



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 05:40 AM BST

PDB ID : 6PIU  
Title : Crystal structure of HCV NS3/4A D168A protease in complex with P4-P5-6 (NR03-68)  
Authors : Zephyr, J.; Schiffer, C.A.  
Deposited on : 2019-06-27  
Resolution : 2.28 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) : 1.13  
EDS : **FAILED**  
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) : 2.14.4.dev1

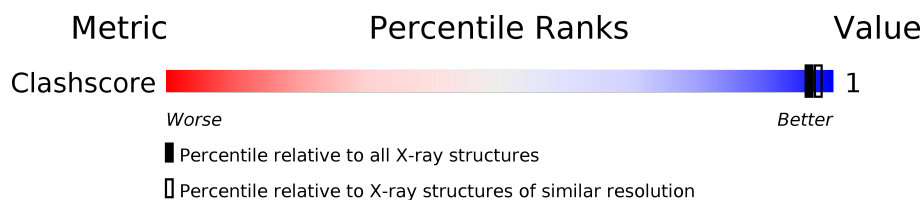
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	7711 (2.30-2.26)

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 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	220	 88% • 10%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3016 atoms, of which 1446 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	197	Total	C	H	N	O	S	0	0	0
			2776	876	1365	255	272	8			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	963	MET	-	initiating methionine	UNP A0A0B4WYC6
A	964	GLY	-	expression tag	UNP A0A0B4WYC6
A	965	SER	-	expression tag	UNP A0A0B4WYC6
A	966	SER	-	expression tag	UNP A0A0B4WYC6
A	967	HIS	-	expression tag	UNP A0A0B4WYC6
A	968	HIS	-	expression tag	UNP A0A0B4WYC6
A	969	HIS	-	expression tag	UNP A0A0B4WYC6
A	970	HIS	-	expression tag	UNP A0A0B4WYC6
A	971	HIS	-	expression tag	UNP A0A0B4WYC6
A	972	HIS	-	expression tag	UNP A0A0B4WYC6
A	973	SER	-	expression tag	UNP A0A0B4WYC6
A	974	SER	-	expression tag	UNP A0A0B4WYC6
A	975	GLY	-	expression tag	UNP A0A0B4WYC6
A	976	LEU	-	expression tag	UNP A0A0B4WYC6
A	977	VAL	-	expression tag	UNP A0A0B4WYC6
A	978	PRO	-	expression tag	UNP A0A0B4WYC6
A	979	ARG	-	expression tag	UNP A0A0B4WYC6
A	980	GLY	-	expression tag	UNP A0A0B4WYC6
A	981	SER	-	expression tag	UNP A0A0B4WYC6
A	982	HIS	-	expression tag	UNP A0A0B4WYC6
A	983	MET	-	expression tag	UNP A0A0B4WYC6
A	984	ALA	-	expression tag	UNP A0A0B4WYC6
A	985	SER	-	expression tag	UNP A0A0B4WYC6
A	986	MET	-	expression tag	UNP A0A0B4WYC6
A	987	LYS	-	expression tag	UNP A0A0B4WYC6
A	988	LYS	-	expression tag	UNP A0A0B4WYC6
A	989	LYS	-	expression tag	UNP A0A0B4WYC6

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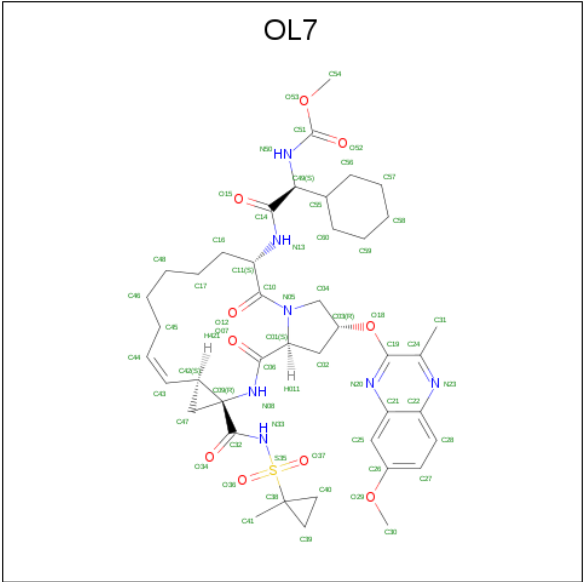
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Chain	Residue	Modelled	Actual	Comment	Reference
A	990	GLY	-	expression tag	UNP A0A0B4WYC6
A	991	SER	-	expression tag	UNP A0A0B4WYC6
A	992	VAL	-	expression tag	UNP A0A0B4WYC6
A	993	VAL	-	expression tag	UNP A0A0B4WYC6
A	994	ILE	-	expression tag	UNP A0A0B4WYC6
A	995	VAL	-	expression tag	UNP A0A0B4WYC6
A	996	GLY	-	expression tag	UNP A0A0B4WYC6
A	997	ARG	-	expression tag	UNP A0A0B4WYC6
A	998	ILE	-	expression tag	UNP A0A0B4WYC6
A	999	ASN	-	expression tag	UNP A0A0B4WYC6
A	1000	LEU	-	expression tag	UNP A0A0B4WYC6
A	1001	SER	-	expression tag	UNP A0A0B4WYC6
A	1002	GLY	-	expression tag	UNP A0A0B4WYC6
A	1003	ASP	-	expression tag	UNP A0A0B4WYC6
A	1013	GLU	LEU	conflict	UNP A0A0B4WYC6
A	1014	GLU	LEU	conflict	UNP A0A0B4WYC6
A	1017	GLN	ILE	conflict	UNP A0A0B4WYC6
A	1018	GLU	ILE	conflict	UNP A0A0B4WYC6
A	1021	GLN	LEU	conflict	UNP A0A0B4WYC6
A	1047	SER	CYS	conflict	UNP A0A0B4WYC6
A	1052	LEU	CYS	conflict	UNP A0A0B4WYC6
A	1072	THR	ILE	conflict	UNP A0A0B4WYC6
A	1086	GLN	PRO	conflict	UNP A0A0B4WYC6
A	1159	SER	CYS	conflict	UNP A0A0B4WYC6
A	1168	ALA	ASP	engineered mutation	UNP A0A0B4WYC6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

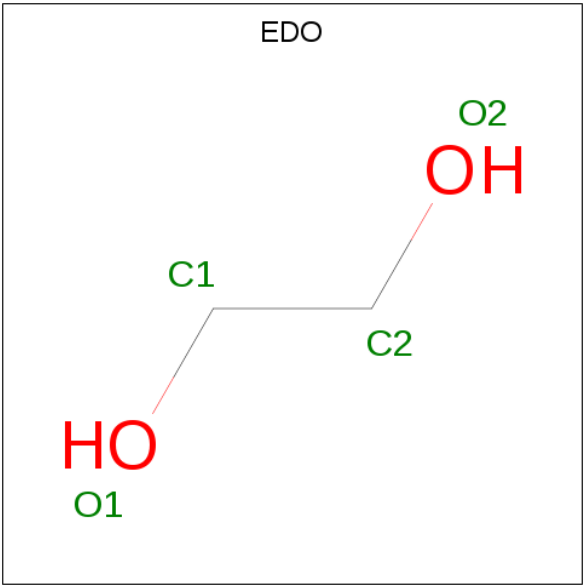
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is methyl [(1S)-1-cyclohexyl-2-{{[(2R,6S,12Z,13aS,14aR,16aS)-2-[(7-methoxy-3-methylquinoxalin-2-yl)oxy]-14a-{{[(1-methylcyclopropyl)sulfonyl]carbamoyl}-5,16-dioxo-1,2,3,5,6,7,8,9,10,11,13a,14,14a,15,16,16a-hexadecahydrocyclopropa[e]pyrrolo[1,2-a][1,4]diazacyclopentadecin-6-yl]amino}-2-oxoethyl]carbamate (three-letter code: OL7) (formula: C<sub>42</sub>H<sub>57</sub>N<sub>7</sub>O<sub>10</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			117	42	57	7	10	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		

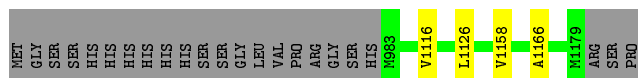
### 3 Residue-property plots [i](#)

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. 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 failed to run properly.

- Molecule 1: NS3 protease

Chain A:  88% • 10%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.81Å 59.65Å 58.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.40 – 2.28	Depositor
% Data completeness (in resolution range)	99.7 (27.40-2.28)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, $R_{free}$	0.193 , 0.235	Depositor
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.158	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
Total number of atoms	3016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, OL7

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	0.26	0/1435	0.48	0/1955

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	1411	1365	1384	3	0
2	A	1	0	0	0	0
3	A	60	57	0	0	0
4	A	16	24	24	0	0
5	A	82	0	0	0	0
All	All	1570	1446	1408	3	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 1.

All (3) 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:1158:VAL:HB	1:A:1166:ALA:HB3	1.81	0.62
1:A:1116:VAL:HG22	1:A:1126:LEU:HD23	1.91	0.53
1:A:1116:VAL:HG22	1:A:1126:LEU:CD2	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
4	EDO	A	1206	-	3,3,3	0.45	0	2,2,2	0.63	0
4	EDO	A	1205	-	3,3,3	0.46	0	2,2,2	0.41	0
3	OL7	A	1202	-	62,66,66	4.65	31 (50%)	84,98,98	2.70	19 (22%)
4	EDO	A	1204	-	3,3,3	0.43	0	2,2,2	0.59	0
4	EDO	A	1203	-	3,3,3	0.45	0	2,2,2	0.46	0

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
4	EDO	A	1206	-	-	1/1/1/1	-
4	EDO	A	1205	-	-	1/1/1/1	-
3	OL7	A	1202	-	-	8/62/103/103	0/6/7/7
4	EDO	A	1204	-	-	1/1/1/1	-
4	EDO	A	1203	-	-	1/1/1/1	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	OL7	C24-N23	11.04	1.46	1.32
3	A	1202	OL7	C02-C03	-10.23	1.30	1.52
3	A	1202	OL7	C25-C26	9.81	1.54	1.37
3	A	1202	OL7	C25-C21	9.46	1.56	1.41
3	A	1202	OL7	C04-C03	8.87	1.67	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	OL7	C47-C09-N08	13.53	135.97	117.80
3	A	1202	OL7	O37-S35-O36	-9.40	101.49	120.57
3	A	1202	OL7	O53-C51-N50	5.63	120.68	110.80
3	A	1202	OL7	C47-C42-C43	-5.28	106.68	120.03
3	A	1202	OL7	C32-N33-S35	-5.17	115.73	124.08

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	OL7	C14-C49-C55-C56

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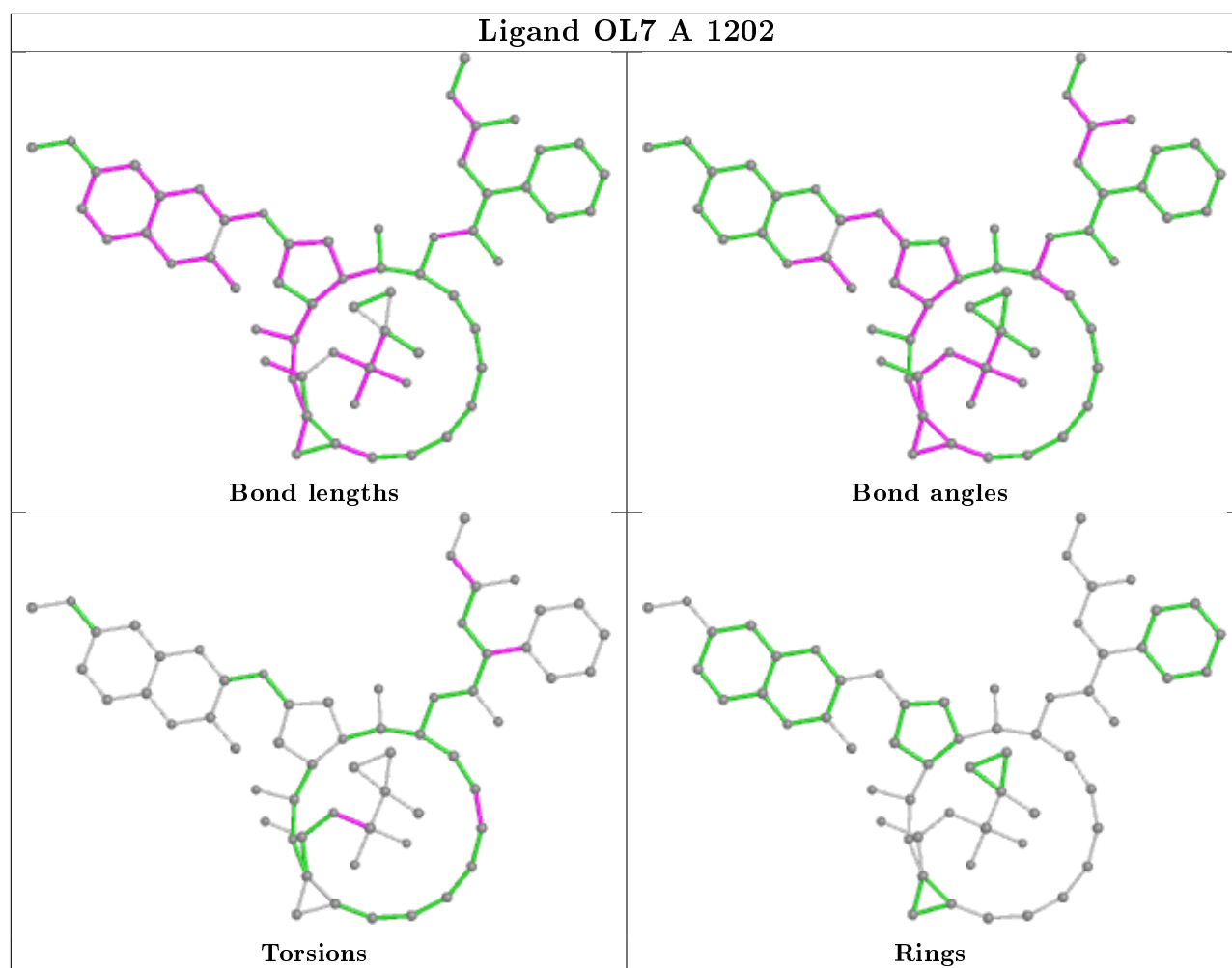
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Mol	Chain	Res	Type	Atoms
3	A	1202	OL7	C14-C49-C55-C60
3	A	1202	OL7	N50-C49-C55-C56
3	A	1202	OL7	N50-C49-C55-C60
3	A	1202	OL7	N50-C51-O53-C54

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.