



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:33 PM UTC

PDB ID : 1EY2 / pdb_00001ey2
Title : HUMAN HOMOGENTISATE DIOXYGENASE WITH FE(II)
Authors : Timm, D.E.; Titus, G.P.; Penalva, M.A.; Mueller, H.A.; de Cordoba, S.M.
Deposited on : 2000-05-05
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

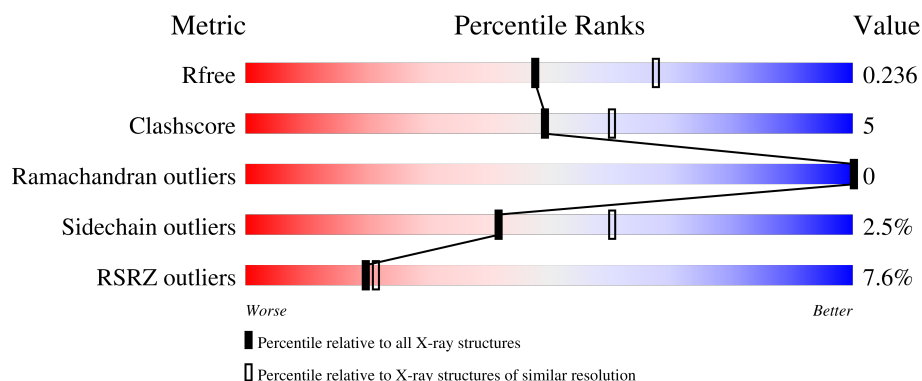
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	471	7% 77% 11% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3544 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 HOMOGENITISATE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	Se	0	0	0
			3311	2123	566	603	10	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MSE	-	expression tag	UNP Q93099
A	-24	GLY	-	expression tag	UNP Q93099
A	-23	HIS	-	expression tag	UNP Q93099
A	-22	HIS	-	expression tag	UNP Q93099
A	-21	HIS	-	expression tag	UNP Q93099
A	-20	HIS	-	expression tag	UNP Q93099
A	-19	HIS	-	expression tag	UNP Q93099
A	-18	HIS	-	expression tag	UNP Q93099
A	-17	HIS	-	expression tag	UNP Q93099
A	-16	HIS	-	expression tag	UNP Q93099
A	-15	HIS	-	expression tag	UNP Q93099
A	-14	HIS	-	expression tag	UNP Q93099
A	-13	SER	-	expression tag	UNP Q93099
A	-12	SER	-	expression tag	UNP Q93099
A	-11	GLY	-	expression tag	UNP Q93099
A	-10	HIS	-	expression tag	UNP Q93099
A	-9	ILE	-	expression tag	UNP Q93099
A	-8	ASP	-	expression tag	UNP Q93099
A	-7	ASP	-	expression tag	UNP Q93099
A	-6	ASP	-	expression tag	UNP Q93099
A	-5	ASP	-	expression tag	UNP Q93099
A	-4	LYS	-	expression tag	UNP Q93099
A	-3	HIS	-	expression tag	UNP Q93099
A	-2	MSE	-	expression tag	UNP Q93099
A	-1	GLY	-	expression tag	UNP Q93099
A	0	SER	-	expression tag	UNP Q93099
A	1	MSE	MET	engineered mutation	UNP Q93099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	142	MSE	MET	engineered mutation	UNP Q93099
A	172	MSE	MET	engineered mutation	UNP Q93099
A	186	MSE	MET	engineered mutation	UNP Q93099
A	283	MSE	MET	engineered mutation	UNP Q93099
A	339	MSE	MET	engineered mutation	UNP Q93099
A	343	MSE	MET	engineered mutation	UNP Q93099
A	368	MSE	MET	engineered mutation	UNP Q93099
A	396	MSE	MET	engineered mutation	UNP Q93099
A	399	MSE	MET	engineered mutation	UNP Q93099

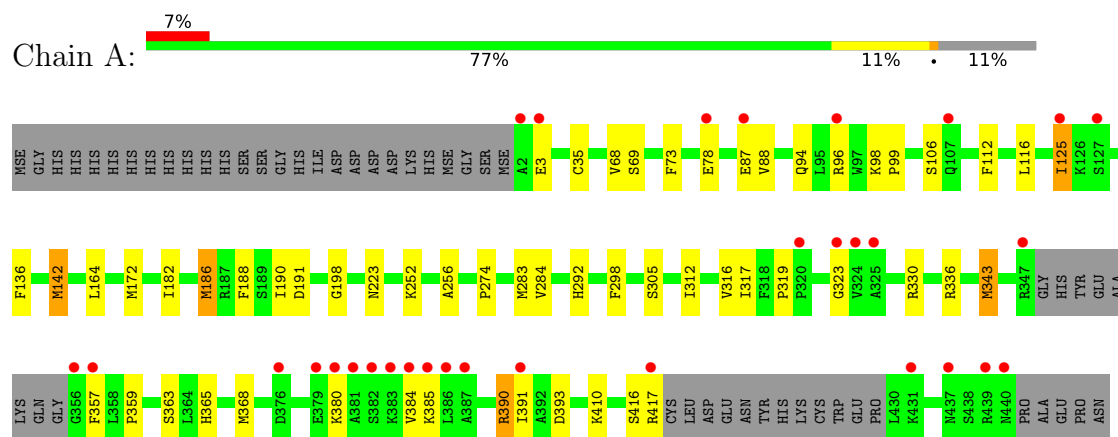
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	232	Total O 232 232	0	0

- Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.81Å 157.81Å 95.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.30) 99.7 (30.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.193 , 0.242 0.189 , 0.236	Depositor DCC
R_{free} test set	1579 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.65	6/3400 (0.2%)	1.02	12/4600 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	MSE	SE-CE	-11.93	1.59	1.95
1	A	186	MSE	SE-CE	-8.24	1.70	1.95
1	A	172	MSE	SE-CE	-6.83	1.75	1.95
1	A	343	MSE	SE-CE	-6.12	1.77	1.95
1	A	368	MSE	SE-CE	-5.91	1.77	1.95
1	A	186	MSE	CG-SE	-5.82	1.77	1.95

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	PRO	N-CA-C	6.83	119.03	110.70
1	A	312	ILE	N-CA-C	-6.58	104.35	110.53
1	A	125	ILE	N-CA-C	6.40	116.55	110.53
1	A	416	SER	N-CA-C	6.09	118.39	110.53
1	A	385	LYS	N-CA-C	-5.55	101.64	109.96
1	A	319	PRO	CA-C-N	5.39	125.66	119.83
1	A	319	PRO	C-N-CA	5.39	125.66	119.83
1	A	223	ASN	CA-C-N	5.37	125.44	119.32
1	A	223	ASN	C-N-CA	5.37	125.44	119.32
1	A	305	SER	N-CA-C	-5.14	102.40	110.36
1	A	284	VAL	N-CA-C	5.02	115.71	108.93
1	A	336	ARG	N-CA-C	-5.01	100.29	108.76

There are no chirality outliers.

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	3311	0	3213	35	0
2	A	1	0	0	0	0
3	A	232	0	0	4	0
All	All	3544	0	3213	35	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.

All (35) 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:112:PHE:HB3	1:A:142:MSE:HE2	1.45	0.98
1:A:94:GLN:HE22	1:A:96:ARG:HH21	1.30	0.78
1:A:142:MSE:HE3	1:A:190:ILE:H	1.51	0.75
1:A:283:MSE:HG3	3:A:2049:HOH:O	1.86	0.75
1:A:142:MSE:HE3	1:A:190:ILE:N	2.09	0.67
1:A:94:GLN:HE22	1:A:96:ARG:NH2	1.92	0.67
1:A:96:ARG:HH11	1:A:357:PHE:HD2	1.44	0.64
1:A:96:ARG:HD3	1:A:363:SER:HB3	1.81	0.61
1:A:98:LYS:HG2	1:A:417:ARG:HH21	1.72	0.54
1:A:292:HIS:HD2	1:A:330:ARG:O	1.91	0.53
1:A:380:LYS:O	1:A:384:VAL:HG13	2.09	0.52
1:A:390:ARG:HD3	1:A:393:ASP:OD2	2.11	0.51
1:A:125:ILE:HG22	3:A:2208:HOH:O	2.10	0.51
1:A:142:MSE:HE3	1:A:190:ILE:HB	1.94	0.49
1:A:298:PHE:HB3	1:A:317:ILE:O	2.12	0.48
1:A:87:GLU:HB2	1:A:410:LYS:HE3	1.95	0.48
1:A:78:GLU:HG3	3:A:2134:HOH:O	2.14	0.48
1:A:98:LYS:HG3	1:A:417:ARG:HE	1.80	0.46
1:A:87:GLU:HG3	1:A:410:LYS:HG3	1.98	0.46
1:A:164:LEU:HB3	1:A:191:ASP:HB2	1.98	0.46
1:A:94:GLN:NE2	1:A:365:HIS:NE2	2.64	0.46
1:A:136:PHE:CZ	1:A:198:GLY:HA3	2.50	0.46
1:A:87:GLU:HG3	1:A:88:VAL:HG23	1.97	0.45
1:A:323:GLY:HA3	1:A:391:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:HIS:CD2	1:A:330:ARG:O	2.70	0.45
1:A:73:PHE:CD2	1:A:256:ALA:HB2	2.52	0.44
1:A:186:MSE:SE	1:A:274:PRO:HG3	2.68	0.44
1:A:142:MSE:CE	1:A:190:ILE:HB	2.48	0.42
1:A:35:CYS:HB3	3:A:2102:HOH:O	2.19	0.42
1:A:98:LYS:HG2	1:A:417:ARG:NH2	2.35	0.42
1:A:323:GLY:HA3	1:A:391:ILE:CD1	2.50	0.42
1:A:182:ILE:HG21	1:A:188:PHE:CD2	2.56	0.41
1:A:78:GLU:OE2	1:A:252:LYS:HA	2.21	0.40
1:A:96:ARG:NH1	1:A:357:PHE:CD2	2.86	0.40
1:A:298:PHE:HB2	1:A:316:VAL:HG13	2.04	0.40

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	413/471 (88%)	400 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	361/394 (92%)	352 (98%)	9 (2%)	42 60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	68	VAL
1	A	69	SER
1	A	99	PRO
1	A	106	SER
1	A	116	LEU
1	A	343	MSE
1	A	359	PRO
1	A	390	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	94	GLN
1	A	175	GLN
1	A	183	GLN
1	A	258	GLN
1	A	292	HIS
1	A	433	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	410/471 (87%)	0.02	31 (7%) 20 21	14, 29, 60, 75	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ARG	4.5
1	A	379	GLU	4.5
1	A	440	ASN	4.5
1	A	356	GLY	4.3
1	A	78	GLU	4.1
1	A	380	LYS	4.1
1	A	2	ALA	3.8
1	A	417	ARG	3.5
1	A	439	ARG	3.3
1	A	325	ALA	3.3
1	A	376	ASP	3.0
1	A	107	GLN	2.9
1	A	385	LYS	2.9
1	A	391	ILE	2.9
1	A	431	LYS	2.8
1	A	383	LYS	2.7
1	A	127	SER	2.6
1	A	3	GLU	2.5
1	A	87	GLU	2.5
1	A	347	ARG	2.4
1	A	382	SER	2.4
1	A	324	VAL	2.3
1	A	386	LEU	2.2
1	A	381	ALA	2.2
1	A	387	ALA	2.2
1	A	323	GLY	2.2
1	A	357	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	384	VAL	2.1
1	A	437	ASN	2.1
1	A	320	PRO	2.1
1	A	125	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE2	A	1001	1/1	0.95	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.