



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:04 PM UTC

PDB ID : 2WXJ / pdb_00002wxj
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

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

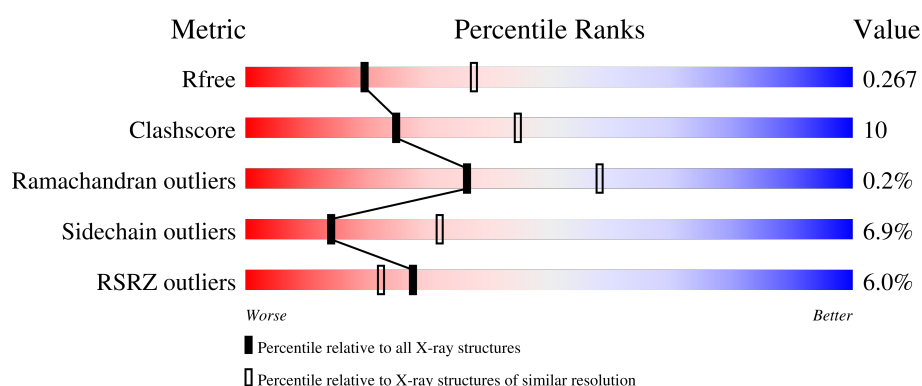
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	5% 67% 18% 13%

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.88Å 64.79Å 117.71Å 90.00° 103.21° 90.00°	Depositor
Resolution (Å)	66.52 – 2.60 66.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (66.52-2.60) 99.5 (66.52-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.58Å)	Xtriage
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 (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6723	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage'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.*

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: 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	0.71	4/6776 (0.1%)	0.90	9/9142 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	VAL	C-N	9.50	1.46	1.33
1	A	930	VAL	CA-CB	6.31	1.60	1.53
1	A	316	LEU	C-N	6.26	1.43	1.33
1	A	478	VAL	C-O	6.05	1.31	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	912	PHE	N-CA-C	11.53	123.41	111.07
1	A	930	VAL	N-CA-C	7.97	115.81	107.76
1	A	334	ASN	N-CA-C	7.83	118.22	107.73
1	A	750	THR	CB-CA-C	-5.84	101.77	114.10
1	A	111	LYS	N-CA-C	-5.56	106.85	113.97
1	A	332	LYS	N-CA-C	5.27	116.29	108.86
1	A	329	GLU	N-CA-C	5.12	115.29	108.38
1	A	442	TRP	CA-C-N	5.04	124.97	119.78
1	A	442	TRP	C-N-CA	5.04	124.97	119.78

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	127	0
2	A	41	0	28	3	0
3	A	49	0	0	3	0
All	All	6723	0	6643	130	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 10.

All (130) 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:549:LEU:HG	1:A:564:MET:HE1	1.54	0.85
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.59	0.83
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.63	0.81
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:756:MET:HE3	1:A:781:GLY:HA3	1.66	0.75
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:CG	1:A:564:MET:HE1	2.22	0.70
1:A:913:GLY:HA2	3:A:2026:HOH:O	1.91	0.69
1:A:387:MET:HE3	1:A:590:CYS:CB	2.23	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:386:ARG:HG3	1:A:387:MET:HE2	1.78	0.65
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:387:MET:HE3	1:A:590:CYS:SG	2.40	0.61
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:212:MET:HE1	1:A:253:ASN:HB3	1.84	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:387:MET:CE	1:A:590:CYS:HB3	2.36	0.55
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.72	0.55
1:A:753:ASP:O	1:A:753:ASP:CG	2.49	0.55
1:A:330:GLY:C	1:A:369:PRO:HD2	2.32	0.54
1:A:330:GLY:HA2	1:A:470:ALA:O	2.08	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
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:756:MET:HE3	1:A:781:GLY:CA	2.37	0.53
1:A:534:MET:HA	1:A:534:MET:HE2	1.91	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:754:SER:O	1:A:755:LYS:C	2.53	0.51
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.26	0.51
1:A:512:ARG:NH2	1:A:538:VAL:HG22	2.26	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:386:ARG:CG	1:A:387:MET:HE2	2.41	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:702:SER:O	1:A:706:THR:HG22	2.13	0.49
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.77	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:109:VAL:HG13	1:A:110:LYS:N	2.25	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:512:ARG:HH21	1:A:516:GLU:CD	2.21	0.48
1:A:894:ARG:HD3	1:A:909:HIS:ND1	2.29	0.47
1:A:898:ASN:HD22	1:A:898:ASN:C	2.22	0.47
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.50	0.47
1:A:549:LEU:CD1	1:A:564:MET:HE1	2.45	0.46
1:A:340:LYS:HG3	1:A:364:ASN:HA	1.98	0.46
1:A:334:ASN:CG	1:A:335:ALA:H	2.23	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
1:A:112:LEU:O	1:A:115:SER:OG	2.33	0.45
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:212:MET:HE3	1:A:253:ASN:HA	1.99	0.44
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:532:TRP:HZ3	1:A:564:MET:HE2	1.84	0.43
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:750:THR:HG22	1:A:751:PHE:H	1.84	0.43
1:A:208:SER:C	1:A:210:LYS:H	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1500:RW3:NBA	2:A:1500:RW3:HAN	2.34	0.43
1:A:915:PHE:C	1:A:915:PHE:CD1	2.97	0.42
1:A:475:LEU:HA	1:A:476:PRO:HD3	1.78	0.42
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.34	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:131:LEU:O	1:A:132:ARG:C	2.62	0.42
1:A:585:PHE:C	1:A:587:PHE:H	2.29	0.41
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: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:419:ALA:HB3	1:A:441:MET:HE3	2.02	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:699:VAL:HG21	1:A:715:MET:HE2	2.02	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:907:LEU:C	1:A:907:LEU:HD23	2.46	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%)	36 58

All (2) Ramachandran outliers are listed below:

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

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	728/827 (88%)	678 (93%)	50 (7%)	14	32

All (50) 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	214	LEU
1	A	223	LYS
1	A	230	GLN
1	A	270	LEU
1	A	317	TRP
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	360	SER
1	A	418	ILE
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	525	GLU
1	A	537	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	804	GLU
1	A	843	ASN
1	A	855	LEU
1	A	898	ASN
1	A	901	ILE
1	A	907	LEU
1	A	915	PHE
1	A	930	VAL
1	A	935	THR
1	A	937	ASP
1	A	951	GLU
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	155	GLN
1	A	193	ASN
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	351	ASN
1	A	364	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	431	GLN
1	A	617	GLN
1	A	721	GLN
1	A	786	GLN
1	A	851	ASN
1	A	895	HIS
1	A	898	ASN
1	A	914	HIS
1	A	940	HIS
1	A	943	GLN
1	A	948	ASN

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	RW3	A	1500	-	47,47,47	3.74	25 (53%)	67,69,69	3.10	26 (38%)

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	-	-	3/16/26/26	0/7/7/7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	RW3	CBN-SBJ	-15.19	1.57	1.75
2	A	1500	RW3	NAV-NBA	-8.46	1.20	1.36
2	A	1500	RW3	C6-NAV	-8.18	1.28	1.35
2	A	1500	RW3	CBD-CBB	-6.64	1.39	1.49
2	A	1500	RW3	CBN-NBM	-5.30	1.30	1.38
2	A	1500	RW3	CBF-SBJ	-5.00	1.64	1.74
2	A	1500	RW3	CAM-CAE	-4.51	1.35	1.42
2	A	1500	RW3	CBG-NBO	-4.18	1.31	1.39
2	A	1500	RW3	CBL-NBM	-3.67	1.29	1.37
2	A	1500	RW3	C5-C6	-3.64	1.36	1.40
2	A	1500	RW3	CBB-NBA	-3.08	1.29	1.33
2	A	1500	RW3	C2-N3	-3.07	1.28	1.33
2	A	1500	RW3	CAE-NAF	-3.03	1.32	1.37
2	A	1500	RW3	CBH-CBG	-3.02	1.35	1.40
2	A	1500	RW3	CAO-CAG	-3.01	1.37	1.42
2	A	1500	RW3	C5-C4	-2.73	1.39	1.42
2	A	1500	RW3	CBE-CBD	-2.73	1.35	1.39
2	A	1500	RW3	CAN-CAM	-2.60	1.36	1.42
2	A	1500	RW3	C2-N1	-2.41	1.29	1.33
2	A	1500	RW3	CBG-CBF	-2.30	1.36	1.40
2	A	1500	RW3	C4-NAZ	-2.27	1.28	1.34
2	A	1500	RW3	C4-N3	-2.26	1.29	1.35
2	A	1500	RW3	C5-CBB	-2.18	1.38	1.44
2	A	1500	RW3	C6-N1	-2.10	1.30	1.34
2	A	1500	RW3	CAD-CAE	-2.10	1.38	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	RW3	CBF-SBJ-CBN	9.11	96.76	88.33
2	A	1500	RW3	C5-CBB-NBA	-8.03	104.68	110.19
2	A	1500	RW3	CBB-NBA-NAV	8.02	113.53	106.02
2	A	1500	RW3	C5-C6-N1	-6.91	119.63	126.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	RW3	SBJ-CBN-NBO	-6.02	109.82	117.06
2	A	1500	RW3	CBL-NBM-CBN	-5.56	114.90	124.05
2	A	1500	RW3	CBC-CBF-CBG	-5.30	118.05	121.99
2	A	1500	RW3	NAF-CAG-NAH	-4.64	113.86	117.62
2	A	1500	RW3	N1-C6-NAV	4.46	132.30	125.34
2	A	1500	RW3	CAR-CAO-CAG	4.38	127.23	122.67
2	A	1500	RW3	N3-C2-N1	-4.38	121.95	128.58
2	A	1500	RW3	CBC-CBF-SBJ	4.32	136.85	126.07
2	A	1500	RW3	CAP-NAH-CAA	4.22	121.06	111.57
2	A	1500	RW3	CAO-CAR-NAV	-3.97	108.77	112.80
2	A	1500	RW3	C2-N1-C6	3.84	121.22	111.83
2	A	1500	RW3	CAR-NAV-NBA	3.78	122.91	119.98
2	A	1500	RW3	SBJ-CBN-NBM	3.43	127.87	121.87
2	A	1500	RW3	CAG-NAF-CAE	3.41	123.48	116.11
2	A	1500	RW3	CBG-CBF-SBJ	-3.15	105.09	109.75
2	A	1500	RW3	CBD-CBB-NBA	3.04	122.87	118.91
2	A	1500	RW3	CBE-CBD-CBC	-2.90	115.89	119.25
2	A	1500	RW3	CAJ-NAI-CAQ	-2.54	105.80	110.63
2	A	1500	RW3	CBG-NBO-CBN	2.53	114.65	108.66
2	A	1500	RW3	CAR-CAO-CAN	-2.34	116.13	122.06
2	A	1500	RW3	CAD-CAE-NAF	2.28	122.02	118.69
2	A	1500	RW3	CAM-CAE-NAF	-2.20	119.22	122.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

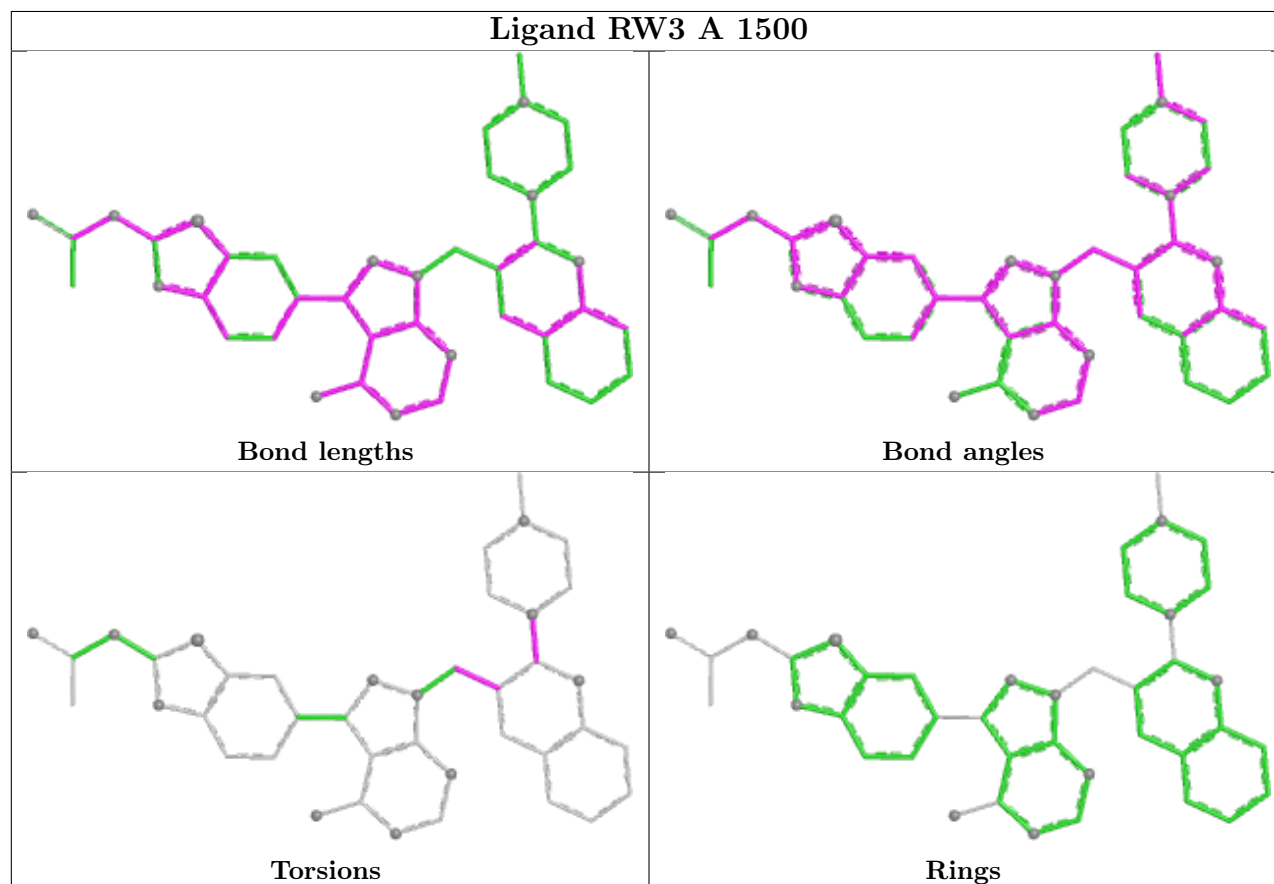
There are no ring outliers.

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 ⓘ

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%)	0.18	49 (5%)	27 22	2, 11, 23, 35	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	ASN	8.3
1	A	479	ALA	7.2
1	A	316	LEU	5.8
1	A	428	TYR	5.4
1	A	482	PRO	5.0
1	A	494	LEU	4.7
1	A	511	LEU	4.2
1	A	478	VAL	4.0
1	A	429	LYS	3.7
1	A	1027	TRP	3.7
1	A	846	ALA	3.7
1	A	487	ALA	3.6
1	A	770	SER	3.4
1	A	386	ARG	3.2
1	A	445	VAL	3.2
1	A	318	SER	2.9
1	A	319	LEU	2.9
1	A	334	ASN	2.9
1	A	486	PRO	2.8
1	A	317	TRP	2.8
1	A	491	ILE	2.8
1	A	843	ASN	2.7
1	A	1024	ARG	2.7
1	A	514	ILE	2.6
1	A	366	CYS	2.6
1	A	339	MET	2.6
1	A	270	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	427	ASP	2.5
1	A	517	ARG	2.5
1	A	484	TYR	2.5
1	A	388	ALA	2.4
1	A	485	PHE	2.4
1	A	434	THR	2.3
1	A	373	GLN	2.3
1	A	991	CYS	2.2
1	A	387	MET	2.2
1	A	771	ALA	2.2
1	A	513	GLU	2.1
1	A	463	PRO	2.1
1	A	430	ASP	2.1
1	A	937	ASP	2.1
1	A	435	GLY	2.1
1	A	395	TYR	2.1
1	A	426	PHE	2.1
1	A	335	ALA	2.0
1	A	490	LYS	2.0
1	A	432	LEU	2.0
1	A	524	TYR	2.0
1	A	341	LEU	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 [\(i\)](#)

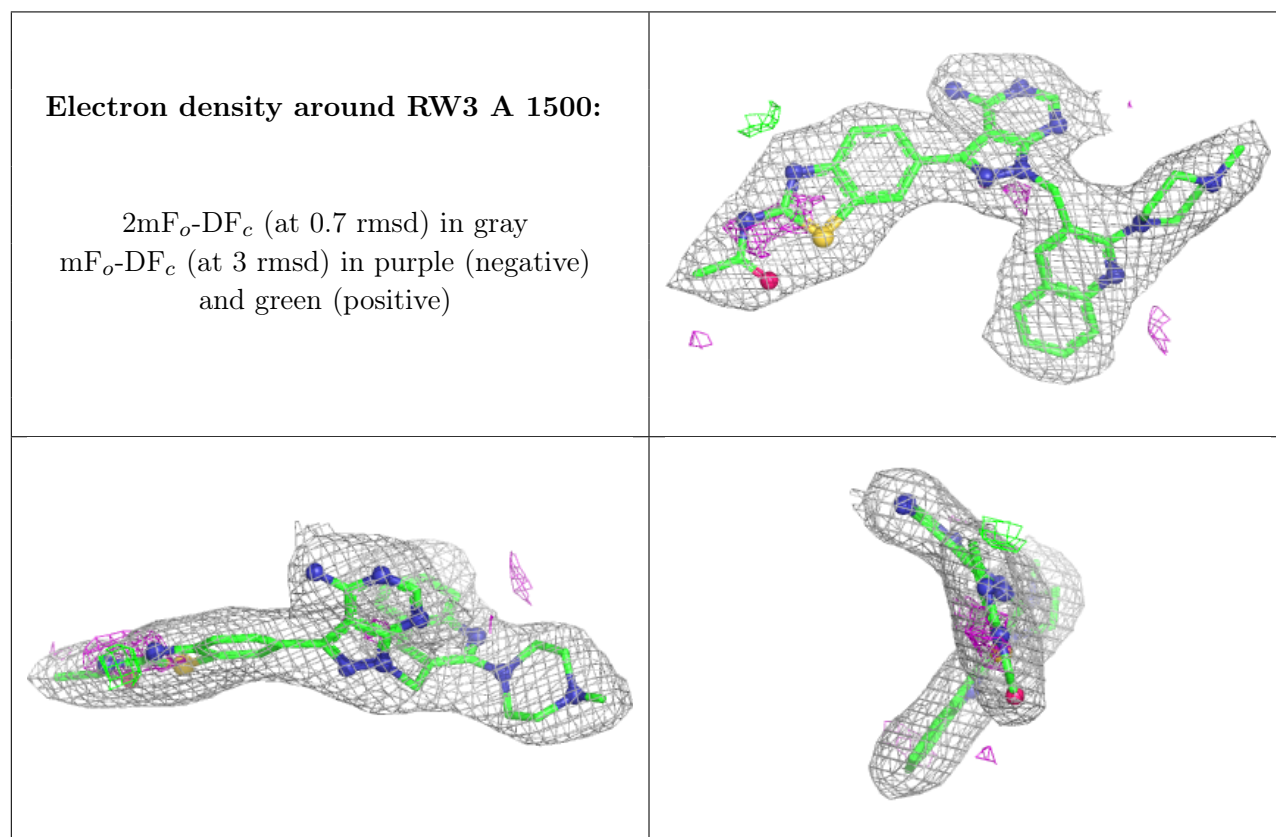
There are no oligosaccharides in this entry.

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	RW3	A	1500	41/41	0.94	0.08	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.