

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 10:42 PM EDT

PDB ID	:	6U1H
Title	:	Thermus thermophilus D-alanine-D-alanine ligase in complex with ADP, phos-
		phate, $Mg2+$ and $K+$
Authors	:	Pederick, J.L.; Bruning, J.B.
Deposited on	:	2019-08-15
Resolution	:	2.20 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
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)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9924 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	324	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	А	324	2424	1576	405	438	5	0	0	U
1	В	318	Total	С	Ν	0	S	0	1	0
	D	310	2365	1536	394	431	4	0	1	0
1	С	322	Total	С	Ν	0	S	0	0	0
	U	322	2410	1572	393	440	5	0	0	0
1	Л	205	Total	С	Ν	0	S	0	0	0
	305	2289	1489	386	409	5	0	0	0	

• Molecule 1 is a protein called D-alanine–D-alanine ligase.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	MET	-	initiating methionine	UNP Q5SHZ3
А	0	GLU	-	expression tag	UNP Q5SHZ3
А	320	HIS	-	expression tag	UNP Q5SHZ3
А	321	HIS	-	expression tag	UNP Q5SHZ3
А	322	HIS	-	expression tag	UNP Q5SHZ3
A	323	HIS	-	expression tag	UNP Q5SHZ3
А	324	HIS	-	expression tag	UNP Q5SHZ3
А	325	HIS	-	expression tag	UNP Q5SHZ3
В	-1	MET	-	initiating methionine	UNP Q5SHZ3
В	0	GLU	-	expression tag	UNP Q5SHZ3
В	320	HIS	-	expression tag	UNP Q5SHZ3
В	321	HIS	-	expression tag	UNP Q5SHZ3
В	322	HIS	-	expression tag	UNP Q5SHZ3
В	323	HIS	-	expression tag	UNP Q5SHZ3
В	324	HIS	-	expression tag	UNP Q5SHZ3
В	325	HIS	-	expression tag	UNP Q5SHZ3
С	-1	MET	-	initiating methionine	UNP Q5SHZ3
С	0	GLU	-	expression tag	UNP Q5SHZ3
С	320	HIS	-	expression tag	UNP Q5SHZ3
С	321	HIS	-	expression tag	UNP Q5SHZ3
С	322	HIS	-	expression tag	UNP Q5SHZ3

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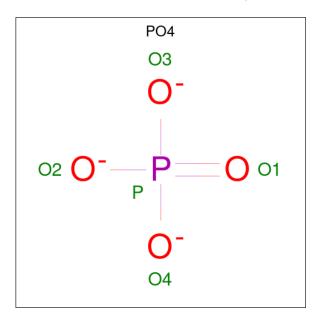
Chain	Residue	Modelled	Actual	Comment	Reference
С	323	HIS	-	expression tag	UNP Q5SHZ3
С	324	HIS	-	expression tag	UNP Q5SHZ3
С	325	HIS	-	expression tag	UNP Q5SHZ3
D	-1	MET	-	initiating methionine	UNP Q5SHZ3
D	0	GLU	-	expression tag	UNP Q5SHZ3
D	320	HIS	-	expression tag	UNP Q5SHZ3
D	321	HIS	-	expression tag	UNP Q5SHZ3
D	322	HIS	-	expression tag	UNP Q5SHZ3
D	323	HIS	-	expression tag	UNP Q5SHZ3
D	324	HIS	-	expression tag	UNP Q5SHZ3
D	325	HIS	-	expression tag	UNP Q5SHZ3

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• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mg 2 2	0	0
2	В	1	Total Mg 1 1	0	0
2	С	2	Total Mg 2 2	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



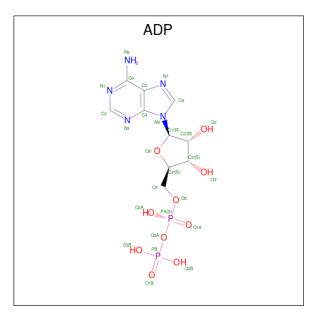


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total K 1 1	0	0
4	С	1	Total K 1 1	0	0

• Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
5	А	1	Total	С	Ν	Ο	Р	0	0	
0	Π	1	27	10	5	10	2	0	0	
5	В	1	Total	С	Ν	Ο	Р	0	0	
5	D	D	T	27	10	5	10	2	0	0
5	С	1	Total	С	Ν	Ο	Р	0	0	
5	U	1	27	10	5	10	2	0	0	
5	Л	1	Total	С	Ν	Ο	Р	0	0	
5	5 D	1	27	10	5	10	2	0	0	

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	93	Total O 93 93	0	0
6	В	68	Total O 68 68	0	0
6	С	76	Total O 76 76	0	0
6	D	74	Total O 74 74	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	55.29Å 68.62Å 91.65Å	Depositor
a, b, c, α , β , γ	69.55° 78.97° 66.10°	Depositor
Resolution (Å)	42.43 - 2.20	Depositor
% Data completeness	96.9 (42.43-2.20)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.52 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.218 , 0.265	Depositor
Wilson B-factor $(Å^2)$	33.6	Xtriage
Anisotropy	0.447	Xtriage
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9924	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.97% 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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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



Mol	Iol Type Chain Res Link		Bo	Bond lengths			Bond angles			
IVIOI	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	PO4	С	403	2	4,4,4	0.85	0	$6,\!6,\!6$	0.52	0
5	ADP	А	405	2	$24,\!29,\!29$	0.97	1 (4%)	$29,\!45,\!45$	1.31	4 (13%)
5	ADP	В	402	2	24,29,29	0.97	1 (4%)	29,45,45	1.35	4 (13%)
5	ADP	С	405	2	24,29,29	0.98	1 (4%)	29,45,45	1.32	4 (13%)
3	PO4	А	403	2	4,4,4	0.87	0	$6,\!6,\!6$	0.50	0
5	ADP	D	401	-	$24,\!29,\!29$	0.98	1 (4%)	$29,\!45,\!45$	1.27	4 (13%)

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).

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
5	ADP	D	401	-	-	1/12/32/32	0/3/3/3
5	ADP	В	402	2	-	0/12/32/32	0/3/3/3
5	ADP	А	405	2	-	0/12/32/32	0/3/3/3
5	ADP	С	405	2	-	0/12/32/32	0/3/3/3

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	ADP	C5-C4	2.52	1.47	1.40
5	А	405	ADP	C5-C4	2.46	1.47	1.40
5	В	402	ADP	C5-C4	2.45	1.47	1.40
5	С	405	ADP	C5-C4	2.45	1.47	1.40

All (4) bond length outliers are listed below:

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\mathbf{Ideal}(^{o})$
5	А	405	ADP	N3-C2-N1	-3.20	123.68	128.68
5	С	405	ADP	N3-C2-N1	-3.16	123.75	128.68
5	В	402	ADP	N3-C2-N1	-3.11	123.81	128.68
5	В	402	ADP	PA-O3A-PB	-3.09	122.21	132.83
5	D	401	ADP	N3-C2-N1	-2.88	124.17	128.68
5	С	405	ADP	PA-O3A-PB	-2.87	122.98	132.83
5	С	405	ADP	C3'-C2'-C1'	2.83	105.23	100.98
5	А	405	ADP	C4-C5-N7	-2.72	106.57	109.40

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	D	401	ADP	PA-O3A-PB	-2.71	123.52	132.83
5	А	405	ADP	PA-O3A-PB	-2.71	123.53	132.83
5	В	402	ADP	C4-C5-N7	-2.70	106.59	109.40
5	D	401	ADP	C4-C5-N7	-2.60	106.69	109.40
5	В	402	ADP	C3'-C2'-C1'	2.34	104.51	100.98
5	А	405	ADP	C3'-C2'-C1'	2.24	104.36	100.98
5	С	405	ADP	C4-C5-N7	-2.20	107.11	109.40
5	D	401	ADP	C3'-C2'-C1'	2.16	104.23	100.98

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There are no chirality outliers.

All (1) torsion outliers are listed below:

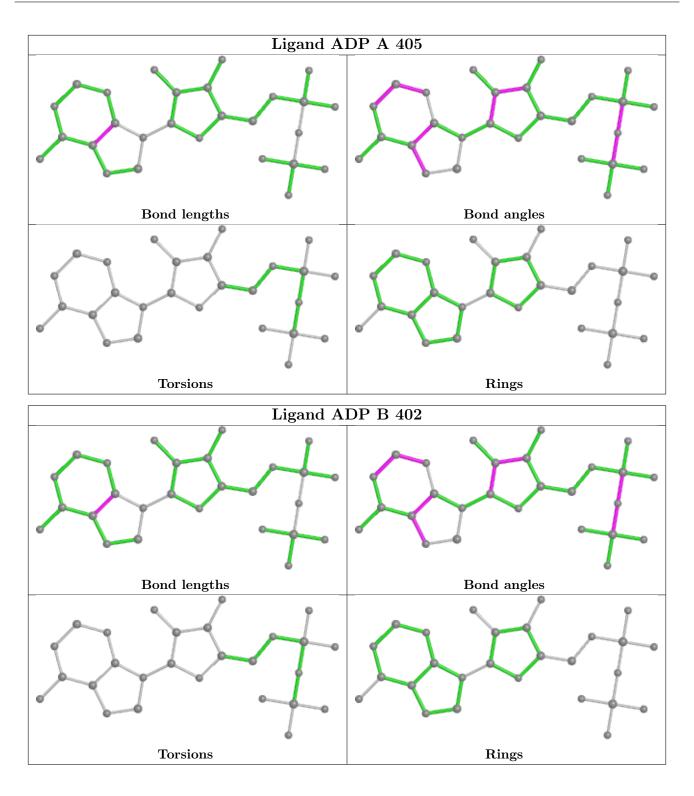
Mol	Chain	Res	Type	Atoms
5	D	401	ADP	PB-O3A-PA-O2A

There are no ring outliers.

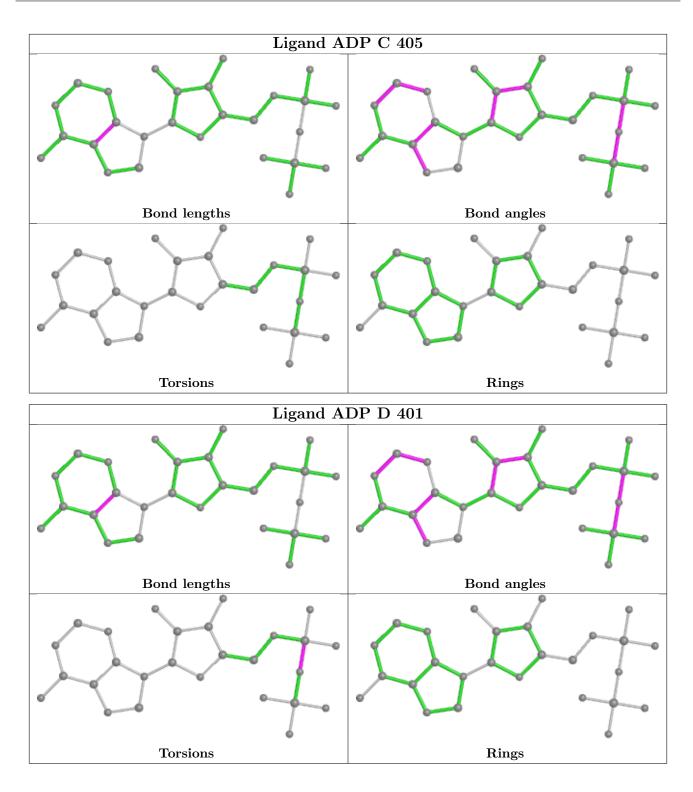
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









4.7 Other polymers (i)

There are no such residues in this entry.



4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

