



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 1EYB / pdb_00001eyb
Title : CRYSTAL STRUCTURE OF APO HUMAN HOMOGENTISATE DIOXY-
GENASE
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Deposited on : 2000-05-05
Resolution : 1.90 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

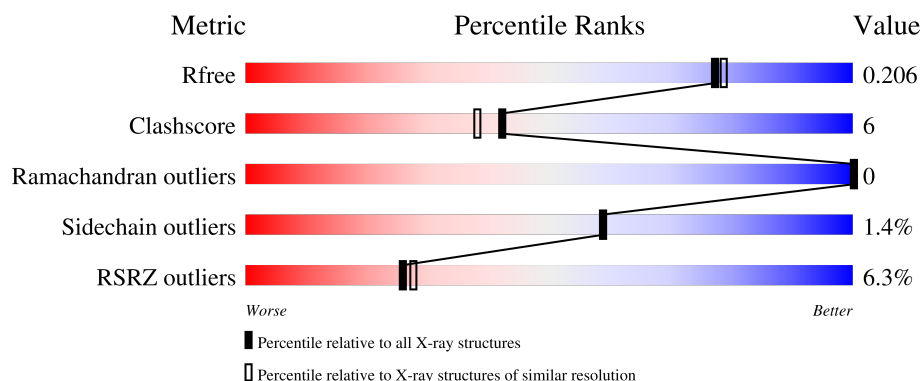
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3786 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
			3303	2120	565	599	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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	483	Total O 483 483	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	158.38Å 158.38Å 93.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.90) 92.7 (30.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.222 0.178 , 0.206	Depositor DCC
R_{free} test set	2581 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3786	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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 [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	A	0.61	6/3392 (0.2%)	1.18	16/4590 (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	-7.26	1.73	1.95
1	A	396	MSE	SE-CE	-5.75	1.78	1.95
1	A	399	MSE	SE-CE	-5.70	1.78	1.95
1	A	172	MSE	SE-CE	-5.44	1.79	1.95
1	A	343	MSE	SE-CE	-5.23	1.79	1.95
1	A	339	MSE	SE-CE	-5.11	1.80	1.95

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	CD-NE-CZ	22.60	156.04	124.40
1	A	343	MSE	CA-CB-CG	10.12	134.34	114.10
1	A	307	ARG	NE-CZ-NH1	8.39	129.89	121.50
1	A	314	ASP	CA-CB-CG	8.07	120.67	112.60
1	A	86	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	307	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	A	63	ARG	CD-NE-CZ	6.26	133.16	124.40
1	A	335	HIS	CA-CB-CG	6.13	119.94	113.80
1	A	238	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	A	400	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	434	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	112	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	365	HIS	CA-CB-CG	5.24	119.03	113.80
1	A	238	GLN	CB-CG-CD	5.17	121.40	112.60
1	A	68	VAL	CB-CA-C	-5.17	101.92	111.79
1	A	346	ILE	CA-C-O	5.06	126.13	120.71

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	3303	0	3202	41	0
2	A	483	0	0	12	1
All	All	3786	0	3202	41	1

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 6.

All (41) 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	1.32	1.10
1:A:343:MSE:SE	2:A:1480:HOH:O	2.35	0.93
1:A:87:GLU:HG3	1:A:88:VAL:HG23	1.56	0.85
1:A:337:ASN:HD22	1:A:339:MSE:H	1.25	0.85
1:A:87:GLU:HB2	1:A:410:LYS:HE3	1.66	0.76
1:A:112:PHE:CB	1:A:142:MSE:HE2	2.13	0.75
1:A:142:MSE:HE3	1:A:190:ILE:HB	1.69	0.75
1:A:375:ALA:O	1:A:379:GLU:HG2	1.86	0.75
1:A:142:MSE:HE3	1:A:190:ILE:CB	2.25	0.67
1:A:337:ASN:ND2	1:A:339:MSE:H	1.96	0.60
1:A:343:MSE:CG	2:A:1480:HOH:O	2.50	0.59
1:A:65:LEU:HD13	2:A:1282:HOH:O	2.04	0.56
1:A:343:MSE:HG2	2:A:1480:HOH:O	2.05	0.56
1:A:335:HIS:HB3	1:A:371:HIS:NE2	2.22	0.54
1:A:430:LEU:N	2:A:1485:HOH:O	2.40	0.54
1:A:337:ASN:HD22	1:A:339:MSE:N	2.01	0.52
1:A:379:GLU:O	1:A:383:LYS:HG2	2.08	0.52
1:A:84:ASN:ND2	1:A:87:GLU:HB3	2.26	0.51
1:A:142:MSE:HE3	1:A:190:ILE:N	2.28	0.49
1:A:383:LYS:HE3	2:A:1243:HOH:O	2.14	0.47
1:A:365:HIS:CD2	2:A:1371:HOH:O	2.68	0.47
1:A:383:LYS:HG3	2:A:1243:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:N	1:A:331:PRO:CD	2.81	0.44
1:A:98:LYS:HG2	2:A:1110:HOH:O	2.17	0.44
1:A:142:MSE:CE	1:A:190:ILE:HB	2.42	0.44
1:A:104:LYS:HE2	2:A:1209:HOH:O	2.17	0.43
1:A:104:LYS:HD3	1:A:195:GLU:OE2	2.18	0.43
1:A:87:GLU:HB2	1:A:410:LYS:CE	2.44	0.43
1:A:182:ILE:HD13	1:A:188:PHE:CG	2.54	0.42
1:A:26:PRO:HB3	1:A:32:PRO:HG3	2.01	0.42
1:A:313:ALA:HA	1:A:401:GLU:O	2.20	0.42
1:A:53:ARG:NH2	2:A:1321:HOH:O	2.52	0.42
1:A:63:ARG:HD3	1:A:66:PRO:HA	2.02	0.41
1:A:171:LYS:HE3	1:A:233:TRP:CE2	2.54	0.41
1:A:182:ILE:HG21	1:A:188:PHE:CD2	2.55	0.41
1:A:7:ILE:HG13	1:A:231:ILE:HG22	2.03	0.41
1:A:142:MSE:HE3	1:A:190:ILE:H	1.84	0.41
1:A:358:LEU:HB3	1:A:359:PRO:HD2	2.02	0.41
1:A:375:ALA:HA	1:A:430:LEU:HD23	2.03	0.41
1:A:335:HIS:HB3	1:A:371:HIS:CE1	2.56	0.40
1:A:238:GLN:CD	2:A:1479:HOH:O	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1067:HOH:O	2:A:1326:HOH:O[10_665]	2.12	0.08

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%)	402 (97%)	11 (3%)	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 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	358/394 (91%)	353 (99%)	5 (1%)	59 59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	95	LEU
1	A	116	LEU
1	A	177	ASN
1	A	337	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	38	ASN
1	A	84	ASN
1	A	94	GLN
1	A	128	ASN
1	A	162	ASN
1	A	175	GLN
1	A	238	GLN
1	A	247	ASN
1	A	258	GLN
1	A	292	HIS
1	A	337	ASN
1	A	365	HIS
1	A	440	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 oligosaccharides 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 ⓘ

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%)	0.20	26 (6%)	26 27	16, 23, 42, 57	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	6.7
1	A	88	VAL	5.7
1	A	356	GLY	5.0
1	A	87	GLU	5.0
1	A	2	ALA	4.5
1	A	79	GLY	4.3
1	A	379	GLU	4.2
1	A	78	GLU	4.1
1	A	417	ARG	4.0
1	A	347	ARG	3.8
1	A	440	ASN	3.4
1	A	371	HIS	3.3
1	A	27	GLU	3.1
1	A	98	LYS	2.9
1	A	106	SER	2.7
1	A	338	CYS	2.7
1	A	376	ASP	2.6
1	A	335	HIS	2.6
1	A	250	GLN	2.5
1	A	238	GLN	2.5
1	A	85	TRP	2.5
1	A	3	GLU	2.4
1	A	439	ARG	2.4
1	A	109	LYS	2.3
1	A	357	PHE	2.2
1	A	414	LYS	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.