

# Full wwPDB X-ray Structure Validation Report (i)

#### Mar 6, 2024 - 01:11 PM EST

PDB ID	:	8UHO
Title	:	Crystal structure of SARS CoV-2 3CL protease in complex with $GSK4365096A$
Authors	:	Concha, N.O.; Williams, S.P.
Deposited on		
Resolution	:	2.02 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* 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 (1)) were used in the production of this report:

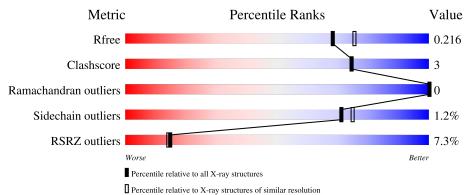
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	:::::::::::::::::::::::::::::::::::::::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.02 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	$10434 \ (2.04-2.00)$
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	А	306	<sup>2%</sup> 93%	5%•
1	В	306	91%	8%



# 2 Entry composition (i)

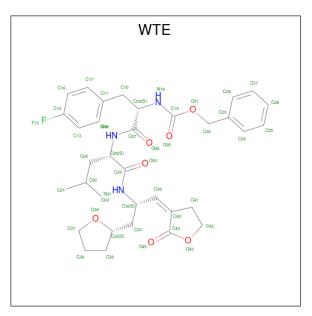
There are 3 unique types of molecules in this entry. The entry contains 9427 atoms, of which 4534 are hydrogens and 0 are deuteriums.

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	А	301	Total 4552	C 1460	Н 2244	N 392	0 434	S 22	0	0	0
1	В	305	Total 4506	C 1460	Н 2206	N 388	0 431	S 21	0	0	0

• Molecule 2 is N-[(benzyloxy)carbonyl]-4-fluoro-L-phenylalanyl-N-[(2S,3Z)-1-[(2S)-oxolan-2-yl]-3-(2-oxooxolan-3-ylidene)propan-2-yl]-L-leucinamide (three-letter code: WTE) (formula:  $C_{34}H_{42}FN_3O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	А	1	Total 87	-			0 7	0	0
2	В	1	Total 87	-		Н 42	O 7	0	0

• Molecule 3 is water.

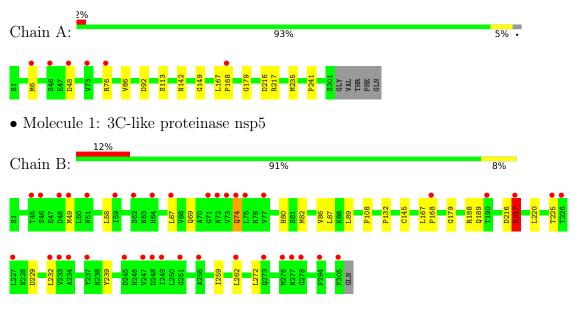


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	117	Total O 117 117	0	0
3	В	78	Total O 78 78	0	0



# 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



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.72Å 100.40Å 103.12Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	41.02 - 2.02	Depositor
Resolution (A)	41.02 - 2.02	EDS
% Data completeness	98.5 (41.02-2.02)	Depositor
(in resolution range)	98.5(41.02-2.02)	EDS
R <sub>merge</sub>	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.57 (at 2.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
$R, R_{free}$	0.184 , $0.217$	Depositor
II, II, <i>free</i>	0.183 , $0.216$	DCC
$R_{free}$ test set	1998 reflections $(4.35\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	24.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.45 , $54.4$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9427	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: WTE

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.36	0/2359	0.59	0/3209	
1	В	0.45	2/2352~(0.1%)	0.65	3/3205~(0.1%)	
All	All	0.41	2/4711~(0.0%)	0.62	3/6414~(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	А	0	1
1	В	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	В	217	ARG	CB-CG	6.33	1.69	1.52
1	В	74	GLN	CD-NE2	5.66	1.47	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	217	ARG	CG-CD-NE	12.04	137.07	111.80
1	В	74	GLN	CB-CA-C	9.57	129.54	110.40
1	В	217	ARG	NE-CZ-NH2	-5.43	117.59	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	217	ARG	Sidechain
1	В	217	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	А	2308	2244	2244	6	0
1	В	2300	2206	2204	23	0
2	А	45	42	0	1	0
2	В	45	42	0	2	0
3	А	117	0	0	0	1
3	В	78	0	0	1	1
All	All	4893	4534	4448	29	1

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 (29) 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:SG	2:B:401:WTE:C39	2.77	0.72
1:B:229:ASP:HA	1:B:232:LEU:HD12	1.83	0.60
1:B:49:MET:HB3	1:B:189:GLN:HG3	1.84	0.60
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.85	0.58
1:A:142:ASN:ND2	2:A:401:WTE:F15	2.25	0.58
1:B:217:ARG:HH11	1:B:220:LEU:CD1	2.19	0.56
1:A:76:ARG:NH2	1:A:92:ASP:OD2	2.40	0.54
1:B:67:LEU:HD11	1:B:74:GLN:HG3	1.92	0.52
1:B:87:LEU:HD21	1:B:89:LEU:HD21	1.91	0.51
1:B:145:CYS:SG	2:B:401:WTE:N31	2.84	0.50
1:B:217:ARG:NH1	1:B:220:LEU:CD1	2.73	0.50
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.48	0.49
1:B:225:THR:O	1:B:262:LEU:HB3	2.13	0.48
1:A:86:VAL:HG23	1:A:179:GLY:HA2	1.96	0.48
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.95	0.48
1:A:113:SER:O	1:A:149:GLY:HA2	2.16	0.46



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:82:MET:HE3	3:B:551:HOH:O	2.16	0.45	
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.98	0.45	
1:B:225:THR:HG22	1:B:262:LEU:O	2.17	0.45	
1:B:217:ARG:HH11	1:B:220:LEU:HD11	1.79	0.45	
1:B:58:LEU:HD11	1:B:80:HIS:HD2	1.82	0.44	
1:B:69:GLN:NE2	1:B:74:GLN:HE21	2.15	0.44	
1:B:225:THR:O	1:B:262:LEU:HD13	2.19	0.43	
1:B:67:LEU:CD1	1:B:74:GLN:HG3	2.49	0.43	
1:B:69:GLN:NE2	1:B:74:GLN:NE2	2.66	0.43	
1:A:235:MET:CE	1:A:241:PRO:HG3	2.50	0.42	
1:B:217:ARG:HB3	1:B:220:LEU:HD12	2.02	0.41	
1:B:220:LEU:HD22	1:B:259:ILE:HD13	2.03	0.41	
1:B:108:PRO:HB3	1:B:132:PRO:HA	2.04	0.40	

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:573:HOH:O	3:B:578:HOH:O[2_555]	1.73	0.47

### 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	nalysed Favoured Allowed		Outliers	Perce	$\mathbf{ntiles}$
1	А	299/306~(98%)	292~(98%)	7~(2%)	0	100	100
1	В	303/306~(99%)	298 (98%)	5 (2%)	0	100	100
All	All	602/612~(98%)	590~(98%)	12 (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	Analysed Rotameric Outliers		Percentiles		
1	А	255/263~(97%)	252~(99%)	3~(1%)	71 75		
1	В	247/263~(94%)	244 (99%)	3 (1%)	71 75		
All	All	502/526~(95%)	496 (99%)	6 (1%)	71 75		

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

Mol	Chain	Res	Type
1	А	6	MET
1	А	48	ASP
1	А	216	ASP
1	В	188	ARG
1	В	216	ASP
1	В	217	ARG

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

Mol	Chain	Res	Type
1	А	69	GLN
1	В	69	GLN
1	В	74	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 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).

Mal	Mol Type Chain Re		Chain Res Link		B	Bond lengths			ond ang	gles
IVIOI			nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	WTE	В	401	-	48,48,48	<b>3.94</b>	9 (18%)	58,64,64	2.07	11 (18%)
2	WTE	А	401	1	48,48,48	4.02	10 (20%)	58,64,64	1.69	9 (15%)

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	WTE	В	401	-	-	11/40/58/58	0/4/4/4
2	WTE	А	401	1	-	9/40/58/58	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	401	WTE	C39-C40	23.61	1.54	1.33
2	В	401	WTE	C39-C40	22.92	1.54	1.33
2	В	401	WTE	C07-N06	7.91	1.51	1.34
2	А	401	WTE	C07-N06	7.30	1.50	1.34
2	А	401	WTE	C19-N18	5.97	1.49	1.34
2	В	401	WTE	C29-N31	5.81	1.46	1.34
2	В	401	WTE	C19-N18	5.45	1.48	1.34
2	В	401	WTE	O43-C44	5.30	1.44	1.36
2	А	401	WTE	C29-N31	5.24	1.45	1.34
2	А	401	WTE	O43-C44	4.85	1.44	1.36



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	401	WTE	O21-C19	4.85	1.44	1.35
2	В	401	WTE	O21-C19	4.52	1.43	1.35
2	А	401	WTE	C22-C23	3.01	1.57	1.50
2	В	401	WTE	C22-C23	2.95	1.57	1.50
2	В	401	WTE	C10-C11	2.74	1.57	1.51
2	А	401	WTE	C10-C11	2.35	1.57	1.51
2	В	401	WTE	O08-C07	-2.18	1.19	1.23
2	А	401	WTE	O08-C07	-2.16	1.19	1.23
2	А	401	WTE	O30-C29	-2.06	1.19	1.23

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All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	401	WTE	O43-C44-O45	6.62	129.43	121.07
2	А	401	WTE	O21-C19-N18	6.27	123.24	110.50
2	В	401	WTE	O38-C34-C33	-5.67	102.18	108.95
2	В	401	WTE	O45-C44-C40	-5.41	121.20	129.72
2	В	401	WTE	C32-N31-C29	-4.95	114.01	123.15
2	В	401	WTE	C02-C04-C05	-4.85	102.09	115.43
2	А	401	WTE	O43-C44-O45	4.36	126.58	121.07
2	А	401	WTE	O20-C19-N18	-4.20	117.97	124.85
2	В	401	WTE	O21-C19-N18	4.00	118.63	110.50
2	В	401	WTE	O20-C19-N18	-3.06	119.83	124.85
2	А	401	WTE	O45-C44-C40	-2.97	125.04	129.72
2	А	401	WTE	O21-C19-O20	-2.87	118.74	124.25
2	А	401	WTE	C02-C04-C05	-2.83	107.66	115.43
2	В	401	WTE	C42-O43-C44	-2.79	108.37	110.74
2	В	401	WTE	C29-C05-N06	-2.51	104.33	111.16
2	А	401	WTE	C32-N31-C29	-2.49	118.56	123.15
2	А	401	WTE	C10-C09-C07	2.48	116.69	110.25
2	В	401	WTE	C16-C14-C13	-2.18	119.93	122.83
2	А	401	WTE	C07-C09-N18	-2.17	105.24	111.16
2	В	401	WTE	C09-C07-N06	2.15	121.42	116.70

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	401	WTE	N18-C19-O21-C22
2	А	401	WTE	O20-C19-O21-C22
2	А	401	WTE	N31-C32-C39-C40
2	А	401	WTE	C32-C39-C40-C41



Mol	Chain	Res	Type	Atoms
2	В	401	WTE	C33-C32-C39-C40
2	В	401	WTE	C32-C33-C34-C35
2	В	401	WTE	C32-C33-C34-O38
2	В	401	WTE	C32-C39-C40-C41
2	В	401	WTE	C39-C32-C33-C34
2	В	401	WTE	N31-C32-C33-C34
2	А	401	WTE	C09-C10-C11-C17
2	А	401	WTE	C09-C10-C11-C12
2	В	401	WTE	O08-C07-C09-N18
2	В	401	WTE	N06-C07-C09-N18
2	В	401	WTE	C09-C10-C11-C17
2	В	401	WTE	N31-C32-C39-C40
2	В	401	WTE	C09-C10-C11-C12
2	А	401	WTE	N06-C07-C09-N18
2	А	401	WTE	C33-C32-C39-C40
2	А	401	WTE	C32-C33-C34-C35

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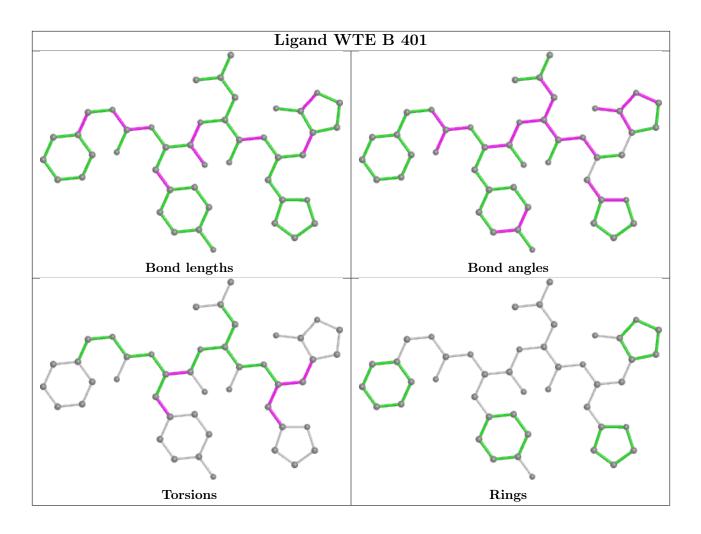
There are no ring outliers.

2 monomers are involved in 3 short contacts:

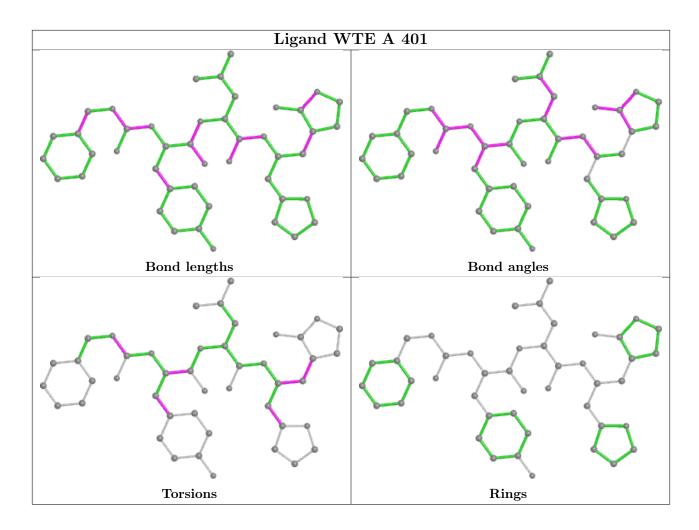
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	WTE	2	0
2	А	401	WTE	1	0

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 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 (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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	301/306~(98%)	0.07	6 (1%) 65 64	15, 27, 42, 67	0
1	В	305/306~(99%)	0.66	38 (12%) 3 3	16, 34, 57, 75	1 (0%)
All	All	606/612~(99%)	0.37	44 (7%) 15 14	15, 29, 53, 75	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	232	LEU	4.5
1	В	72	ASN	4.5
1	В	278	GLY	4.3
1	В	46	SER	4.1
1	В	62	SER	3.7
1	В	227	LEU	3.6
1	В	237	TYR	3.5
1	В	45	THR	3.5
1	В	48	ASP	3.4
1	А	73	VAL	3.4
1	В	74	GLN	3.2
1	В	262	LEU	3.1
1	В	305	PHE	3.1
1	В	226	THR	3.0
1	В	51	ASN	3.0
1	В	67	LEU	2.9
1	В	64	HIS	2.8
1	В	77	VAL	2.6
1	В	168	PRO	2.6
1	В	217	ARG	2.5
1	В	225	THR	2.5
1	В	248	ASP	2.5
1	В	59	ILE	2.5
1	А	48	ASP	2.5



Mol	Chain	Res	Type	RSRZ
1	В	73	VAL	2.5
1	В	190	THR	2.4
1	В	255	ALA	2.4
1	В	251	GLY	2.4
1	В	294	PHE	2.4
1	В	245	ASP	2.4
1	А	6	MET	2.2
1	В	75	LEU	2.2
1	В	71	GLY	2.2
1	В	247	VAL	2.1
1	В	234	ALA	2.1
1	В	249	ILE	2.1
1	А	46	SER	2.1
1	В	276	MET	2.1
1	В	277	ASN	2.1
1	А	76	ARG	2.1
1	В	233	VAL	2.1
1	А	168	PRO	2.0
1	В	273	GLN	2.0
1	В	49	MET	2.0

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#### 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.

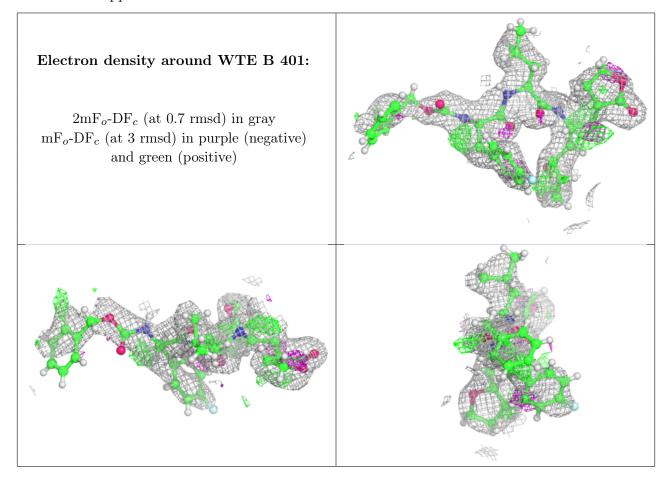
### 6.4 Ligands (i)

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,  $95^{th}$  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.

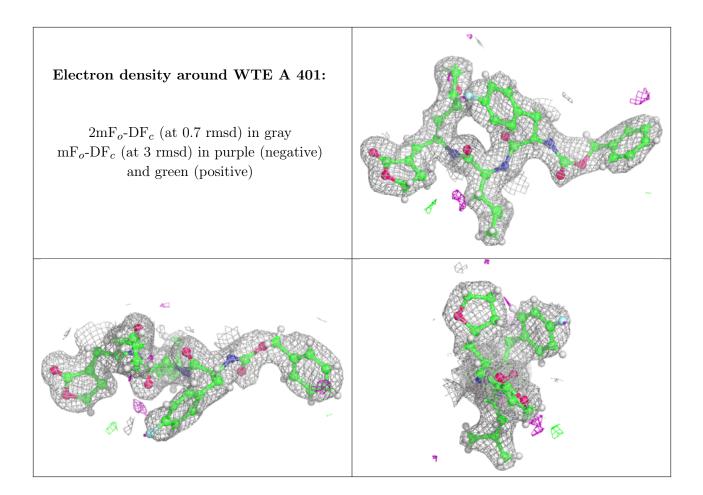
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	WTE	В	401	45/45	0.82	0.27	$28,\!50,\!81,\!99$	0
2	WTE	А	401	45/45	0.94	0.16	18,29,49,55	0



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.

