



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 07:07 pm GMT

PDB ID : 7NEO  
Title : Crystal Structure of SARS-CoV-2 main protease (Nsp5) in complex with compound 15  
Authors : Talibov, V.O.  
Deposited on : 2021-02-04  
Resolution : 1.64 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

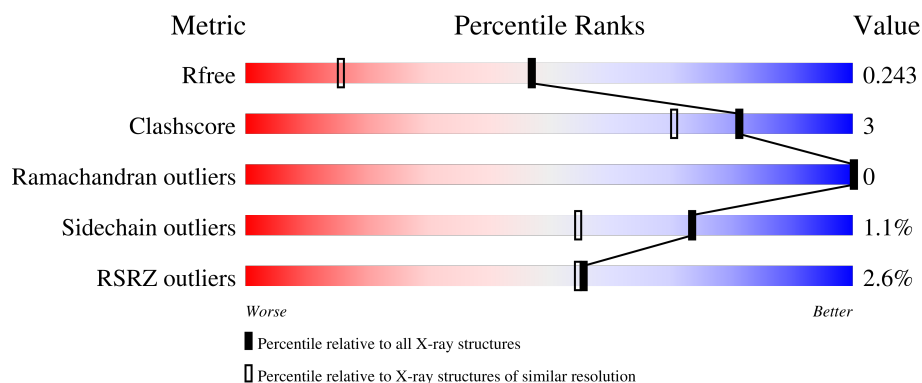
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

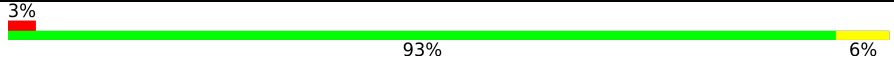
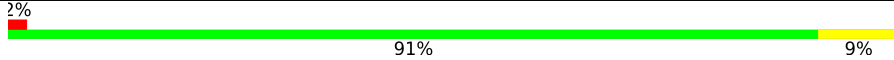
The reported resolution of this entry is 1.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	AAA	306	
1	BBB	306	

## 2 Entry composition [i](#)

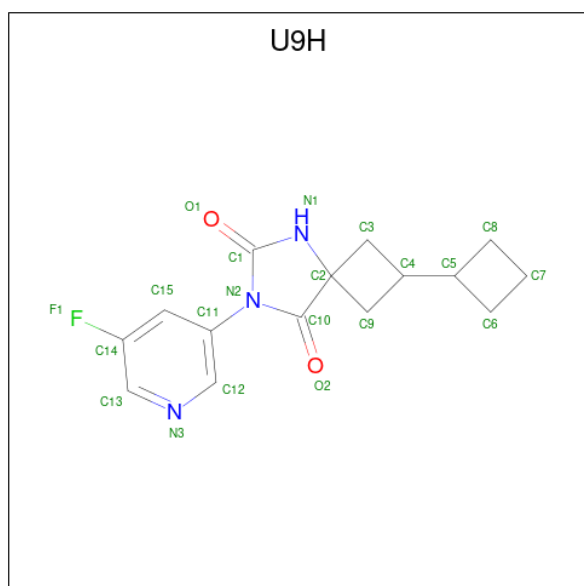
There are 4 unique types of molecules in this entry. The entry contains 5343 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	305	Total	C	N	O	S	0	6	0
			2391	1512	405	451	23			
1	BBB	305	Total	C	N	O	S	0	8	0
			2390	1514	404	448	24			

- Molecule 2 is 2-cyclobutyl-7-(5-fluoropyridin-3-yl)-5,7-diazaspiro[3.4]octane-6,8-dione (three-letter code: U9H) (formula:  $C_{15}H_{16}FN_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	0	0
			21	15	1	3	2		
2	BBB	1	Total	C	F	N	O	0	0
			21	15	1	3	2		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
3	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
3	BBB	1	Total	C	O	S	0	0
			4	2	1	1		
3	BBB	1	Total	C	O	S	0	0
			4	2	1	1		
3	BBB	1	Total	C	O	S	0	0
			4	2	1	1		
3	BBB	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	221	Total	O	0	0
			221	221		
4	BBB	271	Total	O	0	0
			271	271		

### 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



- Molecule 1: 3C-like proteinase nsp5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.57Å 53.82Å 114.77Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	48.63 – 1.64 48.58 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-1.64) 99.0 (48.58-1.64)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.201 , 0.239 0.209 , 0.243	Depositor DCC
$R_{free}$ test set	3165 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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 94.48 % 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 2.7686e-09. 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: DMS, U9H

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	AAA	0.74	0/2444	0.88	0/3321
1	BBB	0.72	0/2443	0.87	0/3319
All	All	0.73	0/4887	0.87	0/6640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	AAA	2391	0	2326	10	0
1	BBB	2390	0	2332	15	0
2	AAA	21	0	0	0	0
2	BBB	21	0	0	0	0
3	AAA	8	0	12	0	0
3	BBB	20	0	30	0	0
4	AAA	221	0	0	2	0
4	BBB	271	0	0	5	0
All	All	5343	0	4700	25	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 3.

All (25) 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:BBB:189:GLN:OE1	4:BBB:502:HOH:O	2.04	0.74
1:BBB:41:HIS:NE2	4:BBB:501:HOH:O	1.94	0.74
1:BBB:40:ARG:HA	1:BBB:87:LEU:HG	1.84	0.60
1:AAA:86:VAL:HG13	1:AAA:179:GLY:HA2	1.91	0.52
1:BBB:50:LEU:HD12	1:BBB:51:ASN:N	2.28	0.49
1:BBB:145:CYS:SG	4:BBB:501:HOH:O	2.23	0.47
1:AAA:256:GLN:NE2	4:AAA:510:HOH:O	2.46	0.47
1:AAA:113:SER:O	1:AAA:149:GLY:HA2	2.15	0.46
1:BBB:113:SER:O	1:BBB:149:GLY:HA2	2.16	0.46
1:AAA:24:THR:HG23	4:AAA:503:HOH:O	2.17	0.43
1:BBB:101:TYR:HA	1:BBB:157:VAL:O	2.18	0.43
1:AAA:218:TRP:CE3	1:AAA:279:ARG:CZ	3.02	0.43
1:BBB:21:THR:HB	1:BBB:67:LEU:HB2	2.00	0.42
1:BBB:207:TRP:CE2	1:BBB:288[A]:GLU:HB3	2.55	0.42
1:AAA:36:VAL:HG21	1:AAA:68:VAL:HG11	2.02	0.42
1:BBB:115:LEU:HD11	1:BBB:122:PRO:HB3	2.02	0.42
1:AAA:121:SER:HA	1:AAA:122:PRO:HD3	1.88	0.41
1:BBB:109:GLY:HA2	1:BBB:200:ILE:HD13	2.02	0.41
1:BBB:69:GLN:HG2	1:BBB:71:GLY:O	2.20	0.41
1:AAA:126:TYR:HE1	1:AAA:128[B]:CYS:SG	2.43	0.41
1:AAA:109:GLY:HA2	1:AAA:200:ILE:HD13	2.03	0.41
1:AAA:6:MET:HE3	1:AAA:6:MET:HB2	1.93	0.40
1:BBB:24:THR:CG2	4:BBB:509:HOH:O	2.69	0.40
1:BBB:24:THR:HG22	4:BBB:509:HOH:O	2.21	0.40
1:BBB:153:ASP:C	1:BBB:153:ASP:OD1	2.59	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	AAA	307/306 (100%)	303 (99%)	4 (1%)	0	100	100
1	BBB	307/306 (100%)	302 (98%)	5 (2%)	0	100	100
All	All	614/612 (100%)	605 (98%)	9 (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	AAA	266/263 (101%)	264 (99%)	2 (1%)	81	68
1	BBB	266/263 (101%)	262 (98%)	4 (2%)	65	42
All	All	532/526 (101%)	526 (99%)	6 (1%)	73	55

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	27	LEU
1	AAA	154	TYR
1	BBB	27	LEU
1	BBB	46	SER
1	BBB	154	TYR
1	BBB	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	DMS	BBB	403	-	3,3,3	0.31	0	3,3,3	0.03	0
3	DMS	BBB	402	-	3,3,3	0.29	0	3,3,3	0.07	0
3	DMS	BBB	404	-	3,3,3	0.28	0	3,3,3	0.22	0
3	DMS	AAA	402	-	3,3,3	0.32	0	3,3,3	0.20	0
3	DMS	BBB	405	-	3,3,3	0.26	0	3,3,3	0.11	0
2	U9H	BBB	401	-	22,24,24	0.80	1 (4%)	24,37,37	1.09	2 (8%)
3	DMS	BBB	406	-	3,3,3	0.36	0	3,3,3	0.17	0
2	U9H	AAA	401	-	22,24,24	0.87	1 (4%)	24,37,37	1.12	2 (8%)
3	DMS	AAA	403	-	3,3,3	0.39	0	3,3,3	0.15	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
2	U9H	BBB	401	-	-	2/8/43/43	0/4/4/4
2	U9H	AAA	401	-	-	1/8/43/43	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	U9H	C2-C10	-3.34	1.49	1.52
2	BBB	401	U9H	C2-C10	-2.61	1.50	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	U9H	C3-C4-C9	2.93	90.20	87.49
2	AAA	401	U9H	C2-N1-C1	-2.85	111.73	113.48
2	BBB	401	U9H	C3-C4-C9	2.61	89.90	87.49
2	BBB	401	U9H	C2-N1-C1	-2.49	111.95	113.48

There are no chirality outliers.

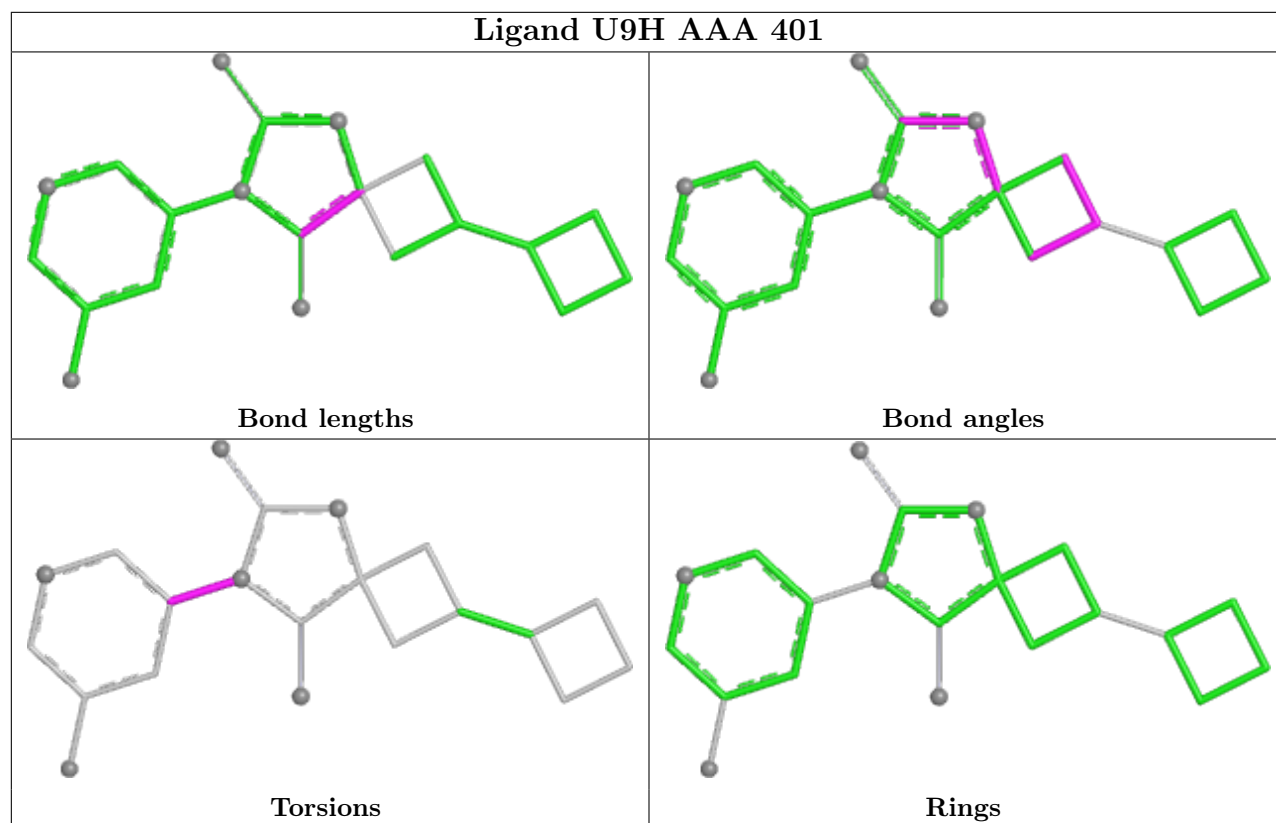
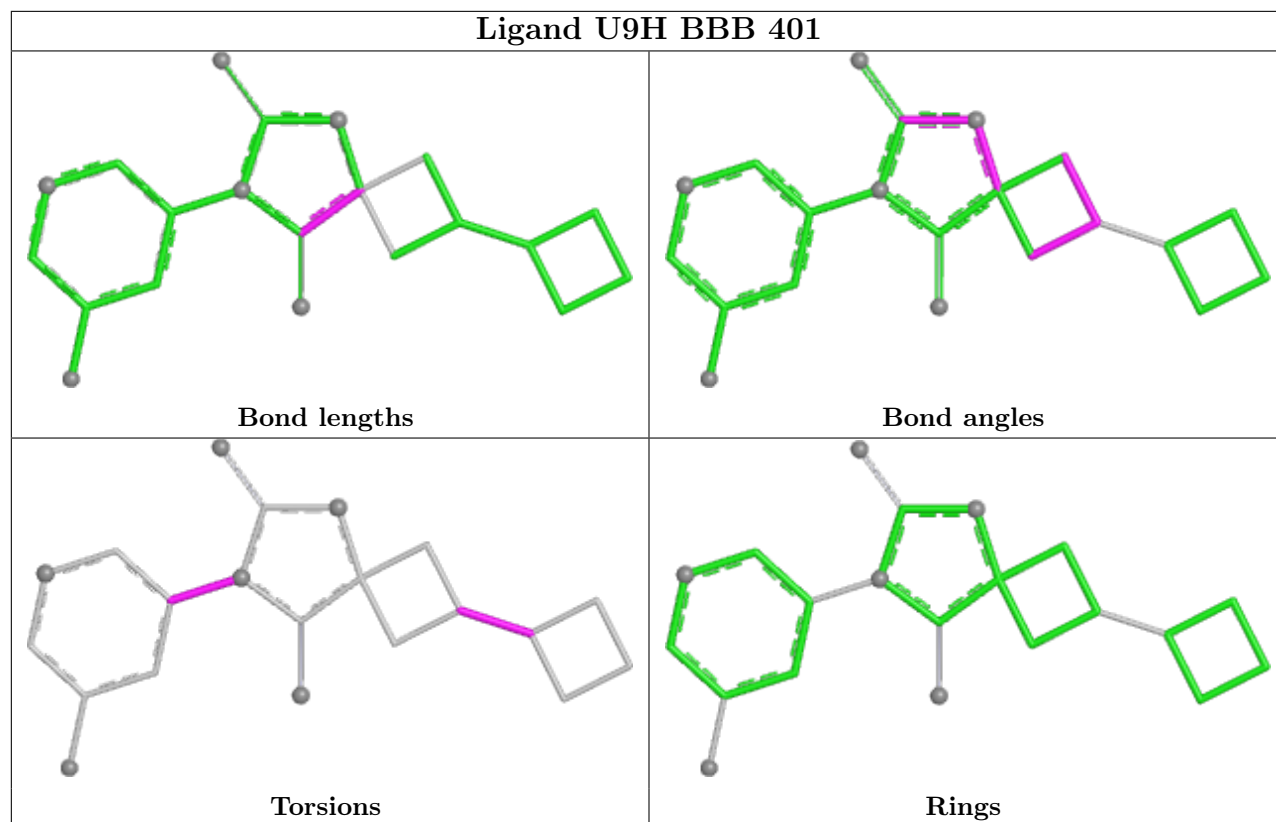
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	401	U9H	C9-C4-C5-C8
2	BBB	401	U9H	C12-C11-N2-C1
2	AAA	401	U9H	C12-C11-N2-C1

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 [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, 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	AAA	305/306 (99%)	0.08	9 (2%) 50 48	9, 19, 38, 52	0
1	BBB	305/306 (99%)	-0.13	7 (2%) 60 60	8, 15, 34, 52	0
All	All	610/612 (99%)	-0.02	16 (2%) 56 55	8, 17, 36, 52	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	154	TYR	5.7
1	AAA	154	TYR	4.6
1	BBB	305	PHE	4.4
1	AAA	302	GLY	3.9
1	BBB	303	VAL	3.6
1	BBB	302	GLY	3.4
1	AAA	305	PHE	3.3
1	AAA	303	VAL	3.0
1	AAA	304	THR	2.7
1	BBB	294	PHE	2.7
1	BBB	304	THR	2.5
1	AAA	47	GLU	2.4
1	AAA	66	PHE	2.3
1	BBB	50	LEU	2.1
1	AAA	294	PHE	2.1
1	AAA	232	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

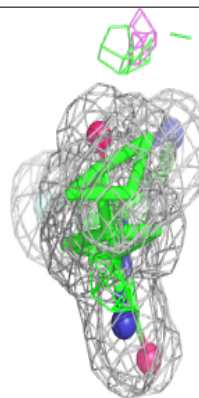
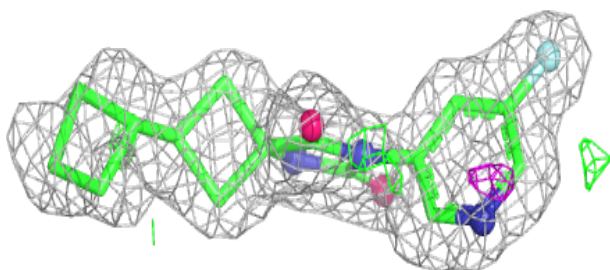
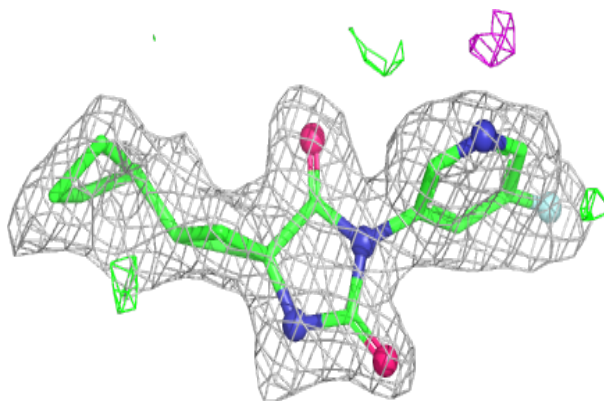
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMS	BBB	405	4/4	0.80	0.23	57,60,63,66	0
3	DMS	BBB	406	4/4	0.83	0.21	35,43,45,50	0
3	DMS	BBB	403	4/4	0.85	0.22	39,42,47,49	0
3	DMS	BBB	402	4/4	0.87	0.18	36,42,44,45	0
3	DMS	AAA	402	4/4	0.87	0.14	37,40,40,44	0
2	U9H	BBB	401	21/21	0.90	0.11	17,22,36,39	0
2	U9H	AAA	401	21/21	0.91	0.11	17,22,40,41	0
3	DMS	AAA	403	4/4	0.97	0.11	25,26,26,27	0
3	DMS	BBB	404	4/4	0.98	0.08	18,18,19,19	0

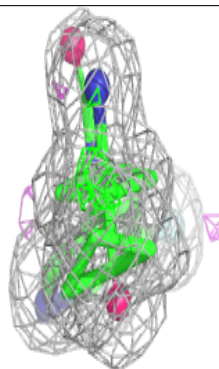
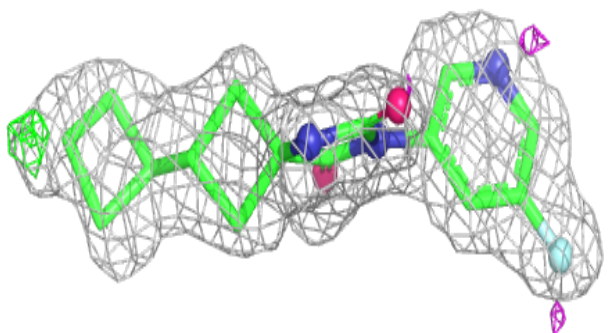
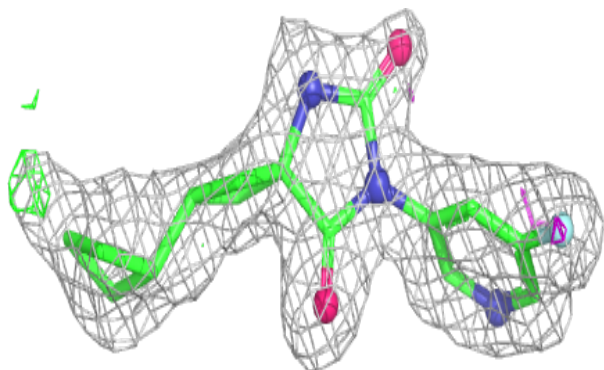
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around U9H BBB 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 U9H AAA 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 [i](#)

There are no such residues in this entry.