Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 11:05 am BST

PDB ID	:	7OL1
Title	:	The X-ray structure of L-threonine dehydrogenase from the common hospital pathogen Clostridium difficile.
Authors	:	Guo, J.; Cooper, J.B.
Deposited on	:	2021-05-18
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

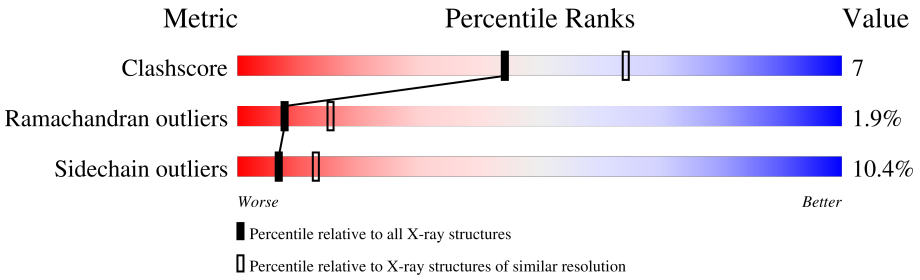
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	339	75% 17% • 6%
1	B	339	68% 24% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5142 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 L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2515	1602	411	488	14			
1	B	319	Total	C	N	O	S	0	0	0
			2515	1602	411	488	14			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A346VYB9
A	-19	GLY	-	expression tag	UNP A0A346VYB9
A	-18	HIS	-	expression tag	UNP A0A346VYB9
A	-17	HIS	-	expression tag	UNP A0A346VYB9
A	-16	HIS	-	expression tag	UNP A0A346VYB9
A	-15	HIS	-	expression tag	UNP A0A346VYB9
A	-14	HIS	-	expression tag	UNP A0A346VYB9
A	-13	HIS	-	expression tag	UNP A0A346VYB9
A	-12	HIS	-	expression tag	UNP A0A346VYB9
A	-11	HIS	-	expression tag	UNP A0A346VYB9
A	-10	HIS	-	expression tag	UNP A0A346VYB9
A	-9	HIS	-	expression tag	UNP A0A346VYB9
A	-8	SER	-	expression tag	UNP A0A346VYB9
A	-7	SER	-	expression tag	UNP A0A346VYB9
A	-6	GLY	-	expression tag	UNP A0A346VYB9
A	-5	HIS	-	expression tag	UNP A0A346VYB9
A	-4	ILE	-	expression tag	UNP A0A346VYB9
A	-3	GLU	-	expression tag	UNP A0A346VYB9
A	-2	GLY	-	expression tag	UNP A0A346VYB9
A	-1	ARG	-	expression tag	UNP A0A346VYB9
A	0	HIS	-	expression tag	UNP A0A346VYB9
B	-20	MET	-	initiating methionine	UNP A0A346VYB9
B	-19	GLY	-	expression tag	UNP A0A346VYB9
B	-18	HIS	-	expression tag	UNP A0A346VYB9
B	-17	HIS	-	expression tag	UNP A0A346VYB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP A0A346VYB9
B	-15	HIS	-	expression tag	UNP A0A346VYB9
B	-14	HIS	-	expression tag	UNP A0A346VYB9
B	-13	HIS	-	expression tag	UNP A0A346VYB9
B	-12	HIS	-	expression tag	UNP A0A346VYB9
B	-11	HIS	-	expression tag	UNP A0A346VYB9
B	-10	HIS	-	expression tag	UNP A0A346VYB9
B	-9	HIS	-	expression tag	UNP A0A346VYB9
B	-8	SER	-	expression tag	UNP A0A346VYB9
B	-7	SER	-	expression tag	UNP A0A346VYB9
B	-6	GLY	-	expression tag	UNP A0A346VYB9
B	-5	HIS	-	expression tag	UNP A0A346VYB9
B	-4	ILE	-	expression tag	UNP A0A346VYB9
B	-3	GLU	-	expression tag	UNP A0A346VYB9
B	-2	GLY	-	expression tag	UNP A0A346VYB9
B	-1	ARG	-	expression tag	UNP A0A346VYB9
B	0	HIS	-	expression tag	UNP A0A346VYB9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	56	Total O 56 56	0	0
2	B	56	Total O 56 56	0	0

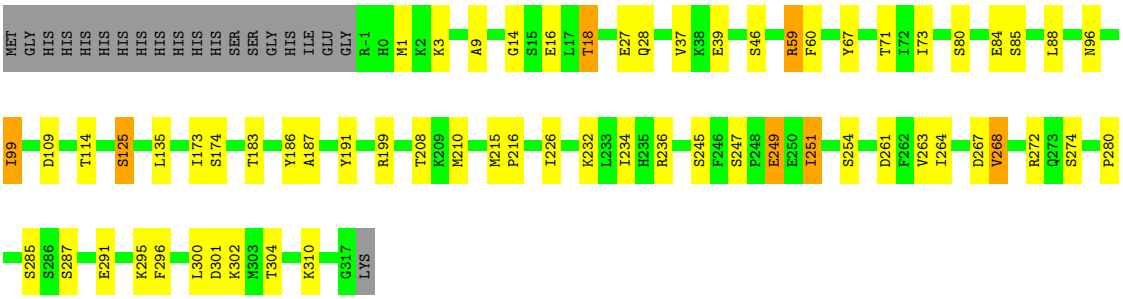
3 Residue-property plots (i)

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.

Note EDS was not executed.

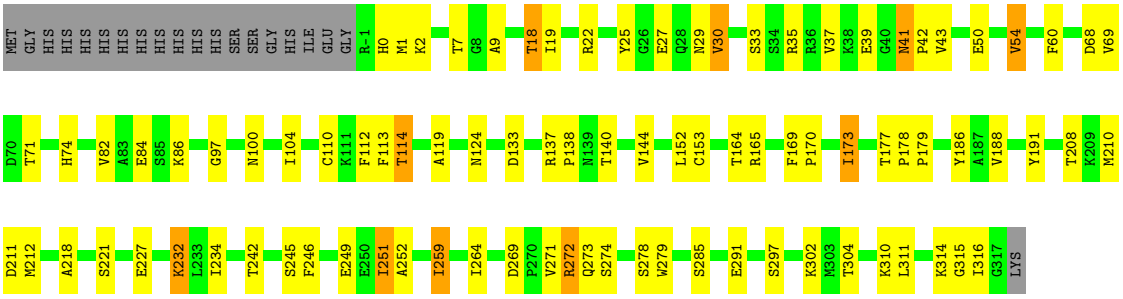
- Molecule 1: L-threonine 3-dehydrogenase

Chain A:



- Molecule 1: L-threonine 3-dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.87Å 180.87Å 88.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.28 – 2.60	Depositor
% Data completeness (in resolution range)	97.3 (63.28-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5142	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.77	0/2567	0.97	3/3469 (0.1%)
1	B	0.79	1/2567 (0.0%)	0.98	1/3469 (0.0%)
All	All	0.78	1/5134 (0.0%)	0.97	4/6938 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	GLU	CD-OE2	7.77	1.34	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	59	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	249	GLU	CB-CA-C	5.34	121.07	110.40
1	B	110	CYS	CB-CA-C	-5.05	100.30	110.40

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	2515	0	2501	25	0
1	B	2515	0	2501	42	0
2	A	56	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	56	0	0	0	0
All	All	5142	0	5002	66	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 7.

All (66) 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:252:ALA:HB2	1:B:264:ILE:HD11	1.64	0.80
1:A:14:GLY:O	1:A:18:THR:HG23	1.84	0.77
1:A:125:SER:OG	1:A:135:LEU:O	2.02	0.76
1:A:1:MET:HE3	1:A:71:THR:HG21	1.69	0.75
1:B:252:ALA:HB2	1:B:264:ILE:CD1	2.20	0.72
1:B:218:ALA:O	1:B:221:SER:HB3	1.94	0.68
1:A:3:LYS:HE3	1:A:67:TYR:O	1.94	0.67
1:A:1:MET:CE	1:A:71:THR:HG21	2.27	0.64
1:B:33:SER:HA	1:B:50:GLU:O	1.96	0.64
1:B:114:THR:HG21	1:B:153:CYS:SG	2.39	0.63
1:B:173:ILE:CG2	1:B:188:VAL:HG22	2.29	0.62
1:B:7:THR:OG1	1:B:74:HIS:HA	1.99	0.61
1:B:173:ILE:HG23	1:B:188:VAL:HG22	1.84	0.60
1:A:1:MET:CE	1:A:73:ILE:HD11	2.32	0.59
1:A:1:MET:HE1	1:A:73:ILE:HD11	1.83	0.59
1:B:54:VAL:HG13	1:B:97:GLY:HA2	1.84	0.59
1:B:9:ALA:HB1	1:B:18:THR:HG21	1.85	0.58
1:B:22:ARG:HG3	1:B:30:VAL:HG21	1.85	0.57
1:B:232:LYS:HD3	1:B:291:GLU:O	2.04	0.56
1:A:1:MET:CE	1:A:226:ILE:HD13	2.35	0.56
1:A:135:LEU:HD11	1:B:133:ASP:HB3	1.88	0.56
1:A:251:ILE:HG23	1:A:300:LEU:HD11	1.86	0.56
1:A:1:MET:HE3	1:A:226:ILE:HD13	1.89	0.55
1:B:19:ILE:HD11	1:B:42:PRO:HB2	1.89	0.54
1:B:311:LEU:O	1:B:316:ILE:HG13	2.06	0.54
1:B:54:VAL:HG13	1:B:97:GLY:CA	2.38	0.54
1:A:3:LYS:CE	1:A:67:TYR:O	2.58	0.52
1:B:25:TYR:O	1:B:29:ASN:ND2	2.40	0.51
1:B:191:TYR:HE1	1:B:304:THR:HG23	1.77	0.49
1:B:211:ASP:O	1:B:212:MET:HG2	2.12	0.49
1:B:0:HIS:HA	1:B:227:GLU:HG2	1.93	0.49
1:B:7:THR:HA	1:B:33:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASP:C	1:B:212:MET:HG2	2.34	0.48
1:B:186:TYR:CE2	1:B:251:ILE:HD11	2.48	0.48
1:A:210:MET:O	1:A:245:SER:HA	2.12	0.48
1:B:140:THR:O	1:B:144:VAL:HG23	2.13	0.48
1:B:113:PHE:HA	1:B:165:ARG:O	2.14	0.48
1:B:119:ALA:HA	1:B:279:TRP:NE1	2.29	0.48
1:B:259:ILE:HG22	1:B:259:ILE:O	2.15	0.47
1:A:96:ASN:HA	1:A:99:ILE:HG22	1.98	0.46
1:B:208:THR:HG21	1:B:273:GLN:HE22	1.81	0.46
1:A:191:TYR:HE1	1:A:304:THR:HG23	1.80	0.46
1:B:1:MET:HE3	1:B:71:THR:HG21	1.96	0.46
1:A:9:ALA:HB1	1:A:18:THR:HG21	1.97	0.45
1:A:215:MET:N	1:A:216:PRO:HD2	2.32	0.45
1:A:295:LYS:O	1:A:296:PHE:HB3	2.17	0.45
1:B:22:ARG:HG3	1:B:30:VAL:CG2	2.47	0.45
1:B:169:PHE:HA	1:B:170:PRO:HD2	1.87	0.44
1:B:208:THR:HG21	1:B:273:GLN:NE2	2.33	0.44
1:A:16:GLU:OE2	1:A:174:SER:HB2	2.18	0.44
1:B:41:ASN:HD22	1:B:43:VAL:H	1.65	0.43
1:B:191:TYR:CE1	1:B:304:THR:HG23	2.53	0.43
1:A:208:THR:O	1:A:247:SER:HA	2.17	0.43
1:B:242:THR:HG22	1:B:285:SER:OG	2.17	0.43
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.82	0.43
1:B:137:ARG:N	1:B:138:PRO:CD	2.82	0.43
1:A:234:ILE:N	1:A:291:GLU:OE1	2.41	0.42
1:A:287:SER:HB3	1:A:291:GLU:OE2	2.20	0.42
1:A:173:ILE:CD1	1:A:187:ALA:HB3	2.50	0.41
1:B:177:THR:HA	1:B:178:PRO:HD2	1.91	0.41
1:B:100:ASN:O	1:B:104:ILE:HG13	2.21	0.41
1:B:173:ILE:HG23	1:B:188:VAL:CG2	2.48	0.41
1:A:173:ILE:HD11	1:A:187:ALA:HB3	2.02	0.41
1:B:112:PHE:O	1:B:164:THR:HA	2.21	0.41
1:B:245:SER:O	1:B:246:PHE:HB3	2.21	0.41
1:B:269:ASP:OD2	1:B:272:ARG:HD2	2.22	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	317/339 (94%)	286 (90%)	27 (8%)	4 (1%)	12 24
1	B	317/339 (94%)	278 (88%)	31 (10%)	8 (2%)	5 9
All	All	634/678 (94%)	564 (89%)	58 (9%)	12 (2%)	8 15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	B	124	ASN
1	B	249	GLU
1	A	46	SER
1	B	68	ASP
1	B	179	PRO
1	A	280	PRO
1	B	27	GLU
1	B	297	SER
1	B	315	GLY
1	A	268	VAL
1	B	271	VAL

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	278/295 (94%)	246 (88%)	32 (12%)	5 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	278/295 (94%)	252 (91%)	26 (9%)	8 17
All	All	556/590 (94%)	498 (90%)	58 (10%)	7 13

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	27	GLU
1	A	28	GLN
1	A	37	VAL
1	A	59	ARG
1	A	60	PHE
1	A	80	SER
1	A	84	GLU
1	A	85	SER
1	A	99	ILE
1	A	109	ASP
1	A	114	THR
1	A	125	SER
1	A	183	THR
1	A	186	TYR
1	A	199	ARG
1	A	232	LYS
1	A	236	ARG
1	A	249	GLU
1	A	251	ILE
1	A	254	SER
1	A	261	ASP
1	A	263	VAL
1	A	264	ILE
1	A	267	ASP
1	A	268	VAL
1	A	272	ARG
1	A	274	SER
1	A	285	SER
1	A	301	ASP
1	A	302	LYS
1	A	310	LYS
1	B	2	LYS
1	B	18	THR
1	B	30	VAL
1	B	35	ARG

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Mol	Chain	Res	Type
1	B	37	VAL
1	B	39	GLU
1	B	41	ASN
1	B	54	VAL
1	B	60	PHE
1	B	69	VAL
1	B	82	VAL
1	B	86	LYS
1	B	114	THR
1	B	152	LEU
1	B	173	ILE
1	B	210	MET
1	B	232	LYS
1	B	234	ILE
1	B	251	ILE
1	B	259	ILE
1	B	272	ARG
1	B	274	SER
1	B	278	SER
1	B	302	LYS
1	B	310	LYS
1	B	314	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	128	ASN
1	B	41	ASN
1	B	157	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 monosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.