



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 08:19 PM EDT

PDB ID : 2XNI  
Title : Protein-ligand complex of a novel macrocyclic HCV NS3 protease inhibitor derived from amino cyclic boronates  
Authors : Li, X.; Zhang, Y.-K.; Liu, Y.; Ding, C.Z.; Zhou, Y.; Li, Q.; Plattner, J.J.; Baker, S.J.; Zhang, S.; Kazmierski, W.M.; Wright, L.L.; Smith, G.K.; Grimes, R.M.; Crosby, R.M.; Creech, K.L.; Carballo, L.H.; Slater, M.J.; Jarvest, R.L.; Thommes, P.; Hubbard, J.A.; Convery, M.A.; Nassau, P.M.; McDowell, W.; Skarzynski, T.J.; Qian, X.; Fan, D.; Liao, L.; Ni, Z.-J.; Pennicott, L.E.; Zou, W.; Wright, J.  
Deposited on : 2010-08-02  
Resolution : 3.30 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.

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

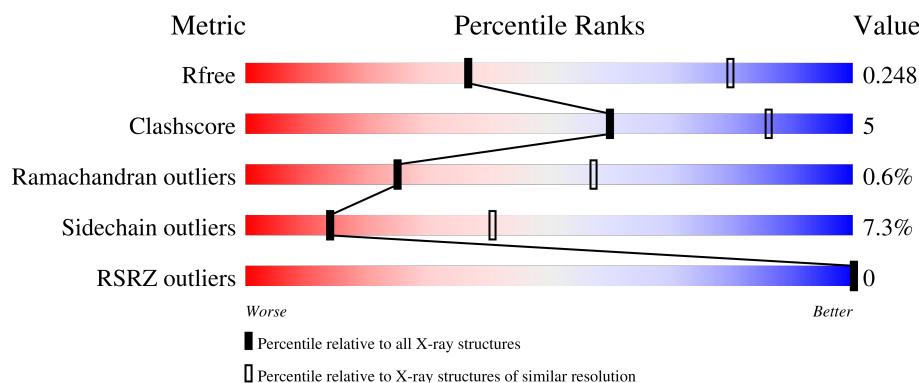
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	198	
1	B	198	

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CCP4 : 7.0.044 (Gargrove)  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
2	C	23	<div><div></div><div>83%</div><div>9%</div><div>9%</div></div>
2	D	23	<div><div></div><div>57%</div><div>13%</div><div>30%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2844 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 NS3 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1339	835	244	251	9			
1	B	153	Total	C	N	O	S	0	0	0
			1136	710	206	212	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP C1KHZ7
A	-8	SER	-	expression tag	UNP C1KHZ7
A	-7	MET	-	expression tag	UNP C1KHZ7
A	-6	THR	-	expression tag	UNP C1KHZ7
A	-5	GLY	-	expression tag	UNP C1KHZ7
A	-4	GLY	-	expression tag	UNP C1KHZ7
A	-3	GLN	-	expression tag	UNP C1KHZ7
A	-2	GLN	-	expression tag	UNP C1KHZ7
A	-1	MET	-	expression tag	UNP C1KHZ7
A	0	GLY	-	expression tag	UNP C1KHZ7
A	181	GLY	-	expression tag	UNP C1KHZ7
A	182	SER	-	expression tag	UNP C1KHZ7
A	183	HIS	-	expression tag	UNP C1KHZ7
A	184	HIS	-	expression tag	UNP C1KHZ7
A	185	HIS	-	expression tag	UNP C1KHZ7
A	186	HIS	-	expression tag	UNP C1KHZ7
A	187	HIS	-	expression tag	UNP C1KHZ7
A	188	HIS	-	expression tag	UNP C1KHZ7
A	40	THR	ALA	conflict	UNP C1KHZ7
A	153	LEU	ILE	conflict	UNP C1KHZ7
B	-9	ALA	-	expression tag	UNP C1KHZ7
B	-8	SER	-	expression tag	UNP C1KHZ7
B	-7	MET	-	expression tag	UNP C1KHZ7
B	-6	THR	-	expression tag	UNP C1KHZ7
B	-5	GLY	-	expression tag	UNP C1KHZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP C1KHZ7
B	-3	GLN	-	expression tag	UNP C1KHZ7
B	-2	GLN	-	expression tag	UNP C1KHZ7
B	-1	MET	-	expression tag	UNP C1KHZ7
B	0	GLY	-	expression tag	UNP C1KHZ7
B	181	GLY	-	expression tag	UNP C1KHZ7
B	182	SER	-	expression tag	UNP C1KHZ7
B	183	HIS	-	expression tag	UNP C1KHZ7
B	184	HIS	-	expression tag	UNP C1KHZ7
B	185	HIS	-	expression tag	UNP C1KHZ7
B	186	HIS	-	expression tag	UNP C1KHZ7
B	187	HIS	-	expression tag	UNP C1KHZ7
B	188	HIS	-	expression tag	UNP C1KHZ7
B	40	THR	ALA	conflict	UNP C1KHZ7
B	153	LEU	ILE	conflict	UNP C1KHZ7

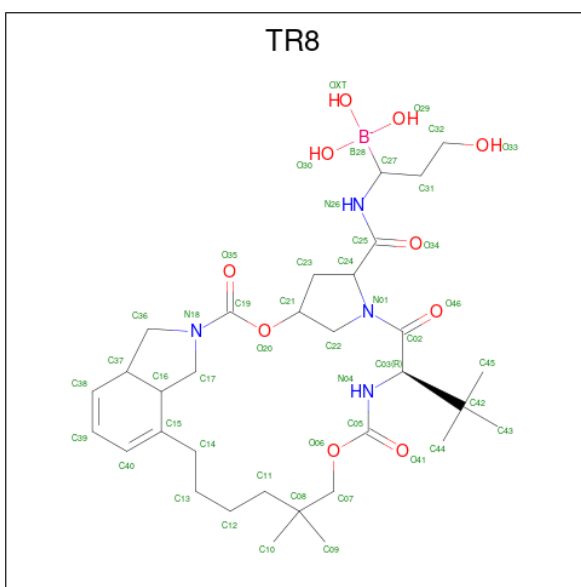
- Molecule 2 is a protein called NS4A COFACTOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	0	0	0
			149	99	27	23			
2	D	16	Total	C	N	O	0	0	0
			108	70	20	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	LYS	-	expression tag	UNP C9WU77
C	20	LYS	-	expression tag	UNP C9WU77
C	40	LYS	-	expression tag	UNP C9WU77
C	41	LYS	-	expression tag	UNP C9WU77
D	19	LYS	-	expression tag	UNP C9WU77
D	20	LYS	-	expression tag	UNP C9WU77
D	40	LYS	-	expression tag	UNP C9WU77
D	41	LYS	-	expression tag	UNP C9WU77

- Molecule 3 is (1-[(10-tert-butyl-15,15-dimethyl-3,9,12-trioxo-6,7,9,10,11,12,14,15,16,17,18,19,23,23a-tetradecahydro-1H,5H-2,23:5,8-dimethano-4,13,2,8,11-benzodioxatriazacycloheptosin-7(3H)-yl)carbonyl]amino}-3-hydroxypropyl)(trihydroxy)borate(1-) (three-letter code: TR8) (formula: C<sub>32</sub>H<sub>52</sub>BN<sub>4</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			46	1	32	4	9		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	24	Total	O	0	0
			24	24		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	O	0	0
			4	4		
6	D	4	Total	O	0	0
			4	4		



- Molecule 1: NS3 PROTEASE

[illegible]

- Molecule 1: NS3 PROTEASE

T98	T108	R109	R123	I132	G137	S138	S139	C145	P146	L153	F154	R155	V158	D168	L175	R180	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	ALA	SER	THR	GLY	GLN	GLN	GLY	ALA	PRO	ILE	THR	ALA	ALA	TYR	GLN	GLN	THR	ARG	GLY	LEU	LEU	GLY	CYS	ILE	ILE	THR	SER	LEU	THR	GLY	ARG	ASP	LYS	ASN	Q28	I35	T42	F43	L44	V55	S66	Q73	T76	D81	W85	T95	P96	C97
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- Molecule 2: NS4A COFACTOR

LYS K20 R28 S32 K40 LYS

- Molecule 2: NS4A COFACTOR

LYS  
LYS  
G21  
S22  
V26  
S32  
A36  
ILE  
ILE  
PRO  
LYS  
LYS



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	233.29Å 233.29Å 78.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	117.04 – 3.30 116.64 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (117.04-3.30) 99.7 (116.64-3.30)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.202 , 0.249 0.201 , 0.248	Depositor DCC
$R_{free}$ test set	588 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 91.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: ZN, TR8, MG

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	0.47	0/1365	0.63	0/1861
1	B	0.48	0/1160	0.64	0/1583
2	C	0.47	0/150	0.61	0/201
2	D	0.52	0/108	0.68	0/145
All	All	0.48	0/2783	0.64	0/3790

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	1339	0	1354	14	0
1	B	1136	0	1140	12	0
2	C	149	0	180	0	0
2	D	108	0	125	2	0
3	A	46	0	49	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	30	0	0	0	0
6	B	24	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
All	All	2844	0	2848	26	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 5.

The worst 5 of 26 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:123:ARG:HH12	1:B:158:VAL:HG21	1.46	0.79
1:A:176:GLU:HB3	1:A:180:ARG:NH1	2.04	0.72
1:A:77:ASN:ND2	1:A:80:GLN:HG3	2.09	0.68
1:A:82:LEU:HD21	1:A:175:LEU:HD23	1.81	0.62
1:A:77:ASN:HB2	1:A:178:THR:CG2	2.32	0.60

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	179/198 (90%)	169 (94%)	9 (5%)	1 (1%)	25	57
1	B	151/198 (76%)	141 (93%)	10 (7%)	0	100	100
2	C	19/23 (83%)	18 (95%)	0	1 (5%)	2	12
2	D	14/23 (61%)	13 (93%)	1 (7%)	0	100	100
All	All	363/442 (82%)	341 (94%)	20 (6%)	2 (1%)	25	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
2	C	32	SER

### 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	A	146/159 (92%)	135 (92%)	11 (8%)	13	39
1	B	125/159 (79%)	116 (93%)	9 (7%)	14	41
2	C	17/19 (90%)	16 (94%)	1 (6%)	19	49
2	D	12/19 (63%)	11 (92%)	1 (8%)	11	36
All	All	300/356 (84%)	278 (93%)	22 (7%)	14	41

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	THR
1	B	132	ILE
1	B	123	ARG
1	B	155	ARG
1	A	103	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	ASN

### 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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	TR8	A	1181	1	45,49,50	2.06	9 (20%)	57,72,75	1.47	6 (10%)

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
3	TR8	A	1181	1	-	10/50/89/91	0/3/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1181	TR8	C40-C15	6.22	1.40	1.33
3	A	1181	TR8	C37-C38	-5.80	1.40	1.50
3	A	1181	TR8	C16-C15	-5.79	1.41	1.52
3	A	1181	TR8	C16-C37	-3.88	1.40	1.54
3	A	1181	TR8	C39-C38	3.04	1.40	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1181	TR8	O20-C19-N18	5.29	115.88	111.24
3	A	1181	TR8	C23-C21-C22	4.39	107.35	103.69
3	A	1181	TR8	C14-C15-C40	-3.21	116.64	121.51
3	A	1181	TR8	C03-C02-N01	2.48	121.42	118.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1181	TR8	C36-N18-C19	2.20	130.44	123.86

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

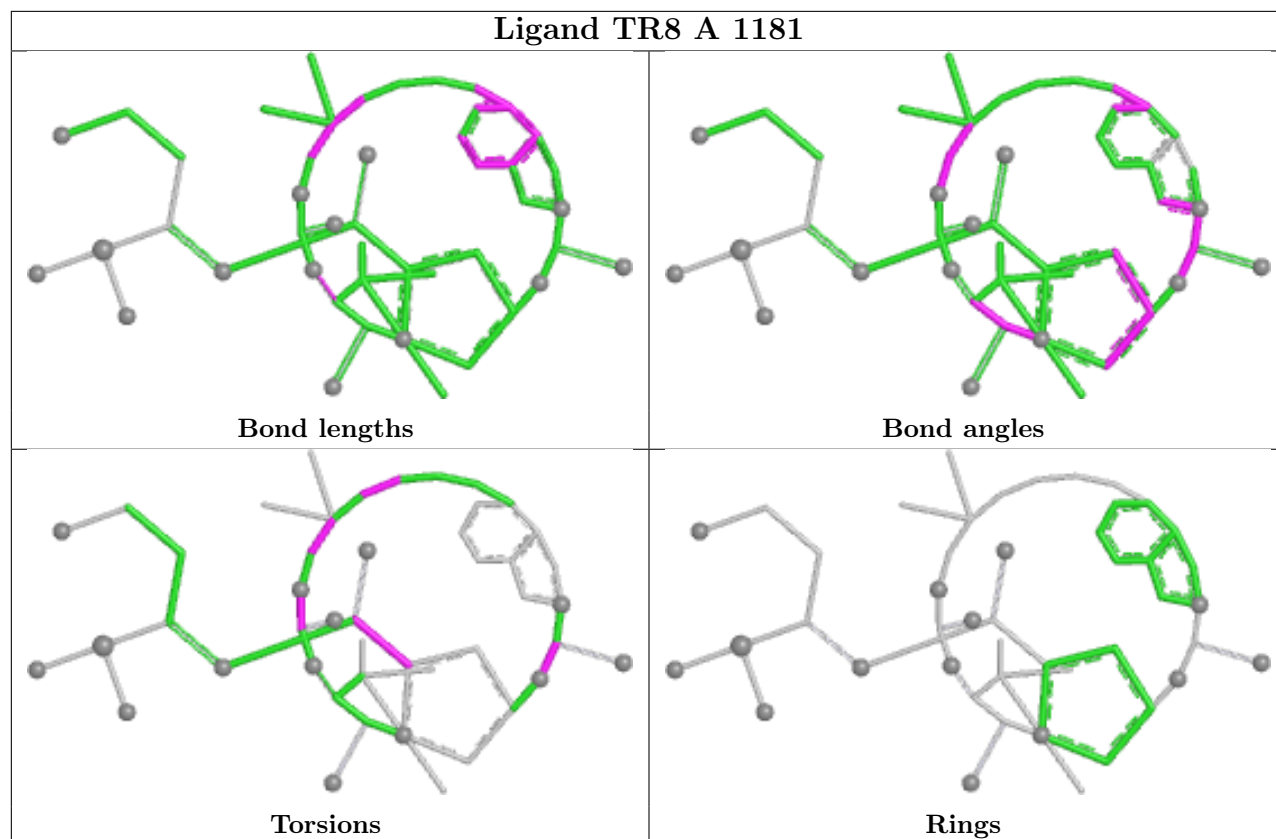
Mol	Chain	Res	Type	Atoms
3	A	1181	TR8	O06-C07-C08-C11
3	A	1181	TR8	N18-C19-O20-C21
3	A	1181	TR8	O35-C19-O20-C21
3	A	1181	TR8	O41-C05-O06-C07
3	A	1181	TR8	N04-C05-O06-C07

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1181	TR8	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 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	181/198 (91%)	0.35	0 100 100	40, 58, 76, 84	0
1	B	153/198 (77%)	0.34	0 100 100	57, 75, 96, 107	0
2	C	21/23 (91%)	0.31	0 100 100	44, 56, 72, 78	0
2	D	16/23 (69%)	0.27	0 100 100	50, 57, 64, 64	0
All	All	371/442 (83%)	0.34	0 100 100	40, 65, 91, 107	0

There are no RSRZ outliers to report.

### 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
5	MG	A	1183	1/1	0.86	0.13	57,57,57,57	0
3	TR8	A	1181	46/47	0.94	0.38	71,87,90,91	0
5	MG	C	1041	1/1	0.97	0.10	59,59,59,59	0
4	ZN	B	1181	1/1	0.99	0.20	59,59,59,59	0

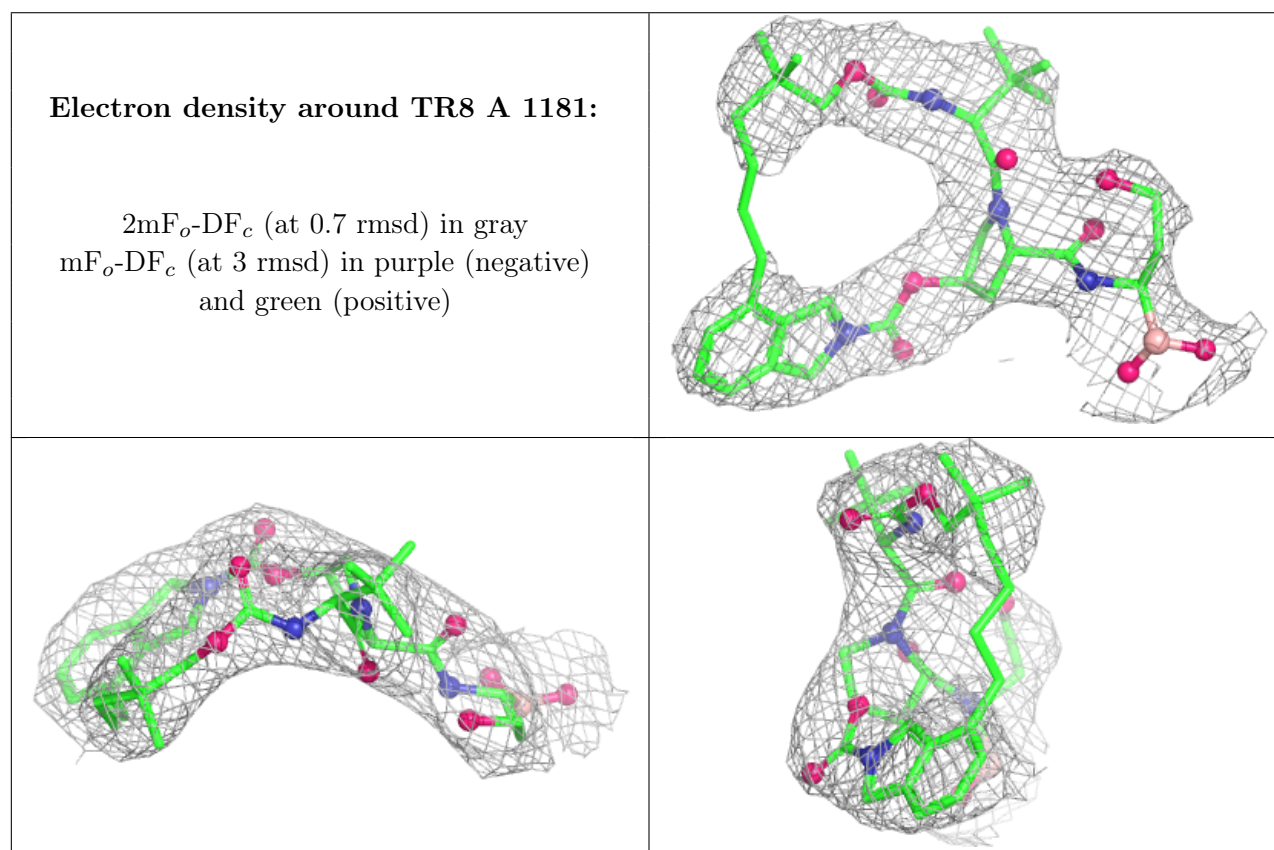
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	A	1182	1/1	1.00	0.19	63,63,63,63	0

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.