



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:09 PM UTC

PDB ID : 5T2B / pdb_00005t2b
Title : mPI3Kd IN COMPLEX WITH 5e
Authors : Petersen, J.; Terstige, I.; Perry, M.; Svensson, T.; Tyrchan, C.; Lindmark, H.; Oster, L.
Deposited on : 2016-08-23
Resolution : 2.30 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

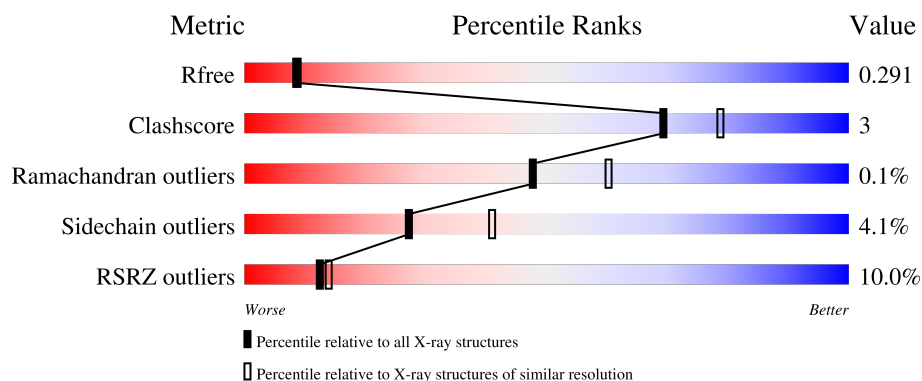
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	9% 75% 11% 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6693 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.

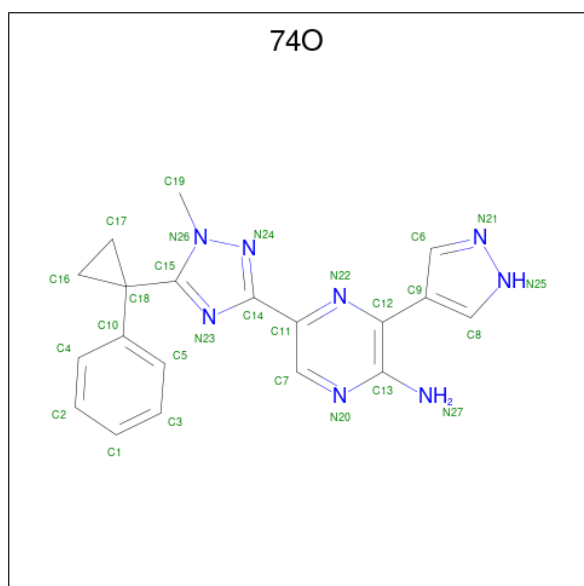
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	0	0
			6621	4248	1124	1196	53			

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 5-[1-methyl-5-(1-phenylcyclopropyl)-1,2,4-triazol-3-yl]-3-(1 {H}-pyrazol-4-yl)pyrazin-2-amine (CCD ID: 740) (formula: C₁₉H₁₈N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			27	19	8		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.79Å 64.50Å 115.98Å 90.00° 103.36° 90.00°	Depositor
Resolution (Å)	49.93 – 2.30 49.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.93-2.30) 97.7 (49.93-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.222 , 0.271 0.236 , 0.291	Depositor DCC
R_{free} test set	2243 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6693	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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:
74O

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	0.80	1/6763 (0.0%)	1.34	23/9123 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	715	MET	SD-CE	-5.41	1.66	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	8.48	122.28	113.80
1	A	745	CYS	CA-C-N	6.31	128.74	120.60
1	A	745	CYS	C-N-CA	6.31	128.74	120.60
1	A	422	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	935	THR	CA-C-N	5.53	127.69	120.28
1	A	935	THR	C-N-CA	5.53	127.69	120.28
1	A	798	ASP	CA-C-N	5.49	127.47	120.56
1	A	798	ASP	C-N-CA	5.49	127.47	120.56
1	A	813	TYR	CA-C-N	5.46	125.16	119.92
1	A	813	TYR	C-N-CA	5.46	125.16	119.92
1	A	792	GLN	CA-C-N	5.42	127.54	120.28
1	A	792	GLN	C-N-CA	5.42	127.54	120.28
1	A	219	CYS	CA-C-N	5.35	127.45	120.28
1	A	219	CYS	C-N-CA	5.35	127.45	120.28
1	A	444	SER	CA-C-N	5.28	131.19	121.70
1	A	444	SER	C-N-CA	5.28	131.19	121.70
1	A	736	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	472	VAL	N-CA-CB	5.10	117.11	110.99
1	A	456	ALA	CA-C-N	5.05	124.90	120.10
1	A	456	ALA	C-N-CA	5.05	124.90	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	VAL	N-CA-C	-5.02	105.53	111.00
1	A	797	MET	CA-C-N	5.02	127.00	120.28
1	A	797	MET	C-N-CA	5.02	127.00	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	6621	0	6604	46	0
2	A	27	0	0	1	0
3	A	45	0	0	0	0
All	All	6693	0	6604	46	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 (46) 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	1.52	0.91
1:A:756:MET:HE2	1:A:781:GLY:HA3	1.58	0.83
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.73	0.70
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.82	0.60
1:A:343:VAL:H	1:A:360:SER:HB3	1.67	0.60
1:A:1002:LEU:HB3	1:A:1004:LEU:HD23	1.84	0.58
1:A:553:THR:HG21	1:A:564:MET:HG2	1.85	0.57
1:A:894:ARG:HA	1:A:898:ASN:HD21	1.72	0.54
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.91	0.53
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.91	0.53
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.91	0.53
1:A:712:LYS:HE3	1:A:750:THR:HB	1.92	0.52
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.93	0.51
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:HIS:HB2	1:A:738:SER:HA	1.92	0.51
1:A:344:GLN:HB2	1:A:395:TYR:HE1	1.76	0.51
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.94	0.48
1:A:271:THR:O	1:A:273:HIS:HD2	1.97	0.47
1:A:929:ARG:HH22	1:A:1001:SER:HA	1.79	0.47
1:A:213:PRO:O	1:A:217:MET:HG3	2.16	0.46
1:A:806:LEU:HB2	1:A:962:ARG:HH21	1.80	0.46
1:A:118:SER:HB3	1:A:124:GLY:HA2	1.98	0.46
1:A:383:ASP:HB3	1:A:556:ASN:O	2.16	0.46
1:A:553:THR:HG22	1:A:564:MET:HE3	1.98	0.46
1:A:808:LEU:HD11	1:A:963:ALA:HB2	1.99	0.45
1:A:549:LEU:HG	1:A:564:MET:CE	2.35	0.45
1:A:777:ILE:HB	1:A:825:ILE:HB	1.99	0.45
1:A:390:LEU:HB3	1:A:423:LEU:HD12	1.98	0.45
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.99	0.45
1:A:394:LEU:HD22	1:A:441:MET:HE1	1.98	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.99	0.44
1:A:900:MET:HE1	2:A:1101:74O:C14	2.49	0.43
1:A:419:ALA:HB1	1:A:441:MET:HB3	2.00	0.43
1:A:549:LEU:CG	1:A:564:MET:HE1	2.36	0.43
1:A:194:VAL:HG21	1:A:216:LEU:HD21	2.01	0.42
1:A:172:GLU:HG3	1:A:263:CYS:SG	2.60	0.42
1:A:247:HIS:CD2	1:A:740:LEU:HD21	2.55	0.42
1:A:331:ARG:HG3	1:A:470:ALA:HB3	2.01	0.42
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.85	0.42
1:A:328:ILE:HB	1:A:472:VAL:HG23	2.02	0.41
1:A:332:LYS:HB3	1:A:469:ALA:HB1	2.01	0.41
1:A:587:PHE:HB3	1:A:592:VAL:HG11	2.02	0.41
1:A:761:ILE:HB	1:A:776:ILE:HG13	2.02	0.41
1:A:332:LYS:HG2	1:A:394:LEU:HD21	2.02	0.41
1:A:349:HIS:HB2	1:A:354:LEU:HD21	2.01	0.41
1:A:855:LEU:HD22	1:A:941:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

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	796/939 (85%)	774 (97%)	21 (3%)	1 (0%)	48 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ILE

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%)	696 (96%)	30 (4%)	27 41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	188	ARG
1	A	190	LEU
1	A	203	PHE
1	A	263	CYS
1	A	270	LEU
1	A	291	ASN
1	A	316	LEU
1	A	317	TRP
1	A	325	ILE
1	A	332	LYS
1	A	340	LYS
1	A	356	LYS
1	A	363	VAL
1	A	368	GLU
1	A	511	LEU

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Mol	Chain	Res	Type
1	A	514	ILE
1	A	530	LEU
1	A	553	THR
1	A	634	LEU
1	A	726	GLU
1	A	743	GLU
1	A	841	LYS
1	A	855	LEU
1	A	898	ASN
1	A	915	PHE
1	A	937	ASP
1	A	998	LEU
1	A	1004	LEU
1	A	1017	VAL

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	155	GLN
1	A	193	ASN
1	A	247	HIS
1	A	267	HIS
1	A	273	HIS
1	A	278	HIS
1	A	289	GLN
1	A	291	ASN
1	A	344	GLN
1	A	422	ASN
1	A	610	GLN
1	A	710	GLN
1	A	721	GLN
1	A	898	ASN
1	A	906	GLN
1	A	918	ASN
1	A	943	GLN
1	A	944	GLN
1	A	949	ASN

5.3.3 RNA ⓘ

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](#)

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	74O	A	1101	-	30,31,31	1.23	6 (20%)	35,46,46	1.40	5 (14%)

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	74O	A	1101	-	-	5/14/24/24	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	74O	C12-C13	-2.75	1.38	1.42
2	A	1101	74O	C15-N26	2.52	1.36	1.34
2	A	1101	74O	C12-C9	-2.49	1.45	1.48
2	A	1101	74O	C13-N27	2.30	1.40	1.34
2	A	1101	74O	C18-C10	-2.29	1.49	1.53
2	A	1101	74O	C11-C14	-2.03	1.44	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74O	C17-C18-C10	3.42	122.57	118.58
2	A	1101	74O	C17-C18-C16	2.89	59.74	58.45
2	A	1101	74O	C12-C9-C8	-2.84	123.45	127.65
2	A	1101	74O	C12-C13-N20	2.67	121.22	119.78
2	A	1101	74O	C7-N20-C13	-2.31	116.41	118.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

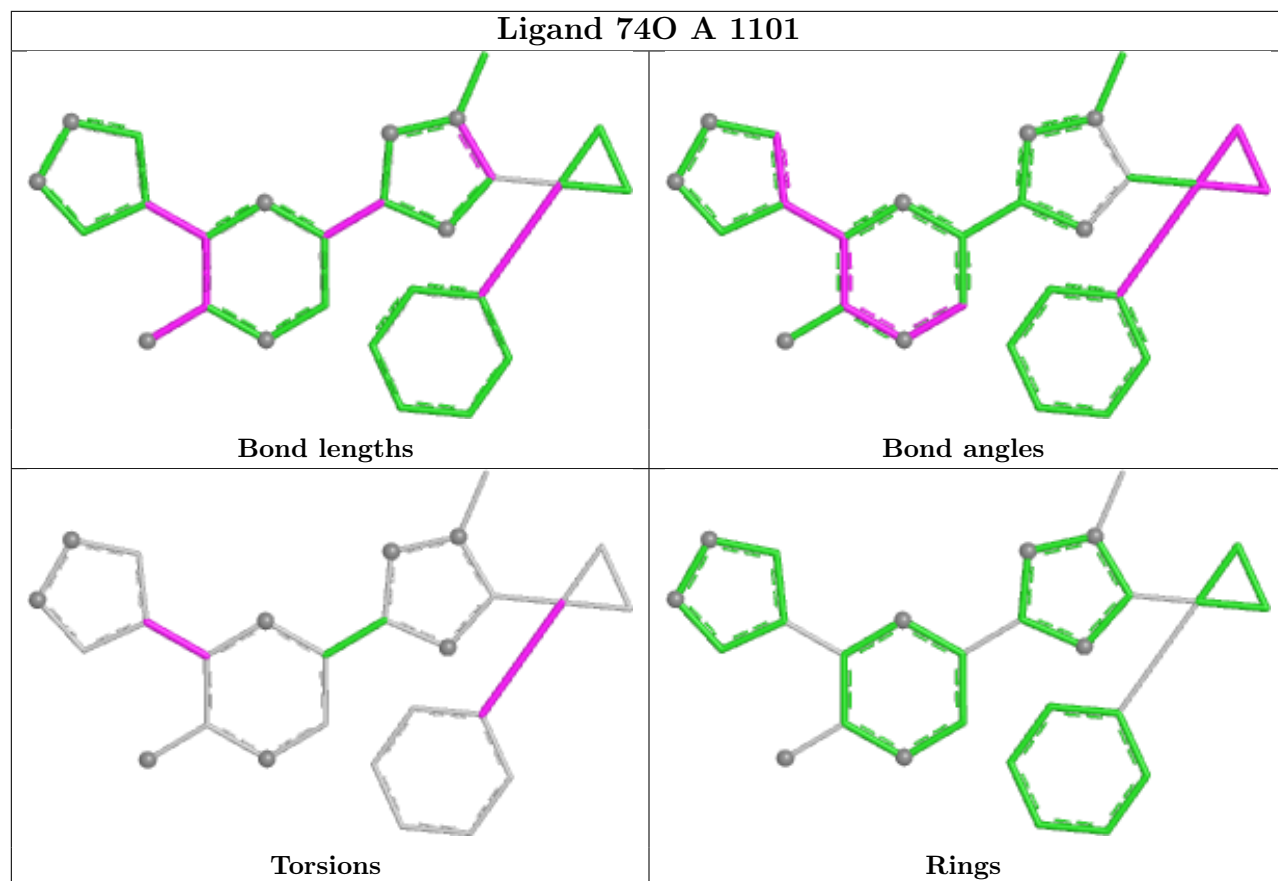
Mol	Chain	Res	Type	Atoms
2	A	1101	74O	N22-C12-C9-C8
2	A	1101	74O	C13-C12-C9-C8
2	A	1101	74O	C4-C10-C18-C15
2	A	1101	74O	C5-C10-C18-C15
2	A	1101	74O	C13-C12-C9-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	74O	1	0

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	820/939 (87%)	0.72	82 (10%) 12 14	24, 47, 79, 149	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	8.4
1	A	316	LEU	7.5
1	A	479	ALA	6.4
1	A	1027	TRP	5.2
1	A	511	LEU	4.8
1	A	317	TRP	4.6
1	A	919	PHE	4.5
1	A	445	VAL	4.5
1	A	398	VAL	4.2
1	A	365	VAL	4.1
1	A	332	LYS	4.1
1	A	173	PRO	4.0
1	A	478	VAL	3.9
1	A	334	ASN	3.9
1	A	517	ARG	3.9
1	A	936	TYR	3.5
1	A	109	VAL	3.4
1	A	377	PHE	3.4
1	A	333	VAL	3.4
1	A	515	LEU	3.3
1	A	341	LEU	3.3
1	A	230	GLN	3.3
1	A	227	VAL	3.1
1	A	488	LEU	3.1
1	A	533	LYS	3.1
1	A	323	PHE	3.1
1	A	1023	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	3.0
1	A	226	THR	2.9
1	A	530	LEU	2.8
1	A	318	SER	2.8
1	A	767	GLU	2.8
1	A	331	ARG	2.8
1	A	371	TRP	2.8
1	A	471	LEU	2.7
1	A	512	ARG	2.7
1	A	491	ILE	2.7
1	A	257	CYS	2.7
1	A	591	TYR	2.7
1	A	483	VAL	2.7
1	A	228	PHE	2.6
1	A	291	ASN	2.6
1	A	714	MET	2.6
1	A	476	PRO	2.6
1	A	319	LEU	2.5
1	A	516	GLU	2.5
1	A	381	VAL	2.5
1	A	514	ILE	2.5
1	A	474	TYR	2.5
1	A	523	LEU	2.5
1	A	189	ALA	2.5
1	A	452	LEU	2.5
1	A	369	PRO	2.5
1	A	935	THR	2.4
1	A	494	LEU	2.4
1	A	601	ARG	2.4
1	A	482	PRO	2.3
1	A	1026	SER	2.3
1	A	396	ALA	2.3
1	A	930	VAL	2.3
1	A	847	THR	2.3
1	A	929	ARG	2.2
1	A	1025	GLU	2.2
1	A	897	ASP	2.2
1	A	937	ASP	2.2
1	A	1012	LEU	2.2
1	A	342	VAL	2.2
1	A	339	MET	2.2
1	A	892	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	132	ARG	2.1
1	A	934	LEU	2.1
1	A	529	ASP	2.1
1	A	843	ASN	2.1
1	A	853	ASP	2.1
1	A	203	PHE	2.1
1	A	560	ASP	2.1
1	A	330	GLY	2.1
1	A	477	GLU	2.1
1	A	846	ALA	2.1
1	A	470	ALA	2.0
1	A	569	CYS	2.0
1	A	473	ILE	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](#)

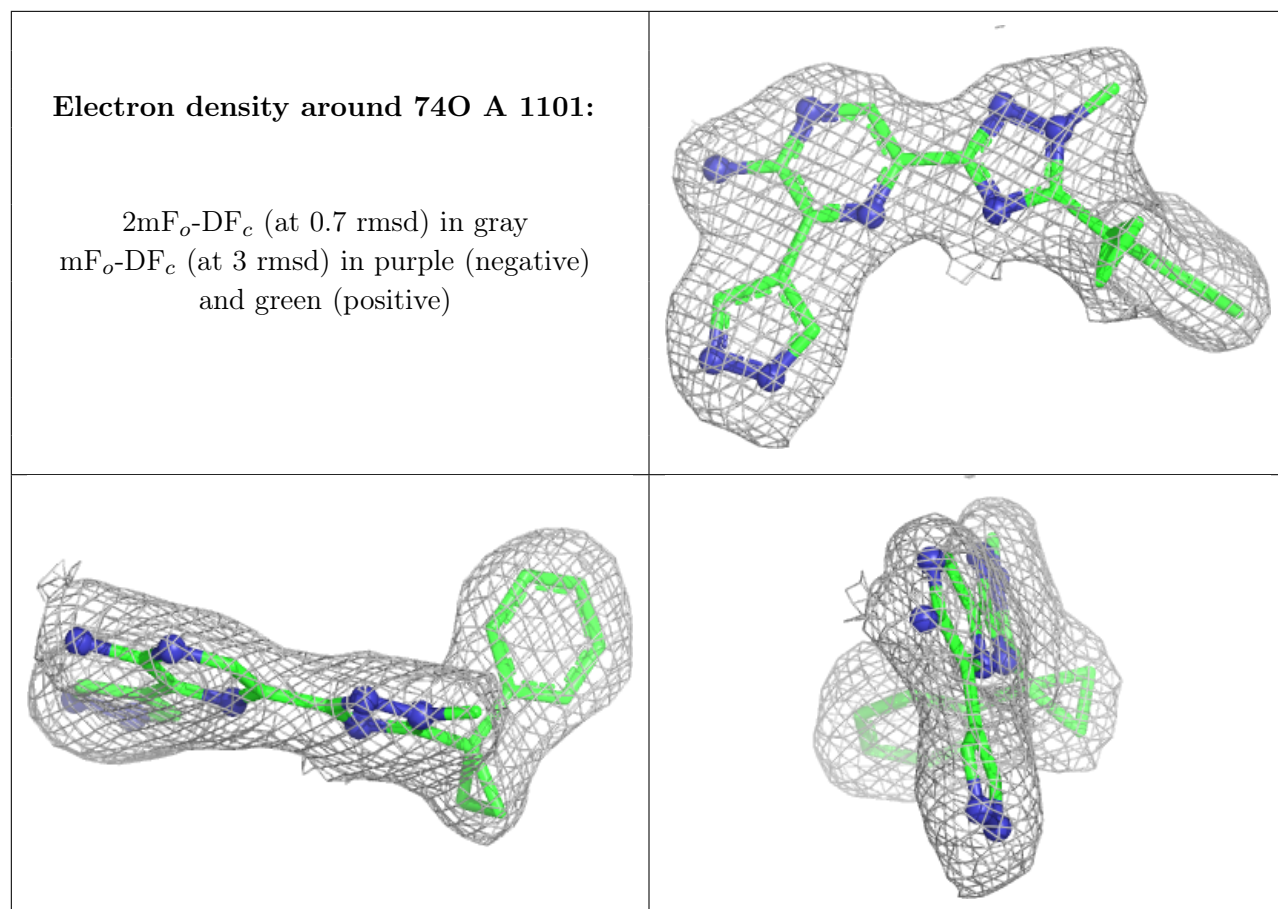
There are no oligosaccharides in this entry.

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	74O	A	1101	27/27	0.95	0.07	24,29,35,37	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.