



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:40 am BST

PDB ID : 5T2L  
Title : mPI3Kd IN COMPLEX WITH 7I  
Authors : Petersen, J.; Terstige, I.; Perry, M.; Svensson, T.; Tyrchan, C.; Lindmark, H.; Oster, L.  
Deposited on : 2016-08-23  
Resolution : 2.55 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.

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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 : 2.11  
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) : 2.11

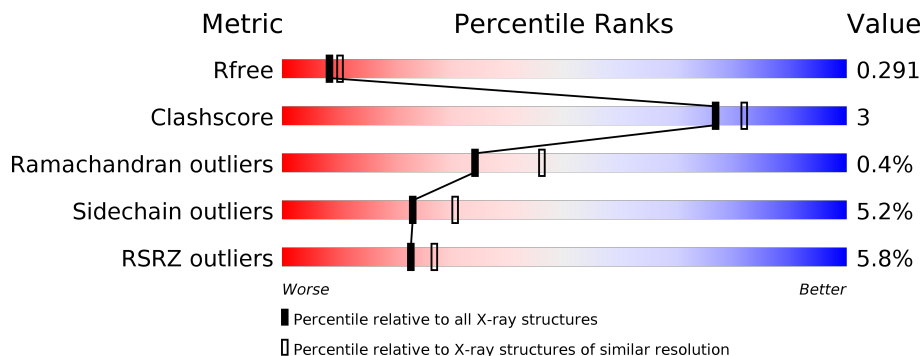
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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 6765 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.

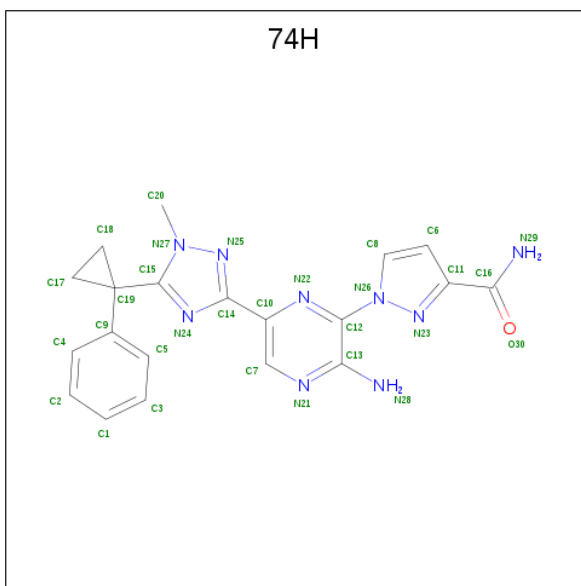
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	830	6675	4279	1134	1207	55	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is 1-[3-azanyl-6-[1-methyl-5-(1-phenylcyclopropyl)-1,2,4-triazol-3-yl]pyrazin-2-yl]pyrazole-3-carboxamide (three-letter code: 74H) (formula: C<sub>20</sub>H<sub>19</sub>N<sub>9</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	20	9	1	0	0

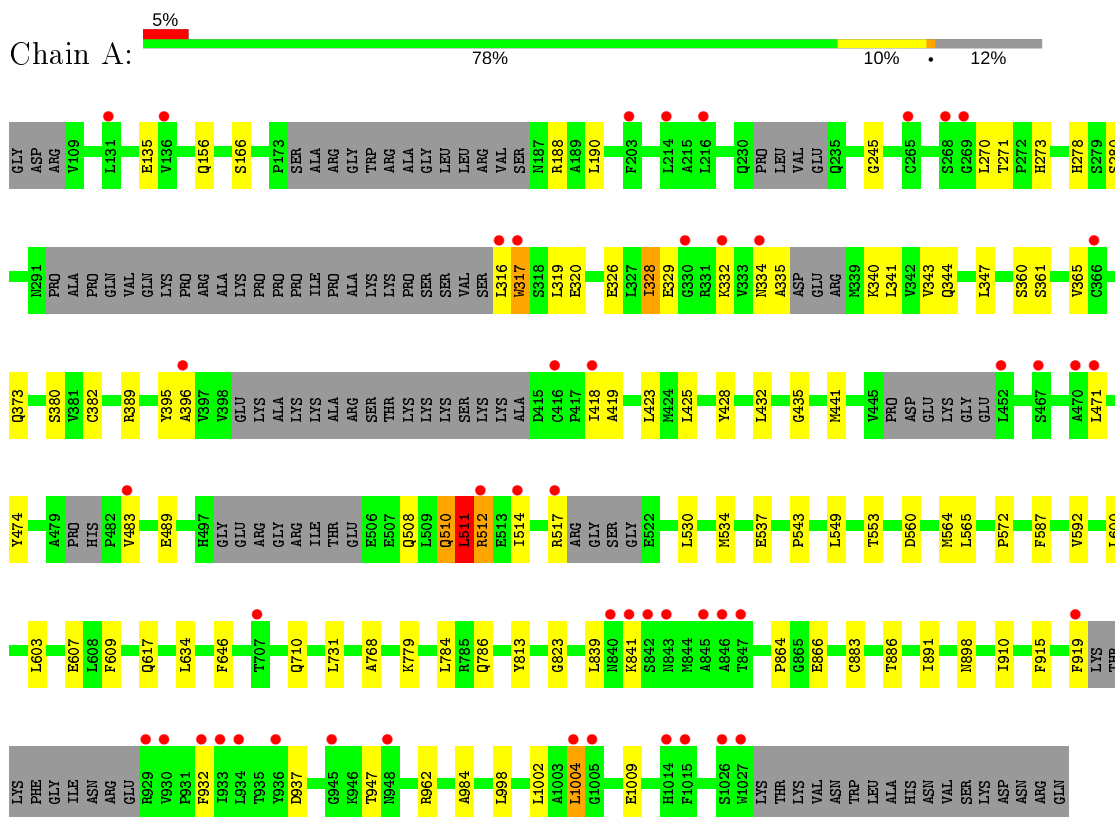
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	A	60	Total O 60 60	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.55Å 142.19Å 218.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.69 – 2.55 51.26 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (54.69-2.55) 98.5 (51.26-2.55)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.55Å)	Xtrriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.228 , 0.279 0.233 , 0.291	Depositor DCC
$R_{free}$ test set	1627 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtrriage
Anisotropy	0.475	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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: 74H

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	0.49	0/6821	0.69	1/9204 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	510	GLN	C-N-CA	6.69	138.43	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	6675	0	6637	40	0
2	A	30	0	0	0	0
3	A	60	0	0	0	0
All	All	6765	0	6637	40	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 (40) 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:510:GLN:HA	1:A:512:ARG:H	1.56	0.71
1:A:361:SER:H	1:A:373:GLN:HE22	1.44	0.65
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.77	0.65
1:A:347:LEU:HD21	1:A:425:LEU:HD11	1.84	0.59
1:A:512:ARG:HH12	1:A:537:GLU:HB2	1.66	0.59
1:A:319:LEU:HD11	1:A:483:VAL:HG11	1.85	0.58
1:A:549:LEU:HG	1:A:564:MET:CE	2.34	0.58
1:A:317:TRP:HA	1:A:382:CYS:HB2	1.86	0.57
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.92	0.51
1:A:603:LEU:HD22	1:A:607:GLU:HB3	1.91	0.51
1:A:886:THR:HA	1:A:891:ILE:HD12	1.92	0.51
1:A:609:PHE:HE1	1:A:646:PHE:CD2	2.30	0.50
1:A:587:PHE:HB3	1:A:592:VAL:HG11	1.93	0.50
1:A:549:LEU:HG	1:A:564:MET:HE3	1.92	0.50
1:A:883:CYS:HB3	1:A:932:PHE:CZ	2.47	0.50
1:A:343:VAL:H	1:A:360:SER:HB3	1.78	0.49
1:A:508:GLN:O	1:A:511:LEU:HB2	2.12	0.49
1:A:271:THR:O	1:A:273:HIS:HD2	1.97	0.48
1:A:779:LYS:HD3	1:A:784:LEU:HD21	1.95	0.47
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.97	0.47
1:A:432:LEU:HB3	1:A:483:VAL:HG23	1.96	0.47
1:A:278:HIS:CD2	1:A:280:SER:H	2.35	0.45
1:A:334:ASN:ND2	1:A:335:ALA:H	2.15	0.44
1:A:361:SER:N	1:A:373:GLN:HE22	2.14	0.44
1:A:419:ALA:HB1	1:A:441:MET:HB3	1.99	0.44
1:A:1002:LEU:HB3	1:A:1004:LEU:HD23	2.00	0.43
1:A:512:ARG:NH1	1:A:534:MET:HB3	2.33	0.43
1:A:328:ILE:HG22	1:A:329:GLU:HG2	2.01	0.43
1:A:344:GLN:HB2	1:A:395:TYR:HE1	1.84	0.42
1:A:549:LEU:HG	1:A:564:MET:HE1	2.00	0.42
1:A:341:LEU:HG	1:A:365:VAL:HG22	2.02	0.42
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.55	0.42
1:A:543:PRO:HB3	1:A:572:PRO:HG2	2.02	0.42
1:A:347:LEU:CD2	1:A:425:LEU:HD11	2.49	0.41
1:A:813:TYR:OH	1:A:910:ILE:HA	2.20	0.41
1:A:320:GLU:HA	1:A:380:SER:OG	2.20	0.41
1:A:334:ASN:ND2	1:A:335:ALA:N	2.69	0.41
1:A:396:ALA:HB2	1:A:418:ILE:HD11	2.03	0.40
1:A:600:LEU:O	1:A:603:LEU:HB2	2.22	0.40
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.85	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	809/939 (86%)	780 (96%)	26 (3%)	3 (0%)	34	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	LEU
1	A	328	ILE
1	A	435	GLY

### 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	729/827 (88%)	691 (95%)	38 (5%)	23	30

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	166	SER
1	A	188	ARG
1	A	190	LEU
1	A	270	LEU
1	A	316	LEU
1	A	317	TRP
1	A	332	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	340	LYS
1	A	389	ARG
1	A	423	LEU
1	A	471	LEU
1	A	489	GLU
1	A	511	LEU
1	A	512	ARG
1	A	514	ILE
1	A	517	ARG
1	A	530	LEU
1	A	553	THR
1	A	560	ASP
1	A	565	LEU
1	A	634	LEU
1	A	710	GLN
1	A	731	LEU
1	A	786	GLN
1	A	839	LEU
1	A	841	LYS
1	A	864	PRO
1	A	866	GLU
1	A	898	ASN
1	A	915	PHE
1	A	919	PHE
1	A	937	ASP
1	A	947	THR
1	A	962	ARG
1	A	998	LEU
1	A	1004	LEU
1	A	1009	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	116	GLN
1	A	170	GLN
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	373	GLN

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Mol	Chain	Res	Type
1	A	617	GLN
1	A	836	ASN
1	A	840	ASN
1	A	898	ASN
1	A	914	HIS
1	A	918	ASN
1	A	976	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	74H	A	1101	-	30,34,34	1.46	6 (20%)	33,51,51	1.18	4 (12%)

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	74H	A	1101	-	-	3/10/28/28	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74H	C11-C16	-4.30	1.45	1.50
2	A	1101	74H	C19-C9	-3.27	1.49	1.54
2	A	1101	74H	N23-N26	-2.54	1.34	1.39
2	A	1101	74H	C12-N26	-2.35	1.40	1.44
2	A	1101	74H	C13-N28	2.33	1.40	1.34
2	A	1101	74H	C16-N29	2.32	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74H	O30-C16-C11	2.91	122.04	119.61
2	A	1101	74H	C14-N24-C15	2.80	104.35	101.21
2	A	1101	74H	C2-C4-C9	2.71	123.60	120.76
2	A	1101	74H	N24-C15-N27	-2.36	108.34	113.51

There are no chirality outliers.

All (3) torsion outliers are listed below:

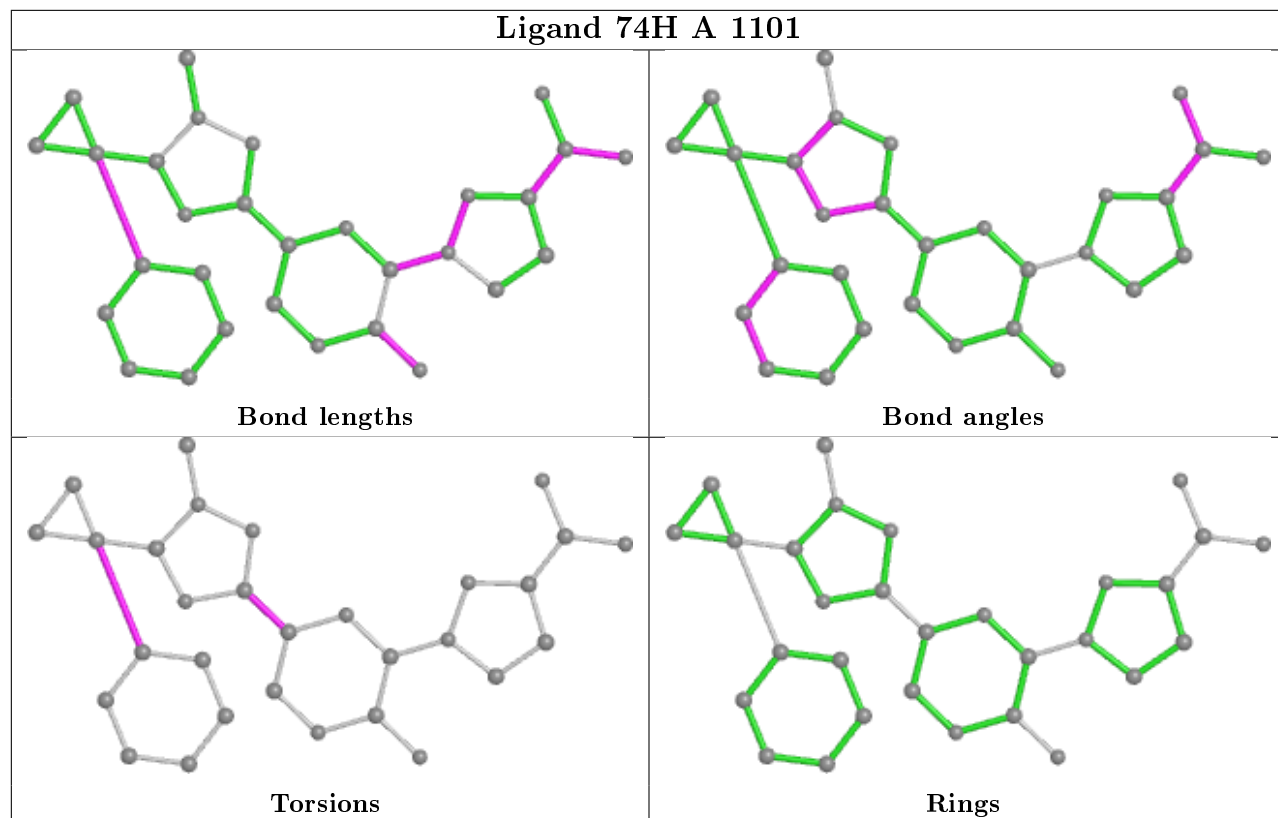
Mol	Chain	Res	Type	Atoms
2	A	1101	74H	C15-C19-C9-C4
2	A	1101	74H	C15-C19-C9-C5
2	A	1101	74H	N22-C10-C14-N24

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	830/939 (88%)	0.39	48 (5%) <span style="border: 1px solid red; padding: 2px;">23</span> <span style="border: 1px solid red; padding: 2px;">27</span>	8, 32, 64, 116	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	TRP	6.3
1	A	919	PHE	6.0
1	A	932	PHE	5.9
1	A	1005	GLY	5.6
1	A	846	ALA	5.5
1	A	517	ARG	5.5
1	A	843	ASN	5.2
1	A	470	ALA	5.0
1	A	452	LEU	4.6
1	A	332	LYS	4.6
1	A	845	ALA	4.1
1	A	936	TYR	4.1
1	A	930	VAL	3.8
1	A	396	ALA	3.7
1	A	330	GLY	3.6
1	A	842	SER	3.6
1	A	840	ASN	3.5
1	A	512	ARG	3.4
1	A	933	ILE	3.4
1	A	268	SER	3.2
1	A	467	SER	3.2
1	A	934	LEU	3.2
1	A	841	LYS	3.1
1	A	1026	SER	3.0
1	A	418	ILE	3.0
1	A	269	GLY	3.0
1	A	707	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	216	LEU	2.9
1	A	1004	LEU	2.8
1	A	136	VAL	2.7
1	A	847	THR	2.7
1	A	1027	TRP	2.7
1	A	203	PHE	2.6
1	A	416	CYS	2.6
1	A	948	ASN	2.6
1	A	366	CYS	2.5
1	A	334	ASN	2.5
1	A	1015	PHE	2.5
1	A	483	VAL	2.4
1	A	1014	HIS	2.4
1	A	929	ARG	2.4
1	A	131	LEU	2.3
1	A	514	ILE	2.3
1	A	214	LEU	2.2
1	A	945	GLY	2.2
1	A	316	LEU	2.1
1	A	471	LEU	2.1
1	A	265	CYS	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](#)

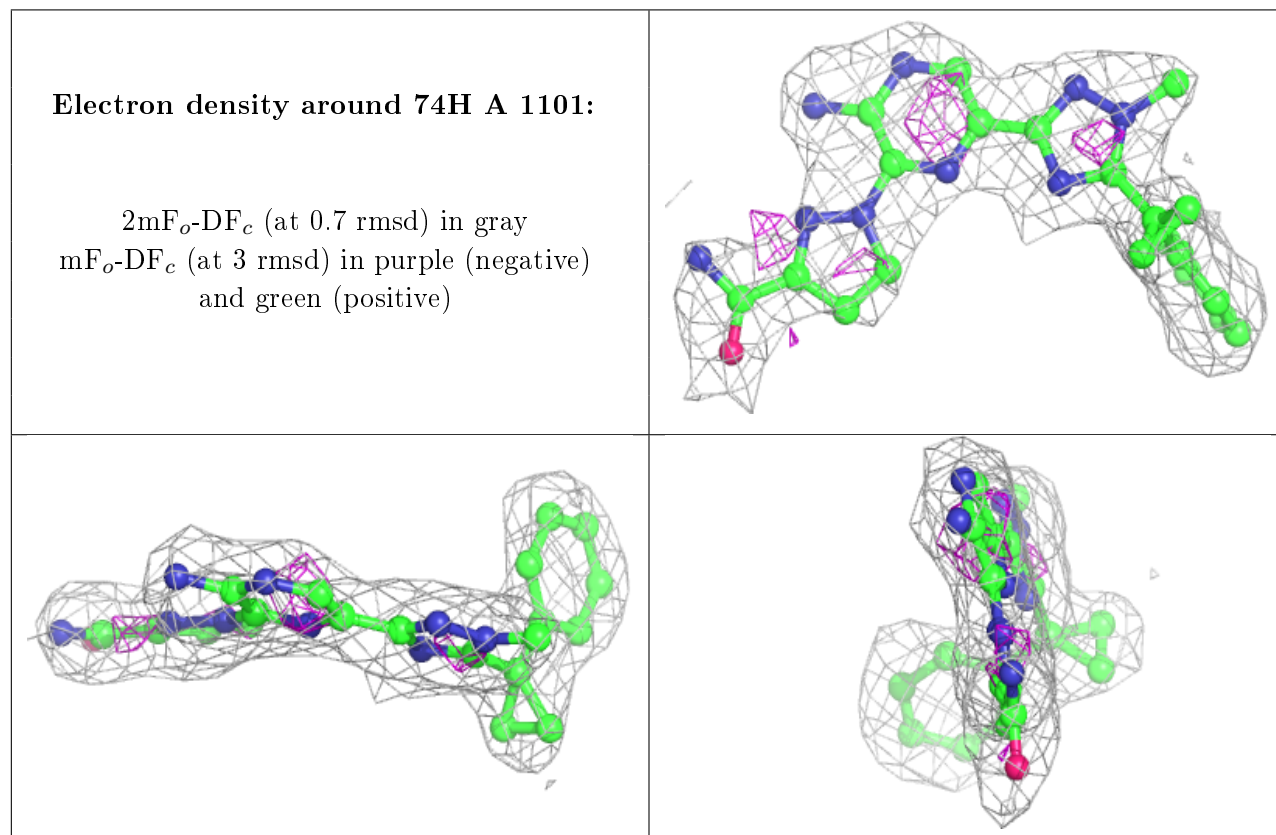
There are no carbohydrates in this entry.

## 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	74H	A	1101	30/30	0.95	0.18	8,25,27,28	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.