



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:27 am BST

PDB ID : 3L17
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 : 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 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 : 2.11
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) : 2.11

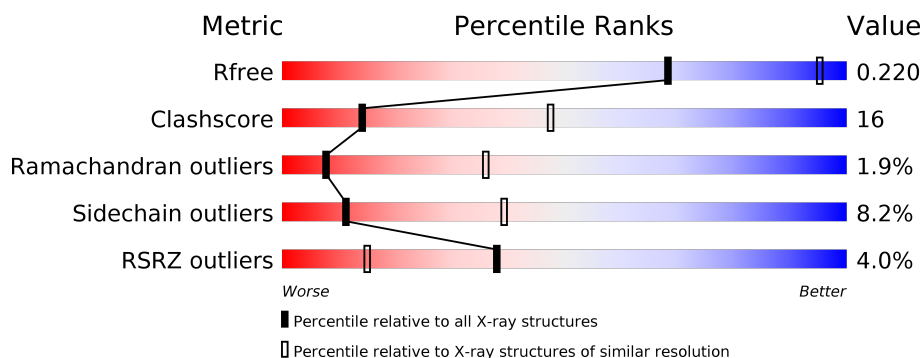
1 Overall quality at a glance

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}	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 on 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	966	<div> <div>4%</div> <div>57%</div> <div>26%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6854 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.

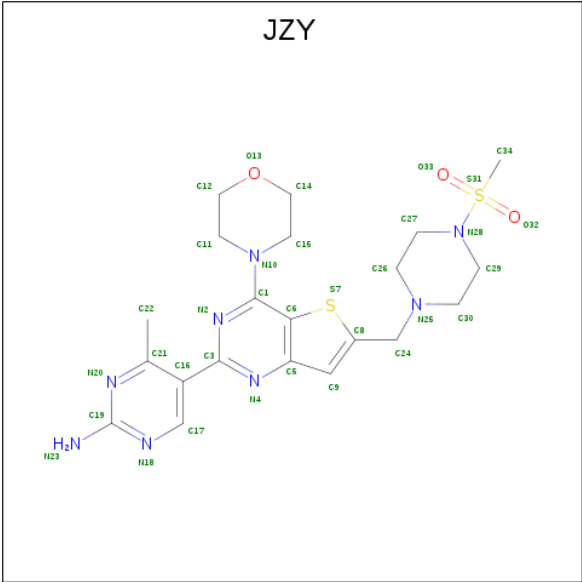
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6820	4376	1164	1244	36			

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

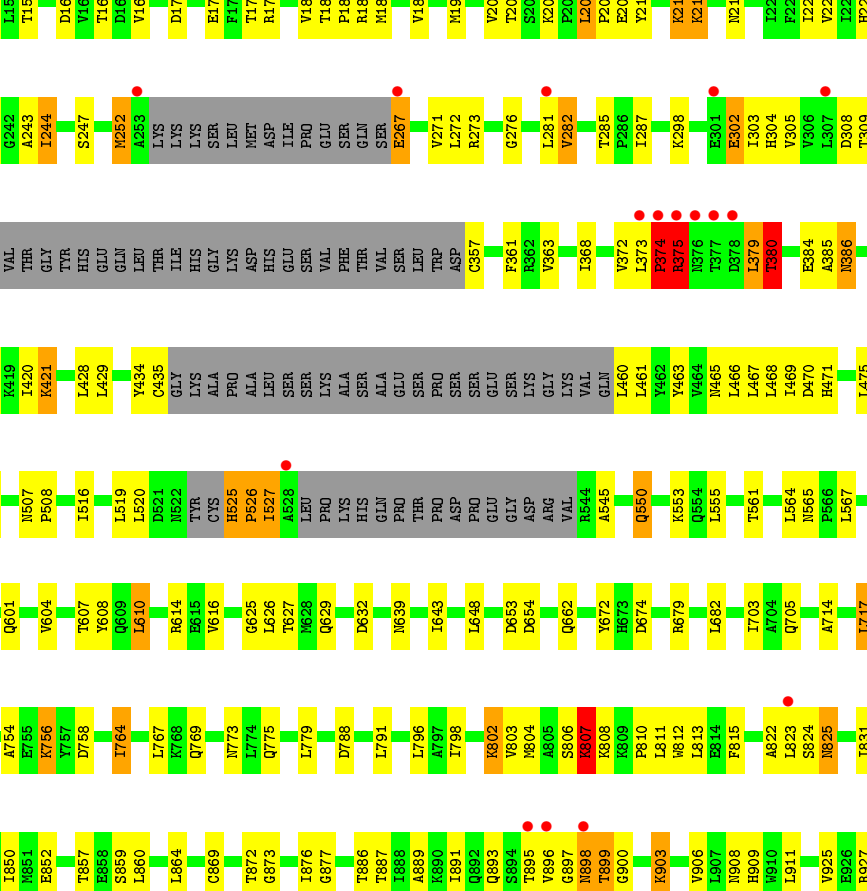
- Molecule 2 is 4-methyl-5-(6-{[4-(methylsulfonyl)piperazin-1-yl]methyl}-4-morpholin-4-ylthieno[3,2-d]pyrimidin-2-yl)pyrimidin-2-amine (three-letter code: JZY) (formula: C₂₁H₂₈N₈O₃S₂).



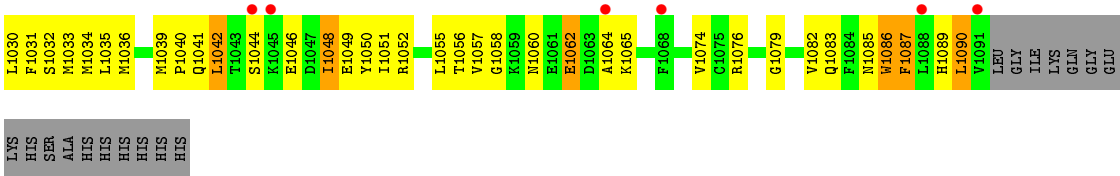
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	21	8	3	2		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

- Chain A: 



The visualization displays the distribution of Chain A across various amino acid codes. The bar chart indicates the following distribution: 4% (red), 57% (green), 26% (yellow), and 13% (grey). The amino acid codes are organized into rows and columns, with some cells containing multiple codes. The bar chart is positioned below the grid, with each column of the grid corresponding to a segment of the bar chart.



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.09 Å 67.73 Å 107.45 Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	45.18 – 3.00 41.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.18-3.00) 98.0 (41.19-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.271 0.224 , 0.220	Depositor DCC
R_{free} test set	1051 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	91.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 92.3	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	0.94	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: JZY

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	0.58	0/6966	0.66	0/9422

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	1086	TRP	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	6820	0	6855	213	0
2	A	34	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6854	0	6883	214	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 16.

All (214) 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:583:LEU:HD22	1:A:610:LEU:HD22	1.21	1.17
1:A:469:ILE:HD13	1:A:527:ILE:HD11	1.29	1.11
1:A:583:LEU:HD22	1:A:610:LEU:CD2	1.94	0.97
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.58	0.85
1:A:1055:LEU:O	1:A:1056:THR:HG22	1.77	0.83
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.60	0.83
1:A:469:ILE:HD13	1:A:527:ILE:CD1	2.07	0.83
1:A:181:VAL:HG12	1:A:185:MET:CE	2.12	0.79
1:A:583:LEU:CD2	1:A:610:LEU:HD22	2.07	0.79
1:A:898:ASN:O	1:A:900:GLY:N	2.17	0.78
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.66	0.77
1:A:576:TRP:O	1:A:579:ARG:HD3	1.85	0.77
1:A:202:VAL:HG13	1:A:285:THR:HG21	1.68	0.76
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.50	0.76
1:A:276:GLY:HA2	1:A:822:ALA:HB2	1.66	0.76
1:A:798:ILE:HD12	1:A:798:ILE:H	1.51	0.73
1:A:895:THR:OG1	1:A:903:LYS:NZ	2.16	0.73
1:A:1056:THR:HG23	1:A:1056:THR:O	1.88	0.72
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.71	0.71
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.73	0.70
1:A:1056:THR:HG21	1:A:1064:ALA:CB	2.21	0.70
1:A:788:ASP:OD2	1:A:791:LEU:HD12	1.92	0.69
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.23	0.68
1:A:386:ASN:N	1:A:386:ASN:HD22	1.90	0.68
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.59	0.67
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.76	0.67
1:A:368:ILE:HG22	1:A:516:ILE:HD12	1.76	0.67
1:A:385:ALA:C	1:A:386:ASN:HD22	1.98	0.66
2:A:1:JZY:H11A	2:A:1:JZY:S7	2.37	0.65
1:A:379:LEU:HD12	1:A:435:CYS:O	1.97	0.65
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.64	0.65
1:A:373:LEU:HD12	1:A:374:PRO:N	2.12	0.64
1:A:384:GLU:HG2	1:A:386:ASN:HD21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HD12	1:A:435:CYS:C	2.19	0.64
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.79	0.63
1:A:935:TYR:O	1:A:939:THR:HG22	1.98	0.63
1:A:501:LYS:HD2	1:A:1041:GLN:HE22	1.63	0.62
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.13	0.62
1:A:181:VAL:HG12	1:A:185:MET:HE1	1.81	0.62
1:A:368:ILE:HG22	1:A:516:ILE:CD1	2.30	0.62
1:A:745:VAL:O	1:A:749:ILE:HD13	1.99	0.62
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.81	0.62
1:A:210:TYR:O	1:A:213:LYS:HD3	1.99	0.62
1:A:276:GLY:CA	1:A:822:ALA:HB2	2.29	0.62
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.00	0.62
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.82	0.61
1:A:891:ILE:O	1:A:906:VAL:HG11	2.01	0.61
1:A:825:ASN:N	1:A:825:ASN:ND2	2.46	0.61
1:A:860:LEU:HD11	1:A:1015:LYS:HB3	1.80	0.61
1:A:608:TYR:CE1	1:A:639:ASN:ND2	2.69	0.60
1:A:997:THR:HG21	1:A:1076:ARG:NH1	2.16	0.60
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.84	0.59
1:A:466:LEU:HD11	1:A:476:ARG:CD	2.32	0.59
1:A:1056:THR:HG21	1:A:1064:ALA:HB2	1.83	0.59
1:A:767:LEU:HG	1:A:803:VAL:HG23	1.84	0.59
1:A:824:SER:C	1:A:825:ASN:HD22	2.06	0.59
1:A:893:GLN:HG3	1:A:897:GLY:HA3	1.85	0.59
1:A:469:ILE:CD1	1:A:527:ILE:HD11	2.19	0.58
1:A:210:TYR:O	1:A:213:LYS:CD	2.51	0.58
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.39	0.58
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.84	0.58
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.33	0.58
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.69	0.58
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.50	0.57
1:A:1014:VAL:HG13	1:A:1065:LYS:HG3	1.87	0.57
1:A:380:THR:HA	1:A:403:PRO:HA	1.87	0.57
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.05	0.56
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.40	0.56
1:A:756:LYS:HG2	1:A:807:LYS:HA	1.88	0.56
1:A:895:THR:O	1:A:903:LYS:NZ	2.37	0.55
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.45	0.55
1:A:886:THR:HG22	1:A:887:THR:O	2.05	0.55
1:A:741:MET:CE	1:A:779:LEU:HA	2.37	0.55
1:A:228:THR:HG22	1:A:229:THR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:OD2	1:A:471:HIS:NE2	2.39	0.55
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.37	0.55
1:A:434:TYR:CZ	1:A:460:LEU:HD13	2.42	0.54
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.27	0.54
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.89	0.54
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.37	0.54
1:A:207:LEU:HD23	1:A:208:PRO:CD	2.38	0.54
1:A:1035:LEU:HD12	1:A:1048:ILE:CD1	2.35	0.54
1:A:741:MET:HE1	1:A:779:LEU:HA	1.90	0.53
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.91	0.53
1:A:887:THR:HG21	1:A:889:ALA:HB3	1.91	0.53
1:A:935:TYR:O	1:A:939:THR:CG2	2.56	0.53
1:A:1031:PHE:O	1:A:1034:MET:HB3	2.09	0.52
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.09	0.52
1:A:550:GLN:HE21	1:A:553:LYS:HD2	1.73	0.52
1:A:555:LEU:HD11	1:A:575:LEU:HD12	1.92	0.52
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.44	0.52
1:A:1033:MET:HA	1:A:1036:MET:HE3	1.91	0.52
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.91	0.52
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.45	0.52
1:A:703:ILE:HD11	1:A:714:ALA:HA	1.90	0.52
1:A:182:THR:HB	1:A:183:PRO:HD3	1.91	0.52
1:A:887:THR:HG22	1:A:889:ALA:N	2.25	0.52
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.92	0.51
1:A:150:PHE:O	1:A:153:GLN:HB3	2.10	0.51
1:A:825:ASN:N	1:A:825:ASN:HD22	2.06	0.51
1:A:1082:VAL:HA	1:A:1085:ASN:HB3	1.92	0.51
1:A:625:GLY:O	1:A:629:GLN:HG3	2.11	0.51
1:A:583:LEU:O	1:A:616:VAL:HG11	2.11	0.51
1:A:808:LYS:NZ	1:A:836:ASP:OD1	2.41	0.51
1:A:717:LEU:HD22	1:A:721:LEU:HG	1.92	0.51
1:A:1087:PHE:CD1	1:A:1089:HIS:HB3	2.47	0.50
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.40	0.50
1:A:198:MET:SD	1:A:282:VAL:HG11	2.51	0.50
1:A:802:LYS:HG2	1:A:812:TRP:HB3	1.92	0.50
1:A:233:ILE:N	1:A:233:ILE:HD12	2.27	0.50
1:A:373:LEU:N	1:A:374:PRO:CD	2.75	0.50
1:A:1056:THR:HG21	1:A:1064:ALA:HB1	1.93	0.50
1:A:1014:VAL:HG11	1:A:1065:LYS:HD2	1.93	0.50
1:A:850:ILE:HD13	1:A:1030:LEU:CD1	2.42	0.49
1:A:373:LEU:HD12	1:A:374:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.94	0.49
1:A:947:ARG:NH2	1:A:963:ILE:O	2.45	0.49
1:A:214:LYS:HD3	1:A:214:LYS:O	2.13	0.49
1:A:475:LEU:H	1:A:525:HIS:N	2.11	0.49
1:A:804:MET:HB2	1:A:810:PRO:HG2	1.94	0.49
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.94	0.49
1:A:587:LYS:HA	1:A:626:LEU:HD11	1.94	0.48
1:A:418:ILE:HD13	1:A:418:ILE:N	2.28	0.48
1:A:239:ASP:O	1:A:287:ILE:HG23	2.14	0.48
1:A:184:ARG:O	1:A:188:VAL:HG23	2.14	0.48
1:A:519:LEU:HD12	1:A:520:LEU:N	2.27	0.48
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.96	0.48
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.96	0.48
1:A:273:ARG:O	1:A:305:VAL:HG22	2.13	0.48
1:A:184:ARG:HH21	1:A:321:GLU:CG	2.27	0.47
1:A:555:LEU:CD1	1:A:575:LEU:HD12	2.43	0.47
1:A:804:MET:CE	1:A:831:ILE:HG23	2.43	0.47
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.13	0.47
1:A:267:GLU:OE2	1:A:267:GLU:N	2.47	0.47
1:A:272:LEU:HD22	1:A:305:VAL:CG1	2.45	0.47
1:A:997:THR:HG22	1:A:998:SER:N	2.30	0.47
1:A:386:ASN:N	1:A:386:ASN:ND2	2.61	0.47
1:A:1055:LEU:O	1:A:1056:THR:CG2	2.54	0.47
1:A:163:THR:O	1:A:165:VAL:HG13	2.15	0.47
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.79	0.47
1:A:741:MET:HE2	1:A:741:MET:HB2	1.80	0.46
1:A:705:GLN:NE2	1:A:873:GLY:O	2.48	0.46
1:A:466:LEU:HD11	1:A:476:ARG:HD2	1.96	0.46
1:A:937:VAL:O	1:A:941:VAL:HG23	2.16	0.46
1:A:155:THR:HG23	1:A:161:ASP:HA	1.97	0.46
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.79	0.46
1:A:567:LEU:HD22	1:A:571:ASP:HB3	1.98	0.46
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.31	0.46
1:A:629:GLN:NE2	1:A:1025:ASN:HD22	2.15	0.45
1:A:203:THR:OG1	1:A:205:LYS:HG3	2.16	0.45
1:A:632:ASP:C	1:A:632:ASP:OD1	2.55	0.45
1:A:1032:SER:HB3	1:A:1048:ILE:HG21	1.97	0.45
1:A:1021:ARG:NH2	1:A:1056:THR:HG23	2.31	0.45
1:A:222:ILE:CD1	1:A:303:ILE:HD12	2.46	0.45
1:A:935:TYR:O	1:A:939:THR:HB	2.17	0.44
1:A:205:LYS:HE2	1:A:654:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:N	1:A:1042:LEU:HD13	2.27	0.44
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.14	0.44
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.18	0.44
1:A:997:THR:HG21	1:A:1076:ARG:HH11	1.82	0.44
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.53	0.44
1:A:217:ASN:OD1	1:A:217:ASN:N	2.50	0.43
1:A:240:THR:H	1:A:243:ALA:HB3	1.83	0.43
1:A:174:GLU:OE2	1:A:177:ARG:NH1	2.51	0.43
1:A:887:THR:HG22	1:A:889:ALA:HB3	1.99	0.43
1:A:309:THR:HG23	1:A:310:PRO:HD2	1.99	0.43
1:A:764:ILE:HA	1:A:764:ILE:HD13	1.94	0.43
1:A:796:LEU:HD21	1:A:815:PHE:CZ	2.54	0.43
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.83	0.43
1:A:1057:VAL:HG12	1:A:1058:GLY:N	2.34	0.43
1:A:850:ILE:HD13	1:A:1030:LEU:HD13	2.00	0.43
1:A:945:GLY:O	1:A:985:PHE:HA	2.18	0.43
1:A:1074:VAL:O	1:A:1074:VAL:HG12	2.19	0.43
1:A:240:THR:HG23	1:A:241:PRO:CD	2.40	0.43
1:A:421:LYS:HE2	1:A:526:PRO:HG2	2.00	0.43
1:A:873:GLY:C	1:A:876:ILE:HG22	2.40	0.42
1:A:925:VAL:O	1:A:929:VAL:HG23	2.19	0.42
1:A:244:ILE:HA	1:A:247:SER:HB3	2.01	0.42
1:A:561:THR:HB	1:A:565:ASN:HD22	1.84	0.42
1:A:233:ILE:HG22	1:A:234:LYS:O	2.18	0.42
1:A:775:GLN:HE22	1:A:796:LEU:N	2.18	0.42
1:A:743:GLN:O	1:A:747:LEU:HD12	2.19	0.42
1:A:756:LYS:HZ1	1:A:807:LYS:HB3	1.84	0.42
1:A:1089:HIS:O	1:A:1090:LEU:C	2.57	0.42
1:A:604:VAL:O	1:A:607:THR:HB	2.19	0.42
1:A:519:LEU:HD12	1:A:520:LEU:O	2.19	0.42
1:A:1000:LYS:HA	1:A:1076:ARG:NH2	2.35	0.41
1:A:391:GLN:HE21	1:A:391:GLN:HB3	1.69	0.41
1:A:395:CYS:HB2	1:A:418:ILE:HG12	2.02	0.41
1:A:240:THR:CG2	1:A:241:PRO:HD2	2.41	0.41
1:A:357:CYS:N	1:A:421:LYS:HD3	2.35	0.41
1:A:852:GLU:HG3	1:A:864:LEU:HD12	2.01	0.41
1:A:955:THR:OG1	1:A:957:THR:HG22	2.20	0.41
1:A:497:PHE:O	1:A:1042:LEU:HD11	2.21	0.41
1:A:824:SER:C	1:A:825:ASN:ND2	2.72	0.41
1:A:507:ASN:HA	1:A:508:PRO:HD2	1.91	0.41
1:A:1050:TYR:C	1:A:1050:TYR:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:ASP:O	1:A:654:ASP:C	2.58	0.41
1:A:380:THR:O	1:A:435:CYS:HA	2.21	0.41
1:A:564:LEU:O	1:A:565:ASN:C	2.59	0.41
1:A:405:THR:OG1	1:A:407:GLU:O	2.39	0.41
1:A:373:LEU:N	1:A:374:PRO:HD2	2.35	0.41
1:A:470:ASP:OD1	1:A:470:ASP:C	2.59	0.41
1:A:576:TRP:O	1:A:579:ARG:CD	2.63	0.41
1:A:1042:LEU:CD2	1:A:1042:LEU:C	2.90	0.40
1:A:1082:VAL:O	1:A:1086:TRP:N	2.54	0.40
1:A:308:ASP:N	1:A:308:ASP:OD1	2.55	0.40
1:A:375:ARG:HE	1:A:375:ARG:N	2.18	0.40
1:A:379:LEU:CD1	1:A:435:CYS:O	2.69	0.40
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.36	0.40
1:A:1060:ASN:HD22	1:A:1062:GLU:HG2	1.86	0.40
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.51	0.40
1:A:898:ASN:C	1:A:900:GLY:N	2.75	0.40
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	739 (90%)	70 (8%)	16 (2%)	8 36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	PRO
1	A	527	ILE
1	A	758	ASP
1	A	899	THR

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Mol	Chain	Res	Type
1	A	1090	LEU
1	A	374	PRO
1	A	807	LYS
1	A	1044	SER
1	A	1087	PHE
1	A	252	MET
1	A	375	ARG
1	A	380	THR
1	A	754	ALA
1	A	545	ALA
1	A	896	VAL
1	A	1079	GLY

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	756/864 (88%)	694 (92%)	62 (8%)	11	39

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	207	LEU
1	A	213	LYS
1	A	214	LYS
1	A	226	ARG
1	A	236	SER
1	A	244	ILE
1	A	252	MET
1	A	267	GLU
1	A	281	LEU
1	A	282	VAL
1	A	298	LYS
1	A	302	GLU
1	A	321	GLU

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Mol	Chain	Res	Type
1	A	322	GLU
1	A	372	VAL
1	A	374	PRO
1	A	375	ARG
1	A	379	LEU
1	A	380	THR
1	A	386	ASN
1	A	391	GLN
1	A	404	PHE
1	A	410	TRP
1	A	421	LYS
1	A	525	HIS
1	A	550	GLN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	662	GLN
1	A	679	ARG
1	A	682	LEU
1	A	717	LEU
1	A	756	LYS
1	A	764	ILE
1	A	769	GLN
1	A	773	ASN
1	A	802	LYS
1	A	806	SER
1	A	807	LYS
1	A	823	LEU
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	857	THR
1	A	869	CYS
1	A	898	ASN
1	A	899	THR
1	A	903	LYS
1	A	909	HIS
1	A	911	LEU

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Mol	Chain	Res	Type
1	A	1026	LEU
1	A	1042	LEU
1	A	1046	GLU
1	A	1048	ILE
1	A	1049	GLU
1	A	1062	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	295	HIS
1	A	304	HIS
1	A	386	ASN
1	A	396	GLN
1	A	432	GLN
1	A	550	GLN
1	A	554	GLN
1	A	601	GLN
1	A	629	GLN
1	A	646	GLN
1	A	705	GLN
1	A	743	GLN
1	A	769	GLN
1	A	825	ASN
1	A	834	HIS
1	A	898	ASN
1	A	908	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1023	HIS
1	A	1041	GLN
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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	JZY	A	1	-	36,38,38	1.88	4 (11%)	42,56,56	3.34	26 (61%)

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	JZY	A	1	-	-	8/17/36/36	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	JZY	S31-N28	-7.70	1.53	1.63
2	A	1	JZY	C16-C21	5.27	1.49	1.41
2	A	1	JZY	C34-S31	-3.69	1.67	1.75
2	A	1	JZY	C1-N2	2.28	1.35	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	JZY	O33-S31-O32	-8.49	106.49	118.59
2	A	1	JZY	O32-S31-N28	7.00	112.91	107.03
2	A	1	JZY	C30-C29-N28	-6.44	103.99	108.91
2	A	1	JZY	C30-N25-C26	5.55	121.32	108.83
2	A	1	JZY	C27-N28-S31	5.02	122.48	116.30
2	A	1	JZY	C3-N4-C5	4.57	119.60	116.50
2	A	1	JZY	C16-C21-N20	-4.51	118.25	122.10
2	A	1	JZY	C29-N28-S31	4.28	121.56	116.30
2	A	1	JZY	C24-N25-C26	4.12	120.23	111.06
2	A	1	JZY	C19-N20-C21	3.79	119.88	116.79
2	A	1	JZY	C15-N10-C11	3.76	119.83	111.52
2	A	1	JZY	N4-C3-N2	-3.70	123.21	126.11
2	A	1	JZY	C26-C27-N28	-3.64	106.13	108.91
2	A	1	JZY	C29-N28-C27	3.42	115.95	112.17
2	A	1	JZY	C24-N25-C30	3.31	118.42	111.06
2	A	1	JZY	C16-C17-N18	-3.25	119.38	124.49
2	A	1	JZY	C6-C1-N2	-3.06	114.91	122.60
2	A	1	JZY	C1-N2-C3	3.06	123.35	116.17
2	A	1	JZY	C17-N18-C19	2.75	121.54	116.44
2	A	1	JZY	C6-C1-N10	2.70	126.95	121.57
2	A	1	JZY	N18-C19-N20	-2.40	122.78	125.70
2	A	1	JZY	O33-S31-C34	2.39	111.65	108.44
2	A	1	JZY	C12-C11-N10	-2.26	105.85	110.02
2	A	1	JZY	C5-C6-S7	-2.26	108.92	111.84
2	A	1	JZY	C22-C21-N20	2.04	119.64	116.49
2	A	1	JZY	O33-S31-N28	2.01	108.72	107.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

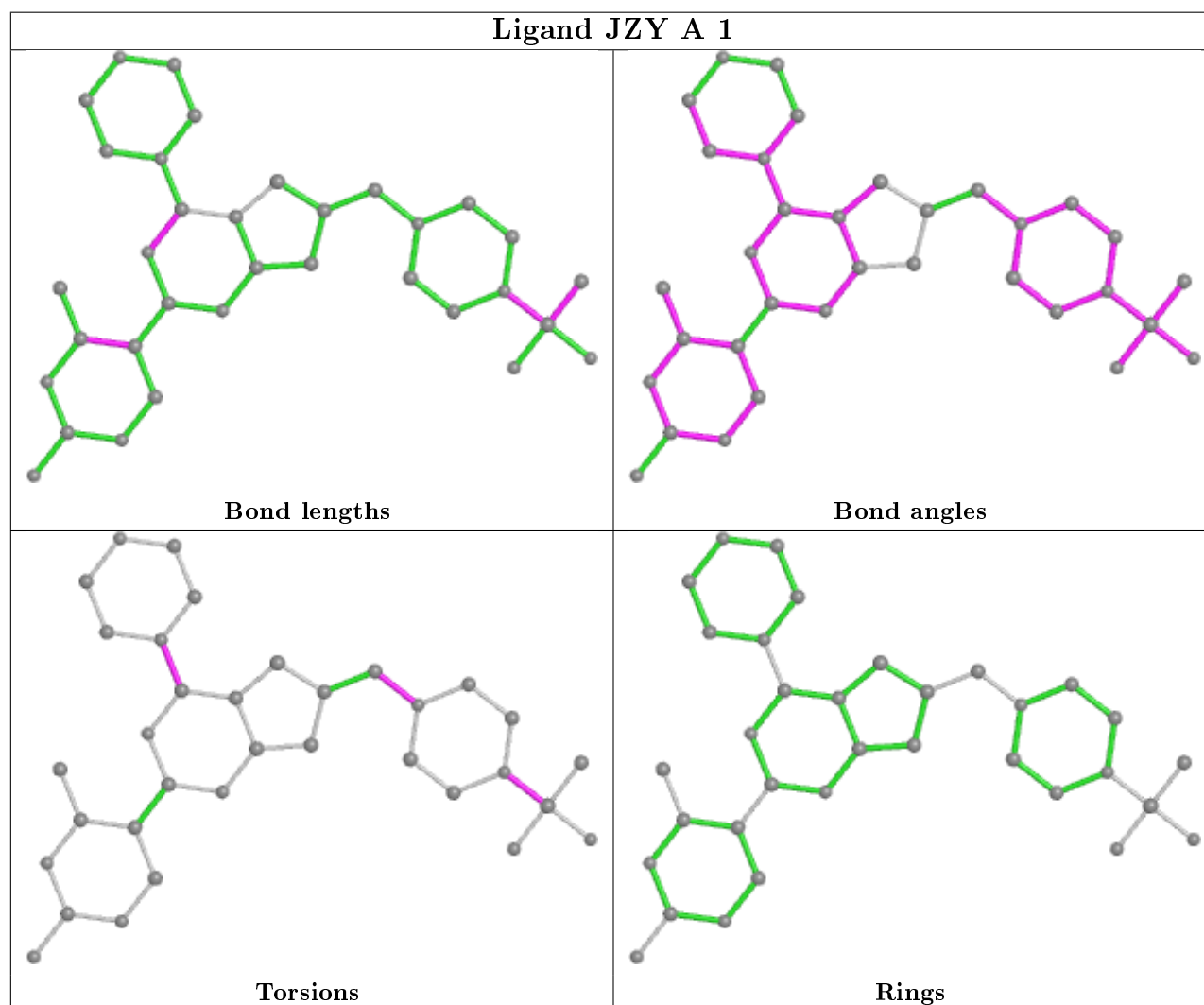
Mol	Chain	Res	Type	Atoms
2	A	1	JZY	N2-C1-N10-C11
2	A	1	JZY	C6-C1-N10-C11
2	A	1	JZY	C8-C24-N25-C26
2	A	1	JZY	C27-N28-S31-O33
2	A	1	JZY	C29-N28-S31-O32
2	A	1	JZY	C27-N28-S31-C34
2	A	1	JZY	C29-N28-S31-O33
2	A	1	JZY	C29-N28-S31-C34

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	JZY	1	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

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, 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	841/966 (87%)	0.10	34 (4%) 38 15	89, 101, 110, 125	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	7.5
1	A	376	ASN	7.1
1	A	143	MET	6.6
1	A	898	ASN	5.6
1	A	1091	VAL	5.3
1	A	377	THR	4.4
1	A	375	ARG	4.3
1	A	1088	LEU	3.8
1	A	235	VAL	3.4
1	A	220	ILE	3.2
1	A	253	ALA	3.0
1	A	823	LEU	2.9
1	A	997	THR	2.8
1	A	281	LEU	2.8
1	A	374	PRO	2.7
1	A	995	MET	2.6
1	A	225	HIS	2.6
1	A	404	PHE	2.6
1	A	1045	LYS	2.5
1	A	1064	ALA	2.4
1	A	221	PHE	2.4
1	A	896	VAL	2.4
1	A	895	THR	2.4
1	A	987	LEU	2.3
1	A	267	GLU	2.3
1	A	233	ILE	2.3
1	A	307	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	2.3
1	A	378	ASP	2.3
1	A	373	LEU	2.2
1	A	489	GLY	2.2
1	A	301	GLU	2.1
1	A	1068	PHE	2.0
1	A	1000	LYS	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](#)

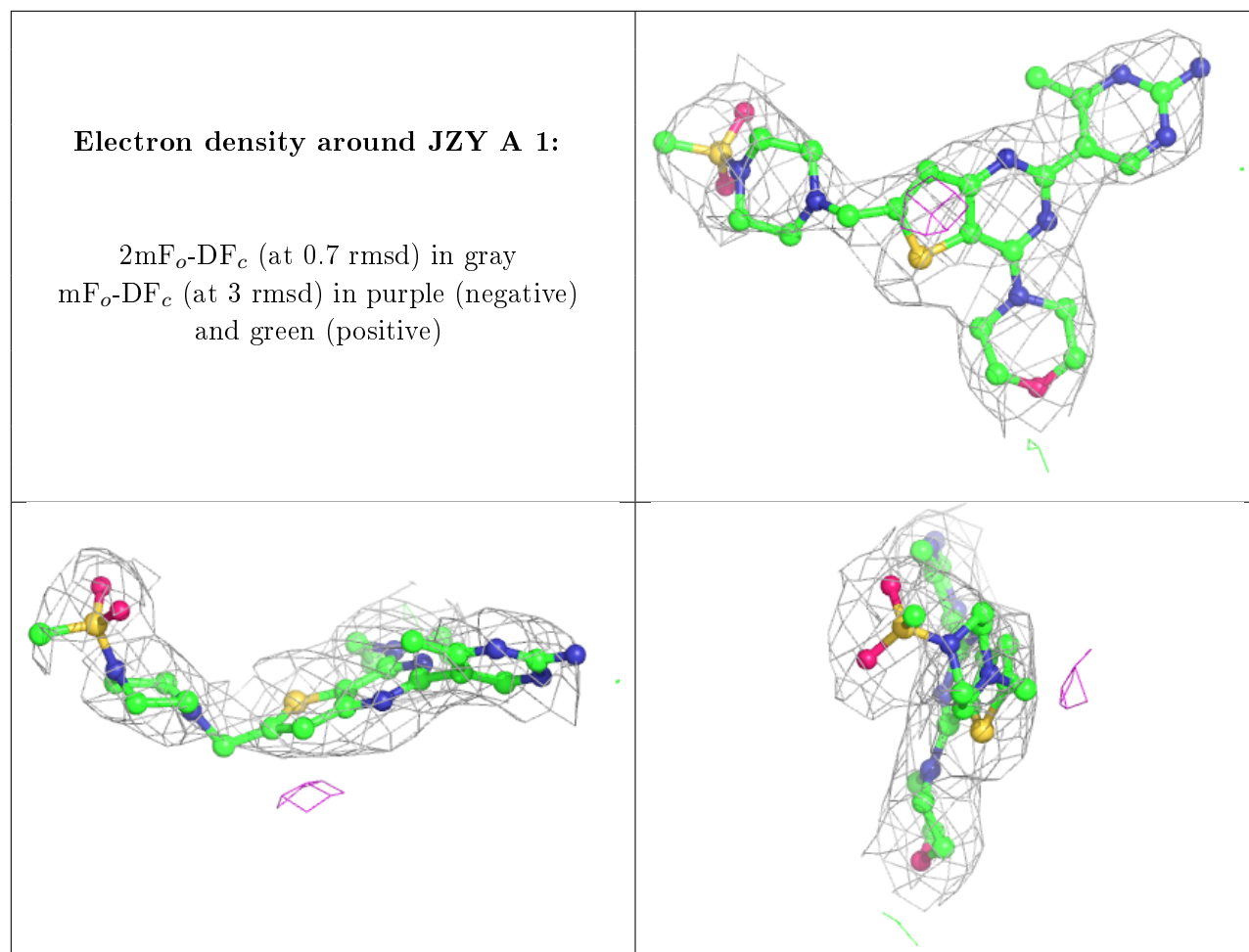
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
2	JZY	A	1	34/34	0.94	0.19	93,97,105,106	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.