



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 09:21 AM UTC

PDB ID : 3L13 / pdb_00003l13
Title : Crystal Structures of Pan-PI3-Kinase and Dual Pan-PI3-Kinase/mTOR Inhibitors
Authors : Murray, J.M.; Wiesmann, C.
Deposited on : 2009-12-10
Resolution : 3.00 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

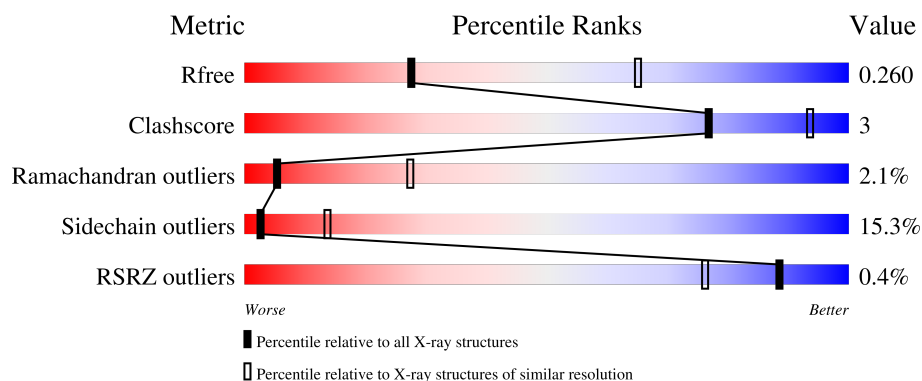
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	960	 69% 17% • 12%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6846 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.

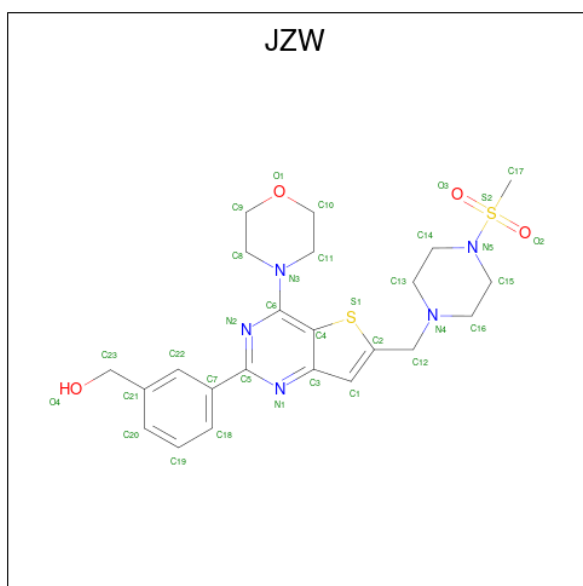
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6812	4371	1164	1242	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736

- Molecule 2 is [3-(6-{[4-(methylsulfonyl)piperazin-1-yl]methyl}-4-morpholin-4-ylthieno[3,2-d]pyrimidin-2-yl)phenyl]methanol (CCD ID: JZW) (formula: C₂₃H₂₉N₅O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	23	5	4	2		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.36Å 67.74Å 107.15Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.00) 99.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.275 0.219 , 0.260	Depositor DCC
R_{free} test set	1064 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6846	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JZW

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	0.60	0/6958	0.85	0/9412

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	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	6812	0	6843	39	0
2	A	34	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6846	0	6872	40	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 (40) 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:204:SER:OG	1:A:652:GLU:OE2	1.95	0.84
1:A:576:TRP:O	1:A:579:ARG:HD3	1.93	0.68
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.47	0.63
1:A:576:TRP:O	1:A:579:ARG:CD	2.54	0.56
1:A:373:LEU:N	1:A:374:PRO:CD	2.69	0.55
1:A:837:ASP:OD2	1:A:840:GLN:NE2	2.39	0.55
1:A:181:VAL:O	1:A:185:MET:HG3	2.07	0.54
1:A:680:PHE:O	1:A:684:ARG:HG2	2.07	0.54
2:A:1:JZW:H8A	2:A:1:JZW:S1	2.48	0.53
1:A:1086:TRP:O	1:A:1087:PHE:HB2	2.11	0.51
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.11	0.50
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.45	0.49
1:A:470:ASP:C	1:A:470:ASP:OD1	2.56	0.49
1:A:1086:TRP:O	1:A:1087:PHE:CB	2.61	0.48
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.96	0.47
1:A:878:MET:C	1:A:879:ILE:HG13	2.38	0.47
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.97	0.47
1:A:802:LYS:NZ	2:A:1:JZW:O3	2.44	0.47
1:A:632:ASP:C	1:A:632:ASP:OD1	2.58	0.46
1:A:895:THR:O	1:A:897:GLY:N	2.48	0.46
1:A:624:VAL:O	1:A:628:MET:HG2	2.16	0.46
1:A:467:LEU:O	1:A:476:ARG:NH1	2.49	0.45
1:A:805:ALA:O	1:A:806:SER:HB3	2.16	0.45
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.98	0.44
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.50	0.44
1:A:898:ASN:C	1:A:900:GLY:N	2.76	0.44
1:A:947:ARG:NH2	1:A:963:ILE:O	2.51	0.44
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.53	0.43
1:A:231:GLN:HE21	1:A:231:GLN:HA	1.83	0.43
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.54	0.43
1:A:625:GLY:O	1:A:629:GLN:HG3	2.18	0.43
1:A:935:TYR:O	1:A:939:THR:HB	2.18	0.43
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.19	0.42
1:A:766:GLN:HE21	1:A:766:GLN:HB3	1.70	0.42
1:A:706:SER:O	1:A:710:GLN:HB3	2.19	0.42
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	2.02	0.41
1:A:893:GLN:O	1:A:894:SER:C	2.64	0.40
1:A:614:ARG:NH1	1:A:646:GLN:HE22	2.19	0.40
1:A:947:ARG:NH2	1:A:964:ASP:O	2.55	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	825/960 (86%)	766 (93%)	42 (5%)	17 (2%)	5	27

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	806	SER
1	A	896	VAL
1	A	898	ASN
1	A	899	THR
1	A	1040	PRO
1	A	894	SER
1	A	1087	PHE
1	A	227	SER
1	A	239	ASP
1	A	776	ASN
1	A	376	ASN
1	A	775	GLN
1	A	778	GLN
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	999	GLY
1	A	545	ALA
1	A	526	PRO

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	754/858 (88%)	639 (85%)	115 (15%)	3 14

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	153	GLN
1	A	164	ASP
1	A	168	VAL
1	A	174	GLU
1	A	194	LYS
1	A	202	VAL
1	A	204	SER
1	A	207	LEU
1	A	213	LYS
1	A	214	LYS
1	A	215	ILE
1	A	219	CYS
1	A	226	ARG
1	A	231	GLN
1	A	234	LYS
1	A	240	THR
1	A	252	MET
1	A	267	GLU
1	A	271	VAL
1	A	277	ARG
1	A	278	ASP
1	A	282	VAL

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Mol	Chain	Res	Type
1	A	287	ILE
1	A	298	LYS
1	A	306	VAL
1	A	319	ARG
1	A	370	ILE
1	A	372	VAL
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	379	LEU
1	A	381	VAL
1	A	388	GLN
1	A	391	GLN
1	A	395	CYS
1	A	472	ARG
1	A	477	ARG
1	A	515	SER
1	A	520	LEU
1	A	525	HIS
1	A	527	ILE
1	A	549	ASN
1	A	550	GLN
1	A	554	GLN
1	A	574	LEU
1	A	575	LEU
1	A	583	LEU
1	A	587	LYS
1	A	603	ILE
1	A	610	LEU
1	A	626	LEU
1	A	638	GLU
1	A	647	LYS
1	A	650	SER
1	A	662	GLN
1	A	682	LEU
1	A	701	SER
1	A	717	LEU
1	A	728	MET
1	A	749	ILE
1	A	756	LYS
1	A	760	SER
1	A	761	SER

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Mol	Chain	Res	Type
1	A	763	VAL
1	A	764	ILE
1	A	767	LEU
1	A	770	LYS
1	A	778	GLN
1	A	779	LEU
1	A	784	ARG
1	A	823	LEU
1	A	825	ASN
1	A	828	ILE
1	A	838	LEU
1	A	840	GLN
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	850	ILE
1	A	865	LEU
1	A	871	SER
1	A	875	LYS
1	A	878	MET
1	A	883	LYS
1	A	887	THR
1	A	888	ILE
1	A	899	THR
1	A	903	LYS
1	A	907	LEU
1	A	912	LYS
1	A	915	SER
1	A	926	GLU
1	A	927	ARG
1	A	946	ASP
1	A	960	LEU
1	A	967	HIS
1	A	988	THR
1	A	1002	THR
1	A	1008	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1044	SER

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Mol	Chain	Res	Type
1	A	1046	GLU
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1077	ASP
1	A	1081	THR
1	A	1085	ASN
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	291	GLN
1	A	389	HIS
1	A	391	GLN
1	A	396	GLN
1	A	550	GLN
1	A	600	GLN
1	A	609	GLN
1	A	634	ASN
1	A	646	GLN
1	A	743	GLN
1	A	766	GLN
1	A	840	GLN
1	A	908	ASN
1	A	951	ASN
1	A	1083	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

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	JZW	A	1	-	37,38,38	2.37	9 (24%)	49,55,55	2.58	18 (36%)

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	JZW	A	1	-	-	6/20/38/38	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	JZW	S2-N5	-6.21	1.53	1.63
2	A	1	JZW	C3-C1	-6.07	1.33	1.42
2	A	1	JZW	C3-C4	-6.03	1.34	1.40
2	A	1	JZW	C5-N1	4.55	1.44	1.34
2	A	1	JZW	C5-N2	4.42	1.44	1.34
2	A	1	JZW	C17-S2	-3.78	1.67	1.75
2	A	1	JZW	C2-S1	-3.55	1.67	1.74
2	A	1	JZW	C4-S1	-3.34	1.67	1.74
2	A	1	JZW	C15-N5	-2.42	1.45	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	JZW	O3-S2-O2	-7.06	107.90	118.46
2	A	1	JZW	C12-N4-C16	6.30	120.95	111.14
2	A	1	JZW	C17-S2-N5	5.84	114.14	107.27
2	A	1	JZW	N2-C5-N1	-5.05	116.83	125.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	JZW	C15-C16-N4	-4.98	100.61	110.65
2	A	1	JZW	C14-N5-S2	3.95	123.06	116.71
2	A	1	JZW	C15-N5-C14	3.81	116.50	112.12
2	A	1	JZW	C2-C12-N4	3.65	119.91	112.46
2	A	1	JZW	C4-C6-N2	-3.63	118.00	122.33
2	A	1	JZW	C4-S1-C2	-3.38	90.07	91.92
2	A	1	JZW	C7-C5-N1	3.24	122.75	117.40
2	A	1	JZW	C16-N4-C13	2.61	114.46	108.84
2	A	1	JZW	C1-C3-N1	-2.60	122.16	129.98
2	A	1	JZW	C6-N2-C5	2.56	121.92	115.92
2	A	1	JZW	C12-N4-C13	2.48	115.00	111.14
2	A	1	JZW	C8-N3-C6	2.33	126.82	118.92
2	A	1	JZW	C9-C8-N3	-2.11	105.94	109.93
2	A	1	JZW	O1-C9-C8	-2.04	107.38	111.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	JZW	C14-N5-S2-O2
2	A	1	JZW	C14-N5-S2-O3
2	A	1	JZW	C15-N5-S2-O3
2	A	1	JZW	C14-N5-S2-C17
2	A	1	JZW	C15-N5-S2-C17
2	A	1	JZW	C2-C12-N4-C16

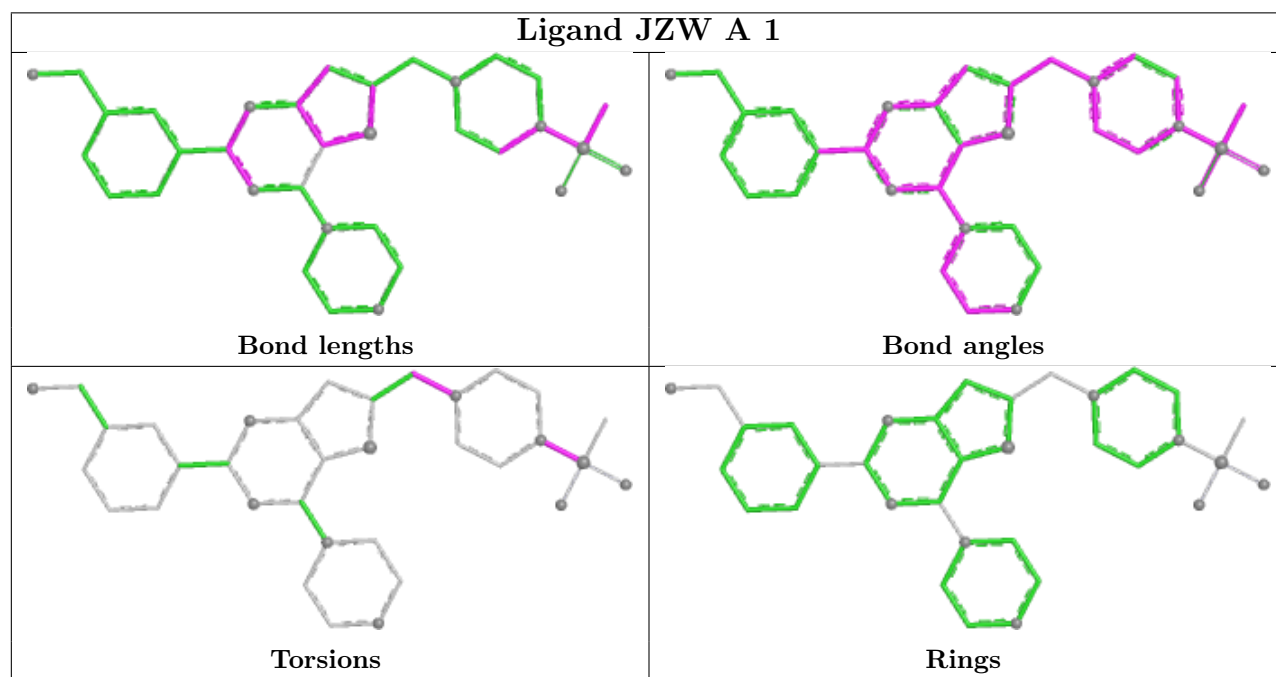
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	JZW	2	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, 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	841/960 (87%)	-0.38	3 (0%) 88 76	27, 40, 47, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	5.4
1	A	376	ASN	2.2
1	A	1089	HIS	2.1

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.

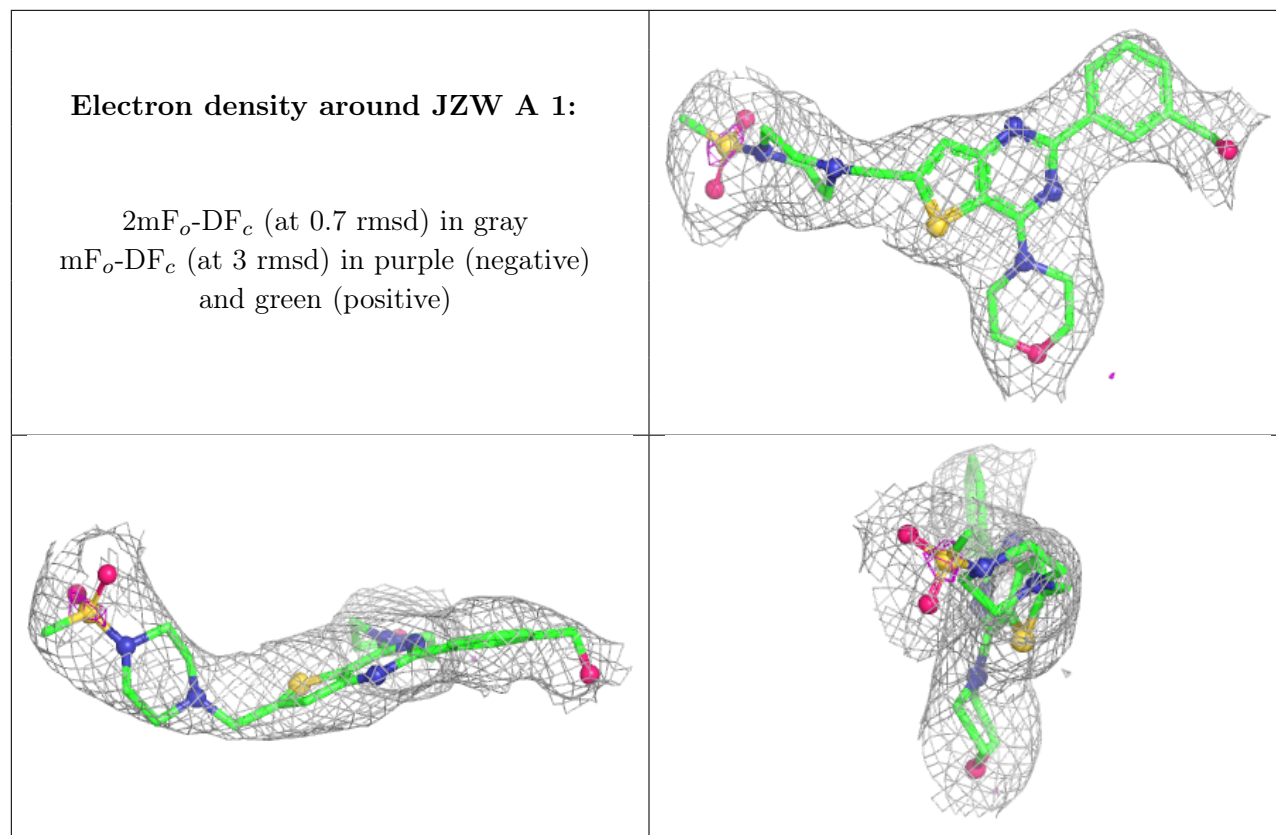
6.4 Ligands [i](#)

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	JZW	A	1	34/34	0.92	0.09	77,82,85,88	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 ⓘ

There are no such residues in this entry.