



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:46 AM UTC

PDB ID : 2Z2B / pdb_00002z2b
Title : Deletion 107-116 mutant of dihydroorotase from E. coli
Authors : Lee, M.; Maher, M.J.; Guss, J.M.
Deposited on : 2007-05-17
Resolution : 1.85 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

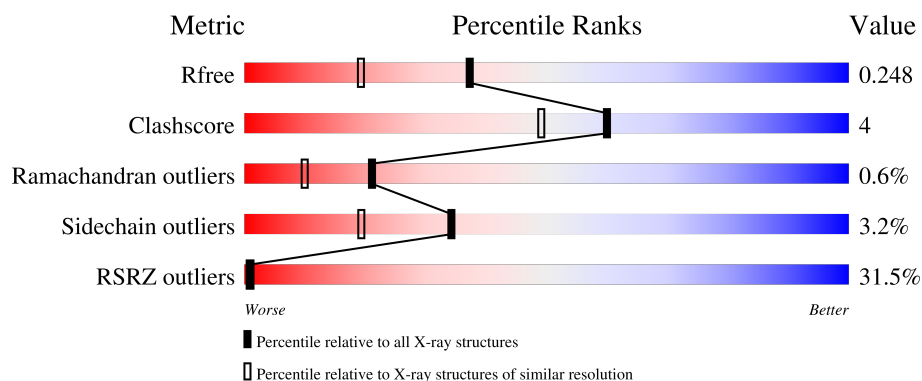
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	337	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2749 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 Dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2611	1656	458	481	16	55	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P05020
A	?	-	ALA	deletion	UNP P05020
A	?	-	THR	deletion	UNP P05020
A	?	-	THR	deletion	UNP P05020
A	?	-	ASN	deletion	UNP P05020
A	?	-	SER	deletion	UNP P05020
A	?	-	SER	deletion	UNP P05020
A	?	-	HIS	deletion	UNP P05020
A	?	-	GLY	deletion	UNP P05020
A	?	-	VAL	deletion	UNP P05020
A	109	VAL	ILE	conflict	UNP P05020

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

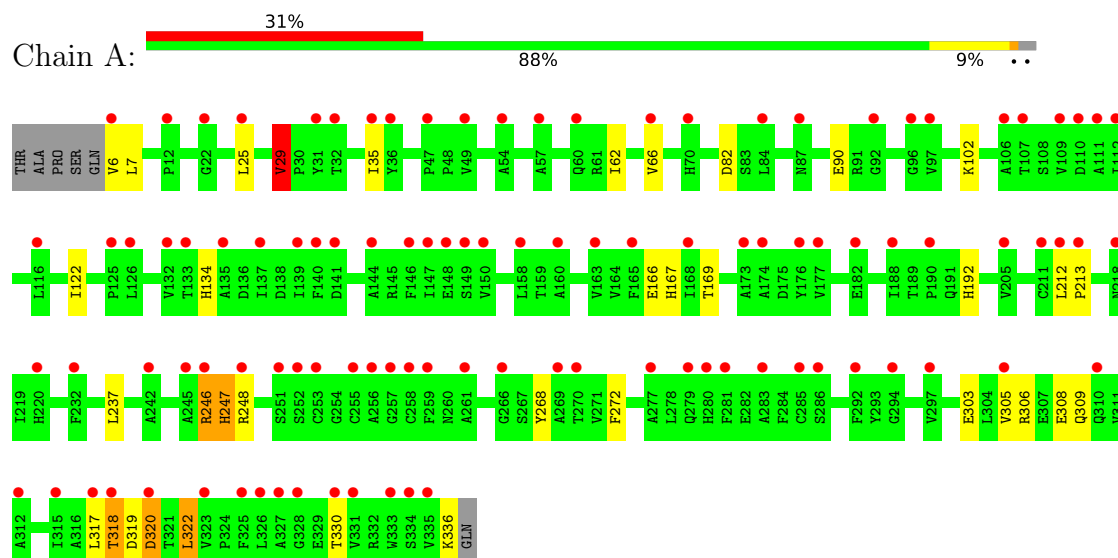
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		

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 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: Dihydroorotase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	52.30Å 52.30Å 216.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.85 40.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.00-1.85) 95.9 (40.00-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.245 0.198 , 0.248	Depositor DCC
R_{free} test set	1430 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2749	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: KCX, ZN

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	0.84	1/2659 (0.0%)	0.90	2/3617 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	CA-CB	5.72	1.56	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	CB-CA-C	-6.07	105.65	111.05
1	A	29	VAL	N-CA-CB	5.71	114.35	110.52

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	2611	0	2578	22	0
2	A	2	0	0	0	0
3	A	136	0	0	1	0
All	All	2749	0	2578	22	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 4.

All (22) 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:246:ARG:C	1:A:248:ARG:H	2.05	0.62
1:A:246:ARG:C	1:A:248:ARG:N	2.61	0.58
1:A:134:HIS:ND1	3:A:1396:HOH:O	2.32	0.57
1:A:25:LEU:HD12	1:A:29:VAL:HG23	1.86	0.56
1:A:246:ARG:CG	1:A:247:HIS:N	2.67	0.56
1:A:7:LEU:O	1:A:303:GLU:HA	2.08	0.54
1:A:246:ARG:O	1:A:248:ARG:N	2.45	0.50
1:A:246:ARG:HG2	1:A:247:HIS:N	2.27	0.50
1:A:6:VAL:HG23	1:A:305:VAL:HG12	1.95	0.47
1:A:317:LEU:CD1	1:A:322:LEU:HB2	2.45	0.47
1:A:62:ILE:O	1:A:66:VAL:HG23	2.17	0.45
1:A:308:GLU:HG3	1:A:330:THR:CG2	2.47	0.44
1:A:317:LEU:O	1:A:318:THR:C	2.61	0.43
1:A:317:LEU:O	1:A:319:ASP:N	2.52	0.43
1:A:237:LEU:HG	1:A:268:TYR:CE1	2.54	0.42
1:A:90:GLU:HG3	1:A:122:ILE:HG21	2.01	0.42
1:A:308:GLU:HG3	1:A:330:THR:HG23	2.00	0.42
1:A:268:TYR:O	1:A:272:PHE:HD1	2.03	0.41
1:A:169:THR:HG22	1:A:192:HIS:CD2	2.56	0.41
1:A:167:HIS:CE1	1:A:213:PRO:HD3	2.56	0.40
1:A:166:GLU:O	1:A:167:HIS:C	2.63	0.40
1:A:212:LEU:HA	1:A:213:PRO:C	2.45	0.40

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	328/337 (97%)	310 (94%)	16 (5%)	2 (1%)	21	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	THR
1	A	320	ASP

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	281/286 (98%)	272 (97%)	9 (3%)	34	19

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

Mol	Chain	Res	Type
1	A	29	VAL
1	A	82	ASP
1	A	246	ARG
1	A	247	HIS
1	A	306	ARG
1	A	309	GLN
1	A	320	ASP
1	A	322	LEU
1	A	336	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	102	1,2	10,11,12	0.88	0	6,12,14	1.48	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	102	1,2	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	KCX	OQ1-CX-NZ	-3.51	119.59	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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	330/337 (97%)	1.71	104 (31%) 1 1	7, 55, 67, 83	12 (3%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	5.0
1	A	144	ALA	4.7
1	A	310	GLN	4.3
1	A	334	SER	4.3
1	A	320	ASP	4.1
1	A	257	GLY	4.1
1	A	6	VAL	4.1
1	A	286	SER	4.0
1	A	112	ILE	3.8
1	A	335	VAL	3.8
1	A	25	LEU	3.7
1	A	256	ALA	3.7
1	A	173	ALA	3.7
1	A	109	VAL	3.5
1	A	333	TRP	3.4
1	A	305	VAL	3.4
1	A	22	GLY	3.3
1	A	328	GLY	3.3
1	A	283	ALA	3.2
1	A	327	ALA	3.1
1	A	182	GLU	3.0
1	A	158	LEU	2.9
1	A	213	PRO	2.8
1	A	232	PHE	2.8
1	A	212	LEU	2.8
1	A	146	PHE	2.7
1	A	258	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	2.7
1	A	312	ALA	2.7
1	A	294	GLY	2.7
1	A	139	ILE	2.7
1	A	315	ILE	2.7
1	A	261	ALA	2.7
1	A	326	LEU	2.7
1	A	47	PRO	2.6
1	A	97	VAL	2.6
1	A	54	ALA	2.6
1	A	160	ALA	2.6
1	A	218	ASN	2.6
1	A	137	ILE	2.6
1	A	252	SER	2.6
1	A	318	THR	2.6
1	A	141	ASP	2.6
1	A	211	CYS	2.5
1	A	96	GLY	2.5
1	A	49	VAL	2.5
1	A	163	VAL	2.5
1	A	176	TYR	2.5
1	A	280	HIS	2.5
1	A	150	VAL	2.5
1	A	106	ALA	2.5
1	A	107	THR	2.4
1	A	135	ALA	2.4
1	A	116	LEU	2.4
1	A	269	ALA	2.4
1	A	66	VAL	2.4
1	A	331	VAL	2.4
1	A	285	CYS	2.4
1	A	147	ILE	2.4
1	A	111	ALA	2.4
1	A	323	VAL	2.4
1	A	149	SER	2.4
1	A	251	SER	2.4
1	A	70	HIS	2.3
1	A	132	VAL	2.3
1	A	188	ILE	2.3
1	A	279	GLN	2.3
1	A	277	ALA	2.2
1	A	253	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	140	PHE	2.2
1	A	259	PHE	2.2
1	A	87	ASN	2.2
1	A	110	ASP	2.2
1	A	330	THR	2.2
1	A	126	LEU	2.2
1	A	266	GLY	2.2
1	A	36	TYR	2.1
1	A	270	THR	2.1
1	A	84	LEU	2.1
1	A	148	GLU	2.1
1	A	12	PRO	2.1
1	A	255	CYS	2.1
1	A	57	ALA	2.1
1	A	242	ALA	2.1
1	A	281	PHE	2.1
1	A	292	PHE	2.1
1	A	325	PHE	2.1
1	A	168	ILE	2.1
1	A	32	THR	2.1
1	A	190	PRO	2.1
1	A	174	ALA	2.1
1	A	165	PHE	2.0
1	A	133	THR	2.0
1	A	92	GLY	2.0
1	A	220	HIS	2.0
1	A	60	GLN	2.0
1	A	297	VAL	2.0
1	A	317	LEU	2.0
1	A	35	ILE	2.0
1	A	31	TYR	2.0
1	A	125	PRO	2.0
1	A	177	VAL	2.0
1	A	246	ARG	2.0
1	A	248	ARG	2.0

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

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
1	KCX	A	102	12/13	0.92	0.15	49,53,58,62	0

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	ZN	A	1337	1/1	0.99	0.19	41,41,41,41	0
2	ZN	A	338	1/1	1.00	0.14	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.