



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:16 PM UTC

PDB ID : 3L17 / pdb_00003l17
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 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

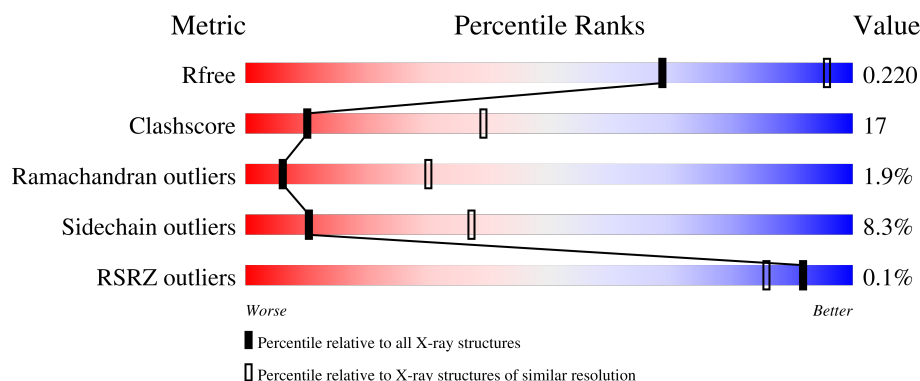
1 Overall quality at a glance

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	966	 56% 26% 13%

2 Entry composition [i](#)

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.

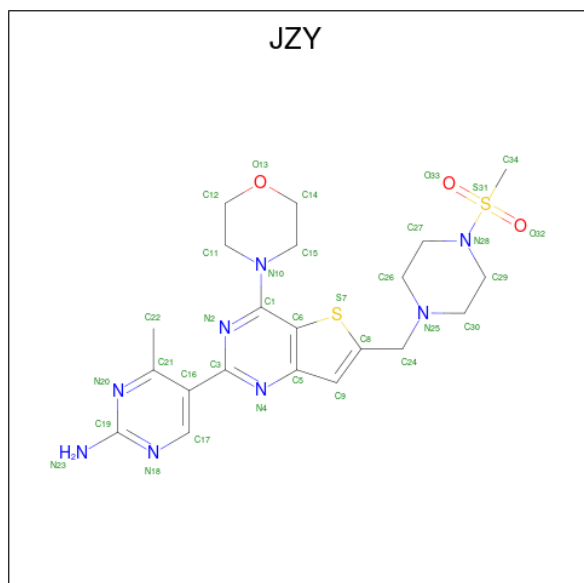
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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-ylthio)no[3,2-d]pyrimidin-2-yl)pyrimidin-2-amine (CCD ID: JZY) (formula: C₂₁H₂₈N₈O₃S₂).



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

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.09Å 67.73Å 107.45Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	45.18 – 3.00 45.18 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.18-3.00) 97.9 (45.18-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.01Å)	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)	0.30 , 85.4	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

5.1 Standard geometry

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	0.72	0/6966	0.87	4/9422 (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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	808	LYS	N-CA-C	-6.82	100.70	110.59
1	A	758	ASP	N-CA-C	5.18	121.84	110.80
1	A	616	VAL	N-CA-C	5.17	115.94	110.72
1	A	1088	LEU	N-CA-C	-5.05	107.27	112.93

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

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	234	0
2	A	34	0	28	2	0
All	All	6854	0	6883	236	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 17.

All (236) 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:181:VAL:HG12	1:A:185:MET:HE2	1.25	1.11
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:741:MET:HE1	1:A:779:LEU:HA	1.49	0.94
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: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:276:GLY:HA2	1:A:822:ALA:HB2	1.66	0.76
1:A:1042:LEU:HD13	1:A:1042:LEU:H	1.50	0.76
1:A:741:MET:HE1	1:A:779:LEU:CA	2.16	0.74
1:A:181:VAL:HG12	1:A:185:MET:CE	2.12	0.74
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:428:LEU:HD22	1:A:465:ASN:HB3	1.71	0.71
1:A:1056:THR:HG23	1:A:1056:THR:O	1.88	0.71
1:A:385:ALA:C	1:A:386:ASN:HD22	1.98	0.70
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:379:LEU:HD12	1:A:435:CYS:C	2.19	0.68
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.23	0.68
1:A:386:ASN:HD22	1:A:386:ASN:N	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1038:GLY:C	1:A:1039:MET:HE2	2.23	0.64
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
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.79	0.63
1:A:824:SER:C	1:A:825:ASN:HD22	2.06	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: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: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:628:MET:HE3	1:A:1030:LEU:CD2	2.31	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:194:LYS:O	1:A:198:MET:HE3	2.02	0.60
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:628:MET:HE3	1:A:1030:LEU:HD21	1.83	0.59
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.84	0.59
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.27	0.59
1:A:466:LEU:HD11	1:A:476:ARG:CD	2.32	0.59
1:A:767:LEU:HG	1:A:803:VAL:HG23	1.84	0.59
1:A:1056:THR:HG21	1:A:1064:ALA:HB2	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:HA	1:A:403:PRO:HA	1.87	0.57
1:A:1034:MET:HG2	1:A:1039:MET:HE3	1.87	0.57
1:A:252:MET:HE3	1:A:252:MET:HA	1.86	0.56
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:171:ASP:OD2	1:A:471:HIS:NE2	2.39	0.55
1:A:228:THR:HG22	1:A:229:THR:N	2.21	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: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:804:MET:HE3	1:A:810:PRO:HB2	1.90	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: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: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: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:223:VAL:HG12	1:A:225:HIS:CE1	2.44	0.52
1:A:808:LYS:NZ	1:A:836:ASP:OD1	2.41	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:HD22	1:A:825:ASN:N	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:717:LEU:HD22	1:A:721:LEU:HG	1.92	0.51
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:PHE:CD1	1:A:1089:HIS:HB3	2.47	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:1038:GLY:HA3	1:A:1039:MET:HE2	1.94	0.49
1:A:373:LEU:HD12	1:A:374:PRO:CD	2.42	0.49
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:O	1:A:214:LYS:HD3	2.13	0.49
1:A:632:ASP:C	1:A:632:ASP:OD1	2.55	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:838:LEU:HD23	1:A:877:GLY:HA3	1.96	0.48
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.96	0.48
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.17	0.48
1:A:804:MET:HE1	1:A:831:ILE:HD13	1.95	0.48
1:A:273:ARG:O	1:A:305:VAL:HG22	2.13	0.48
1:A:830:ILE:HG21	1:A:878:MET:HE3	1.95	0.48
2:A:1:JZY:H22	2:A:1:JZY:N4	2.29	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:873:GLY:C	1:A:876:ILE:HG22	2.40	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:163:THR:O	1:A:165:VAL:HG13	2.15	0.47
1:A:1055:LEU:O	1:A:1056:THR:CG2	2.54	0.47
1:A:1089:HIS:O	1:A:1090:LEU:C	2.57	0.47
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:632:ASP:HB3	1:A:1033:MET:HE2	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:653:ASP:O	1:A:654:ASP:C	2.58	0.46
1:A:1050:TYR:CD2	1:A:1050:TYR:C	2.94	0.46
1:A:564:LEU:O	1:A:565:ASN:C	2.59	0.46
1:A:629:GLN:NE2	1:A:1025:ASN:HD22	2.15	0.45
1:A:470:ASP:OD1	1:A:470:ASP:C	2.59	0.45
1:A:203:THR:OG1	1:A:205:LYS:HG3	2.16	0.45
1:A:1032:SER:HB3	1:A:1048:ILE:HG21	1.97	0.45
1:A:1038:GLY:CA	1:A:1039:MET:HE2	2.47	0.45
1:A:898:ASN:C	1:A:900:GLY:N	2.75	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:824:SER:C	1:A:825:ASN:ND2	2.72	0.45
1:A:361:PHE:CD2	1:A:361:PHE:C	2.94	0.44
1:A:812:TRP:C	1:A:813:LEU:HD23	2.42	0.44
1:A:935:TYR:O	1:A:939:THR:HB	2.17	0.44
1:A:1042:LEU:C	1:A:1042:LEU:CD2	2.90	0.44
1:A:205:LYS:HE2	1:A:654:ASP:OD2	2.17	0.44
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.14	0.44
1:A:1042:LEU:HD13	1:A:1042:LEU:N	2.27	0.44
1:A:386:ASN:N	1:A:386:ASN:ND2	2.61	0.44
1:A:1044:SER:C	1:A:1045:LYS:HZ3	2.26	0.44
1:A:947:ARG:HH22	1:A:964:ASP:C	2.25	0.44
1:A:804:MET:HE1	1:A:831:ILE:CG2	2.47	0.44
1:A:997:THR:HG21	1:A:1076:ARG:HH11	1.82	0.44
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.18	0.44
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.53	0.44
1:A:1055:LEU:C	1:A:1056:THR:HG22	2.41	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:217:ASN:OD1	1:A:217:ASN:N	2.50	0.43
1:A:309:THR:HG23	1:A:310:PRO:HD2	1.99	0.43
1:A:764:ILE:HD13	1:A:764:ILE:HA	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:LEU:HD21	1:A:815:PHE:CZ	2.54	0.43
1:A:850:ILE:HD13	1:A:1030:LEU:HD13	2.00	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:945:GLY:O	1:A:985:PHE:HA	2.18	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:906:VAL:O	1:A:907:LEU:C	2.62	0.43
1:A:1074:VAL:O	1:A:1074:VAL:HG12	2.19	0.43
1:A:192:ASP:C	1:A:192:ASP:OD1	2.61	0.42
1:A:925:VAL:O	1:A:929:VAL:HG23	2.19	0.42
1:A:180:LEU:C	1:A:183:PRO:HD2	2.44	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: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:898:ASN:C	1:A:898:ASN:HD22	2.27	0.42
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:1000:LYS:HA	1:A:1076:ARG:NH2	2.35	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:507:ASN:HA	1:A:508:PRO:HD2	1.91	0.41
1:A:380:THR:O	1:A:435:CYS:HA	2.21	0.41
1:A:373:LEU:N	1:A:374:PRO:HD2	2.35	0.41
1:A:405:THR:OG1	1:A:407:GLU:O	2.39	0.41
1:A:358:ASP:O	1:A:359:ARG:C	2.64	0.41
1:A:576:TRP:O	1:A:579:ARG:CD	2.63	0.41
1:A:308:ASP:N	1:A:308:ASP:OD1	2.55	0.40
1:A:375:ARG:N	1:A:375:ARG:HE	2.18	0.40
1:A:379:LEU:CD1	1:A:435:CYS:O	2.69	0.40
1:A:1082:VAL:O	1:A:1086:TRP:N	2.54	0.40
1:A:419:LYS:O	1:A:420:ILE:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.51	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 [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%)	739 (90%)	70 (8%)	16 (2%)	6	30

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
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%)	693 (92%)	63 (8%)	10	37

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	267	GLU
1	A	271	VAL
1	A	281	LEU
1	A	282	VAL
1	A	298	LYS
1	A	302	GLU
1	A	305	VAL
1	A	309	THR
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	381	VAL
1	A	386	ASN
1	A	391	GLN
1	A	408	VAL
1	A	421	LYS
1	A	525	HIS
1	A	550	GLN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU

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Mol	Chain	Res	Type
1	A	595	SER
1	A	601	GLN
1	A	603	ILE
1	A	610	LEU
1	A	662	GLN
1	A	682	LEU
1	A	703	ILE
1	A	717	LEU
1	A	737	GLN
1	A	764	ILE
1	A	767	LEU
1	A	802	LYS
1	A	806	SER
1	A	807	LYS
1	A	808	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	899	THR
1	A	903	LYS
1	A	909	HIS
1	A	911	LEU
1	A	1025	ASN
1	A	1026	LEU
1	A	1042	LEU
1	A	1045	LYS
1	A	1046	GLU
1	A	1048	ILE
1	A	1062	GLU

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

Mol	Chain	Res	Type
1	A	225	HIS
1	A	291	GLN
1	A	295	HIS
1	A	304	HIS
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	396	GLN
1	A	550	GLN
1	A	554	GLN
1	A	601	GLN
1	A	634	ASN
1	A	743	GLN
1	A	769	GLN
1	A	778	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	1025	ASN
1	A	1041	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	JZY	A	1	-	37,38,38	2.01	6 (16%)	48,56,56	3.25	26 (54%)

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	-	-	5/18/36/36	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	JZY	S31-N28	-6.16	1.53	1.63
2	A	1	JZY	C5-C6	5.86	1.46	1.40
2	A	1	JZY	C16-C21	5.27	1.49	1.41
2	A	1	JZY	C34-S31	-4.02	1.67	1.75
2	A	1	JZY	C6-S7	-3.76	1.66	1.74
2	A	1	JZY	C9-C8	2.10	1.40	1.36

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	JZY	O33-S31-O32	-8.01	106.49	118.46
2	A	1	JZY	O32-S31-N28	7.05	112.91	107.02
2	A	1	JZY	C6-C1-N2	-6.22	114.91	122.33
2	A	1	JZY	C6-S7-C8	6.16	95.28	91.92
2	A	1	JZY	C24-N25-C26	5.84	120.23	111.14
2	A	1	JZY	C30-N25-C26	5.79	121.32	108.84
2	A	1	JZY	C30-C29-N28	-4.68	103.99	108.97
2	A	1	JZY	C24-N25-C30	4.68	118.42	111.14
2	A	1	JZY	C16-C21-N20	-4.51	118.25	122.10
2	A	1	JZY	C24-C8-S7	-4.02	113.80	121.42
2	A	1	JZY	C19-N20-C21	3.79	119.88	116.79
2	A	1	JZY	C15-N10-C11	3.67	119.83	111.57
2	A	1	JZY	C5-N4-C3	3.67	119.60	116.24
2	A	1	JZY	C27-N28-S31	3.60	122.48	116.71
2	A	1	JZY	C29-N28-C27	3.34	115.95	112.12
2	A	1	JZY	C16-C17-N18	-3.25	119.38	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	JZY	C1-N2-C3	3.16	123.35	115.92
2	A	1	JZY	C29-N28-S31	3.02	121.56	116.71
2	A	1	JZY	C17-N18-C19	2.98	121.54	116.29
2	A	1	JZY	C26-C27-N28	-2.67	106.13	108.97
2	A	1	JZY	N18-C19-N20	-2.62	122.78	125.70
2	A	1	JZY	O33-S31-C34	2.45	111.65	108.30
2	A	1	JZY	C24-C8-C9	2.28	134.76	127.51
2	A	1	JZY	C12-C11-N10	-2.15	105.85	109.93
2	A	1	JZY	O33-S31-N28	2.04	108.72	107.02
2	A	1	JZY	C22-C21-N20	2.00	119.64	116.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

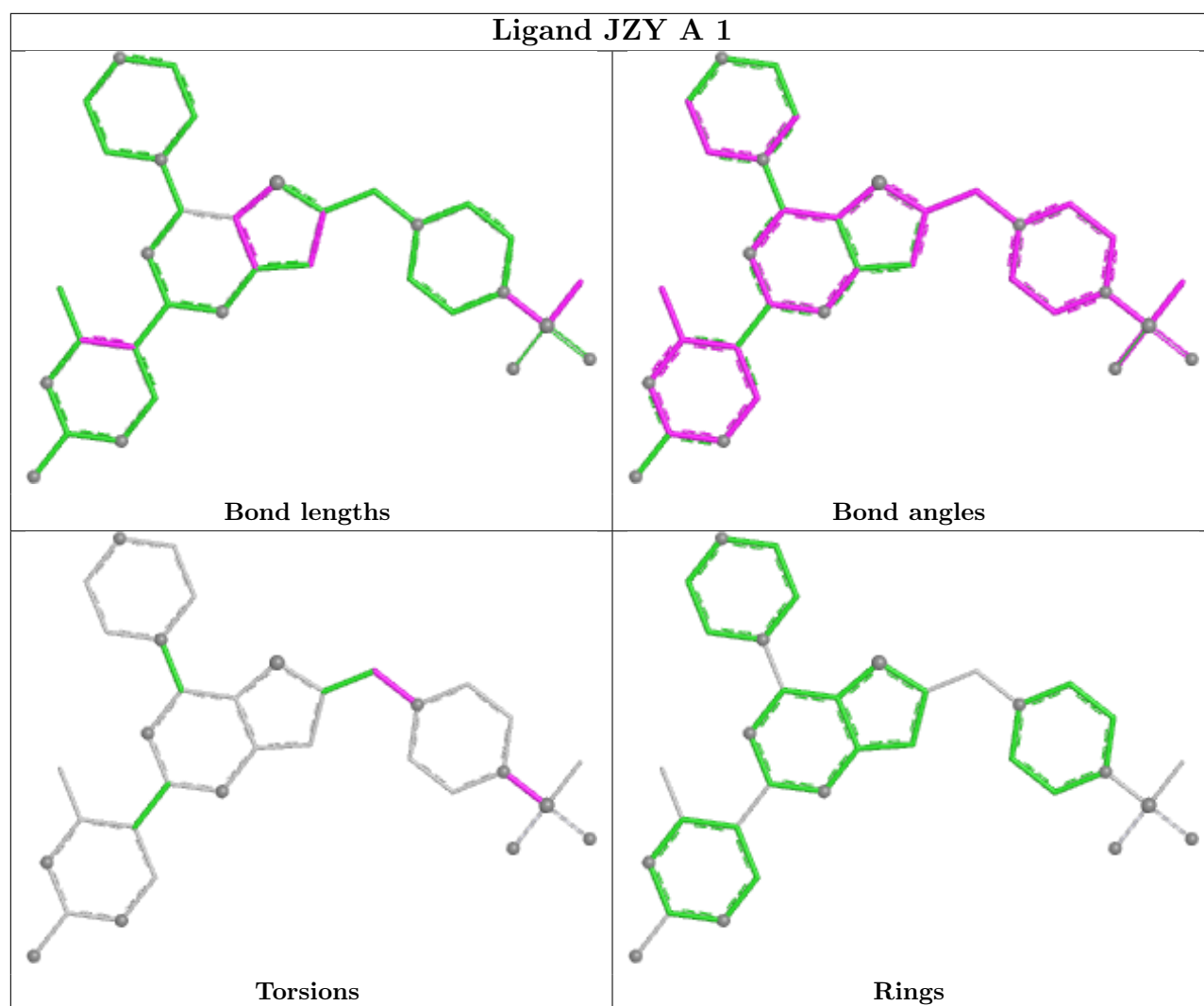
Mol	Chain	Res	Type	Atoms
2	A	1	JZY	C8-C24-N25-C26
2	A	1	JZY	C29-N28-S31-O32
2	A	1	JZY	C27-N28-S31-O33
2	A	1	JZY	C29-N28-S31-O33
2	A	1	JZY	C29-N28-S31-C34

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	JZY	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	841/966 (87%)	-0.26	1 (0%) 92 86	89, 101, 110, 125	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	3.3

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](#)

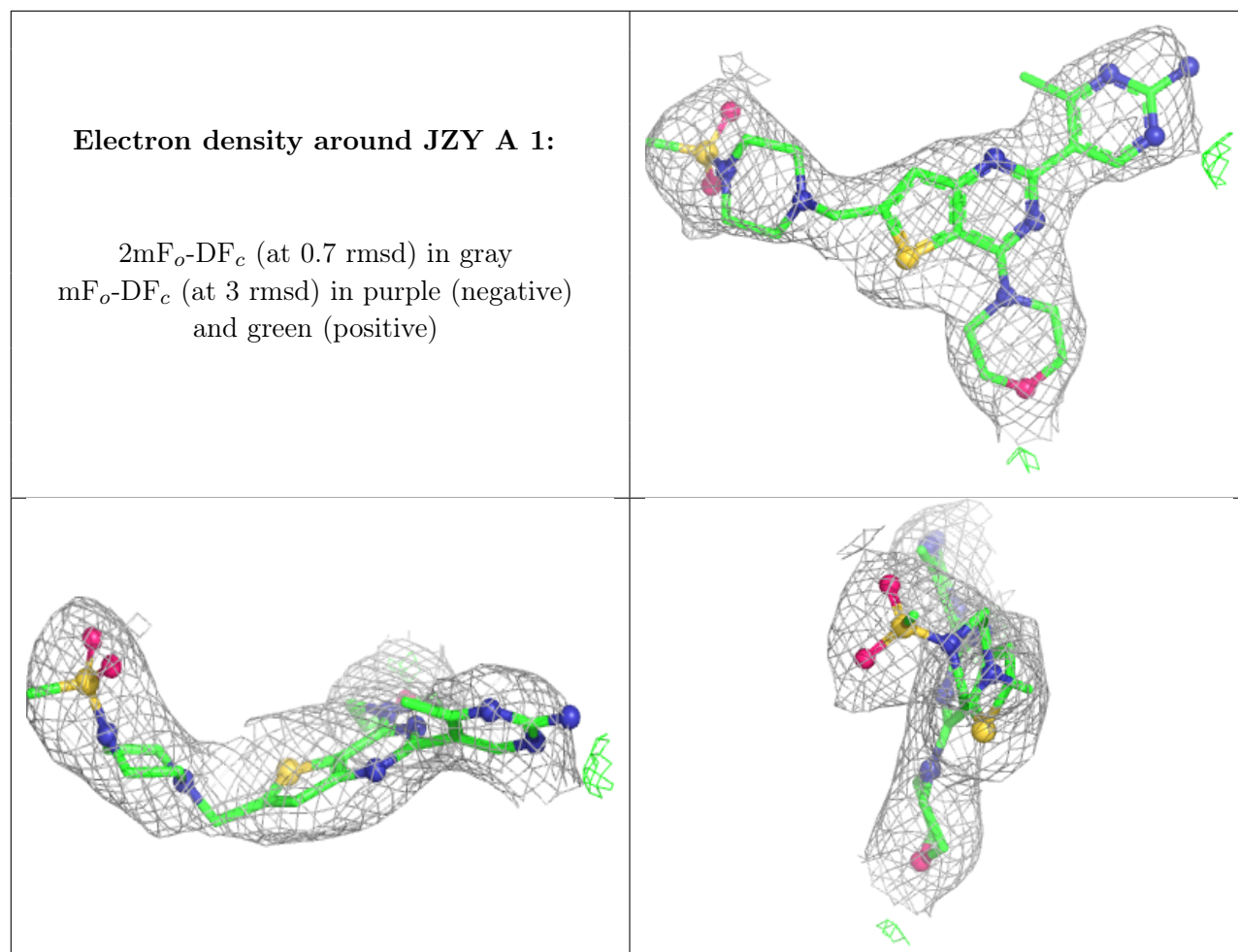
There are no oligosaccharides in this entry.

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	JZY	A	1	34/34	0.95	0.09	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.