



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 12:57 pm BST

PDB ID : 2I1R  
Title : Novel Thiazolones as HCV NS5B Polymerase Inhibitors: Further Designs,  
Synthesis, SAR and X-ray Complex Structure  
Authors : Yao, N.; Yan, S.  
Deposited on : 2006-08-14  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

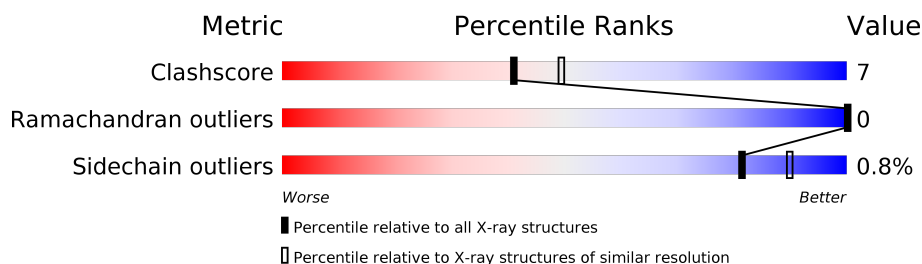
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9003 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 RNA-directed RNA polymerase (NS5B) (P68).

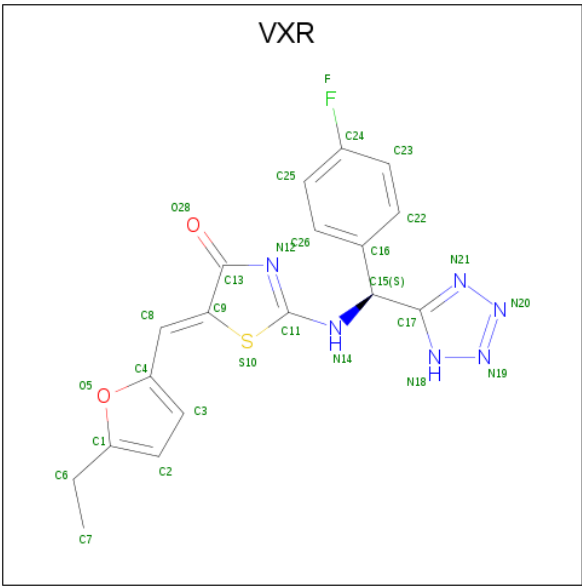
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4352	2747	770	805	30			
1	B	561	Total	C	N	O	S	0	0	0
			4369	2756	775	808	30			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	CLONING ARTIFACT	UNP P26663
A	-4	SER	-	CLONING ARTIFACT	UNP P26663
A	-3	HIS	-	EXPRESSION TAG	UNP P26663
A	-2	HIS	-	EXPRESSION TAG	UNP P26663
A	-1	HIS	-	EXPRESSION TAG	UNP P26663
A	0	HIS	-	EXPRESSION TAG	UNP P26663
A	1	HIS	-	EXPRESSION TAG	UNP P26663
A	2	HIS	-	EXPRESSION TAG	UNP P26663
A	329	VAL	THR	CONFLICT	UNP P26663
A	338	ALA	VAL	CONFLICT	UNP P26663
A	544	GLN	ARG	CONFLICT	UNP P26663
B	-5	ALA	-	CLONING ARTIFACT	UNP P26663
B	-4	SER	-	CLONING ARTIFACT	UNP P26663
B	-3	HIS	-	EXPRESSION TAG	UNP P26663
B	-2	HIS	-	EXPRESSION TAG	UNP P26663
B	-1	HIS	-	EXPRESSION TAG	UNP P26663
B	0	HIS	-	EXPRESSION TAG	UNP P26663
B	1	HIS	-	EXPRESSION TAG	UNP P26663
B	2	HIS	-	EXPRESSION TAG	UNP P26663
B	329	VAL	THR	CONFLICT	UNP P26663
B	338	ALA	VAL	CONFLICT	UNP P26663
B	544	GLN	ARG	CONFLICT	UNP P26663

- Molecule 2 is (5Z)-5-[(5-ETHYL-2-FURYL)METHYLENE]-2-[[S)-(4-FLUOROPHENYL)(1H-TETRAZOL-5-YL)METHYL]AMINO]-1,3-THIAZOL-4(5H)-ONE (three-letter code:

VXR) (formula: C<sub>18</sub>H<sub>15</sub>FN<sub>6</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			28	18	1	6	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			28	18	1	6	2	1		

- Molecule 3 is water.

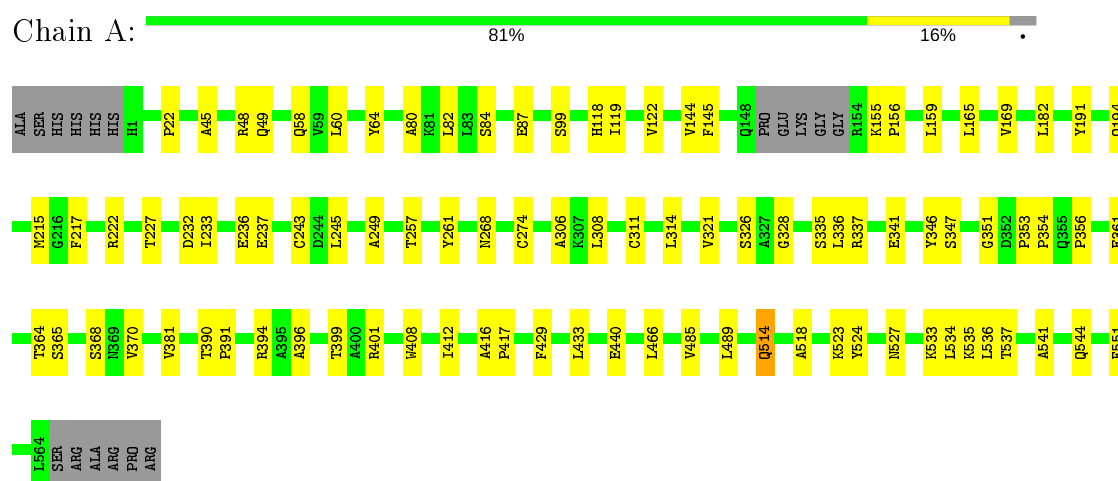
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	111	Total	O	0	0
			111	111		

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

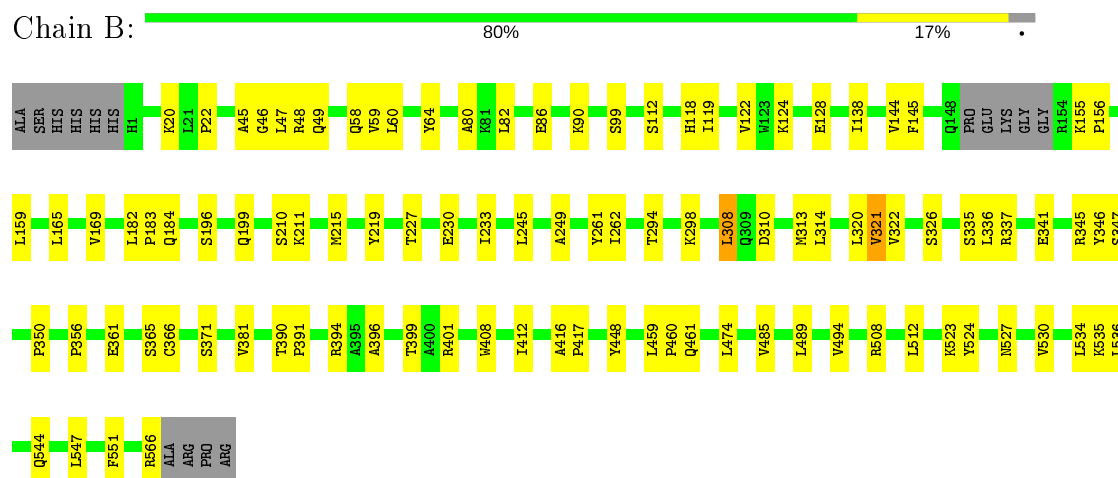
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

#### • Molecule 1: RNA-directed RNA polymerase (NS5B) (P68)



#### • Molecule 1: RNA-directed RNA polymerase (NS5B) (P68)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.60 Å   106.12 Å   126.61 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.2 (20.00-2.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.236 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.32	0/4448	0.57	0/6037
1	B	0.32	0/4465	0.57	0/6059
All	All	0.32	0/8913	0.57	0/12096

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	4352	0	4368	56	0
1	B	4369	0	4386	69	0
2	A	28	0	15	0	0
2	B	28	0	15	0	0
3	A	115	0	0	1	0
3	B	111	0	0	3	0
All	All	9003	0	8784	125	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 7.

The worst 5 of 125 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:A:523:LYS:HE2	1:A:536:LEU:HD12	1.56	0.87
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.56	0.87
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.61	0.81
1:A:535:LYS:HD2	1:A:536:LEU:N	1.96	0.81
1:A:535:LYS:HD2	1:A:536:LEU:H	1.49	0.77

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	555/576 (96%)	541 (98%)	14 (2%)	0	100	100
1	B	557/576 (97%)	541 (97%)	16 (3%)	0	100	100
All	All	1112/1152 (96%)	1082 (97%)	30 (3%)	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	476/489 (97%)	473 (99%)	3 (1%)	86	93
1	B	478/489 (98%)	473 (99%)	5 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	954/978 (98%)	946 (99%)	8 (1%)	81	90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	LEU
1	B	321	VAL
1	B	308	LEU
1	A	514	GLN
1	B	112	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	B	110	ASN
1	B	461	GLN
1	A	544	GLN
1	B	374	HIS

### 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 carbohydrates 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	VXR	A	600	-	23,31,31	2.06	9 (39%)	30,43,43	3.91	11 (36%)
2	VXR	B	600	-	23,31,31	1.98	8 (34%)	30,43,43	3.95	12 (40%)

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	VXR	A	600	-	-	2/11/30/30	0/4/4/4
2	VXR	B	600	-	-	1/11/30/30	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	VXR	C11-S10	-4.15	1.67	1.73
2	A	600	VXR	C11-S10	-4.03	1.67	1.73
2	A	600	VXR	C11-N12	-3.56	1.26	1.31
2	B	600	VXR	C13-C9	-3.13	1.46	1.50
2	A	600	VXR	C13-C9	-3.12	1.46	1.50

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	VXR	S10-C11-N12	-11.56	105.18	115.85
2	A	600	VXR	S10-C11-N12	-11.10	105.60	115.85
2	B	600	VXR	C13-C9-S10	-9.74	103.74	109.12
2	A	600	VXR	C13-C9-S10	-9.71	103.76	109.12
2	A	600	VXR	C9-C13-N12	-7.32	109.72	113.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	VXR	C2-C1-C6-C7
2	B	600	VXR	C17-C15-N14-C11

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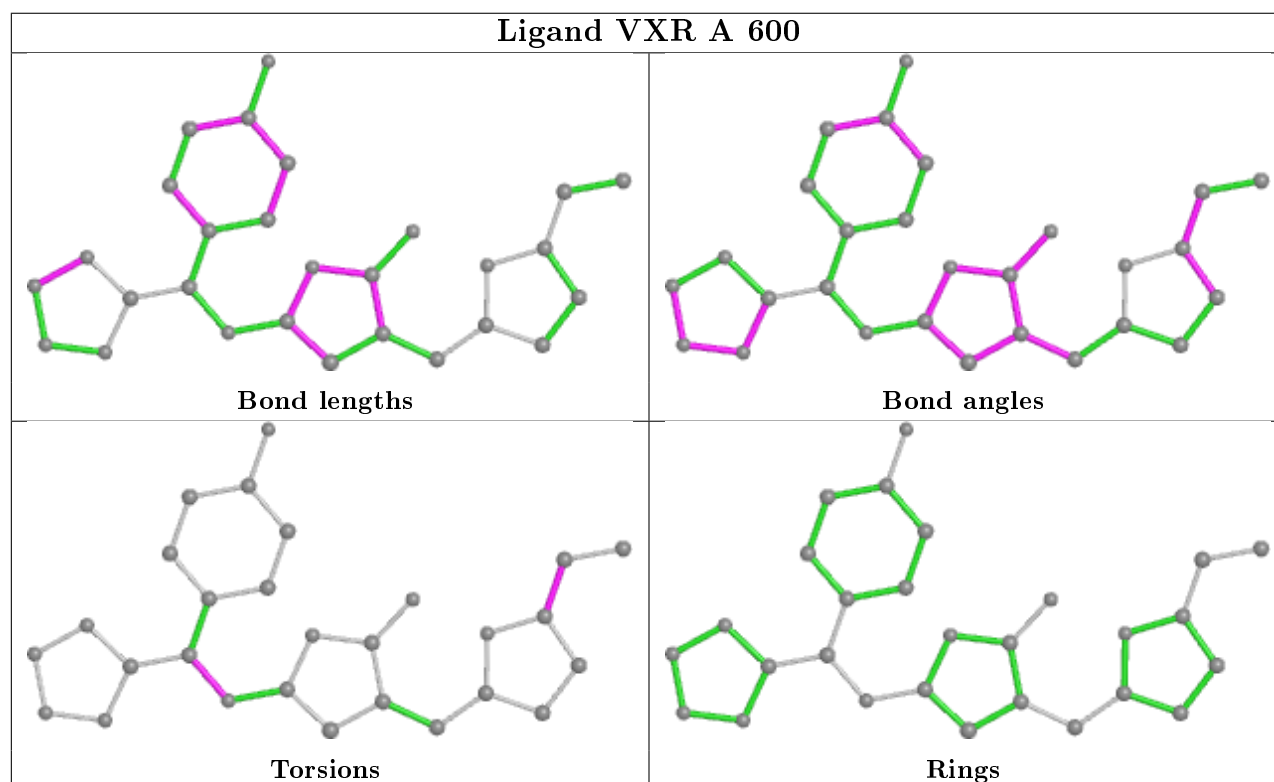
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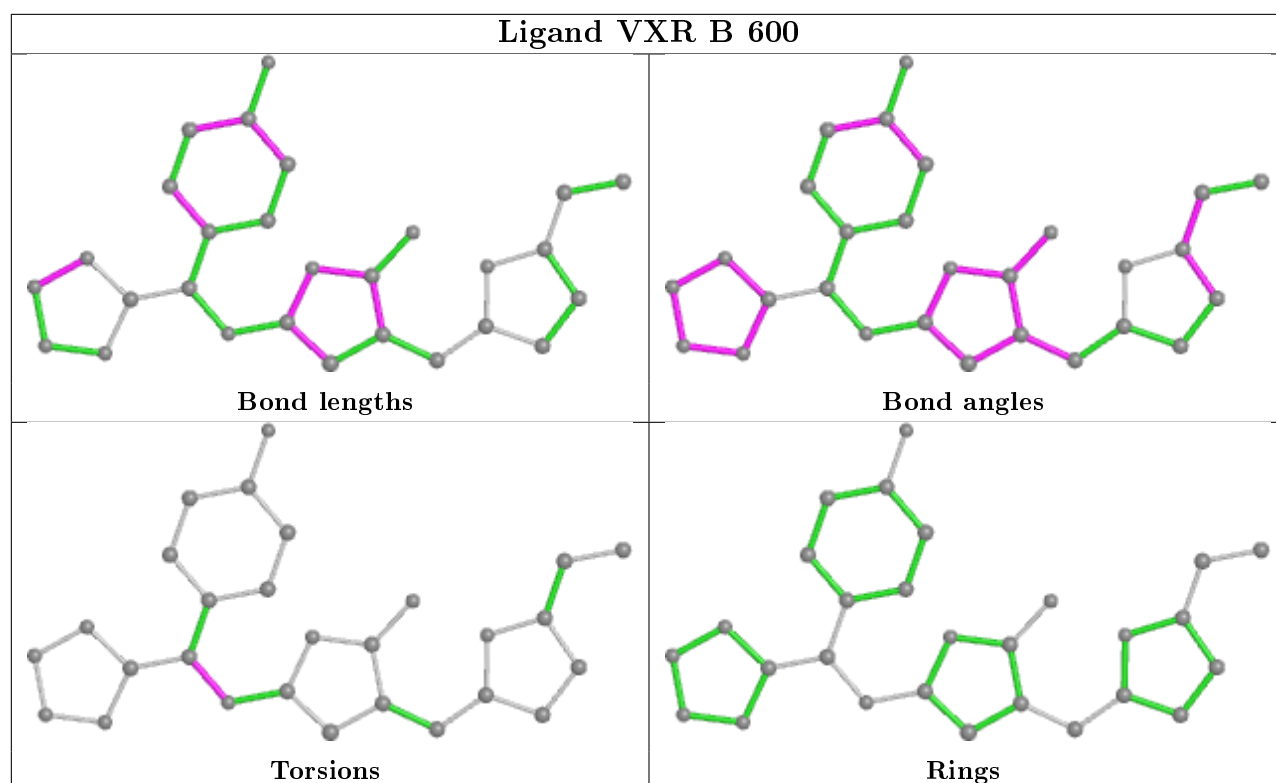
Mol	Chain	Res	Type	Atoms
2	A	600	VXR	C17-C15-N14-C11

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.