



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 03:23 PM EDT

PDB ID : 6EYZ  
Title : PI3 kinase delta in complex with 4-Fluorophenyl 5-(4-(5-((4-isopropylpiperazin-1-yl)methyl)oxazol-2-yl)-1H-indazol-6-yl)-2-methoxynicotinate  
Authors : Convery, M.A.; Campos, S.; Dalton, S.E.  
Deposited on : 2017-11-13  
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](mailto: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

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
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) : 2.37.1

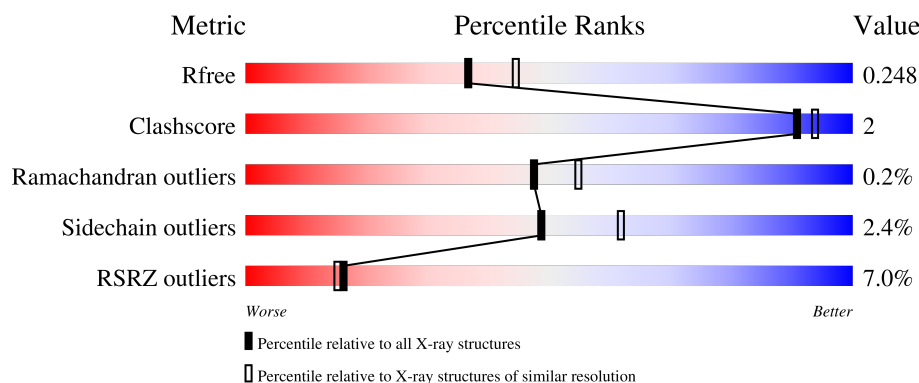
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1051	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7281 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.

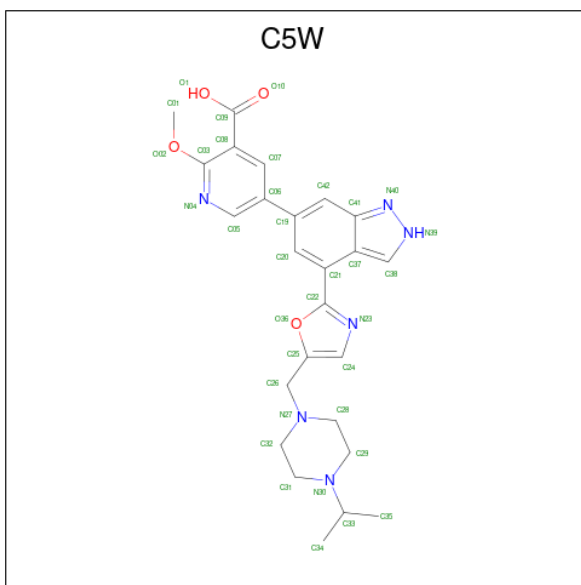
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6940	4434	1190	1262	54			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLU	-	insertion	UNP Q3UDT3
A	100	ASN	-	insertion	UNP Q3UDT3
A	101	LEU	-	insertion	UNP Q3UDT3
A	102	TYR	-	insertion	UNP Q3UDT3
A	103	PHE	-	insertion	UNP Q3UDT3
A	104	GLN	-	insertion	UNP Q3UDT3
A	105	GLY	-	insertion	UNP Q3UDT3

- Molecule 2 is 2-methoxy-5-[4-[5-[(4-propan-2-ylpiperazin-1-yl)methyl]-1,3-oxazol-2-yl]-2 {H}-indazol-6-yl]pyridine-3-carboxylic acid (three-letter code: C5W) (formula: C<sub>25</sub>H<sub>28</sub>N<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	25	6	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	307	Total O 307 307	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.83Å 64.58Å 116.41Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	54.06 – 2.20 54.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (54.06-2.20) 98.5 (54.06-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.190 , 0.237 0.203 , 0.248	Depositor DCC
$R_{free}$ test set	2577 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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: C5W

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	0.51	0/7090	0.65	0/9571

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 [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	A	6940	0	6910	24	0
2	A	34	0	0	0	0
3	A	307	0	0	1	0
All	All	7281	0	6910	24	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 2.

All (24) 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:A:350:GLY:HA3	1:A:588:PRO:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:HG13	1:A:552:VAL:HG21	1.81	0.61
1:A:349:HIS:HB2	1:A:354:LEU:HD21	1.84	0.58
1:A:341:LEU:HG	1:A:365:VAL:HG22	1.85	0.58
1:A:929:ARG:HH22	1:A:1001:SER:HA	1.72	0.55
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.91	0.53
1:A:695:LEU:HD23	1:A:759:LEU:HD13	1.90	0.53
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.92	0.52
1:A:703:SER:HA	3:A:1331:HOH:O	2.11	0.50
1:A:902:ARG:HD3	1:A:906:GLN:HB2	1.93	0.50
1:A:209:THR:HB	1:A:257:CYS:HB3	1.96	0.47
1:A:618:VAL:HG11	1:A:980:LEU:HD22	1.98	0.46
1:A:500:ARG:HE	1:A:536:HIS:HB3	1.82	0.45
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.52	0.44
1:A:991:CYS:SG	1:A:993:LYS:HG2	2.57	0.44
1:A:758:PRO:HB3	1:A:779:LYS:HG2	2.00	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.00	0.43
1:A:191:LEU:O	1:A:272:PRO:HD2	2.19	0.42
1:A:135:GLU:HG2	1:A:625:LEU:HD12	2.01	0.41
1:A:326:GLU:HB3	1:A:474:TYR:HB3	2.01	0.41
1:A:245:GLY:HA3	1:A:768:ALA:HB2	2.02	0.41
1:A:194:VAL:HG21	1:A:216:LEU:HD21	2.01	0.41
1:A:203:PHE:HE1	1:A:227:VAL:HG21	1.86	0.40
1:A:173:PRO:HB3	1:A:799:VAL:HG13	2.02	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	846/1051 (80%)	823 (97%)	21 (2%)	2 (0%)	47 55

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	328	ILE
1	A	379	ILE

### 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	760/931 (82%)	742 (98%)	18 (2%)	49 62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	264	SER
1	A	267	HIS
1	A	283	LEU
1	A	416	CYS
1	A	430	ASP
1	A	439	LEU
1	A	459	VAL
1	A	523	LEU
1	A	525	GLU
1	A	696	ASN
1	A	767	GLU
1	A	779	LYS
1	A	787	ASP
1	A	795	GLN
1	A	895	HIS
1	A	915	PHE
1	A	1029	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	C5W	A	1101	1	33,38,39	0.78	1 (3%)	37,54,56	1.14	2 (5%)

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	C5W	A	1101	1	-	4/15/30/32	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	C5W	C26-C25	-2.19	1.49	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	C5W	C19-C42-C41	-3.52	118.36	121.44
2	A	1101	C5W	C26-C25-C24	3.28	135.48	128.93

There are no chirality outliers.

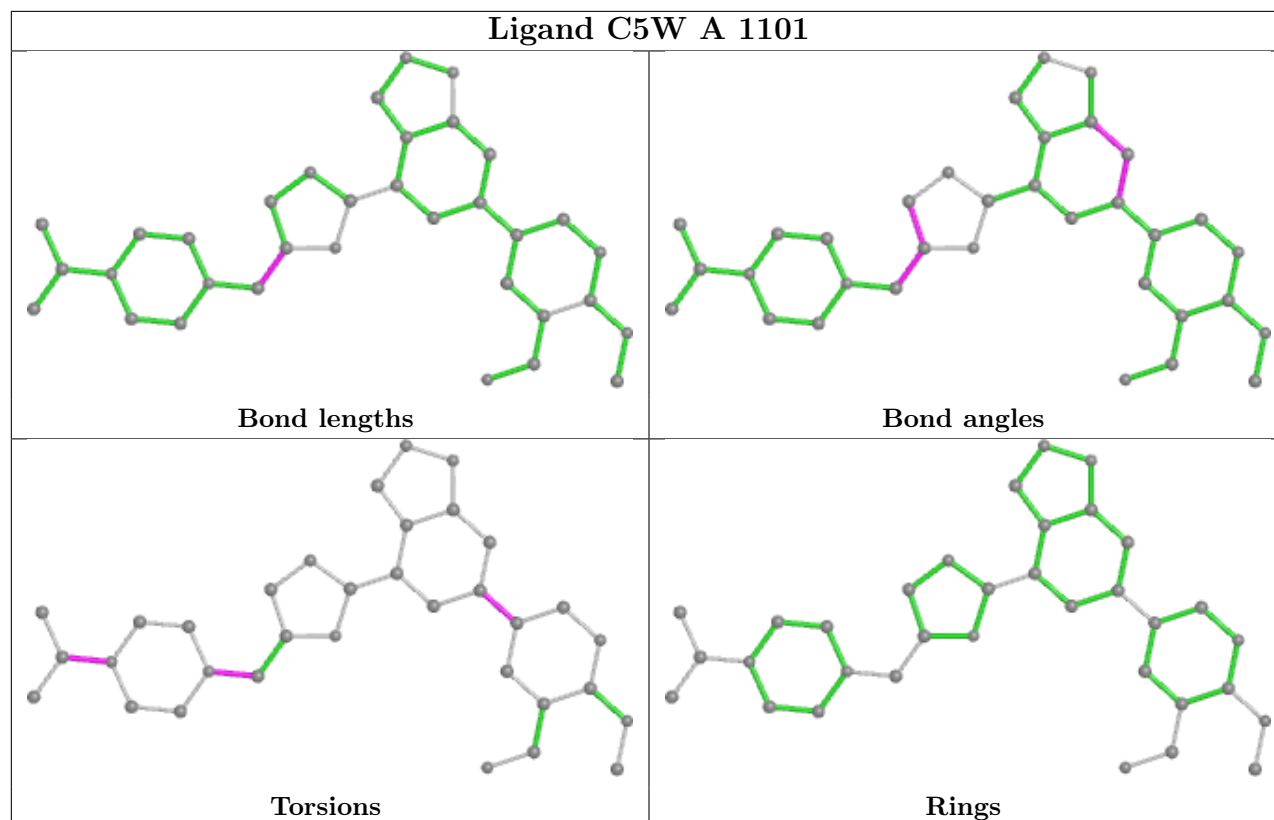
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	C5W	C25-C26-N27-C32
2	A	1101	C5W	C07-C06-C19-C42
2	A	1101	C5W	C34-C33-N30-C29
2	A	1101	C5W	C07-C06-C19-C20

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.



## 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	862/1051 (82%)	0.44	60 (6%)	16 15	35, 64, 111, 177	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	LEU	7.6
1	A	506	GLU	6.5
1	A	1031	VAL	6.3
1	A	531	VAL	4.6
1	A	1030	LYS	4.5
1	A	233	VAL	4.2
1	A	323	PHE	4.2
1	A	507	GLU	4.1
1	A	530	LEU	3.8
1	A	503	ILE	3.8
1	A	514	ILE	3.8
1	A	232	LEU	3.7
1	A	361	SER	3.6
1	A	341	LEU	3.6
1	A	1027	TRP	3.4
1	A	529	ASP	3.4
1	A	1005	GLY	3.4
1	A	365	VAL	3.3
1	A	292	PRO	3.3
1	A	471	LEU	3.3
1	A	505	GLU	3.3
1	A	396	ALA	3.3
1	A	108	ARG	3.1
1	A	228	PHE	3.1
1	A	370	VAL	3.1
1	A	472	VAL	3.0
1	A	511	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	504	THR	2.9
1	A	474	TYR	2.9
1	A	517	ARG	2.9
1	A	496	ARG	2.9
1	A	395	TYR	2.8
1	A	371	TRP	2.8
1	A	523	LEU	2.8
1	A	522	GLU	2.8
1	A	936	TYR	2.7
1	A	710	GLN	2.6
1	A	358	VAL	2.5
1	A	534	MET	2.5
1	A	1024	ARG	2.5
1	A	483	VAL	2.4
1	A	491	ILE	2.4
1	A	524	TYR	2.3
1	A	477	GLU	2.3
1	A	443	PRO	2.2
1	A	480	PRO	2.2
1	A	515	LEU	2.2
1	A	513	GLU	2.2
1	A	366	CYS	2.2
1	A	189	ALA	2.1
1	A	330	GLY	2.1
1	A	225	ALA	2.1
1	A	1013	LYS	2.1
1	A	109	VAL	2.1
1	A	234	GLU	2.1
1	A	329	GLU	2.1
1	A	846	ALA	2.1
1	A	203	PHE	2.1
1	A	521	GLY	2.1
1	A	342	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

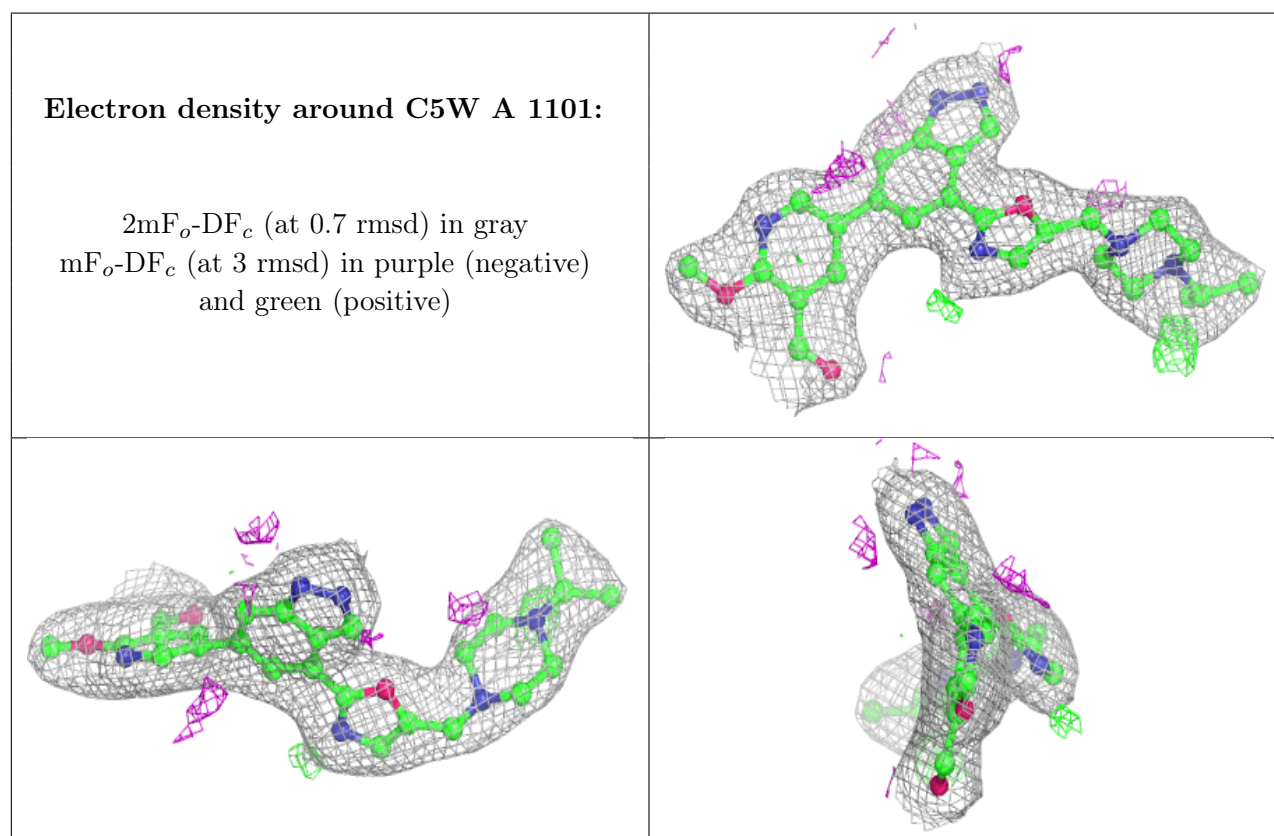
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C5W	A	1101	34/35	0.97	0.18	30,40,51,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.