wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2026 – 01:21 pm GMT

PDB ID	:	9T1T / pdb_00009t1t
Title	:	Crystal Structure of the correct enantiomer bound to the PH domain of Btk
Authors	:	Brear, P.; West, R.M.; Nicolescu, R.C.B.; Blaszczyk, B.K.; Deingruber, T.; Sanders, M.G.; Perez-Areales, F.J.; Spring, D.R.; Hyvonen, M.
Deposited on	:	2025-10-22
Resolution	:	1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

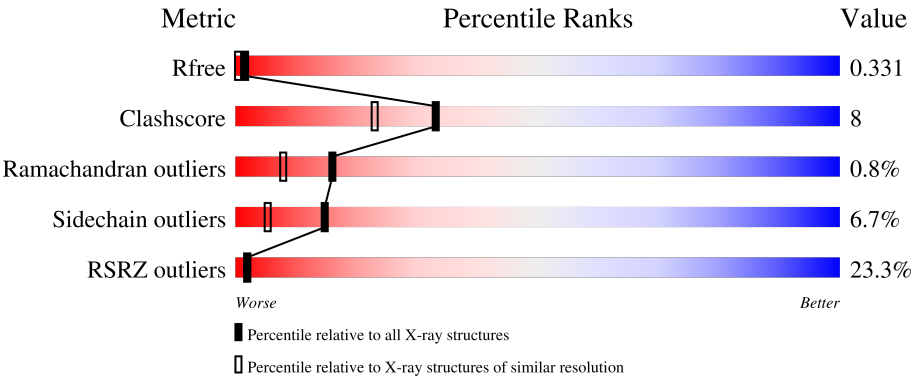
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	169	16% 68% 21% 7% 5%
1	C	169	12% 72% 18% •• 8%
1	G	169	28% 75% 19% • 5%
1	J	169	32% 64% 29% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1JS0	C	201	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5510 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 Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	1	0
			1347	865	234	242	6			
1	C	156	Total	C	N	O	S	0	0	0
			1300	840	224	230	6			
1	G	161	Total	C	N	O	S	0	1	0
			1343	865	230	242	6			
1	J	162	Total	C	N	O	S	0	0	0
			1344	867	230	241	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	SER	CYS	engineered mutation	UNP Q06187
C	145	SER	CYS	engineered mutation	UNP Q06187
G	145	SER	CYS	engineered mutation	UNP Q06187
J	145	SER	CYS	engineered mutation	UNP Q06187

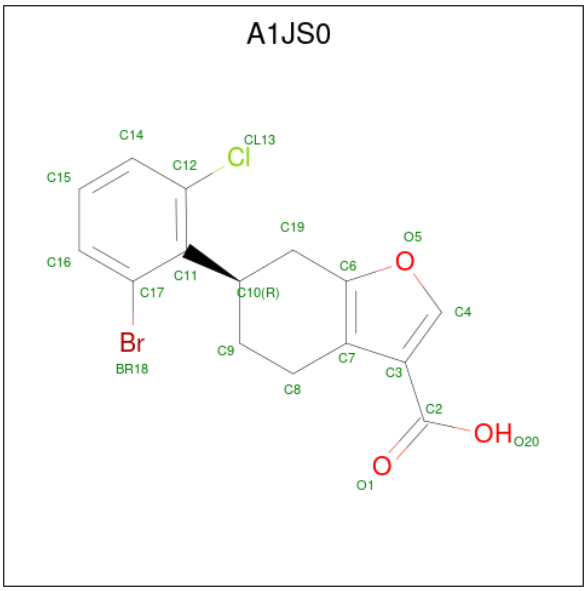
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0

- Molecule 4 is (6 {R})-6-(2-bromanyl-6-chloranyl-phenyl)-4,5,6,7-tetrahydro-1-benzofuran-3-carboxylic acid (CCD ID: A1JS0) (formula: $C_{15}H_{12}BrClO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Br C Cl O 20 1 15 1 3	0	0

- Molecule 5 is water.

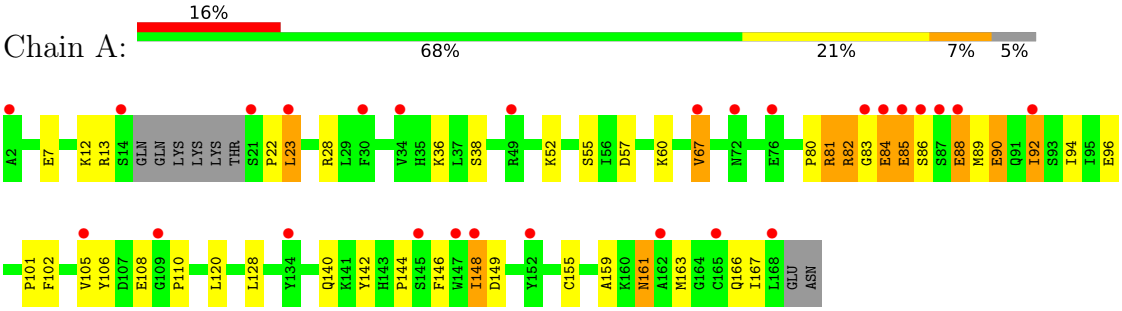
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	C	46	Total O 46 46	0	0
5	G	22	Total O 22 22	0	0
5	J	24	Total O 24 24	0	0

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.

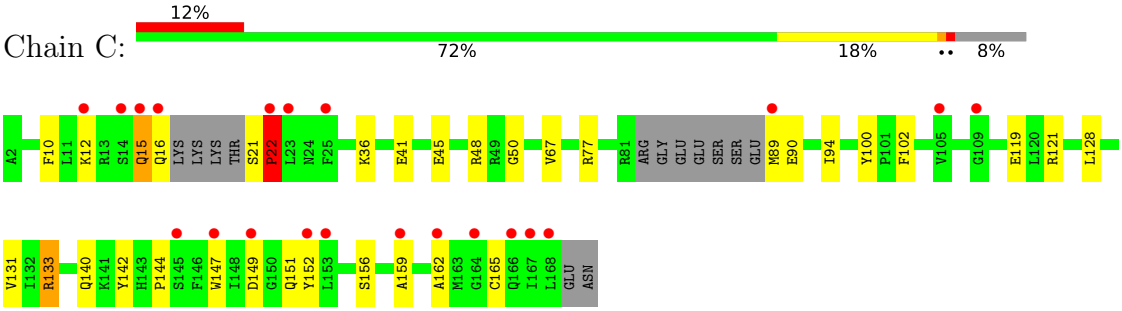
• Molecule 1: Tyrosine-protein kinase BTK

Chain A:



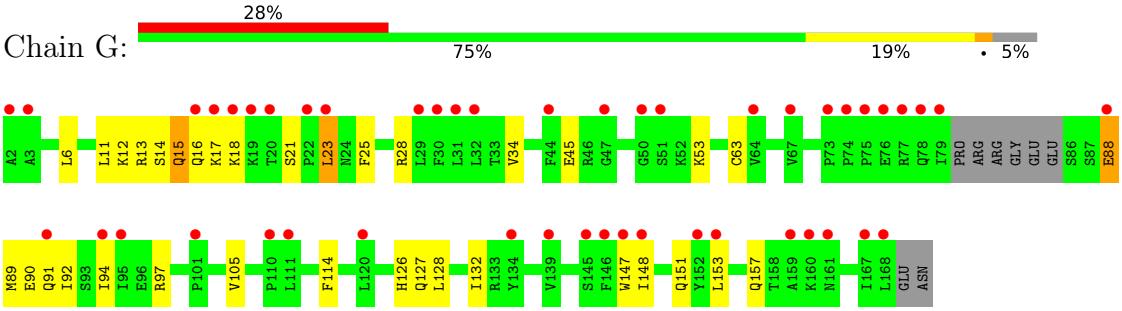
• Molecule 1: Tyrosine-protein kinase BTK

Chain C:



• Molecule 1: Tyrosine-protein kinase BTK

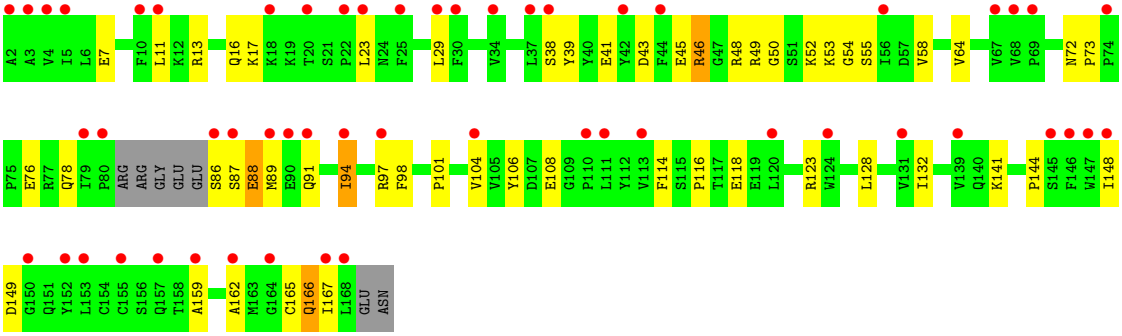
Chain G:



• Molecule 1: Tyrosine-protein kinase BTK

Chain J:




A2 A3 V4 I5 L6 E7 F10 L11 K12 R13 Q16 K17 K18 K19 T20 S21 P22 L23 N24 F25 L29 F30 V34 L37 S38 Y39 Y40 E41 Y42 D43 F44 E45 R46 G47 R48 R49 G50 S51 K52 K53 G54 S55 I56 D57 V58 V64 V67 V68 P69 N72 P73 P74
P75 E76 R77 Q78 I79 P80 ARG ARG GLY GLU GLU S86 S87 E88 M89 E90 Q91 I94 R97 F98 P101 V104 V105 Y106 D107 E108 G109 P110 L111 Y112 V113 F114 S115 P116 T117 E118 E119 L120 R123 W124 L128 V131 I132 V139 Q140 K141 P144 S145 F146 W147 I148
D149 G150 Q151 Y152 L153 C154 C155 S156 Q157 T158 A159 A162 M163 G164 C165 Q166 I167 L168 GLU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.13Å 66.62Å 79.83Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	28.66 – 1.96 28.66 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.5 (28.66-1.96) 93.4 (28.66-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.97Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.296 , 0.367 0.285 , 0.331	Depositor DCC
R_{free} test set	2060 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% 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: A1JS0, MG, ZN

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	0.88	0/1380	1.21	6/1861 (0.3%)
1	C	0.88	0/1332	1.20	3/1797 (0.2%)
1	G	0.80	0/1375	1.12	0/1853
1	J	0.79	0/1377	1.11	2/1857 (0.1%)
All	All	0.84	0/5464	1.16	11/7368 (0.1%)

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	3
1	C	0	4
1	G	0	1
1	J	0	3
All	All	0	11

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	PHE	CA-CB-CG	6.66	120.46	113.80
1	C	100	TYR	CB-CA-C	6.47	116.93	110.33
1	C	102	PHE	CA-CB-CG	6.15	119.95	113.80
1	A	102	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	146	PHE	CB-CA-C	-5.75	99.77	109.83

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	A	81	ARG	Sidechain
1	A	82	ARG	Sidechain
1	C	48	ARG	Sidechain
1	C	77	ARG	Sidechain

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	1347	0	1347	21	0
1	C	1300	0	1306	19	0
1	G	1343	0	1353	23	0
1	J	1344	0	1356	28	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	G	1	0	0	0	0
4	C	20	0	0	5	0
5	A	58	0	0	0	0
5	C	46	0	0	1	0
5	G	22	0	0	1	0
5	J	24	0	0	0	0
All	All	5510	0	5362	84	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 8.

The worst 5 of 84 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:67:VAL:HG13	1:A:101:PRO:HB2	1.50	0.92
1:C:12:LYS:NZ	4:C:201:A1JS0:C8	2.47	0.78
1:C:12:LYS:HZ3	4:C:201:A1JS0:C8	2.00	0.75
1:J:159:ALA:HB3	1:J:162:ALA:HB2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:GLU:HG3	5:G:320:HOH:O	1.95	0.67

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	158/169 (94%)	145 (92%)	12 (8%)	1 (1%)	21 12
1	C	150/169 (89%)	147 (98%)	2 (1%)	1 (1%)	18 10
1	G	158/169 (94%)	145 (92%)	10 (6%)	3 (2%)	6 1
1	J	158/169 (94%)	148 (94%)	10 (6%)	0	100 100
All	All	624/676 (92%)	585 (94%)	34 (5%)	5 (1%)	16 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	C	22	PRO
1	G	15	GLN
1	G	89	MET
1	G	88	GLU

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	151/158 (96%)	133 (88%)	18 (12%)	5 1
1	C	146/158 (92%)	140 (96%)	6 (4%)	27 17
1	G	152/158 (96%)	146 (96%)	6 (4%)	28 18
1	J	152/158 (96%)	142 (93%)	10 (7%)	15 5
All	All	601/632 (95%)	561 (93%)	40 (7%)	15 5

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	97	ARG
1	J	88	GLU
1	G	147	TRP
1	J	45	GLU
1	J	97	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	126	HIS
1	G	127	GLN
1	J	16	GLN
1	G	151	GLN
1	C	126	HIS

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)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	A1JS0	C	201	-	22,22,22	0.56	0	25,32,32	1.05	1 (4%)

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
4	A1JS0	C	201	-	1/1/2/2	3/8/17/17	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	201	A1JS0	O5-C6-C19	4.05	124.04	119.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	201	A1JS0	C10

All (3) torsion outliers are listed below:

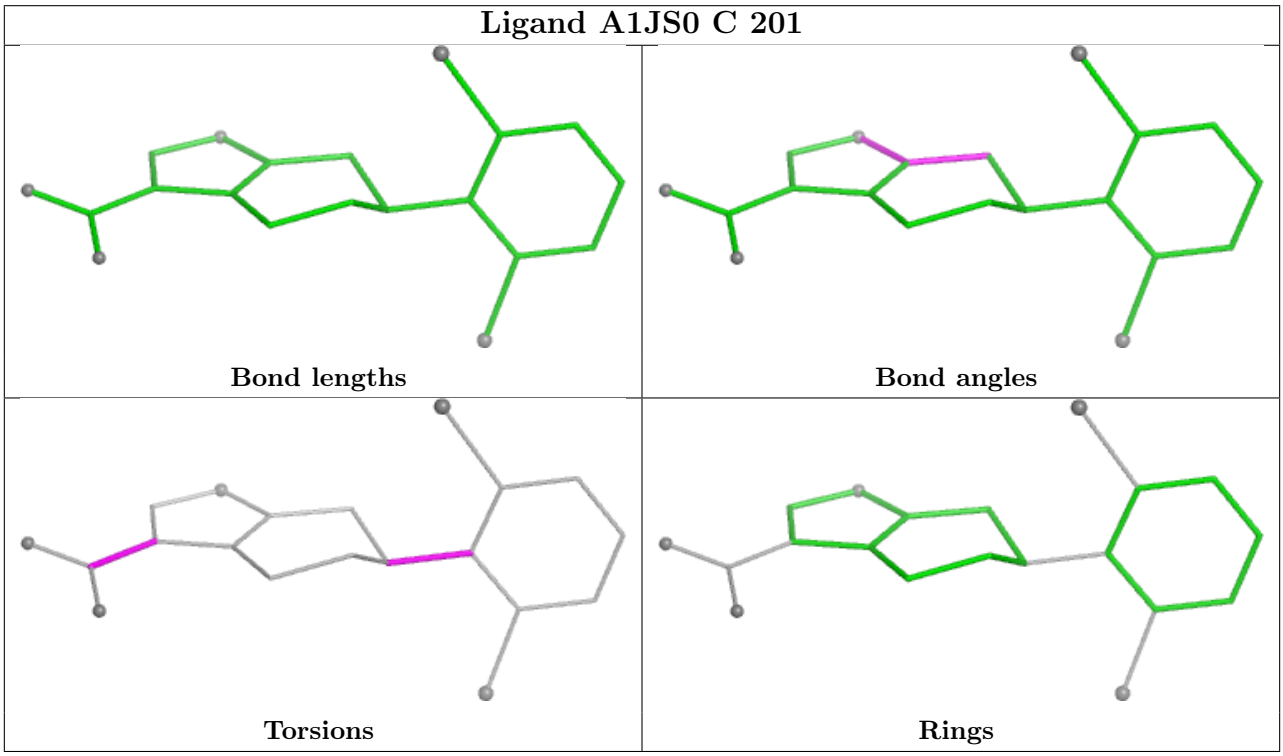
Mol	Chain	Res	Type	Atoms
4	C	201	A1JS0	C19-C10-C11-C17
4	C	201	A1JS0	O1-C2-C3-C7
4	C	201	A1JS0	O20-C2-C3-C7

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	A1JS0	5	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.



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

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	161/169 (95%)	1.19	27 (16%)	4	4	21, 52, 76, 97	1 (0%)
1	C	156/169 (92%)	1.03	21 (13%)	7	7	29, 46, 69, 109	0
1	G	161/169 (95%)	1.74	47 (29%)	1	1	45, 71, 100, 107	1 (0%)
1	J	162/169 (95%)	1.79	54 (33%)	1	0	30, 75, 98, 104	0
All	All	640/676 (94%)	1.44	149 (23%)	2	2	21, 63, 95, 109	2 (0%)

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	PRO	6.3
1	G	79	ILE	5.9
1	C	168	LEU	5.1
1	G	159	ALA	4.8
1	G	20	THR	4.8

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

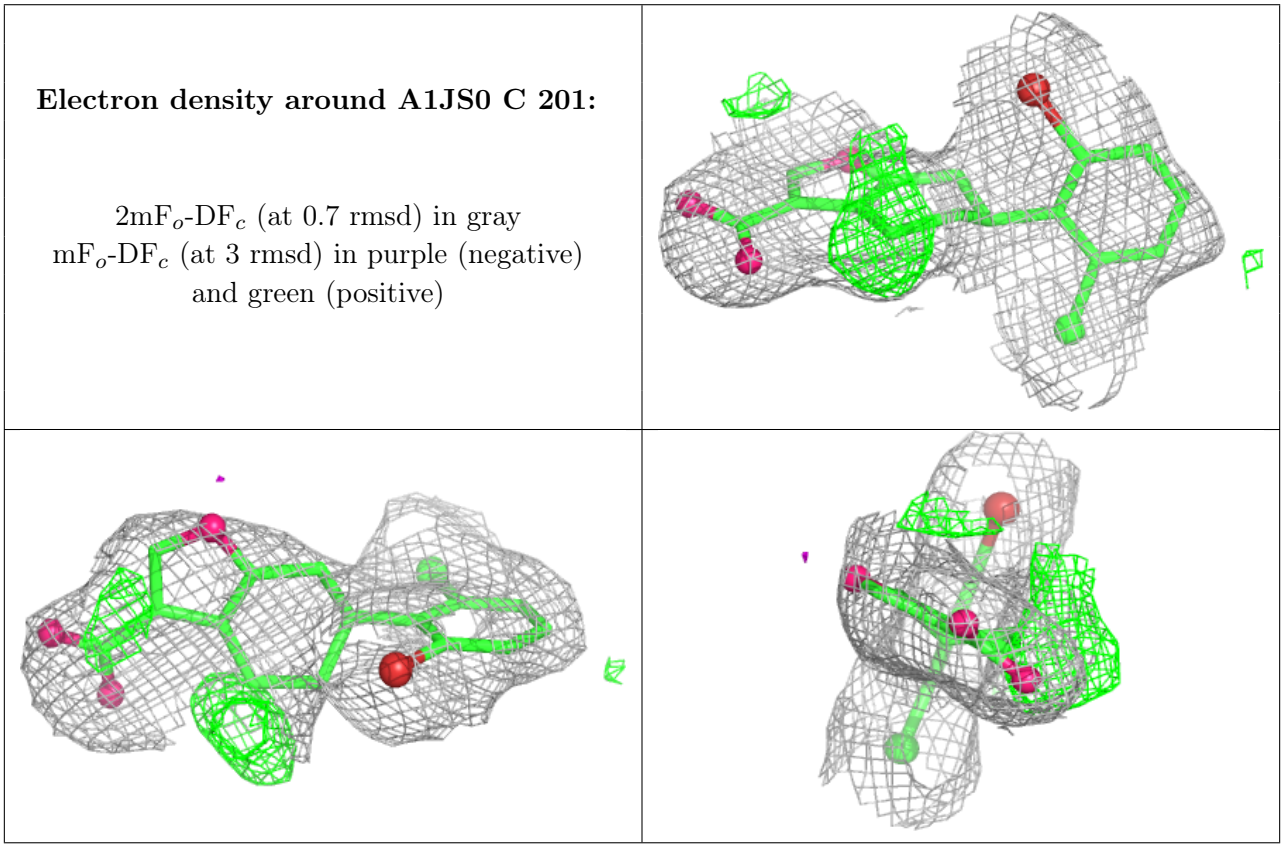
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	G	202	1/1	0.81	0.14	55,55,55,55	0
4	A1JS0	C	201	20/20	0.83	0.14	74,77,82,84	0
3	MG	A	202	1/1	0.87	0.09	41,41,41,41	0
2	ZN	J	201	1/1	0.95	0.09	62,62,62,62	0
2	ZN	G	201	1/1	0.96	0.07	56,56,56,56	0
2	ZN	C	202	1/1	0.97	0.05	45,45,45,45	0
2	ZN	A	201	1/1	0.97	0.09	48,48,48,48	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 A1JS0 C 201:

$2mF_o$-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.