



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:09 PM EDT

PDB ID : 5T27  
Title : mPI3Kd IN COMPLEX WITH 5d  
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Deposited on : 2016-08-23  
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](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

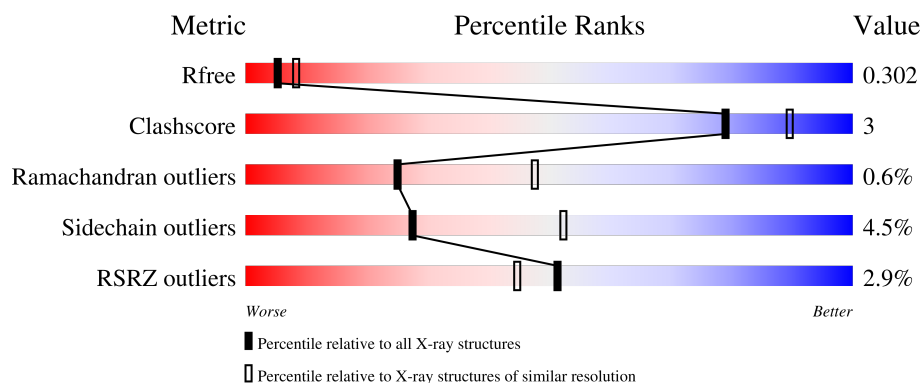
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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  $\geq 3$ , 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	939	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6676 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.

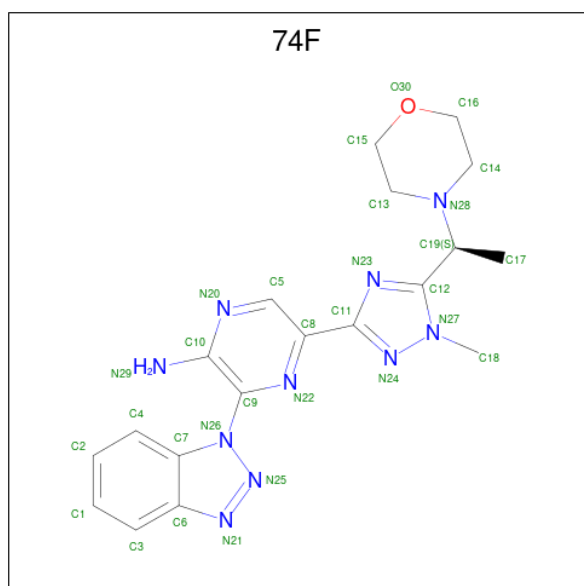
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	819	6628	4249	1127	1200	52	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	510A	GLN	-	insertion	UNP O35904

- Molecule 2 is 3-(benzotriazol-1-yl)-5-[1-methyl-5-[(1 {S})-1-morpholin-4-ylethyl]-1,2,4-triazol-1-yl]pyrazin-2-amine (three-letter code: 74F) (formula: C<sub>19</sub>H<sub>22</sub>N<sub>10</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	19	10	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.79Å 143.66Å 219.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.65 – 2.60 43.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.65-2.60) 98.5 (43.65-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.252 , 0.296 0.256 , 0.302	Depositor DCC
$R_{free}$ test set	1575 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: 74F

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	0.43	0/6768	0.64	2/9126 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	332	LYS	C-N-CA	5.95	136.57	121.70
1	A	333	VAL	C-N-CA	5.45	135.32	121.70

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	6628	0	6599	37	0
2	A	30	0	0	0	0
3	A	18	0	0	0	0
All	All	6676	0	6599	37	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 3.

All (37) 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:424:MET:O	1:A:433:LYS:NZ	2.06	0.86
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.61	0.82
1:A:507:THR:HA	1:A:509:GLU:H	1.50	0.76
1:A:361:SER:H	1:A:373:GLN:HE22	1.33	0.76
1:A:549:LEU:HG	1:A:564:MET:CE	2.30	0.61
1:A:434:THR:HA	1:A:475:LEU:HB3	1.85	0.59
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.85	0.58
1:A:549:LEU:HG	1:A:564:MET:HE1	1.87	0.56
1:A:192:VAL:HG11	1:A:216:LEU:HD11	1.86	0.56
1:A:895:HIS:H	1:A:898:ASN:HD21	1.55	0.53
1:A:319:LEU:HD11	1:A:483:VAL:HG11	1.92	0.52
1:A:434:THR:HG21	1:A:477:GLU:HA	1.91	0.52
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.92	0.51
1:A:436:GLU:O	1:A:437:ARG:HD2	2.13	0.49
1:A:209:THR:HB	1:A:257:CYS:HB3	1.95	0.48
1:A:340:LYS:HD3	1:A:362:GLU:HB3	1.95	0.48
1:A:779:LYS:HE2	1:A:784:LEU:HD21	1.96	0.47
1:A:614:GLN:O	1:A:618:VAL:HG23	2.15	0.47
1:A:110:LYS:HE2	1:A:144:ARG:HH22	1.80	0.46
1:A:419:ALA:HB1	1:A:441:MET:HB3	1.98	0.46
1:A:343:VAL:H	1:A:360:SER:HB3	1.81	0.46
1:A:549:LEU:HG	1:A:564:MET:HE3	1.99	0.45
1:A:225:ALA:HB1	1:A:230:GLN:HB2	1.99	0.45
1:A:434:THR:HA	1:A:475:LEU:CB	2.45	0.44
1:A:512:ARG:HH11	1:A:534:MET:HB3	1.83	0.44
1:A:691:LYS:HG3	1:A:727:ALA:HB3	2.00	0.43
1:A:205:PHE:HE1	1:A:223:LYS:HG3	1.83	0.43
1:A:895:HIS:H	1:A:898:ASN:ND2	2.16	0.42
1:A:317:TRP:HA	1:A:382:CYS:HB2	2.02	0.42
1:A:116:GLN:HB3	1:A:679:MET:CE	2.50	0.41
1:A:610:GLN:HE22	1:A:799:VAL:HG21	1.83	0.41
1:A:786:GLN:OE1	1:A:988:GLU:HG3	2.20	0.41
1:A:698:PHE:CZ	1:A:714:MET:HB3	2.55	0.41
1:A:341:LEU:HD12	1:A:369:PRO:HG3	2.02	0.41
1:A:369:PRO:HG2	1:A:371:TRP:CH2	2.56	0.41
1:A:331:ARG:HD2	1:A:470:ALA:HB3	2.02	0.40
1:A:425:LEU:O	1:A:433:LYS:HG3	2.21	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	791/939 (84%)	762 (96%)	24 (3%)	5 (1%)	25	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	A	334	ASN
1	A	229	ARG
1	A	328	ILE
1	A	332	LYS

### 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	727/827 (88%)	694 (96%)	33 (4%)	27	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	119	LEU
1	A	156	GLN
1	A	166	SER
1	A	191	LEU
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	317	TRP
1	A	332	LYS
1	A	333	VAL
1	A	338	ARG
1	A	356	LYS
1	A	374	ARG
1	A	430	ASP
1	A	512	ARG
1	A	514	ILE
1	A	516	GLU
1	A	517	ARG
1	A	530	LEU
1	A	559	GLU
1	A	560	ASP
1	A	565	LEU
1	A	610	GLN
1	A	731	LEU
1	A	743	GLU
1	A	839	LEU
1	A	851	ASN
1	A	855	LEU
1	A	898	ASN
1	A	915	PHE
1	A	965	THR
1	A	998	LEU
1	A	1009	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	258	HIS
1	A	278	HIS
1	A	291	ASN
1	A	373	GLN
1	A	610	GLN
1	A	617	GLN
1	A	780	ASN
1	A	795	GLN
1	A	898	ASN
1	A	914	HIS

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Mol	Chain	Res	Type
1	A	918	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	74F	A	1101	-	29,34,34	1.00	2 (6%)	33,49,49	1.38	6 (18%)

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	74F	A	1101	-	-	3/9/24/24	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74F	C10-N29	2.63	1.40	1.34
2	A	1101	74F	C12-N23	-2.06	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74F	C9-N26-N25	2.84	122.37	117.81
2	A	1101	74F	C1-C3-C6	-2.58	116.38	120.08
2	A	1101	74F	N21-N25-N26	2.40	109.05	106.37
2	A	1101	74F	O30-C16-C14	-2.35	106.61	111.80
2	A	1101	74F	C2-C4-C7	-2.26	115.11	119.44
2	A	1101	74F	N23-C12-N27	-2.05	107.53	111.22

There are no chirality outliers.

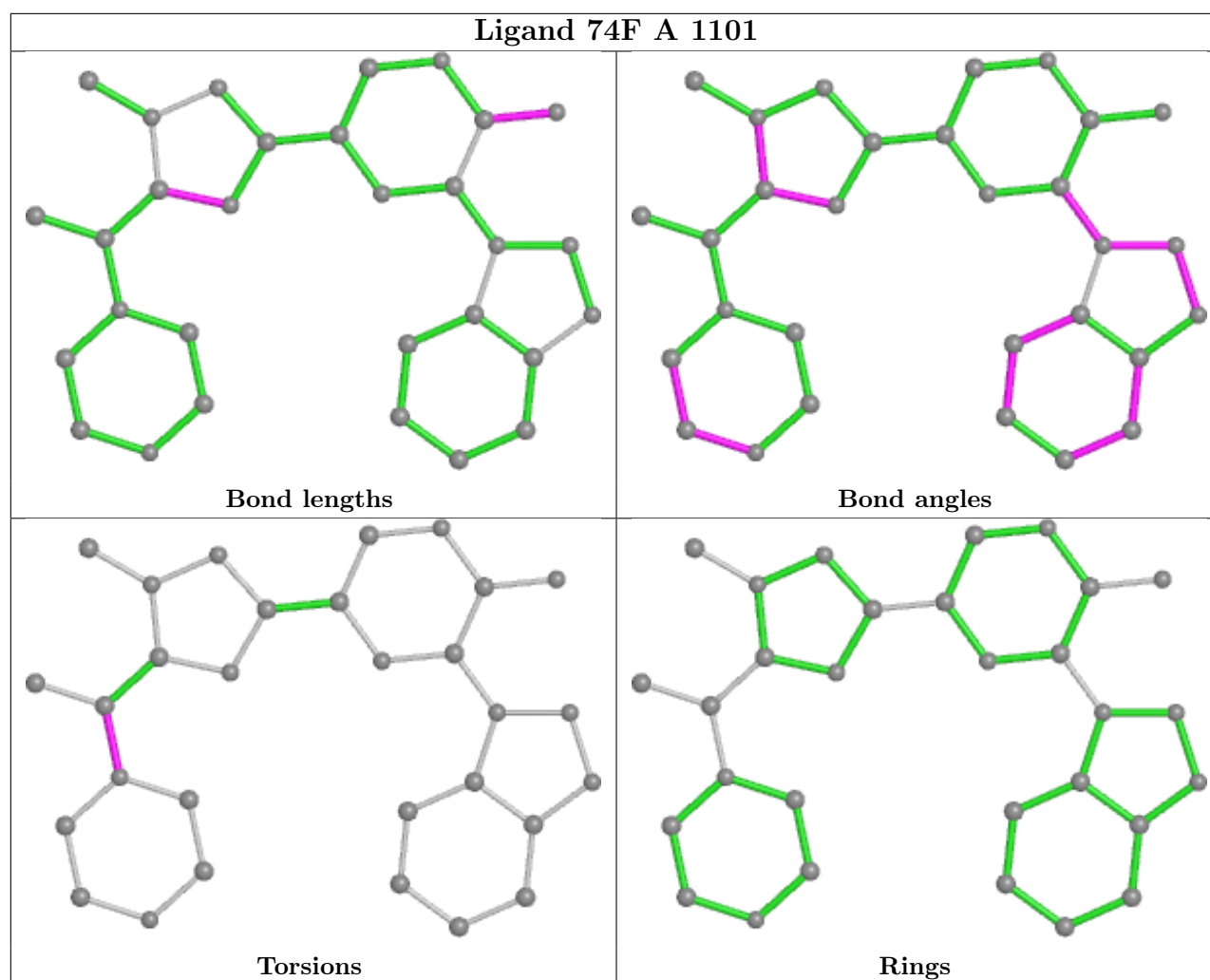
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	74F	C12-C19-N28-C13
2	A	1101	74F	C12-C19-N28-C14
2	A	1101	74F	C17-C19-N28-C13

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	819/939 (87%)	0.19	24 (2%)	51	45	21, 52, 86, 133	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	TRP	6.5
1	A	330	GLY	5.1
1	A	334	ASN	4.4
1	A	394	LEU	4.1
1	A	470	ALA	3.7
1	A	341	LEU	3.4
1	A	767	GLU	3.2
1	A	203	PHE	3.2
1	A	396	ALA	2.9
1	A	467	SER	2.9
1	A	847	THR	2.7
1	A	471	LEU	2.7
1	A	933	ILE	2.6
1	A	205	PHE	2.5
1	A	364	ASN	2.5
1	A	226	THR	2.4
1	A	517	ARG	2.4
1	A	417	PRO	2.3
1	A	264	SER	2.3
1	A	363	VAL	2.1
1	A	216	LEU	2.1
1	A	768	ALA	2.1
1	A	932	PHE	2.1
1	A	945	GLY	2.1

## 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](#)

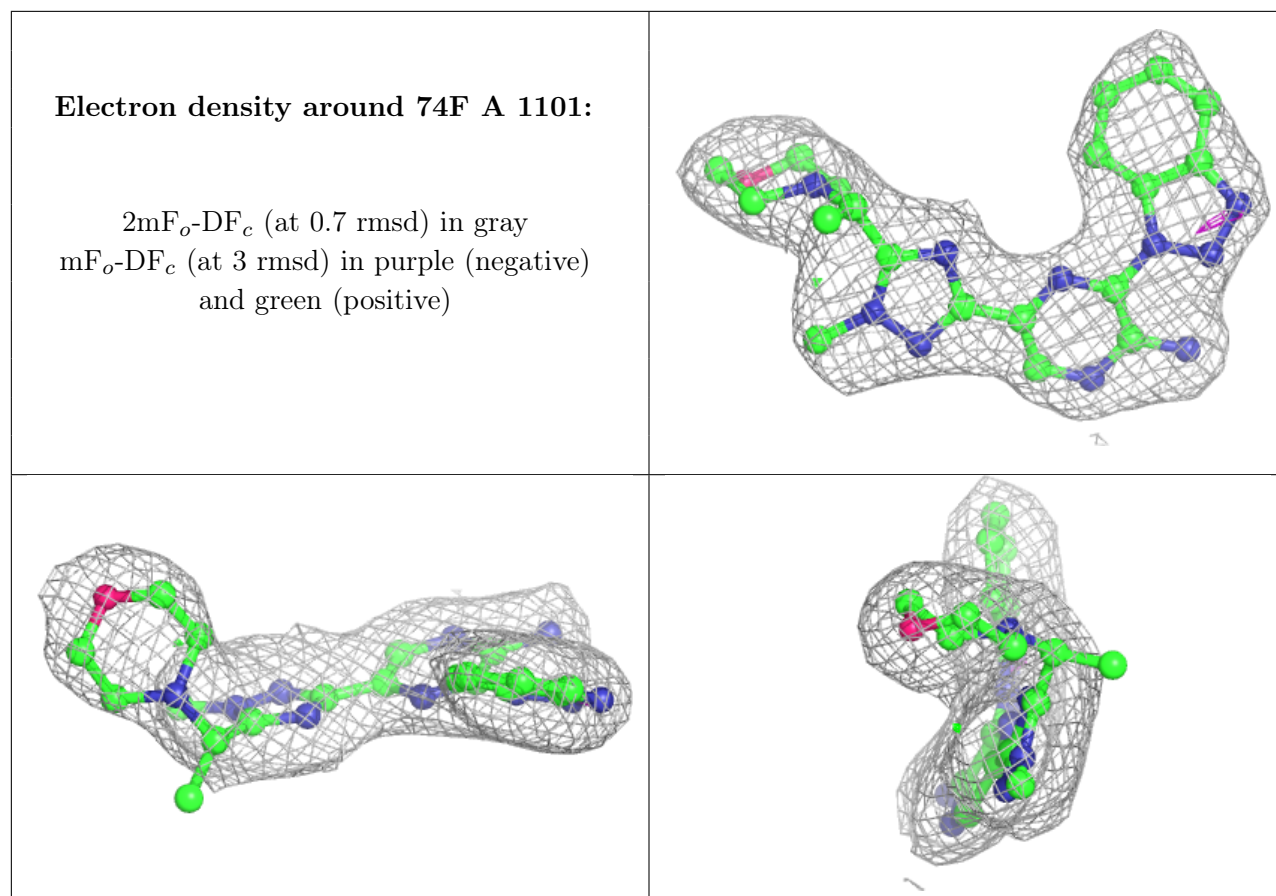
There are no monosaccharides in this entry.

## 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	74F	A	1101	30/30	0.94	0.19	26,41,50,52	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 ⓘ

There are no such residues in this entry.