



# Full wwPDB X-ray Structure Validation Report

Dec 13, 2023 – 08:42 am GMT

PDB ID : 2WXJ  
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with INK654.  
Authors : Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.  
Deposited on : 2009-11-09  
Resolution : 2.60 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](mailto: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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

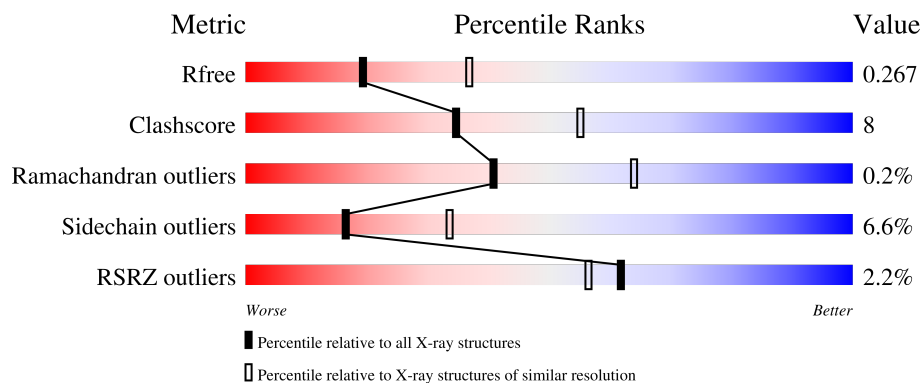
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2%      69%      16%      •      13%</p>





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.88Å 64.79Å 117.71Å 90.00° 103.21° 90.00°	Depositor
Resolution (Å)	66.52 – 2.60 58.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (66.52-2.60) 99.3 (58.73-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.5.0046	Depositor
R, $R_{free}$	0.210 , 0.264 0.213 , 0.267	Depositor DCC
$R_{free}$ test set	1018 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6723	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: RW3

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	0.59	2/6776 (0.0%)	0.64	2/9142 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	CYS	CB-SG	-6.08	1.72	1.82
1	A	478	VAL	C-N	5.48	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	907	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	423	LEU	CA-CB-CG	5.47	127.88	115.30

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	6633	0	6615	108	0
2	A	41	0	28	3	0
3	A	49	0	0	3	0
All	All	6723	0	6643	111	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 8.

All (111) 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:837:ILE:CD1	1:A:901:ILE:HD11	1.95	0.95
1:A:110:LYS:O	1:A:110:LYS:HG3	1.65	0.93
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.34	0.92
2:A:1500:RW3:OBI	2:A:1500:RW3:SBJ	2.30	0.88
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.58	0.86
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.60	0.84
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.59	0.83
1:A:367:SER:HB3	1:A:369:PRO:HD3	1.62	0.80
1:A:779:LYS:NZ	1:A:782:ASP:OD2	2.15	0.79
1:A:837:ILE:HD12	1:A:901:ILE:HD11	1.65	0.77
1:A:367:SER:HB3	1:A:369:PRO:CD	2.17	0.74
1:A:109:VAL:CG1	1:A:110:LYS:N	2.50	0.74
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.85	0.74
1:A:512:ARG:HD3	1:A:534:MET:HG3	1.70	0.73
1:A:549:LEU:HG	1:A:564:MET:HE3	1.73	0.70
1:A:913:GLY:HA2	3:A:2026:HOH:O	1.91	0.69
1:A:212:MET:HE1	1:A:253:ASN:HB3	1.75	0.68
1:A:110:LYS:HZ2	1:A:144:ARG:HH12	1.42	0.67
1:A:549:LEU:HG	1:A:564:MET:CE	2.26	0.66
1:A:145:GLN:O	1:A:149:GLU:HG3	1.97	0.65
1:A:858:TRP:CZ3	1:A:901:ILE:HD13	2.32	0.64
1:A:146:PHE:CE1	1:A:631:LYS:HE3	2.33	0.64
1:A:109:VAL:N	3:A:2001:HOH:O	2.31	0.63
1:A:836:ASN:ND2	3:A:2036:HOH:O	2.32	0.63
1:A:109:VAL:HG12	1:A:110:LYS:N	2.14	0.63
1:A:110:LYS:O	1:A:110:LYS:CG	2.46	0.62
1:A:317:TRP:HA	1:A:382:CYS:HB2	1.83	0.60
1:A:109:VAL:HG12	1:A:110:LYS:H	1.67	0.60
1:A:367:SER:HB3	1:A:369:PRO:N	2.17	0.59
1:A:154:ARG:HA	1:A:157:LEU:HG	1.85	0.59
1:A:1007:THR:OG1	1:A:1010:GLU:HB2	2.02	0.58
1:A:1006:LYS:HB3	1:A:1010:GLU:HB3	1.88	0.56
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.72	0.55
1:A:330:GLY:HA2	1:A:470:ALA:O	2.08	0.54
1:A:387:MET:CE	1:A:590:CYS:HB3	2.36	0.54
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.43	0.54
1:A:1013:LYS:HG3	1:A:1014:HIS:N	2.21	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:O	1:A:382:CYS:HB3	2.08	0.54
1:A:343:VAL:H	1:A:360:SER:HB2	1.73	0.53
1:A:512:ARG:O	1:A:515:LEU:HG	2.09	0.53
1:A:914:HIS:HD2	1:A:988:GLU:OE2	1.92	0.53
1:A:1012:LEU:O	1:A:1016:ARG:HG3	2.09	0.53
1:A:432:LEU:HB3	1:A:483:VAL:HG23	1.91	0.52
1:A:895:HIS:H	1:A:898:ASN:HD21	1.57	0.52
1:A:917:GLY:HA3	1:A:997:TYR:CE1	2.45	0.52
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.91	0.52
1:A:435:GLY:O	1:A:475:LEU:N	2.42	0.52
1:A:901:ILE:HD12	1:A:901:ILE:O	2.10	0.52
1:A:953:PHE:O	1:A:956:PHE:HB3	2.10	0.52
1:A:587:PHE:HB3	1:A:592:VAL:HG11	1.92	0.51
1:A:212:MET:CE	1:A:253:ASN:HB3	2.40	0.51
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.92	0.51
1:A:618:VAL:HG12	1:A:629:LEU:CD2	2.40	0.51
1:A:918:ASN:OD1	1:A:988:GLU:HG2	2.10	0.51
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.93	0.51
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.26	0.51
1:A:753:ASP:O	1:A:753:ASP:CG	2.49	0.51
1:A:512:ARG:NH2	1:A:538:VAL:HG22	2.26	0.50
1:A:109:VAL:HG13	1:A:110:LYS:N	2.25	0.50
1:A:962:ARG:HG2	1:A:962:ARG:NH1	2.11	0.50
1:A:435:GLY:HA2	1:A:475:LEU:O	2.12	0.50
1:A:213:PRO:O	1:A:217:MET:HG3	2.12	0.50
1:A:211:ASP:O	1:A:256:LEU:HG	2.12	0.49
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.78	0.49
1:A:387:MET:HG3	1:A:589:ASP:HA	1.94	0.49
1:A:330:GLY:C	1:A:369:PRO:HD2	2.32	0.49
1:A:702:SER:O	1:A:706:THR:HG22	2.13	0.49
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.46	0.49
1:A:271:THR:O	1:A:273:HIS:HD2	1.95	0.48
1:A:710:GLN:O	1:A:714:MET:HG2	2.14	0.48
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.95	0.48
1:A:838:GLN:NE2	1:A:937:ASP:OD2	2.47	0.48
1:A:894:ARG:HD3	1:A:909:HIS:ND1	2.29	0.47
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.50	0.47
1:A:754:SER:O	1:A:755:LYS:C	2.53	0.46
1:A:340:LYS:HG3	1:A:364:ASN:HA	1.98	0.46
1:A:842:SER:O	1:A:844:MET:HG2	2.15	0.46
1:A:832:ASP:OD1	1:A:833:THR:N	2.48	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:HIS:O	1:A:720:ARG:HG3	2.17	0.45
1:A:330:GLY:O	1:A:369:PRO:HD2	2.17	0.45
1:A:930:VAL:HG13	1:A:997:TYR:OH	2.17	0.45
1:A:603:LEU:HD22	1:A:607:GLU:HB3	1.99	0.44
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.98	0.44
1:A:938:PHE:N	1:A:938:PHE:CD1	2.84	0.44
1:A:846:ALA:HA	1:A:857:ASN:HB3	1.99	0.44
1:A:703:SER:OG	1:A:757:LYS:HE2	2.19	0.43
1:A:371:TRP:O	1:A:373:GLN:HG2	2.18	0.43
1:A:735:LEU:HD13	1:A:826:GLU:HB2	2.00	0.43
1:A:512:ARG:HH21	1:A:516:GLU:CD	2.21	0.43
1:A:750:THR:HG22	1:A:751:PHE:H	1.84	0.43
2:A:1500:RW3:NBA	2:A:1500:RW3:HAN	2.34	0.43
1:A:475:LEU:HA	1:A:476:PRO:HD3	1.78	0.42
1:A:898:ASN:HD22	1:A:898:ASN:C	2.22	0.42
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.34	0.42
1:A:387:MET:HE2	1:A:590:CYS:SG	2.60	0.42
1:A:225:ALA:O	1:A:230:GLN:N	2.53	0.42
2:A:1500:RW3:HAZ2	2:A:1500:RW3:HBE	1.84	0.42
1:A:618:VAL:HG21	1:A:980:LEU:HD22	2.01	0.41
1:A:256:LEU:O	1:A:262:ILE:HB	2.20	0.41
1:A:334:ASN:CG	1:A:335:ALA:H	2.23	0.41
1:A:326:GLU:HB3	1:A:474:TYR:HB3	2.02	0.41
1:A:236:PRO:HD2	1:A:237:GLU:OE1	2.20	0.41
1:A:895:HIS:H	1:A:898:ASN:ND2	2.17	0.41
1:A:214:LEU:HD11	1:A:237:GLU:HG3	2.02	0.41
1:A:325:ILE:HD11	1:A:375:LEU:HD12	2.02	0.41
1:A:534:MET:O	1:A:537:GLU:HG2	2.21	0.41
1:A:151:ALA:HB2	1:A:674:GLY:O	2.21	0.40
1:A:154:ARG:NH2	1:A:674:GLY:O	2.54	0.40
1:A:837:ILE:HD11	1:A:901:ILE:CD1	2.41	0.40
1:A:917:GLY:HA2	1:A:930:VAL:CG1	2.52	0.40
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.64	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	800/940 (85%)	759 (95%)	39 (5%)	2 (0%)	41 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	755	LYS
1	A	770	SER

### 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	728/827 (88%)	680 (93%)	48 (7%)	16 33

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	111	LYS
1	A	188	ARG
1	A	190	LEU
1	A	203	PHE
1	A	223	LYS
1	A	230	GLN
1	A	291	ASN
1	A	317	TRP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	331	ARG
1	A	332	LYS
1	A	340	LYS
1	A	352	GLU
1	A	360	SER
1	A	382	CYS
1	A	423	LEU
1	A	478	VAL
1	A	489	GLU
1	A	511	LEU
1	A	514	ILE
1	A	517	ARG
1	A	523	LEU
1	A	525	GLU
1	A	553	THR
1	A	563	GLN
1	A	586	SER
1	A	594	SER
1	A	599	SER
1	A	618	VAL
1	A	634	LEU
1	A	744	VAL
1	A	750	THR
1	A	753	ASP
1	A	755	LYS
1	A	757	LYS
1	A	779	LYS
1	A	843	ASN
1	A	852	LYS
1	A	855	LEU
1	A	870	ARG
1	A	898	ASN
1	A	915	PHE
1	A	930	VAL
1	A	935	THR
1	A	937	ASP
1	A	962	ARG
1	A	986	LEU
1	A	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	247	HIS
1	A	273	HIS
1	A	291	ASN
1	A	344	GLN
1	A	431	GLN
1	A	617	GLN
1	A	786	GLN
1	A	898	ASN
1	A	914	HIS
1	A	943	GLN

### 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 monosaccharides 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	RW3	A	1500	-	39,47,47	2.03	14 (35%)	43,69,69	2.22	13 (30%)

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	RW3	A	1500	-	-	2/10/26/26	0/7/7/7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	RW3	CAM-CAE	-4.33	1.35	1.42
2	A	1500	RW3	CBH-CBG	-3.83	1.35	1.41
2	A	1500	RW3	CBN-NBM	-3.78	1.30	1.36
2	A	1500	RW3	C6-N1	-3.74	1.30	1.35
2	A	1500	RW3	CBL-NBM	-3.47	1.29	1.36
2	A	1500	RW3	CAO-CAG	-2.99	1.37	1.42
2	A	1500	RW3	C2-N3	-2.91	1.28	1.33
2	A	1500	RW3	CAE-NAF	-2.91	1.32	1.37
2	A	1500	RW3	CBE-CBD	-2.76	1.35	1.41
2	A	1500	RW3	C5-C6	-2.60	1.36	1.43
2	A	1500	RW3	CAN-CAM	-2.56	1.36	1.42
2	A	1500	RW3	CBG-NBO	-2.30	1.31	1.38
2	A	1500	RW3	CAP-NAH	-2.13	1.43	1.46
2	A	1500	RW3	CAD-CAE	-2.01	1.38	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	RW3	CBC-CBF-SBJ	5.87	136.85	125.10
2	A	1500	RW3	NAF-CAG-NAH	-5.29	113.86	117.62
2	A	1500	RW3	CBG-CBF-SBJ	-5.10	105.09	111.85
2	A	1500	RW3	CAP-NAH-CAA	4.32	121.06	111.52
2	A	1500	RW3	N1-C2-N3	-4.30	121.95	128.68
2	A	1500	RW3	CAG-NAF-CAE	3.49	123.48	116.11
2	A	1500	RW3	CAJ-NAI-CAQ	-3.25	105.80	110.66
2	A	1500	RW3	OBI-CBL-NBM	-2.59	119.64	123.04
2	A	1500	RW3	CBF-CBG-NBO	2.42	113.67	108.04
2	A	1500	RW3	CAD-CAE-NAF	2.18	122.02	118.69
2	A	1500	RW3	CAR-CAO-CAN	-2.12	116.13	120.88
2	A	1500	RW3	CAM-CAE-NAF	-2.04	119.22	122.26
2	A	1500	RW3	CBK-CBL-NBM	2.04	117.97	114.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

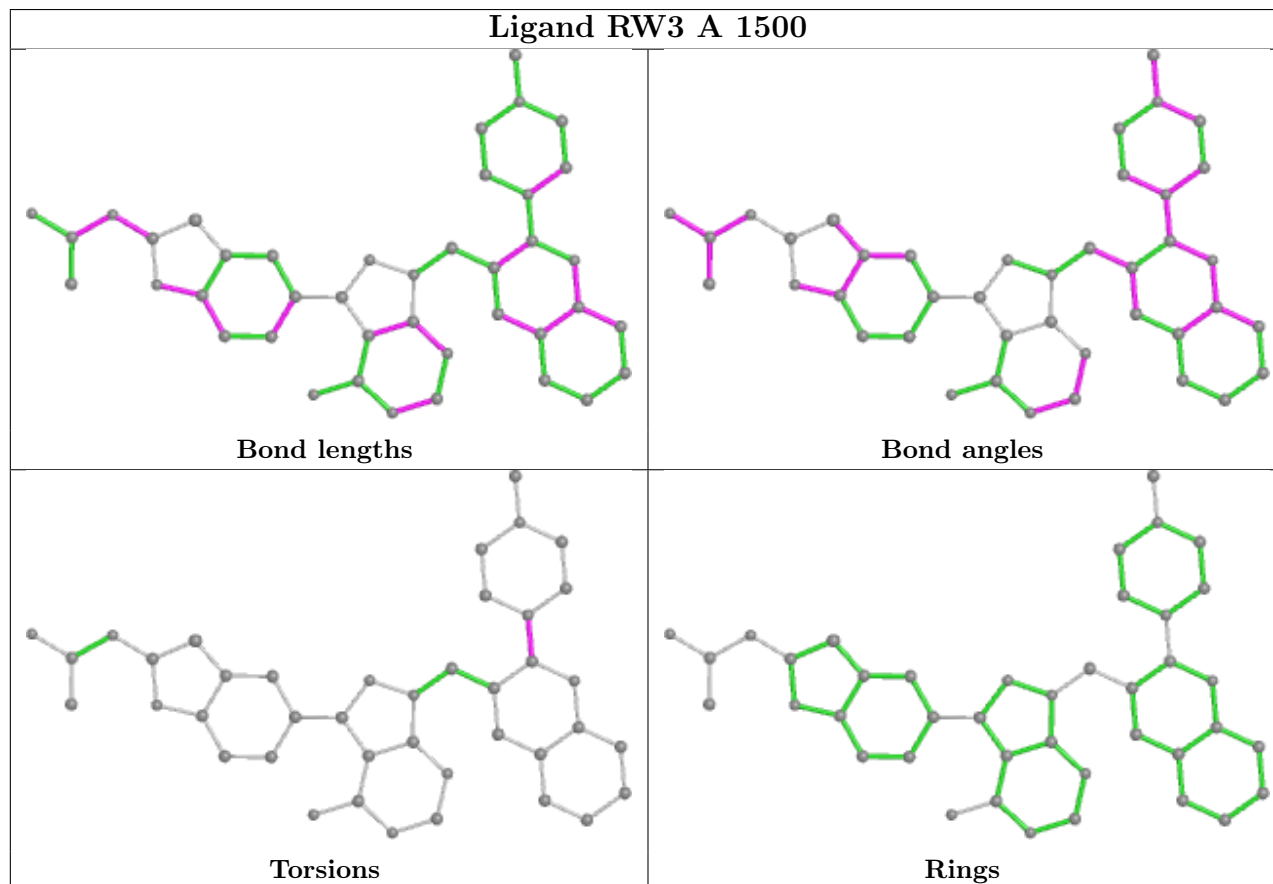
Mol	Chain	Res	Type	Atoms
2	A	1500	RW3	NAF-CAG-NAH-CAP
2	A	1500	RW3	CAO-CAG-NAH-CAP

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	RW3	3	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	822/940 (87%)	-0.07	18 (2%) 62 56	2, 11, 23, 35	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	TRP	6.2
1	A	319	LEU	3.6
1	A	341	LEU	3.5
1	A	270	LEU	3.3
1	A	322	PRO	3.2
1	A	377	PHE	3.2
1	A	846	ALA	3.2
1	A	334	ASN	2.7
1	A	330	GLY	2.5
1	A	323	PHE	2.5
1	A	227	VAL	2.4
1	A	366	CYS	2.4
1	A	843	ASN	2.4
1	A	394	LEU	2.3
1	A	492	LEU	2.3
1	A	514	ILE	2.0
1	A	488	LEU	2.0
1	A	770	SER	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](#)

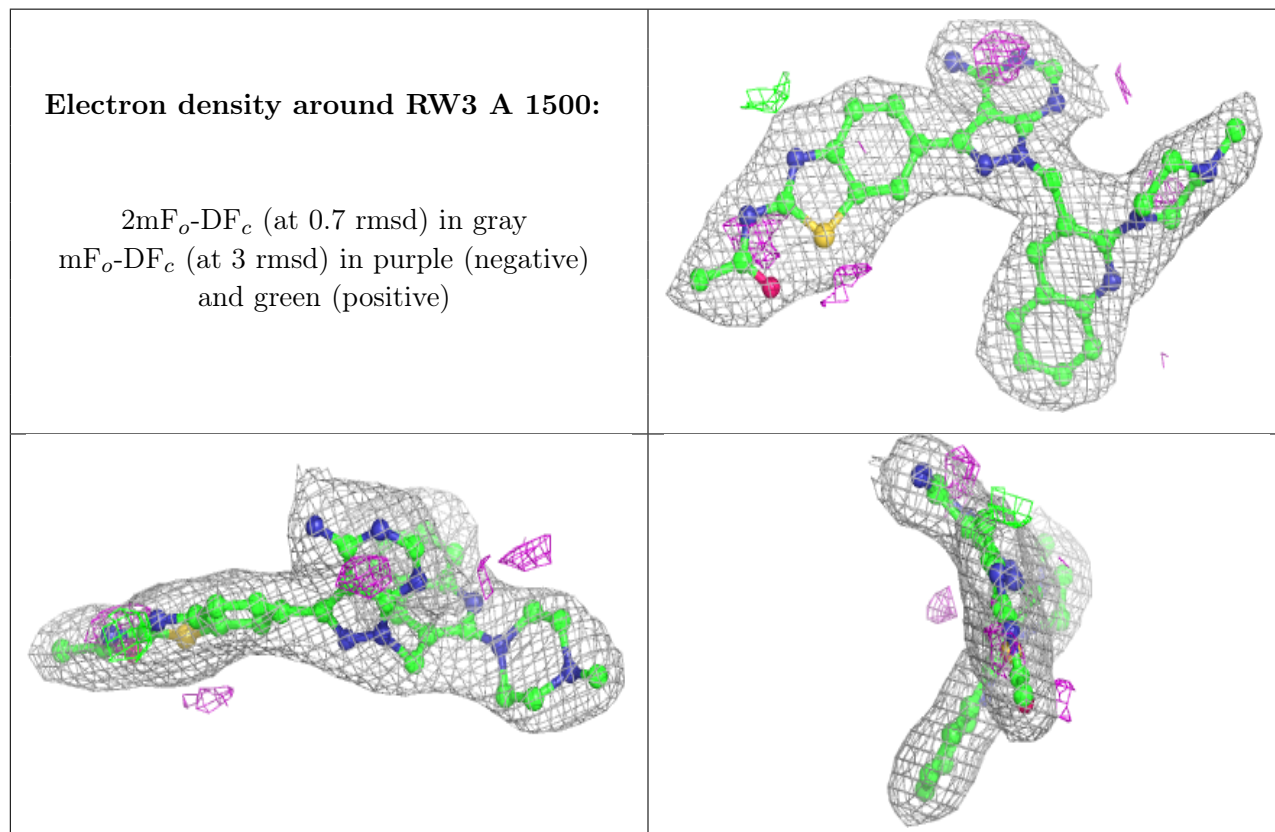
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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	RW3	A	1500	41/41	0.96	0.14	19,25,31,34	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.