



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:40 am BST

PDB ID : 5EIK
Title : Structure of a Trimeric Intracellular Cation channel from *C. elegans* in the absence of Ca²⁺
Authors : Hu, M.H.; Yang, H.T.; Liu, Z.F.
Deposited on : 2015-10-30
Resolution : 2.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

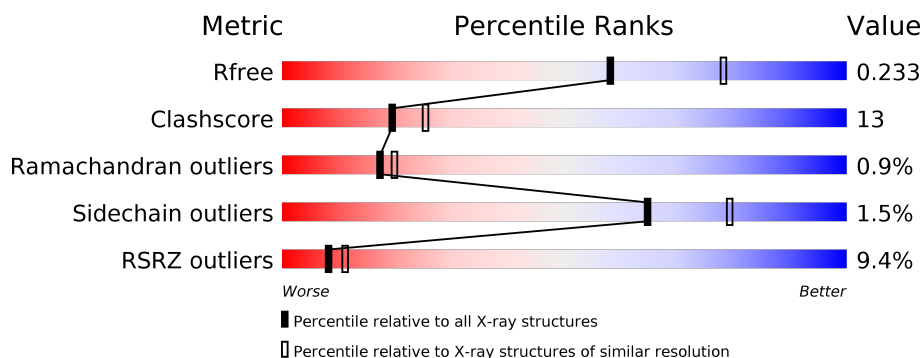
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	258	<div> <div>9%</div> <div>71%</div> <div>18%</div> <div>9%</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
3	CPL	A	302	-	-	-	X
6	DMU	A	309	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMU	A	310	-	-	-	X
6	DMU	A	311	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2202 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.

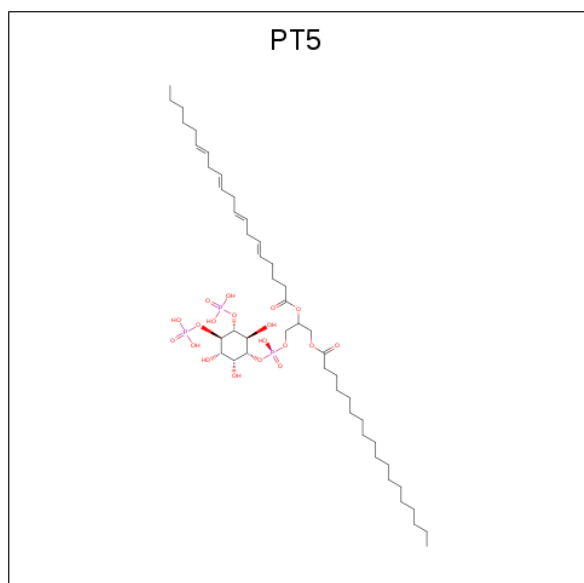
- Molecule 1 is a protein called Uncharacterized protein Y57A10A.28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1851	1225	304	312	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

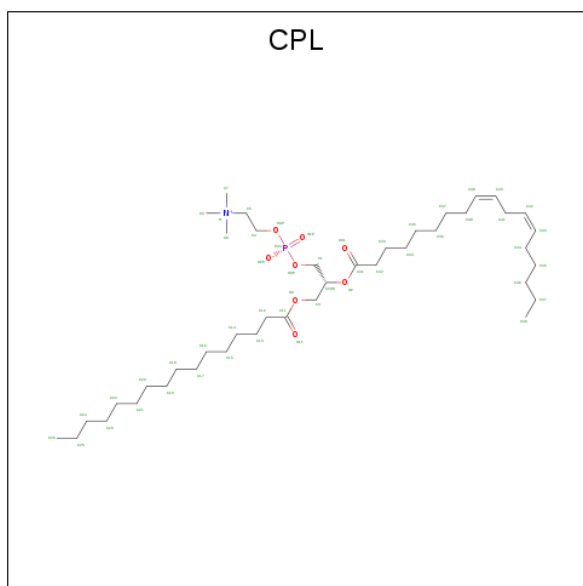
Chain	Residue	Modelled	Actual	Comment	Reference
A	253	HIS	-	expression tag	UNP Q9NA73
A	254	HIS	-	expression tag	UNP Q9NA73
A	255	HIS	-	expression tag	UNP Q9NA73
A	256	HIS	-	expression tag	UNP Q9NA73
A	257	HIS	-	expression tag	UNP Q9NA73
A	258	HIS	-	expression tag	UNP Q9NA73

- Molecule 2 is (1S)-2-[[[(R)-hydroxy{[(1R,2R,3S,4R,5R,6S)-2,3,6-trihydroxy-4,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (8E,11E)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: C₄₇H₈₅O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			61	39	19	3		

- Molecule 3 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

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

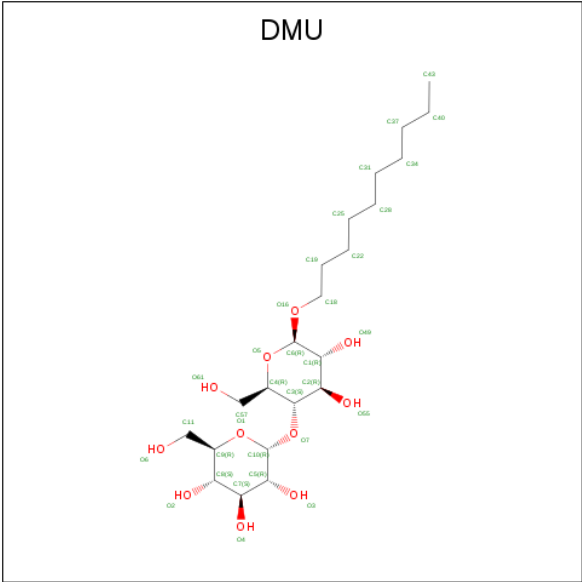
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			33	22	11		
6	A	1	Total	C	O	0	0
			33	22	11		
6	A	1	Total	C	O	0	0
			33	22	11		
6	A	1	Total	C	O	0	0
			33	22	11		

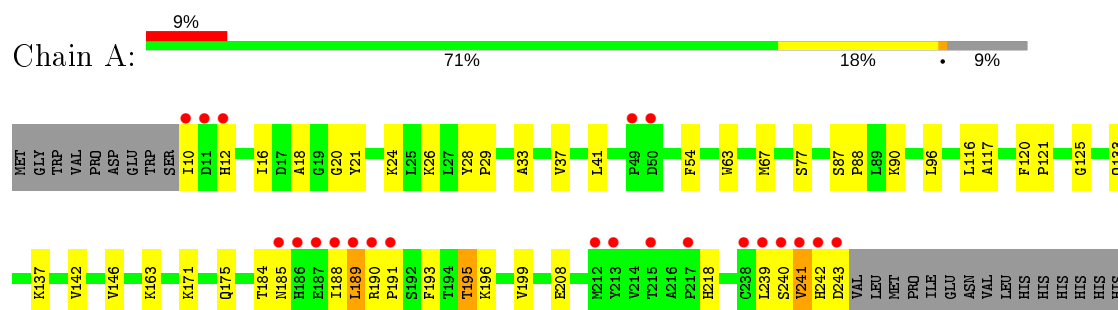
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	88	Total	O	0	0
			88	88		

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: Uncharacterized protein Y57A10A.28



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	126.34Å 126.34Å 135.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 23.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.30) 99.0 (23.54-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.249 0.198 , 0.233	Depositor DCC
R_{free} test set	901 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 95.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2202	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PT5, MG, CPL, DMU, ACT

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	0.36	0/1907	0.55	0/2597

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	1851	0	1879	46	0
2	A	61	0	58	0	0
3	A	49	0	71	3	0
4	A	1	0	0	0	0
5	A	20	0	15	0	0
6	A	132	0	165	13	0
7	A	88	0	0	0	0
All	All	2202	0	2188	55	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.

All (55) 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)
6:A:309:DMU:H35	6:A:309:DMU:H30	1.26	1.17
3:A:302:CPL:H201	6:A:309:DMU:O3	1.75	0.85
6:A:312:DMU:H30	6:A:312:DMU:H35	1.62	0.81
1:A:189:LEU:O	1:A:191:PRO:HD3	1.87	0.75
1:A:26:LYS:HZ2	1:A:28:TYR:H	1.34	0.72
6:A:309:DMU:H35	6:A:309:DMU:C57	2.14	0.72
1:A:133:GLN:OE1	1:A:137:LYS:HE2	1.89	0.71
1:A:241:VAL:O	1:A:241:VAL:HG22	1.94	0.68
1:A:125:GLY:HA3	6:A:310:DMU:H23	1.77	0.67
1:A:239:LEU:CG	1:A:240:SER:H	2.08	0.67
1:A:188:ILE:HG23	1:A:190:ARG:HG2	1.79	0.65
1:A:26:LYS:NZ	1:A:28:TYR:H	1.95	0.65
1:A:239:LEU:HD21	1:A:242:HIS:H	1.62	0.64
1:A:239:LEU:HG	1:A:240:SER:H	1.62	0.63
6:A:309:DMU:C9	6:A:309:DMU:H30	2.18	0.63
1:A:239:LEU:CD1	1:A:240:SER:H	2.13	0.61
1:A:239:LEU:HD23	1:A:243:ASP:HB2	1.82	0.61
1:A:87:SER:HB2	1:A:88:PRO:HD3	1.80	0.61
1:A:239:LEU:HD12	1:A:240:SER:H	1.68	0.59
1:A:239:LEU:HG	1:A:240:SER:N	2.17	0.59
1:A:18:ALA:O	1:A:21:TYR:HB3	2.05	0.57
1:A:117:ALA:HB2	6:A:311:DMU:H24	1.85	0.57
1:A:239:LEU:CG	1:A:240:SER:N	2.68	0.56
1:A:188:ILE:HG12	1:A:189:LEU:N	2.22	0.55
1:A:96:LEU:HD11	3:A:302:CPL:H142	1.90	0.54
6:A:311:DMU:H30	6:A:311:DMU:H35	1.90	0.54
1:A:96:LEU:CD2	6:A:309:DMU:H4	2.39	0.52
1:A:63:TRP:CZ2	1:A:67:MET:HG3	2.44	0.52
1:A:37:VAL:O	1:A:41:LEU:HG	2.12	0.50
1:A:10:ILE:O	1:A:10:ILE:HG12	2.10	0.50
1:A:87:SER:HA	1:A:90:LYS:HD3	1.94	0.50
1:A:193:PHE:CD1	1:A:193:PHE:N	2.80	0.49
1:A:120:PHE:HB3	1:A:121:PRO:HD3	1.95	0.48
1:A:77:SER:HB2	1:A:163:LYS:HD3	1.96	0.48
1:A:239:LEU:HD21	1:A:242:HIS:N	2.26	0.47
1:A:208:GLU:HG3	1:A:218:HIS:CD2	2.49	0.47
1:A:188:ILE:HG12	1:A:189:LEU:H	1.79	0.46
1:A:12:HIS:O	1:A:16:ILE:HG13	2.16	0.46
1:A:195:THR:O	1:A:199:VAL:HG23	2.15	0.46
1:A:241:VAL:CG2	1:A:241:VAL:O	2.63	0.45
1:A:33:ALA:O	1:A:37:VAL:HG23	2.17	0.45
1:A:239:LEU:CD2	1:A:243:ASP:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:O	1:A:146:VAL:HG23	2.17	0.44
1:A:20:GLY:O	1:A:24:LYS:HD3	2.17	0.44
1:A:54:PHE:CD1	1:A:54:PHE:C	2.92	0.43
1:A:239:LEU:HD11	1:A:242:HIS:CD2	2.53	0.43
1:A:171:LYS:O	1:A:175:GLN:HG3	2.18	0.42
6:A:310:DMU:O55	6:A:310:DMU:H36	2.19	0.42
1:A:196:LYS:HB2	1:A:196:LYS:HE3	1.85	0.42
1:A:63:TRP:CE2	1:A:67:MET:HG3	2.55	0.42
1:A:184:THR:O	1:A:184:THR:HG23	2.20	0.42
6:A:311:DMU:H36	6:A:311:DMU:O55	2.21	0.41
1:A:189:LEU:CD1	1:A:189:LEU:O	2.69	0.41
1:A:116:LEU:HD23	6:A:311:DMU:H22	2.03	0.41
3:A:302:CPL:H201	6:A:309:DMU:H38	1.81	0.40

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	232/258 (90%)	219 (94%)	11 (5%)	2 (1%)	17	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	241	VAL

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	203/226 (90%)	200 (98%)	3 (2%)	65 79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PRO
1	A	189	LEU
1	A	195	THR

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

Mol	Chain	Res	Type
1	A	136	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
6	DMU	A	310	1	34,34,34	1.56	4 (11%)	45,45,45	1.60	6 (13%)
6	DMU	A	311	-	34,34,34	1.15	5 (14%)	45,45,45	1.52	6 (13%)
2	PT5	A	301	-	61,61,69	1.83	14 (22%)	75,79,87	1.08	3 (4%)
5	ACT	A	307	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
5	ACT	A	308	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
3	CPL	A	302	-	48,48,51	1.58	3 (6%)	53,56,59	2.50	8 (15%)
5	ACT	A	304	-	1,3,3	1.89	0	0,3,3	0.00	-
5	ACT	A	306	-	1,3,3	2.00	0	0,3,3	0.00	-
6	DMU	A	312	-	34,34,34	1.20	3 (8%)	45,45,45	1.24	5 (11%)
6	DMU	A	309	-	34,34,34	1.44	4 (11%)	45,45,45	1.25	7 (15%)
5	ACT	A	305	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-

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
6	DMU	A	310	1	-	8/19/59/59	0/2/2/2
6	DMU	A	311	-	-	9/19/59/59	0/2/2/2
2	PT5	A	301	-	-	24/58/82/90	0/1/1/1
3	CPL	A	302	-	-	26/52/52/55	-
6	DMU	A	312	-	-	6/19/59/59	0/2/2/2
6	DMU	A	309	-	-	9/19/59/59	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	CPL	O3-C11	6.21	1.51	1.33
3	A	302	CPL	O2-C31	6.10	1.51	1.34
6	A	310	DMU	O7-C3	6.02	1.59	1.43
2	A	301	PT5	P5-O51	5.60	1.68	1.50
6	A	309	DMU	O2-C8	-4.21	1.33	1.43
2	A	301	PT5	C16-C15	4.20	1.56	1.31
2	A	301	PT5	C22-C21	3.93	1.54	1.31
2	A	301	PT5	P1-O11	3.83	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PT5	P1-O13	3.69	1.74	1.59
2	A	301	PT5	O18-C11	3.61	1.43	1.33
2	A	301	PT5	P4-O42	3.59	1.62	1.50
6	A	309	DMU	O16-C6	3.46	1.46	1.40
2	A	301	PT5	C24-C25	3.43	1.55	1.29
6	A	310	DMU	C2-C3	3.39	1.61	1.52
6	A	309	DMU	C8-C7	3.26	1.60	1.52
6	A	312	DMU	O1-C10	3.26	1.50	1.41
2	A	301	PT5	P5-O53	3.13	1.66	1.54
6	A	312	DMU	O2-C8	-3.02	1.35	1.43
6	A	311	DMU	O3-C5	2.81	1.49	1.43
3	A	302	CPL	C1-C2	2.80	1.59	1.50
6	A	311	DMU	C7-C5	2.62	1.59	1.52
6	A	312	DMU	O16-C6	2.56	1.44	1.40
6	A	310	DMU	O1-C10	2.52	1.48	1.41
2	A	301	PT5	P5-O5	2.49	1.64	1.59
6	A	311	DMU	C8-C7	2.46	1.58	1.52
6	A	309	DMU	C8-C9	-2.38	1.48	1.53
6	A	310	DMU	O16-C6	2.34	1.44	1.40
2	A	301	PT5	C36-C35	-2.33	1.38	1.51
6	A	311	DMU	C2-C3	2.24	1.58	1.52
5	A	307	ACT	CH3-C	2.23	1.51	1.48
2	A	301	PT5	P4-O4	2.22	1.63	1.59
6	A	311	DMU	O16-C6	2.21	1.44	1.40
2	A	301	PT5	C2-C1	2.11	1.58	1.52
5	A	305	ACT	CH3-C	2.06	1.51	1.48
5	A	308	ACT	CH3-C	2.06	1.51	1.48
2	A	301	PT5	O18-C9	2.04	1.49	1.45

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	CPL	C8-N-C7	-10.51	81.95	108.97
3	A	302	CPL	C8-N-C6	-10.19	82.78	108.97
6	A	310	DMU	C10-O7-C3	-7.32	99.85	117.96
3	A	302	CPL	C8-N-C5	-5.81	86.14	109.92
6	A	311	DMU	O3-C5-C7	-4.56	99.81	110.35
6	A	311	DMU	C18-O16-C6	-4.05	107.12	113.84
6	A	310	DMU	C18-O16-C6	-3.84	107.47	113.84
3	A	302	CPL	C2-O2-C31	3.83	127.22	117.79
3	A	302	CPL	C7-N-C6	3.76	118.63	108.97
3	A	302	CPL	C6-N-C5	3.65	124.83	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	312	DMU	C18-O16-C6	-3.45	108.12	113.84
6	A	311	DMU	C10-O7-C3	-3.42	109.50	117.96
3	A	302	CPL	O2-C31-C32	3.29	118.58	111.50
3	A	302	CPL	P-O4P-C4	-3.27	105.50	121.59
6	A	312	DMU	C10-O7-C3	-2.95	110.65	117.96
6	A	310	DMU	O7-C3-C2	2.83	114.82	107.28
6	A	311	DMU	C6-O5-C4	-2.80	108.19	113.69
6	A	309	DMU	C10-O7-C3	-2.80	111.03	117.96
2	A	301	PT5	C39-C38-C37	2.79	128.61	114.42
6	A	310	DMU	C6-O5-C4	-2.75	108.29	113.69
6	A	311	DMU	O7-C10-C5	2.74	115.19	108.10
6	A	312	DMU	O1-C9-C11	2.62	112.95	106.44
6	A	312	DMU	O2-C8-C9	2.51	115.53	109.30
6	A	309	DMU	O7-C10-C5	2.48	114.52	108.10
6	A	309	DMU	O1-C9-C8	2.38	114.02	109.69
2	A	301	PT5	C5-C6-C1	2.37	113.88	108.96
6	A	310	DMU	O7-C10-O1	2.29	117.08	110.67
6	A	312	DMU	O1-C9-C8	2.28	113.83	109.69
6	A	309	DMU	C6-O5-C4	-2.28	109.22	113.69
2	A	301	PT5	O1-C1-C2	2.12	113.60	108.66
6	A	310	DMU	O7-C3-C4	-2.12	103.64	109.45
6	A	309	DMU	O2-C8-C7	-2.09	105.53	110.35
6	A	309	DMU	O7-C10-O1	-2.05	104.96	110.67
6	A	309	DMU	C10-O1-C9	2.04	117.68	113.69
6	A	311	DMU	O1-C9-C11	2.03	111.48	106.44

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PT5	O16-C8-C9-O18
2	A	301	PT5	C12-C10-O16-C8
2	A	301	PT5	C19-C20-C21-C22
3	A	302	CPL	O4P-C4-C5-N
3	A	302	CPL	C32-C31-O2-C2
3	A	302	CPL	O31-C31-O2-C2
6	A	309	DMU	O5-C6-O16-C18
6	A	309	DMU	C19-C18-O16-C6
2	A	301	PT5	O17-C10-O16-C8
3	A	302	CPL	C41-C42-C43-C44
6	A	309	DMU	C1-C6-O16-C18
2	A	301	PT5	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	A	302	CPL	C31-C32-C33-C34
3	A	302	CPL	C11-C12-C13-C14
6	A	309	DMU	O16-C18-C19-C22
6	A	311	DMU	C25-C28-C31-C34
6	A	312	DMU	C19-C22-C25-C28
6	A	309	DMU	C25-C28-C31-C34
2	A	301	PT5	C14-C15-C16-C17
2	A	301	PT5	C38-C39-C40-C41
2	A	301	PT5	C36-C37-C38-C39
3	A	302	CPL	C32-C33-C34-C35
6	A	311	DMU	C28-C31-C34-C37
6	A	311	DMU	C31-C34-C37-C40
3	A	302	CPL	C4-C5-N-C8
3	A	302	CPL	C17-C18-C19-C20
3	A	302	CPL	C15-C16-C17-C18
3	A	302	CPL	C18-C19-C20-C21
2	A	301	PT5	C33-C34-C35-C36
6	A	312	DMU	C22-C25-C28-C31
2	A	301	PT5	C20-C21-C22-C23
2	A	301	PT5	C12-C13-C14-C15
6	A	310	DMU	C25-C28-C31-C34
3	A	302	CPL	C35-C36-C37-C38
3	A	302	CPL	C4-C5-N-C7
6	A	310	DMU	C18-C19-C22-C25
2	A	301	PT5	C31-C32-C33-C34
3	A	302	CPL	C16-C17-C18-C19
2	A	301	PT5	C35-C36-C37-C38
3	A	302	CPL	C33-C34-C35-C36
3	A	302	CPL	C19-C20-C21-C22
3	A	302	CPL	C36-C37-C38-C39
3	A	302	CPL	C12-C11-O3-C3
6	A	311	DMU	C34-C37-C40-C43
2	A	301	PT5	O13-C7-C8-O16
6	A	310	DMU	O16-C18-C19-C22
3	A	302	CPL	C22-C23-C24-C25
3	A	302	CPL	O11-C11-O3-C3
6	A	309	DMU	C34-C37-C40-C43
3	A	302	CPL	C38-C39-C40-C41
3	A	302	CPL	C20-C21-C22-C23
2	A	301	PT5	C7-C8-C9-O18
2	A	301	PT5	C40-C41-C42-C43
2	A	301	PT5	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
6	A	310	DMU	C31-C34-C37-C40
6	A	310	DMU	C34-C37-C40-C43
6	A	309	DMU	O1-C10-O7-C3
6	A	310	DMU	C4-C3-O7-C10
6	A	312	DMU	C25-C28-C31-C34
3	A	302	CPL	C21-C22-C23-C24
2	A	301	PT5	O13-C7-C8-C9
6	A	310	DMU	C2-C3-O7-C10
6	A	312	DMU	O5-C6-O16-C18
3	A	302	CPL	C1-O3P-P-O4P
3	A	302	CPL	C34-C35-C36-C37
6	A	309	DMU	C31-C34-C37-C40
6	A	311	DMU	C3-C4-C57-O61
6	A	309	DMU	C5-C10-O7-C3
6	A	311	DMU	C22-C25-C28-C31
3	A	302	CPL	C13-C14-C15-C16
2	A	301	PT5	C16-C17-C18-C19
6	A	312	DMU	C31-C34-C37-C40
2	A	301	PT5	O19-C11-O18-C9
2	A	301	PT5	C31-C11-O18-C9
6	A	312	DMU	C1-C6-O16-C18
6	A	311	DMU	C4-C3-O7-C10
6	A	311	DMU	C19-C22-C25-C28
2	A	301	PT5	C13-C14-C15-C16
2	A	301	PT5	O18-C11-C31-C32
6	A	310	DMU	C28-C31-C34-C37
6	A	311	DMU	C2-C3-O7-C10
2	A	301	PT5	O19-C11-C31-C32

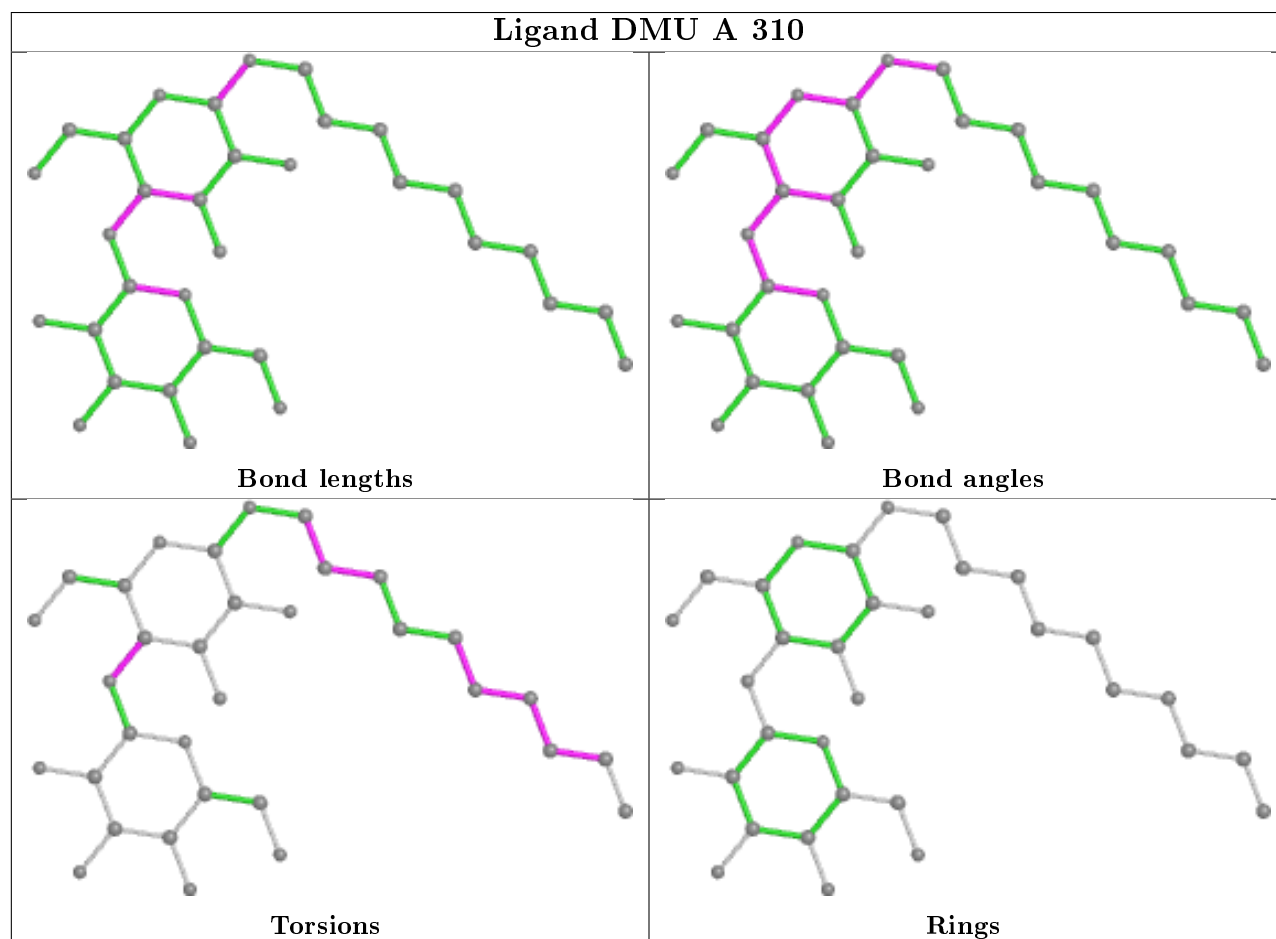
There are no ring outliers.

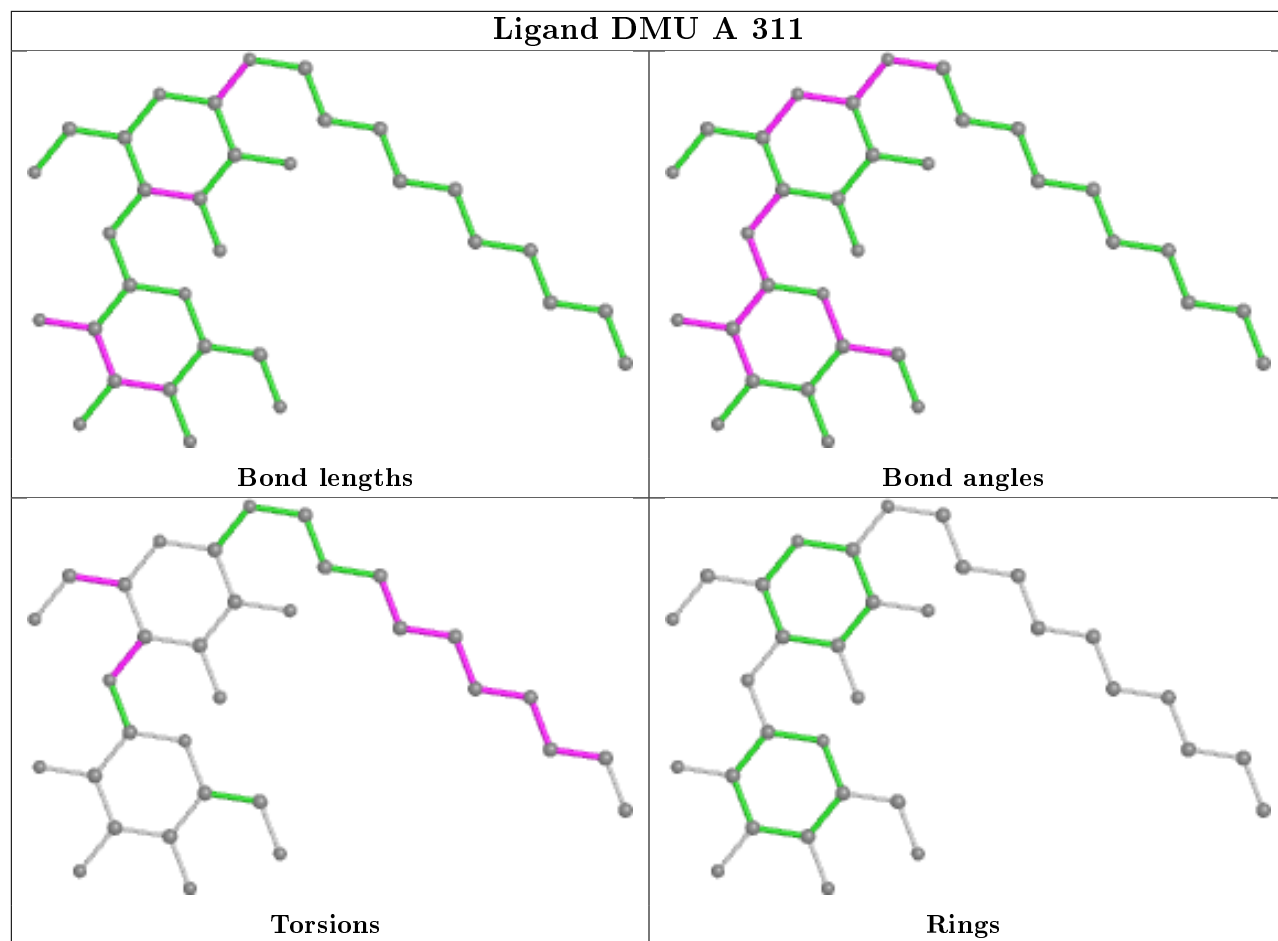
5 monomers are involved in 14 short contacts:

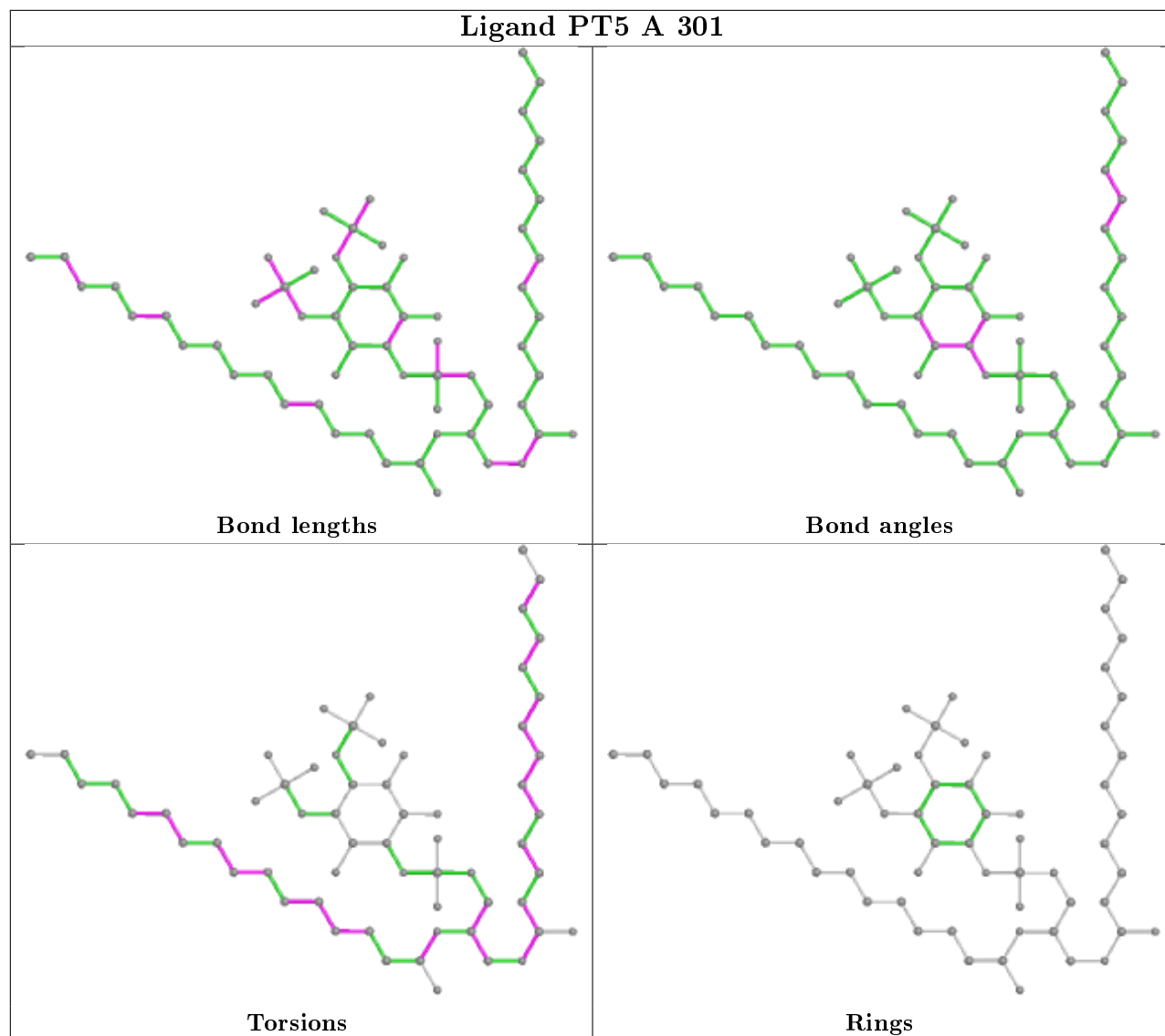
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	310	DMU	2	0
6	A	311	DMU	4	0
3	A	302	CPL	3	0
6	A	312	DMU	1	0
6	A	309	DMU	6	0

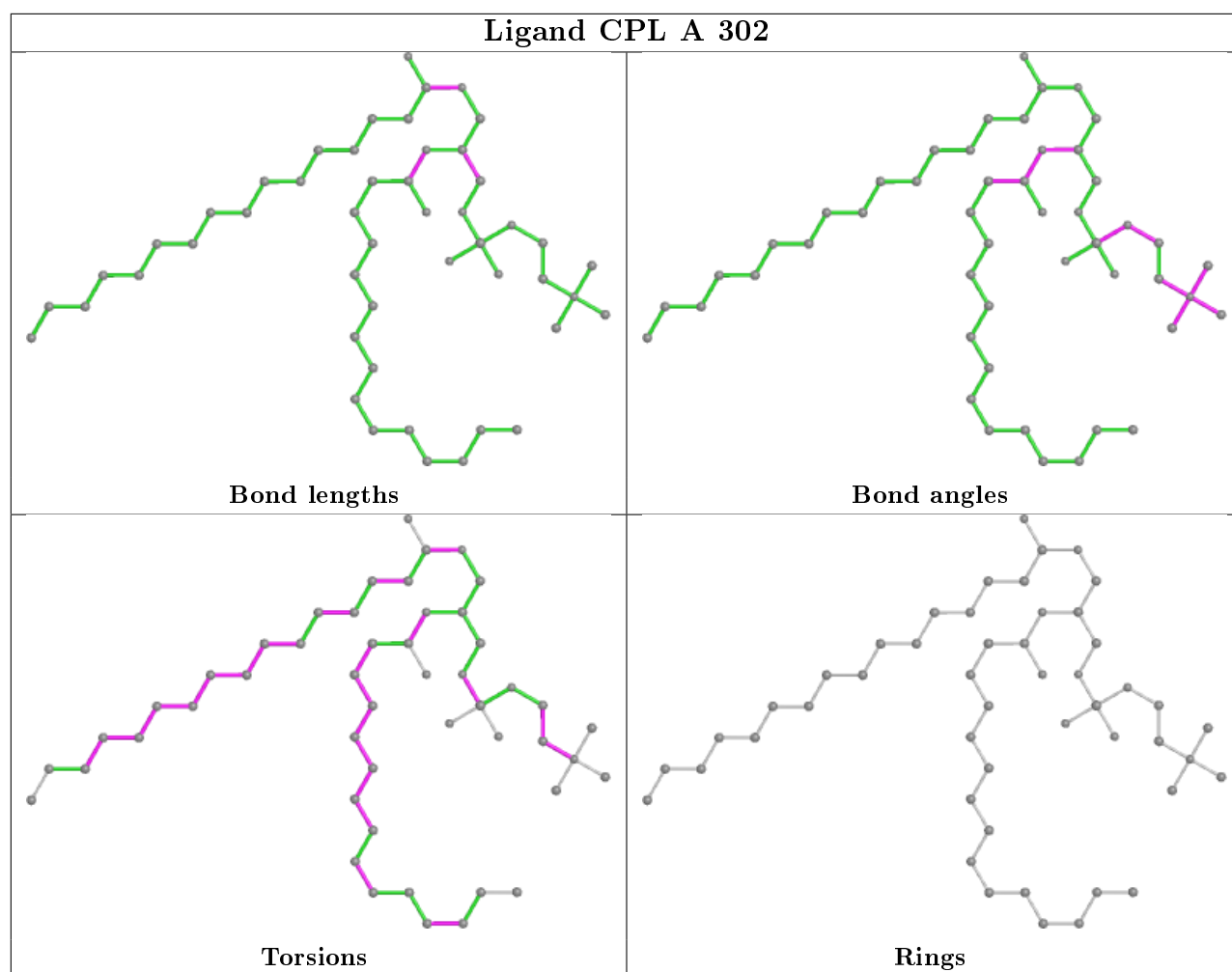
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

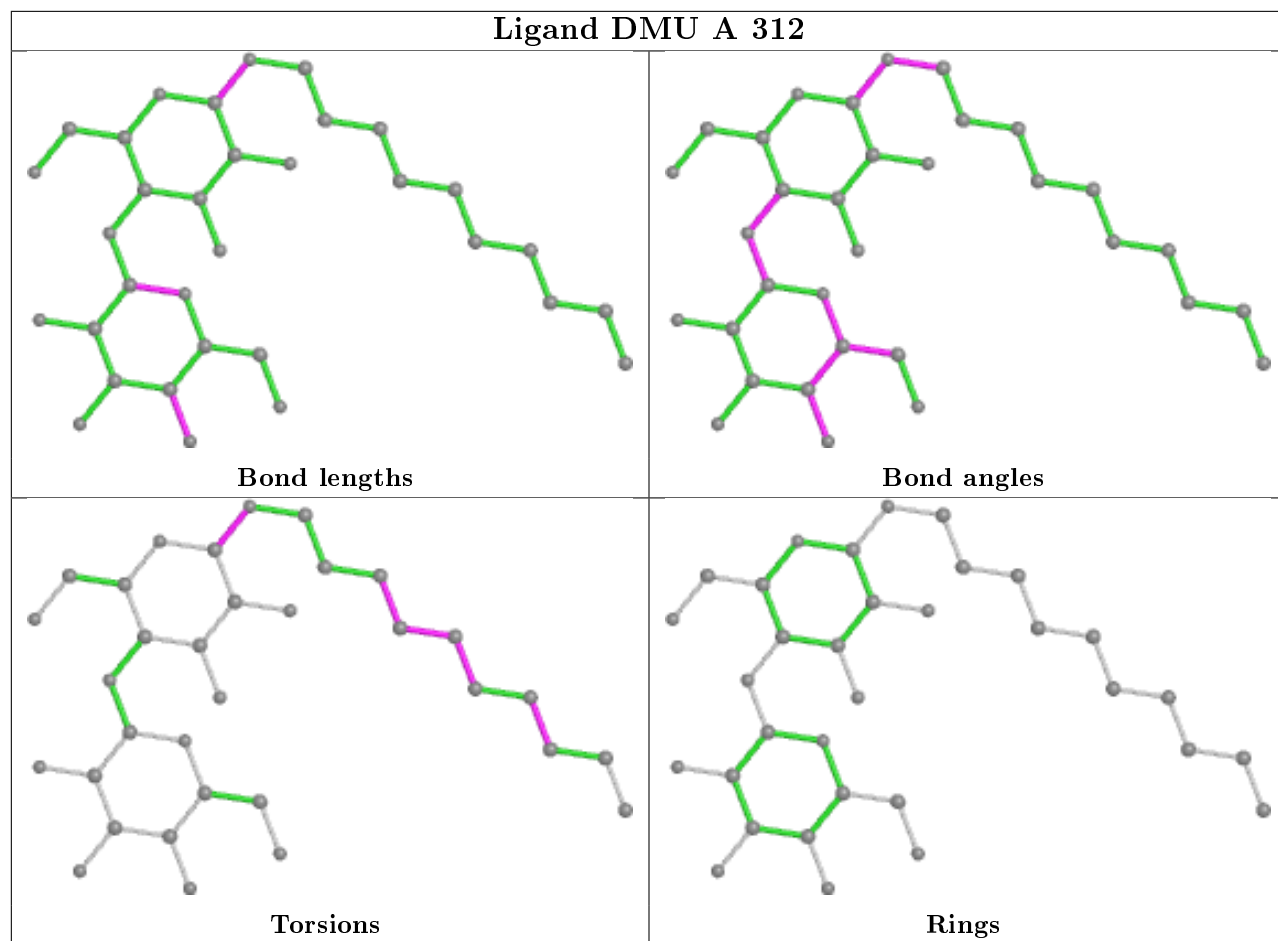
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

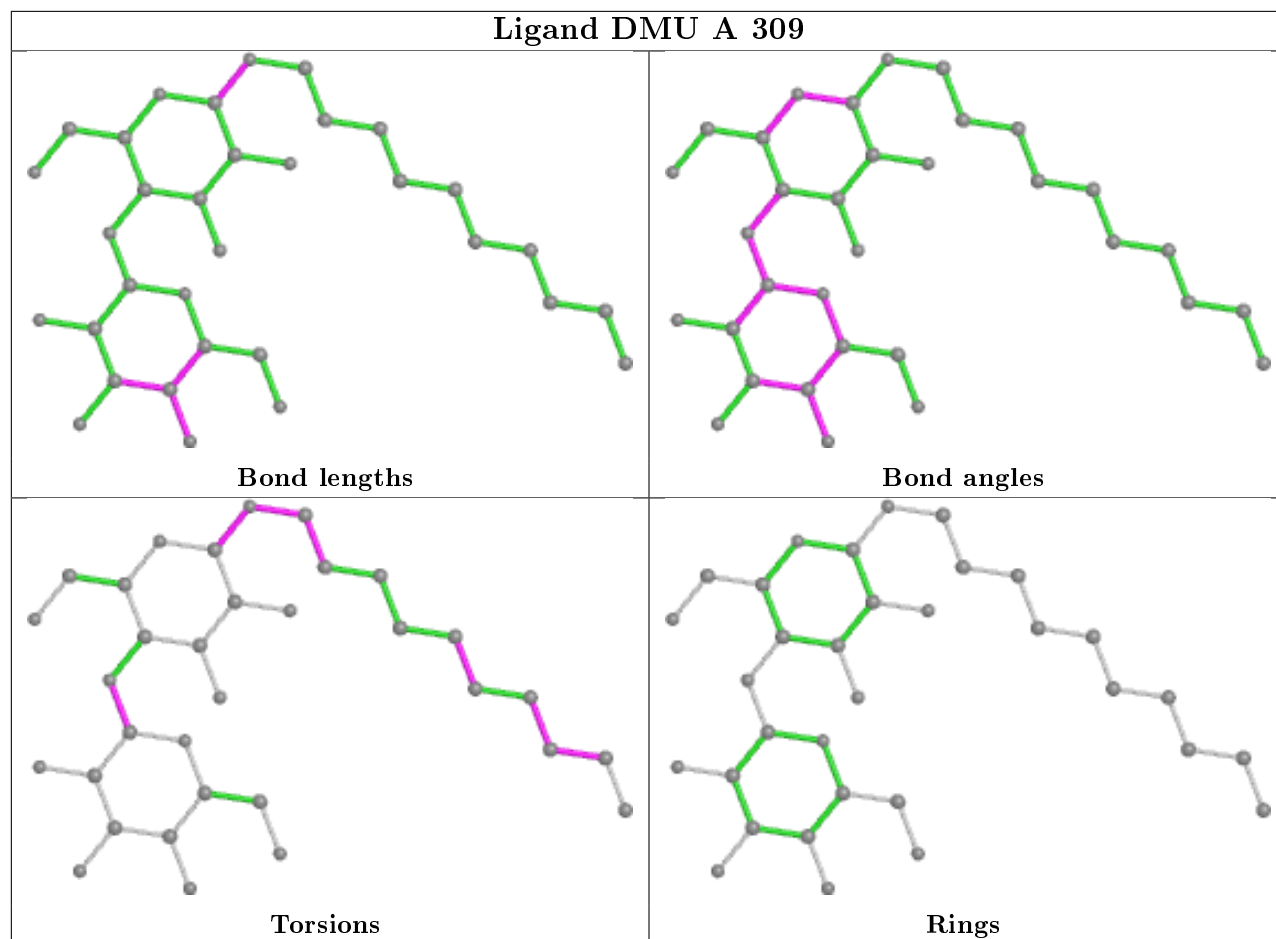












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	234/258 (90%)	0.47	22 (9%) 8 11	30, 45, 133, 170	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	LEU	11.1
1	A	188	ILE	9.5
1	A	240	SER	8.1
1	A	242	HIS	7.7
1	A	241	VAL	7.4
1	A	10	ILE	7.3
1	A	190	ARG	7.1
1	A	213	TYR	6.8
1	A	239	LEU	5.8
1	A	187	GLU	5.3
1	A	185	ASN	5.1
1	A	186	HIS	5.0
1	A	12	HIS	4.5
1	A	243	ASP	4.3
1	A	11	ASP	4.3
1	A	212	MET	2.9
1	A	50	ASP	2.8
1	A	191	PRO	2.6
1	A	217	PRO	2.6
1	A	215	THR	2.5
1	A	238	CYS	2.5
1	A	49	PRO	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

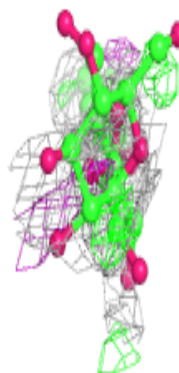
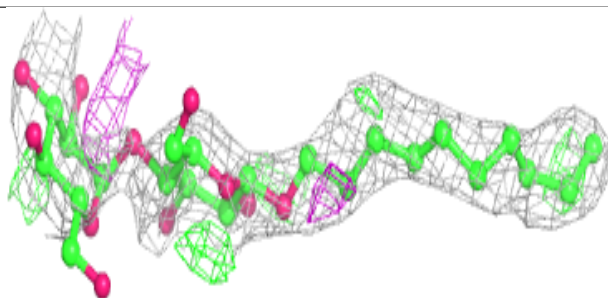
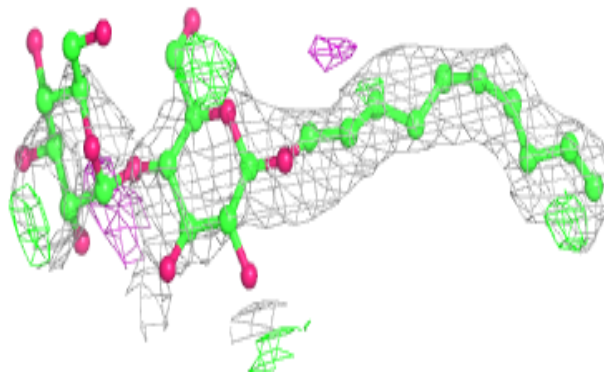
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DMU	A	311	33/33	0.25	0.47	65,114,121,126	0
3	CPL	A	302	49/52	0.35	0.40	115,147,165,169	0
6	DMU	A	309	33/33	0.54	0.49	73,116,124,130	0
5	ACT	A	304	4/4	0.55	0.30	131,132,133,133	0
6	DMU	A	310	33/33	0.65	0.41	73,101,117,123	0
6	DMU	A	312	33/33	0.68	0.32	50,85,113,136	0
5	ACT	A	308	4/4	0.70	0.30	115,118,119,119	0
5	ACT	A	305	4/4	0.72	0.26	129,129,131,132	0
5	ACT	A	307	4/4	0.77	0.26	89,92,94,95	0
5	ACT	A	306	4/4	0.84	0.33	126,128,129,129	0
2	PT5	A	301	61/69	0.89	0.20	37,63,88,97	0
4	MG	A	303	1/1	0.94	0.47	92,92,92,92	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.

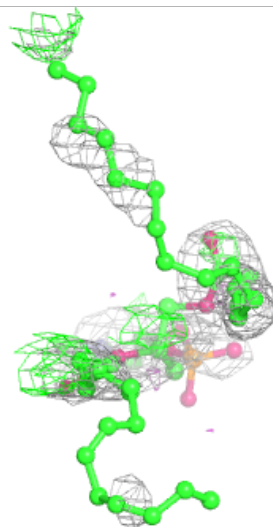
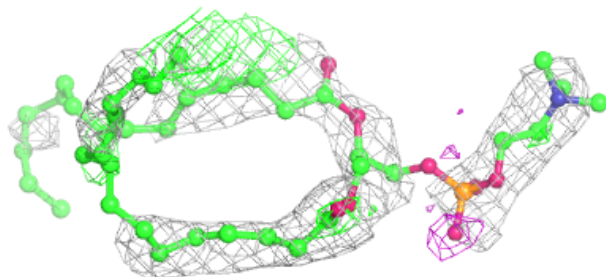
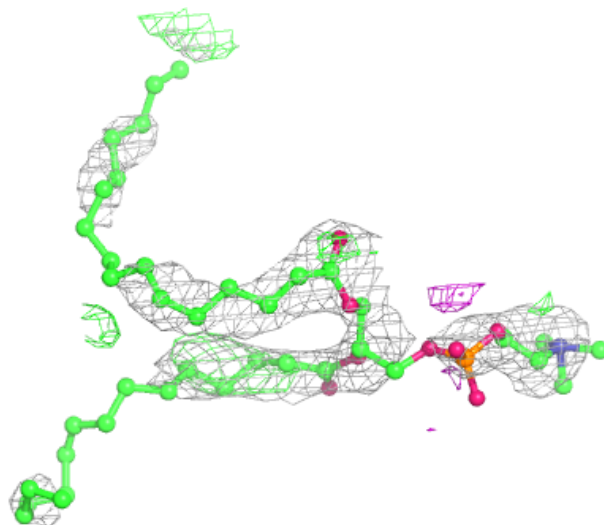
Electron density around DMU A 311:

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



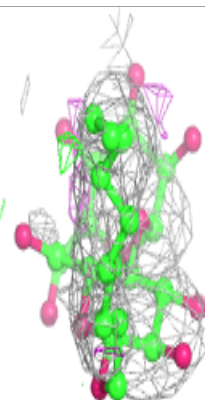
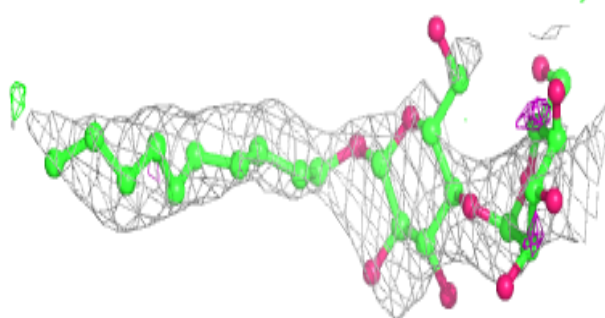
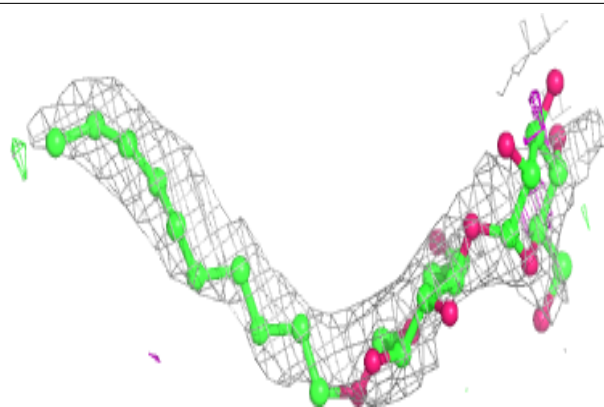
Electron density around CPL A 302:

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

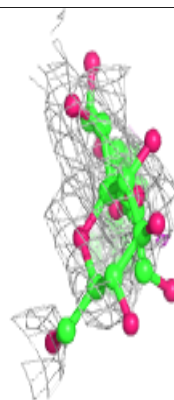
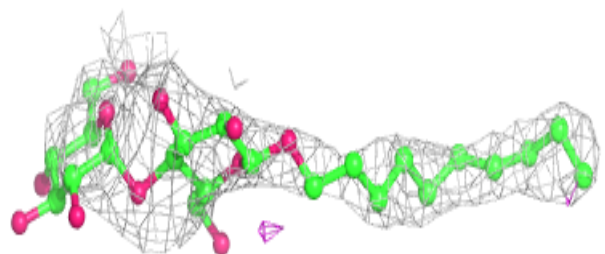
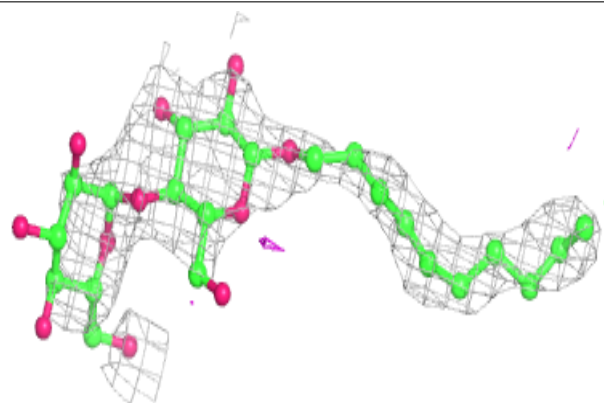


Electron density around DMU A 309:

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

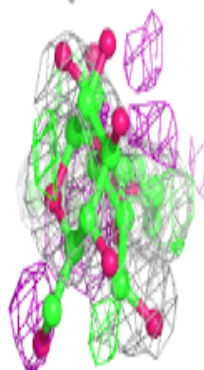
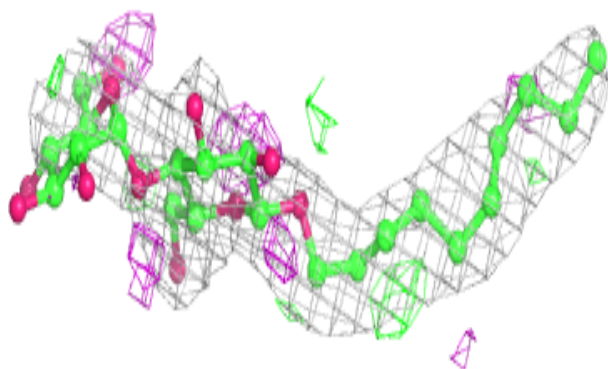
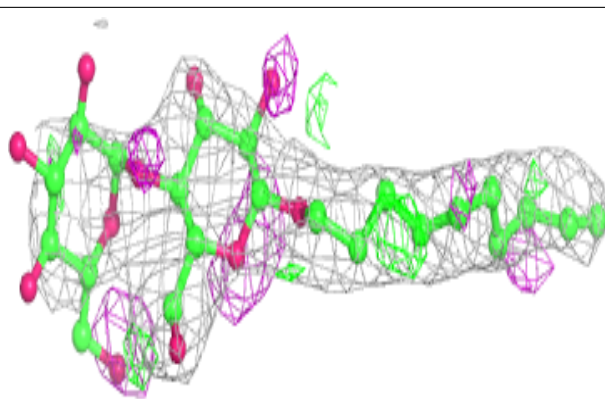
**Electron density around DMU A 310:**

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

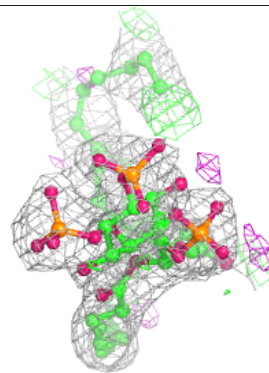
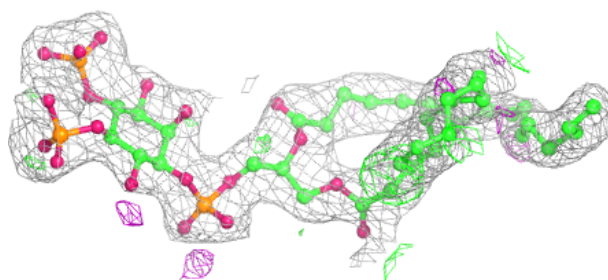
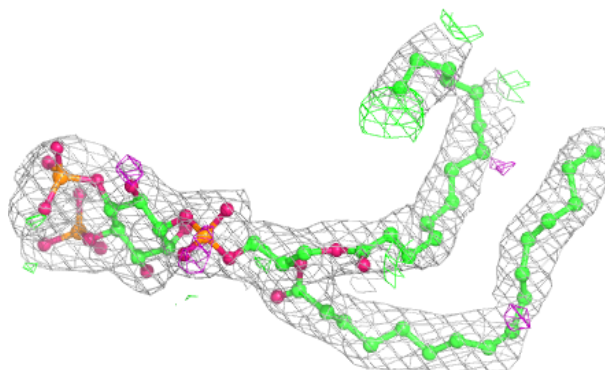


Electron density around DMU A 312:

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

**Electron density around PT5 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)



6.5 Other polymers

There are no such residues in this entry.