



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 1, 2021 – 12:10 pm GMT

PDB ID : 7POW  
Title : Crystal structure of phosphatidyl serine synthase (PSS) in transition state.  
Authors : Yildiz, O.; Centola, M.  
Deposited on : 2021-09-10  
Resolution : 2.51 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 : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

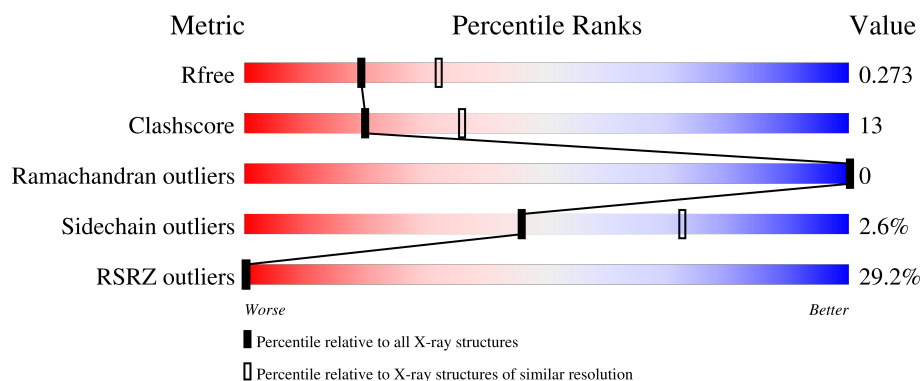
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	204	<div> <div>25%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	B	204	<div> <div>31%</div> <div>72%</div> <div>27%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	307	-	-	X	-
6	OLC	A	310	-	-	-	X
6	OLC	A	312	-	-	-	X
6	OLC	B	309	-	-	-	X
8	SER	B	306	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3613 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.

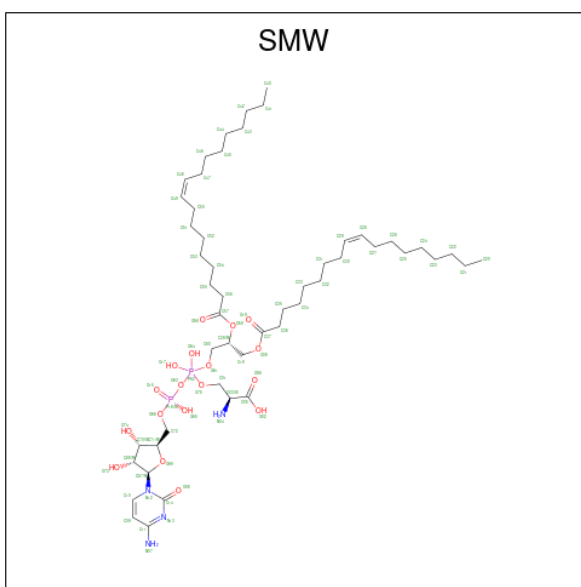
- Molecule 1 is a protein called CDP-diacylglycerol--serine O-phosphatidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	Se	0	0	0
			1551	1043	235	264	5	4			
1	B	204	Total	C	N	O	S	Se	0	1	0
			1582	1065	240	268	5	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q58609
A	-1	PRO	-	expression tag	UNP Q58609
A	0	HIS	-	expression tag	UNP Q58609
B	-2	ALA	-	expression tag	UNP Q58609
B	-1	PRO	-	expression tag	UNP Q58609
B	0	HIS	-	expression tag	UNP Q58609

- Molecule 2 is (2S)-2-amino-3-[[[(2R,3S,4R,5R)-5-(4-amino-2-oxo-pyrimidin-1-yl)-3,4-dihydroxy-tetrahydrofuran-2-yl]methoxy-hydroxy-phosphoryl]oxy-[(2R)-2,3-bis[[[(Z)-octadec-9-enoyl]oxy]propoxy]-dihydroxy-lambda<sup>5</sup>-phosphanyl]oxy-propanoic acid (three-letter code: SMW) (formula: C<sub>51</sub>H<sub>92</sub>N<sub>4</sub>O<sub>18</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			75	51	4	18	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

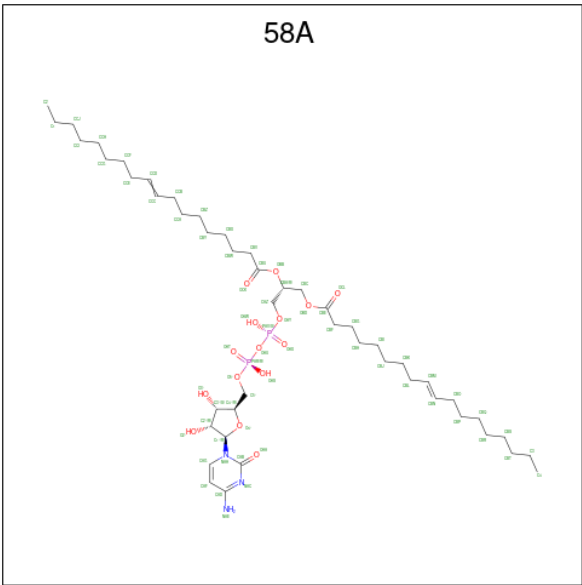
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	B	2	Total	Cl	0	0
			2	2		

- # OLC
- 
- The chemical structure of OLC (Oleic acid) is shown. It consists of a long hydrocarbon chain with a double bond (C9=C10) and a carboxylic acid group (C1=O19, O20). The chain is labeled with carbon atoms C1 through C18. The carboxylic acid group is labeled with O19, O20, and C21. The structure is drawn in a zig-zag conformation, with the double bond in the middle of the chain. The carboxylic acid group is at the right end, and the hydrocarbon chain extends to the left. The structure is labeled with 'OLC' at the top.

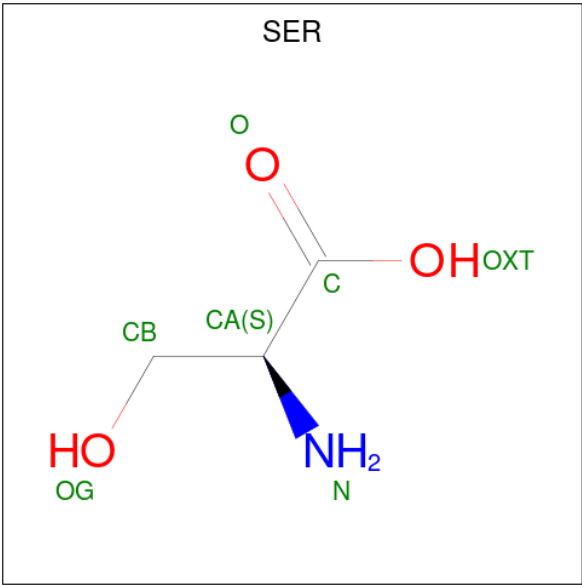
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	B	1	Total 25	C 21	O 4	0	0
6	B	1	Total 25	C 21	O 4	0	0
6	B	1	Total 25	C 21	O 4	0	0
6	B	1	Total 25	C 21	O 4	0	0

- Molecule 7 is 5'-O-[(R)-{[(S)-{(2R)-2,3-bis[(9E)-octadec-9-enoyloxy]propoxy}(hydroxy)phosphoryl]oxy} (hydroxy)phosphoryl]cytidine (three-letter code: 58A) (formula: C<sub>48</sub>H<sub>85</sub>N<sub>3</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	64	44	3	15	2	0	0

- Molecule 8 is SERINE (three-letter code: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	7	3	1	3	0	0

- Molecule 9 is water.

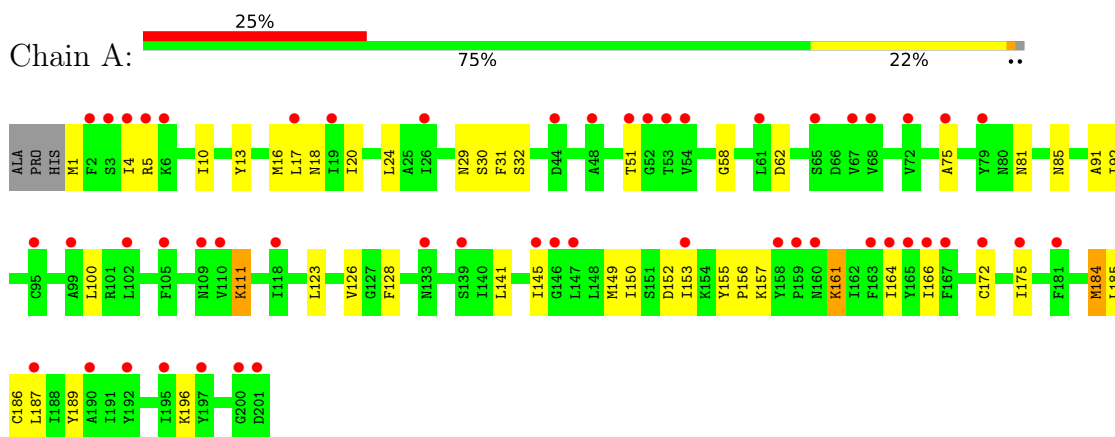
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	44	Total 44	O 44	0	0
9	B	30	Total 30	O 30	0	0



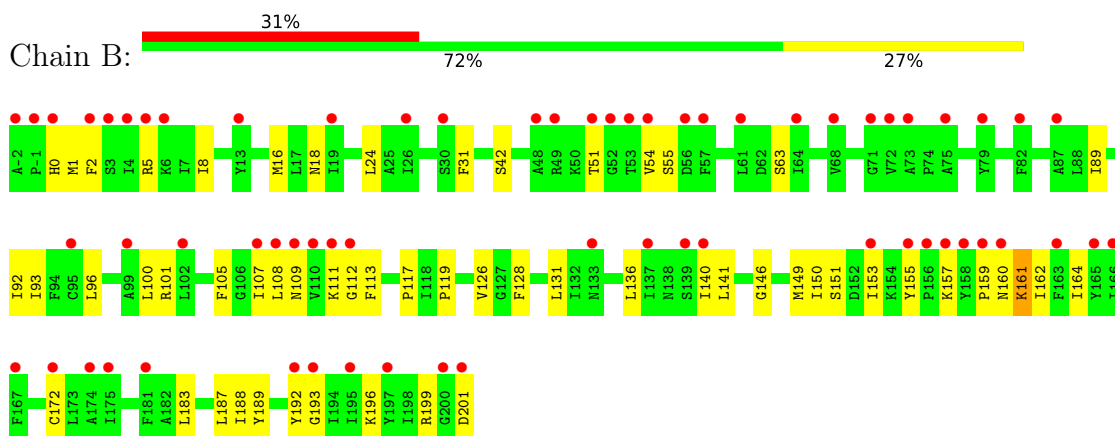
### 3 Residue-property plots [i](#)

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: CDP-diacylglycerol--serine O-phosphatidyltransferase



- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.35Å 61.22Å 79.31Å 90.00° 118.72° 90.00°	Depositor
Resolution (Å)	38.04 – 2.51 38.04 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.04-2.51) 99.9 (38.04-2.51)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.215 , 0.276 0.216 , 0.273	Depositor DCC
$R_{free}$ test set	782 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.51 % 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 3.7851e-03. 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: CA, OLC, SMW, MG, CL, 58A

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	0.42	0/1579	0.56	0/2140
1	B	0.39	0/1615	0.58	0/2189
All	All	0.41	0/3194	0.57	0/4329

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	1551	0	1655	41	0
1	B	1582	0	1683	51	0
2	A	75	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	4	0
5	B	2	0	0	1	0
6	A	150	0	240	15	0
6	B	100	0	160	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	64	0	69	6	0
8	B	7	0	4	1	0
9	A	44	0	0	1	0
9	B	30	0	0	1	0
All	All	3613	0	3811	92	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 13.

The worst 5 of 92 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:100:LEU:HD21	1:B:16:MSE:HE2	1.64	0.77
1:B:162:ILE:H	1:B:162:ILE:HD12	1.52	0.74
1:A:196:LYS:NZ	9:A:401:HOH:O	2.20	0.73
1:A:5:ARG:NH1	6:B:310:OLC:O25	2.23	0.72
6:A:312:OLC:H18A	6:B:307:OLC:H16A	1.72	0.72

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	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
1	B	203/204 (100%)	198 (98%)	5 (2%)	0	100	100
All	All	402/408 (98%)	393 (98%)	9 (2%)	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	170/168 (101%)	164 (96%)	6 (4%)	36	62
1	B	173/168 (103%)	171 (99%)	2 (1%)	71	88
All	All	343/336 (102%)	335 (98%)	8 (2%)	46	76

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

Mol	Chain	Res	Type
1	B	161	LYS
1	B	18	ASN
1	A	164	ILE
1	A	161	LYS
1	A	184	MSE

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

Mol	Chain	Res	Type
1	A	81	ASN

### 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

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

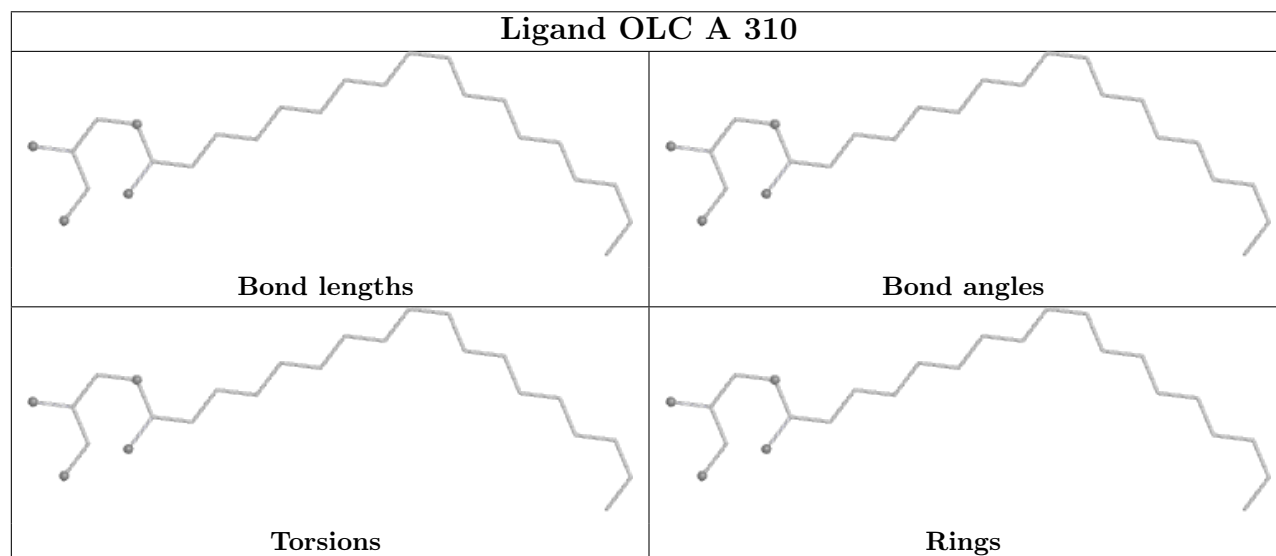
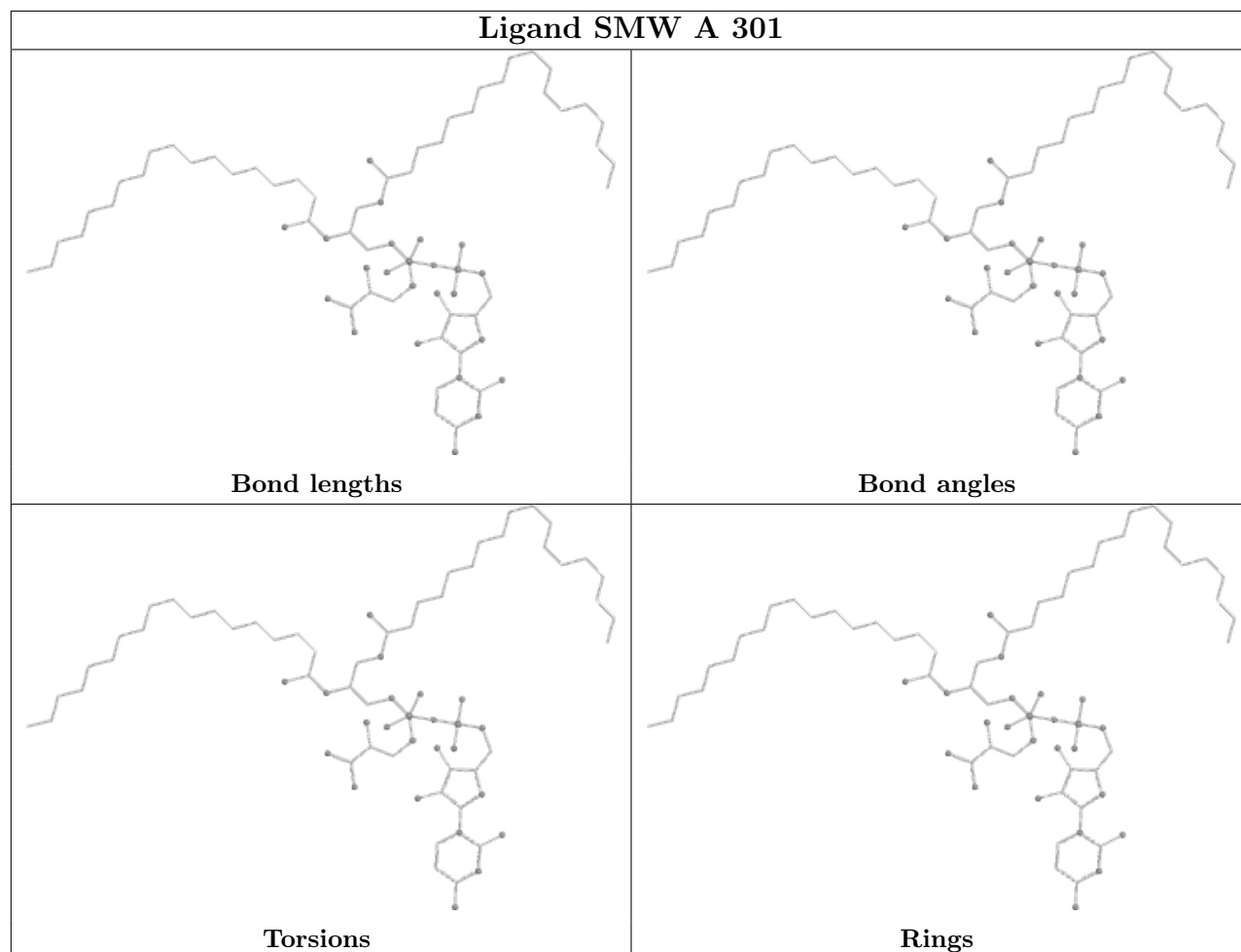
There are no chirality outliers.

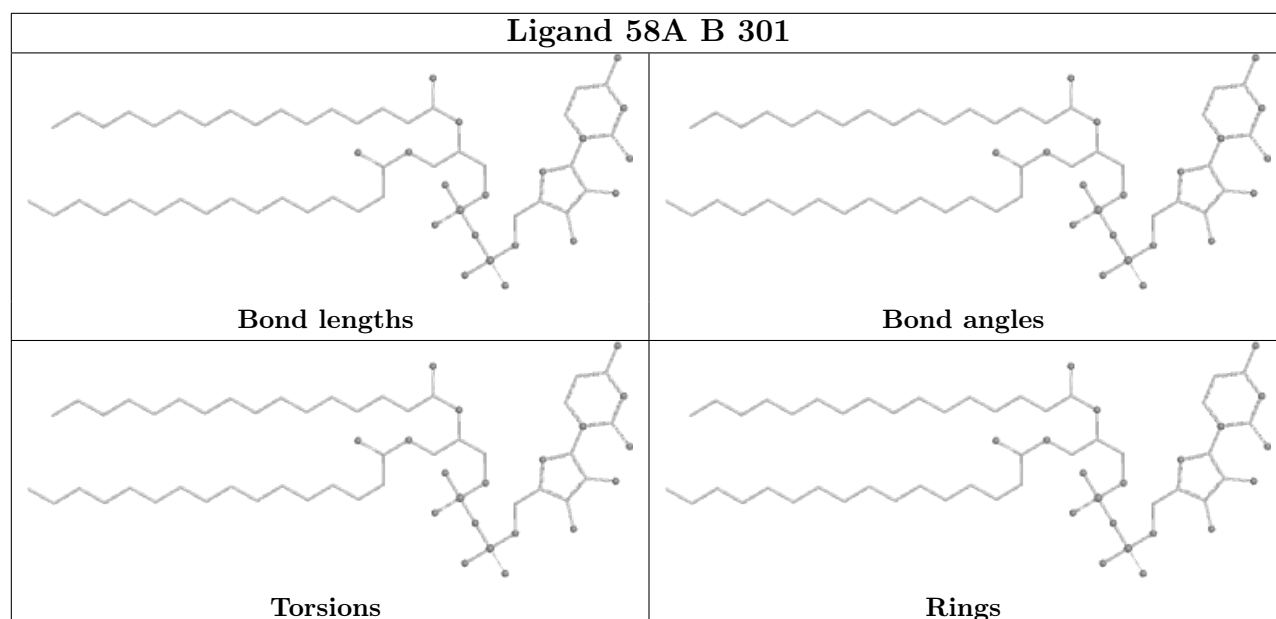
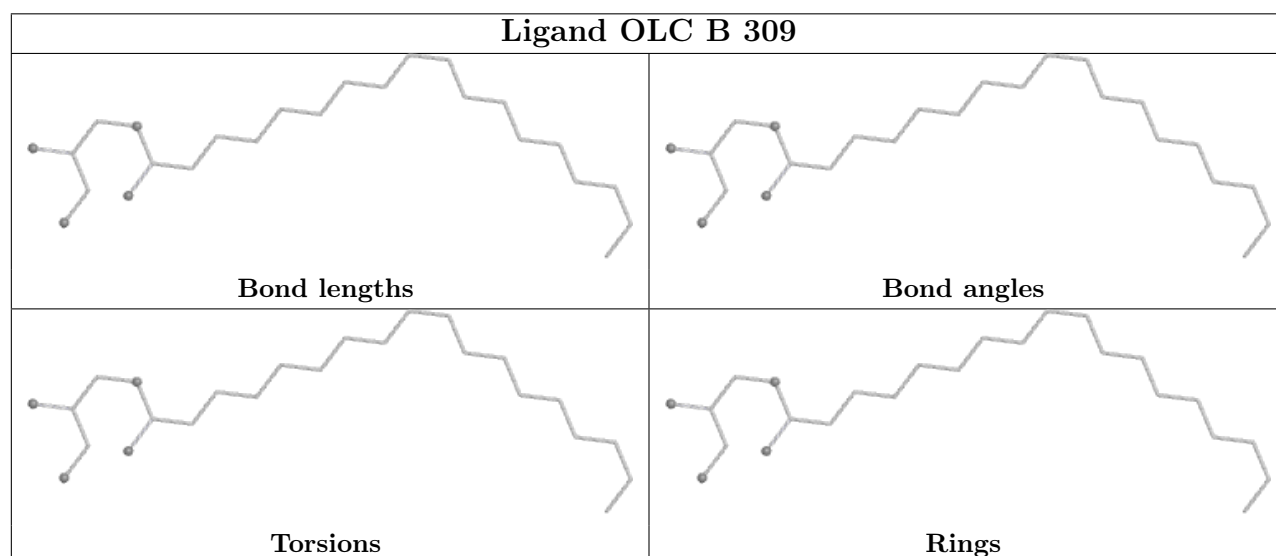
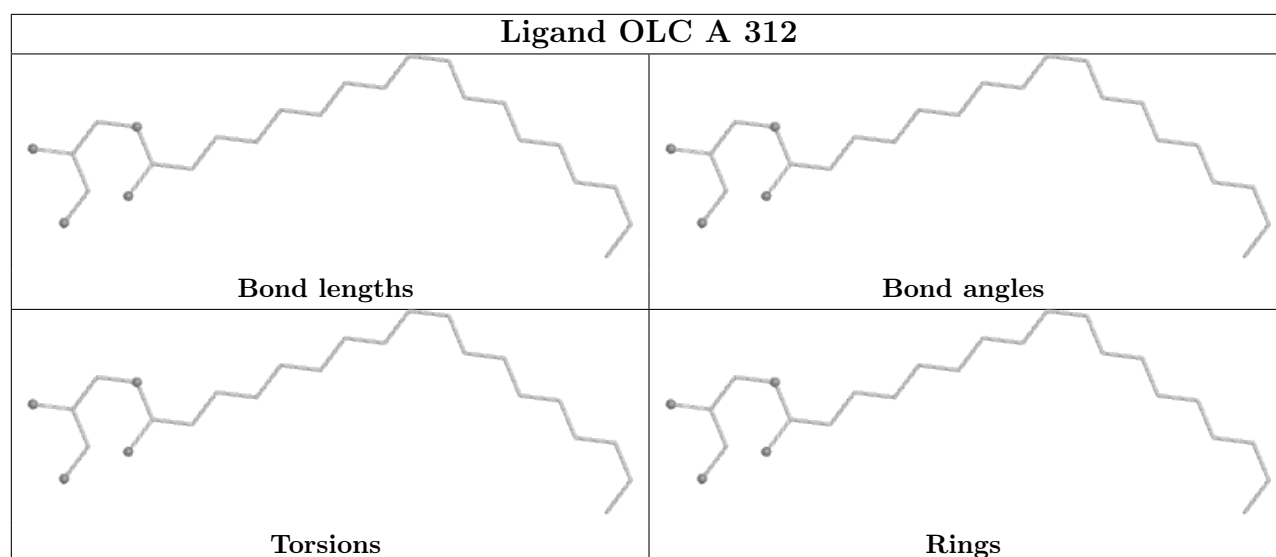
There are no torsion outliers.

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 [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	197/204 (96%)	1.60	52 (26%) 0 0	15, 24, 50, 104	0
1	B	200/204 (98%)	1.88	64 (32%) 0 0	16, 25, 71, 118	0
All	All	397/408 (97%)	1.74	116 (29%) 0 0	15, 24, 57, 118	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	PRO	11.7
1	B	109	ASN	10.6
1	B	-1	PRO	10.0
1	B	110	VAL	9.5
1	B	0	HIS	9.0

### 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](#)

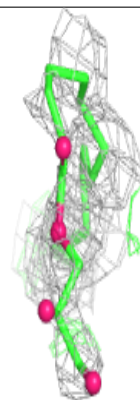
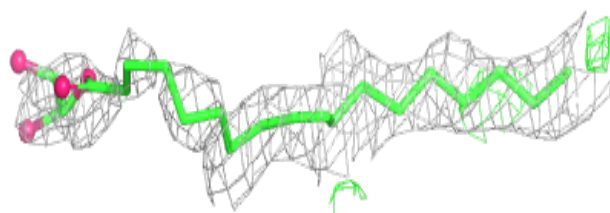
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
6	OLC	A	313	25/25	0.32	0.35	34,57,70,74	0
6	OLC	B	309	25/25	0.36	0.42	37,51,72,79	0
6	OLC	A	310	25/25	0.47	0.41	37,50,70,84	0
6	OLC	A	312	25/25	0.49	0.42	38,49,65,77	0
6	OLC	A	311	25/25	0.53	0.37	38,50,65,71	0
4	MG	A	303	1/1	0.58	0.28	26,26,26,26	0
6	OLC	A	309	25/25	0.59	0.31	42,53,64,71	0
6	OLC	B	310	25/25	0.63	0.39	45,60,73,76	0
6	OLC	B	307	25/25	0.64	0.28	33,46,61,68	0
6	OLC	B	308	25/25	0.67	0.31	19,33,47,50	0
6	OLC	A	308	25/25	0.72	0.30	18,34,44,51	0
8	SER	B	306	7/7	0.73	0.40	58,60,68,70	0
2	SMW	A	301	75/75	0.74	0.31	21,36,47,53	0
7	58A	B	301	64/68	0.77	0.30	17,34,50,63	0
4	MG	B	303	1/1	0.85	0.30	28,28,28,28	0
5	CL	A	306	1/1	0.88	0.19	38,38,38,38	0
5	CL	A	305	1/1	0.90	0.18	32,32,32,32	0
5	CL	A	307	1/1	0.91	0.28	41,41,41,41	0
5	CL	B	305	1/1	0.94	0.11	35,35,35,35	0
3	CA	B	302	1/1	0.95	0.08	30,30,30,30	0
5	CL	A	304	1/1	0.96	0.31	29,29,29,29	0
3	CA	A	302	1/1	0.97	0.09	28,28,28,28	0
5	CL	B	304	1/1	0.99	0.19	33,33,33,33	0

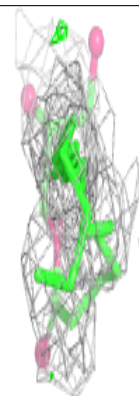
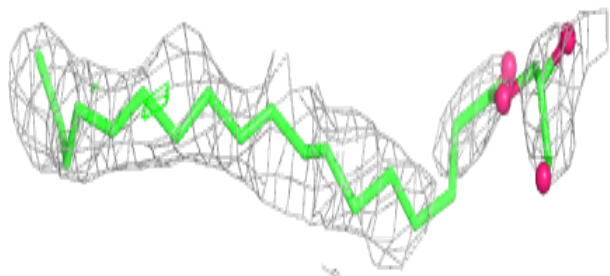
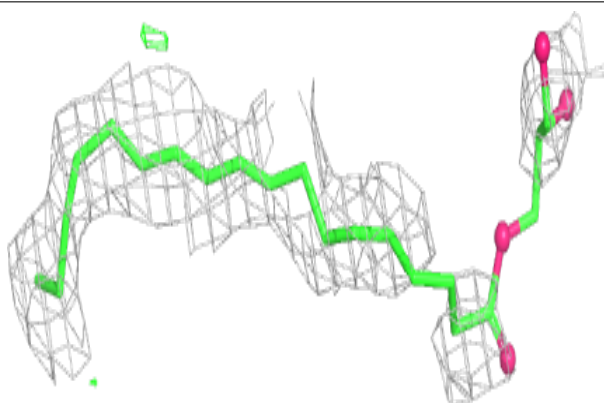
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around OLC B 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

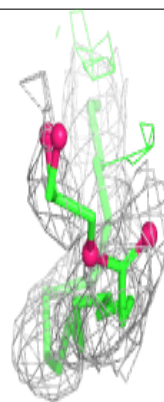
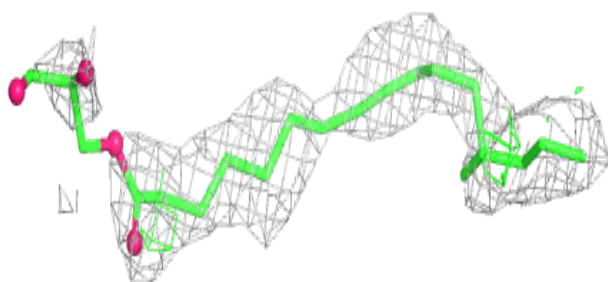
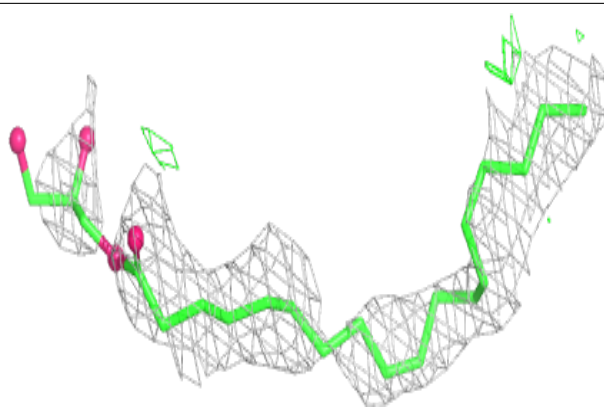
**Electron density around OLC A 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

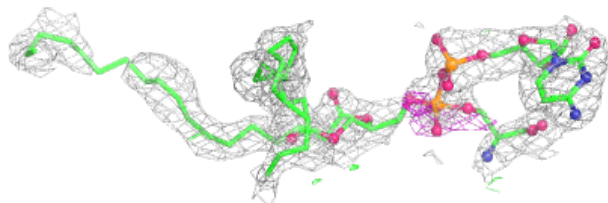
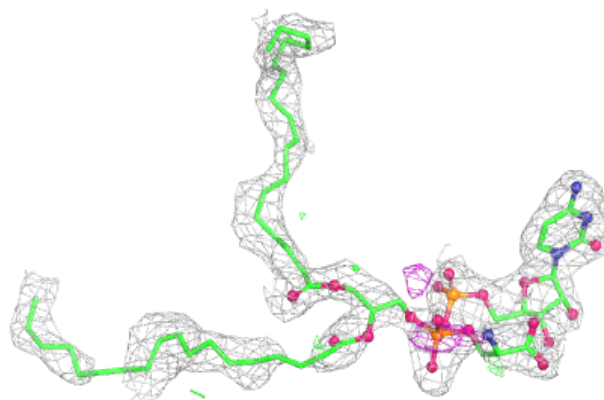


**Electron density around OLC A 312:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

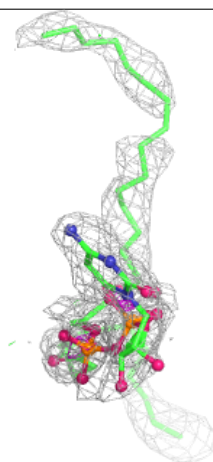
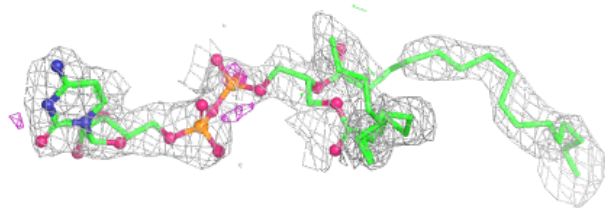
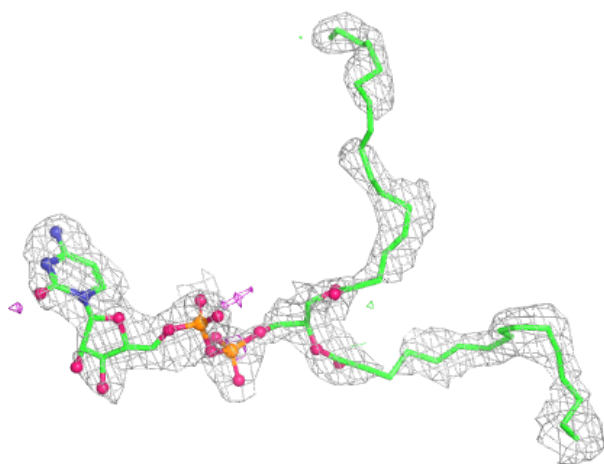
**Electron density around SMW A 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 58A B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.