

Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 07:21 AM EDT

PDB ID 2Z25

> Title : Thr110Val dihydroorotase from E. coli

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2007-05-17 Deposited on

1.87 Å(reported) Resolution

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 (i) 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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

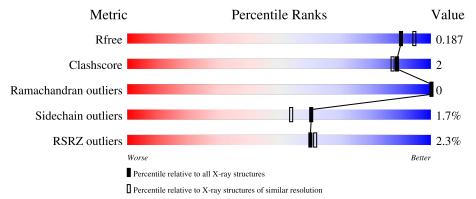
Validation Pipeline (wwPDB-VP) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
R_{free}	130704	9470 (1.90-1.86)		
Clashscore	141614	10282 (1.90-1.86)		
Ramachandran outliers	138981	10152 (1.90-1.86)		
Sidechain outliers	138945	10152 (1.90-1.86)		
RSRZ outliers	127900	9303 (1.90-1.86)		

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 <=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	347	94%	5% •				
1	В	347	93%	5% ••				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6087 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.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	343	Total 2698	C 1706	N 478	O 498	S 16	4	2	0
1	В	343	Total 2694	C 1703	N 475	O 500	S 16	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

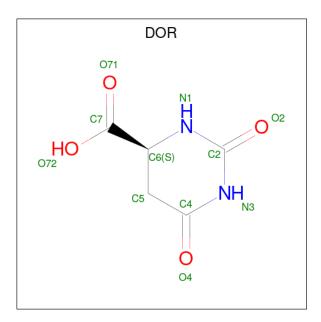
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	VAL	THR	engineered mutation	UNP P05020
A	119	VAL	ILE	conflict	UNP P05020
В	110	VAL	THR	engineered mutation	UNP P05020
В	119	VAL	ILE	conflict	UNP P05020

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

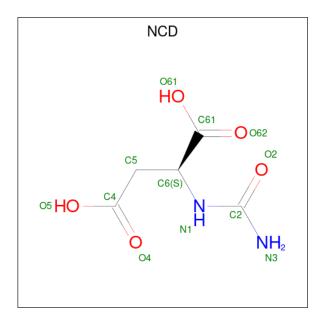
• Molecule 3 is (4S)-2,6-DIOXOHEXAHYDROPYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: DOR) (formula: $C_5H_6N_2O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 11	C 5	N 2	O 4	0	0

 \bullet Molecule 4 is N-CARBAMOYL-L-ASPARTATE (three-letter code: NCD) (formula: $C_5H_8N_2O_5).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 12	C 5	N 2	O 5	0	0

• Molecule 5 is water.



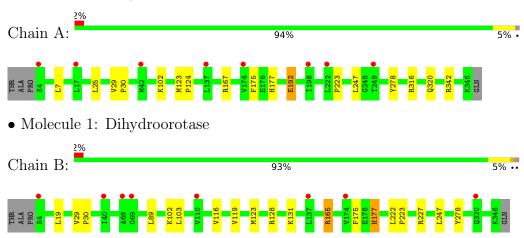
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	385	Total O 385 385	0	0
5	В	283	Total O 283 283	0	0



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 (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	51.45Å 78.97Å 180.53Å	Donositon	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	40.00 - 1.87	Depositor	
Resolution (A)	39.10 - 1.87	EDS	
% Data completeness	98.4 (40.00-1.87)	Depositor	
(in resolution range)	98.3 (39.10-1.87)	EDS	
R_{merge}	0.05	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.99 (at 1.87Å)	Xtriage	
Refinement program	REFMAC 5.2.0005	Depositor	
P. P.	0.147 , 0.185	Depositor	
R, R_{free}	0.158 , 0.187	DCC	
R_{free} test set	3091 reflections (5.08%)	wwPDB-VP	
Wilson B-factor (Å ²)	23.8	Xtriage	
Anisotropy	0.227	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 41.4	EDS	
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	6087	wwPDB-VP	
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DOR, KCX, NCD

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.51	0/2750	0.65	0/3742	
1	В	0.46	0/2743	0.64	$2/3732 \ (0.1\%)$	
All	All	0.49	0/5493	0.64	2/7474 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	165	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	В	165	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2698	0	2662	7	0
1	В	2694	0	2653	11	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
3	A	11	0	5	1	0
4	В	12	0	6	1	0
5	A	385	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	283	0	0	2	0
All	All	6087	0	5326	20	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 2.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	$-$ overlap (\mathring{A})
1:A:316:ARG:NH2	1:A:342:ARG:HD2	2.10	0.66
1:A:25:LEU:C	1:A:25:LEU:HD23	2.26	0.56
1:B:103:LEU:CD1	1:B:116:VAL:HG21	2.40	0.52
1:A:192:GLU:H	1:A:192:GLU:CD	2.13	0.51
3:A:1410:DOR:C4	5:A:1551:HOH:O	2.59	0.50
1:A:177:HIS:CE1	1:A:223:PRO:HD3	2.47	0.49
1:B:227:ARG:HG2	5:B:2427:HOH:O	2.13	0.49
1:B:103:LEU:HD13	1:B:116:VAL:HG21	1.95	0.47
1:B:29:VAL:CG2	1:B:30:PRO:HD3	2.45	0.46
1:B:165:ARG:HD2	5:B:2439:HOH:O	2.17	0.45
1:B:119:VAL:CG1	1:B:123:MET:HE1	2.46	0.45
1:B:177:HIS:CE1	1:B:223:PRO:HD3	2.52	0.45
1:B:19:LEU:HD22	1:B:29:VAL:HG12	1.99	0.44
4:B:2410:NCD:H31	4:B:2410:NCD:C4	2.31	0.44
1:A:29:VAL:N	1:A:30:PRO:CD	2.82	0.43
1:B:222:LEU:HA	1:B:223:PRO:C	2.39	0.42
1:A:123:MET:N	1:A:124:PRO:CD	2.84	0.41
1:B:247:LEU:HG	1:B:278:TYR:CE1	2.56	0.41
1:A:247:LEU:HG	1:A:278:TYR:CE1	2.56	0.41
1:B:29:VAL:HG22	1:B:30:PRO:HD3	2.03	0.41

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	Perce	entiles
1	A	341/347 (98%)	328 (96%)	13 (4%)	0	100	100
1	В	340/347 (98%)	325 (96%)	15 (4%)	0	100	100
All	All	681/694 (98%)	653 (96%)	28 (4%)	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	291/294 (99%)	286 (98%)	5 (2%)	60 54
1	В	291/294 (99%)	286 (98%)	5 (2%)	60 54
All	All	582/588 (99%)	572 (98%)	10 (2%)	60 54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	167	ARG
1	A	175	PHE
1	A	192	GLU
1	A	320	GLN
1	В	89	LEU
1	В	128	ARG
1	В	131	LYS
1	В	175	PHE
1	В	177	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	319	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)

2 non-standard protein/DNA/RNA residues are 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	B	Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
1	KCX	В	102	1,2	9,11,12	0.97	0	5,12,14	1.60	1 (20%)	
1	KCX	A	102	1,2	9,11,12	0.87	0	5,12,14	1.25	1 (20%)	

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	В	102	1,2	-	0/9/10/12	-
1	KCX	A	102	1,2	-	0/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	В	102	KCX	OQ1-CX-NZ	-3.51	119.52	124.96
1	A	102	KCX	OQ1-CX-NZ	-2.40	121.23	124.96

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	Bo	Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NCD	В	2410	2	11,11,11	1.08	0	13,14,14	1.26	1 (7%)	
3	DOR	A	1410	-	11,11,11	1.17	1 (9%)	12,15,15	1.99	4 (33%)	

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
4	NCD	В	2410	2	-	4/12/12/12	-
3	DOR	A	1410	-	-	0/4/16/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
3	A	1410	DOR	O72-C7	-2.03	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1410	DOR	C4-N3-C2	-4.82	121.86	125.73

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1410	DOR	O2-C2-N1	-2.39	118.16	122.92
3	A	1410	DOR	N3-C2-N1	2.19	118.42	116.12
4	В	2410	NCD	O2-C2-N3	-2.13	119.56	123.22
3	A	1410	DOR	O4-C4-C5	-2.13	118.48	122.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	2410	NCD	C61-C6-N1-C2
4	В	2410	NCD	C4-C5-C6-C61
4	В	2410	NCD	O2-C2-N1-C6
4	В	2410	NCD	N3-C2-N1-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	2410	NCD	1	0
3	A	1410	DOR	1	0

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)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	342/347 (98%)	0.27	8 (2%) 60 62	22, 28, 38, 47	1 (0%)
1	В	342/347 (98%)	0.28	8 (2%) 60 62	21, 28, 40, 56	2 (0%)
All	All	684/694 (98%)	0.27	16 (2%) 60 62	21, 28, 39, 56	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	68	ALA	3.7
1	A	137	LEU	3.4
1	В	4	SER	2.9
1	A	174	VAL	2.5
1	В	110	VAL	2.5
1	В	137	LEU	2.5
1	В	320	GLN	2.4
1	A	4	SER	2.4
1	A	198	ILE	2.3
1	В	69	GLY	2.3
1	В	40	ILE	2.3
1	A	17	LEU	2.2
1	A	222	LEU	2.1
1	A	42	MET	2.1
1	A	249	THR	2.1
1	В	174	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	KCX	A	102	12/13	0.95	0.17	24,27,30,34	0
1	KCX	В	102	12/13	0.95	0.16	22,25,30,30	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	DOR	A	1410	11/11	0.96	0.13	20,22,34,42	0
4	NCD	В	2410	12/12	0.96	0.10	21,24,31,33	0
2	ZN	В	400	1/1	1.00	0.07	24,24,24,24	0
2	ZN	В	401	1/1	1.00	0.09	24,24,24,24	0
2	ZN	A	400	1/1	1.00	0.09	20,20,20,20	0
2	ZN	A	401	1/1	1.00	0.08	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.

