



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 07:19 am BST

PDB ID : 4RW3  
Title : Structural insights into substrate binding of brown spider venom class II phospholipases D  
Authors : Coronado, M.A.; Ullah, A.; da Silva, L.S.; Chaves-Moreira, D.; Vuitika, L.; Chaim, O.M.; Veiga, S.S.; Chahine, J.; Murakami, M.T.; Arni, R.K.  
Deposited on : 2014-12-01  
Resolution : 1.72 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 : 2.11  
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) : 2.11

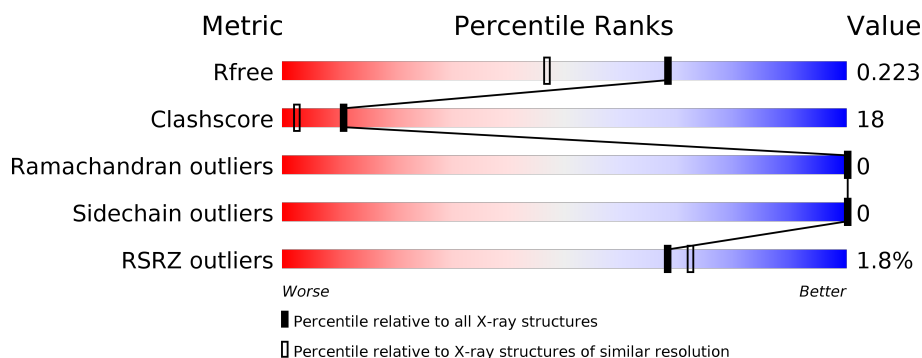
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	302	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </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
10	TDA	A	313	-	-	X	-
4	IPD	A	304	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OCA	A	306	-	-	X	-
8	DKA	A	312	-	-	X	-
9	PLM	A	309	-	-	X	-
9	PLM	A	311	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 2558 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 Phospholipase D LiSicTox-alphaIA1bii.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	2	7	0
			2241	1412	395	426	8			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P0CE82
A	-20	GLY	-	EXPRESSION TAG	UNP P0CE82
A	-19	SER	-	EXPRESSION TAG	UNP P0CE82
A	-18	SER	-	EXPRESSION TAG	UNP P0CE82
A	-17	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-16	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-15	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-14	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-13	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-12	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-11	SER	-	EXPRESSION TAG	UNP P0CE82
A	-10	SER	-	EXPRESSION TAG	UNP P0CE82
A	-9	GLY	-	EXPRESSION TAG	UNP P0CE82
A	-8	LEU	-	EXPRESSION TAG	UNP P0CE82
A	-7	VAL	-	EXPRESSION TAG	UNP P0CE82
A	-6	PRO	-	EXPRESSION TAG	UNP P0CE82
A	-5	ARG	-	EXPRESSION TAG	UNP P0CE82
A	-4	GLY	-	EXPRESSION TAG	UNP P0CE82
A	-3	SER	-	EXPRESSION TAG	UNP P0CE82
A	-2	HIS	-	EXPRESSION TAG	UNP P0CE82
A	-1	MET	-	EXPRESSION TAG	UNP P0CE82
A	0	LEU	-	EXPRESSION TAG	UNP P0CE82
A	1	GLU	-	EXPRESSION TAG	UNP P0CE82

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

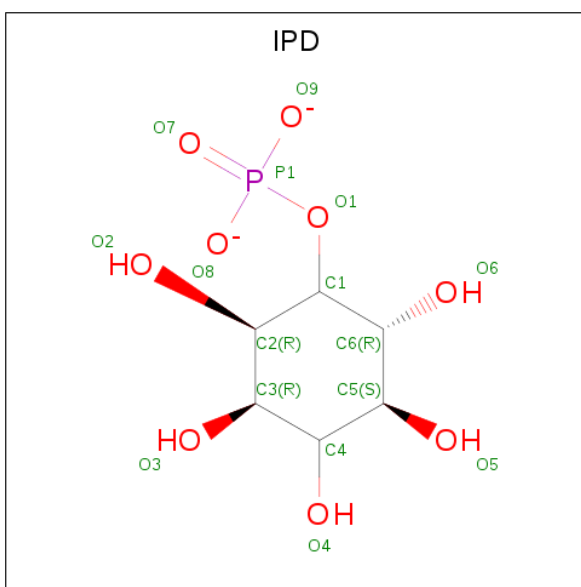
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is D-MYO-INOSITOL-1-PHOSPHATE (three-letter code: IPD) (formula:  $C_6H_{11}O_9P$ ).



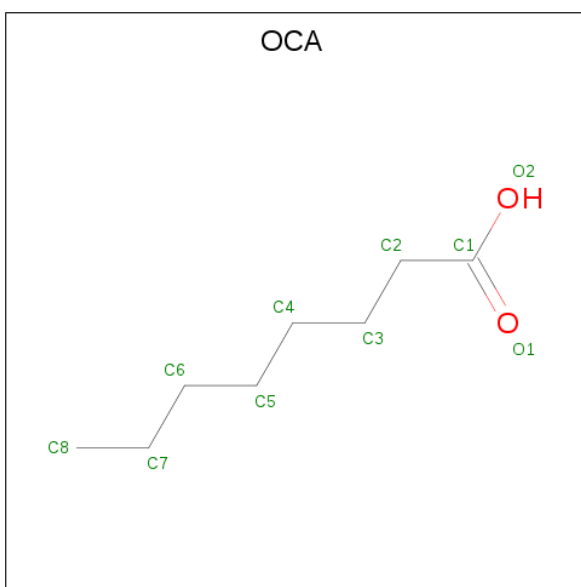
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



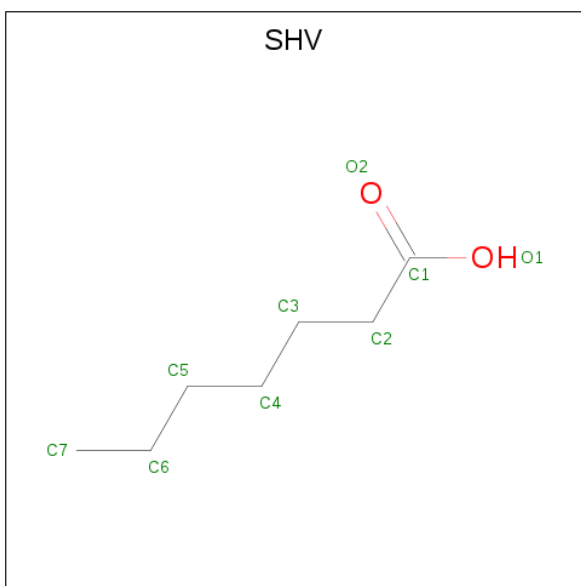
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula:  $C_8H_{16}O_2$ ).



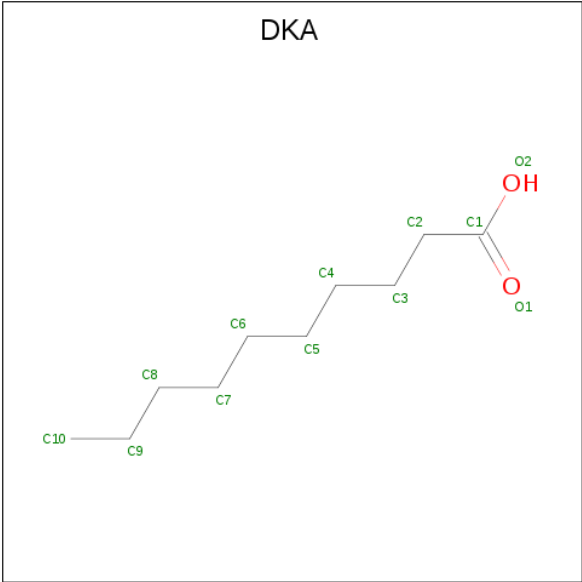
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	8	2		

- Molecule 7 is HEPTANOIC ACID (three-letter code: SHV) (formula:  $C_7H_{14}O_2$ ).



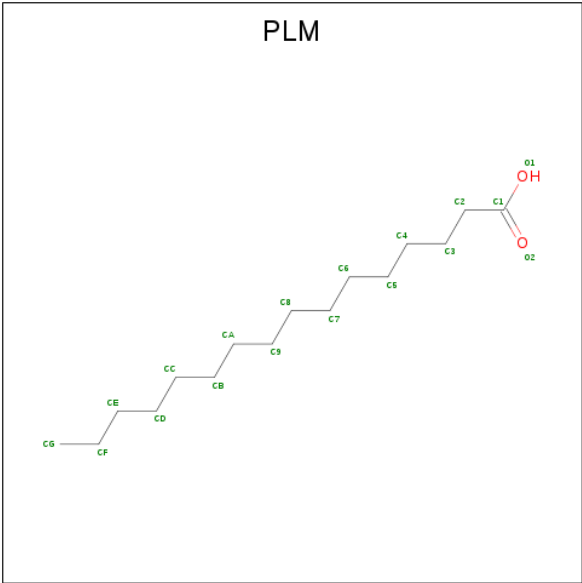
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	7	2		

- Molecule 8 is DECANOIC ACID (three-letter code: DKA) (formula:  $C_{10}H_{20}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	10	2		
8	A	1	Total	C	O	0	0
			12	10	2		

- Molecule 9 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			18	16	2		
9	A	1	Total	C	O	0	0
			18	16	2		

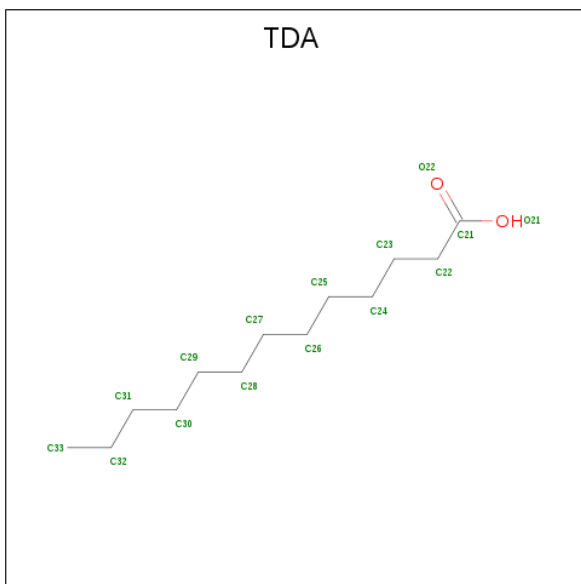
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 10 is N-TRIDECANOIC ACID (three-letter code: TDA) (formula:  $C_{13}H_{26}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			15	13	2		

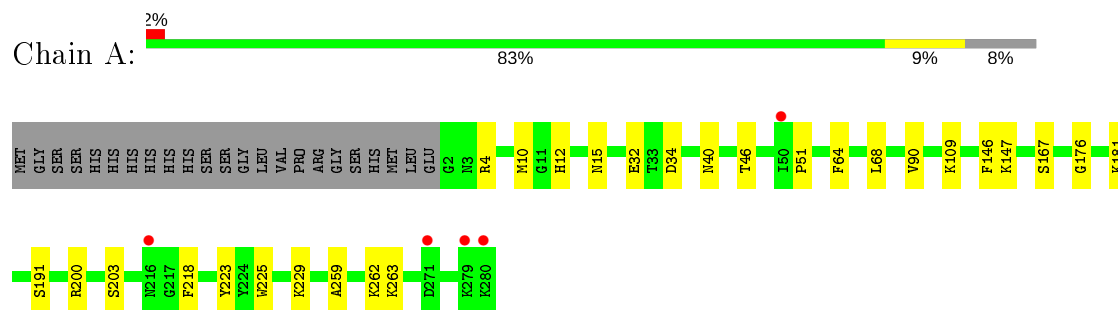
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	168	Total	O	0	0
			168	168		

### 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 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: Phospholipase D LiSicTox-alphaIA1bii



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.81Å 49.30Å 56.30Å 90.00° 105.83° 90.00°	Depositor
Resolution (Å)	30.00 – 1.72 23.64 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.72) 99.9 (23.64-1.72)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.183 , 0.223 0.185 , 0.223	Depositor DCC
$R_{free}$ test set	2808 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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: GOL, MG, IPD, SHV, OCA, TDA, DKA, PLM, PEG

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	0.52	1/2306 (0.0%)	0.62	0/3122

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	PHE	C-N	-5.80	1.20	1.34

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	2241	0	2180	80	0
2	A	1	0	0	0	0
3	A	14	0	20	1	0
4	A	16	0	8	9	0
5	A	6	0	8	0	0
6	A	10	0	15	10	0
7	A	9	0	13	2	0
8	A	24	0	38	16	0
9	A	54	0	93	26	0
10	A	15	0	25	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	168	0	0	4	0
All	All	2558	0	2400	87	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 18.

All (87) 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:229:LYS:HE3	9:A:309:PLM:CD	1.62	1.29
1:A:181:LYS:NZ	10:A:313:TDA:H281	1.50	1.24
1:A:229:LYS:NZ	9:A:309:PLM:HD1	1.56	1.19
1:A:147:LYS:HE2	8:A:312:DKA:H61	1.31	1.13
1:A:229:LYS:HZ1	9:A:309:PLM:HD1	1.10	1.08
1:A:181:LYS:HZ1	10:A:313:TDA:H281	0.96	1.07
1:A:229:LYS:CE	9:A:309:PLM:HD2	1.83	1.07
1:A:229:LYS:CE	9:A:309:PLM:CD	2.31	1.07
1:A:147:LYS:HD2	8:A:312:DKA:H81	1.37	1.06
1:A:181:LYS:NZ	10:A:313:TDA:H251	1.71	1.06
1:A:181:LYS:HZ1	10:A:313:TDA:C28	1.71	1.04
1:A:181:LYS:HZ2	10:A:313:TDA:H251	0.86	1.01
1:A:147:LYS:CE	8:A:312:DKA:H61	1.90	1.00
1:A:263:LYS:CE	6:A:306:OCA:H51	1.94	0.98
1:A:109:LYS:HZ1	9:A:311:PLM:H82	1.33	0.93
1:A:229:LYS:HE3	9:A:309:PLM:HD2	0.93	0.93
1:A:229:LYS:CE	9:A:309:PLM:HD1	1.99	0.92
1:A:181:LYS:HZ2	10:A:313:TDA:C25	1.81	0.88
1:A:181:LYS:NZ	10:A:313:TDA:H312	1.90	0.85
1:A:109:LYS:NZ	9:A:311:PLM:H82	1.92	0.83
1:A:147:LYS:HE3	8:A:312:DKA:H31	1.63	0.81
1:A:229:LYS:HZ2	9:A:309:PLM:HG2	1.46	0.81
1:A:263:LYS:NZ	6:A:306:OCA:H51	1.95	0.80
1:A:147:LYS:HE3	8:A:312:DKA:C3	2.13	0.79
1:A:181:LYS:HZ2	10:A:313:TDA:H281	1.50	0.76
1:A:229:LYS:NZ	9:A:309:PLM:HG2	2.02	0.75
1:A:181:LYS:NZ	10:A:313:TDA:C28	2.38	0.75
1:A:263:LYS:HE3	6:A:306:OCA:H51	1.67	0.75
1:A:218:PHE:HB2	7:A:307:SHV:H51	1.69	0.74
1:A:109:LYS:HE2	9:A:311:PLM:H61	1.71	0.73
9:A:311:PLM:HG2	9:A:311:PLM:O1	1.90	0.71
1:A:147:LYS:HE2	8:A:312:DKA:C6	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:HZ1	10:A:313:TDA:H312	1.52	0.71
1:A:229:LYS:HZ1	9:A:309:PLM:CD	1.97	0.71
1:A:225:TRP:CD2	4:A:304:IPD:O8	2.45	0.69
1:A:147:LYS:CE	8:A:312:DKA:H32	2.23	0.68
1:A:225:TRP:CG	4:A:304:IPD:O8	2.46	0.68
1:A:259:ALA:HB1	6:A:306:OCA:H81	1.77	0.66
1:A:109:LYS:HZ2	9:A:311:PLM:HC1	1.60	0.66
1:A:109:LYS:CE	9:A:311:PLM:H61	2.26	0.65
1:A:181:LYS:HZ1	10:A:313:TDA:C31	2.09	0.64
6:A:306:OCA:H72	11:A:422:HOH:O	1.98	0.63
1:A:203[B]:SER:OG	3:A:302:PEG:H22	1.99	0.62
1:A:263:LYS:HZ1	6:A:306:OCA:H21	1.62	0.62
1:A:229:LYS:HZ2	9:A:309:PLM:CG	2.13	0.62
1:A:51:PRO:HB2	8:A:308:DKA:H22	1.82	0.61
1:A:262:LYS:HZ3	9:A:310:PLM:HC2	1.66	0.59
1:A:147:LYS:CE	8:A:312:DKA:C3	2.79	0.59
1:A:263:LYS:NZ	6:A:306:OCA:C5	2.68	0.57
1:A:147:LYS:CD	8:A:312:DKA:H81	2.26	0.56
1:A:147:LYS:HD2	8:A:312:DKA:C8	2.26	0.56
1:A:15:ASN:HB3	1:A:46:THR:O	2.06	0.55
1:A:181:LYS:HZ3	10:A:313:TDA:H312	1.70	0.55
1:A:4[A]:ARG:HD3	11:A:402:HOH:O	2.06	0.55
1:A:12:HIS:NE2	4:A:304:IPD:H5	2.23	0.53
1:A:167:SER:HB2	4:A:304:IPD:O9	2.08	0.53
1:A:147:LYS:HE3	8:A:312:DKA:H61	1.86	0.53
1:A:40:ASN:HB3	9:A:311:PLM:H91	1.91	0.53
1:A:191:SER:HB3	1:A:223:TYR:CZ	2.43	0.52
1:A:223:TYR:OH	4:A:304:IPD:O7	2.15	0.52
1:A:51:PRO:CB	8:A:308:DKA:H22	2.40	0.52
1:A:34:ASP:O	1:A:46:THR:HA	2.12	0.49
1:A:109:LYS:HZ1	9:A:311:PLM:H61	1.76	0.49
9:A:311:PLM:CG	9:A:311:PLM:O1	2.60	0.49
10:A:313:TDA:H251	10:A:313:TDA:H281	1.61	0.48
1:A:259:ALA:CB	6:A:306:OCA:H81	2.44	0.48
1:A:263:LYS:HE2	6:A:306:OCA:H72	1.96	0.48
8:A:312:DKA:C10	11:A:469:HOH:O	2.62	0.48
1:A:225:TRP:CD1	4:A:304:IPD:O8	2.67	0.47
1:A:263:LYS:HZ1	6:A:306:OCA:H51	1.78	0.47
1:A:167:SER:HA	1:A:191:SER:OG	2.14	0.47
9:A:309:PLM:HG2	9:A:309:PLM:HD1	1.73	0.47
8:A:312:DKA:H101	11:A:469:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:MET:CE	1:A:90:VAL:HG21	2.45	0.46
1:A:225:TRP:CZ3	4:A:304:IPD:H2	2.51	0.45
1:A:225:TRP:CE2	4:A:304:IPD:O8	2.69	0.45
1:A:262:LYS:HZ3	9:A:310:PLM:H81	1.82	0.45
1:A:147:LYS:HE3	8:A:312:DKA:H32	1.86	0.44
1:A:181:LYS:NZ	10:A:313:TDA:C31	2.68	0.44
1:A:32:GLU:OE2	4:A:304:IPD:O6	2.29	0.44
1:A:109:LYS:NZ	9:A:311:PLM:H61	2.33	0.44
1:A:4[B]:ARG:NE	1:A:262:LYS:O	2.52	0.43
1:A:229:LYS:HZ3	9:A:309:PLM:C6	2.32	0.43
1:A:64:PHE:CE2	1:A:68:LEU:HD11	2.53	0.42
1:A:262:LYS:NZ	9:A:310:PLM:H81	2.34	0.42
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.84	0.42
1:A:176:GLY:O	7:A:307:SHV:H22	2.21	0.41

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	284/302 (94%)	282 (99%)	2 (1%)	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	241/254 (95%)	241 (100%)	0	100	100

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

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	116	GLN
1	A	121	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z  > 2$
8	DKA	A	308	-	8,11,11	0.33	0	7,11,11	0.32	0
10	TDA	A	313	-	11,14,14	0.16	0	10,14,14	0.52	0
3	PEG	A	303	-	6,6,6	0.48	0	5,5,5	0.23	0
9	PLM	A	311	-	14,17,17	0.24	0	13,17,17	0.63	0
9	PLM	A	310	-	14,17,17	0.21	0	13,17,17	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	305	-	5,5,5	0.27	0	5,5,5	0.36	0
8	DKA	A	312	-	8,11,11	0.26	0	7,11,11	0.70	0
4	IPD	A	304	2	16,16,16	4.63	1 (6%)	24,25,25	3.98	6 (25%)
7	SHV	A	307	-	5,8,8	0.26	0	4,8,8	0.25	0
9	PLM	A	309	-	14,17,17	0.24	0	13,17,17	0.87	0
6	OCA	A	306	-	6,9,9	0.19	0	5,9,9	0.36	0
3	PEG	A	302	-	6,6,6	0.43	0	5,5,5	0.49	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
8	DKA	A	308	-	-	1/7/9/9	-
10	TDA	A	313	-	-	7/10/12/12	-
3	PEG	A	303	-	-	4/4/4/4	-
9	PLM	A	311	-	-	10/13/15/15	-
9	PLM	A	310	-	-	7/13/15/15	-
5	GOL	A	305	-	-	4/4/4/4	-
8	DKA	A	312	-	-	4/7/9/9	-
4	IPD	A	304	2	-	0/5/29/29	0/1/1/1
7	SHV	A	307	-	-	1/4/6/6	-
9	PLM	A	309	-	-	11/13/15/15	-
6	OCA	A	306	-	-	3/5/7/7	-
3	PEG	A	302	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	IPD	O4-C4	-18.40	0.99	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	IPD	O4-C4-C3	15.29	145.70	110.35
4	A	304	IPD	O6-C6-C1	-8.47	87.51	109.94
4	A	304	IPD	O6-C6-C5	5.73	123.60	110.35
4	A	304	IPD	O4-C4-C5	-3.82	101.52	110.35
4	A	304	IPD	C6-C5-C4	2.36	114.94	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	IPD	C3-C2-C1	2.34	115.02	109.68

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	313	TDA	C21-C22-C23-C24
5	A	305	GOL	O1-C1-C2-C3
5	A	305	GOL	C1-C2-C3-O3
8	A	312	DKA	C1-C2-C3-C4
9	A	309	PLM	C1-C2-C3-C4
3	A	303	PEG	O1-C1-C2-O2
8	A	312	DKA	C3-C4-C5-C6
10	A	313	TDA	C25-C26-C27-C28
9	A	311	PLM	C5-C6-C7-C8
9	A	310	PLM	C8-C9-CA-CB
8	A	312	DKA	C6-C7-C8-C9
10	A	313	TDA	C26-C27-C28-C29
9	A	309	PLM	C8-C9-CA-CB
8	A	308	DKA	C3-C4-C5-C6
9	A	311	PLM	C6-C7-C8-C9
9	A	309	PLM	C3-C4-C5-C6
6	A	306	OCA	C2-C3-C4-C5
6	A	306	OCA	C4-C5-C6-C7
9	A	311	PLM	C8-C9-CA-CB
9	A	311	PLM	C3-C4-C5-C6
9	A	310	PLM	CA-CB-CC-CD
5	A	305	GOL	O1-C1-C2-O2
5	A	305	GOL	O2-C2-C3-O3
9	A	309	PLM	C4-C5-C6-C7
9	A	309	PLM	CC-CD-CE-CF
9	A	309	PLM	C6-C7-C8-C9
10	A	313	TDA	C22-C23-C24-C25
3	A	302	PEG	O1-C1-C2-O2
7	A	307	SHV	C2-C3-C4-C5
9	A	309	PLM	C2-C3-C4-C5
10	A	313	TDA	C24-C25-C26-C27
10	A	313	TDA	C30-C31-C32-C33
9	A	309	PLM	CA-CB-CC-CD
9	A	309	PLM	CB-CC-CD-CE
9	A	310	PLM	C2-C3-C4-C5
9	A	310	PLM	CB-CC-CD-CE

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Mol	Chain	Res	Type	Atoms
8	A	312	DKA	C4-C5-C6-C7
9	A	311	PLM	C9-CA-CB-CC
9	A	310	PLM	C3-C4-C5-C6
9	A	310	PLM	C4-C5-C6-C7
9	A	309	PLM	CD-CE-CF-CG
3	A	303	PEG	O2-C3-C4-O4
3	A	303	PEG	C4-C3-O2-C2
9	A	311	PLM	CC-CD-CE-CF
9	A	311	PLM	CA-CB-CC-CD
9	A	309	PLM	C5-C6-C7-C8
9	A	310	PLM	C5-C6-C7-C8
3	A	303	PEG	C1-C2-O2-C3
9	A	311	PLM	CB-CC-CD-CE
6	A	306	OCA	C3-C4-C5-C6
9	A	311	PLM	C4-C5-C6-C7
9	A	311	PLM	C7-C8-C9-CA
10	A	313	TDA	C29-C30-C31-C32

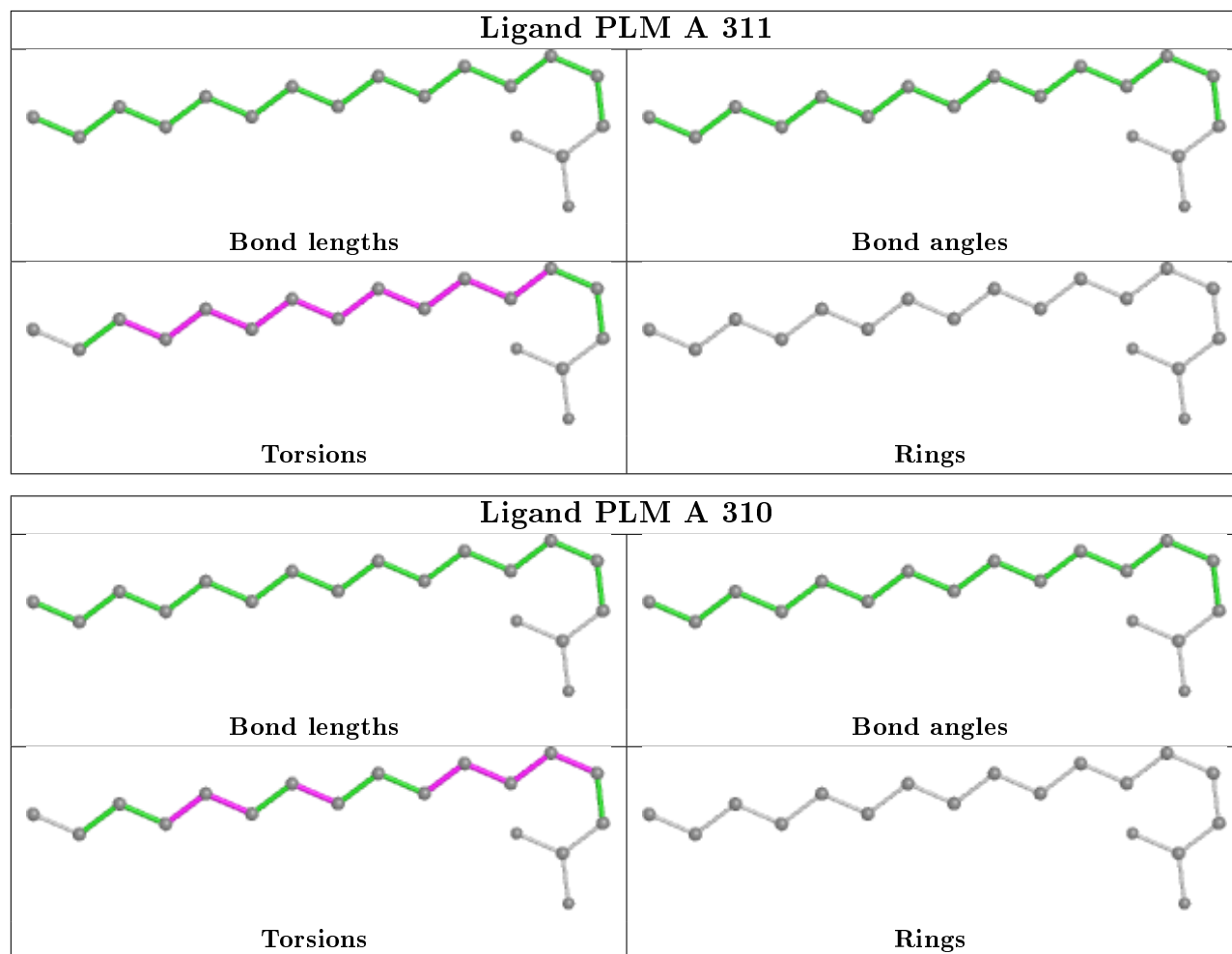
There are no ring outliers.

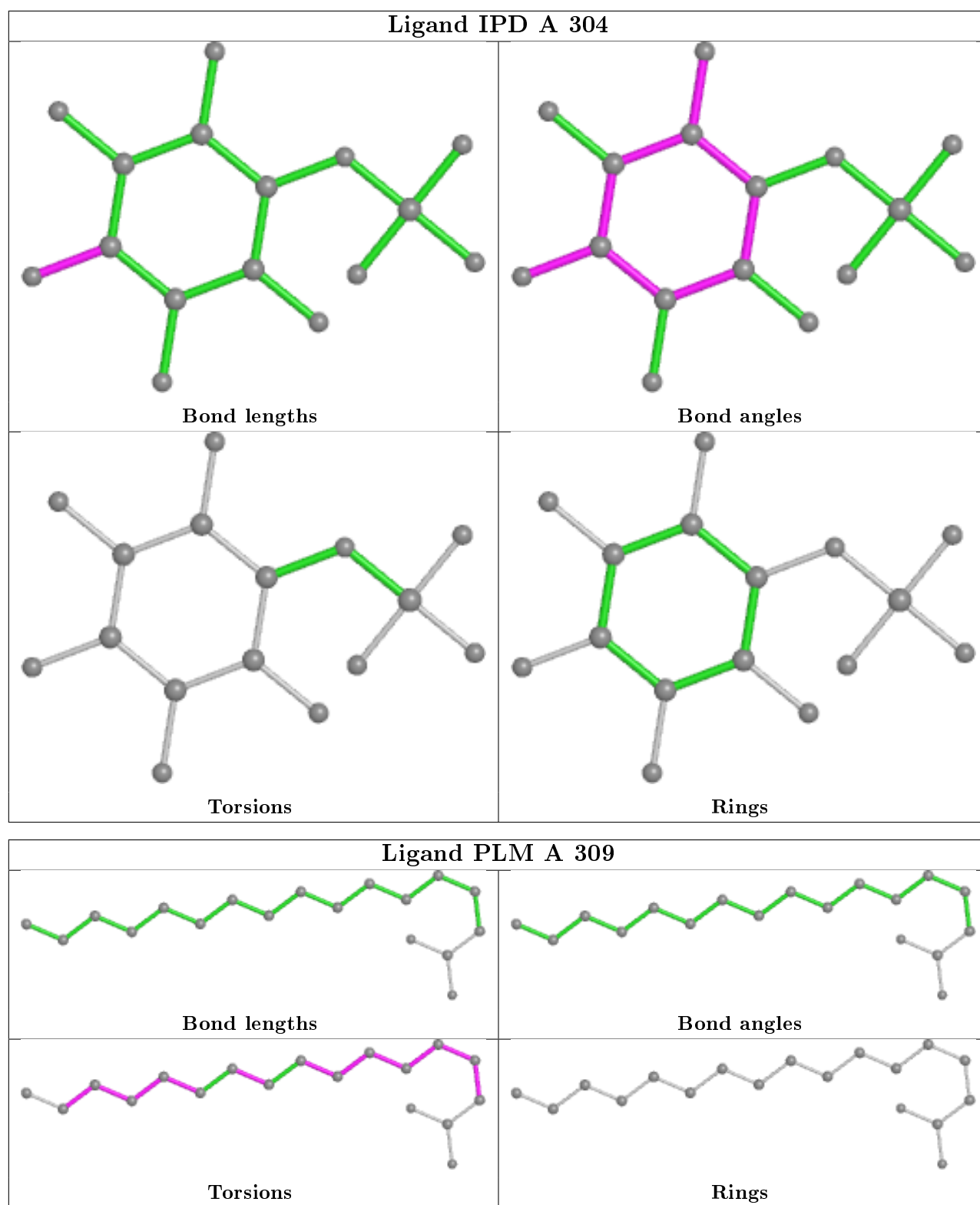
10 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	308	DKA	2	0
10	A	313	TDA	14	0
9	A	311	PLM	10	0
9	A	310	PLM	3	0
8	A	312	DKA	14	0
4	A	304	IPD	9	0
7	A	307	SHV	2	0
9	A	309	PLM	13	0
6	A	306	OCA	10	0
3	A	302	PEG	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	279/302 (92%)	0.01	5 (1%) 68 72	11, 16, 25, 49	6 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	LYS	4.5
1	A	50	ILE	2.8
1	A	216	ASN	2.7
1	A	279	LYS	2.1
1	A	271	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 carbohydrates 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.

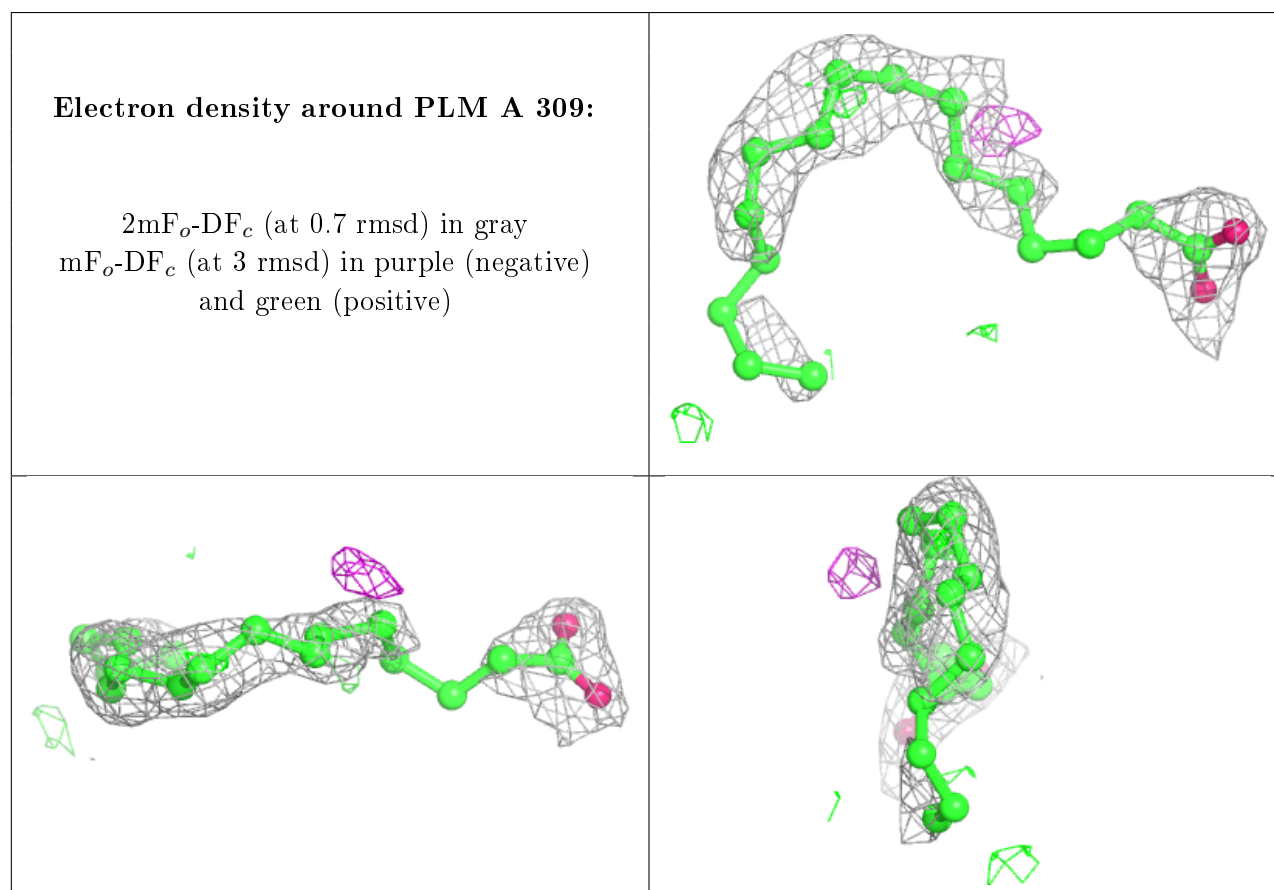
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	TDA	A	313	15/15	0.43	0.28	41,46,51,51	0
8	DKA	A	312	12/12	0.51	0.25	50,55,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PLM	A	309	18/18	0.61	0.25	36,44,48,48	0
4	IPD	A	304	16/16	0.62	0.39	19,24,40,49	8
5	GOL	A	305	6/6	0.67	0.25	40,42,42,43	0
9	PLM	A	310	18/18	0.69	0.24	38,44,52,52	0
6	OCA	A	306	10/10	0.71	0.23	47,51,55,56	0
3	PEG	A	302	7/7	0.73	0.30	45,46,48,49	0
7	SHV	A	307	9/9	0.75	0.22	45,47,51,52	0
8	DKA	A	308	12/12	0.75	0.19	43,45,50,50	0
3	PEG	A	303	7/7	0.78	0.24	47,48,48,49	0
9	PLM	A	311	18/18	0.81	0.20	21,25,34,34	0
2	MG	A	301	1/1	0.97	0.07	12,12,12,12	0

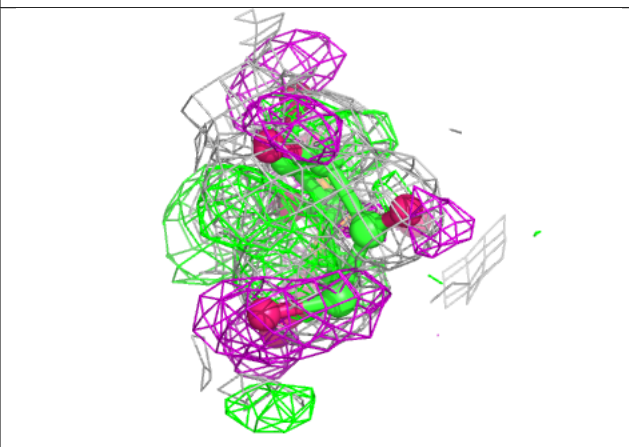
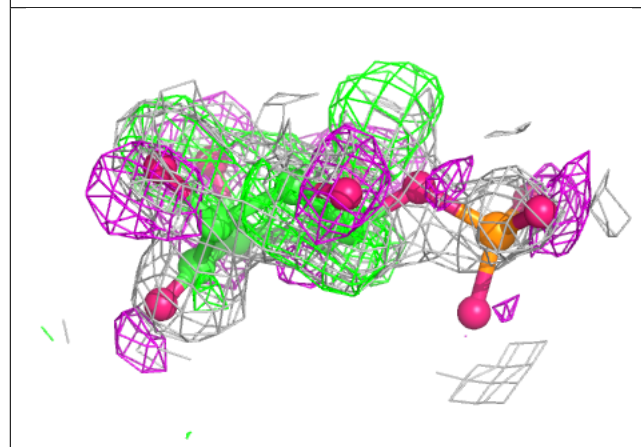
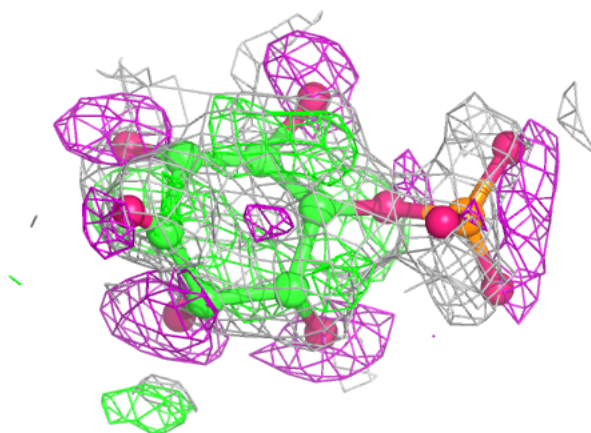
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





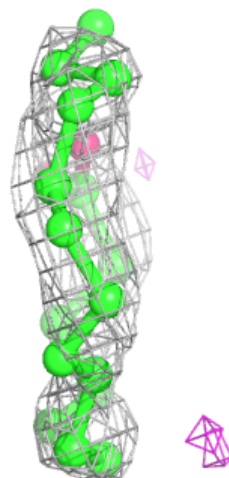
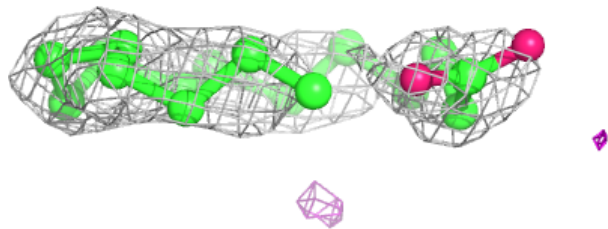
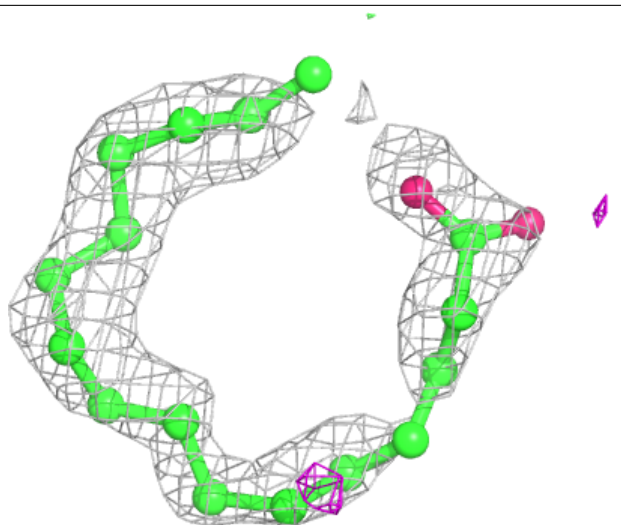
**Electron density around IPD A 304:**

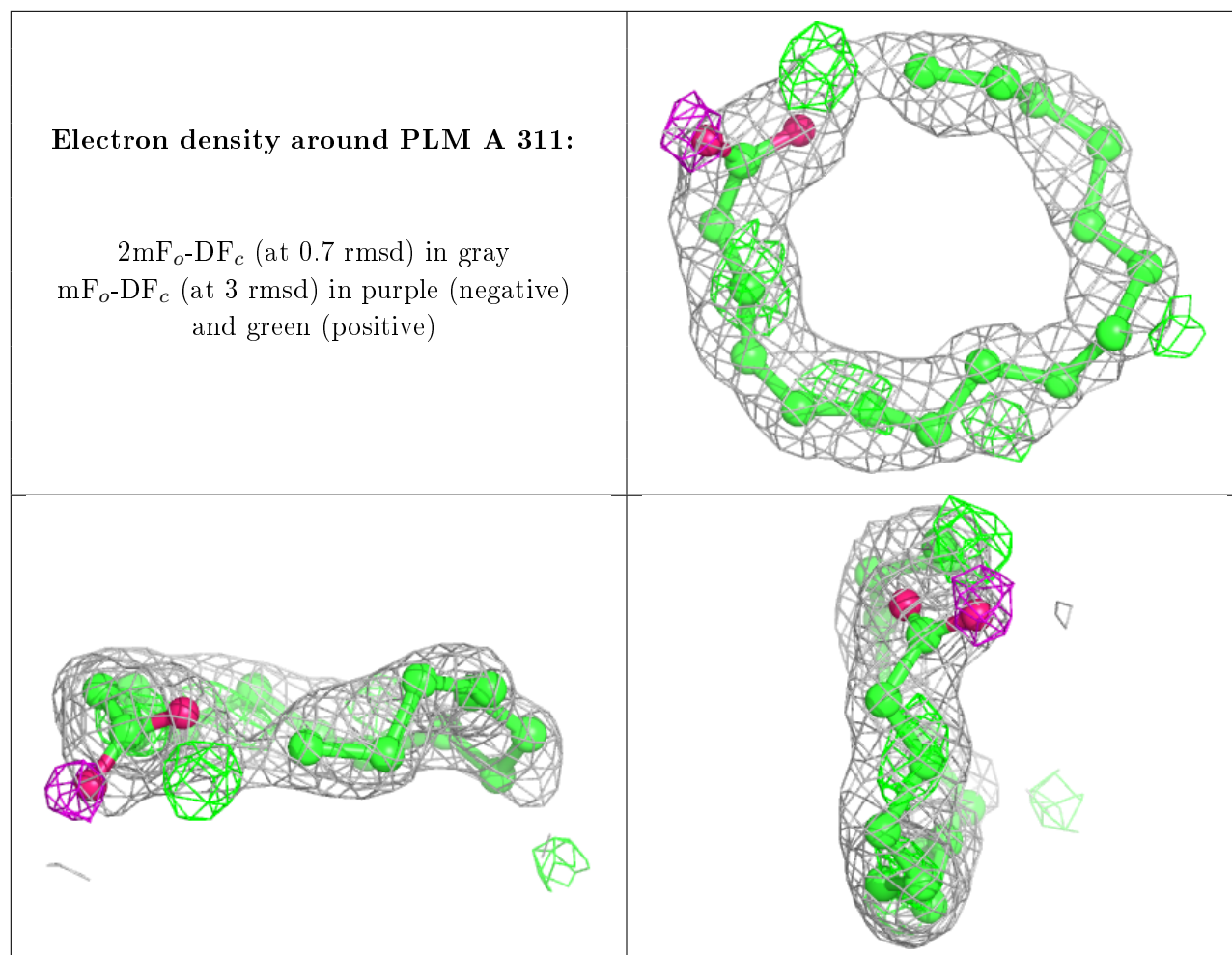
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PLM 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.