	99.07	113.10
1	F	390	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	281	LEU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLN	Peptide
1	C	429	ALA	Peptide
1	D	388	ALA	Peptide
1	E	383	MET	Peptide
1	E	423	TYR	Peptide

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	3371	0	3304	166	0
1	B	3395	0	3332	140	0
1	C	3395	0	3332	200	0
1	D	3370	0	3309	175	0
1	E	3403	0	3344	208	0
1	F	3393	0	3325	216	0
2	A	45	0	0	5	0
2	B	55	0	0	7	0
2	C	61	0	0	12	0
2	D	60	0	0	2	0
2	E	46	0	0	6	0
2	F	46	0	0	1	0
All	All	20640	0	19946	1065	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 26.

The worst 5 of 1065 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:F:355:THR:C	1:F:357:LEU:HA	1.62	1.18
1:D:283:GLU:HA	1:D:284:ILE:HB	1.27	1.13
1:D:356:GLU:HA	1:D:358:PHE:N	1.62	1.12
1:D:356:GLU:HA	1:D:358:PHE:H	1.01	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:GLU:HB3	1:C:357:LEU:C	1.73	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	442/448 (99%)	399 (90%)	33 (8%)	10 (2%)	6	16
1	B	445/448 (99%)	407 (92%)	29 (6%)	9 (2%)	7	19
1	C	445/448 (99%)	390 (88%)	43 (10%)	12 (3%)	5	12
1	D	440/448 (98%)	380 (86%)	44 (10%)	16 (4%)	3	7
1	E	446/448 (100%)	386 (86%)	42 (9%)	18 (4%)	3	6
1	F	445/448 (99%)	377 (85%)	56 (13%)	12 (3%)	5	12
All	All	2663/2688 (99%)	2339 (88%)	247 (9%)	77 (3%)	4	10

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	49	LEU
1	A	205	ILE
1	A	289	ASP
1	A	328	VAL

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	340/343 (99%)	302 (89%)	38 (11%)	6	13
1	B	342/343 (100%)	309 (90%)	33 (10%)	8	19
1	C	342/343 (100%)	310 (91%)	32 (9%)	8	20
1	D	339/343 (99%)	310 (91%)	29 (9%)	10	24
1	E	343/343 (100%)	304 (89%)	39 (11%)	5	13
1	F	341/343 (99%)	304 (89%)	37 (11%)	6	14
All	All	2047/2058 (100%)	1839 (90%)	208 (10%)	7	17

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	206	ARG
1	E	167	LEU
1	F	381	LEU
1	D	263	SER
1	D	435	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	402	HIS
1	F	40	HIS
1	D	435	GLN
1	E	360	GLN
1	F	244	GLN

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 monosaccharides 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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	444/448 (99%)	-0.42	9 (2%)	65	67	42, 66, 105, 141	0
1	B	447/448 (99%)	-0.35	9 (2%)	65	67	41, 64, 92, 147	0
1	C	447/448 (99%)	-0.31	7 (1%)	72	74	44, 62, 109, 156	0
1	D	444/448 (99%)	-0.46	5 (1%)	80	82	43, 66, 105, 148	0
1	E	448/448 (100%)	-0.23	11 (2%)	57	59	47, 66, 98, 144	0
1	F	447/448 (99%)	-0.17	9 (2%)	65	67	47, 73, 107, 145	0
All	All	2677/2688 (99%)	-0.32	50 (1%)	66	69	41, 66, 104, 156	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	ASP	5.5
1	B	290	GLY	4.6
1	B	281	LEU	4.5
1	B	286	ALA	4.0
1	B	288	ARG	3.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.