



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:26 AM UTC

PDB ID : 5T7F / pdb_00005t7f
Title : PI3Kdelta in complex with the inhibitor GS-643624
Authors : Somoza, J.R.; Villasenor, A.
Deposited on : 2016-09-04
Resolution : 2.60 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

<http://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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

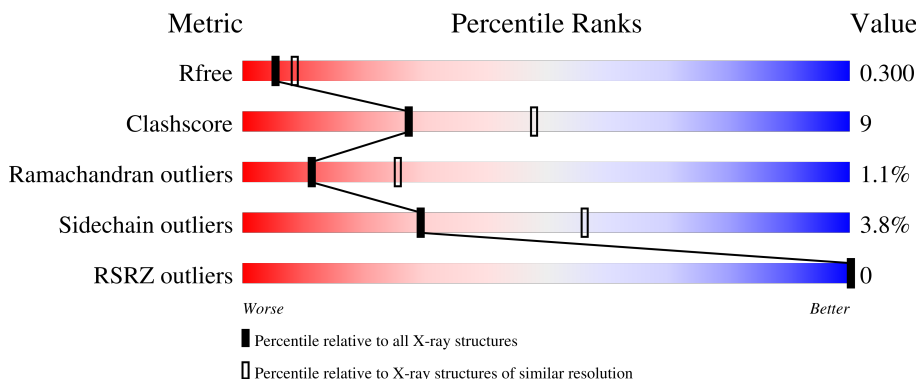
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	 68% 17% • 13%
1	B	939	 67% 17% •• 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13339 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.

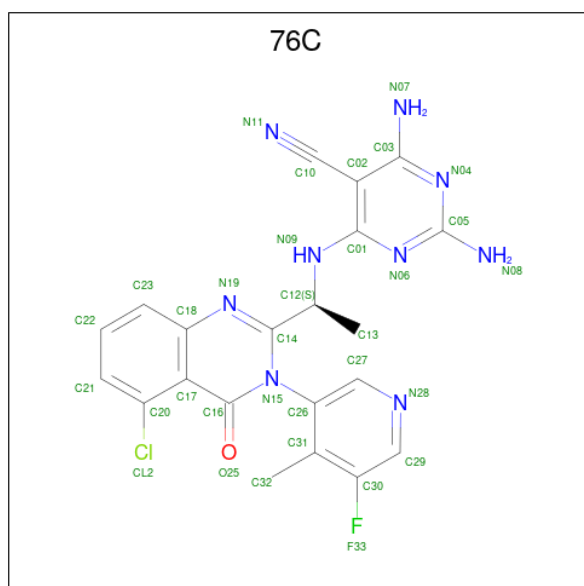
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total	C	N	O	S	0	0	0
			6603	4233	1121	1195	54			
1	B	816	Total	C	N	O	S	0	0	0
			6575	4216	1114	1191	54			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 2,4-bis(azanyl)-6-[[[(1 {S})-1-[5-chloranyl-3-(5-fluoranyl-4-methyl-pyridin-3-yl)-4-oxidanylidene-quinazolin-2-yl]ethyl]amino]pyrimidine-5-carbonitrile (CCD ID: 76C) (formula: C₂₁H₁₇ClFN₉O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 33	C 21	Cl 1	F 1	N 9	O 1	0	0
2	B	1	Total 33	C 21	Cl 1	F 1	N 9	O 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total 48	O 48	0	0
3	B	47	Total 47	O 47	0	0

LYS	GLU	K755	Y524	T434	K356
VAL	RS29	A768	L530	G435	S360
ASN	V930	P931	M534	M441	S361
TRP	F932	I777	E537	V445	E362
LEU	I933	N760	L549	PRD	V363
ALA	I934	R785	K557	ASP	N364
HIS	T935	Q786	H558	GLU	V365
ASN	Y936	Q792	E559	LYS	C366
VAL	D937	L808	M564	GLY	S367
SER	L938	T822	L574	GLU	E368
LYS	R939	I825	D589	P369	P369
ASP	Q944	T833	C590	V370	V370
ASN	R945	I834	Y591	W371	W371
ARG	R946	Q838	V592	K372	K372
GLN	R947	K841	G593	Q373	Q373
	R948	S842	S594	R374	R374
	R949	N843	F595	L375	L375
	R950	M844	A596		
	R951	R847	I597	R386	R386
	R952	K852	S599	M387	M387
	R953	L855	Q614	L390	L390
	R954	L856	V618	A393	A393
	R955	K860	Y621	L394	L394
	R956	C883	E669	Y395	Y395
	R957	V884	R673	A396	A396
	R958	H895	Q674	V397	V397
	R959	H896	H677	V398	V398
	R960	D897	M683	GLU	GLU
	R961	M900	E687	LYS	LYS
	R962	F915	K693	ALA	ALA
	R963	G917	L740	ALA	ALA
	R964	R918	L741	ALA	ALA
	R965	PHE	E742	D415	D415
	R966	LYS	T750	I418	I418
	R967	THR	F751	A421	A421
	R968	LYS		L425	L425
	R969	LYS		F426	F426
	R970	PHE		D427	D427
	R971	GLY		Y428	Y428
	R972	ILE		Q431	Q431
	R973	ASN			
	R974	ARG			
	R975	THR			
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.23Å 142.79Å 221.07Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	45.90 – 2.60 45.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.4 (45.90-2.60) 86.1 (45.90-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.294 0.239 , 0.300	Depositor DCC
R_{free} test set	1983 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13339	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 76C

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	0.28	0/6741	0.73	6/9090 (0.1%)
1	B	0.33	0/6715	0.77	14/9059 (0.2%)
All	All	0.31	0/13456	0.75	20/18149 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	5

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	N-CA-C	11.38	124.91	108.86
1	B	1010	GLU	N-CA-C	-8.69	102.23	112.92
1	B	332	LYS	N-CA-C	8.27	123.95	108.65
1	B	332	LYS	CB-CG-CD	-7.32	94.46	111.30
1	B	949	ASN	CA-C-N	7.22	129.96	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1012	LEU	Peptide
1	B	1013	LYS	Peptide
1	B	1014	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	B	331	ARG	Peptide
1	B	366	CYS	Peptide

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	A	6603	0	6597	106	0
1	B	6575	0	6565	133	1
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	A	48	0	0	3	0
3	B	47	0	0	2	0
All	All	13339	0	13162	239	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 9.

The worst 5 of 239 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:331:ARG:HD3	1:A:368:GLU:HB3	1.56	0.85
1:A:193:ASN:ND2	1:A:202:SER:OG	2.10	0.84
1:A:883:CYS:HB3	1:A:932:PHE:HZ	1.44	0.81
1:B:387:MET:HE3	1:B:590:CYS:HB3	1.66	0.78
1:B:557:LYS:HE3	1:B:559:GLU:HG2	1.65	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:B:356:LYS:NZ	1:B:843:ASN:O[3_555]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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	794/939 (85%)	752 (95%)	36 (4%)	6 (1%)	16	34
1	B	794/939 (85%)	740 (93%)	43 (5%)	11 (1%)	9	19
All	All	1588/1878 (85%)	1492 (94%)	79 (5%)	17 (1%)	11	25

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	367	SER
1	B	1012	LEU
1	A	333	VAL
1	A	366	CYS
1	B	755	LYS

5.3.2 Protein sidechains

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	726/827 (88%)	697 (96%)	29 (4%)	28	55
1	B	723/827 (87%)	697 (96%)	26 (4%)	31	58
All	All	1449/1654 (88%)	1394 (96%)	55 (4%)	29	56

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	951	GLU

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Mol	Chain	Res	Type
1	B	340	LYS
1	B	1014	HIS
1	B	944	GLN
1	B	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	721	GLN
1	B	1020	ASN
1	B	976	HIS
1	B	193	ASN
1	B	536	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 oligosaccharides in this entry.

5.6 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	76C	B	1101	-	35,36,36	1.10	5 (14%)	41,53,53	1.55	3 (7%)
2	76C	A	1101	-	35,36,36	1.10	5 (14%)	41,53,53	1.54	4 (9%)

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	76C	B	1101	-	-	0/10/14/14	0/4/4/4
2	76C	A	1101	-	-	0/10/14/14	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	76C	C01-N09	3.30	1.40	1.35
2	A	1101	76C	C01-N09	3.29	1.40	1.35
2	B	1101	76C	C05-N08	2.33	1.38	1.33
2	A	1101	76C	C05-N08	2.32	1.38	1.33
2	A	1101	76C	C03-N07	2.13	1.39	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	76C	C17-C20-CL2	4.29	125.14	119.62
2	B	1101	76C	C17-C20-CL2	4.28	125.14	119.62
2	A	1101	76C	C31-C26-N15	4.21	122.66	119.05
2	B	1101	76C	C31-C26-N15	4.20	122.64	119.05
2	B	1101	76C	N15-C14-N19	-2.20	122.31	124.21

There are no chirality outliers.

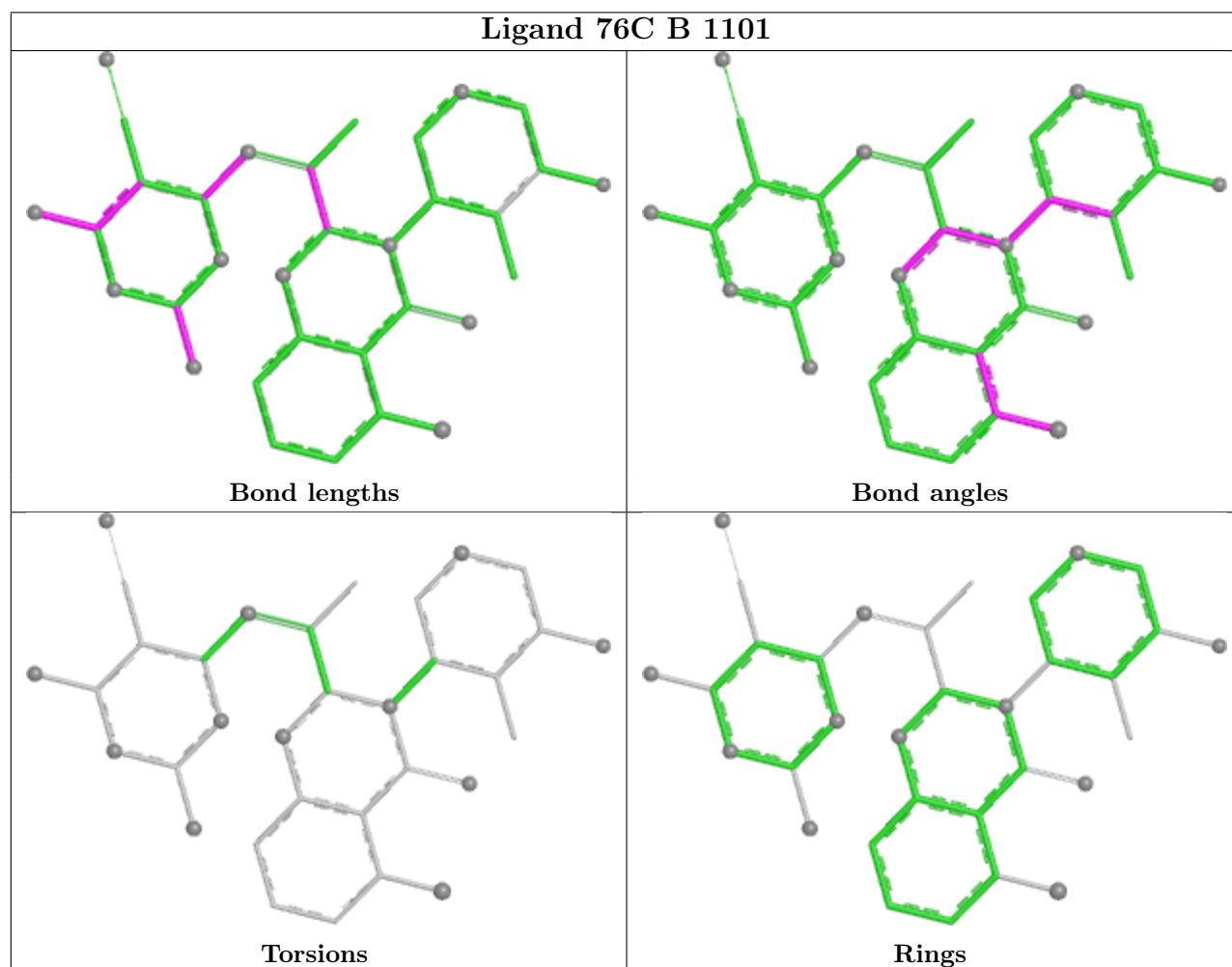
There are no torsion outliers.

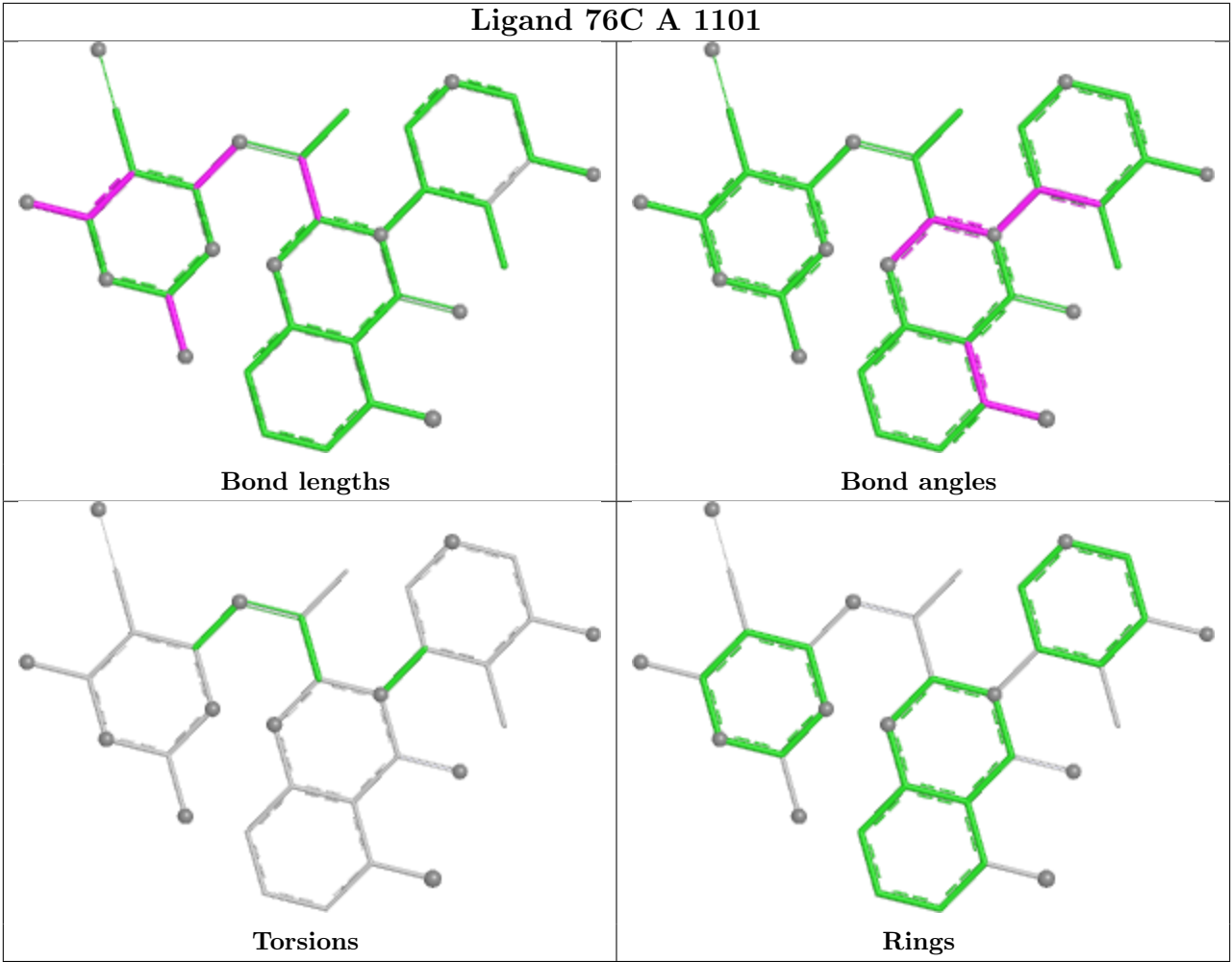
There are no ring outliers.

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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	155:GLN	C	156:GLN	N	6.51
1	A	156:GLN	C	157:LEU	N	6.22

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	819/939 (87%)	-1.09	0 100 100	38, 61, 89, 110	0
1	B	816/939 (86%)	-1.06	0 100 100	37, 61, 92, 118	0
All	All	1635/1878 (87%)	-1.07	0 100 100	37, 61, 90, 118	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

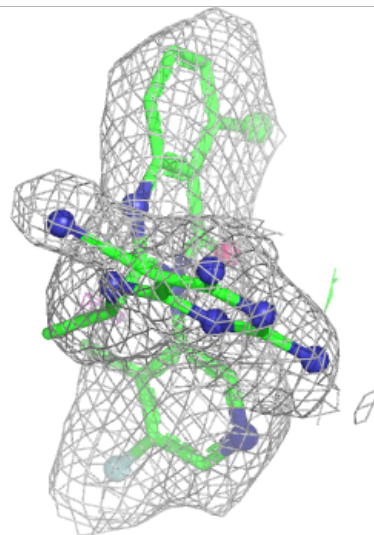
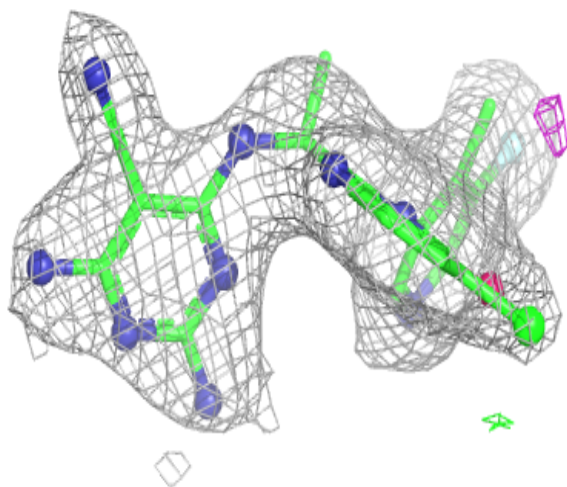
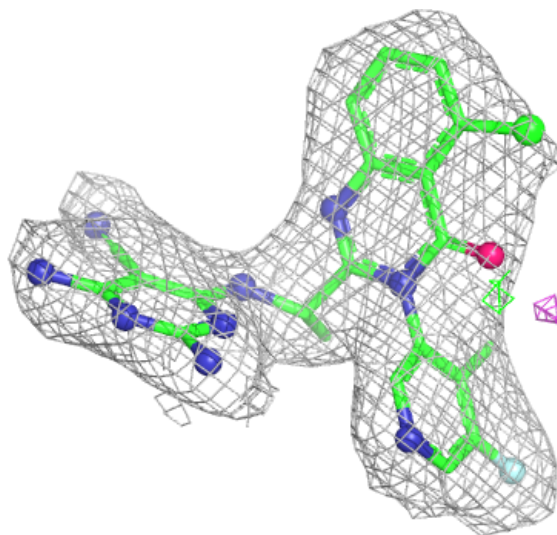
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	76C	A	1101	33/33	0.99	0.04	36,45,56,70	0
2	76C	B	1101	33/33	0.99	0.04	36,46,56,73	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.

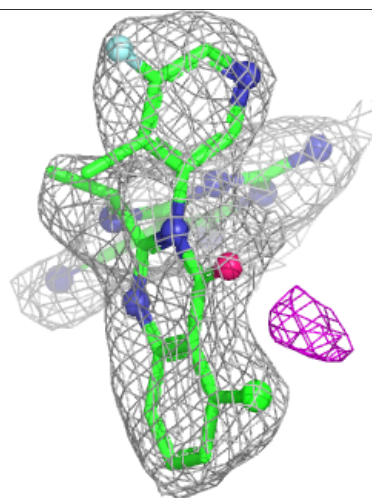
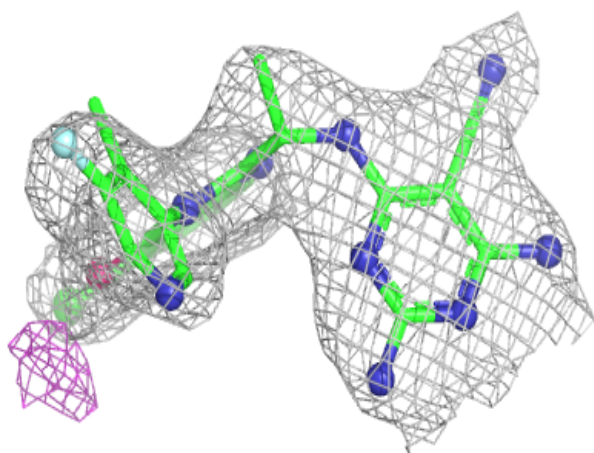
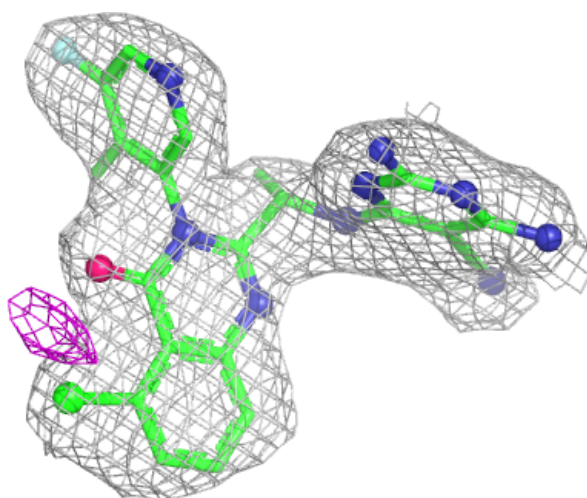
Electron density around 76C A 1101:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 76C B 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.