



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5T2L / pdb_00005t2l
Title : mPI3Kd IN COMPLEX WITH 7l
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

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

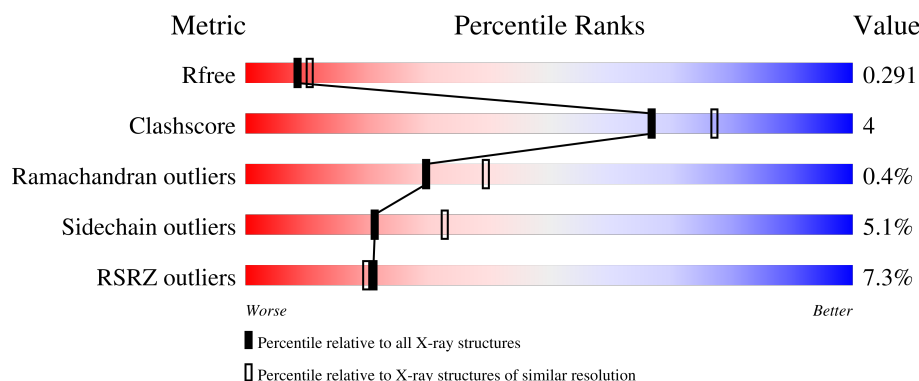
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	6% 75% 12% 12%

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.

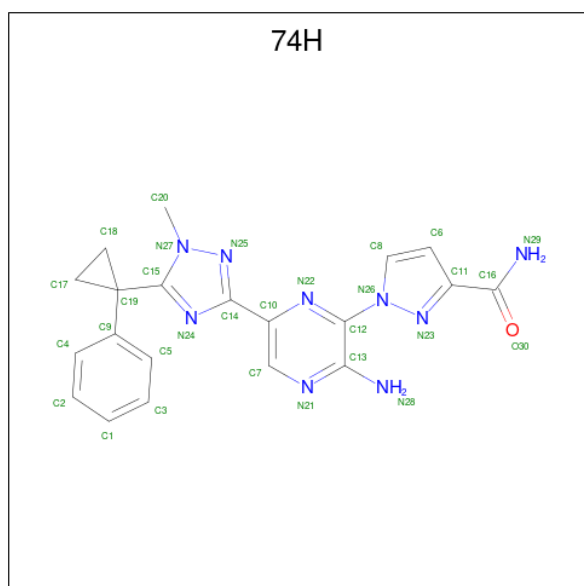
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

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

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 (CCD ID: 74H) (formula: C₂₀H₁₉N₉O).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total 60	O 60	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.55Å 142.19Å 218.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.69 – 2.55 54.69 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (54.69-2.55) 98.5 (54.69-2.55)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.55Å)	Xtriage
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 ²)	35.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6765	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage'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.*

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: 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	0.85	2/6821 (0.0%)	1.41	28/9204 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	MET	SD-CE	-7.77	1.60	1.79
1	A	333	VAL	CA-C	5.25	1.59	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	GLN	CA-C-N	9.29	138.43	121.70
1	A	510	GLN	C-N-CA	9.29	138.43	121.70
1	A	494	LEU	CA-C-N	8.78	129.87	120.03
1	A	494	LEU	C-N-CA	8.78	129.87	120.03
1	A	332	LYS	N-CA-C	7.87	121.36	109.63
1	A	915	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	955	ARG	N-CA-C	-6.32	104.31	111.14
1	A	197	GLU	N-CA-C	6.03	118.35	111.11
1	A	715	MET	N-CA-C	-5.86	104.81	111.14
1	A	291	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	496	ARG	CA-C-N	5.78	132.11	121.70
1	A	496	ARG	C-N-CA	5.78	132.11	121.70
1	A	135	GLU	CA-C-N	5.78	127.84	120.56
1	A	135	GLU	C-N-CA	5.78	127.84	120.56
1	A	675	SER	CA-C-N	5.65	127.78	120.44
1	A	675	SER	C-N-CA	5.65	127.78	120.44
1	A	509	LEU	CA-C-N	5.62	131.82	121.70
1	A	509	LEU	C-N-CA	5.62	131.82	121.70
1	A	991	CYS	N-CA-C	5.56	115.63	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	GLU	CA-C-N	5.38	127.50	120.28
1	A	507	GLU	C-N-CA	5.38	127.50	120.28
1	A	457	GLY	CA-C-N	5.38	128.48	120.90
1	A	457	GLY	C-N-CA	5.38	128.48	120.90
1	A	464	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	433	LYS	CA-C-N	5.05	130.79	121.85
1	A	433	LYS	C-N-CA	5.05	130.79	121.85
1	A	949	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	135	GLU	CB-CG-CD	5.04	121.18	112.60

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	49	0
2	A	30	0	0	1	0
3	A	60	0	0	0	0
All	All	6765	0	6637	49	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 4.

All (49) 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	1.42	0.99
1:A:510:GLN:HA	1:A:512:ARG:H	1.56	0.71
1:A:756:MET:HE2	1:A:781:GLY:HA3	1.77	0.67
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:549:LEU:CG	1:A:564:MET:HE1	2.24	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD11	1:A:483:VAL:HG11	1.85	0.58
1:A:317:TRP:HA	1:A:382:CYS:HB2	1.86	0.57
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.89	0.54
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: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:386:ARG:HG3	1:A:387:MET:HE2	1.95	0.49
1:A:553:THR:CG2	1:A:564:MET:HE3	2.43	0.48
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.79	0.48
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:110:LYS:HZ3	1:A:144:ARG:HH12	1.64	0.46
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:710:GLN:O	1:A:714:MET:HE2	2.18	0.43
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:698:PHE:HZ	1:A:714:MET:HE3	1.85	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:394:LEU:HD22	1:A:441:MET:HE1	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:900:MET:HE1	2:A:1101:74H:C14	2.51	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%)	30	39

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%)	692 (95%)	37 (5%)	21	33

All (37) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	340	LYS
1	A	363	VAL
1	A	389	ARG
1	A	423	LEU
1	A	471	LEU
1	A	475	LEU
1	A	489	GLU
1	A	511	LEU
1	A	514	ILE
1	A	515	LEU
1	A	517	ARG
1	A	522	GLU
1	A	530	LEU
1	A	553	THR
1	A	560	ASP
1	A	565	LEU
1	A	634	LEU
1	A	676	THR
1	A	710	GLN
1	A	731	LEU
1	A	766	GLU
1	A	786	GLN
1	A	839	LEU
1	A	841	LYS
1	A	866	GLU
1	A	898	ASN
1	A	915	PHE
1	A	919	PHE
1	A	947	THR
1	A	962	ARG
1	A	1004	LEU
1	A	1009	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	193	ASN
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	373	GLN
1	A	422	ASN
1	A	464	ASN
1	A	536	HIS
1	A	541	HIS
1	A	563	GLN
1	A	617	GLN
1	A	685	GLN
1	A	840	ASN
1	A	857	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 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	74H	A	1101	-	32,34,34	1.18	4 (12%)	40,51,51	1.28	6 (15%)

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	-	-	2/17/28/28	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74H	C15-N27	3.09	1.37	1.34
2	A	1101	74H	C11-C16	-2.69	1.45	1.48
2	A	1101	74H	C19-C9	-2.30	1.49	1.53
2	A	1101	74H	C13-N28	2.26	1.40	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74H	C2-C4-C9	2.80	123.60	120.75
2	A	1101	74H	C18-C19-C9	2.43	121.42	118.58
2	A	1101	74H	C18-C19-C17	2.21	59.44	58.45
2	A	1101	74H	C12-N26-C8	-2.18	122.58	126.38
2	A	1101	74H	C16-C11-N23	2.12	123.08	120.38
2	A	1101	74H	C12-N26-N23	2.02	125.47	121.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

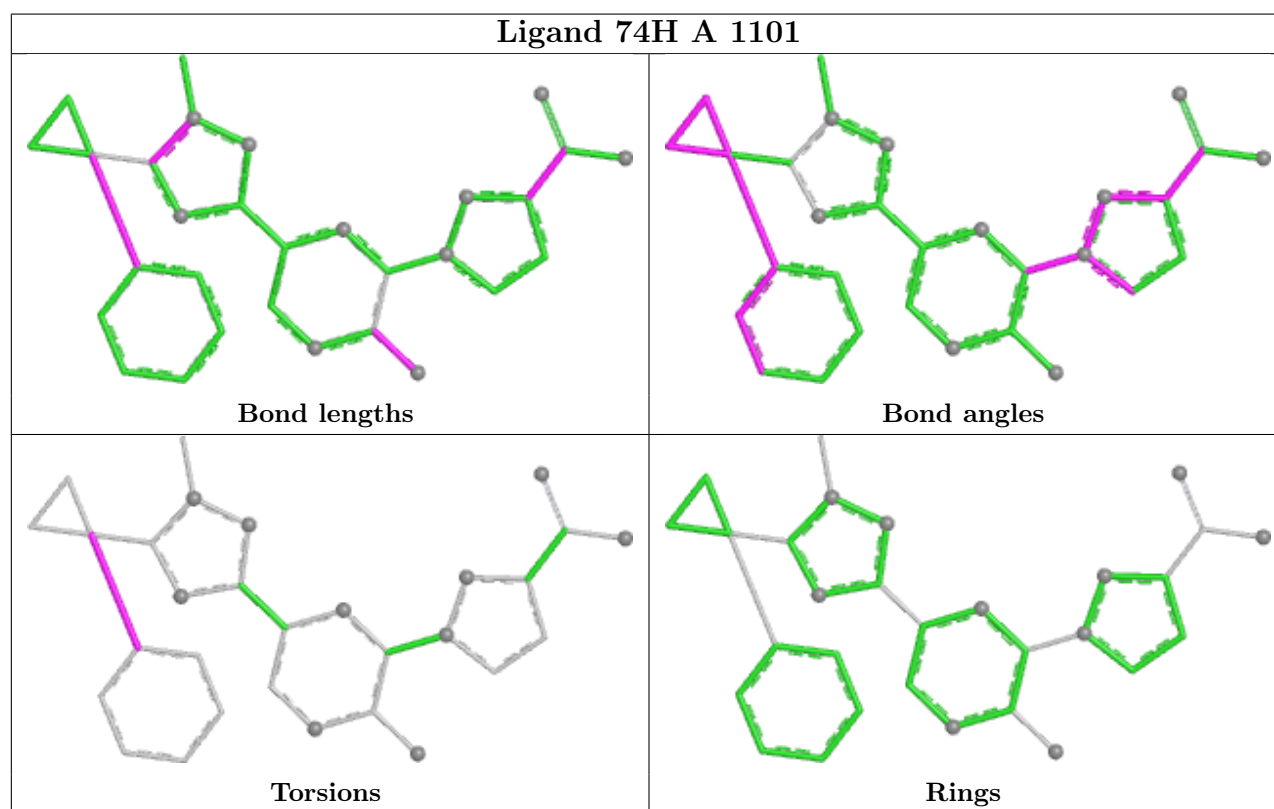
Mol	Chain	Res	Type	Atoms
2	A	1101	74H	C15-C19-C9-C4
2	A	1101	74H	C15-C19-C9-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	74H	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	830/939 (88%)	0.53	61 (7%) 21 20	8, 32, 64, 116	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1027	TRP	6.8
1	A	919	PHE	6.7
1	A	317	TRP	5.9
1	A	316	LEU	5.5
1	A	332	LYS	5.2
1	A	479	ALA	5.0
1	A	335	ALA	4.9
1	A	932	PHE	4.4
1	A	933	ILE	4.1
1	A	268	SER	4.1
1	A	398	VAL	4.1
1	A	846	ALA	4.1
1	A	497	HIS	4.1
1	A	517	ARG	3.9
1	A	1004	LEU	3.9
1	A	840	ASN	3.8
1	A	230	GLN	3.8
1	A	993	LYS	3.7
1	A	512	ARG	3.7
1	A	1005	GLY	3.6
1	A	936	TYR	3.5
1	A	445	VAL	3.4
1	A	841	LYS	3.3
1	A	452	LEU	3.2
1	A	930	VAL	3.2
1	A	1026	SER	3.1
1	A	269	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	845	ALA	3.0
1	A	291	ASN	3.0
1	A	514	ILE	3.0
1	A	467	SER	2.8
1	A	203	PHE	2.8
1	A	929	ARG	2.7
1	A	1009	GLU	2.7
1	A	842	SER	2.7
1	A	511	LEU	2.6
1	A	918	ASN	2.6
1	A	333	VAL	2.6
1	A	187	ASN	2.6
1	A	843	ASN	2.5
1	A	934	LEU	2.4
1	A	415	ASP	2.4
1	A	707	THR	2.4
1	A	931	PRO	2.3
1	A	515	LEU	2.3
1	A	523	LEU	2.3
1	A	516	GLU	2.3
1	A	1014	HIS	2.3
1	A	522	GLU	2.3
1	A	1015	PHE	2.3
1	A	847	THR	2.2
1	A	509	LEU	2.2
1	A	483	VAL	2.2
1	A	330	GLY	2.2
1	A	870	ARG	2.2
1	A	266	LEU	2.2
1	A	839	LEU	2.2
1	A	489	GLU	2.1
1	A	173	PRO	2.1
1	A	265	CYS	2.1
1	A	506	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

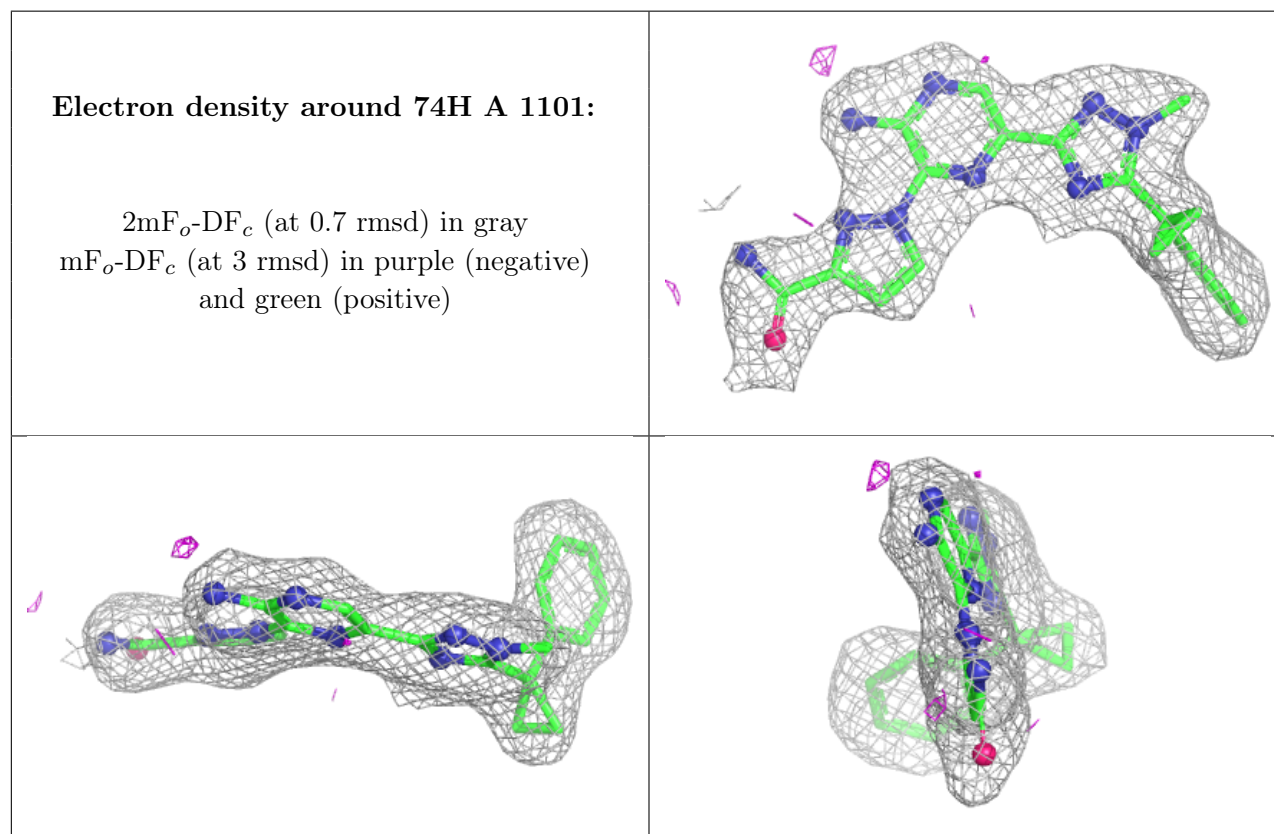
There are no oligosaccharides in this entry.

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	74H	A	1101	30/30	0.94	0.08	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.