



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 PM UTC

PDB ID : 6MUL / pdb_00006mul
Title : Murine PI3K delta kinsae domain - cpd 1
Authors : Fischmann, T.O.
Deposited on : 2018-10-23
Resolution : 3.09 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

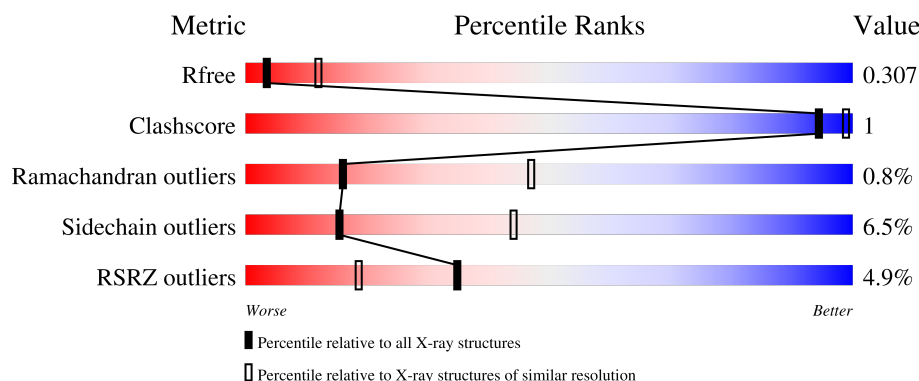
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	940	3% 79% 8% 13%
1	B	940	6% 79% 8% 13%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13340 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.

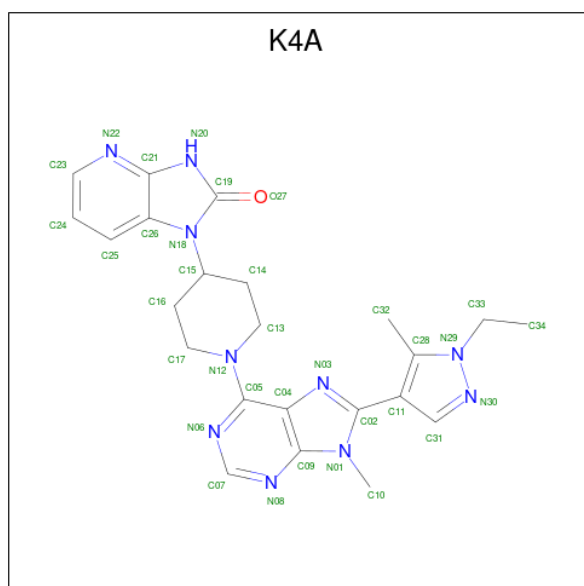
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	2	1
			6640	4256	1128	1201	55			
1	B	822	Total	C	N	O	S	0	1	1
			6632	4253	1126	1199	54			

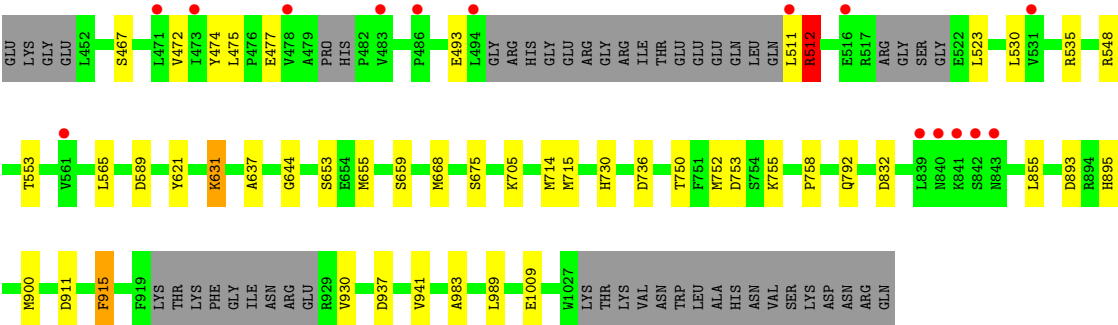
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q3UDT3
B	105	GLY	-	expression tag	UNP Q3UDT3

- Molecule 2 is 1-{1-[8-(1-ethyl-5-methyl-1H-pyrazol-4-yl)-9-methyl-9H-purin-6-yl]piperidin-4-yl}-1,3-dihydro-2H-imidazo[4,5-b]pyridin-2-one (CCD ID: K4A) (formula: $C_{23}H_{26}N_{10}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	23	10	1		
2	B	1	Total	C	N	O	0	0
			34	23	10	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.03Å 219.11Å 78.24Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	36.52 – 3.09 36.52 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.52-3.09) 99.3 (36.52-3.09)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, R_{free}	0.248 , 0.292 0.260 , 0.307	Depositor DCC
R_{free} test set	1776 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13340	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: K4A

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	0.86	1/6783 (0.0%)	1.14	8/9151 (0.1%)
1	B	0.86	1/6775 (0.0%)	1.16	11/9141 (0.1%)
All	All	0.86	2/13558 (0.0%)	1.15	19/18292 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	736	ASP	C-N	5.20	1.39	1.34
1	A	564	MET	SD-CE	-5.05	1.67	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	SER	CA-C-N	16.65	140.58	122.26
1	B	367	SER	C-N-CA	16.65	140.58	122.26
1	A	367	SER	CA-C-N	12.73	136.72	122.59
1	A	367	SER	C-N-CA	12.73	136.72	122.59
1	A	368	GLU	N-CA-C	-11.36	92.38	109.30
1	B	368	GLU	N-CA-C	-10.82	86.80	108.12
1	A	366	CYS	N-CA-C	9.62	125.09	113.16
1	B	915	PHE	CA-CB-CG	9.15	122.95	113.80
1	A	915	PHE	CA-CB-CG	8.98	122.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	VAL	N-CA-CB	6.88	118.21	110.72
1	B	367	SER	N-CA-C	6.80	119.40	109.07
1	B	512	ARG	N-CA-C	6.49	120.68	113.21
1	B	422	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	472	VAL	N-CA-CB	5.59	118.27	110.56
1	A	366	CYS	CA-C-O	-5.44	112.70	119.28
1	B	367	SER	CA-C-O	5.37	127.13	121.33
1	A	365	VAL	N-CA-C	5.36	120.50	109.34
1	B	435	GLY	CA-C-N	-5.30	115.14	122.30
1	B	435	GLY	C-N-CA	-5.30	115.14	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	THR	Peptide

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	6640	0	6615	19	0
1	B	6632	0	6612	17	0
2	A	34	0	0	0	0
2	B	34	0	0	1	0
All	All	13340	0	13227	34	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 1.

All (34) 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:434:THR:O	1:A:475:LEU:O	1.90	0.90
1:B:434:THR:O	1:B:475:LEU:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:THR:O	1:A:475:LEU:CB	2.44	0.64
1:A:270:LEU:HD11	1:A:770:SER:HB2	1.82	0.61
1:A:434:THR:O	1:A:475:LEU:HB2	2.06	0.55
1:A:752:MET:HE2	1:A:754:SER:HB3	1.90	0.53
1:A:335:ALA:HB3	1:B:126:HIS:CG	2.43	0.53
1:B:752:MET:HG3	1:B:758:PRO:HG2	1.91	0.52
1:A:143:MET:HE1	1:A:631:LYS:CD	2.42	0.50
1:A:434:THR:O	1:A:475:LEU:HB3	2.12	0.48
1:B:621:TYR:CE1	1:B:983:ALA:HB2	2.48	0.48
1:B:143:MET:HE1	1:B:631:LYS:CD	2.44	0.48
1:B:715:MET:HE1	1:B:750:THR:O	2.13	0.48
1:A:335:ALA:HB3	1:B:126:HIS:ND1	2.28	0.48
1:A:621:TYR:CE1	1:A:983:ALA:HB2	2.49	0.47
1:B:143:MET:HE1	1:B:631:LYS:HD3	1.97	0.46
1:B:435:GLY:O	1:B:474:TYR:HA	2.15	0.46
1:A:832:ASP:C	1:A:900:MET:HE3	2.42	0.45
1:B:832:ASP:C	1:B:900:MET:HE3	2.43	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.00	0.44
1:A:859:LEU:HD21	1:A:901:ILE:HD11	1.99	0.44
1:B:637:ALA:HB1	1:B:644:GLY:HA2	2.00	0.44
1:A:143:MET:HE1	1:A:631:LYS:HD3	2.00	0.43
1:A:435:GLY:O	1:A:474:TYR:HA	2.19	0.42
1:A:358:VAL:HG22	1:A:377:PHE:CE1	2.54	0.42
1:B:358:VAL:HG22	1:B:377:PHE:CE1	2.54	0.42
1:B:512:ARG:HD2	1:B:512:ARG:C	2.45	0.42
1:B:434:THR:O	1:B:475:LEU:CB	2.68	0.42
1:B:937:ASP:O	1:B:941:VAL:HG23	2.20	0.41
1:A:937:ASP:O	1:A:941:VAL:HG23	2.20	0.41
1:B:752:MET:HE1	2:B:9001:K4A:C32	2.51	0.41
1:A:719:MET:HE1	1:A:749:CYS:SG	2.60	0.41
1:A:655:MET:CG	1:A:668:MET:HE1	2.51	0.41
1:B:655:MET:CG	1:B:668:MET:HE1	2.51	0.41

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	802/940 (85%)	748 (93%)	48 (6%)	6 (1%)	18	49
1	B	801/940 (85%)	744 (93%)	51 (6%)	6 (1%)	18	49
All	All	1603/1880 (85%)	1492 (93%)	99 (6%)	12 (1%)	16	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	434	THR
1	B	535	ARG
1	A	328	ILE
1	A	434	THR
1	A	535	ARG
1	A	755	LYS
1	B	755	LYS
1	A	730	HIS
1	B	331	ARG
1	B	730	HIS
1	A	331	ARG
1	B	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	729/827 (88%)	683 (94%)	46 (6%)	16	45
1	B	728/827 (88%)	679 (93%)	49 (7%)	15	43
All	All	1457/1654 (88%)	1362 (94%)	95 (6%)	15	44

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	118	SER
1	A	170	GLN
1	A	190	LEU
1	A	201	GLU
1	A	221	LEU
1	A	229	ARG
1	A	247	HIS
1	A	250	LEU
1	A	257	CYS
1	A	270	LEU
1	A	275	THR
1	A	325	ILE
1	A	329	GLU
1	A	332	LYS
1	A	342	VAL
1	A	365	VAL
1	A	423	LEU
1	A	467	SER
1	A	472	VAL
1	A	477	GLU
1	A	493	GLU
1	A	511	LEU
1	A	523	LEU
1	A	530	LEU
1	A	548	ARG
1	A	553	THR
1	A	565	LEU
1	A	589	ASP
1	A	631	LYS
1	A	653	SER
1	A	659	SER
1	A	675	SER
1	A	705	LYS
1	A	714	MET
1	A	753	ASP
1	A	792	GLN
1	A	855	LEU
1	A	893	ASP
1	A	895	HIS
1	A	910	ILE
1	A	911	ASP
1	A	915	PHE

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Mol	Chain	Res	Type
1	A	930	VAL
1	A	989	LEU
1	A	1009	GLU
1	B	113	ILE
1	B	170	GLN
1	B	190	LEU
1	B	201	GLU
1	B	221	LEU
1	B	229	ARG
1	B	247	HIS
1	B	250	LEU
1	B	257	CYS
1	B	270	LEU
1	B	275	THR
1	B	325	ILE
1	B	332	LYS
1	B	334	ASN
1	B	340	LYS
1	B	342	VAL
1	B	365	VAL
1	B	366	CYS
1	B	367	SER
1	B	368	GLU
1	B	423	LEU
1	B	445	VAL
1	B	467	SER
1	B	477	GLU
1	B	493	GLU
1	B	511	LEU
1	B	512	ARG
1	B	523	LEU
1	B	530	LEU
1	B	548	ARG
1	B	553	THR
1	B	565	LEU
1	B	589	ASP
1	B	631	LYS
1	B	653	SER
1	B	659	SER
1	B	675	SER
1	B	705	LYS
1	B	714	MET

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Mol	Chain	Res	Type
1	B	753	ASP
1	B	792	GLN
1	B	855	LEU
1	B	893	ASP
1	B	895	HIS
1	B	911	ASP
1	B	915	PHE
1	B	930	VAL
1	B	989	LEU
1	B	1009	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	A	422	ASN
1	A	685	GLN
1	A	780	ASN
1	A	792	GLN
1	B	422	ASN
1	B	558	HIS
1	B	685	GLN
1	B	792	GLN
1	B	996	GLN

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

2 ligands are 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	K4A	A	9001	-	39,39,39	0.97	2 (5%)	51,58,58	1.60	6 (11%)
2	K4A	B	9001	-	39,39,39	1.10	3 (7%)	51,58,58	1.78	8 (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	K4A	A	9001	-	-	2/14/24/24	0/6/6/6
2	K4A	B	9001	-	-	2/14/24/24	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9001	K4A	C02-N01	4.76	1.42	1.37
2	A	9001	K4A	C02-N01	4.17	1.42	1.37
2	A	9001	K4A	C19-N18	3.82	1.46	1.38
2	B	9001	K4A	C19-N18	3.75	1.46	1.38
2	B	9001	K4A	C11-C02	-2.65	1.42	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9001	K4A	C26-N18-C19	-8.22	103.71	109.24
2	A	9001	K4A	C26-N18-C19	-7.60	104.13	109.24
2	A	9001	K4A	O27-C19-N18	-4.25	122.55	125.89
2	B	9001	K4A	C09-C04-C05	-3.99	111.79	115.91
2	B	9001	K4A	O27-C19-N18	-3.67	123.01	125.89
2	B	9001	K4A	C04-C05-N06	3.60	126.03	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9001	K4A	C09-N01-C02	-3.55	104.26	106.22
2	A	9001	K4A	C09-C04-C05	-3.28	112.52	115.91
2	B	9001	K4A	C33-N29-N30	2.96	123.00	119.22
2	A	9001	K4A	C04-C05-N06	2.88	124.53	118.55
2	A	9001	K4A	N20-C19-N18	2.68	109.92	106.69
2	B	9001	K4A	C05-C04-N03	2.46	137.19	133.36
2	B	9001	K4A	N20-C19-N18	2.32	109.48	106.69
2	A	9001	K4A	C33-N29-N30	2.08	121.88	119.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

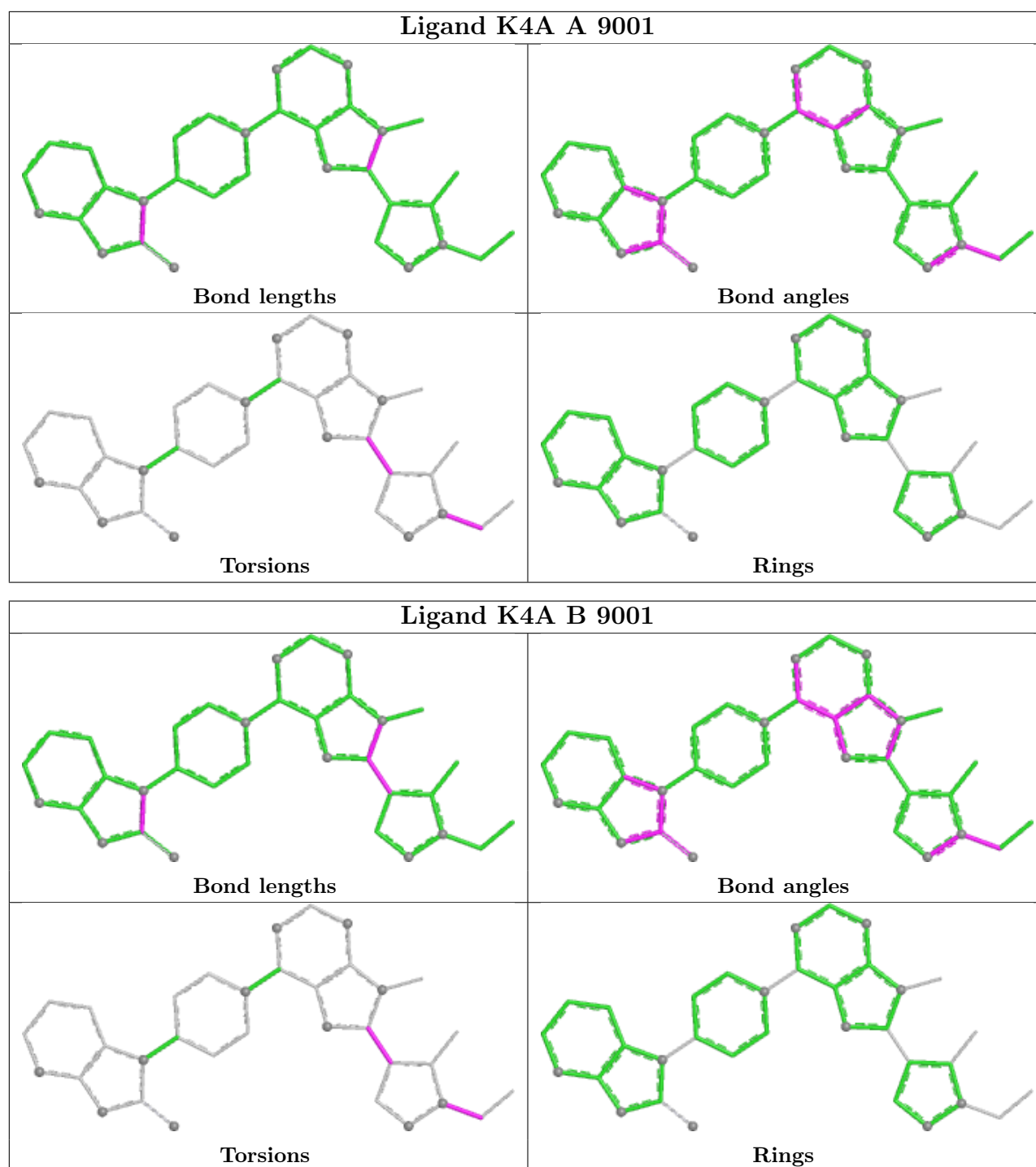
Mol	Chain	Res	Type	Atoms
2	A	9001	K4A	N01-C02-C11-C31
2	B	9001	K4A	N01-C02-C11-C31
2	A	9001	K4A	C34-C33-N29-N30
2	B	9001	K4A	C34-C33-N29-N30

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9001	K4A	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	822/940 (87%)	0.45	26 (3%)	50 30	25, 82, 129, 168	2 (0%)
1	B	822/940 (87%)	0.44	54 (6%)	24 13	25, 78, 134, 165	1 (0%)
All	All	1644/1880 (87%)	0.45	80 (4%)	35 18	25, 80, 131, 168	3 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	840	ASN	6.3
1	B	840	ASN	5.5
1	B	343	VAL	4.7
1	B	317	TRP	4.2
1	B	230	GLN	4.0
1	B	347	LEU	3.9
1	B	316	LEU	3.9
1	B	432	LEU	3.9
1	B	205	PHE	3.8
1	A	317	TRP	3.7
1	A	841	LYS	3.7
1	B	377	PHE	3.5
1	A	445	VAL	3.5
1	B	378	ASP	3.5
1	A	335	ALA	3.4
1	A	316	LEU	3.4
1	B	842	SER	3.4
1	B	366	CYS	3.4
1	B	841	LYS	3.3
1	B	494	LEU	3.3
1	B	511	LEU	3.3
1	A	568	LEU	3.2
1	B	839	LEU	3.0
1	B	425	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	381	VAL	3.0
1	A	433	LYS	2.9
1	A	388	ALA	2.9
1	B	426	PHE	2.9
1	A	191	LEU	2.8
1	A	192	VAL	2.8
1	A	531	VAL	2.8
1	B	354	LEU	2.8
1	B	384	LEU	2.7
1	B	516	GLU	2.7
1	A	377	PHE	2.7
1	A	591	TYR	2.7
1	A	560	ASP	2.7
1	A	319	LEU	2.6
1	B	325	ILE	2.6
1	B	323	PHE	2.6
1	B	375	LEU	2.6
1	B	324	SER	2.6
1	B	365	VAL	2.6
1	B	319	LEU	2.6
1	B	433	LYS	2.6
1	B	390	LEU	2.5
1	B	478	VAL	2.5
1	B	843	ASN	2.4
1	A	839	LEU	2.4
1	B	203	PHE	2.4
1	B	531	VAL	2.4
1	A	843	ASN	2.3
1	B	110	LYS	2.3
1	B	330	GLY	2.3
1	B	486	PRO	2.3
1	B	344	GLN	2.3
1	A	471	LEU	2.3
1	B	318	SER	2.3
1	B	561	VAL	2.2
1	B	334	ASN	2.2
1	B	379	ILE	2.2
1	B	150	ALA	2.2
1	B	355	CYS	2.2
1	B	192	VAL	2.2
1	B	388	ALA	2.2
1	B	358	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	483	VAL	2.1
1	A	147	CYS	2.1
1	A	515	LEU	2.1
1	B	394	LEU	2.1
1	B	423	LEU	2.1
1	A	251	TYR	2.1
1	A	512	ARG	2.0
1	B	473	ILE	2.0
1	A	432	LEU	2.0
1	A	641	ARG	2.0
1	B	471	LEU	2.0
1	B	360	SER	2.0
1	A	153	HIS	2.0
1	B	349	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](#)

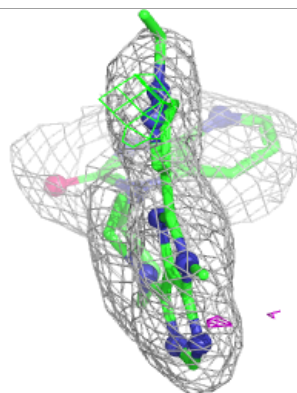
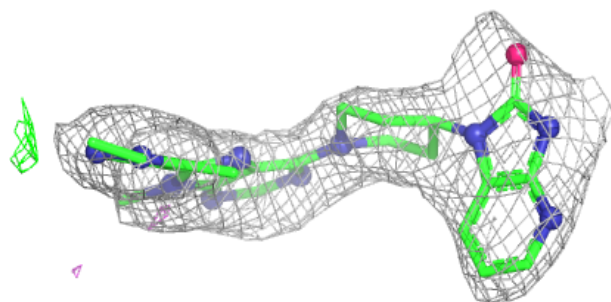
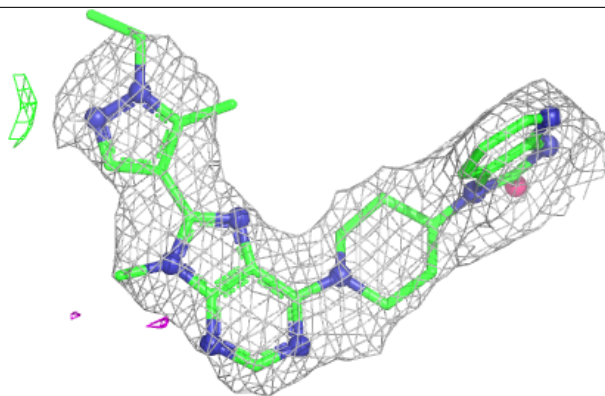
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	K4A	A	9001	34/34	0.88	0.11	35,45,61,66	0
2	K4A	B	9001	34/34	0.92	0.09	31,42,58,60	0

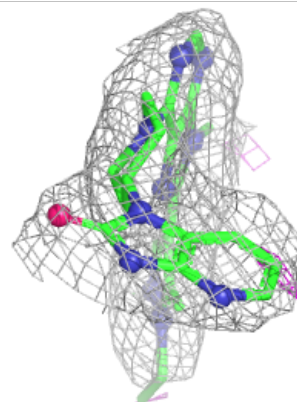
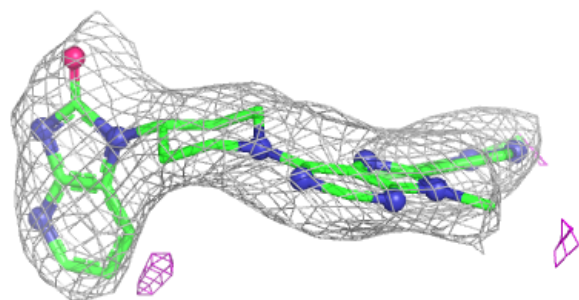
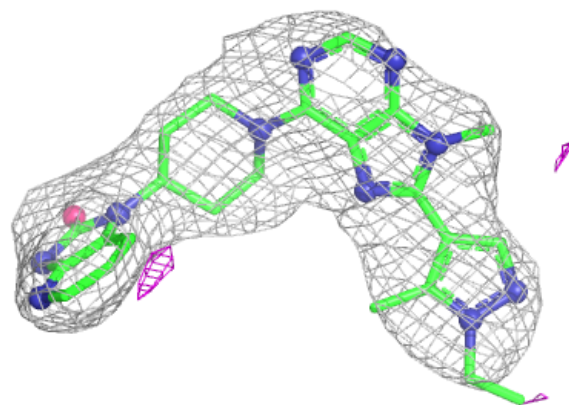
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around K4A A 9001:

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

**Electron density around K4A B 9001:**

$2mF_o-DF_c$ (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.