



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:16 PM UTC

PDB ID : 5T2G / pdb_00005t2g
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

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

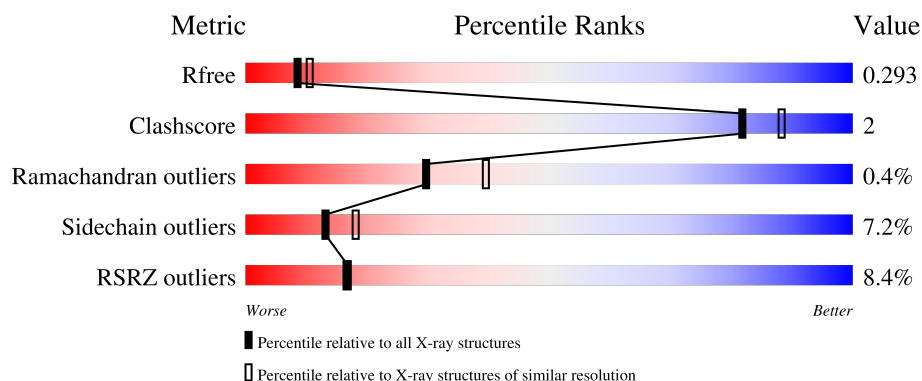
1 Overall quality at a glance

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	7% 75% 11% 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6697 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.

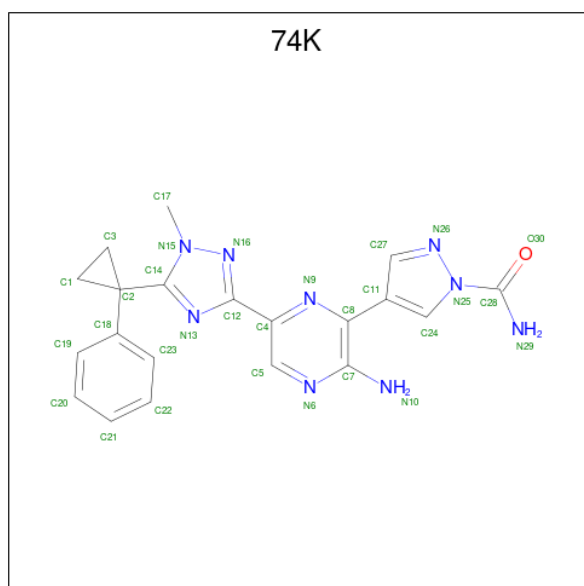
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	0	0
			6618	4246	1124	1194	54			

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 4-[3-azanyl-6-[1-methyl-5-(1-phenylcyclopropyl)-1,2,4-triazol-3-yl]pyrazin-2-yl]pyrazole-1-carboxamide (CCD ID: 74K) (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	49	Total	O	0	0
			49	49		

- 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, α , β , γ	64.59Å 142.16Å 221.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.84 – 2.55 56.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.84-2.55) 99.9 (56.84-2.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.234 , 0.278 0.247 , 0.293	Depositor DCC
R_{free} test set	1688 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6697	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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: 74K

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	0.83	2/6760 (0.0%)	1.37	22/9118 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	MET	SD-CE	-7.57	1.60	1.79
1	A	757	LYS	CA-CB	5.76	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	8.23	122.03	113.80
1	A	427	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	898	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	291	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	798	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	715	MET	N-CA-C	-5.53	105.33	111.36
1	A	930	VAL	N-CA-CB	5.40	116.01	110.23
1	A	664	PHE	CA-C-N	5.37	125.94	119.98
1	A	664	PHE	C-N-CA	5.37	125.94	119.98
1	A	151	ALA	CA-C-N	5.32	127.67	120.44
1	A	151	ALA	C-N-CA	5.32	127.67	120.44
1	A	213	PRO	CA-C-N	5.30	127.64	120.38
1	A	213	PRO	C-N-CA	5.30	127.64	120.38
1	A	991	CYS	N-CA-C	5.21	115.02	108.45
1	A	472	VAL	N-CA-CB	5.19	116.38	110.72
1	A	828	VAL	N-CA-C	-5.18	99.64	107.73
1	A	556	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	766	GLU	CA-C-N	5.04	127.03	120.28
1	A	766	GLU	C-N-CA	5.04	127.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	LYS	CA-C-N	5.03	130.75	121.85
1	A	433	LYS	C-N-CA	5.03	130.75	121.85
1	A	897	ASP	CA-CB-CG	5.01	117.61	112.60

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	6618	0	6604	33	0
2	A	30	0	0	1	0
3	A	49	0	0	0	0
All	All	6697	0	6604	33	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 2.

All (33) 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	1.49	0.94
1:A:549:LEU:HG	1:A:564:MET:CE	2.27	0.62
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.85	0.58
1:A:756:MET:HG2	1:A:780:ASN:O	2.05	0.56
1:A:162:TRP:CE3	1:A:286:ARG:HG3	2.41	0.55
1:A:317:TRP:HA	1:A:382:CYS:HB2	1.89	0.55
1:A:549:LEU:CG	1:A:564:MET:HE1	2.32	0.54
1:A:553:THR:HG21	1:A:564:MET:HG2	1.89	0.54
1:A:1002:LEU:HB3	1:A:1004:LEU:HD23	1.89	0.54
1:A:756:MET:HG2	1:A:781:GLY:HA3	1.91	0.53
1:A:834:ILE:HD11	1:A:901:ILE:HD11	1.90	0.52
1:A:192:VAL:HG13	1:A:272:PRO:HB2	1.91	0.52
1:A:719:MET:HE1	1:A:749:CYS:SG	2.49	0.51
1:A:883:CYS:HB3	1:A:932:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.93	0.49
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.94	0.49
1:A:512:ARG:HG2	1:A:530:LEU:HD12	1.94	0.49
1:A:568:LEU:HA	1:A:571:TRP:HB2	1.94	0.49
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.77	0.49
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.78	0.48
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.48	0.47
1:A:113:ILE:HA	1:A:116:GLN:HE21	1.79	0.47
1:A:647:LEU:O	1:A:651:LEU:HG	2.18	0.44
1:A:620:LYS:HG2	1:A:660:VAL:HG11	2.00	0.43
1:A:169:LEU:HD22	1:A:259:PHE:HE1	1.83	0.43
1:A:808:LEU:HD11	1:A:963:ALA:HB2	2.01	0.43
1:A:340:LYS:HG2	1:A:362:GLU:HB3	2.00	0.43
1:A:209:THR:HB	1:A:257:CYS:HB3	2.00	0.42
1:A:886:THR:HA	1:A:891:ILE:HD12	2.01	0.42
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	2.01	0.42
1:A:278:HIS:CD2	1:A:280:SER:H	2.39	0.41
1:A:870:ARG:HA	1:A:870:ARG:HD2	1.91	0.40
1:A:752:MET:HE1	2:A:1101:74K:O30	2.20	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	796/939 (85%)	764 (96%)	29 (4%)	3 (0%)	30 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ILE
1	A	742	GLU

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Mol	Chain	Res	Type
1	A	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%)	674 (93%)	52 (7%)	13	18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	190	LEU
1	A	203	PHE
1	A	216	LEU
1	A	247	HIS
1	A	260	GLN
1	A	270	LEU
1	A	274	LEU
1	A	316	LEU
1	A	317	TRP
1	A	325	ILE
1	A	329	GLU
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	344	GLN
1	A	365	VAL
1	A	394	LEU
1	A	398	VAL
1	A	423	LEU
1	A	439	LEU
1	A	471	LEU
1	A	472	VAL
1	A	475	LEU

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Mol	Chain	Res	Type
1	A	483	VAL
1	A	512	ARG
1	A	514	ILE
1	A	516	GLU
1	A	517	ARG
1	A	530	LEU
1	A	553	THR
1	A	568	LEU
1	A	576	VAL
1	A	586	SER
1	A	617	GLN
1	A	634	LEU
1	A	722	GLU
1	A	748	GLN
1	A	756	MET
1	A	757	LYS
1	A	841	LYS
1	A	855	LEU
1	A	898	ASN
1	A	915	PHE
1	A	930	VAL
1	A	951	GLU
1	A	962	ARG
1	A	986	LEU
1	A	998	LEU
1	A	1004	LEU
1	A	1027	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	126	HIS
1	A	155	GLN
1	A	170	GLN
1	A	193	ASN
1	A	235	GLN
1	A	278	HIS
1	A	334	ASN
1	A	536	HIS
1	A	773	ASN
1	A	780	ASN

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Mol	Chain	Res	Type
1	A	898	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	74K	A	1101	-	32,34,34	1.12	1 (3%)	35,51,51	2.24	10 (28%)

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	74K	A	1101	-	-	5/18/28/28	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74K	C8-C11	2.03	1.50	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74K	N16-C12-N13	-6.47	108.30	114.71
2	A	1101	74K	C27-N26-N25	5.78	109.47	103.81
2	A	1101	74K	C17-N15-N16	3.57	124.63	119.29
2	A	1101	74K	C12-N16-N15	3.39	107.20	103.09
2	A	1101	74K	C5-N6-C7	3.20	121.74	118.64
2	A	1101	74K	O30-C28-N29	-3.17	116.46	122.63
2	A	1101	74K	C8-N9-C4	3.16	122.17	118.01
2	A	1101	74K	C4-C12-N16	3.00	127.40	123.38
2	A	1101	74K	C3-C2-C1	2.65	59.63	58.45
2	A	1101	74K	C4-C5-N6	-2.05	118.93	122.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	74K	C24-C11-C8-N9
2	A	1101	74K	C24-C11-C8-C7
2	A	1101	74K	C19-C18-C2-C14
2	A	1101	74K	C23-C18-C2-C14
2	A	1101	74K	C27-C11-C8-C7

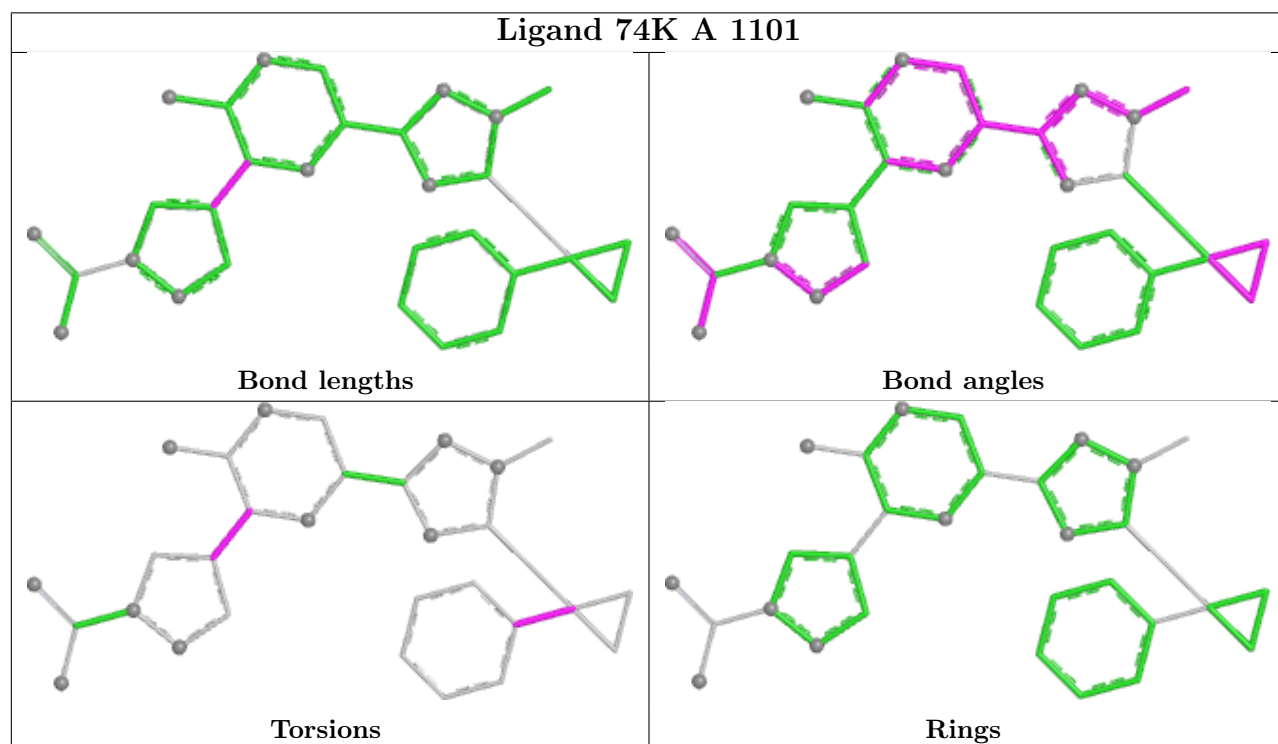
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	74K	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%)	0.65	69 (8%) 17 16	17, 43, 81, 149	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	7.0
1	A	1027	TRP	6.3
1	A	398	VAL	6.0
1	A	479	ALA	5.6
1	A	919	PHE	5.3
1	A	335	ALA	5.3
1	A	511	LEU	5.1
1	A	317	TRP	4.9
1	A	494	LEU	4.8
1	A	445	VAL	4.5
1	A	357	THR	4.3
1	A	332	LYS	4.2
1	A	333	VAL	3.9
1	A	373	GLN	3.9
1	A	515	LEU	3.7
1	A	328	ILE	3.4
1	A	512	ARG	3.3
1	A	173	PRO	3.2
1	A	1004	LEU	3.2
1	A	190	LEU	3.1
1	A	366	CYS	3.1
1	A	318	SER	3.1
1	A	945	GLY	3.1
1	A	230	GLN	3.0
1	A	347	LEU	3.0
1	A	397	VAL	3.0
1	A	932	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	334	ASN	2.9
1	A	517	ARG	2.9
1	A	491	ILE	2.8
1	A	483	VAL	2.8
1	A	530	LEU	2.8
1	A	514	ILE	2.8
1	A	478	VAL	2.8
1	A	993	LYS	2.8
1	A	844	MET	2.7
1	A	379	ILE	2.7
1	A	206	GLN	2.6
1	A	264	SER	2.6
1	A	377	PHE	2.5
1	A	523	LEU	2.5
1	A	226	THR	2.4
1	A	492	LEU	2.4
1	A	341	LEU	2.4
1	A	358	VAL	2.3
1	A	485	PHE	2.3
1	A	381	VAL	2.3
1	A	532	TRP	2.3
1	A	846	ALA	2.3
1	A	369	PRO	2.3
1	A	936	TYR	2.3
1	A	325	ILE	2.2
1	A	356	LYS	2.2
1	A	995	ILE	2.2
1	A	364	ASN	2.1
1	A	266	LEU	2.1
1	A	538	VAL	2.1
1	A	361	SER	2.1
1	A	378	ASP	2.1
1	A	319	LEU	2.1
1	A	1023	LEU	2.1
1	A	841	LYS	2.1
1	A	486	PRO	2.1
1	A	549	LEU	2.0
1	A	359	SER	2.0
1	A	563	GLN	2.0
1	A	985	GLY	2.0
1	A	1005	GLY	2.0
1	A	153	HIS	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](#)

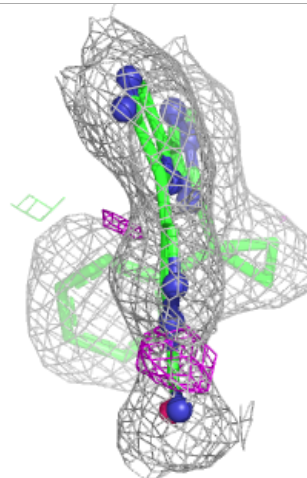
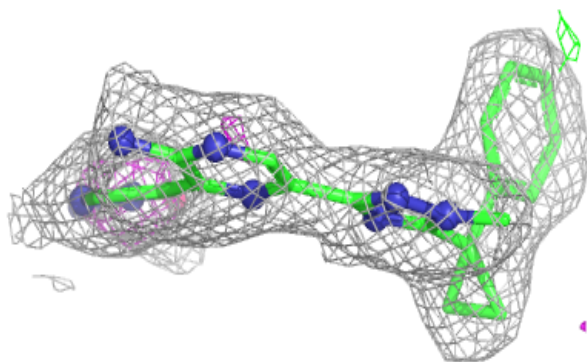
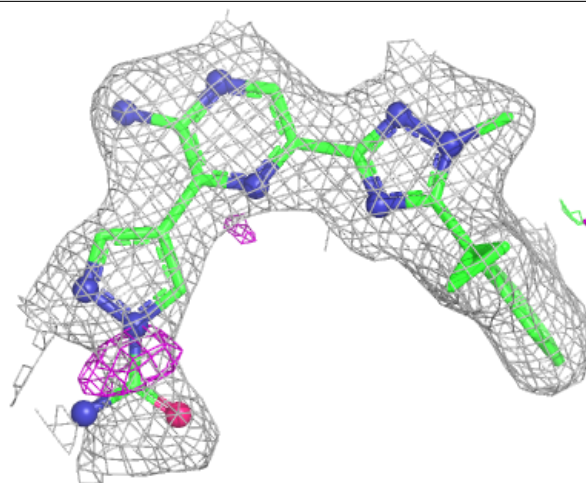
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	74K	A	1101	30/30	0.92	0.10	19,27,50,55	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 74K 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.