



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2021 – 07:03 am BST

PDB ID : 7OIJ
Title : mPI3Kd in complex with an inhibitor
Authors : Petersen, J.
Deposited on : 2021-05-11
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.23.1

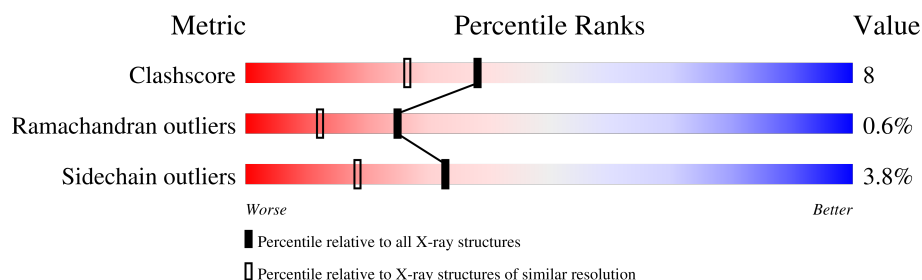
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	AAA	1084	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6982 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	827	Total	C	N	O	S	3	1	0
			6678	4281	1131	1211	55			

There are 41 discrepancies between the modelled and reference sequences:

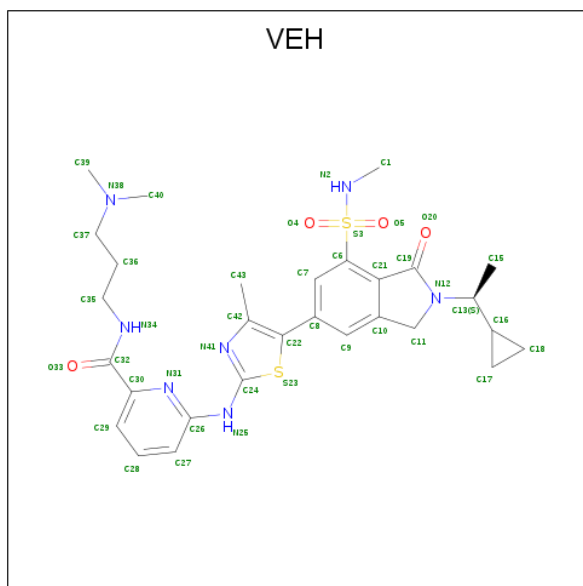
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	-	expression tag	UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	ASN	-	expression tag	UNP O35904
AAA	-32	HIS	-	expression tag	UNP O35904
AAA	-31	ASN	-	expression tag	UNP O35904
AAA	-30	HIS	-	expression tag	UNP O35904
AAA	-29	ASN	-	expression tag	UNP O35904
AAA	-28	HIS	-	expression tag	UNP O35904
AAA	-27	ASN	-	expression tag	UNP O35904
AAA	-26	HIS	-	expression tag	UNP O35904
AAA	-25	ASN	-	expression tag	UNP O35904
AAA	-24	ASP	-	expression tag	UNP O35904
AAA	-23	TYR	-	expression tag	UNP O35904
AAA	-22	ASP	-	expression tag	UNP O35904
AAA	-21	ILE	-	expression tag	UNP O35904
AAA	-20	PRO	-	expression tag	UNP O35904
AAA	-19	THR	-	expression tag	UNP O35904
AAA	-18	THR	-	expression tag	UNP O35904
AAA	-17	GLU	-	expression tag	UNP O35904
AAA	-16	ASN	-	expression tag	UNP O35904
AAA	-15	LEU	-	expression tag	UNP O35904
AAA	-14	TYR	-	expression tag	UNP O35904

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression tag	UNP O35904
AAA	99	GLU	-	insertion	UNP O35904
AAA	100	ASN	-	insertion	UNP O35904
AAA	101	LEU	-	insertion	UNP O35904
AAA	102	TYR	-	insertion	UNP O35904
AAA	103	PHE	-	insertion	UNP O35904
AAA	104	GLN	-	insertion	UNP O35904
AAA	105	GLY	-	insertion	UNP O35904
AAA	510A	GLN	-	insertion	UNP O35904

- Molecule 2 is 6-[[5-[2-[(1S)-1-cyclopropylethyl]-7-(methylsulfonyl)-1-oxidanylidene-3H-is oindol-5-yl]-4-methyl-1,3-thiazol-2-yl]amino]-N-[3-(dimethylamino)propyl]pyridine-2-carbo xamide (three-letter code: VEH) (formula: C₂₉H₃₇N₇O₄S₂) (labeled as "Ligand of Interest" by depositor).

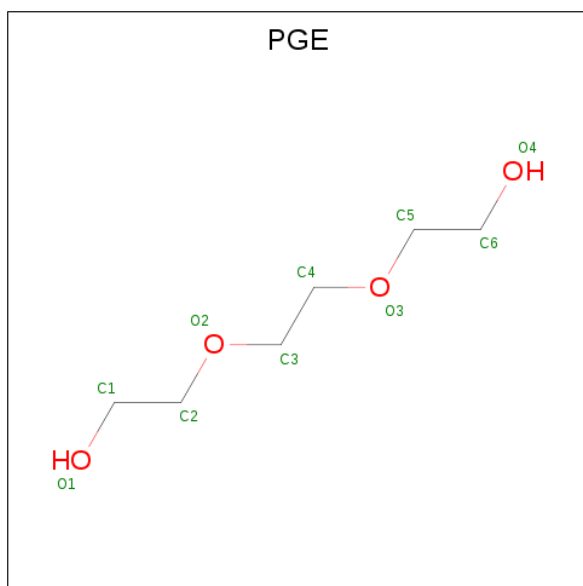


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	S	0	0
			42	29	7	4	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Na 1 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	257	Total O 257 257	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.81Å 64.84Å 116.58Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	42.97 – 1.80	Depositor
% Data completeness (in resolution range)	99.2 (42.97-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6982	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VEH, NA, PGE

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	AAA	0.71	0/6824	0.81	0/9207

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	6678	0	6656	101	1
2	AAA	42	0	0	1	0
3	AAA	1	0	0	0	0
4	AAA	4	0	5	1	0
5	AAA	257	0	0	3	0
All	All	6982	0	6661	102	1

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 8.

The worst 5 of 102 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:AAA:495:ILE:HG23	1:AAA:563:GLN:HA	1.38	1.05
1:AAA:495:ILE:CG2	1:AAA:563:GLN:HA	2.02	0.90
1:AAA:495:ILE:HD13	1:AAA:562:ALA:O	1.78	0.84
1:AAA:495:ILE:CD1	1:AAA:562:ALA:O	2.28	0.81
1:AAA:367:SER:HB3	1:AAA:368:GLU:C	2.05	0.77

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)
1:AAA:714:MET:SD	1:AAA:714:MET:SD[2_555]	1.48	0.72

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	AAA	806/1084 (74%)	778 (96%)	23 (3%)	5 (1%)	25	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	367	SER
1	AAA	893	ASP
1	AAA	1026	SER
1	AAA	368	GLU
1	AAA	496	THR

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	AAA	734/962 (76%)	706 (96%)	28 (4%)	33	18

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	530	LEU
1	AAA	1026	SER
1	AAA	634	LEU
1	AAA	841	LYS
1	AAA	553	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 3 ligands modelled in this entry, 1 is 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	AAA	1103	-	3,3,9	0.55	0	2,2,8	0.25	0
2	VEH	AAA	1101	-	39,46,46	1.21	2 (5%)	46,68,68	2.61	13 (28%)

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	PGE	AAA	1103	-	-	0/1/1/7	-
2	VEH	AAA	1101	-	-	4/34/50/50	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1101	VEH	C9-C10	-3.42	1.33	1.39
2	AAA	1101	VEH	C29-C30	2.69	1.44	1.39

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1101	VEH	C10-C11-N12	10.77	105.77	102.18
2	AAA	1101	VEH	C11-N12-C19	-8.29	109.71	113.12
2	AAA	1101	VEH	C30-C32-N34	4.00	121.18	115.59
2	AAA	1101	VEH	C13-N12-C19	3.83	127.02	122.91
2	AAA	1101	VEH	C29-C28-C27	-3.01	115.98	120.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

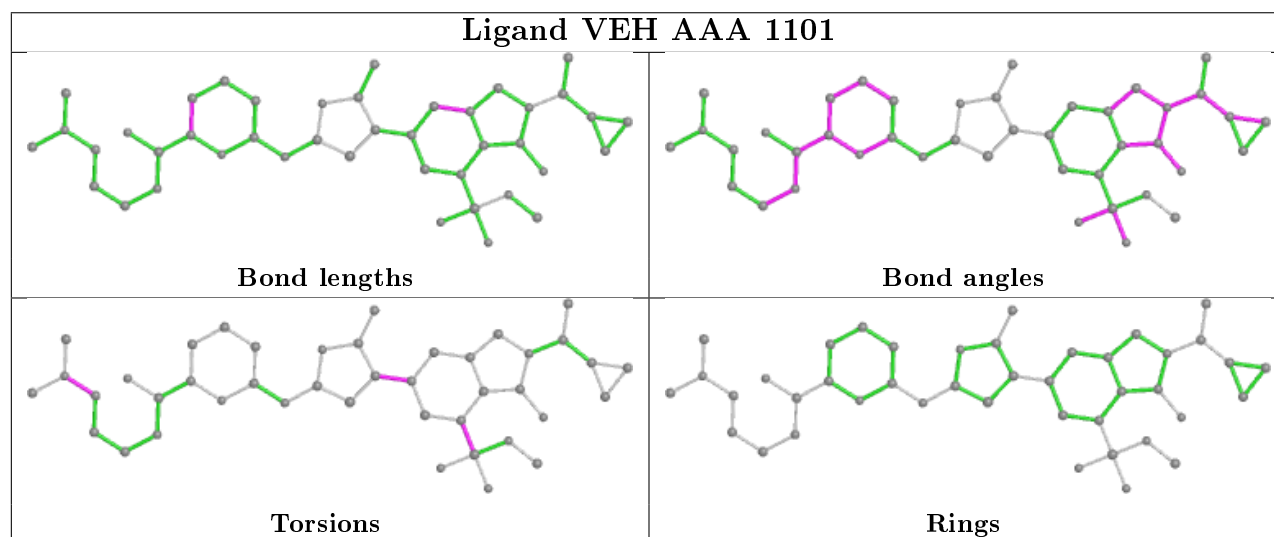
Mol	Chain	Res	Type	Atoms
2	AAA	1101	VEH	C42-C22-C8-C7
2	AAA	1101	VEH	C36-C37-N38-C40
2	AAA	1101	VEH	C21-C6-S3-O4
2	AAA	1101	VEH	C42-C22-C8-C9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	1103	PGE	1	0
2	AAA	1101	VEH	1	0

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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	497:GLU	C	509:GLU	N	21.77

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.