



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2020 – 04:09 PM JST

PDB ID : 6LOY  
Title : crystal structure of alpha-momorcharin in complex with dAMP  
Authors : Fan, X.; Jin, T.  
Deposited on : 2020-01-07  
Resolution : 1.35 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.

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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 : 2.14.6  
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) : 2.14.6

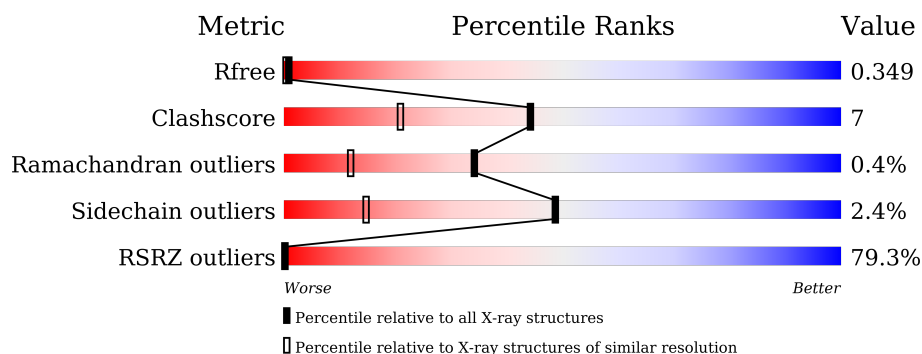
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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  $\leq 5\%$ . 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	286	<div> <div>68%</div> <div>74%</div> <div>11%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

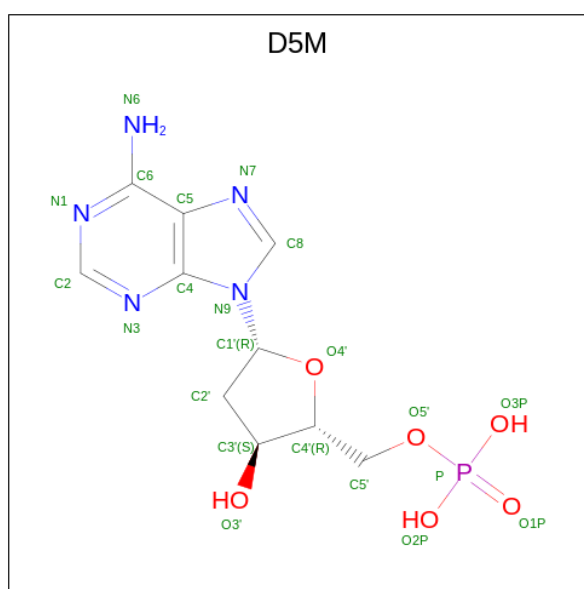
There are 3 unique types of molecules in this entry. The entry contains 2148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosome-inactivating protein momordin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1947	1242	338	364	3	0	2	0

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	22	10	5	6	1	0	0

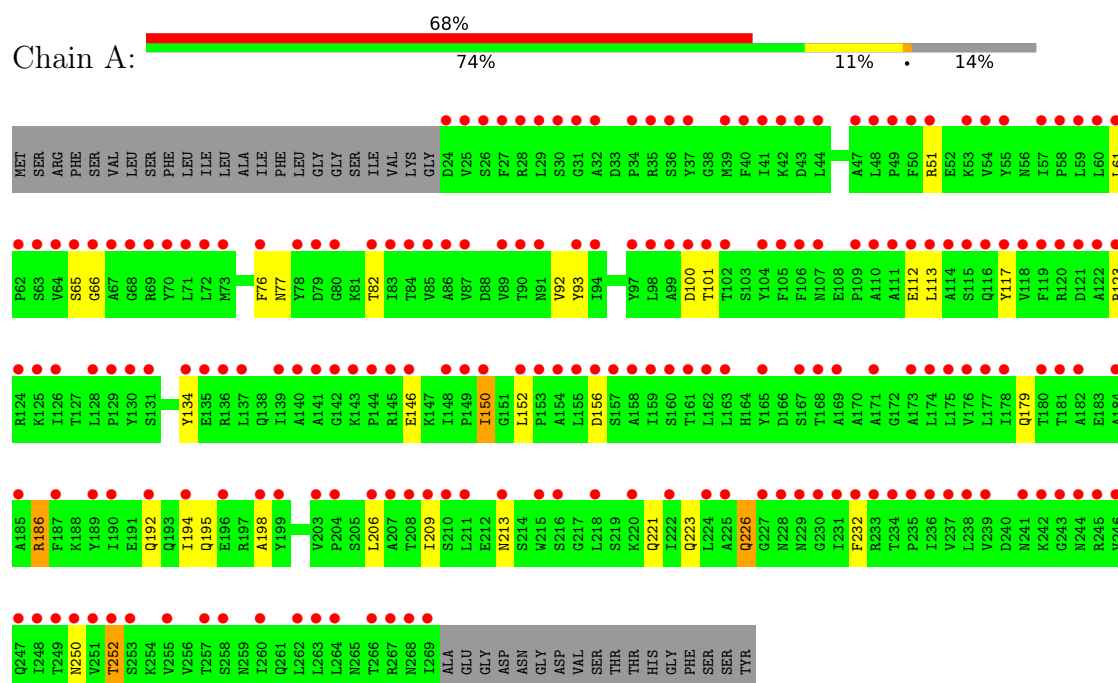
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total	O	0	0
			179	179		

### 3 Residue-property plots

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: Ribosome-inactivating protein momordin I



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.67Å 130.67Å 39.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.95 – 1.35 14.95 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.2 (14.95-1.35) 92.3 (14.95-1.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.300 , 0.349 0.295 , 0.349	Depositor DCC
$R_{free}$ test set	2505 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.71 , 89.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.31% 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: D5M

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	0.81	0/1983	1.00	3/2693 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	186	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	A	252	THR	N-CA-CB	5.19	120.16	110.30
1	A	252	THR	CB-CA-C	-5.07	97.92	111.60

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	1947	0	1981	26	0
2	A	22	0	12	5	0
3	A	179	0	0	2	0
All	All	2148	0	1993	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 7.

All (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:A:152:LEU:HD13	1:A:198:ALA:HA	1.59	0.82
1:A:213:ASN:HA	2:A:301:D5M:O2P	1.98	0.63
1:A:123:ARG:HH21	1:A:123:ARG:HG3	1.65	0.62
1:A:192:GLN:HA	1:A:195:GLN:HE21	1.69	0.57
1:A:209:ILE:HD11	3:A:446:HOH:O	2.08	0.54
1:A:186:ARG:NH1	2:A:301:D5M:H2'1	2.24	0.52
1:A:250:ASN:HD22	1:A:252:THR:H	1.58	0.52
1:A:93:TYR:HA	2:A:301:D5M:C2	2.40	0.52
1:A:150:ILE:CD1	1:A:179:GLN:HB2	2.39	0.51
1:A:51:ARG:HG2	1:A:61:LEU:HD21	1.95	0.49
1:A:206:LEU:O	1:A:209:ILE:HG13	2.15	0.47
1:A:92:VAL:O	2:A:301:D5M:H2	2.16	0.45
1:A:221:GLN:CG	1:A:232:PHE:CG	3.00	0.44
1:A:150:ILE:HD11	1:A:179:GLN:OE1	2.18	0.44
1:A:77:ASN:HB2	1:A:156:ASP:OD1	2.18	0.43
1:A:134:TYR:CE2	2:A:301:D5M:O4'	2.70	0.43
1:A:221:GLN:HG3	1:A:232:PHE:HA	1.98	0.43
1:A:221:GLN:HG3	1:A:232:PHE:CG	2.53	0.43
1:A:150:ILE:CG2	1:A:194:ILE:CD1	2.97	0.43
1:A:76:PHE:CD2	1:A:82:THR:HB	2.54	0.42
1:A:66:GLY:HA2	1:A:117:TYR:CE1	2.54	0.42
1:A:100:ASP:OD2	1:A:101:THR:HG23	2.19	0.41
1:A:152:LEU:HD11	1:A:194:ILE:HG22	2.02	0.41
1:A:206:LEU:HG	3:A:475:HOH:O	2.20	0.41
1:A:250:ASN:ND2	1:A:252:THR:OG1	2.53	0.41
1:A:223:GLN:O	1:A:226:GLN:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	246/286 (86%)	237 (96%)	8 (3%)	1 (0%)	34 12

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN

### 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	211/241 (88%)	206 (98%)	5 (2%)	49 15

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	112	GLU
1	A	113	LEU
1	A	146	GLU
1	A	150	ILE

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

Mol	Chain	Res	Type
1	A	195	GLN
1	A	250	ASN

### 5.3.3 RNA ⓘ

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](#)

1 ligand is 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	D5M	A	301	-	22,24,24	3.24	10 (45%)	24,36,36	2.36	6 (25%)

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	D5M	A	301	-	-	5/6/22/22	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	D5M	C3'-C4'	-8.72	1.29	1.53
2	A	301	D5M	C2'-C1'	-6.73	1.33	1.52
2	A	301	D5M	O4'-C4'	5.24	1.56	1.45
2	A	301	D5M	O4'-C1'	3.97	1.51	1.42
2	A	301	D5M	C2-N1	3.74	1.40	1.33
2	A	301	D5M	C2'-C3'	3.65	1.62	1.52
2	A	301	D5M	C4-N3	3.55	1.40	1.35
2	A	301	D5M	C6-N6	2.54	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	D5M	O3'-C3'	2.16	1.47	1.43
2	A	301	D5M	C5-C4	-2.06	1.35	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	D5M	C5-C6-N6	7.11	131.16	120.35
2	A	301	D5M	N3-C2-N1	-4.88	121.05	128.68
2	A	301	D5M	N6-C6-N1	-4.46	109.31	118.57
2	A	301	D5M	C3'-C2'-C1'	3.21	110.58	102.54
2	A	301	D5M	O2P-P-O5'	2.70	113.92	106.73
2	A	301	D5M	C2'-C1'-N9	-2.31	108.95	114.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

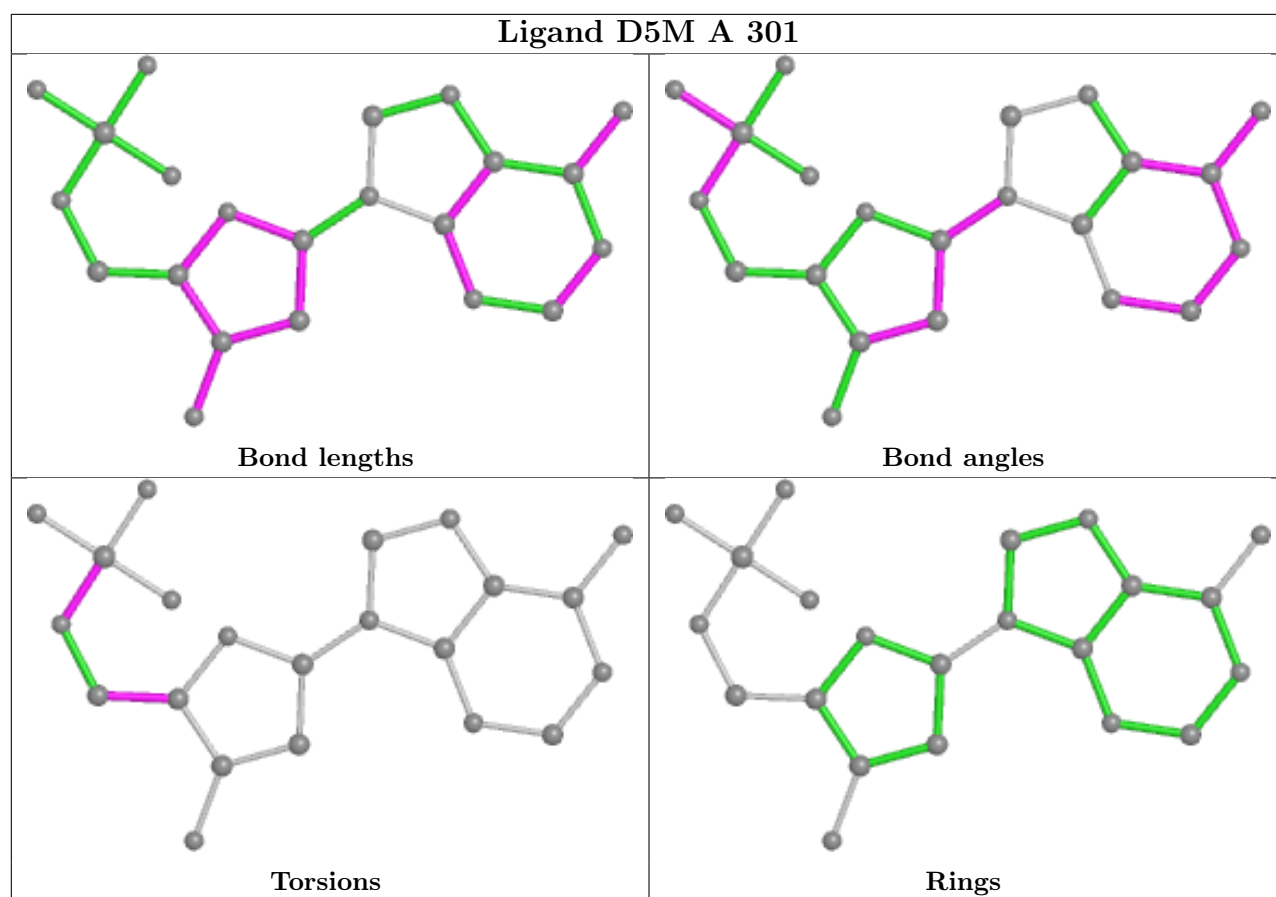
Mol	Chain	Res	Type	Atoms
2	A	301	D5M	C5'-O5'-P-O1P
2	A	301	D5M	C5'-O5'-P-O3P
2	A	301	D5M	C5'-O5'-P-O2P
2	A	301	D5M	C3'-C4'-C5'-O5'
2	A	301	D5M	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	D5M	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	246/286 (86%)	3.20	195 (79%) 0 0	17, 28, 39, 46	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	VAL	8.8
1	A	251	VAL	7.2
1	A	239	VAL	7.1
1	A	118	VAL	6.8
1	A	122	ALA	6.7
1	A	269	ILE	6.7
1	A	139	ILE	6.7
1	A	203	VAL	6.6
1	A	225	ALA	6.4
1	A	236	ILE	5.9
1	A	218	LEU	5.8
1	A	209	ILE	5.8
1	A	117	TYR	5.7
1	A	113	LEU	5.6
1	A	232	PHE	5.6
1	A	163	LEU	5.4
1	A	61	LEU	5.3
1	A	177	LEU	5.3
1	A	110	ALA	5.3
1	A	72	LEU	5.1
1	A	27	PHE	5.1
1	A	101	THR	5.0
1	A	176	VAL	5.0
1	A	141	ALA	5.0
1	A	238	LEU	4.9
1	A	47	ALA	4.8
1	A	60	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	4.8
1	A	153	PRO	4.8
1	A	130	TYR	4.8
1	A	34	PRO	4.7
1	A	50	PHE	4.7
1	A	128	LEU	4.6
1	A	199	TYR	4.5
1	A	159	ILE	4.5
1	A	231	ILE	4.5
1	A	70	TYR	4.5
1	A	173	ALA	4.4
1	A	152	LEU	4.3
1	A	76	PHE	4.3
1	A	119	PHE	4.3
1	A	234	THR	4.3
1	A	67	ALA	4.3
1	A	44	LEU	4.2
1	A	137	LEU	4.2
1	A	168	THR	4.2
1	A	104	TYR	4.2
1	A	29	LEU	4.2
1	A	31	GLY	4.2
1	A	266	THR	4.2
1	A	131	SER	4.1
1	A	189	TYR	4.1
1	A	206	LEU	4.1
1	A	262	LEU	4.1
1	A	175	LEU	4.1
1	A	237	VAL	4.0
1	A	171	ALA	4.0
1	A	252	THR	4.0
1	A	158	ALA	4.0
1	A	241	ASN	4.0
1	A	134	TYR	4.0
1	A	207	ALA	4.0
1	A	150	ILE	4.0
1	A	235	PRO	4.0
1	A	215	TRP	3.9
1	A	94	ILE	3.9
1	A	208	THR	3.9
1	A	154	ALA	3.9
1	A	55	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	93	TYR	3.9
1	A	248	ILE	3.8
1	A	222	ILE	3.8
1	A	32	ALA	3.8
1	A	242	LYS	3.8
1	A	90	THR	3.8
1	A	230	GLY	3.8
1	A	25	VAL	3.7
1	A	85	VAL	3.7
1	A	249	THR	3.7
1	A	211	LEU	3.7
1	A	62	PRO	3.7
1	A	24	ASP	3.7
1	A	54	VAL	3.7
1	A	79	ASP	3.7
1	A	99	ALA	3.7
1	A	41	ILE	3.7
1	A	194	ILE	3.7
1	A	169	ALA	3.6
1	A	143	LYS	3.6
1	A	120	ARG	3.6
1	A	146	GLU	3.6
1	A	115	SER	3.6
1	A	140	ALA	3.6
1	A	106	PHE	3.5
1	A	51	ARG	3.4
1	A	39	MET	3.4
1	A	66	GLY	3.4
1	A	57	ILE	3.4
1	A	142	GLY	3.3
1	A	86	ALA	3.3
1	A	267	ARG	3.3
1	A	174	LEU	3.3
1	A	144	PRO	3.3
1	A	105	PHE	3.3
1	A	37	TYR	3.3
1	A	155	LEU	3.3
1	A	65	SER	3.3
1	A	196	GLU	3.3
1	A	178	ILE	3.3
1	A	181	THR	3.2
1	A	257	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	3.2
1	A	126	ILE	3.2
1	A	114	ALA	3.2
1	A	40	PHE	3.2
1	A	63	SER	3.2
1	A	53	LYS	3.2
1	A	123	ARG	3.2
1	A	263	LEU	3.2
1	A	136	ARG	3.1
1	A	204	PRO	3.1
1	A	30	SER	3.1
1	A	116	GLN	3.1
1	A	83	ILE	3.1
1	A	210	SER	3.1
1	A	162	LEU	3.1
1	A	78	TYR	3.1
1	A	258[A]	SER	3.0
1	A	255	VAL	3.0
1	A	111	ALA	3.0
1	A	84	THR	3.0
1	A	260	ILE	3.0
1	A	43	ASP	3.0
1	A	69	ARG	3.0
1	A	68	GLY	2.9
1	A	187	PHE	2.9
1	A	198	ALA	2.9
1	A	102	THR	2.9
1	A	227	GLY	2.9
1	A	244	ASN	2.9
1	A	80	GLY	2.8
1	A	97	TYR	2.8
1	A	71	LEU	2.8
1	A	82	THR	2.8
1	A	247	GLN	2.8
1	A	59	LEU	2.8
1	A	98	LEU	2.8
1	A	243	GLY	2.8
1	A	58	PRO	2.7
1	A	109	PRO	2.7
1	A	149	PRO	2.7
1	A	228	ASN	2.7
1	A	148	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	165	TYR	2.7
1	A	161	THR	2.6
1	A	184	ALA	2.6
1	A	100	ASP	2.6
1	A	87	VAL	2.6
1	A	129	PRO	2.5
1	A	124	ARG	2.5
1	A	190	ILE	2.5
1	A	125[A]	LYS	2.5
1	A	28	ARG	2.4
1	A	26	SER	2.4
1	A	268	ASN	2.4
1	A	145	ARG	2.4
1	A	182	ALA	2.4
1	A	121	ASP	2.3
1	A	180	THR	2.3
1	A	157	SER	2.3
1	A	107	ASN	2.3
1	A	160	SER	2.3
1	A	264	LEU	2.3
1	A	229	ASN	2.3
1	A	250	ASN	2.3
1	A	73	MET	2.3
1	A	112	GLU	2.3
1	A	48	LEU	2.2
1	A	192	GLN	2.2
1	A	135	GLU	2.2
1	A	89	VAL	2.2
1	A	91	ASN	2.2
1	A	245	ARG	2.2
1	A	36	SER	2.2
1	A	167	SER	2.2
1	A	216	SER	2.2
1	A	185	ALA	2.2
1	A	213	ASN	2.2
1	A	253	SER	2.2
1	A	233	ARG	2.1
1	A	42	LYS	2.1
1	A	49	PRO	2.1
1	A	35	ARG	2.1
1	A	220	LYS	2.1
1	A	156	ASP	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](#)

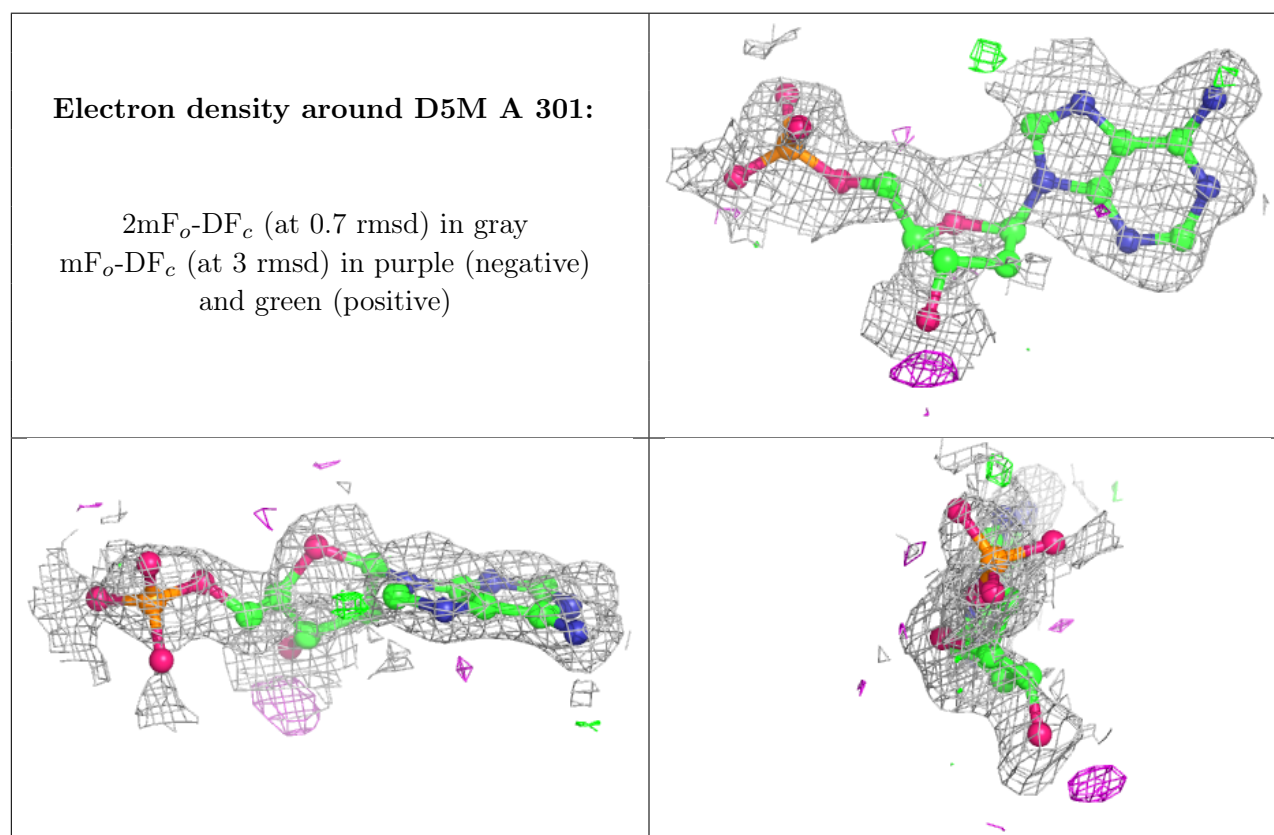
There are no monosaccharides in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
2	D5M	A	301	22/22	0.76	0.23	22,33,43,44	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.