



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2025 – 01:13 pm BST

PDB ID : 9R5Z / pdb\_00009r5z  
Title : Crystal structure of JAK3 with GCL258  
Authors : Wang, G.Q.; Chaikuad, A.; Hillebrand, L.; Gehring, M.; Knapp, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2025-05-11  
Resolution : 1.80 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

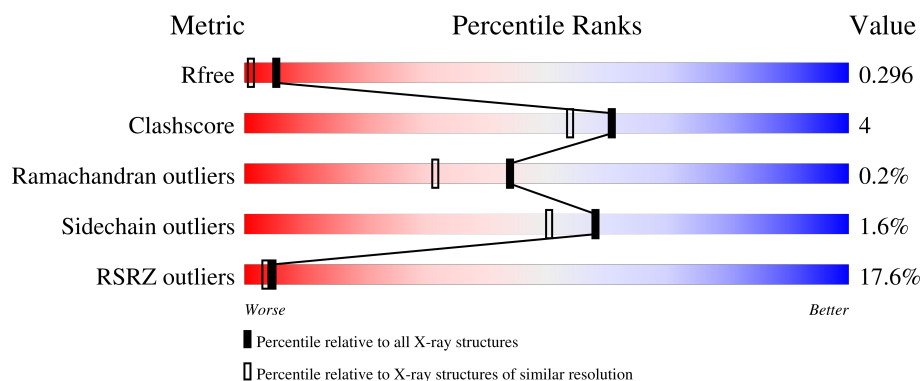
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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  $\geq 3$ , 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	294	<div> <div>26%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
1	B	294	<div> <div>6%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4462 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.

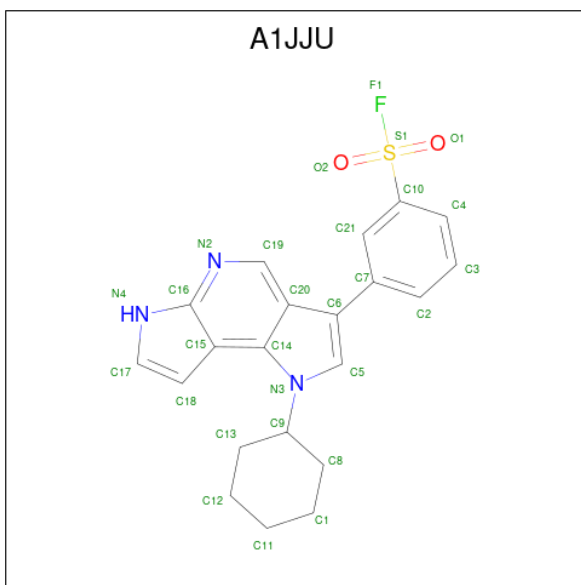
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1988	1277	341	357	13			
1	B	275	Total	C	N	O	S	0	0	0
			2180	1395	381	390	14			

There are 10 discrepancies between the modelled and reference sequences:

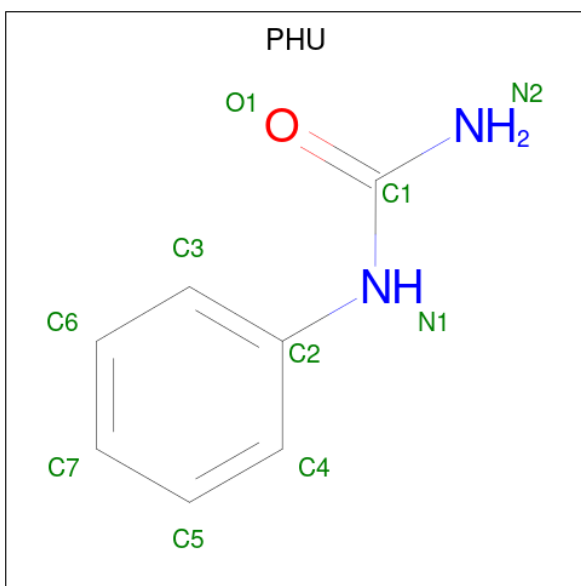
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	SER	-	expression tag	UNP P52333
A	-10	MET	-	expression tag	UNP P52333
A	128	ALA	ASP	conflict	UNP P52333
A	218A	SER	CYS	conflict	UNP P52333
A	225	SER	CYS	conflict	UNP P52333
B	-11	SER	-	expression tag	UNP P52333
B	-10	MET	-	expression tag	UNP P52333
B	128	ALA	ASP	conflict	UNP P52333
B	217B	SER	CYS	conflict	UNP P52333
B	225	SER	CYS	conflict	UNP P52333

- Molecule 2 is 3-(3-cyclohexyl-3,8,10-triazatricyclo[7.3.0.0<sup>2,6</sup>]{2,6}]dodeca-1,4,6,8,11-pentaen-5-yl)benzenesulfonyl fluoride (CCD ID: A1JJU) (formula: C<sub>21</sub>H<sub>20</sub>FN<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			28	21	1	3	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			28	21	1	3	2	1		

- Molecule 3 is 1-phenylurea (CCD ID: PHU) (formula:  $C_7H_8N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	2	1		
3	B	1	Total	C	N	O	0	0
			10	7	2	1		

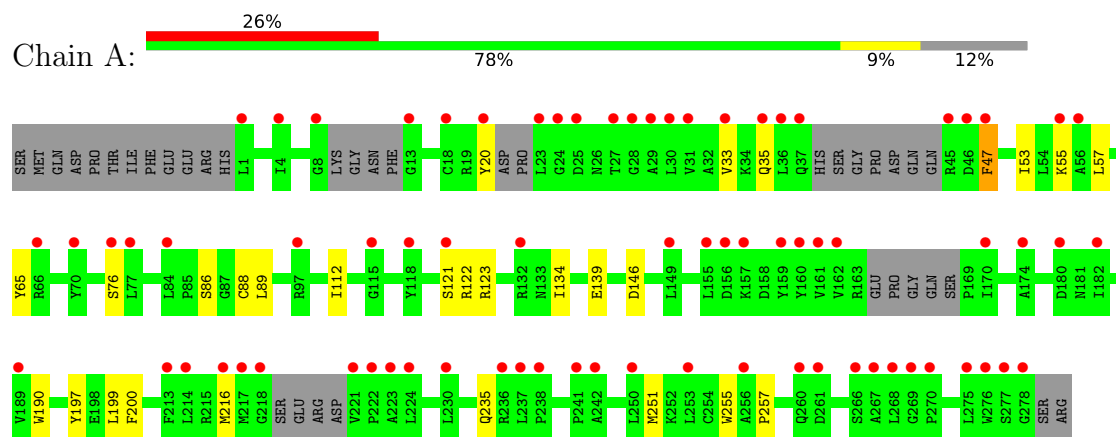
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total 78	O 78	0	0
4	B	140	Total 140	O 140	0	0

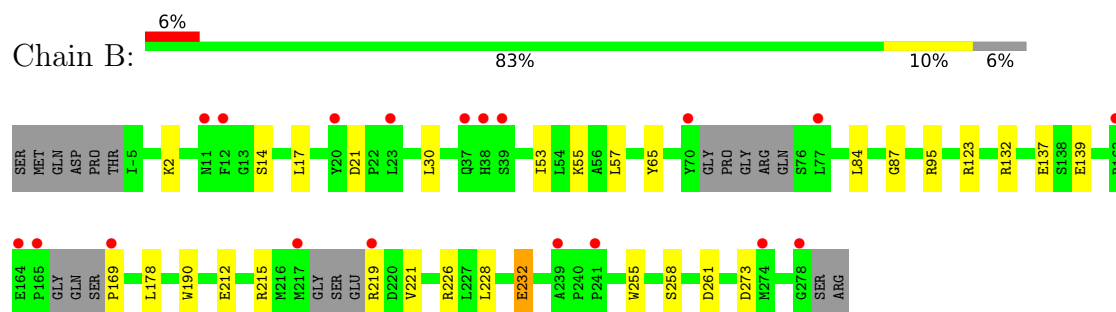
### 3 Residue-property plots [i](#)

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 JAK3



#### • Molecule 1: Tyrosine-protein kinase JAK3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.85Å 62.54Å 101.20Å 90.00° 93.71° 90.00°	Depositor
Resolution (Å)	41.80 – 1.80 41.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.80-1.80) 98.9 (41.80-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.236 , 0.289 0.251 , 0.296	Depositor DCC
$R_{free}$ test set	2393 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8369e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1JJU, PHU

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	0.56	0/2031	1.07	3/2749 (0.1%)
1	B	0.61	0/2231	1.06	2/3016 (0.1%)
All	All	0.59	0/4262	1.07	5/5765 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PHE	CA-CB-CG	8.68	122.48	113.80
1	A	20	TYR	CA-C-O	-7.79	107.56	120.80
1	B	273	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	232	GLU	CB-CA-C	-5.80	101.16	110.79
1	A	200	PHE	CA-CB-CG	-5.18	108.62	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	123	ARG	Sidechain
1	B	132	ARG	Sidechain

## 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	1988	0	1947	18	0
1	B	2180	0	2162	16	0
2	A	28	0	0	0	0
2	B	28	0	0	1	0
3	A	10	0	8	0	0
3	B	10	0	8	0	0
4	A	78	0	0	3	0
4	B	140	0	0	5	0
All	All	4462	0	4125	34	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 4.

All (34) 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:88:CYS:SG	4:A:429:HOH:O	2.55	0.64
1:A:257:PRO:HD2	4:A:449:HOH:O	1.96	0.64
1:A:197:TYR:HD1	1:A:251:MET:HE1	1.62	0.64
1:A:112:ILE:HD13	1:A:134:ILE:HD13	1.80	0.63
1:A:197:TYR:HB2	1:A:251:MET:HE3	1.81	0.62
1:A:216:MET:HE1	1:A:235:GLN:HB3	1.84	0.58
1:B:84:LEU:HD21	1:B:137:GLU:OE1	2.07	0.55
1:B:226:ARG:NE	4:B:403:HOH:O	2.39	0.55
1:A:251:MET:HE2	1:A:255:TRP:CH2	2.44	0.53
1:A:55:LYS:HG3	1:A:65:TYR:CE2	2.43	0.52
1:A:53:ILE:O	1:A:57:LEU:HG	2.12	0.50
1:A:33:VAL:HG12	1:A:35:GLN:NE2	2.27	0.50
1:B:55:LYS:HG3	1:B:65:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HB2	4:A:404:HOH:O	2.11	0.49
1:B:212:GLU:OE2	1:B:215:ARG:NH2	2.46	0.49
1:A:89:LEU:HD21	1:A:199:LEU:HD21	1.94	0.49
1:B:219:ARG:N	4:B:407:HOH:O	2.46	0.48
1:B:84:LEU:CD2	1:B:137:GLU:OE1	2.61	0.47
1:B:95:ARG:NH2	4:B:408:HOH:O	2.47	0.47
1:B:178:LEU:HB2	1:B:228:LEU:HD21	1.97	0.46
1:A:112:ILE:CD1	1:A:134:ILE:HD13	2.45	0.44
1:B:258:SER:OG	1:B:261:ASP:OD2	2.36	0.44
1:B:53:ILE:O	1:B:57:LEU:HG	2.18	0.43
1:A:251:MET:CE	1:A:255:TRP:HH2	2.32	0.42
1:B:169:PRO:HG2	4:B:521:HOH:O	2.19	0.42
1:A:121:SER:OG	1:A:122:ARG:NH1	2.53	0.42
1:B:17:LEU:HD11	1:B:30:LEU:HB3	2.02	0.42
1:B:87:GLY:HA2	2:B:301:A1JJU:C2	2.50	0.42
1:A:190:TRP:CE3	1:A:255:TRP:HA	2.55	0.42
1:B:219:ARG:HA	4:B:449:HOH:O	2.18	0.42
1:A:251:MET:CE	1:A:255:TRP:CH2	3.02	0.42
1:A:197:TYR:HD1	1:A:251:MET:CE	2.31	0.41
1:B:190:TRP:CE3	1:B:255:TRP:HA	2.56	0.41
1:B:2:LYS:CE	1:B:21:ASP:HB3	2.52	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	246/294 (84%)	239 (97%)	6 (2%)	1 (0%)	30	19
1	B	267/294 (91%)	264 (99%)	3 (1%)	0	100	100
All	All	513/588 (87%)	503 (98%)	9 (2%)	1 (0%)	44	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASP

### 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	208/256 (81%)	205 (99%)	3 (1%)	62	56
1	B	235/256 (92%)	231 (98%)	4 (2%)	56	47
All	All	443/512 (86%)	436 (98%)	7 (2%)	58	50

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	A	76	SER
1	A	139	GLU
1	B	14	SER
1	B	139	GLU
1	B	221	VAL
1	B	232	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	96	HIS
1	B	6	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](#)

4 ligands are 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	$\# Z  > 2$
3	PHU	A	302	-	10,10,10	0.27	0	12,12,12	0.38	0
2	A1JJU	A	301	-	27,32,32	0.94	1 (3%)	27,48,48	1.77	8 (29%)
2	A1JJU	B	301	-	27,32,32	0.81	1 (3%)	27,48,48	1.55	3 (11%)
3	PHU	B	302	-	10,10,10	0.24	0	12,12,12	0.27	0

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
3	PHU	A	302	-	-	2/4/4/4	0/1/1/1
2	A1JJU	A	301	-	-	9/10/22/22	0/5/5/5
2	A1JJU	B	301	-	-	5/10/22/22	0/5/5/5
3	PHU	B	302	-	-	2/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A1JJU	C19-N2	3.21	1.34	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A1JJU	C15-C16	-2.16	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	A1JJU	O2-S1-C10	-4.37	106.28	110.74
2	A	301	A1JJU	O2-S1-C10	-4.36	106.29	110.74
2	B	301	A1JJU	C20-C14-C15	-4.04	117.78	121.90
2	A	301	A1JJU	C20-C14-C15	-3.64	118.19	121.90
2	A	301	A1JJU	O1-S1-C10	-3.27	107.40	110.74
2	B	301	A1JJU	O1-S1-C10	-2.95	107.73	110.74
2	A	301	A1JJU	C13-C9-C8	2.56	115.05	110.16
2	A	301	A1JJU	C1-C8-C9	-2.24	108.26	111.57
2	A	301	A1JJU	O1-S1-O2	-2.08	112.57	119.07
2	A	301	A1JJU	C5-N3-C9	2.05	127.30	125.48
2	A	301	A1JJU	C11-C12-C13	2.02	115.53	111.42

There are no chirality outliers.

All (18) torsion outliers are listed below:

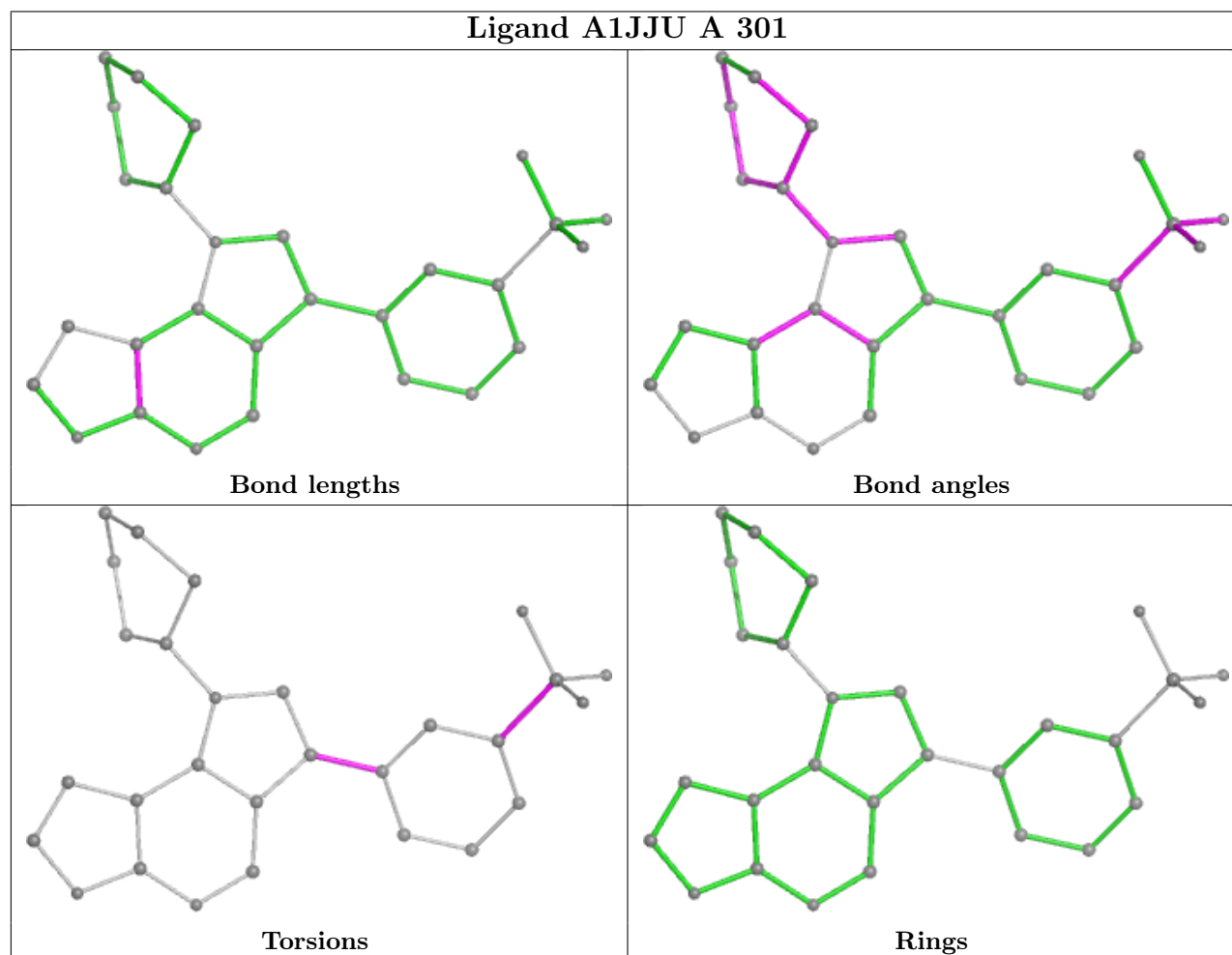
Mol	Chain	Res	Type	Atoms
2	A	301	A1JJU	C5-C6-C7-C2
2	A	301	A1JJU	C20-C6-C7-C2
2	A	301	A1JJU	C4-C10-S1-F1
2	A	301	A1JJU	C4-C10-S1-O2
2	A	301	A1JJU	C4-C10-S1-O1
2	A	301	A1JJU	C21-C10-S1-O2
2	A	301	A1JJU	C21-C10-S1-O1
2	B	301	A1JJU	C5-C6-C7-C2
2	B	301	A1JJU	C20-C6-C7-C2
2	B	301	A1JJU	C4-C10-S1-O2
2	B	301	A1JJU	C21-C10-S1-O2
2	A	301	A1JJU	C21-C10-S1-F1
2	B	301	A1JJU	C4-C10-S1-F1
3	A	302	PHU	C3-C2-N1-C1
3	A	302	PHU	C4-C2-N1-C1
3	B	302	PHU	C3-C2-N1-C1
3	B	302	PHU	C4-C2-N1-C1
2	A	301	A1JJU	C20-C6-C7-C21

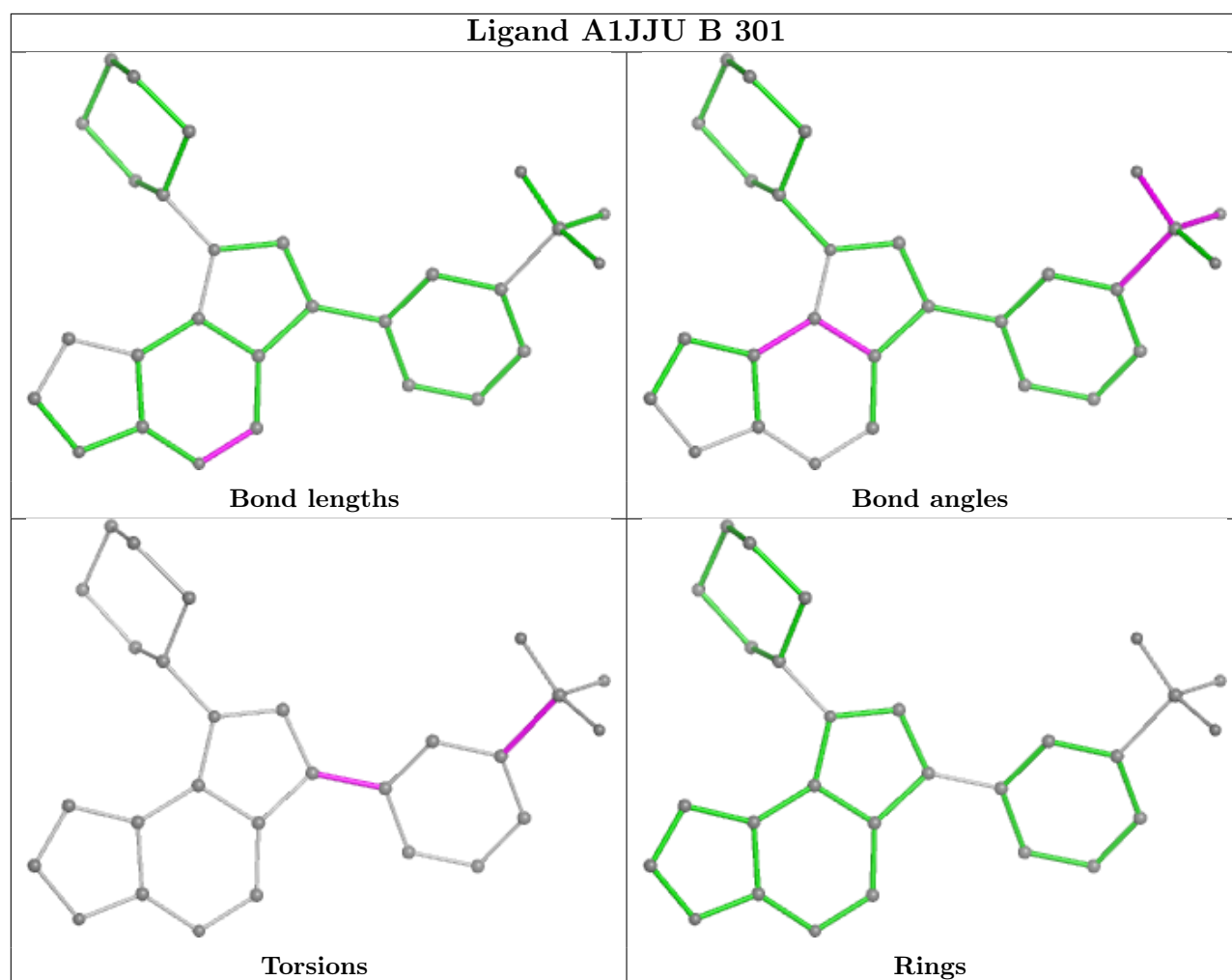
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	A1JJU	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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/294 (87%)	1.59	75 (29%) <b>1</b> <b>1</b>	20, 34, 54, 72	0
1	B	275/294 (93%)	0.46	19 (6%) <b>24</b> <b>21</b>	14, 23, 42, 65	0
All	All	533/588 (90%)	1.01	94 (17%) <b>4</b> <b>3</b>	14, 29, 51, 72	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	THR	5.6
1	A	23	LEU	5.3
1	B	38	HIS	5.1
1	A	24	GLY	5.0
1	A	221	VAL	5.0
1	A	45	ARG	4.5
1	A	18	CYS	4.5
1	A	1	LEU	4.4
1	A	20	TYR	4.3
1	B	70	TYR	4.2
1	A	278	GLY	4.1
1	A	241	PRO	4.0
1	A	29	ALA	4.0
1	A	70	TYR	3.9
1	A	267	ALA	3.9
1	A	155	LEU	3.8
1	B	12	PHE	3.7
1	B	217	MET	3.6
1	B	11	ASN	3.6
1	A	28	GLY	3.5
1	A	13	GLY	3.5
1	A	36	LEU	3.4
1	B	169	PRO	3.4
1	A	213	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	8	GLY	3.3
1	B	219	ARG	3.3
1	A	37	GLN	3.3
1	A	242	ALA	3.2
1	A	97	ARG	3.2
1	A	161	VAL	3.1
1	A	217	MET	3.0
1	A	256	ALA	3.0
1	B	278	GLY	3.0
1	B	241	PRO	2.9
1	A	159	TYR	2.9
1	A	35	GLN	2.9
1	A	30	LEU	2.9
1	A	214	LEU	2.9
1	A	253	LEU	2.9
1	A	47	PHE	2.9
1	A	277	SER	2.9
1	A	182	ILE	2.8
1	A	276	TRP	2.8
1	A	260	GLN	2.8
1	A	270	PRO	2.7
1	A	46	ASP	2.7
1	A	268	LEU	2.7
1	A	162	VAL	2.7
1	A	236	ARG	2.7
1	A	160	TYR	2.6
1	B	165	PRO	2.6
1	A	76	SER	2.6
1	A	118	TYR	2.6
1	B	39	SER	2.6
1	A	31	VAL	2.5
1	B	274	MET	2.5
1	A	4	ILE	2.5
1	A	25	ASP	2.5
1	A	174	ALA	2.5
1	A	250	LEU	2.4
1	B	239	ALA	2.4
1	A	238	PRO	2.4
1	A	132	ARG	2.3
1	A	216	MET	2.3
1	A	157	LYS	2.3
1	B	20	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	66	ARG	2.3
1	A	33	VAL	2.3
1	A	180	ASP	2.3
1	B	37	GLN	2.3
1	A	170	ILE	2.3
1	A	223	ALA	2.3
1	B	164	GLU	2.3
1	A	77	LEU	2.3
1	A	224	LEU	2.3
1	A	149	LEU	2.2
1	A	269	GLY	2.2
1	A	156	ASP	2.2
1	A	56	ALA	2.2
1	A	84	LEU	2.2
1	A	222	PRO	2.2
1	B	163	ARG	2.2
1	A	237	LEU	2.1
1	B	77	LEU	2.1
1	A	55	LYS	2.1
1	A	115	GLY	2.1
1	A	218	GLY	2.1
1	A	189	VAL	2.1
1	A	261	ASP	2.1
1	A	121	SER	2.1
1	A	266	SER	2.1
1	A	275	LEU	2.1
1	A	230	LEU	2.0
1	B	23	LEU	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 oligosaccharides in this entry.

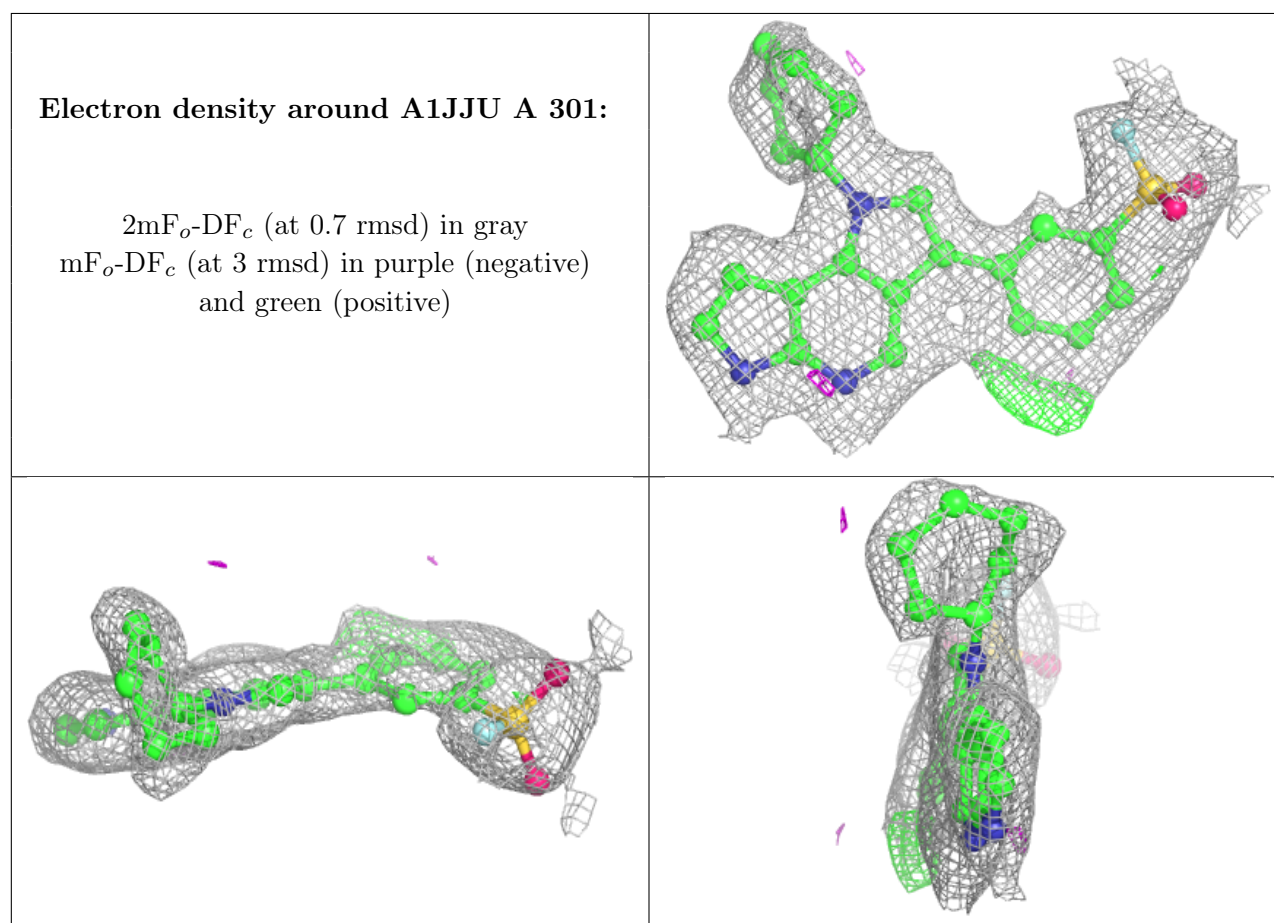
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

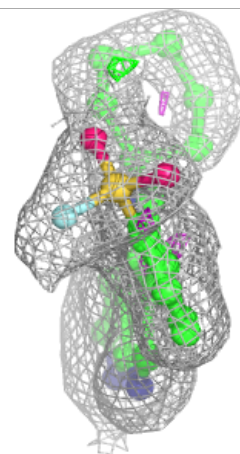
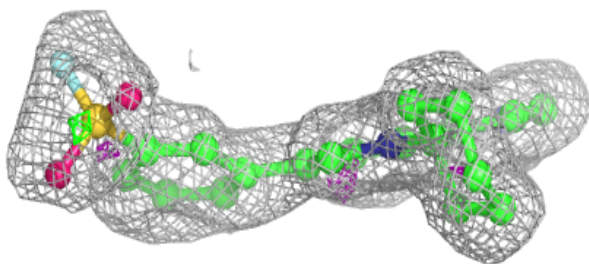
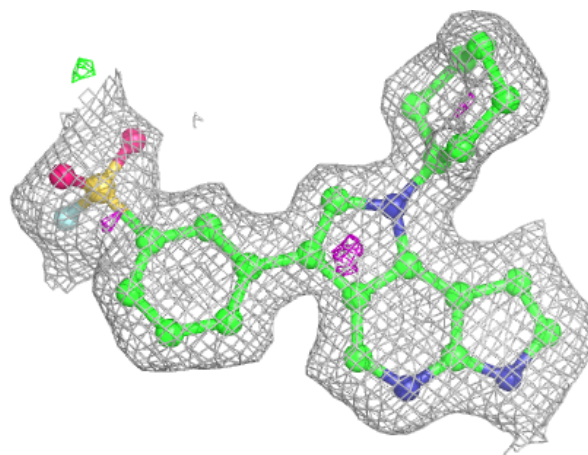
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1JJU	A	301	28/28	0.81	0.14	22,34,59,67	0
3	PHU	A	302	10/10	0.84	0.20	0,0,0,0	0
2	A1JJU	B	301	28/28	0.88	0.11	17,22,46,53	0
3	PHU	B	302	10/10	0.91	0.16	0,0,0,0	0

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 A1JJU B 301:**

$2mF_o-DF_c$  (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.