



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 01:19 AM EDT

PDB ID : 8DIB  
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 : 2.17 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

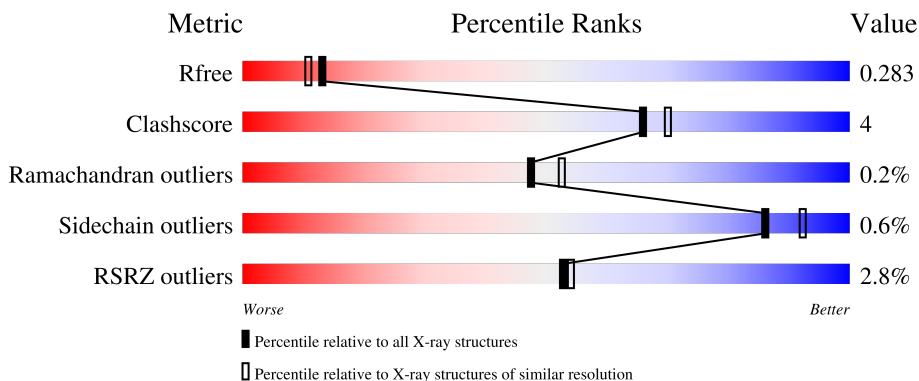
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


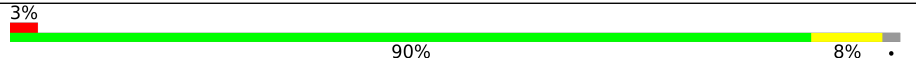
The reported resolution of this entry is 2.17 Å.

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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	
1	B	306	

## 2 Entry composition [i](#)

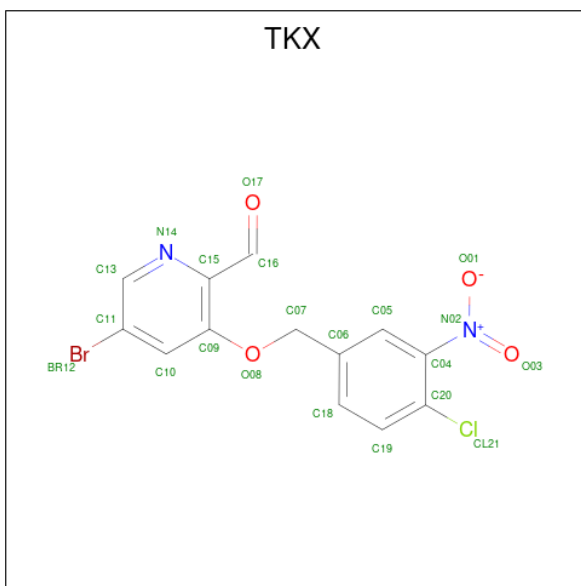
There are 3 unique types of molecules in this entry. The entry contains 4579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	298	Total	C	N	O	S	0	1	0
			2259	1428	385	426	20			
1	B	299	Total	C	N	O	S	0	1	0
			2247	1426	377	424	20			

- Molecule 2 is 5-bromo-3-[(4-chloro-3-nitrophenyl)methoxy]pyridine-2-carbaldehyde (three-letter code: TKX) (formula:  $C_{13}H_8BrClN_2O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	Cl	N			O
2	A	1	Total	Br	C	Cl	N	O	0	0
			21	1	13	1	2	4		
2	B	1	Total	Br	C	Cl	N	O	0	0
			21	1	13	1	2	4		

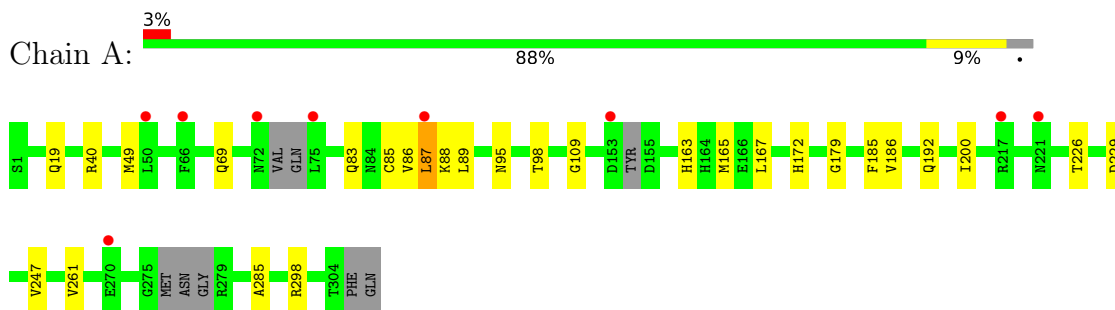
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	20	Total 20	O 20	0	0
3	B	11	Total 11	O 11	0	0

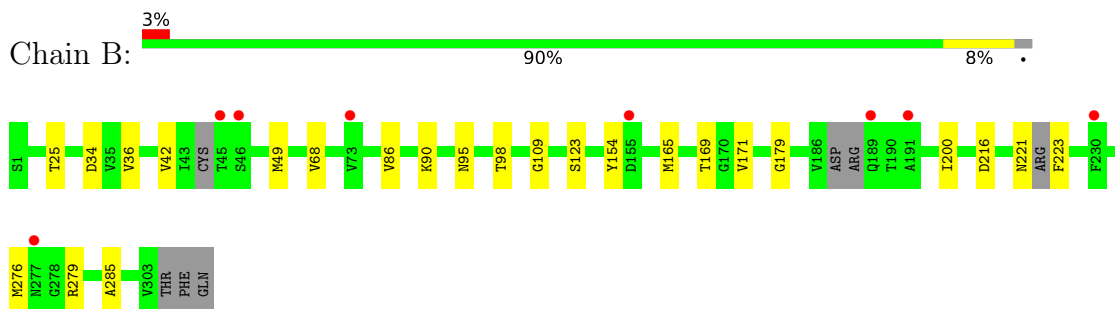
### 3 Residue-property plots [i](#)

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



- Molecule 1: 3C-like proteinase nsp5



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.91Å 53.72Å 115.53Å 90.00° 100.83° 90.00°	Depositor
Resolution (Å)	38.73 – 2.17 39.01 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.73-2.17) 98.3 (39.01-2.17)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.221 , 0.276 0.230 , 0.283	Depositor DCC
$R_{free}$ test set	1343 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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 79.85 % 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 5.0977e-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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.30	0/2306	0.49	0/3138
1	B	0.34	0/2294	0.51	0/3124
All	All	0.32	0/4600	0.50	0/6262

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 [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	A	2259	0	2158	21	0
1	B	2247	0	2151	15	0
2	A	21	0	0	5	0
2	B	21	0	0	5	0
3	A	20	0	0	1	1
3	B	11	0	0	0	0
All	All	4579	0	4309	35	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 4.

All (35) 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:165:MET:HG3	2:B:401:TKX:CL21	2.03	0.96
1:B:165:MET:CG	2:B:401:TKX:CL21	2.52	0.95
1:B:165:MET:SD	2:B:401:TKX:CL21	2.64	0.93
1:A:226:THR:HG23	1:A:229:ASP:H	1.50	0.76
1:A:186:VAL:H	1:A:192:GLN:HE22	1.35	0.75
1:B:165:MET:HG3	2:B:401:TKX:C20	2.22	0.69
1:B:34:ASP:OD2	1:B:90:LYS:NZ	2.26	0.68
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.77	0.67
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.81	0.63
1:A:49:MET:HE3	2:A:401:TKX:C05	2.28	0.62
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.81	0.62
1:A:19:GLN:HB3	1:A:69:GLN:HB3	1.83	0.61
1:A:298:ARG:NH1	3:A:501:HOH:O	2.35	0.60
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.84	0.59
1:A:49:MET:CE	2:A:401:TKX:O01	2.52	0.58
1:A:165:MET:HE3	1:A:167:LEU:HD21	1.88	0.54
1:A:83:GLN:HE21	1:A:88:LYS:HD2	1.74	0.53
1:A:49:MET:HE1	2:A:401:TKX:O01	2.09	0.53
1:A:49:MET:HE1	2:A:401:TKX:N02	2.25	0.51
1:B:49:MET:SD	2:B:401:TKX:O01	2.70	0.49
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.14	0.47
1:A:285:ALA:HB3	1:B:285:ALA:HB3	1.97	0.46
1:B:169:THR:OG1	1:B:171:VAL:HG22	2.16	0.46
1:A:87:LEU:HD13	1:A:89:LEU:HD21	1.98	0.46
1:A:247:VAL:HG13	1:A:261:VAL:HG11	1.97	0.46
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.51	0.45
1:A:165:MET:HE1	1:A:185:PHE:HB3	2.00	0.44
1:B:221:ASN:ND2	1:B:223:PHE:HB2	2.34	0.43
1:A:40:ARG:HD3	1:A:85:CYS:HA	2.00	0.43
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.83	0.42
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.19	0.41
1:B:36:VAL:HG21	1:B:68:VAL:HG11	2.03	0.41
1:A:49:MET:CE	2:A:401:TKX:N02	2.83	0.41
1:B:25:THR:HG21	1:B:42:VAL:HA	2.02	0.41
1:B:276:MET:HE2	1:B:279:ARG:O	2.20	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:507:HOH:O	3:A:518:HOH:O[2_555]	2.11	0.09

### 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	291/306 (95%)	287 (99%)	4 (1%)	0	100	100
1	B	292/306 (95%)	285 (98%)	6 (2%)	1 (0%)	41	43
All	All	583/612 (95%)	572 (98%)	10 (2%)	1 (0%)	47	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	TYR

#### 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	243/263 (92%)	242 (100%)	1 (0%)	91	95
1	B	242/263 (92%)	240 (99%)	2 (1%)	81	89
All	All	485/526 (92%)	482 (99%)	3 (1%)	86	92

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

Mol	Chain	Res	Type
1	A	87	LEU
1	B	123	SER
1	B	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	192	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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	TKX	B	401	1	21,22,22	1.53	5 (23%)	26,30,30	1.52	4 (15%)
2	TKX	A	401	1	21,22,22	1.52	5 (23%)	26,30,30	1.52	4 (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	TKX	B	401	1	-	6/9/11/11	0/2/2/2
2	TKX	A	401	1	-	6/9/11/11	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	TKX	C15-C16	4.30	1.53	1.48
2	A	401	TKX	C15-C16	4.22	1.53	1.48
2	B	401	TKX	O03-N02	-2.84	1.18	1.22
2	A	401	TKX	O03-N02	-2.82	1.18	1.22
2	A	401	TKX	C15-N14	-2.51	1.32	1.35
2	B	401	TKX	C15-N14	-2.47	1.32	1.35
2	A	401	TKX	C20-CL21	2.24	1.79	1.73
2	B	401	TKX	C20-CL21	2.17	1.78	1.73
2	B	401	TKX	BR12-C11	2.06	1.94	1.90
2	A	401	TKX	BR12-C11	2.02	1.94	1.90

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TKX	O17-C16-C15	-4.41	120.05	124.22
2	B	401	TKX	O17-C16-C15	-4.40	120.05	124.22
2	B	401	TKX	C13-N14-C15	3.12	122.21	117.39
2	A	401	TKX	C13-N14-C15	3.09	122.17	117.39
2	A	401	TKX	C16-C15-N14	2.82	119.99	115.41
2	B	401	TKX	C16-C15-N14	2.80	119.95	115.41
2	A	401	TKX	C09-C15-N14	-2.23	120.00	121.73
2	B	401	TKX	C09-C15-N14	-2.22	120.01	121.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TKX	C20-C04-N02-O03
2	A	401	TKX	C05-C04-N02-O03
2	B	401	TKX	C20-C04-N02-O03
2	B	401	TKX	C05-C04-N02-O03
2	A	401	TKX	C15-C09-O08-C07

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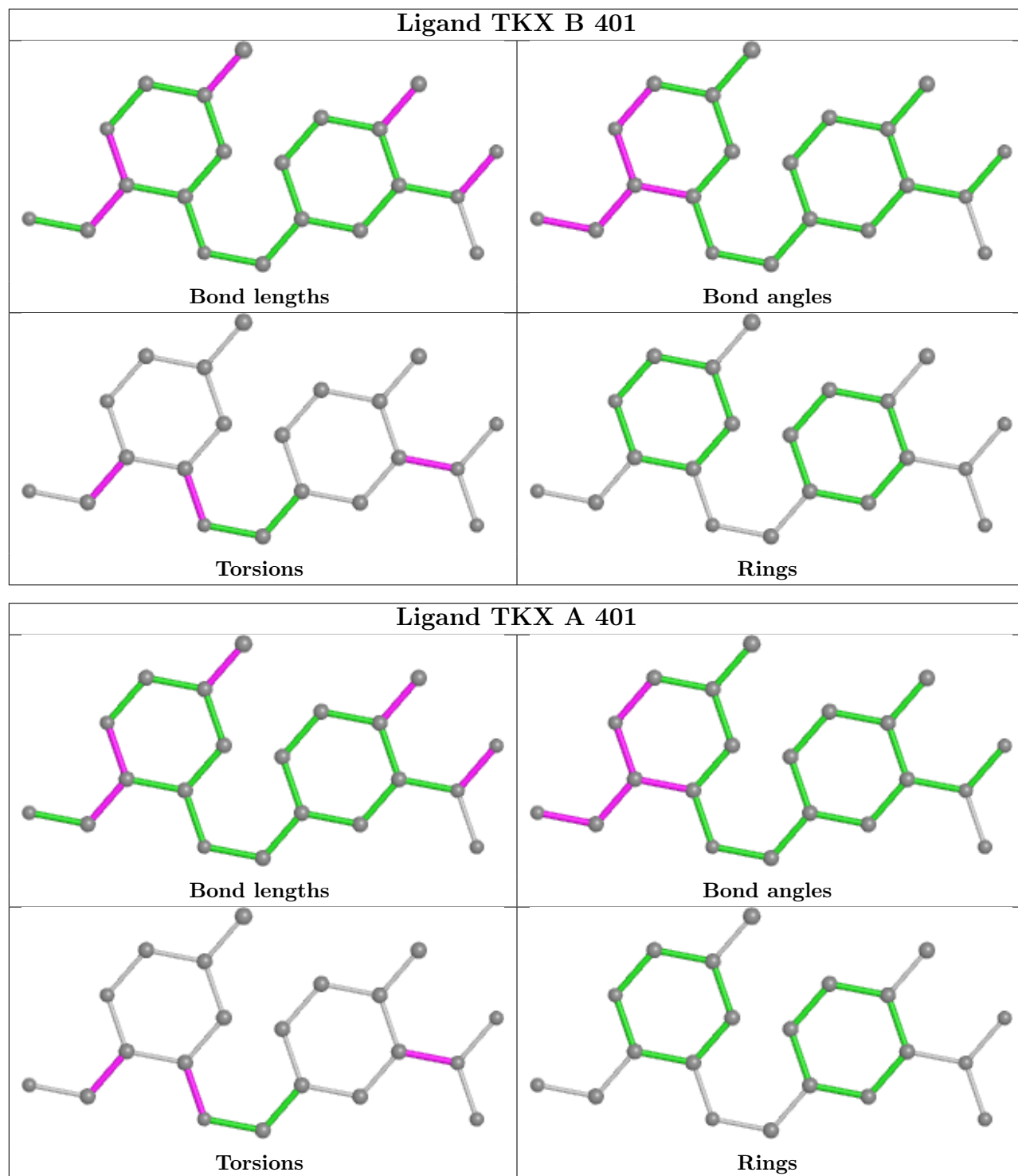
Mol	Chain	Res	Type	Atoms
2	B	401	TKX	C15-C09-O08-C07
2	A	401	TKX	C09-C15-C16-O17
2	B	401	TKX	C09-C15-C16-O17
2	B	401	TKX	C10-C09-O08-C07
2	A	401	TKX	C10-C09-O08-C07
2	A	401	TKX	N14-C15-C16-O17
2	B	401	TKX	N14-C15-C16-O17

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	TKX	5	0
2	A	401	TKX	5	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

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	298/306 (97%)	0.23	9 (3%) 50 51	27, 45, 72, 89	0
1	B	299/306 (97%)	0.23	8 (2%) 54 55	31, 47, 70, 105	0
All	All	597/612 (97%)	0.23	17 (2%) 53 54	27, 46, 72, 105	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	3.3
1	B	155	ASP	3.2
1	B	230	PHE	2.9
1	A	217	ARG	2.8
1	B	189	GLN	2.6
1	A	87	LEU	2.6
1	A	75	LEU	2.6
1	A	72	ASN	2.5
1	A	270	GLU	2.3
1	B	73	VAL	2.3
1	B	46	SER	2.2
1	B	277	ASN	2.2
1	A	153	ASP	2.1
1	B	45	THR	2.1
1	A	66	PHE	2.0
1	A	221	ASN	2.0
1	A	50	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](#)

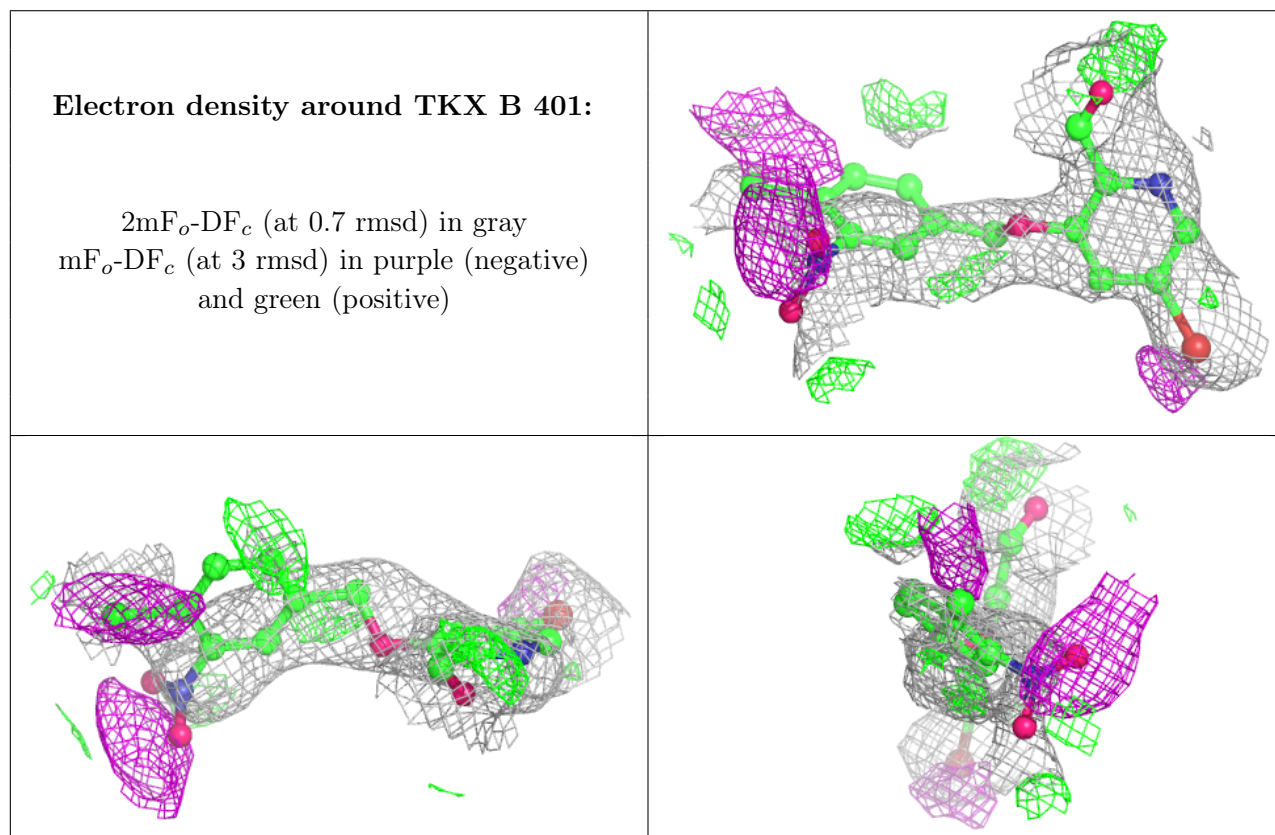
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

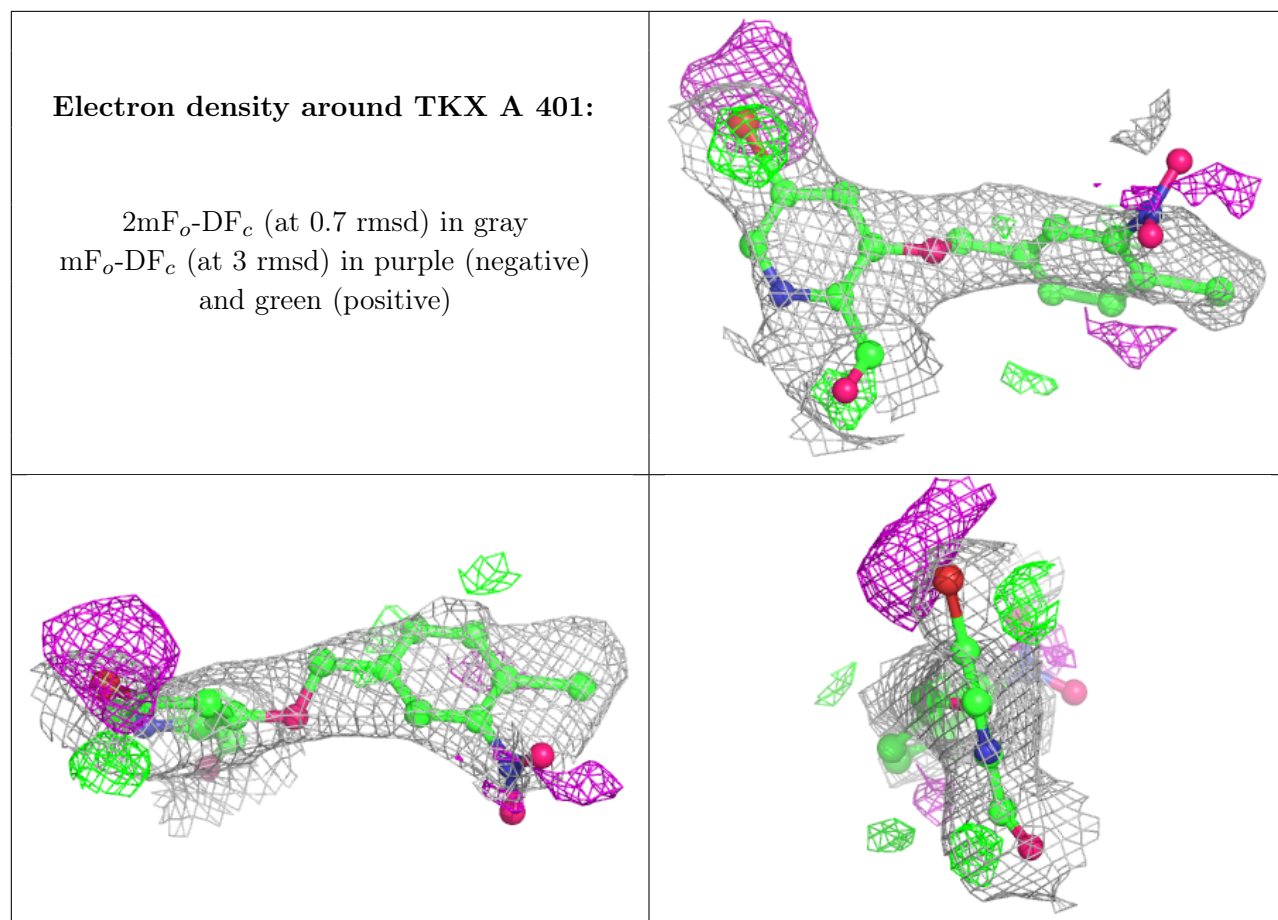
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TKX	B	401	21/21	0.53	0.29	94,96,107,118	0
2	TKX	A	401	21/21	0.73	0.30	94,96,107,118	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.