



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 5T27 / pdb_00005t27
Title : mPI3Kd IN COMPLEX WITH 5d
Authors : Petersen, J.; Terstige, I.; Perry, M.; Svensson, T.; Tyrchan, C.; Lindmark, H.; Oster, L.
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

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

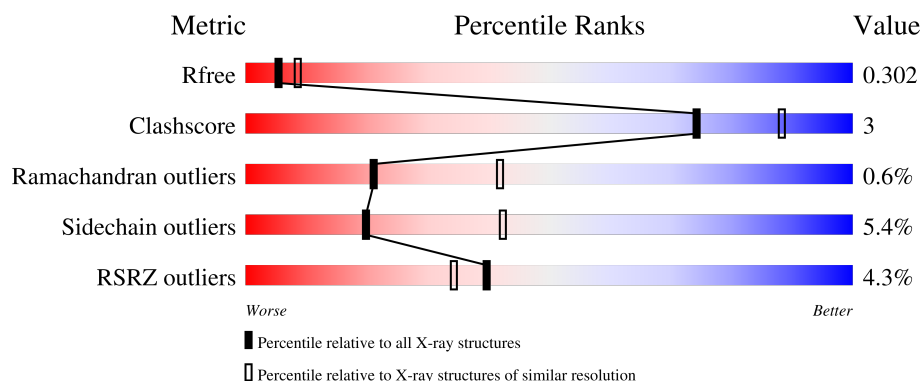
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

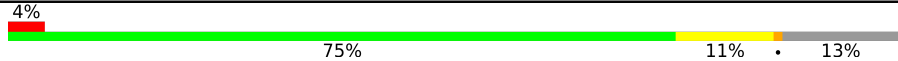
The reported resolution of this entry is 2.60 Å.

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	

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.

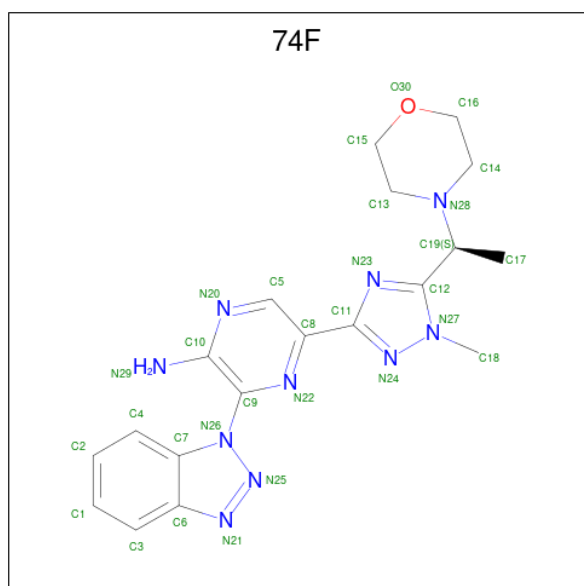
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

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 (CCD ID: 74F) (formula: C₁₉H₂₂N₁₀O).



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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	54.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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: 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	0.76	0/6768	1.36	22/9126 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	9.45	123.25	113.80
1	A	332	LYS	CA-C-N	8.11	136.57	121.97
1	A	332	LYS	C-N-CA	8.11	136.57	121.97
1	A	333	VAL	CA-C-N	7.21	135.32	121.54
1	A	333	VAL	C-N-CA	7.21	135.32	121.54
1	A	507	THR	CA-C-N	6.64	133.66	121.70
1	A	507	THR	C-N-CA	6.64	133.66	121.70
1	A	736	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	698	PHE	CA-C-N	5.54	127.75	120.60
1	A	698	PHE	C-N-CA	5.54	127.75	120.60
1	A	153	HIS	CA-C-N	5.34	127.44	120.28
1	A	153	HIS	C-N-CA	5.34	127.44	120.28
1	A	145	GLN	CA-C-N	5.23	127.29	120.28
1	A	145	GLN	C-N-CA	5.23	127.29	120.28
1	A	982	ARG	CA-C-N	5.13	127.66	120.28
1	A	982	ARG	C-N-CA	5.13	127.66	120.28
1	A	589	ASP	CA-C-N	5.12	127.15	120.28
1	A	589	ASP	C-N-CA	5.12	127.15	120.28
1	A	955	ARG	N-CA-C	-5.08	105.66	111.14
1	A	291	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	149	GLU	CA-C-N	5.00	126.99	120.28
1	A	149	GLU	C-N-CA	5.00	126.99	120.28

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	A	6628	0	6599	41	0
2	A	30	0	0	0	0
3	A	18	0	0	0	0
All	All	6676	0	6599	41	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 (41) 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:549:LEU:HG	1:A:564:MET:HE1	1.35	1.03
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:434:THR:HA	1:A:475:LEU:HB3	1.85	0.59
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.85	0.59
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.85	0.58
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:386:ARG:HG3	1:A:387:MET:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:H	1:A:360:SER:HB3	1.81	0.46
1:A:801:TRP:HZ3	1:A:810:MET:HE2	1.82	0.45
1:A:789:LEU:HD22	1:A:981:MET:HE2	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:214:LEU:HA	1:A:217:MET:HE3	1.99	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:898:ASN:HD22	1:A:898:ASN:C	2.28	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%)	21 42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL

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Mol	Chain	Res	Type
1	A	334	ASN
1	A	229	ARG
1	A	328	ILE
1	A	332	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	727/827 (88%)	688 (95%)	39 (5%)	20	42

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	110	LYS
1	A	119	LEU
1	A	166	SER
1	A	191	LEU
1	A	247	HIS
1	A	270	LEU
1	A	317	TRP
1	A	332	LYS
1	A	333	VAL
1	A	356	LYS
1	A	365	VAL
1	A	374	ARG
1	A	430	ASP
1	A	434	THR
1	A	475	LEU
1	A	512	ARG
1	A	514	ILE
1	A	516	GLU
1	A	517	ARG
1	A	530	LEU
1	A	534	MET

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Mol	Chain	Res	Type
1	A	559	GLU
1	A	565	LEU
1	A	617	GLN
1	A	634	LEU
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	930	VAL
1	A	955	ARG
1	A	965	THR
1	A	990	SER
1	A	998	LEU
1	A	1009	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	137	ASN
1	A	145	GLN
1	A	153	HIS
1	A	187	ASN
1	A	278	HIS
1	A	373	GLN
1	A	422	ASN
1	A	539	GLN
1	A	610	GLN
1	A	617	GLN
1	A	704	GLN
1	A	780	ASN
1	A	795	GLN
1	A	857	ASN
1	A	898	ASN
1	A	914	HIS
1	A	918	ASN
1	A	976	HIS

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 oligosaccharides 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	-	32,34,34	1.26	3 (9%)	37,49,49	1.21	4 (10%)

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	-	-	3/16/24/24	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74F	C12-N27	4.58	1.37	1.34
2	A	1101	74F	N26-N25	-3.18	1.34	1.38
2	A	1101	74F	C10-N29	2.55	1.40	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74F	C13-N28-C19	3.23	118.08	112.53
2	A	1101	74F	C1-C2-C4	2.40	123.20	120.24
2	A	1101	74F	O30-C16-C14	-2.39	106.61	111.77
2	A	1101	74F	C7-N26-C9	-2.23	126.86	129.85

There are no chirality outliers.

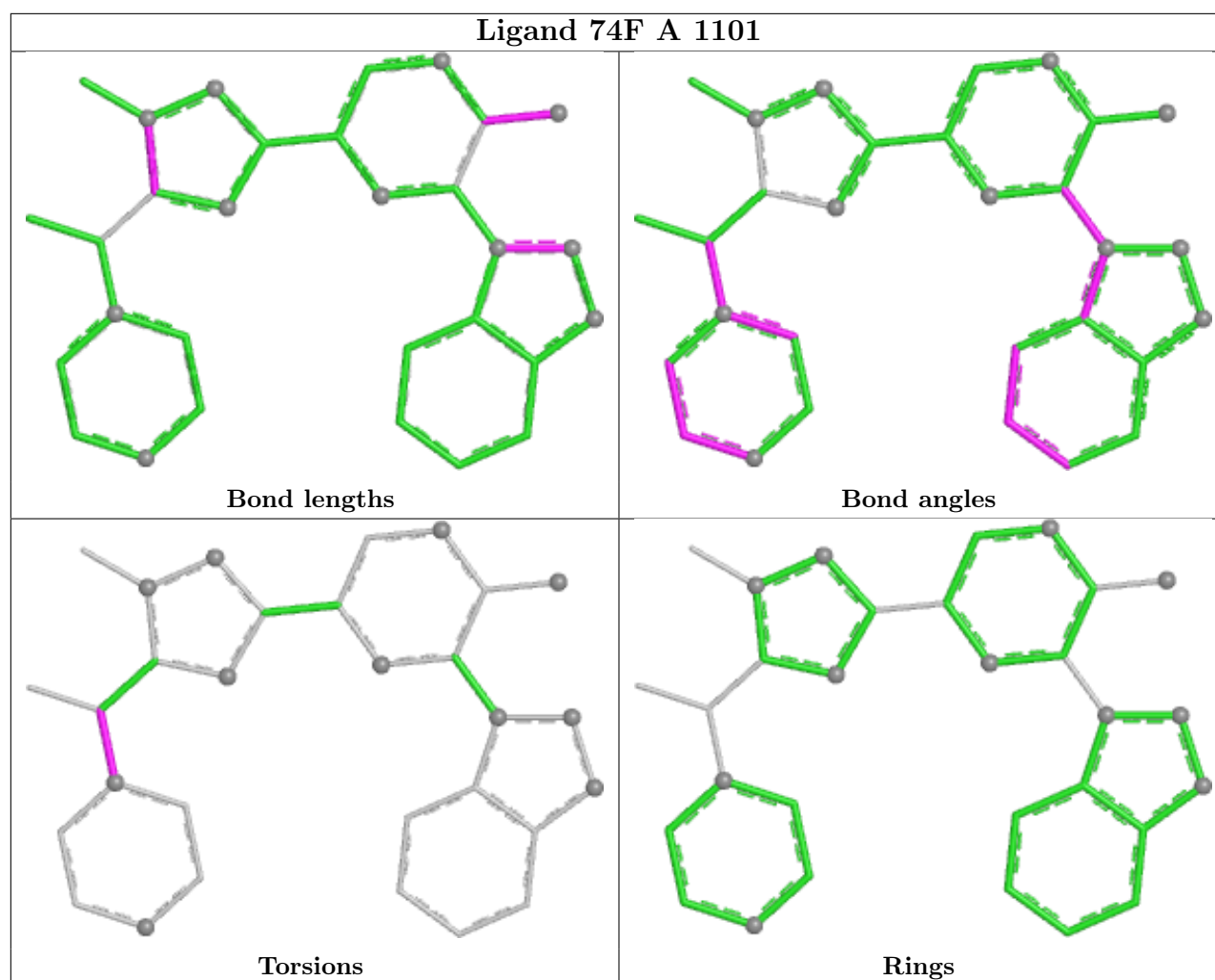
All (3) torsion outliers are listed below:

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, 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%)	0.45	35 (4%) 40 34	21, 52, 86, 133	3 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	6.3
1	A	316	LEU	5.7
1	A	317	TRP	5.1
1	A	1027	TRP	5.1
1	A	919	PHE	5.0
1	A	109	VAL	4.9
1	A	1003	ALA	4.0
1	A	479	ALA	4.0
1	A	398	VAL	3.7
1	A	445	VAL	3.5
1	A	365	VAL	3.2
1	A	507	THR	3.1
1	A	173	PRO	2.9
1	A	226	THR	2.9
1	A	264	SER	2.8
1	A	841	LYS	2.7
1	A	333	VAL	2.7
1	A	962	ARG	2.7
1	A	748	GLN	2.6
1	A	334	ASN	2.6
1	A	768	ALA	2.5
1	A	291	ASN	2.4
1	A	1008	GLU	2.4
1	A	187	ASN	2.3
1	A	478	VAL	2.3
1	A	331	ARG	2.2
1	A	328	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	332	LYS	2.2
1	A	512	ARG	2.1
1	A	847	THR	2.1
1	A	374	ARG	2.0
1	A	119	LEU	2.0
1	A	839	LEU	2.0
1	A	205	PHE	2.0
1	A	511	LEU	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](#)

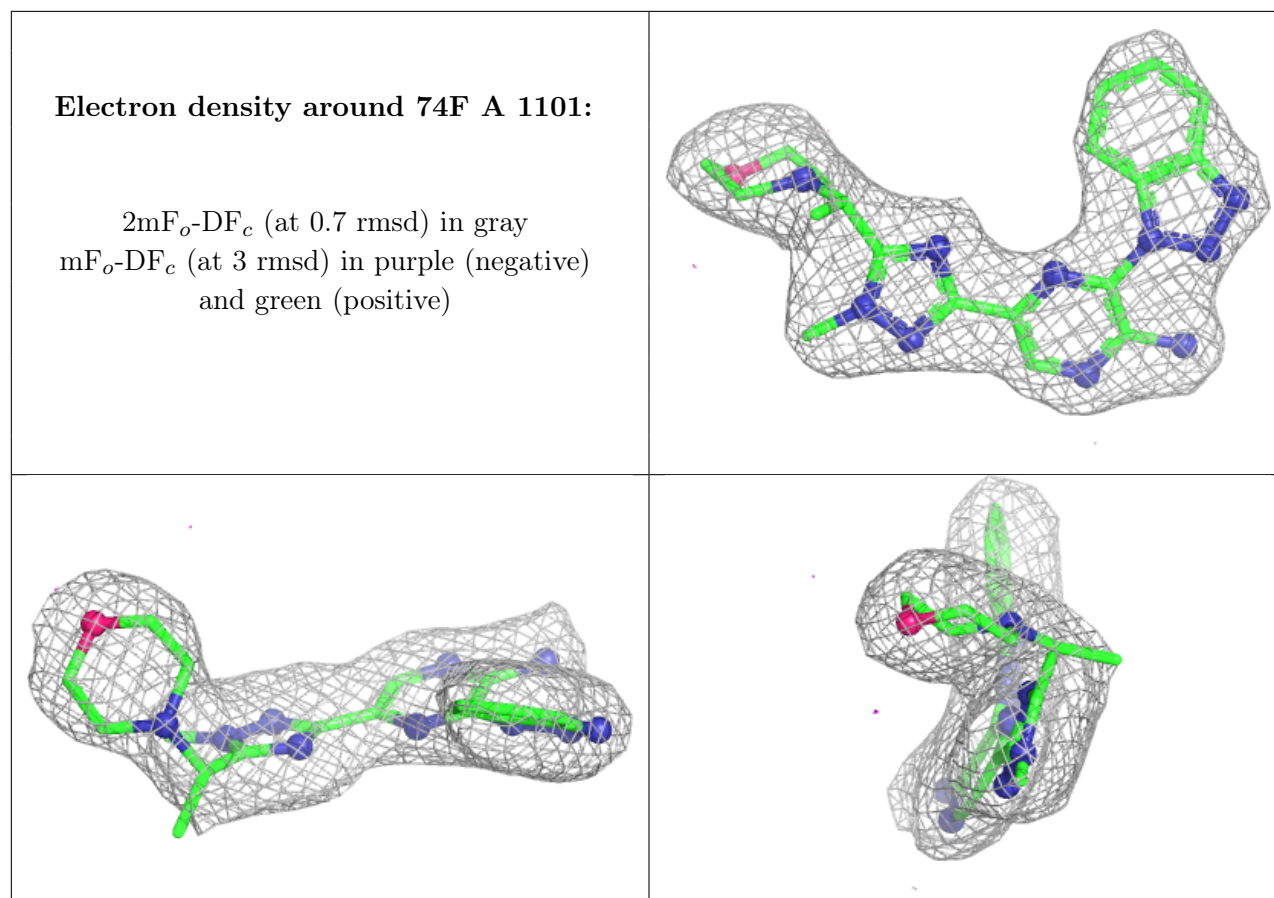
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	74F	A	1101	30/30	0.92	0.10	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.