



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 2, 2025 – 07:40 pm BST

PDB ID : 9RJ8 / pdb\_00009rj8  
Title : SARS-CoV-2 with a bound inhibitor  
Authors : Mac Sweeney, A.  
Deposited on : 2025-06-12  
Resolution : 1.43 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 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

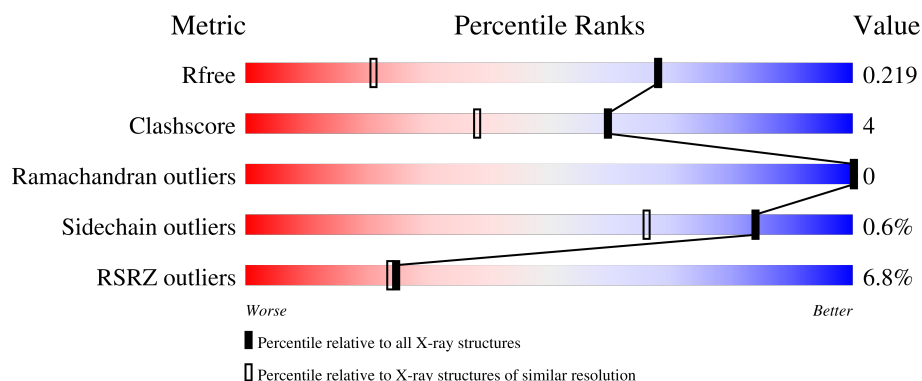
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

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	306	<div> <div>3%</div> <div>91%</div> <div>8% ..</div> </div>
1	B	306	<div> <div>10%</div> <div>88%</div> <div>11% .</div> </div>

## 2 Entry composition [i](#)

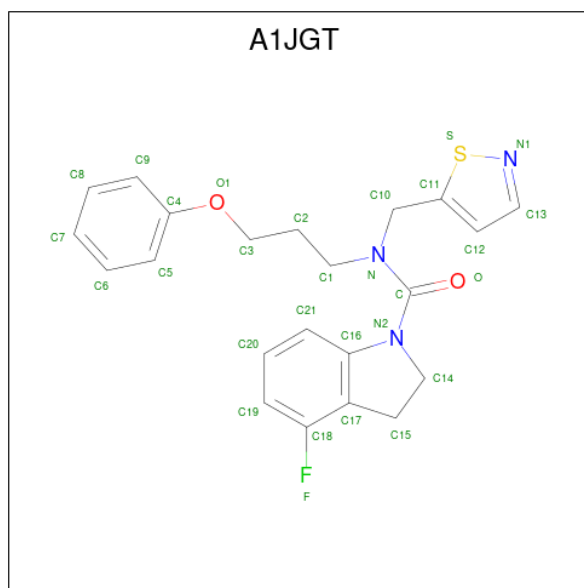
There are 3 unique types of molecules in this entry. The entry contains 9734 atoms, of which 4610 are hydrogens and 0 are deuteriums.

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 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	H	N	O	S	166	0	0
			4625	1475	2292	398	438	22			
1	B	302	Total	C	H	N	O	S	167	3	0
			4597	1467	2274	393	439	24			

- Molecule 2 is 4-fluoranyl- {N}-(3-phenoxypropyl)- {N}-(1,2-thiazol-5-ylmethyl)-2,3-dihydro indole-1-carboxamide (CCD ID: A1JGT) (formula: C<sub>22</sub>H<sub>22</sub>FN<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	S	0	0
			51	22	1	22	3	2	1		
2	B	1	Total	C	F	H	N	O	S	0	0
			51	22	1	22	3	2	1		


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	252	Total 252	O 252	0	0
3	B	158	Total 158	O 158	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.

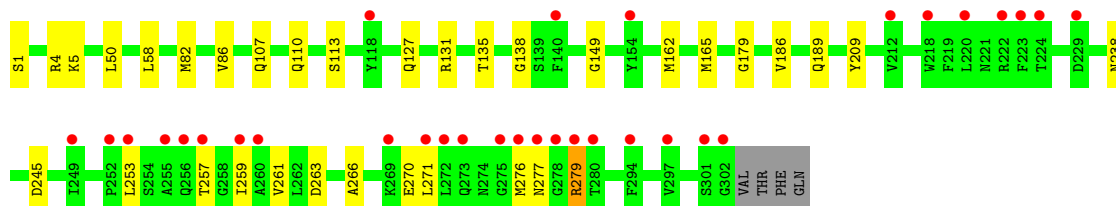
- Molecule 1: 3C-like proteinase nsp5

Chain A:  3% 91% 8% ..



- Molecule 1: 3C-like proteinase nsp5

Chain B:  10% 88% 11% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.80Å 101.81Å 103.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.73 – 1.43 72.73 – 1.43	Depositor EDS
% Data completeness (in resolution range)	74.3 (72.73-1.43) 74.3 (72.73-1.43)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.159 , 0.217 0.167 , 0.219	Depositor DCC
$R_{free}$ test set	6605 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: A1JGT

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	0.62	0/2384	0.96	2/3240 (0.1%)
1	B	0.60	0/2376	0.99	1/3230 (0.0%)
All	All	0.61	0/4760	0.98	3/6470 (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
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	127	GLN	CB-CG-CD	6.23	123.19	112.60
1	B	263	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	187	ASP	CA-CB-CG	5.58	118.18	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	4	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	2333	2292	2283	17	0
1	B	2323	2274	2257	24	0
2	A	29	22	0	0	0
2	B	29	22	0	0	0
3	A	252	0	0	4	0
3	B	158	0	0	3	0
All	All	5124	4610	4540	39	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 (39) 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:B:245:ASP:HB2	3:B:571:HOH:O	1.78	0.82
1:B:107:GLN:H	1:B:110:GLN:HE21	1.27	0.81
1:B:86:VAL:HG22	1:B:162[B]:MET:HE1	1.66	0.78
1:B:165:MET:HE1	1:B:186:VAL:O	1.83	0.77
1:B:86:VAL:HG22	1:B:162[B]:MET:CE	2.28	0.63
1:B:50:LEU:HD12	1:B:189:GLN:HE21	1.65	0.62
1:B:266:ALA:O	1:B:270:GLU:HG2	2.02	0.60
1:A:286:LEU:CD1	3:A:692:HOH:O	2.50	0.59
1:A:165:MET:HE1	1:A:192:GLN:NE2	2.17	0.58
1:B:50:LEU:CD1	1:B:189:GLN:HE21	2.16	0.58
1:A:5:LYS:HD3	3:A:504:HOH:O	2.08	0.54
1:A:166:GLU:OE1	1:B:1:SER:HB2	2.08	0.53
1:B:277:ASN:O	1:B:279:ARG:HG3	2.08	0.53
1:B:58:LEU:HD22	1:B:82:MET:HE3	1.90	0.53
1:B:50:LEU:HD12	1:B:189:GLN:NE2	2.28	0.48
1:B:113:SER:O	1:B:149:GLY:HA2	2.14	0.47
1:B:271:LEU:HD22	1:B:276:MET:HG3	1.97	0.47
1:B:86:VAL:HG23	1:B:179:GLY:HA2	1.97	0.46
1:A:286:LEU:HD22	1:A:286:LEU:C	2.41	0.45
1:A:113:SER:O	1:A:149:GLY:HA2	2.16	0.45
1:A:43:ILE:HB	1:A:61:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:HG23	3:B:521:HOH:O	2.18	0.44
1:B:245:ASP:CB	3:B:571:HOH:O	2.53	0.43
1:A:86:VAL:HG23	1:A:179:GLY:HA2	2.01	0.43
1:A:49:MET:HB3	1:A:189:GLN:HG3	2.01	0.43
1:B:131:ARG:HG2	1:B:135:THR:O	2.19	0.43
1:B:209:TYR:CG	1:B:253:LEU:HB3	2.55	0.42
1:A:47:GLU:H	1:A:47:GLU:CD	2.26	0.42
1:A:164:HIS:HD2	3:A:607:HOH:O	2.03	0.42
1:B:5:LYS:HG3	1:B:127:GLN:HB3	2.01	0.42
1:B:257:THR:CB	1:B:259:ILE:HD12	2.49	0.41
1:A:47:GLU:OE1	1:A:47:GLU:N	2.38	0.41
1:A:62:SER:OG	1:A:64:HIS:CE1	2.73	0.41
1:B:209:TYR:HB2	1:B:253:LEU:HD13	2.02	0.41
1:A:2:GLY:HA3	1:B:138:GLY:O	2.21	0.41
1:A:186:VAL:HG23	1:A:188:ARG:HB3	2.03	0.41
1:A:210:ALA:HB2	1:A:296:VAL:HG13	2.03	0.40
1:A:286:LEU:HD13	3:A:692:HOH:O	2.18	0.40
1:B:82:MET:HE3	1:B:82:MET:HB2	2.00	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	301/306 (98%)	297 (99%)	4 (1%)	0	100	100
1	B	303/306 (99%)	297 (98%)	6 (2%)	0	100	100
All	All	604/612 (99%)	594 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	259/263 (98%)	257 (99%)	2 (1%)	79	58
1	B	257/263 (98%)	256 (100%)	1 (0%)	89	78
All	All	516/526 (98%)	513 (99%)	3 (1%)	84	66

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	286	LEU
1	B	238	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	74	GLN
1	A	107	GLN
1	A	164	HIS
1	A	273	GLN
1	B	72	ASN
1	B	74	GLN
1	B	110	GLN
1	B	189	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

2 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$
2	A1JGT	B	401	-	31,32,32	0.64	1 (3%)	36,43,43	1.51	3 (8%)
2	A1JGT	A	401	-	31,32,32	0.82	2 (6%)	36,43,43	1.20	3 (8%)

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	A1JGT	B	401	-	-	3/18/28/28	0/4/4/4
2	A1JGT	A	401	-	-	3/18/28/28	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1JGT	C12-C11	2.51	1.44	1.37
2	A	401	A1JGT	C-N	2.28	1.41	1.36
2	B	401	A1JGT	C-N	2.25	1.41	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A1JGT	C14-N2-C	6.93	128.96	118.64
2	A	401	A1JGT	C14-N2-C	4.89	125.92	118.64
2	B	401	A1JGT	C13-C12-C11	3.65	111.73	105.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1JGT	C13-C12-C11	3.40	111.30	105.46
2	B	401	A1JGT	C11-C10-N	2.67	118.11	113.65
2	A	401	A1JGT	C11-C10-N	2.43	117.71	113.65

There are no chirality outliers.

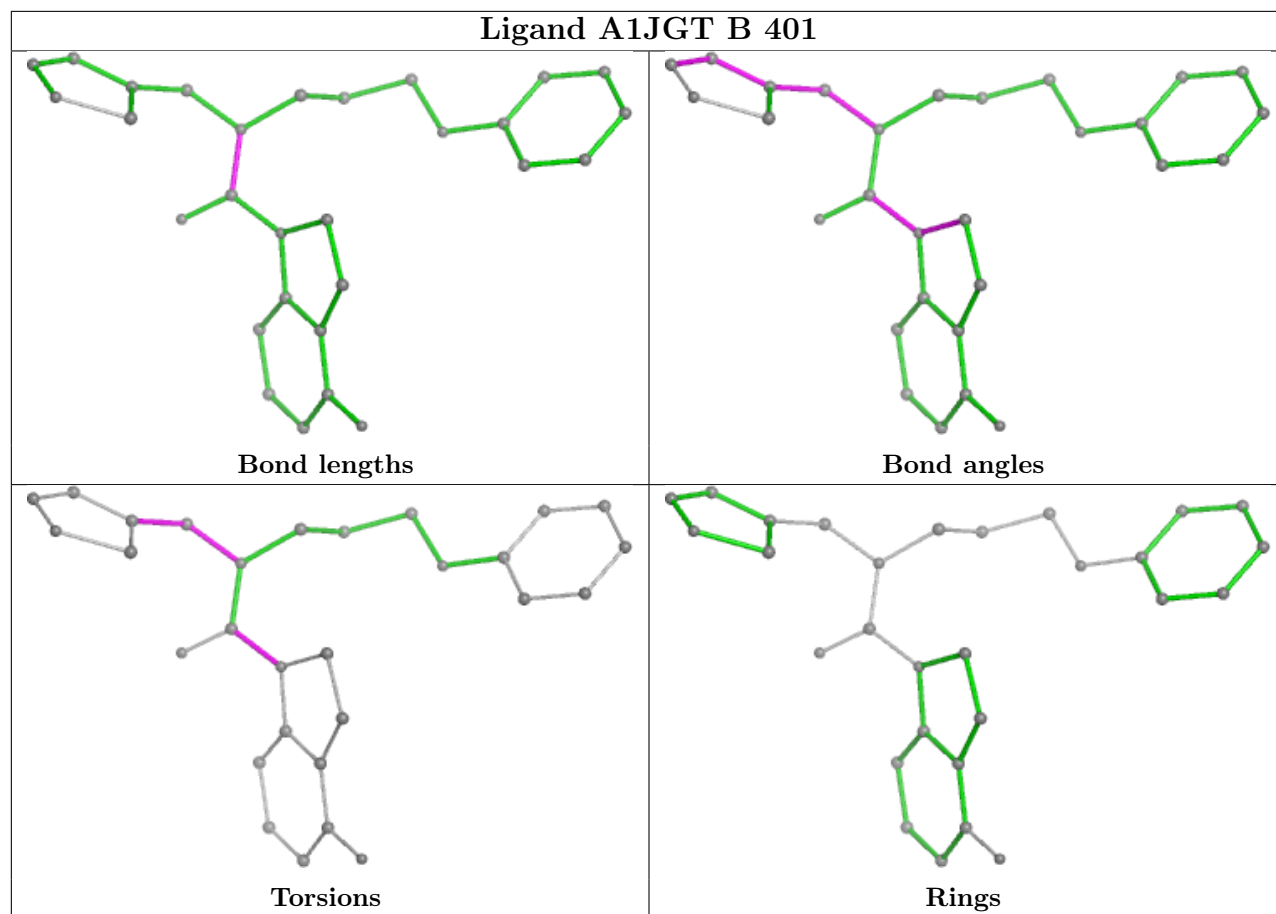
All (6) torsion outliers are listed below:

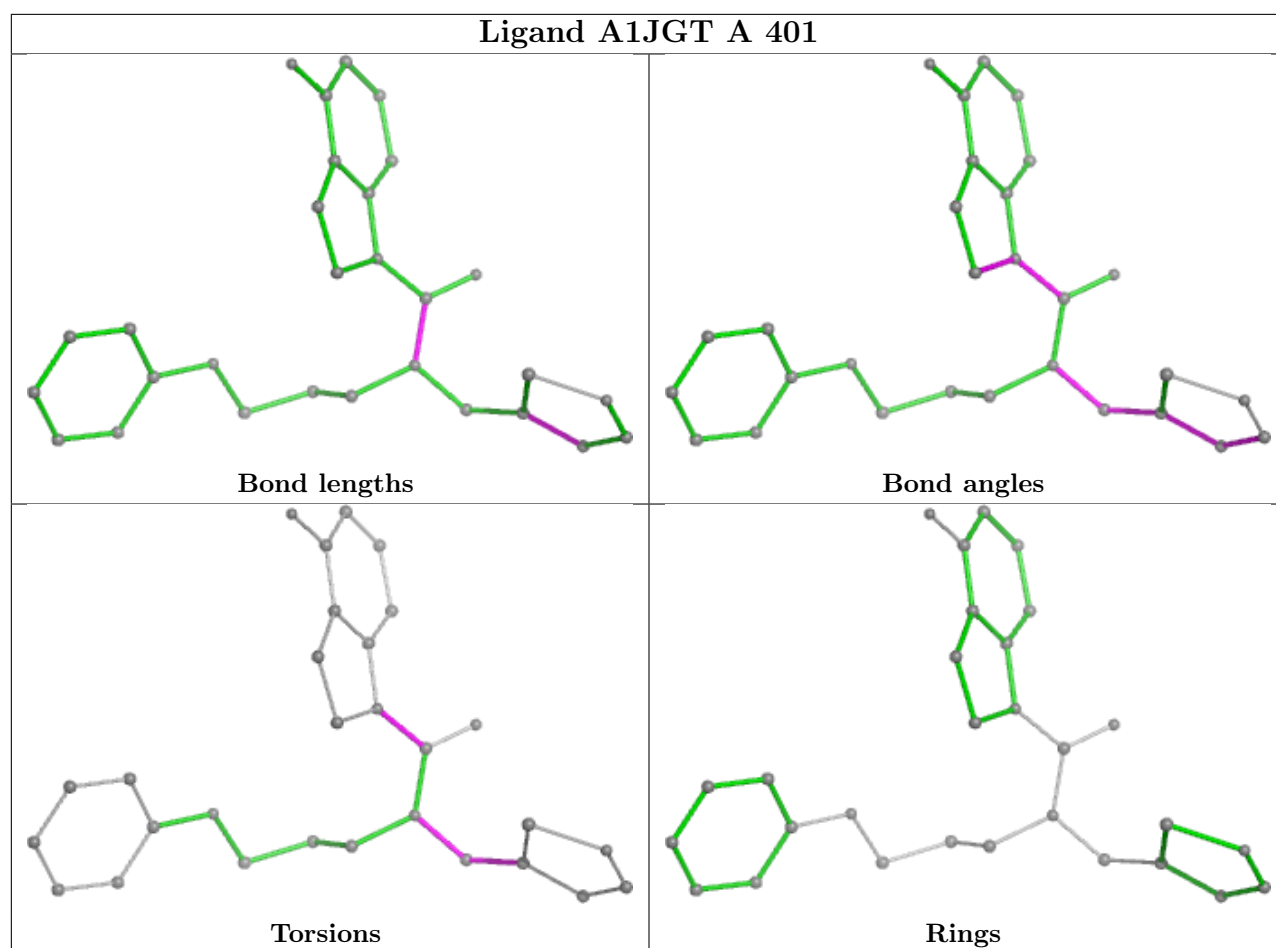
Mol	Chain	Res	Type	Atoms
2	A	401	A1JGT	N-C10-C11-C12
2	A	401	A1JGT	O-C-N2-C16
2	B	401	A1JGT	N-C10-C11-C12
2	A	401	A1JGT	C11-C10-N-C
2	B	401	A1JGT	C11-C10-N-C
2	B	401	A1JGT	O-C-N2-C16

There are no ring outliers.

No monomer is involved in short contacts.

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	303/306 (99%)	-0.16	9 (2%) 52 53	15, 25, 42, 73	0
1	B	302/306 (98%)	0.36	32 (10%) 13 11	11, 32, 59, 103	3 (0%)
All	All	605/612 (98%)	0.10	41 (6%) 25 24	11, 27, 55, 103	3 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	PHE	6.2
1	A	303	VAL	5.4
1	B	278	GLY	4.5
1	B	302	GLY	4.5
1	B	257	THR	4.2
1	B	273	GLN	3.7
1	B	218	TRP	3.6
1	B	140	PHE	3.4
1	B	276	MET	3.4
1	B	279	ARG	3.4
1	A	154	TYR	3.4
1	B	222	ARG	3.3
1	B	280	THR	3.3
1	B	275	GLY	3.3
1	B	154	TYR	3.2
1	B	253	LEU	2.9
1	B	271	LEU	2.9
1	B	255	ALA	2.9
1	A	3	PHE	2.8
1	B	277	ASN	2.8
1	B	252	PRO	2.7
1	A	294	PHE	2.7
1	B	301	SER	2.7
1	A	302	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	212	VAL	2.7
1	B	118	TYR	2.7
1	B	259	ILE	2.6
1	A	189	GLN	2.6
1	A	196	THR	2.5
1	B	249	ILE	2.5
1	A	249	ILE	2.5
1	B	224	THR	2.5
1	B	260	ALA	2.4
1	B	297	VAL	2.3
1	A	286	LEU	2.3
1	B	220	LEU	2.3
1	B	256	GLN	2.2
1	B	272	LEU	2.2
1	B	269	LYS	2.2
1	B	294	PHE	2.1
1	B	229	ASP	2.1

## 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<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.

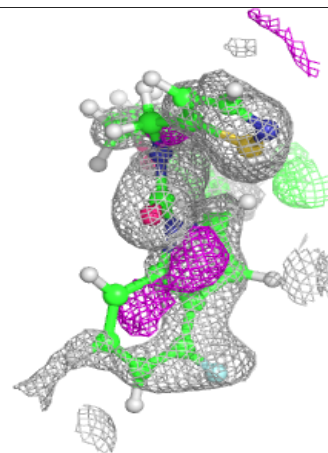
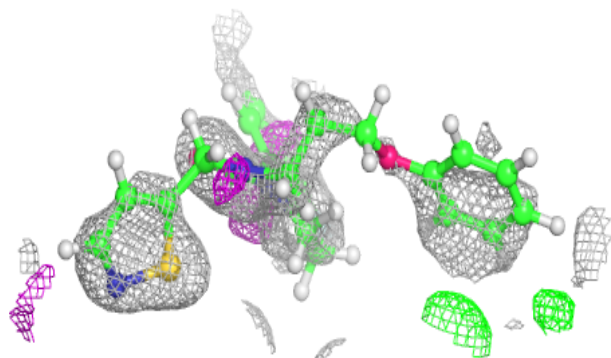
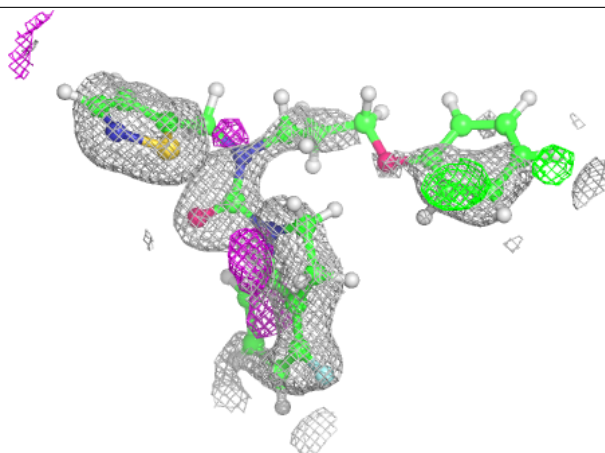
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1JGT	B	401	29/29	0.86	0.17	35,59,75,79	0
2	A1JGT	A	401	29/29	0.93	0.11	32,43,50,54	0

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.



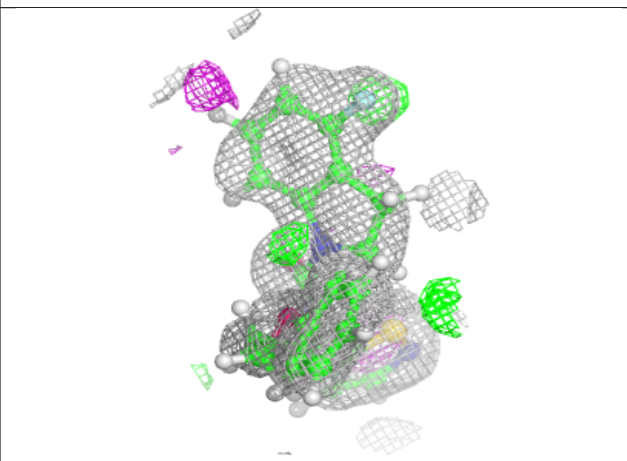
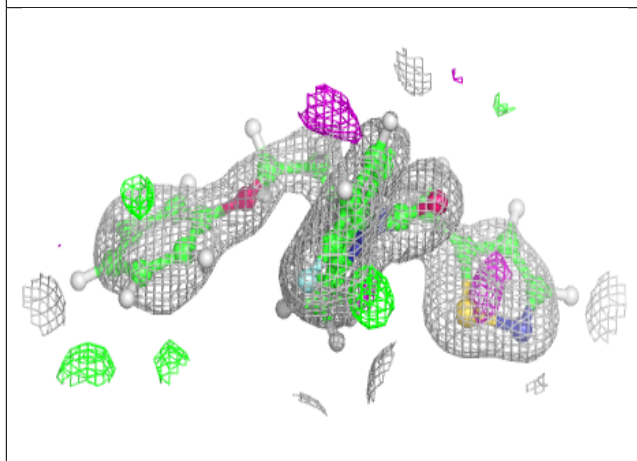
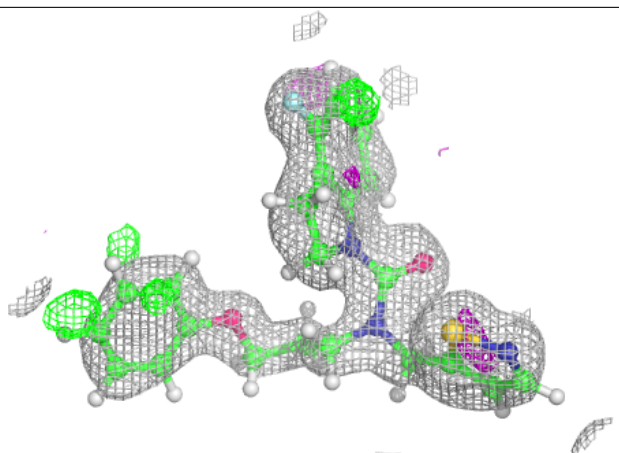
**Electron density around A1JGT B 401:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1JGT A 401:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.