



wwPDB X-ray Structure Validation Summary Report

Oct 4, 2023 – 11:08 PM EDT

PDB ID : 6UNS
Title : Kinase domain of ALK2-K492A/K493A with LDN-193189
Authors : Agnew, C.; Jura, N.
Deposited on : 2019-10-13
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 3 unique types of molecules in this entry. The entry contains 4594 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 Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2250	1433	382	421	14	0	2	0
1	B	290	2272	1445	389	423	15	0	1	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	MET	-	initiating methionine	UNP Q04771
A	171	SER	-	expression tag	UNP Q04771
A	172	TYR	-	expression tag	UNP Q04771
A	173	TYR	-	expression tag	UNP Q04771
A	174	HIS	-	expression tag	UNP Q04771
A	175	HIS	-	expression tag	UNP Q04771
A	176	HIS	-	expression tag	UNP Q04771
A	177	HIS	-	expression tag	UNP Q04771
A	178	HIS	-	expression tag	UNP Q04771
A	179	HIS	-	expression tag	UNP Q04771
A	180	HIS	-	expression tag	UNP Q04771
A	181	HIS	-	expression tag	UNP Q04771
A	182	HIS	-	expression tag	UNP Q04771
A	183	HIS	-	expression tag	UNP Q04771
A	184	ASP	-	expression tag	UNP Q04771
A	185	TYR	-	expression tag	UNP Q04771
A	186	ASP	-	expression tag	UNP Q04771
A	187	ILE	-	expression tag	UNP Q04771
A	188	PRO	-	expression tag	UNP Q04771
A	189	THR	-	expression tag	UNP Q04771
A	190	THR	-	expression tag	UNP Q04771
A	191	GLU	-	expression tag	UNP Q04771
A	192	ASN	-	expression tag	UNP Q04771
A	193	LEU	-	expression tag	UNP Q04771
A	194	TYR	-	expression tag	UNP Q04771

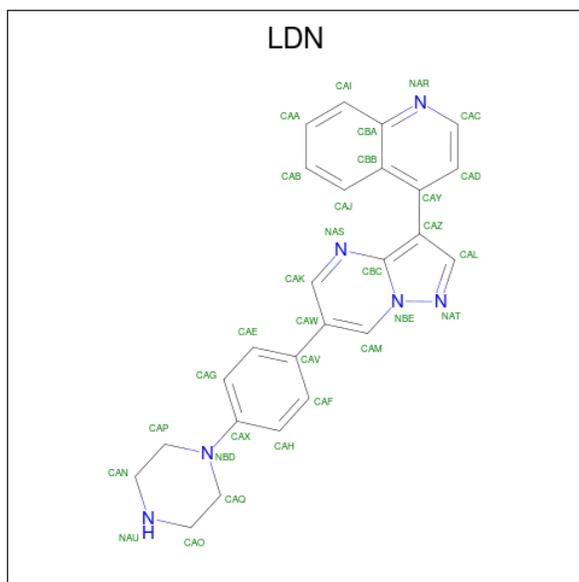
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Chain	Residue	Modelled	Actual	Comment	Reference
A	195	PHE	-	expression tag	UNP Q04771
A	196	GLN	-	expression tag	UNP Q04771
A	197	GLY	-	expression tag	UNP Q04771
A	198	ALA	-	expression tag	UNP Q04771
A	199	MET	-	expression tag	UNP Q04771
A	200	GLY	-	expression tag	UNP Q04771
A	492	ALA	LYS	engineered mutation	UNP Q04771
A	493	ALA	LYS	engineered mutation	UNP Q04771
B	170	MET	-	initiating methionine	UNP Q04771
B	171	SER	-	expression tag	UNP Q04771
B	172	TYR	-	expression tag	UNP Q04771
B	173	TYR	-	expression tag	UNP Q04771
B	174	HIS	-	expression tag	UNP Q04771
B	175	HIS	-	expression tag	UNP Q04771
B	176	HIS	-	expression tag	UNP Q04771
B	177	HIS	-	expression tag	UNP Q04771
B	178	HIS	-	expression tag	UNP Q04771
B	179	HIS	-	expression tag	UNP Q04771
B	180	HIS	-	expression tag	UNP Q04771
B	181	HIS	-	expression tag	UNP Q04771
B	182	HIS	-	expression tag	UNP Q04771
B	183	HIS	-	expression tag	UNP Q04771
B	184	ASP	-	expression tag	UNP Q04771
B	185	TYR	-	expression tag	UNP Q04771
B	186	ASP	-	expression tag	UNP Q04771
B	187	ILE	-	expression tag	UNP Q04771
B	188	PRO	-	expression tag	UNP Q04771
B	189	THR	-	expression tag	UNP Q04771
B	190	THR	-	expression tag	UNP Q04771
B	191	GLU	-	expression tag	UNP Q04771
B	192	ASN	-	expression tag	UNP Q04771
B	193	LEU	-	expression tag	UNP Q04771
B	194	TYR	-	expression tag	UNP Q04771
B	195	PHE	-	expression tag	UNP Q04771
B	196	GLN	-	expression tag	UNP Q04771
B	197	GLY	-	expression tag	UNP Q04771
B	198	ALA	-	expression tag	UNP Q04771
B	199	MET	-	expression tag	UNP Q04771
B	200	GLY	-	expression tag	UNP Q04771
B	492	ALA	LYS	engineered mutation	UNP Q04771
B	493	ALA	LYS	engineered mutation	UNP Q04771

- Molecule 2 is 4-[6-(4-piperazin-1-ylphenyl)pyrazolo[1,5-a]pyrimidin-3-yl]quinoline

(three-letter code: LDN) (formula: C₂₅H₂₂N₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 31 25 6	0	0
2	B	1	Total C N 31 25 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	5	Total O 5 5	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.00Å 83.64Å 137.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.30	Depositor
% Data completeness (in resolution range)	99.9 (48.75-2.30)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.212 , 0.262	Depositor
Wilson B-factor (Å ²)	30.3	Xtrriage
Anisotropy	0.588	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4594	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.63% 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.

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](#)

2 ligands 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LDN	A	501	-	30,36,36	2.09	7 (23%)	35,51,51	3.14	6 (17%)
2	LDN	B	501	-	30,36,36	2.03	7 (23%)	35,51,51	3.27	9 (25%)

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
2	LDN	A	501	-	-	0/4/20/20	0/6/6/6
2	LDN	B	501	-	-	0/4/20/20	0/6/6/6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LDN	CAL-CAZ	-6.70	1.26	1.40
2	B	501	LDN	CAL-CAZ	-6.51	1.27	1.40
2	B	501	LDN	CAZ-CBC	-4.48	1.32	1.43
2	A	501	LDN	CAZ-CBC	-4.16	1.33	1.43
2	A	501	LDN	CAK-NAS	4.06	1.35	1.30

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LDN	CAL-CAZ-CBC	17.45	121.33	105.20
2	A	501	LDN	CAL-CAZ-CBC	16.63	120.57	105.20
2	A	501	LDN	CAK-NAS-CBC	3.68	121.43	116.73
2	B	501	LDN	CAC-NAR-CBA	3.32	122.07	116.93
2	A	501	LDN	CAW-CAK-NAS	-3.29	120.58	125.05

There are no chirality outliers.

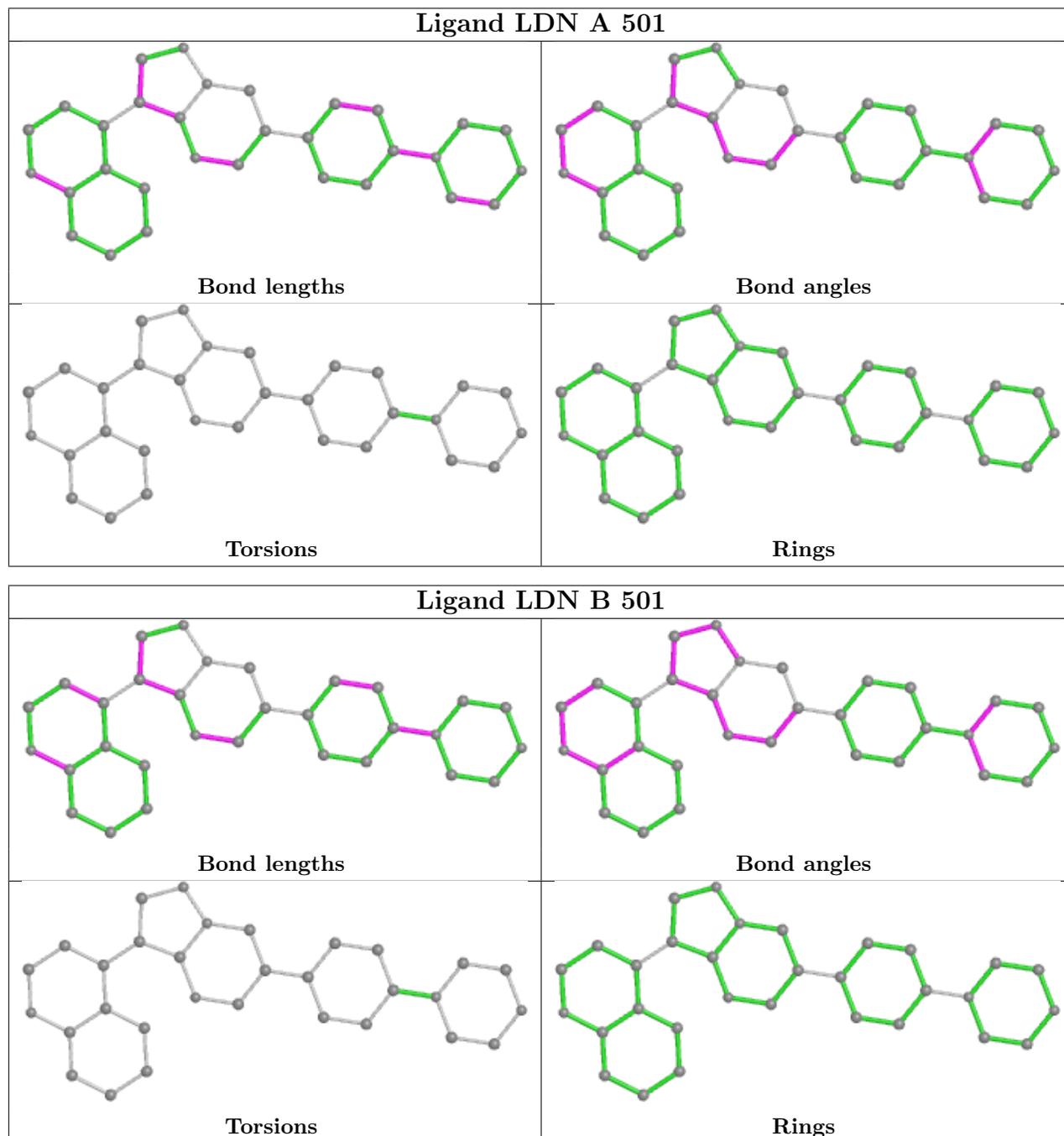
There are no torsion outliers.

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 than 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.