



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:20 pm GMT

PDB ID : 1HRD
Title : GLUTAMATE DEHYDROGENASE
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Deposited on : 1996-04-03
Resolution : 1.96 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 ⓘ symbol.

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 : 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) : recalc28949

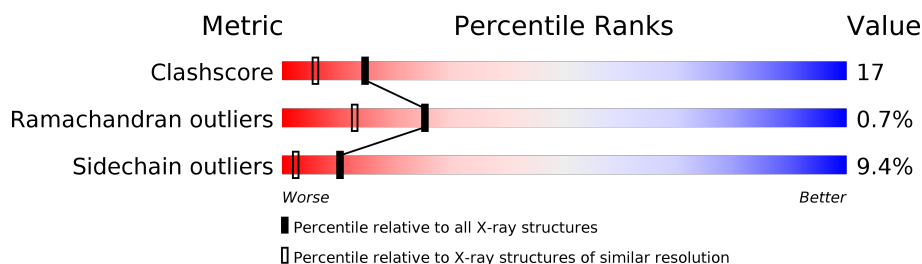
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)

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 $\leq 5\%$. 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	449	 74% 21% .
1	B	449	 63% 28% 9%
1	C	449	 64% 25% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10901 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3460	2198	583	660	19			
1	B	449	Total	C	N	O	S	0	0	0
			3460	2198	583	660	19			
1	C	449	Total	C	N	O	S	0	0	0
			3460	2198	583	660	19			

- Molecule 2 is water.

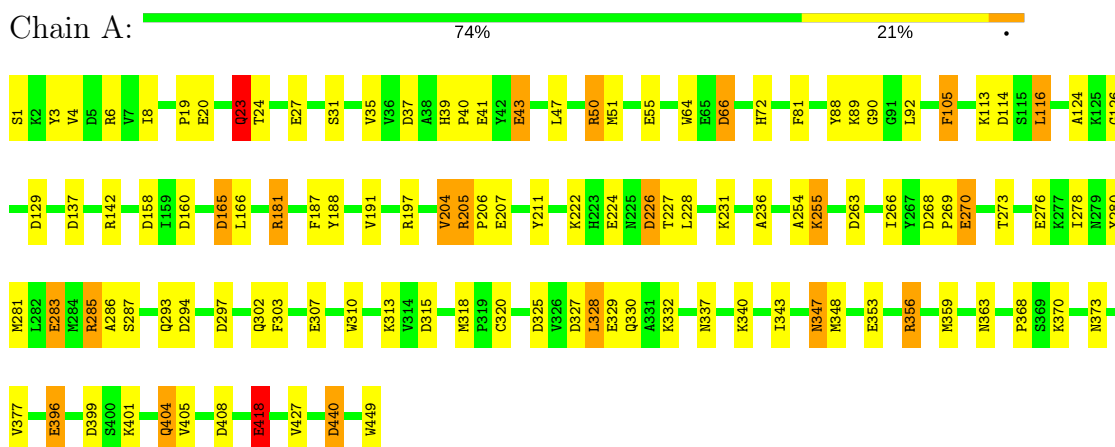
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total	O	0	0
			191	191		
2	B	152	Total	O	0	0
			152	152		
2	C	178	Total	O	0	0
			178	178		

3 Residue-property plots

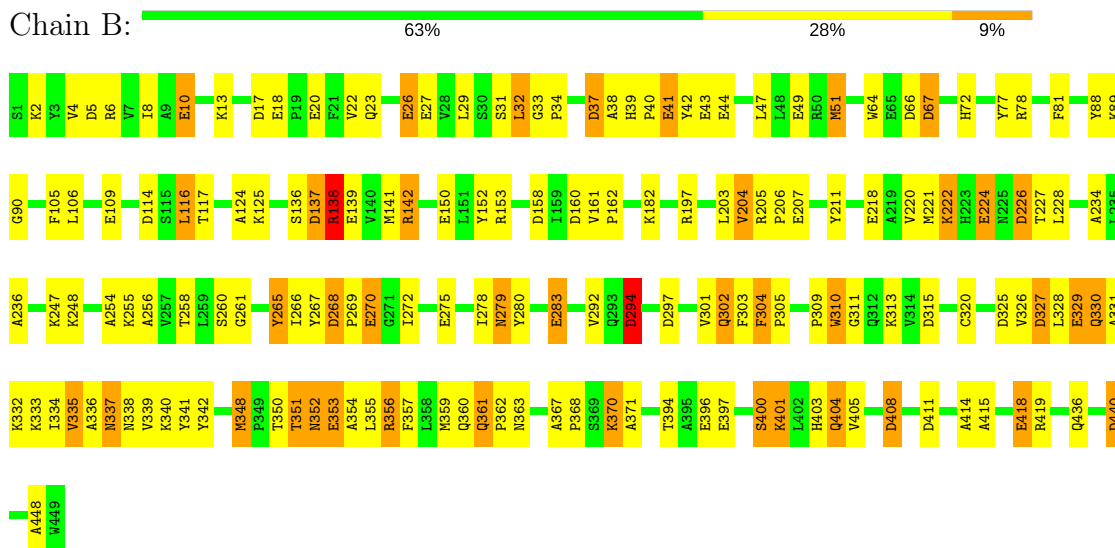
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: GLUTAMATE DEHYDROGENASE



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S1	K113	S260	E329	V433
K2	D114	S261	Q330	Q436
Y3	S115	G262	A331	
V4	L116	P263	V335	V449
D5		A356	A356	
R6	D129	P269	N337	
V7	F130	E270	N338	
I8	D131	G271	V339	
A9	P132	I272	K340	
E10	N133	T273		
V11		T274	N347	
E12	D137	E275	M348	
K13	R138	E276	P349	
	R142	K277	T350	
D17	M148	I278	T351	
E18		N279	N352	
P19		Y280	E353	
E20	R153	M281	A354	
F21		L282	L355	
V22	D158	E283	R356	
	I159	M284	F357	
E26	D160	R285	L358	
E27		A286	M359	
	L166	S287	Q360	
S30		G288	Q361	
	R171	R289	P362	
G33	P34	N290	N363	
V35	E172	K291		
V36	M176	V292	A367	
D37		Q293	P368	
A38	R181	D294	S369	
H39		Y295	K370	
P40	R197	A296	E383	
	L203	D297		
E44	V204	K298	S392	
	R205	F299		
L47	P206		E396	
	E207	Q302	E397	
R50	M51	F303	V398	
	Y215	F304	D399	
E65		P305	S400	
D66	E218	G306		
D67		E307	H403	
	H223	Q312		
K70	E224	K313	D408	
	N225	V314		
V73	D226	D315	D411	
	T227	I316		
R78		I317	E418	
	A234		R419	
F81	L235	C320	Y420	
	A236	Q323	G421	
G86	K247	N324	L422	
A95		D325	V427	
	L252	V326	A428	
F105	A256	D327	I432	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.10Å 151.30Å 94.60Å 90.00° 132.75° 90.00°	Depositor
Resolution (Å)	37.80 – 1.96	Depositor
% Data completeness (in resolution range)	88.0 (37.80-1.96)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10901	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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	0.79	13/3535 (0.4%)	1.28	38/4781 (0.8%)
1	B	0.79	12/3535 (0.3%)	1.31	41/4781 (0.9%)
1	C	0.79	17/3535 (0.5%)	1.28	37/4781 (0.8%)
All	All	0.79	42/10605 (0.4%)	1.29	116/14343 (0.8%)

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	C	2	0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	GLU	CD-OE2	6.64	1.32	1.25
1	B	329	GLU	CD-OE1	6.60	1.32	1.25
1	C	27	GLU	CD-OE2	6.50	1.32	1.25
1	C	270	GLU	CD-OE2	6.41	1.32	1.25
1	A	27	GLU	CD-OE2	6.03	1.32	1.25

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	C	142	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	50	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	A	285	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	66	ASP	CB-CG-OD2	-8.31	110.82	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	278	ILE	CA
1	C	329	GLU	CA

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	3460	0	3390	71	0
1	B	3460	0	3390	144	0
1	C	3460	0	3390	137	0
2	A	191	0	0	2	0
2	B	152	0	0	5	0
2	C	178	0	0	4	0
All	All	10901	0	10170	351	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 17.

The worst 5 of 351 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:A:347:ASN:HD22	1:A:348:MET:N	1.27	1.32
1:B:360:GLN:O	1:B:362:PRO:HD3	1.33	1.24
1:C:280:TYR:O	1:C:283:GLU:HB2	1.44	1.17
1:C:302:GLN:OE1	1:C:302:GLN:HA	1.46	1.10
1:C:323:GLN:OE1	1:C:348:MET:HG2	1.50	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	447/449 (100%)	432 (97%)	14 (3%)	1 (0%)	51	41
1	B	447/449 (100%)	424 (95%)	18 (4%)	5 (1%)	17	6
1	C	447/449 (100%)	420 (94%)	23 (5%)	4 (1%)	20	9
All	All	1341/1347 (100%)	1276 (95%)	55 (4%)	10 (1%)	25	13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	ASN
1	B	204	VAL
1	B	310	TRP
1	B	361	GLN
1	C	289	ARG

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	358/358 (100%)	338 (94%)	20 (6%)	25	11
1	B	358/358 (100%)	318 (89%)	40 (11%)	7	1
1	C	358/358 (100%)	317 (88%)	41 (12%)	6	1
All	All	1074/1074 (100%)	973 (91%)	101 (9%)	10	2

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	328	LEU
1	B	401	LYS
1	C	353	GLU
1	B	337	ASN
1	B	353	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	363	ASN
1	C	23	GLN
1	C	361	GLN
1	B	403	HIS
1	B	404	GLN

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 carbohydrates 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.