



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:33 AM UTC

PDB ID : 6T3B / pdb_00006t3b
Title : Crystal structure of PI3Kgamma with a dihydropurinone inhibitor (compound 4)
Authors : Petersen, J.; Oster, L.; Schimpl, M.; Goldberg, F.W.; Finlay, M.R.V.; Ting, A.K.T.; Beattie, D.; Lamont, G.M.; Fallan, C.; Wrigley, G.L.; Howard, M.R.; Williamson, B.; Davies, B.R.; Cadogan, E.B.; Ramos-Montoya, A.; Dean, E.
Deposited on : 2019-10-10
Resolution : 3.01 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](#) ①) 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

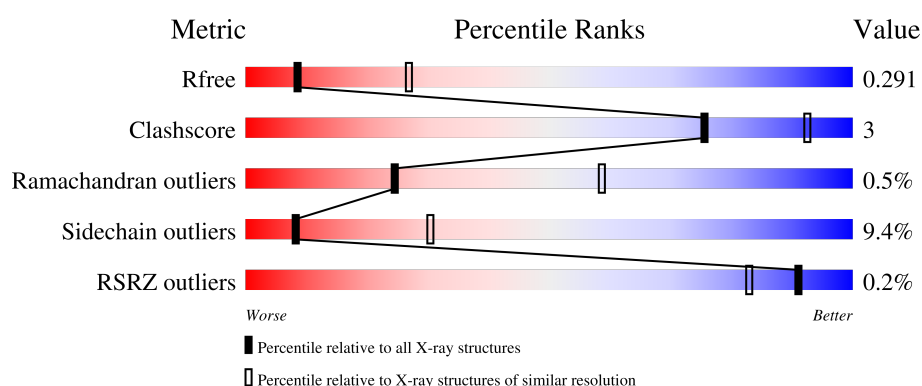
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	966	69% 13% • 17%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6555 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.

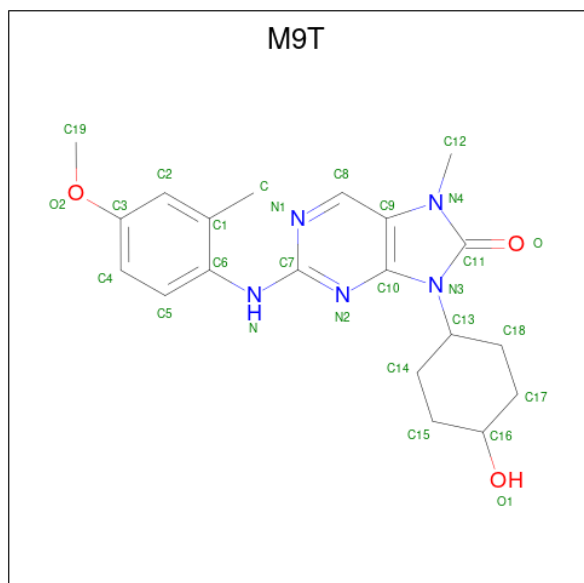
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6527	4197	1114	1182	34			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 2-[(4-methoxy-2-methyl-phenyl)amino]-7-methyl-9-(4-oxidanylcyclohexyl)purine-8-one (CCD ID: M9T) (formula: C₂₀H₂₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	20	5	3		

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.04Å 67.19Å 105.87Å 90.00° 96.64° 90.00°	Depositor
Resolution (Å)	39.90 – 3.01 39.90 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.3 (39.90-3.01) 97.3 (39.90-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.229 , 0.274 0.250 , 0.291	Depositor DCC
R_{free} test set	984 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6555	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: M9T

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	0.73	0/6664	1.28	7/9011 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ILE	CA-C-N	5.51	127.98	120.54
1	A	420	ILE	C-N-CA	5.51	127.98	120.54
1	A	614	ARG	CA-C-N	5.37	127.73	120.38
1	A	614	ARG	C-N-CA	5.37	127.73	120.38
1	A	632	ASP	CA-C-N	5.23	128.01	120.38
1	A	632	ASP	C-N-CA	5.23	128.01	120.38
1	A	594	SER	N-CA-C	-5.20	107.32	113.97

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	6527	0	6557	39	0
2	A	28	0	0	0	0
All	All	6555	0	6557	39	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 (39) 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:365:ILE:HD13	1:A:414:LEU:HD12	1.81	0.62
1:A:508:PRO:HG2	1:A:707:ARG:HE	1.67	0.59
1:A:397:ARG:HB3	1:A:414:LEU:HD22	1.84	0.57
1:A:547:MET:HE1	1:A:555:LEU:HD22	1.87	0.56
1:A:176:THR:HG21	1:A:673:HIS:HB2	1.88	0.56
1:A:222:ILE:HD11	1:A:244:ILE:HG21	1.89	0.54
1:A:743:GLN:HE21	1:A:876:ILE:HG23	1.73	0.54
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.91	0.53
1:A:587:LYS:HA	1:A:626:LEU:HD11	1.89	0.52
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.90	0.52
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.92	0.51
1:A:224:ILE:HD13	1:A:233:ILE:HD12	1.93	0.51
1:A:363:VAL:HG11	1:A:429:LEU:HD11	1.94	0.50
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.93	0.50
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.59	0.50
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.94	0.49
1:A:628:MET:HE1	1:A:662:GLN:HB3	1.95	0.48
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.94	0.48
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.49	0.47
1:A:355:TRP:HA	1:A:421:LYS:HG3	1.96	0.46
1:A:983:VAL:HB	1:A:1082:VAL:HG21	1.98	0.45
1:A:366:ARG:HH21	1:A:519:LEU:HD13	1.82	0.44
1:A:713:PHE:HA	1:A:716:ILE:HD12	2.00	0.43
1:A:211:LEU:HD22	1:A:297:LEU:HB3	2.00	0.43
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.01	0.43
1:A:750:LYS:HE2	1:A:809:LYS:H	1.84	0.42
1:A:200:PRO:HG3	1:A:282:VAL:HG23	2.01	0.42
1:A:842:MET:HE3	1:A:870:ILE:HA	2.01	0.42
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.37	0.42
1:A:844:ILE:HD13	1:A:965:PHE:HB3	2.02	0.42
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.85	0.42
1:A:466:LEU:HD13	1:A:482:LEU:HD11	2.02	0.42
1:A:802:LYS:HG3	1:A:812:TRP:HB3	2.01	0.42
1:A:746:THR:HA	1:A:811:LEU:HD13	2.02	0.42
1:A:596:VAL:HG23	1:A:603:ILE:HG22	2.03	0.41
1:A:777:SER:HB3	1:A:778:GLN:H	1.71	0.41
1:A:222:ILE:HG22	1:A:303:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:HB2	1:A:430:ASN:HB3	2.02	0.41
1:A:928:PHE:HE1	1:A:960:LEU:HD13	1.86	0.41

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	778/966 (80%)	746 (96%)	28 (4%)	4 (0%)	24 59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	ASP
1	A	964	ASP
1	A	874	ASP
1	A	916	PRO

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	721/864 (83%)	653 (91%)	68 (9%)	8 30

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	178	ARG
1	A	180	LEU
1	A	207	LEU
1	A	220	ILE
1	A	223	VAL
1	A	226	ARG
1	A	244	ILE
1	A	245	LEU
1	A	282	VAL
1	A	287	ILE
1	A	302	GLU
1	A	320	LYS
1	A	354	LEU
1	A	365	ILE
1	A	381	VAL
1	A	391	GLN
1	A	475	LEU
1	A	487	ILE
1	A	498	ASN
1	A	501	LYS
1	A	516	ILE
1	A	519	LEU
1	A	531	LYS
1	A	544	ARG
1	A	555	LEU
1	A	574	LEU
1	A	583	LEU
1	A	596	VAL
1	A	610	LEU
1	A	624	VAL
1	A	626	LEU
1	A	646	GLN
1	A	682	LEU
1	A	717	LEU
1	A	721	LEU
1	A	744	LYS
1	A	749	ILE
1	A	767	LEU
1	A	781	GLU
1	A	791	LEU
1	A	792	LYS
1	A	804	MET

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Mol	Chain	Res	Type
1	A	807	LYS
1	A	808	LYS
1	A	842	MET
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	887	THR
1	A	890	LYS
1	A	907	LEU
1	A	911	LEU
1	A	912	LYS
1	A	944	ILE
1	A	957	THR
1	A	963	ILE
1	A	982	ARG
1	A	997	THR
1	A	1013	CYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1045	LYS
1	A	1051	ILE
1	A	1052	ARG
1	A	1063	ASP
1	A	1073	GLU
1	A	1078	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	304	HIS
1	A	389	HIS
1	A	411	ASN
1	A	432	GLN
1	A	465	ASN
1	A	498	ASN
1	A	565	ASN
1	A	601	GLN
1	A	629	GLN
1	A	634	ASN
1	A	662	GLN
1	A	710	GLN

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Mol	Chain	Res	Type
1	A	734	GLN
1	A	743	GLN
1	A	775	GLN
1	A	846	GLN
1	A	892	GLN
1	A	908	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1023	HIS
1	A	1083	GLN
1	A	1085	ASN

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	M9T	A	1201	-	31,31,31	0.75	0	38,45,45	2.55	11 (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	M9T	A	1201	-	-	5/10/20/20	0/4/4/4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	M9T	C9-C10-N2	-10.17	119.33	126.50
2	A	1201	M9T	N1-C7-N2	-5.72	120.89	126.42
2	A	1201	M9T	C13-N3-C11	4.71	130.66	122.61
2	A	1201	M9T	C8-N1-C7	3.81	121.03	115.81
2	A	1201	M9T	C9-N4-C11	-3.65	108.21	110.10
2	A	1201	M9T	N3-C11-N4	3.31	109.68	106.92
2	A	1201	M9T	C12-N4-C11	2.88	126.11	123.59
2	A	1201	M9T	C14-C13-N3	2.50	118.48	112.27
2	A	1201	M9T	C7-N2-C10	2.39	121.65	113.99
2	A	1201	M9T	O-C11-N4	-2.32	124.37	127.21
2	A	1201	M9T	C6-N-C7	-2.21	122.47	129.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

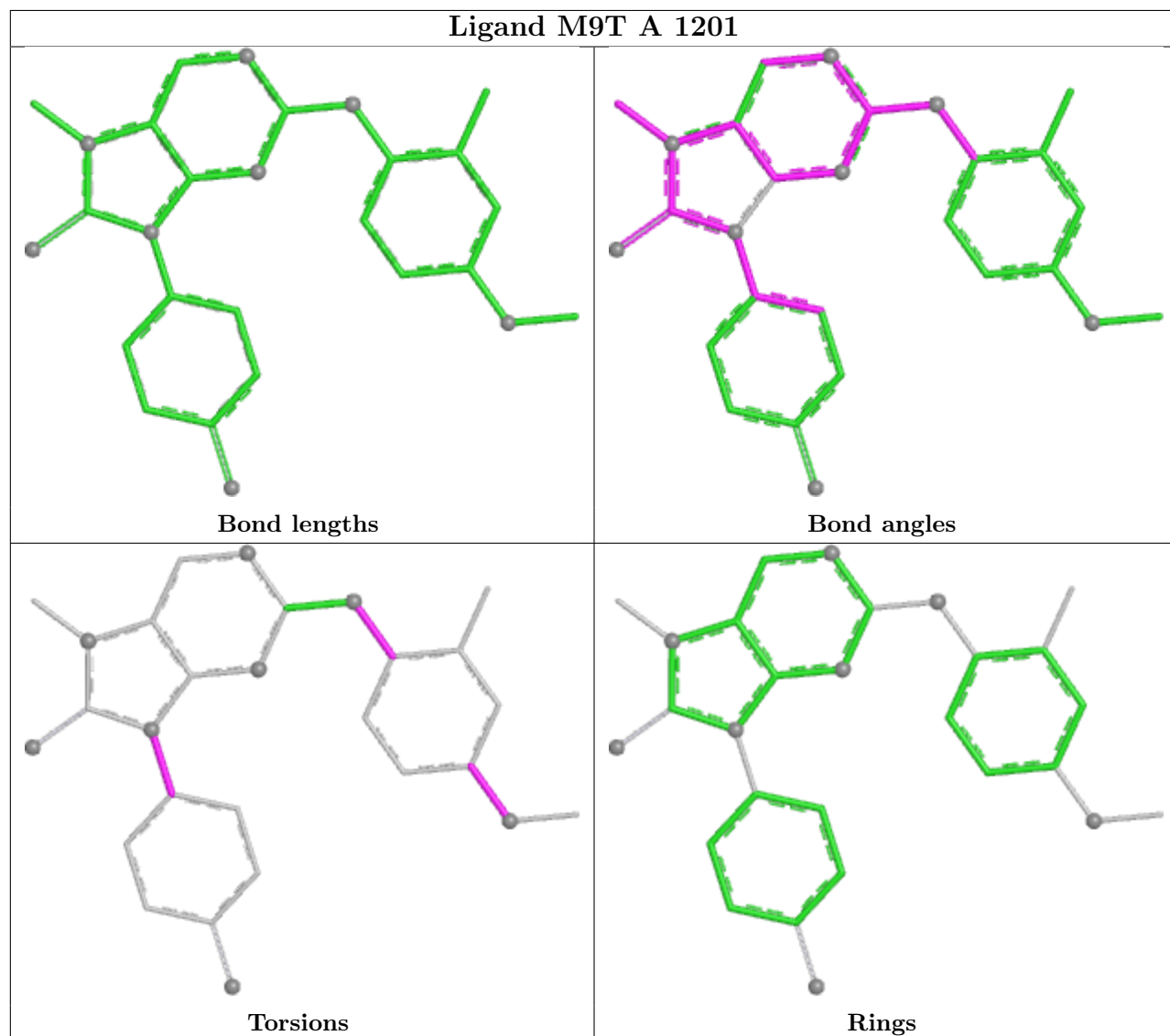
Mol	Chain	Res	Type	Atoms
2	A	1201	M9T	C4-C3-O2-C19
2	A	1201	M9T	C2-C3-O2-C19
2	A	1201	M9T	C1-C6-N-C7
2	A	1201	M9T	C5-C6-N-C7
2	A	1201	M9T	C18-C13-N3-C10

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 [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	804/966 (83%)	-0.14	2 (0%)	91 83	56, 110, 154, 182	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	LEU	2.7
1	A	147	SER	2.2

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](#)

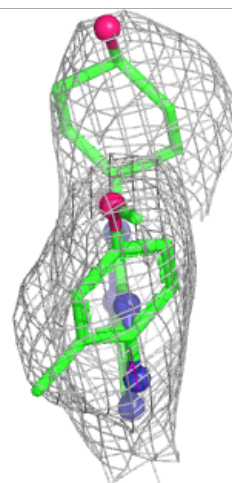
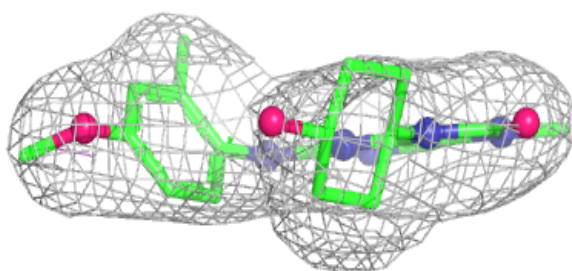
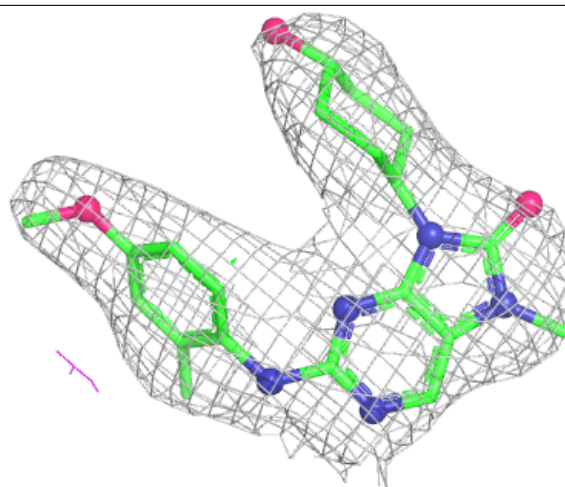
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	M9T	A	1201	28/28	0.88	0.10	80,92,94,95	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 M9T A 1201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.