Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:07 PM EDT

PDB ID	:	3L16
Title	:	Discovery of (thienopyrimidin-2-yl)aminopyrimidines as Potent, Selective, and Orally Available Pan-PI3-Kinase and Dual Pan-PI3-Kinase/mTOR Inhibitors for the Treatment of Cancer
Authors	:	Murray, J.M.; Wiesmann, C.
Deposited on	:	2009-12-10
Resolution	:	2.90 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:

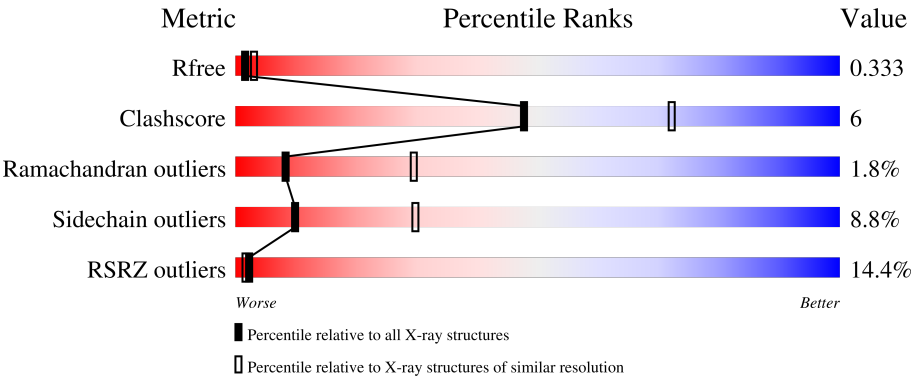
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	966	13% 67% 17% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6845 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.

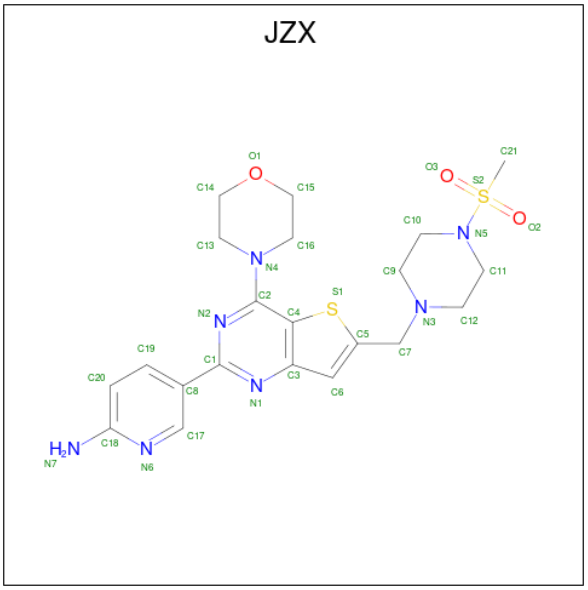
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 5-(6-{[4-(methylsulfonyl)piperazin-1-yl]methyl}-4-morpholin-4-ylthieno[3,2-d] pyrimidin-2-yl)pyridin-2-amine (three-letter code: JZX) (formula: $C_{21}H_{27}N_7O_3S_2$).



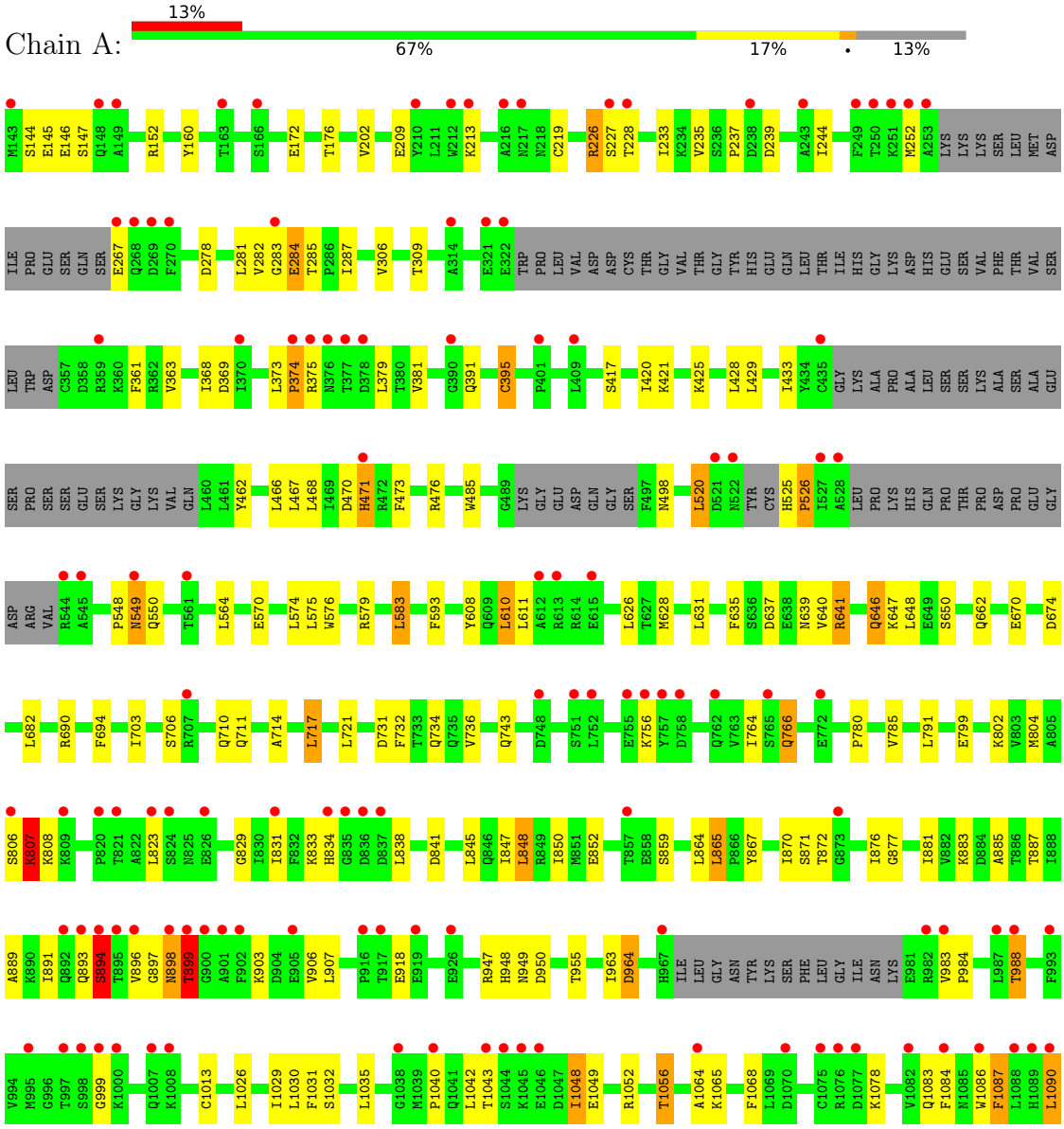
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	21	7	3	2		

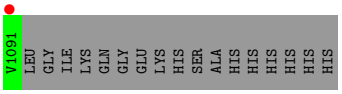
3 Residue-property plots (i)

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:




V1091
LEU
GLY
ILE
LYS
GLN
GLY
GLU
LYS
HIS
SER
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.63Å 67.39Å 106.67Å 90.00° 96.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.90) 98.1 (19.75-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.99 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.238 , 0.295 0.298 , 0.333	Depositor DCC
R_{free} test set	1125 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 94.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6845	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

5.1 Standard geometry

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

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	0.48	0/6958	0.63	1/9412 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	641	ARG	NE-CZ-NH1	-5.91	117.35	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	Peptide
1	A	807	LYS	Peptide

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	6812	0	6843	82	0
2	A	33	0	27	2	0
All	All	6845	0	6870	83	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 6.

All (83) 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:548:PRO:O	1:A:550:GLN:N	2.20	0.73
1:A:395:CYS:SG	1:A:417:SER:OG	2.46	0.73
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.28	0.68
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.77	0.66
1:A:425:LYS:NZ	1:A:473:PHE:CZ	2.56	0.65
1:A:635:PHE:O	1:A:641:ARG:HD2	1.99	0.63
2:A:1:JZX:S1	2:A:1:JZX:H16A	2.38	0.63
1:A:1056:THR:O	1:A:1056:THR:HG23	1.99	0.63
1:A:428:LEU:HD23	1:A:467:LEU:HD23	1.81	0.62
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.48	0.61
1:A:706:SER:O	1:A:710:GLN:HB3	2.02	0.59
1:A:1030:LEU:O	1:A:1031:PHE:C	2.39	0.59
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.02	0.58
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.68	0.58
1:A:806:SER:OG	1:A:807:LYS:N	2.37	0.58
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.86	0.57
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.86	0.57
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.87	0.56
1:A:576:TRP:O	1:A:579:ARG:HD3	2.04	0.55
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.88	0.55
1:A:897:GLY:O	1:A:899:THR:N	2.40	0.55
1:A:847:ILE:O	1:A:850:ILE:N	2.41	0.53
1:A:802:LYS:HE2	2:A:1:JZX:O2	2.08	0.52
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.09	0.52
1:A:1056:THR:O	1:A:1056:THR:CG2	2.58	0.51
1:A:233:ILE:HG22	1:A:235:VAL:HG23	1.94	0.50
1:A:373:LEU:N	1:A:374:PRO:CD	2.75	0.49
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.42	0.49
1:A:703:ILE:HD11	1:A:714:ALA:HA	1.94	0.49
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.43	0.49
1:A:628:MET:O	1:A:631:LEU:N	2.41	0.49
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:PHE:O	1:A:736:VAL:HG23	2.14	0.48
1:A:1086:TRP:O	1:A:1087:PHE:HB2	2.14	0.47
1:A:947:ARG:NH2	1:A:964:ASP:O	2.47	0.47
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.95	0.47
1:A:1086:TRP:CH2	1:A:1090:LEU:HD11	2.50	0.47
1:A:498:ASN:OD1	1:A:498:ASN:C	2.53	0.47
1:A:799:GLU:H	1:A:799:GLU:CD	2.17	0.47
1:A:239:ASP:HB3	1:A:244:ILE:HG23	1.97	0.47
1:A:641:ARG:NE	1:A:670:GLU:OE1	2.41	0.46
1:A:363:VAL:HG13	1:A:363:VAL:O	2.16	0.46
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.98	0.46
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.98	0.45
1:A:887:THR:HG22	1:A:889:ALA:N	2.31	0.45
1:A:893:GLN:O	1:A:894:SER:C	2.54	0.45
1:A:283:GLY:O	1:A:285:THR:N	2.49	0.45
1:A:425:LYS:NZ	1:A:473:PHE:CE2	2.80	0.45
1:A:947:ARG:NH2	1:A:963:ILE:O	2.49	0.45
1:A:1086:TRP:O	1:A:1087:PHE:CB	2.64	0.45
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.99	0.44
1:A:608:TYR:OH	1:A:637:ASP:OD2	2.29	0.44
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.52	0.44
1:A:690:ARG:O	1:A:694:PHE:HD1	2.01	0.44
1:A:284:GLU:HA	1:A:284:GLU:OE1	2.18	0.43
1:A:766:GLN:HE21	1:A:766:GLN:HB3	1.61	0.43
1:A:646:GLN:HE21	1:A:646:GLN:HB3	1.69	0.43
1:A:785:VAL:HG23	1:A:791:LEU:O	2.19	0.43
1:A:834:HIS:HB2	1:A:876:ILE:HD12	2.01	0.43
1:A:1064:ALA:O	1:A:1065:LYS:C	2.57	0.43
1:A:891:ILE:O	1:A:906:VAL:HG11	2.19	0.43
1:A:1030:LEU:O	1:A:1032:SER:N	2.52	0.43
1:A:470:ASP:OD1	1:A:470:ASP:C	2.57	0.43
1:A:226:ARG:O	1:A:228:THR:N	2.52	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.00	0.42
1:A:829:GLY:HA3	1:A:881:ILE:HB	2.01	0.42
1:A:429:LEU:HB2	1:A:468:LEU:HD21	2.00	0.42
1:A:717:LEU:HD22	1:A:721:LEU:HG	2.01	0.42
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.54	0.42
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	2.01	0.42
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.55	0.42
1:A:144:SER:HB3	1:A:147:SER:HB2	2.02	0.42
1:A:865:LEU:HD12	1:A:865:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:HA	1:A:287:ILE:HD11	2.01	0.41
1:A:983:VAL:HG22	1:A:984:PRO:HD2	2.02	0.41
1:A:462:TYR:HA	1:A:485:TRP:O	2.20	0.41
1:A:639:ASN:O	1:A:640:VAL:C	2.56	0.41
1:A:885:ALA:HA	1:A:955:THR:HA	2.03	0.41
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.51	0.41
1:A:160:TYR:OH	1:A:711:GLN:HG2	2.20	0.40
1:A:847:ILE:O	1:A:848:LEU:C	2.59	0.40
1:A:648:LEU:O	1:A:650:SER:N	2.55	0.40
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.57	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	825/966 (85%)	721 (87%)	89 (11%)	15 (2%)	8 29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	A	894	SER
1	A	898	ASN
1	A	1040	PRO
1	A	1087	PHE
1	A	284	GLU
1	A	471	HIS
1	A	899	THR
1	A	964	ASP
1	A	227	SER
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	848	LEU
1	A	526	PRO
1	A	896	VAL
1	A	999	GLY

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	754/864 (87%)	688 (91%)	66 (9%)	10 30

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	152	ARG
1	A	202	VAL
1	A	213	LYS
1	A	219	CYS
1	A	226	ARG
1	A	252	MET
1	A	267	GLU
1	A	278	ASP
1	A	281	LEU
1	A	282	VAL
1	A	306	VAL
1	A	309	THR
1	A	369	ASP
1	A	375	ARG
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	395	CYS
1	A	421	LYS
1	A	520	LEU

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Mol	Chain	Res	Type
1	A	549	ASN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	583	LEU
1	A	610	LEU
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	662	GLN
1	A	682	LEU
1	A	717	LEU
1	A	731	ASP
1	A	764	ILE
1	A	766	GLN
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	841	ASP
1	A	845	LEU
1	A	865	LEU
1	A	870	ILE
1	A	871	SER
1	A	883	LYS
1	A	894	SER
1	A	898	ASN
1	A	899	THR
1	A	903	LYS
1	A	907	LEU
1	A	918	GLU
1	A	988	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1042	LEU
1	A	1043	THR
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1056	THR
1	A	1078	LYS

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Mol	Chain	Res	Type
1	A	1084	PHE
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	291	GLN
1	A	391	GLN
1	A	646	GLN
1	A	705	GLN
1	A	743	GLN
1	A	766	GLN
1	A	769	GLN
1	A	775	GLN
1	A	825	ASN
1	A	834	HIS
1	A	898	ASN
1	A	1007	GLN
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	JZX	A	1	-	34,37,37	1.66	5 (14%)	38,54,54	2.31	12 (31%)

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	JZX	A	1	-	-	1/13/36/36	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	JZX	C2-N2	4.94	1.35	1.30
2	A	1	JZX	C6-C5	-3.91	1.27	1.37
2	A	1	JZX	C21-S2	-3.66	1.67	1.75
2	A	1	JZX	C5-S1	-3.26	1.68	1.74
2	A	1	JZX	C6-C3	-3.11	1.29	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	JZX	O3-S2-O2	-5.96	110.09	118.59
2	A	1	JZX	C5-C7-N3	5.44	124.24	112.78
2	A	1	JZX	C21-S2-N5	5.14	111.81	107.36
2	A	1	JZX	C11-N5-S2	-4.46	110.81	116.30
2	A	1	JZX	C2-N2-C1	3.63	122.55	117.29
2	A	1	JZX	C10-N5-S2	-3.48	112.03	116.30
2	A	1	JZX	C15-C16-N4	-3.30	103.93	110.02
2	A	1	JZX	O2-S2-N5	2.98	109.54	107.03
2	A	1	JZX	C12-N3-C9	2.43	114.30	108.83
2	A	1	JZX	C4-C2-N2	-2.40	116.58	122.60
2	A	1	JZX	C12-C11-N5	-2.27	107.18	108.91
2	A	1	JZX	C8-C17-N6	-2.12	120.09	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	JZX	C11-N5-S2-O3

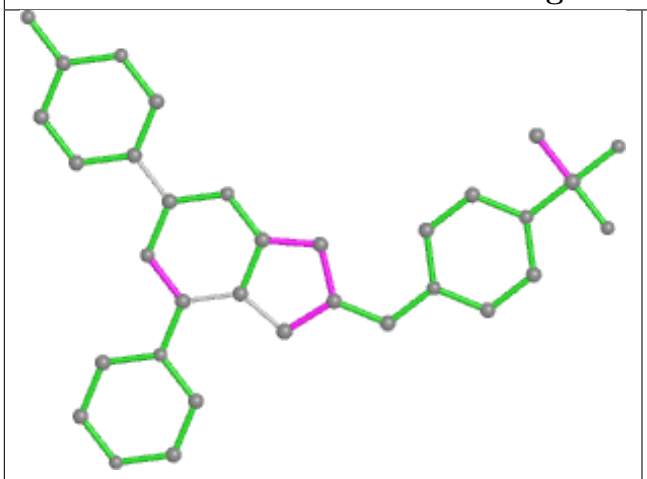
There are no ring outliers.

1 monomer is involved in 2 short contacts:

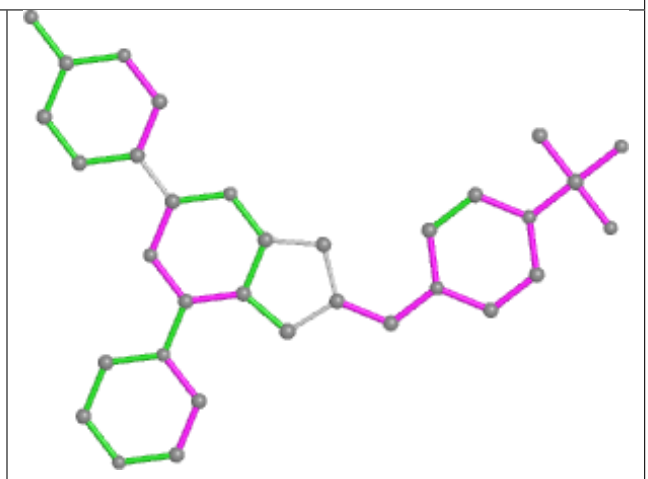
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	JZX	2	0

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.

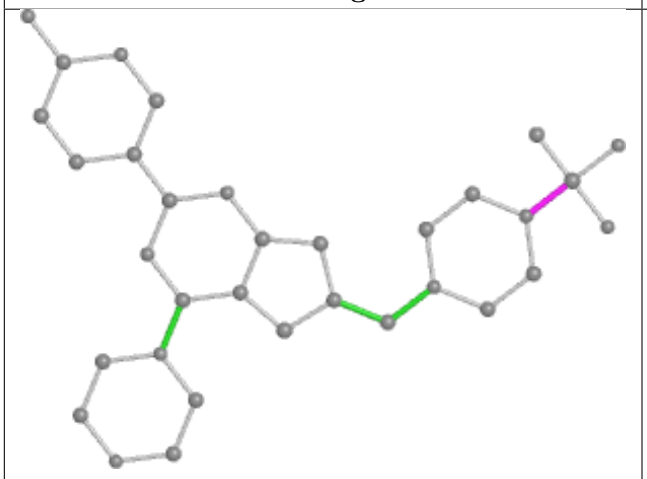
Ligand JZX A 1



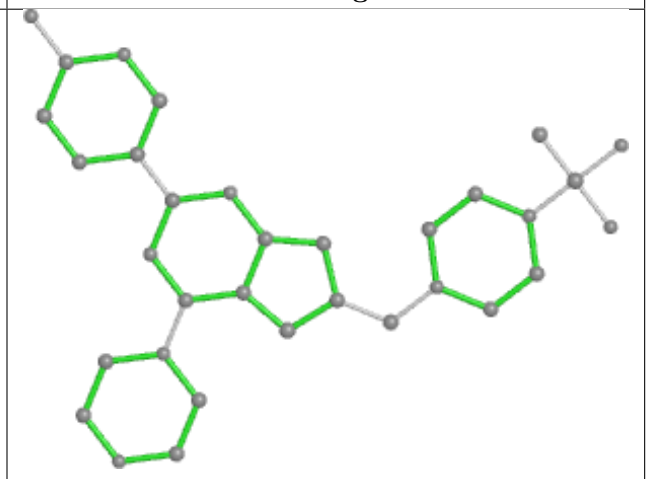
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	841/966 (87%)	0.97	121 (14%) 2 2	11, 71, 109, 143	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	13.7
1	A	322	GLU	12.1
1	A	253	ALA	10.8
1	A	376	ASN	9.1
1	A	1086	TRP	8.8
1	A	267	GLU	8.7
1	A	216	ALA	7.0
1	A	143	MET	6.8
1	A	896	VAL	6.4
1	A	1088	LEU	6.3
1	A	378	ASP	6.2
1	A	1077	ASP	6.2
1	A	823	LEU	5.9
1	A	321	GLU	5.7
1	A	374	PRO	5.7
1	A	268	GLN	5.7
1	A	1091	VAL	5.5
1	A	528	ALA	5.5
1	A	269	ASP	5.5
1	A	895	THR	5.4
1	A	835	GLY	5.4
1	A	983	VAL	5.3
1	A	1043	THR	5.0
1	A	857	THR	4.8
1	A	359	ARG	4.8
1	A	824	SER	4.7
1	A	212	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1075	CYS	4.6
1	A	756	LYS	4.4
1	A	375	ARG	4.4
1	A	1089	HIS	4.3
1	A	213	LYS	4.2
1	A	998	SER	4.2
1	A	148	GLN	4.2
1	A	894	SER	4.1
1	A	919	GLU	4.1
1	A	252	MET	4.0
1	A	757	TYR	4.0
1	A	905	GLU	3.8
1	A	1045	LYS	3.8
1	A	1000	LYS	3.7
1	A	1046	GLU	3.7
1	A	1064	ALA	3.6
1	A	999	GLY	3.6
1	A	916	PRO	3.6
1	A	522	ASN	3.5
1	A	751	SER	3.4
1	A	163	THR	3.4
1	A	987	LEU	3.4
1	A	967	HIS	3.4
1	A	613	ARG	3.4
1	A	612	ALA	3.3
1	A	270	PHE	3.2
1	A	762	GLN	3.2
1	A	544	ARG	3.2
1	A	251	LYS	3.2
1	A	765	SER	3.2
1	A	1007	GLN	3.2
1	A	758	ASP	3.1
1	A	435	CYS	3.1
1	A	982	ARG	3.1
1	A	166	SER	3.0
1	A	527	ILE	2.9
1	A	926	GLU	2.9
1	A	227	SER	2.9
1	A	1090	LEU	2.9
1	A	917	THR	2.9
1	A	377	THR	2.9
1	A	615	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1040	PRO	2.8
1	A	250	THR	2.8
1	A	1076	ARG	2.8
1	A	809	LYS	2.7
1	A	748	ASP	2.7
1	A	820	PRO	2.7
1	A	772	GLU	2.7
1	A	993	PHE	2.6
1	A	898	ASN	2.6
1	A	902	PHE	2.6
1	A	149	ALA	2.6
1	A	549	ASN	2.5
1	A	561	THR	2.5
1	A	806	SER	2.5
1	A	409	LEU	2.5
1	A	899	THR	2.4
1	A	988	THR	2.4
1	A	707	ARG	2.4
1	A	752	LEU	2.4
1	A	900	GLY	2.4
1	A	217	ASN	2.4
1	A	1070	ASP	2.4
1	A	210	TYR	2.4
1	A	1084	PHE	2.3
1	A	893	GLN	2.3
1	A	901	ALA	2.3
1	A	545	ALA	2.3
1	A	238	ASP	2.3
1	A	1008	LYS	2.3
1	A	243	ALA	2.2
1	A	826	GLU	2.2
1	A	370	ILE	2.2
1	A	997	THR	2.2
1	A	390	GLY	2.2
1	A	283	GLY	2.2
1	A	401	PRO	2.2
1	A	1038	GLY	2.1
1	A	249	PHE	2.1
1	A	228	THR	2.1
1	A	1082	VAL	2.1
1	A	831	ILE	2.1
1	A	834	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	821	THR	2.1
1	A	995	MET	2.1
1	A	836	ASP	2.1
1	A	892	GLN	2.1
1	A	873	GLY	2.1
1	A	521	ASP	2.0
1	A	314	ALA	2.0
1	A	755	GLU	2.0
1	A	471	HIS	2.0
1	A	837	ASP	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)

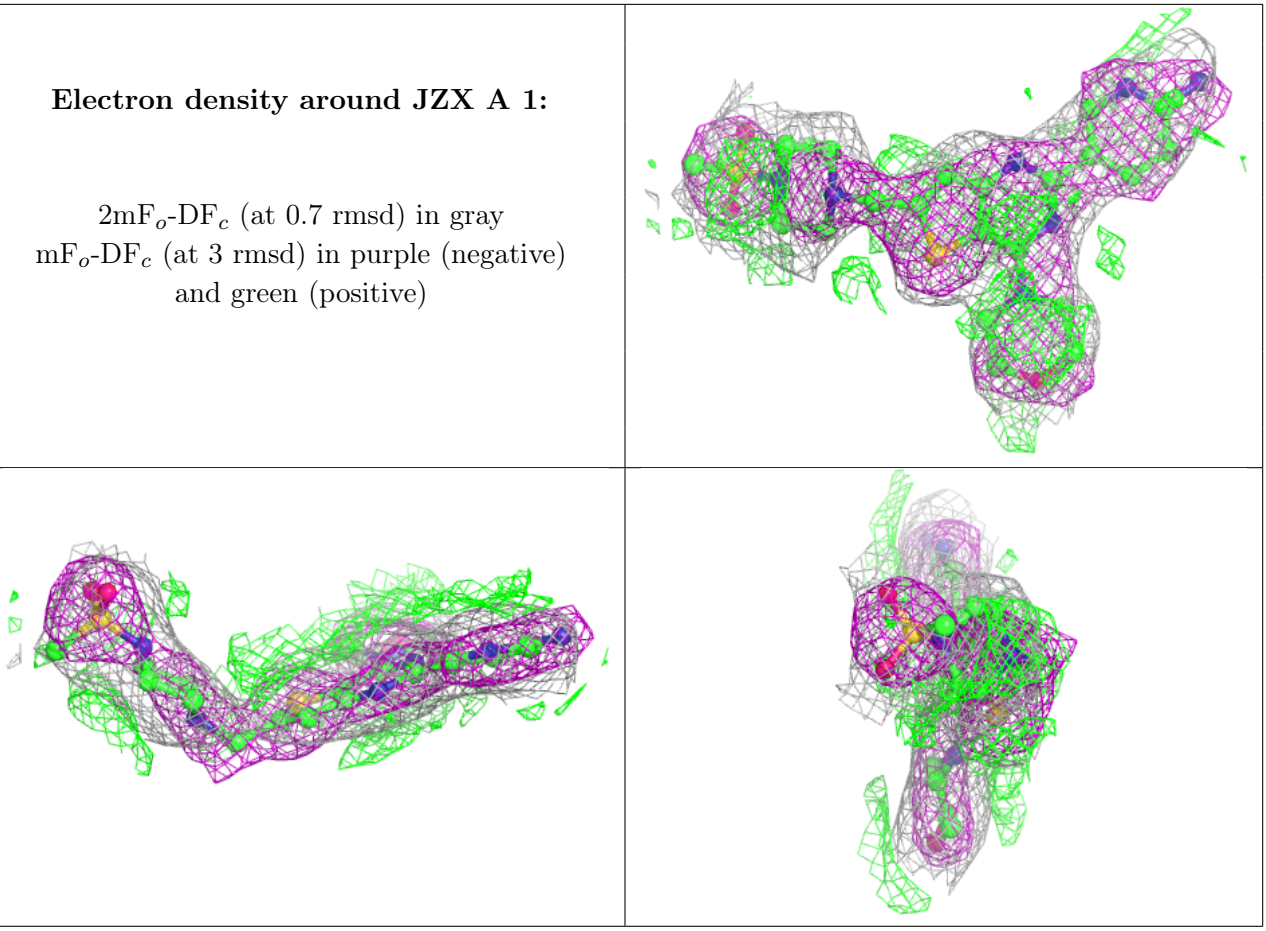
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	JZX	A	1	33/33	0.90	0.34	44,47,70,71	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 JZX 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

There are no such residues in this entry.