

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 09:46 AM EDT

PDB ID	:	105K
Title	:	Crystal structure of Dihydrodipicolinate synthase (TM1521) from Thermotoga
		maritima at 1.80 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2003-09-22
Resolution	:	1.80 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 (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:

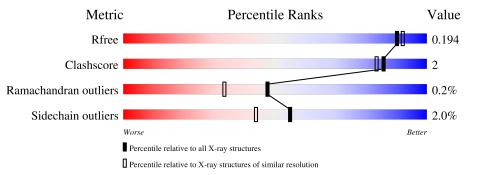
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Mol	Chain	Length	Quality of chain		
1	А	306	88%	8%	•
1	В	306	89%	8%	•



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5064 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	295	Total	С	Ν	Ο	S	0	2	0
	Л	290	2286	1450	396	433	7	0	5	0
1	В	295	Total	С	Ν	0	S	0	1	0
	D	295	2269	1440	390	432	7	0	1	0

• Molecule 1 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-11	MET	-	initiating methionine	UNP Q9X1K9
А	-10	GLY	-	expression tag	UNP Q9X1K9
А	-9	SER	-	expression tag	UNP Q9X1K9
А	-8	ASP	-	expression tag	UNP Q9X1K9
А	-7	LYS	-	expression tag	UNP Q9X1K9
А	-6	ILE	-	expression tag	UNP Q9X1K9
А	-5	HIS	-	expression tag	UNP Q9X1K9
А	-4	HIS	-	expression tag	UNP Q9X1K9
А	-3	HIS	-	expression tag	UNP Q9X1K9
А	-2	HIS	-	expression tag	UNP Q9X1K9
А	-1	HIS	-	expression tag	UNP Q9X1K9
А	0	HIS	-	expression tag	UNP Q9X1K9
В	-11	MET	-	initiating methionine	UNP Q9X1K9
В	-10	GLY	-	expression tag	UNP Q9X1K9
В	-9	SER	-	expression tag	UNP Q9X1K9
В	-8	ASP	-	expression tag	UNP Q9X1K9
В	-7	LYS	-	expression tag	UNP Q9X1K9
В	-6	ILE	-	expression tag	UNP Q9X1K9
В	-5	HIS	-	expression tag	UNP Q9X1K9
В	-4	HIS	-	expression tag	UNP Q9X1K9
В	-3	HIS	-	expression tag	UNP Q9X1K9
В	-2	HIS	-	expression tag	UNP Q9X1K9
В	-1	HIS	-	expression tag	UNP Q9X1K9
В	0	HIS	-	expression tag	UNP Q9X1K9

There are 24 discrepancies between the modelled and reference sequences:





• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	261	Total O 261 261	0	0
3	В	247	Total O 247 247	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. 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. 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: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:	88%	8%	·
MET MET GIX SEP LYS LYS LYS LYS HIS HIS HIS HIS HIS HIS HIS HIS HIS K3 CV102 CV102	q116 K119 D126 1130 L156 K132 L156 K135	K161 K164 N164 P165 D168 D168 R181 S183 S183 D183	V209 M243 L246 N251 P252
• Molecule 1: 4-hydroxy-tetrahydr	odipicolinate synth	ase	
Chain B:	89%	8%) •
MET GLY SER ASP ASP LYS HLS HLS HLS HLS HLS HLS HLS HLS HLS HL	Y132 V142 K155 N156 N156 D166 D166 D166 V209	216 216 241 241 241 1246 1246 1251 1255 1255	L294



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	54.67Å 140.77Å 155.94Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.61 - 1.80	Depositor
Resolution (A)	35.61 - 1.80	EDS
% Data completeness	93.3 (35.61-1.80)	Depositor
(in resolution range)	93.3 (35.61 - 1.80)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$1.67 (at 1.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
D D	0.139 , 0.186	Depositor
R, R_{free}	0.154 , 0.194	DCC
R_{free} test set	2656 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.2	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 53.8	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5064	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 5.15% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: KPI, CA

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.80	0/2317	0.89	6/3141~(0.2%)	
1	В	0.76	0/2293	0.83	2/3114~(0.1%)	
All	All	0.78	0/4610	0.86	8/6255~(0.1%)	

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	166	ASP	CB-CG-OD1	7.85	125.36	118.30
1	А	126	ASP	CB-CG-OD2	6.23	123.91	118.30
1	А	183	ASP	CB-CG-OD2	6.11	123.80	118.30
1	В	168	ASP	CB-CG-OD2	6.10	123.79	118.30
1	А	53	ASP	CB-CG-OD2	5.98	123.68	118.30
1	А	168	ASP	CB-CG-OD2	5.96	123.67	118.30
1	В	166	ASP	CB-CG-OD1	5.83	123.55	118.30
1	А	67	ASP	CB-CG-OD2	5.29	123.06	118.30

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	А	2286	0	2341	11	0

Continued on next page...



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	2269	0	2306	9	0
2	А	1	0	0	0	0
3	А	261	0	0	4	1
3	В	247	0	0	2	1
All	All	5064	0	4647	20	1

Continued from previous page...

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 distance (Å)	Clash overlap (Å)
1:B:36:ASN:ND2	3:B:490:HOH:O	1.86	1.09
1:A:181:ARG:HD2	3:A:833:HOH:O	1.87	0.75
1:B:5:VAL:H	1:B:36:ASN:HD22	1.46	0.64
1:A:116[A]:GLN:OE1	1:A:119[A]:LYS:NZ	2.37	0.57
1:A:168:ASP:OD1	3:A:670:HOH:O	2.18	0.53
1:A:209:VAL:HG21	1:A:243:MET:HG2	1.94	0.49
1:B:102:VAL:HA	1:B:132:TYR:HB3	1.95	0.48
1:A:209:VAL:HG22	1:A:246:LEU:HD12	1.97	0.47
1:B:251:ASN:ND2	1:B:252:PRO:HA	2.29	0.47
1:B:240:ARG:HB3	1:B:241:PRO:HD3	1.97	0.46
1:B:253:ILE:HB	1:B:254:PRO:HD3	1.99	0.45
1:A:36:ASN:ND2	3:A:732:HOH:O	2.48	0.44
1:B:209:VAL:HG22	1:B:246:LEU:HD12	1.99	0.44
1:A:155:LYS:NZ	3:A:833:HOH:O	2.41	0.43
1:A:102:VAL:HA	1:A:132:TYR:HB3	2.00	0.43
1:A:251:ASN:ND2	1:A:252:PRO:HA	2.34	0.42
1:A:150:ILE:HG23	1:A:154:LEU:HD12	2.00	0.42
1:A:164:ASN:HB3	1:A:169:GLN:HG2	2.02	0.42
1:B:161:KPI:H1A	3:B:349:HOH:O	2.20	0.41
1:B:103:THR:HG21	1:B:142:VAL:HG23	2.04	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)
3:A:779:HOH:O	3:B:501:HOH:O[5_545]	2.09	0.11



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	ntiles
1	А	295/306~(96%)	291 (99%)	4 (1%)	0	100	100
1	В	293/306~(96%)	289~(99%)	3~(1%)	1 (0%)	41	27
All	All	588/612~(96%)	580 (99%)	7 (1%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	1	MET

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	Perce	ntiles
1	А	250/263~(95%)	246~(98%)	4 (2%)	62	54
1	В	246/263~(94%)	240 (98%)	6 (2%)	49	36
All	All	496/526~(94%)	486 (98%)	10 (2%)	55	44

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

Mol	Chain	Res	Type
1	А	0	HIS
1	А	43	THR
1	А	93	LYS
1	А	156	ASN
1	В	0	HIS

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	43	THR
1	В	67	ASP
1	В	155	LYS
1	В	156	ASN
1	В	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	90	GLN
1	А	228	ASN
1	А	251	ASN
1	В	36	ASN
1	В	90	GLN
1	В	211	ASN
1	В	216	GLN
1	В	228	ASN
1	В	251	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)

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).

Mal	Mol Type Chain		Res Link		Bos Link Bond lengths		В	ond ang	les	
	Type	Chain	nes	Res Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	KPI	А	161	1	11,13,14	0.91	0	$10,\!15,\!17$	2.05	3 (30%)
1	KPI	В	161	1	11,13,14	1.06	1 (9%)	$10,\!15,\!17$	1.94	3 (30%)

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	KPI	А	161	1	-	0/13/14/16	-
1	KPI	В	161	1	-	0/13/14/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	В	161	KPI	CX2-CX1	-2.64	1.46	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	161	KPI	O2-CX2-CX1	-3.42	117.01	121.38
1	А	161	KPI	C1-CX1-CX2	3.37	121.44	118.17
1	А	161	KPI	CE-NZ-CX1	3.28	130.63	121.70
1	В	161	KPI	CE-NZ-CX1	3.19	130.38	121.70
1	А	161	KPI	CD-CE-NZ	-3.12	104.99	110.66
1	В	161	KPI	CD-CE-NZ	-2.67	105.81	110.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	161	KPI	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

