Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 05:17 AM EDT

PDB ID	:	3L13
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 (i) 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 (i)) were used in the production of this report:

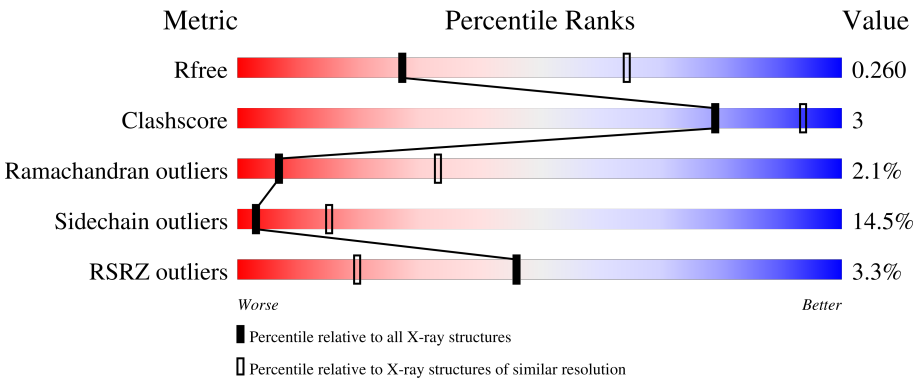
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	3% 68% 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.

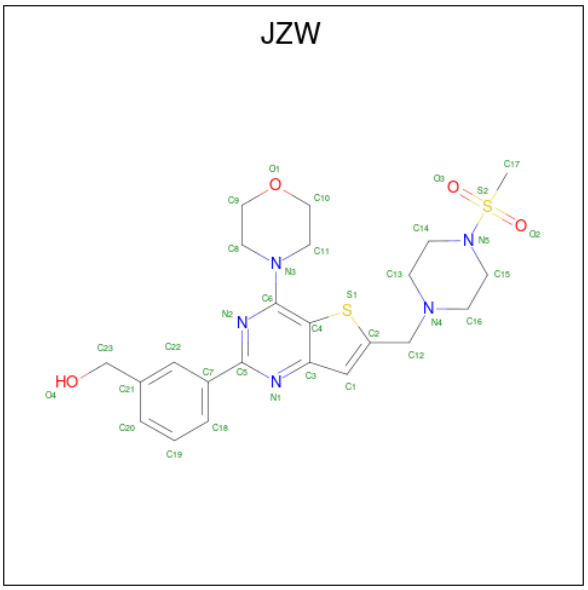
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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

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 (three-letter code: JZW) (formula: $C_{23}H_{29}N_5O_4S_2$).



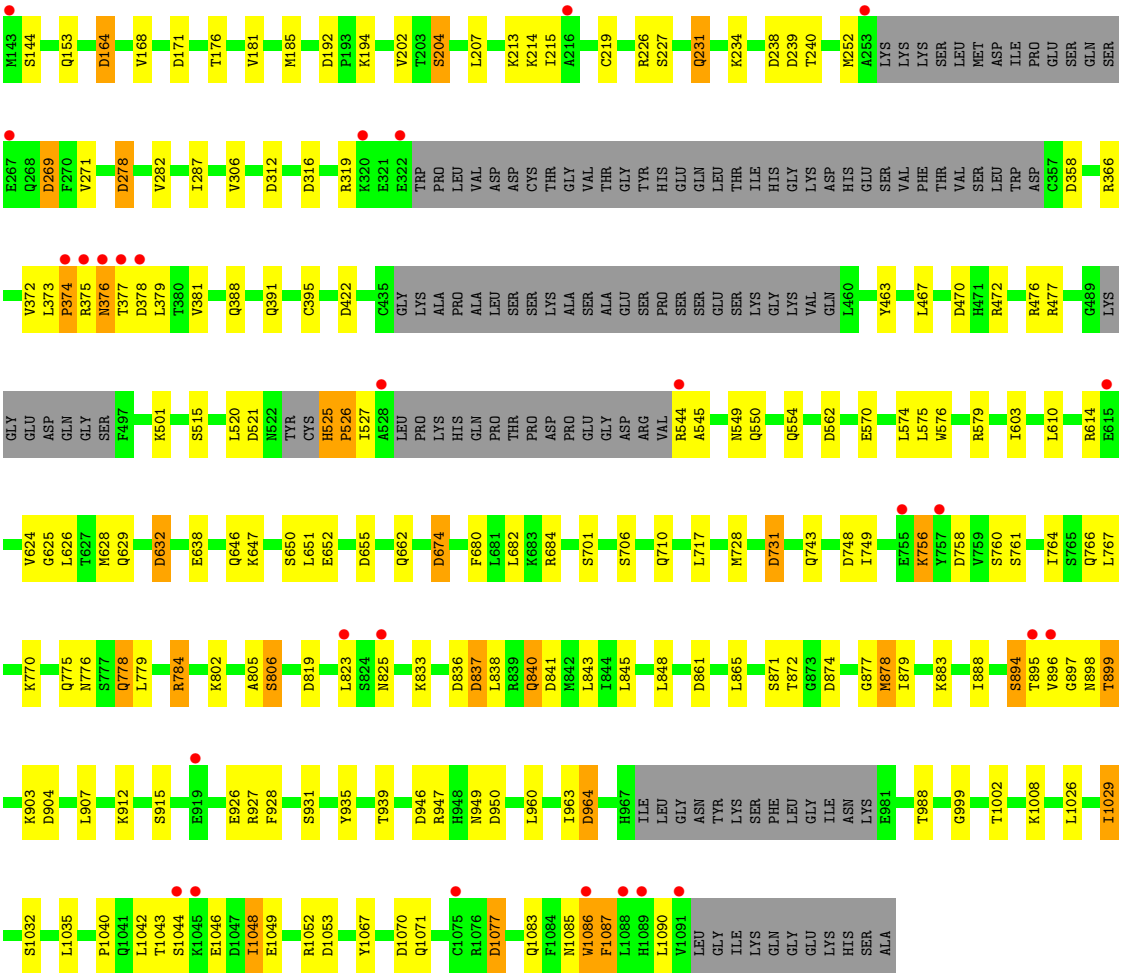
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	34	23	5	4	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain A: 3% 68% 17% • 12%



4 Data and refinement statistics (i)

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 19.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.00) 99.9 (19.92-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.28 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	0/6958	0.73	29/9412 (0.3%)

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.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	192	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	964	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	841	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	874	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	1070	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	819	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	1077	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	632	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	836	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	358	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	837	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	674	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	269	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	950	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	278	ASP	CB-CG-OD2	5.36	123.12	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	164	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	758	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	422	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	521	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	904	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	312	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	1053	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	861	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	238	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	378	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	562	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	748	ASP	CB-CG-OD2	5.11	122.90	118.30

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	38	0
2	A	34	0	29	2	0
All	All	6846	0	6872	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:204:SER:OG	1:A:652:GLU:OE2	1.95	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:470:ASP:C	1:A:470:ASP:OD1	2.56	0.44
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.50	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:878:MET:C	1:A:879:ILE:HG13	2.38	0.42
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.49	0.42
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:632:ASP:C	1:A:632:ASP:OD1	2.58	0.42
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	2.02	0.41
1:A:928:PHE:HA	1:A:931:SER:HG	1.85	0.41
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%)	7 33

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
1	A	999	GLY
1	A	545	ALA
1	A	526	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	754/858 (88%)	645 (86%)	109 (14%)	3 15

All (109) 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	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	269	ASP
1	A	271	VAL
1	A	278	ASP
1	A	282	VAL
1	A	287	ILE
1	A	306	VAL
1	A	319	ARG
1	A	366	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	525	HIS
1	A	527	ILE
1	A	544	ARG
1	A	549	ASN
1	A	550	GLN
1	A	554	GLN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
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	731	ASP
1	A	749	ILE
1	A	756	LYS
1	A	760	SER
1	A	761	SER
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	833	LYS
1	A	838	LEU
1	A	840	GLN
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	871	SER
1	A	878	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	883	LYS
1	A	888	ILE
1	A	894	SER
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	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
1	A	1046	GLU
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1077	ASP
1	A	1085	ASN
1	A	1086	TRP
1	A	1090	LEU

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	231	GLN
1	A	550	GLN
1	A	609	GLN
1	A	646	GLN
1	A	743	GLN
1	A	766	GLN
1	A	778	GLN
1	A	825	ASN
1	A	908	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1083	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	JZW	A	1	-	35,38,38	2.15	9 (25%)	40,55,55	2.69	14 (35%)

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	-	-	6/15/38/38	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	-7.76	1.53	1.63
2	A	1	JZW	C5-N1	4.77	1.44	1.35
2	A	1	JZW	C5-N2	3.86	1.44	1.36
2	A	1	JZW	C2-S1	-3.72	1.67	1.74
2	A	1	JZW	C17-S2	-3.46	1.67	1.75
2	A	1	JZW	C6-N2	2.59	1.33	1.30
2	A	1	JZW	C3-C4	-2.57	1.34	1.42
2	A	1	JZW	C15-N5	-2.38	1.45	1.47
2	A	1	JZW	C1-C3	-2.22	1.33	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	JZW	C17-S2-N5	7.83	114.14	107.36
2	A	1	JZW	O3-S2-O2	-7.50	107.90	118.59
2	A	1	JZW	C14-N5-S2	5.49	123.06	116.30
2	A	1	JZW	C15-C16-N4	-4.89	100.61	110.64
2	A	1	JZW	C12-N4-C16	4.44	120.95	111.06
2	A	1	JZW	C15-N5-C14	3.92	116.50	112.17
2	A	1	JZW	C2-C12-N4	3.38	119.91	112.78
2	A	1	JZW	C6-N2-C5	3.20	121.92	117.29
2	A	1	JZW	C8-N3-C6	2.83	126.82	118.73
2	A	1	JZW	C16-N4-C13	2.50	114.46	108.83
2	A	1	JZW	C4-C6-N3	2.42	126.39	121.57
2	A	1	JZW	C9-C8-N3	-2.21	105.94	110.02
2	A	1	JZW	C16-C15-N5	-2.17	107.25	108.91
2	A	1	JZW	O1-C9-C8	-2.00	107.38	111.80

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

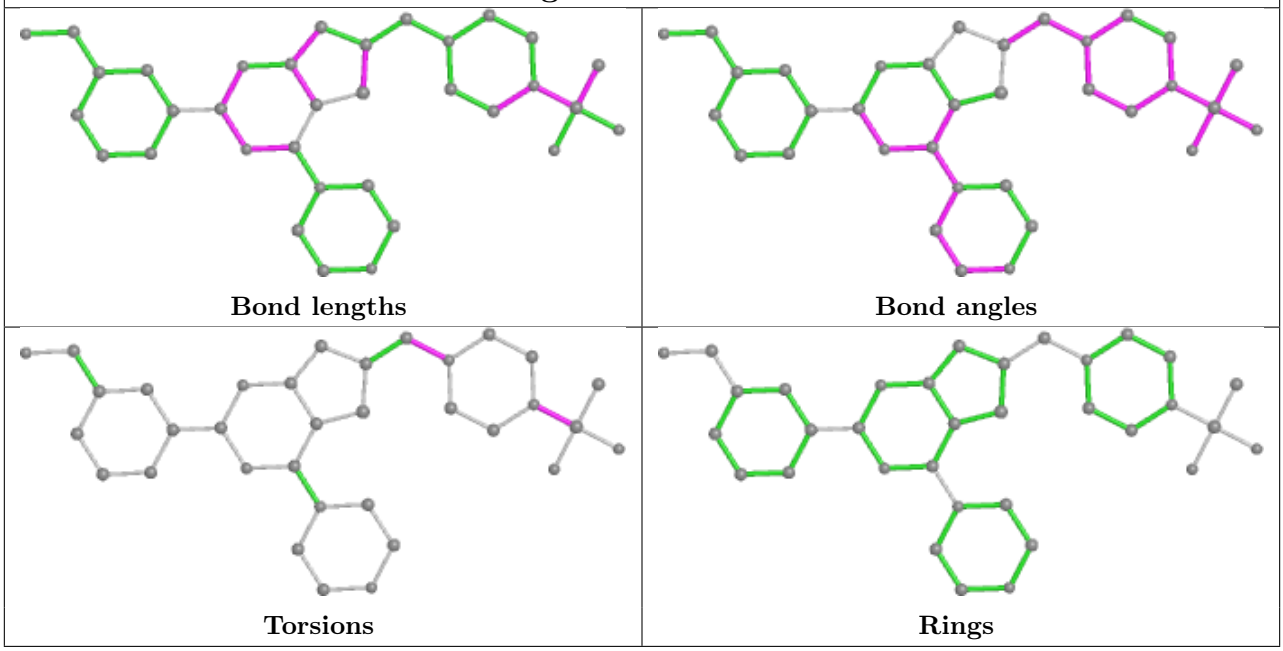
There are no ring outliers.

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 then 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.

Ligand JZW A 1



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%)	-0.18	28 (3%) 46 20	27, 40, 47, 61	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASN	7.8
1	A	1044	SER	7.4
1	A	322	GLU	4.8
1	A	253	ALA	4.7
1	A	895	THR	4.3
1	A	755	GLU	4.1
1	A	377	THR	4.0
1	A	143	MET	3.9
1	A	528	ALA	3.6
1	A	1088	LEU	3.4
1	A	374	PRO	3.2
1	A	544	ARG	3.2
1	A	1089	HIS	3.1
1	A	823	LEU	3.1
1	A	615	GLU	3.1
1	A	375	ARG	2.8
1	A	1075	CYS	2.8
1	A	1086	TRP	2.7
1	A	1045	LYS	2.7
1	A	919	GLU	2.6
1	A	1091	VAL	2.4
1	A	896	VAL	2.4
1	A	825	ASN	2.3
1	A	267	GLU	2.2
1	A	757	TYR	2.2
1	A	216	ALA	2.2
1	A	320	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

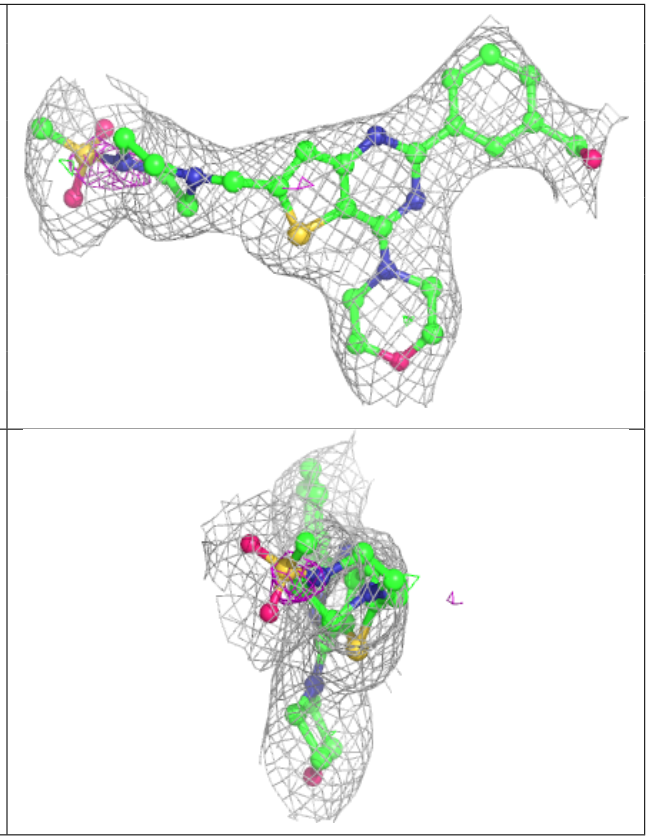
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.89	0.20	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.

Electron density around JZW A 1:

$2mF_o$-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.