



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:16 PM EDT

PDB ID : 8DIF  
Title : Virtual screening for novel SARS-CoV-2 main protease non-covalent and covalent inhibitors  
Authors : Singh, I.; Shoichet, B.K.  
Deposited on : 2022-06-29  
Resolution : 1.98 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

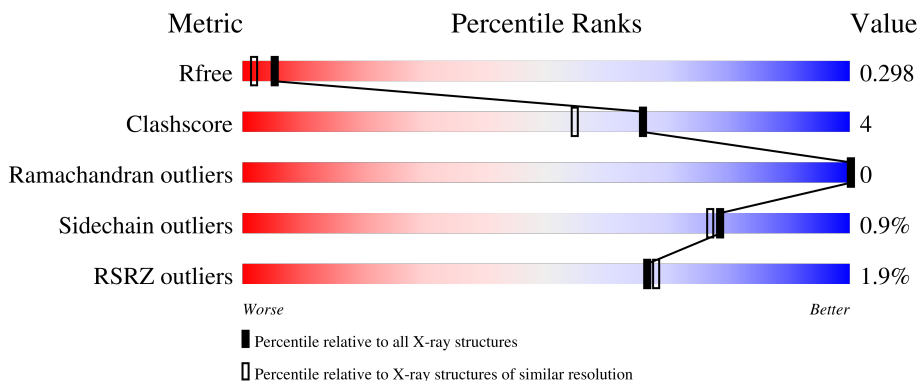
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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  $\geq 3$ , 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	 2% 89% 7% 5%
1	B	306	 2% 85% 10% 5%

## 2 Entry composition [i](#)

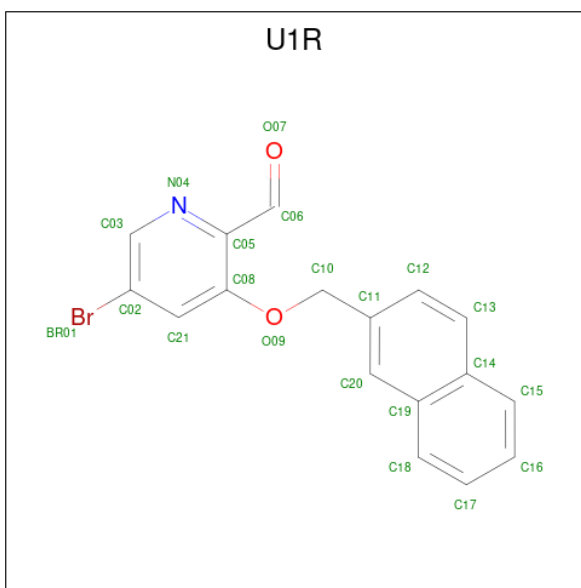
There are 3 unique types of molecules in this entry. The entry contains 4352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	292	Total	C	N	O	S	0	0	0
			2134	1352	359	403	20			
1	B	290	Total	C	N	O	S	0	0	0
			2123	1351	359	393	20			

- Molecule 2 is 5-bromo-3-[(naphthalen-2-yl)methoxy]pyridine-2-carbaldehyde (three-letter code: U1R) (formula: C<sub>17</sub>H<sub>12</sub>BrNO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
2	A	1	Total	Br	C	N	O	0	0
			21	1	17	1	2		
2	B	1	Total	Br	C	N	O	0	0
			21	1	17	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	29	Total O 29 29	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.90Å 53.62Å 115.04Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	56.43 – 1.98 56.43 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (56.43-1.98) 99.2 (56.43-1.98)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.240 , 0.294 0.248 , 0.298	Depositor DCC
$R_{free}$ test set	1838 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.01 % 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 3.0914e-07. 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: U1R

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	0.48	0/2177	0.58	0/2971
1	B	0.56	0/2168	0.62	0/2955
All	All	0.52	0/4345	0.60	0/5926

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	A	2134	0	1985	13	0
1	B	2123	0	1972	21	0
2	A	21	0	0	0	0
2	B	21	0	0	6	0
3	A	24	0	0	0	0
3	B	29	0	0	0	0
All	All	4352	0	3957	33	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 (33) 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:145:CYS:N	2:B:401:U1R:O07	2.19	0.75
1:A:106:ILE:HD12	1:A:106:ILE:C	2.18	0.64
1:A:285:ALA:HB3	1:B:285:ALA:HB3	1.86	0.57
1:A:167:LEU:HD12	1:A:171:VAL:HG23	1.89	0.55
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.88	0.55
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.74	0.53
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.91	0.52
1:B:167:LEU:HD12	1:B:171:VAL:HG23	1.93	0.51
1:A:25:THR:HG21	1:A:42:VAL:HA	1.93	0.50
1:B:188:ARG:O	2:B:401:U1R:C16	2.59	0.50
1:B:49:MET:CE	2:B:401:U1R:C13	2.90	0.49
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.49	0.48
1:B:126:TYR:HE1	1:B:128:CYS:HG	1.60	0.48
1:B:113:SER:O	1:B:149:GLY:HA2	2.14	0.48
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.50	0.47
1:B:17:MET:HG3	1:B:117:CYS:SG	2.55	0.47
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.15	0.46
1:A:113:SER:O	1:A:149:GLY:HA2	2.15	0.46
1:A:126:TYR:HE1	1:A:128:CYS:HG	1.64	0.45
1:A:140:PHE:HD2	1:A:172:HIS:CG	2.36	0.44
1:A:239:TYR:CZ	1:A:272:LEU:HD21	2.53	0.44
1:A:6:MET:HE3	1:A:6:MET:HB2	1.89	0.43
1:B:52:PRO:HG2	1:B:54:TYR:CE2	2.53	0.43
1:A:86:VAL:HG13	1:A:179:GLY:HA2	2.00	0.42
1:A:87:LEU:HD13	1:A:89:LEU:HD21	2.01	0.42
1:B:49:MET:HE1	2:B:401:U1R:C13	2.50	0.41
1:B:117:CYS:O	1:B:144:SER:HA	2.19	0.41
1:B:253:LEU:HD23	1:B:253:LEU:HA	1.84	0.41
1:B:6:MET:HE3	1:B:6:MET:HB2	1.79	0.41
1:B:10:SER:O	1:B:14:GLU:HG3	2.21	0.41
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.56	0.40
1:B:189:GLN:HA	2:B:401:U1R:C16	2.51	0.40
1:B:49:MET:HE2	2:B:401:U1R:C13	2.51	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	280/306 (92%)	275 (98%)	5 (2%)	0	100	100
1	B	278/306 (91%)	270 (97%)	8 (3%)	0	100	100
All	All	558/612 (91%)	545 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	221/263 (84%)	220 (100%)	1 (0%)	88	87
1	B	217/263 (82%)	214 (99%)	3 (1%)	67	62
All	All	438/526 (83%)	434 (99%)	4 (1%)	78	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	B	5	LYS
1	B	27	LEU
1	B	60	ARG

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

### 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 monosaccharides 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	U1R	B	401	1	23,23,23	1.94	7 (30%)	31,31,31	1.28	4 (12%)
2	U1R	A	401	1	23,23,23	1.86	5 (21%)	31,31,31	1.84	6 (19%)

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	U1R	B	401	1	-	4/7/7/7	0/3/3/3
2	U1R	A	401	1	-	2/7/7/7	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	U1R	C03-C02	6.12	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	U1R	C05-C06	-4.24	1.44	1.48
2	A	401	U1R	C03-C02	3.90	1.45	1.38
2	A	401	U1R	C19-C14	-3.16	1.35	1.42
2	B	401	U1R	C21-C08	3.03	1.44	1.38
2	A	401	U1R	C03-N04	-2.75	1.28	1.34
2	B	401	U1R	BR01-C02	2.54	1.95	1.90
2	B	401	U1R	C05-C06	-2.34	1.46	1.48
2	A	401	U1R	O07-C06	-2.18	1.14	1.21
2	B	401	U1R	C19-C14	-2.13	1.37	1.42
2	B	401	U1R	C16-C15	2.12	1.41	1.36
2	B	401	U1R	C12-C11	2.09	1.43	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	U1R	O07-C06-C05	-6.79	117.79	124.22
2	B	401	U1R	O07-C06-C05	-4.53	119.93	124.22
2	A	401	U1R	C03-N04-C05	2.88	121.83	117.39
2	A	401	U1R	C12-C13-C14	-2.71	116.63	120.82
2	B	401	U1R	C06-C05-N04	2.47	119.41	115.41
2	A	401	U1R	O09-C08-C05	2.34	122.38	116.87
2	A	401	U1R	C21-C08-C05	-2.21	117.17	121.24
2	A	401	U1R	C20-C19-C14	2.15	122.03	118.96
2	B	401	U1R	C03-N04-C05	2.15	120.70	117.39
2	B	401	U1R	C10-O09-C08	-2.02	113.79	117.76

There are no chirality outliers.

All (6) torsion outliers are listed below:

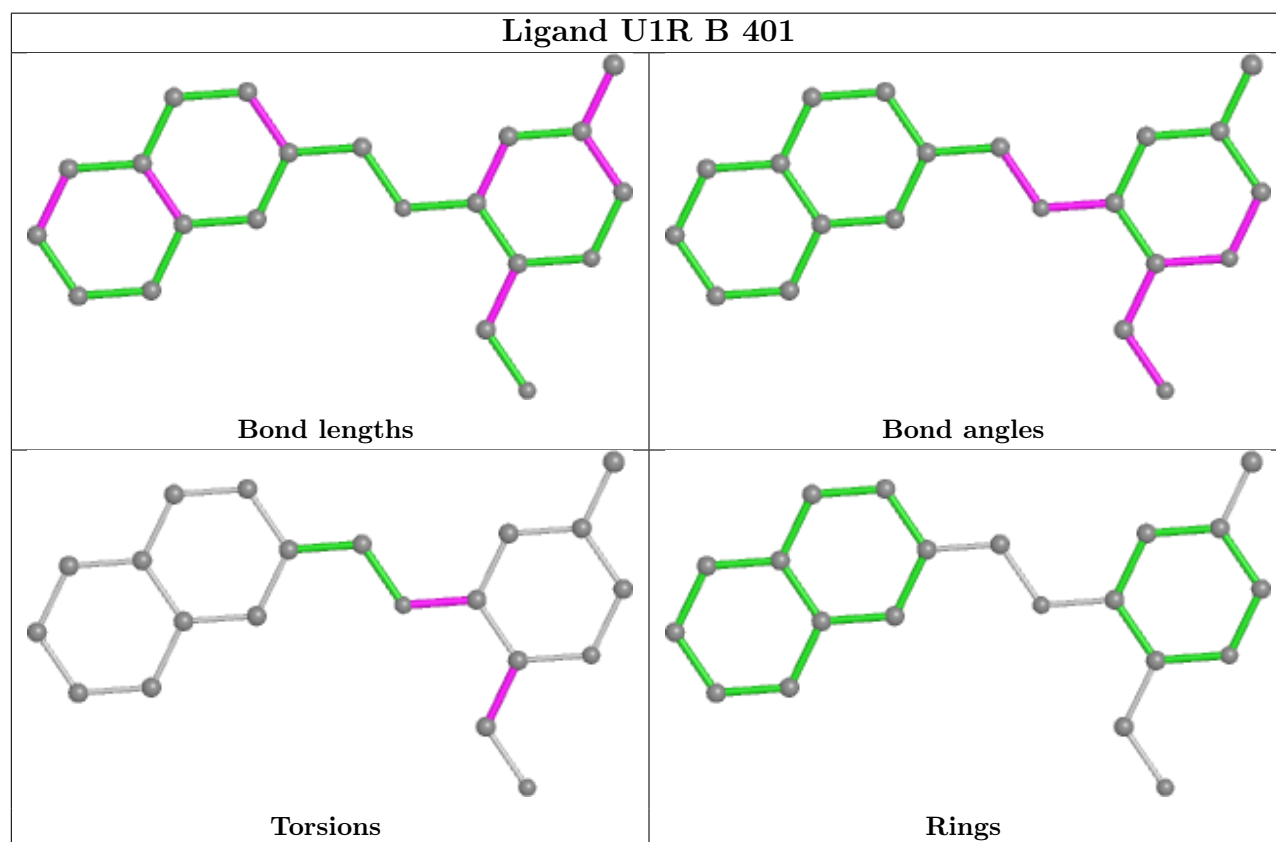
Mol	Chain	Res	Type	Atoms
2	A	401	U1R	N04-C05-C06-O07
2	B	401	U1R	N04-C05-C06-O07
2	B	401	U1R	C05-C08-O09-C10
2	B	401	U1R	C21-C08-O09-C10
2	B	401	U1R	C08-C05-C06-O07
2	A	401	U1R	C08-C05-C06-O07

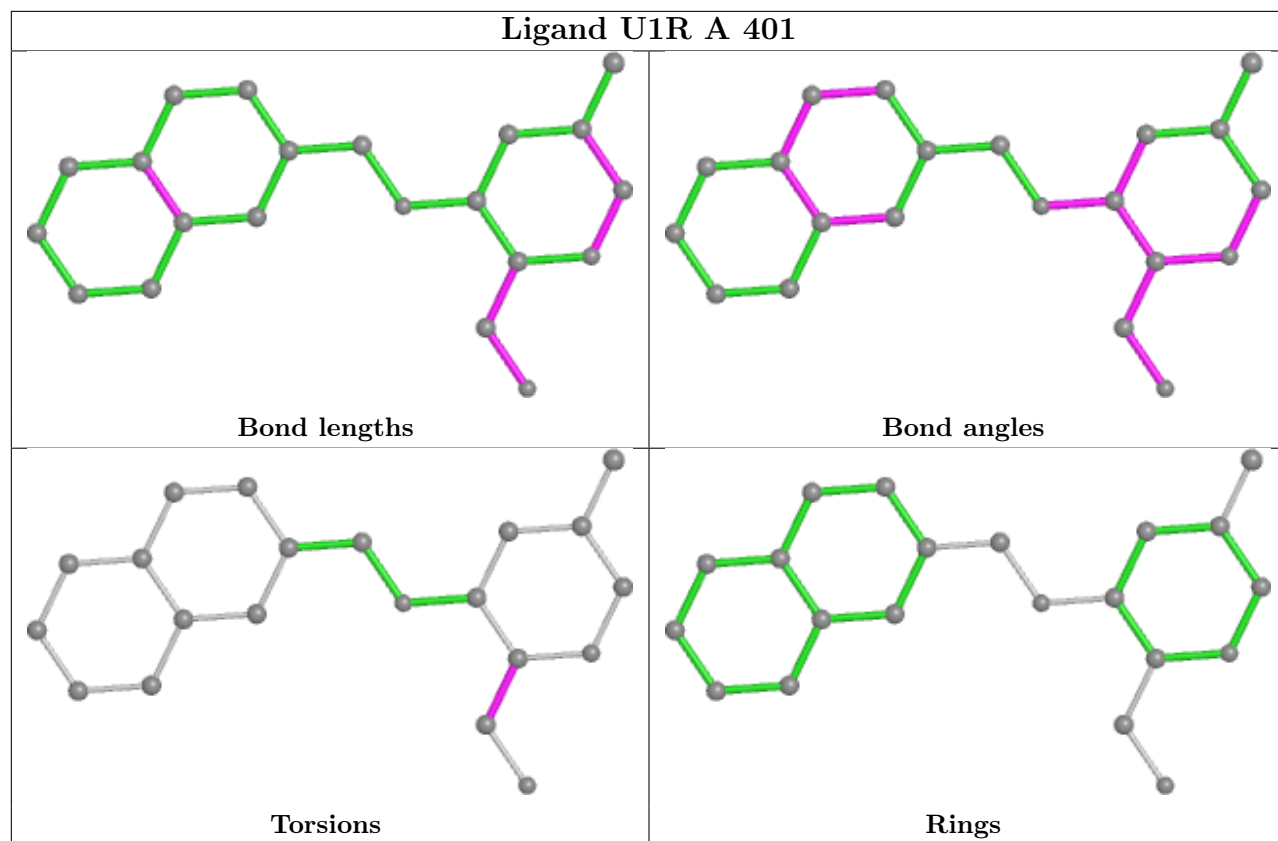
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	U1R	6	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, 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	292/306 (95%)	0.13	6 (2%) 63 65	28, 39, 49, 58	0
1	B	290/306 (94%)	0.14	5 (1%) 70 71	28, 40, 61, 72	0
All	All	582/612 (95%)	0.13	11 (1%) 66 68	28, 39, 55, 72	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	PHE	3.5
1	A	277	ASN	3.4
1	A	229	ASP	2.7
1	A	233	VAL	2.5
1	B	255	ALA	2.5
1	B	303	VAL	2.4
1	A	193	ALA	2.4
1	A	230	PHE	2.2
1	B	87	LEU	2.2
1	A	59	ILE	2.1
1	B	227	LEU	2.1

### 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](#)

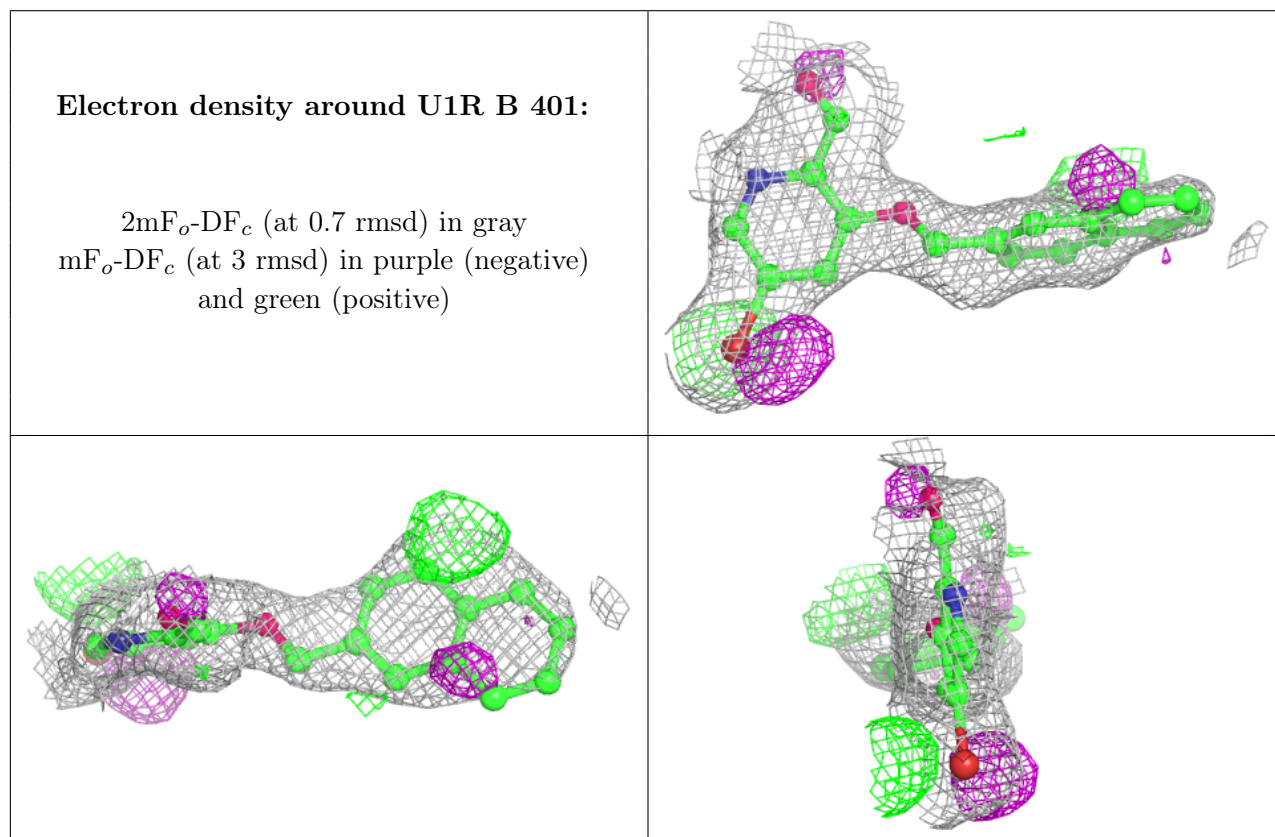
There are no monosaccharides in this entry.

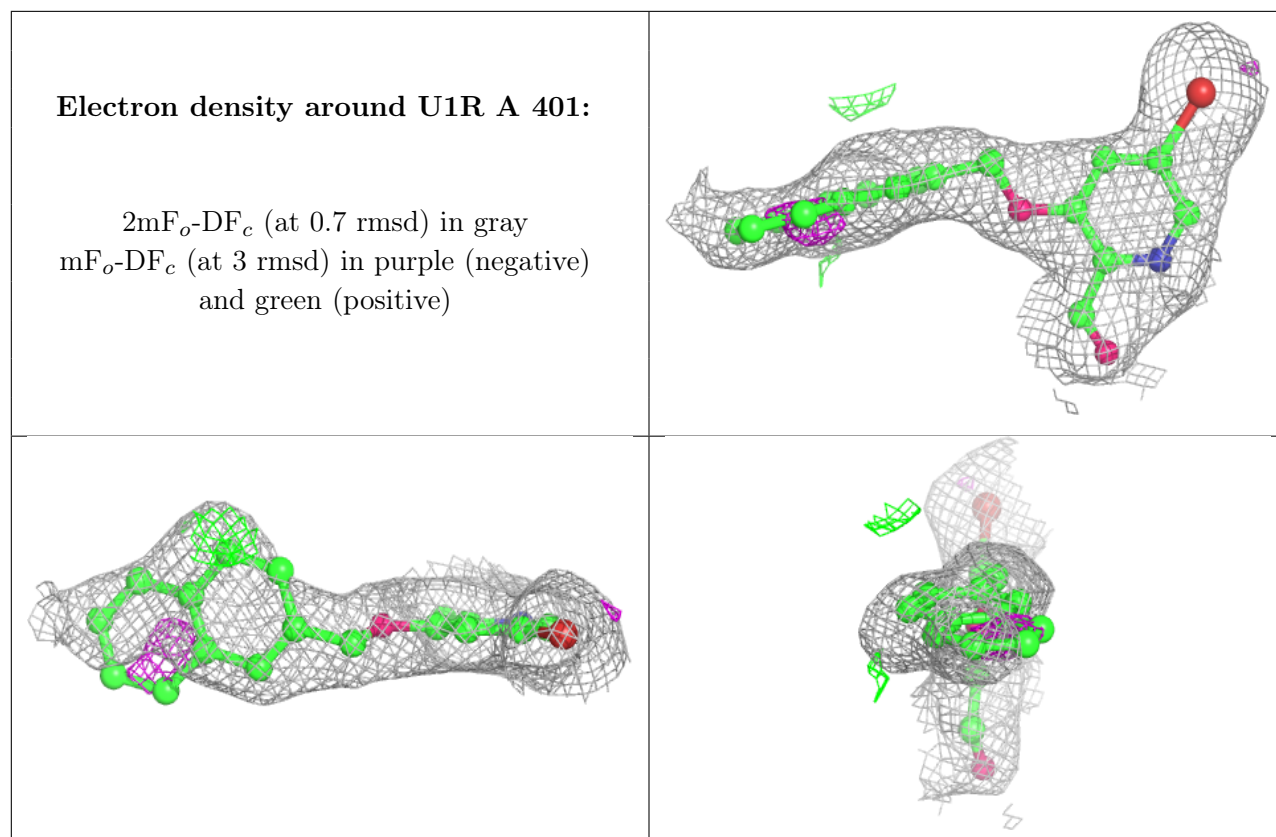
## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
2	U1R	B	401	21/21	0.77	0.20	44,53,58,110	0
2	U1R	A	401	21/21	0.86	0.16	43,50,54,86	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.