



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2022 – 04:54 pm BST

PDB ID : 7PNC  
Title : Dark state structure of Sensory Rhodopsin II solved by serial millisecond crystallography  
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Deposited on : 2021-09-06  
Resolution : 2.20 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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.30  
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) : 2.30

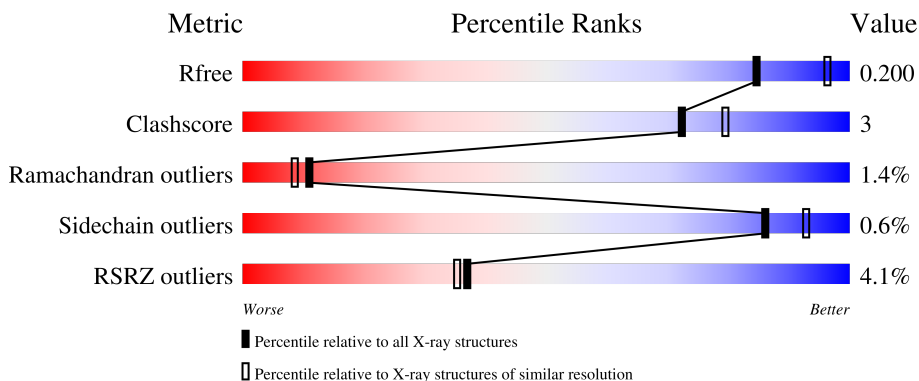
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	249	

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	CL	A	317	-	-	X	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	BOG	A	303	X	-	-	-
4	BOG	A	304	X	-	-	-
4	BOG	A	305	-	-	-	X
4	BOG	A	313	-	-	-	X
4	BOG	A	316	-	-	-	X
5	MPG	A	312	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4172 atoms, of which 2173 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.

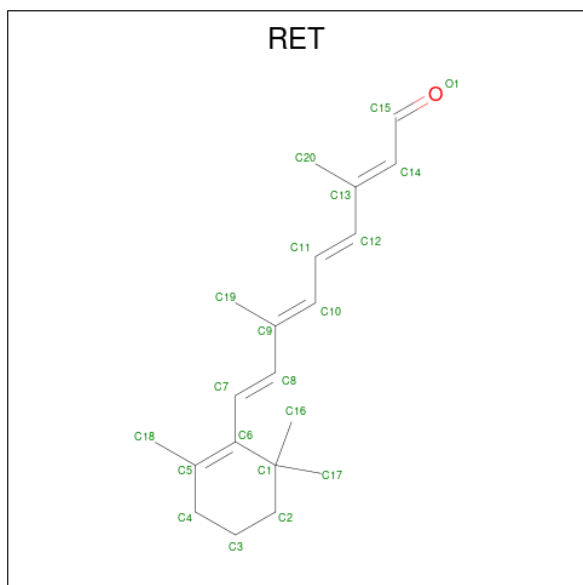
- Molecule 1 is a protein called Sensory rhodopsin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	219	3361	1105	1716	260	273	7	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	expression tag	UNP P42196
A	241	ASN	-	expression tag	UNP P42196
A	242	SER	-	expression tag	UNP P42196
A	243	HIS	-	expression tag	UNP P42196
A	244	HIS	-	expression tag	UNP P42196
A	245	HIS	-	expression tag	UNP P42196
A	246	HIS	-	expression tag	UNP P42196
A	247	HIS	-	expression tag	UNP P42196
A	248	HIS	-	expression tag	UNP P42196
A	249	HIS	-	expression tag	UNP P42196

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O) (labeled as "Ligand of Interest" by depositor).

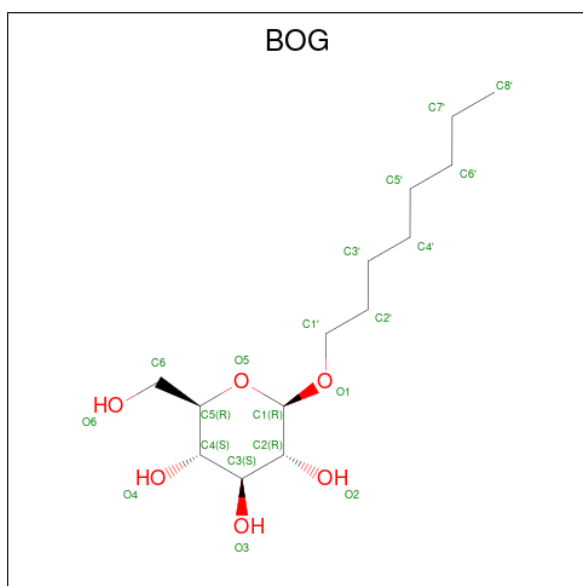


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C H	0	0
			48	20 28		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

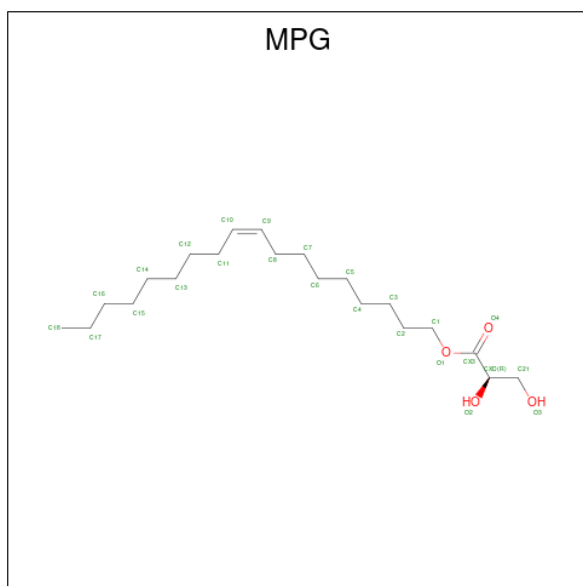
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			48	14	28	6		
4	A	1	Total	C	H	O	0	0
			48	14	28	6		
4	A	1	Total	C	H	O	0	0
			48	14	28	6		
4	A	1	Total	C	H	O	0	0
			48	14	28	6		
4	A	1	Total	C	H	O	0	0
			35	10	19	6		
4	A	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 5 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			65	21	40	4		
5	A	1	Total	C	H	O	0	0
			65	21	40	4		
5	A	1	Total	C	H	O	0	0
			65	21	40	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			43	14	25	4		
5	A	1	Total	C	H	O	0	0
			65	21	40	4		
5	A	1	Total	C	H	O	0	0
			49	16	29	4		

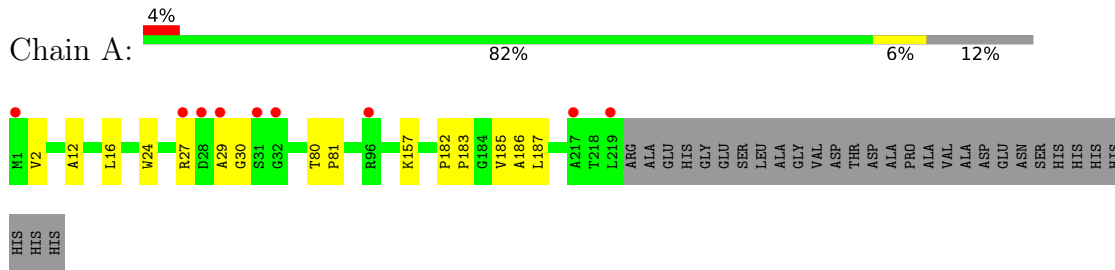
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total	O	0	0
			38	38		

### 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: Sensory rhodopsin-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.75Å 131.70Å 51.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.44 – 2.20 39.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.44-2.20) 99.9 (39.44-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.183 , 0.201 0.183 , 0.200	Depositor DCC
$R_{free}$ test set	781 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtrriage
Anisotropy	0.492	Xtrriage
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>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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: CL, BOG, RET, MPG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/1687	0.44	0/2311

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	1645	1716	1716	7	0
2	A	20	28	27	4	0
3	A	2	0	0	2	0
4	A	156	215	213	2	0
5	A	138	214	210	0	0
6	A	38	0	0	1	0
All	All	1999	2173	2166	14	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 3.

All (14) 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)
3:A:317:CL:CL	6:A:403:HOH:O	2.28	0.88
2:A:301:RET:H171	2:A:301:RET:H8	1.72	0.71
1:A:2:VAL:O	1:A:2:VAL:HG13	2.05	0.55
2:A:301:RET:H171	2:A:301:RET:C8	2.38	0.54
1:A:185:VAL:O	1:A:187:LEU:N	2.46	0.48
2:A:301:RET:H8	2:A:301:RET:H161	1.95	0.47
1:A:80:THR:N	1:A:81:PRO:HD2	2.31	0.45
1:A:12:ALA:O	1:A:16:LEU:HD12	2.18	0.44
1:A:182:PRO:N	1:A:183:PRO:CD	2.82	0.43
4:A:305:BOG:H3'2	4:A:305:BOG:H1	2.01	0.43
4:A:304:BOG:C8'	3:A:317:CL:CL	3.04	0.42
2:A:301:RET:C8	2:A:301:RET:H161	2.48	0.42
1:A:24:TRP:CE2	1:A:27:ARG:HD2	2.56	0.41
1:A:185:VAL:O	1:A:185:VAL:HG23	2.22	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	217/249 (87%)	207 (95%)	7 (3%)	3 (1%)	<b>11</b>   <b>8</b>

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
1	A	30	GLY
1	A	29	ALA

### 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	164/190 (86%)	163 (99%)	1 (1%)	<a href="#">86</a> <a href="#">93</a>

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
2	RET	A	301	1	20,20,21	0.76	1 (5%)	27,27,28	0.35	0
4	BOG	A	316	-	20,20,20	1.33	2 (10%)	25,25,25	0.85	0
5	MPG	A	314	-	19,19,24	1.17	1 (5%)	19,20,25	1.25	1 (5%)
5	MPG	A	309	-	24,24,24	1.08	1 (4%)	24,25,25	1.21	2 (8%)
5	MPG	A	311	-	17,17,24	1.23	1 (5%)	17,18,25	1.29	1 (5%)
4	BOG	A	308	-	20,20,20	1.31	1 (5%)	25,25,25	0.77	0
5	MPG	A	312	-	24,24,24	0.98	1 (4%)	24,25,25	1.21	2 (8%)
4	BOG	A	307	-	20,20,20	1.29	2 (10%)	25,25,25	0.82	1 (4%)
5	MPG	A	310	-	24,24,24	1.01	1 (4%)	24,25,25	1.15	2 (8%)
4	BOG	A	305	-	20,20,20	1.40	2 (10%)	25,25,25	1.04	2 (8%)
4	BOG	A	315	-	16,16,20	1.39	2 (12%)	21,21,25	0.98	1 (4%)
4	BOG	A	303	-	20,20,20	1.11	1 (5%)	25,25,25	0.65	0
5	MPG	A	306	-	24,24,24	0.99	1 (4%)	24,25,25	1.18	1 (4%)
4	BOG	A	313	-	20,20,20	1.31	1 (5%)	25,25,25	0.72	0
4	BOG	A	304	-	20,20,20	1.08	1 (5%)	25,25,25	1.55	5 (20%)

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	RET	A	301	1	-	0/13/30/31	0/1/1/1
4	BOG	A	316	-	-	10/11/31/31	0/1/1/1
5	MPG	A	314	-	-	5/20/20/25	-
5	MPG	A	309	-	-	10/25/25/25	-
5	MPG	A	311	-	-	5/18/18/25	-
4	BOG	A	308	-	-	4/11/31/31	0/1/1/1
5	MPG	A	312	-	-	11/25/25/25	-
4	BOG	A	307	-	-	4/11/31/31	0/1/1/1
5	MPG	A	310	-	-	9/25/25/25	-
4	BOG	A	305	-	-	6/11/31/31	0/1/1/1
4	BOG	A	315	-	-	4/7/27/31	0/1/1/1
4	BOG	A	303	-	2/2/5/5	5/11/31/31	0/1/1/1
5	MPG	A	306	-	-	11/25/25/25	-
4	BOG	A	313	-	-	4/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BOG	A	304	-	2/2/5/5	7/11/31/31	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	305	BOG	O5-C1	4.58	1.53	1.41
4	A	308	BOG	O5-C1	4.49	1.53	1.41
4	A	316	BOG	O5-C1	4.45	1.53	1.41
4	A	313	BOG	O5-C1	4.43	1.53	1.41
4	A	315	BOG	O5-C1	4.40	1.53	1.41
4	A	307	BOG	O5-C1	4.25	1.52	1.41
5	A	314	MPG	O1-CX3	4.03	1.41	1.33
5	A	309	MPG	O1-CX3	3.94	1.41	1.33
5	A	311	MPG	O1-CX3	3.88	1.41	1.33
4	A	304	BOG	O5-C1	3.82	1.51	1.41
4	A	303	BOG	O5-C1	3.81	1.51	1.41
5	A	306	MPG	O1-CX3	3.60	1.40	1.33
5	A	310	MPG	O1-CX3	3.59	1.40	1.33
5	A	312	MPG	O1-CX3	3.51	1.40	1.33
2	A	301	RET	C14-C13	2.85	1.36	1.33
4	A	305	BOG	O1-C1	-2.72	1.35	1.40
4	A	307	BOG	O1-C1	-2.30	1.36	1.40
4	A	316	BOG	O1-C1	-2.14	1.36	1.40
4	A	315	BOG	O1-C1	-2.09	1.36	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	309	MPG	O1-CX3-CXD	4.31	120.28	111.68
4	A	304	BOG	C4-C3-C2	4.16	118.09	110.82
5	A	310	MPG	O1-CX3-CXD	4.15	119.95	111.68
5	A	312	MPG	O1-CX3-CXD	4.12	119.89	111.68
5	A	306	MPG	O1-CX3-CXD	4.10	119.86	111.68
5	A	314	MPG	O1-CX3-CXD	4.07	119.80	111.68
5	A	311	MPG	O1-CX3-CXD	3.86	119.39	111.68
4	A	304	BOG	O1-C1-C2	3.28	113.42	108.30
4	A	305	BOG	O5-C5-C4	2.95	115.05	109.69
5	A	312	MPG	O1-CX3-O4	-2.46	119.47	124.13
4	A	304	BOG	O5-C1-O1	-2.37	104.36	109.97
4	A	304	BOG	C1'-O1-C1	2.32	117.69	113.84
5	A	310	MPG	O1-CX3-O4	-2.32	119.74	124.13
4	A	315	BOG	C3-C4-C5	2.22	114.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	BOG	C6-C5-C4	-2.20	107.86	113.00
4	A	307	BOG	O5-C5-C4	2.06	113.44	109.69
4	A	304	BOG	O3-C3-C4	-2.04	105.62	110.35
5	A	309	MPG	O1-CX3-O4	-2.02	120.30	124.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	303	BOG	C3
4	A	303	BOG	C4
4	A	304	BOG	C3
4	A	304	BOG	C4

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	BOG	O5-C1-O1-C1'
4	A	305	BOG	C2-C1-O1-C1'
4	A	305	BOG	O5-C1-O1-C1'
4	A	316	BOG	C2-C1-O1-C1'
4	A	316	BOG	O5-C1-O1-C1'
5	A	306	MPG	O3-C21-CXD-O2
5	A	306	MPG	O1-CX3-CXD-O2
5	A	309	MPG	O3-C21-CXD-O2
5	A	310	MPG	CXD-CX3-O1-C1
5	A	310	MPG	O4-CX3-O1-C1
5	A	310	MPG	O3-C21-CXD-O2
5	A	314	MPG	O3-C21-CXD-O2
5	A	306	MPG	O4-CX3-O1-C1
5	A	312	MPG	O4-CX3-O1-C1
4	A	315	BOG	O5-C5-C6-O6
4	A	316	BOG	O5-C5-C6-O6
4	A	315	BOG	C4-C5-C6-O6
5	A	306	MPG	CXD-CX3-O1-C1
5	A	312	MPG	CXD-CX3-O1-C1
4	A	303	BOG	C4-C5-C6-O6
5	A	306	MPG	C11-C12-C13-C14
4	A	304	BOG	C2-C1-O1-C1'
4	A	307	BOG	O5-C1-O1-C1'
4	A	303	BOG	O5-C5-C6-O6
5	A	309	MPG	C3-C4-C5-C6
5	A	312	MPG	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	A	305	BOG	O5-C5-C6-O6
5	A	312	MPG	C4-C5-C6-C7
4	A	307	BOG	C2-C1-O1-C1'
5	A	310	MPG	C14-C15-C16-C17
4	A	316	BOG	C3'-C4'-C5'-C6'
4	A	316	BOG	C4-C5-C6-O6
5	A	306	MPG	C3-C4-C5-C6
4	A	308	BOG	C4'-C5'-C6'-C7'
5	A	310	MPG	C1-C2-C3-C4
5	A	314	MPG	C1-C2-C3-C4
5	A	311	MPG	C5-C6-C7-C8
4	A	316	BOG	C1'-C2'-C3'-C4'
4	A	316	BOG	O1-C1'-C2'-C3'
4	A	308	BOG	C2'-C3'-C4'-C5'
4	A	315	BOG	C1'-C2'-C3'-C4'
5	A	312	MPG	C2-C3-C4-C5
5	A	310	MPG	C2-C3-C4-C5
5	A	306	MPG	C4-C5-C6-C7
5	A	309	MPG	C10-C11-C12-C13
4	A	304	BOG	C1'-C2'-C3'-C4'
5	A	311	MPG	O1-C1-C2-C3
4	A	308	BOG	O5-C5-C6-O6
4	A	307	BOG	O1-C1'-C2'-C3'
4	A	305	BOG	O1-C1'-C2'-C3'
4	A	313	BOG	C1'-C2'-C3'-C4'
4	A	315	BOG	O5-C1-O1-C1'
5	A	310	MPG	C6-C7-C8-C9
5	A	312	MPG	C10-C11-C12-C13
4	A	307	BOG	O5-C5-C6-O6
5	A	312	MPG	O4-CX3-CXD-O2
4	A	304	BOG	C2'-C3'-C4'-C5'
5	A	309	MPG	O3-C21-CXD-CX3
4	A	305	BOG	C2'-C1'-O1-C1
4	A	308	BOG	C2'-C1'-O1-C1
4	A	316	BOG	C2'-C1'-O1-C1
5	A	309	MPG	C4-C5-C6-C7
4	A	304	BOG	O1-C1'-C2'-C3'
5	A	309	MPG	C2-C3-C4-C5
5	A	306	MPG	C1-C2-C3-C4
5	A	309	MPG	C11-C12-C13-C14
4	A	304	BOG	O5-C5-C6-O6
4	A	316	BOG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
5	A	309	MPG	C1-C2-C3-C4
5	A	311	MPG	O4-CX3-CXD-O2
5	A	314	MPG	O4-CX3-CXD-O2
4	A	313	BOG	C3'-C4'-C5'-C6'
4	A	313	BOG	C4'-C5'-C6'-C7'
4	A	316	BOG	C5'-C6'-C7'-C8'
4	A	303	BOG	C4'-C5'-C6'-C7'
5	A	306	MPG	C6-C7-C8-C9
5	A	312	MPG	O3-C21-CXD-O2
4	A	303	BOG	C2'-C3'-C4'-C5'
5	A	306	MPG	C13-C14-C15-C16
4	A	303	BOG	C3'-C4'-C5'-C6'
5	A	306	MPG	O4-CX3-CXD-O2
4	A	304	BOG	C4'-C5'-C6'-C7'
5	A	311	MPG	O4-CX3-O1-C1
5	A	314	MPG	C10-C11-C12-C13
4	A	305	BOG	C3'-C4'-C5'-C6'
5	A	311	MPG	C6-C7-C8-C9
5	A	309	MPG	C7-C8-C9-C10
5	A	310	MPG	C9-C10-C11-C12
5	A	310	MPG	C4-C5-C6-C7
5	A	312	MPG	C7-C8-C9-C10
4	A	313	BOG	C4-C5-C6-O6
5	A	314	MPG	O3-C21-CXD-CX3
5	A	312	MPG	C13-C14-C15-C16
5	A	309	MPG	C9-C10-C11-C12
5	A	312	MPG	C9-C10-C11-C12

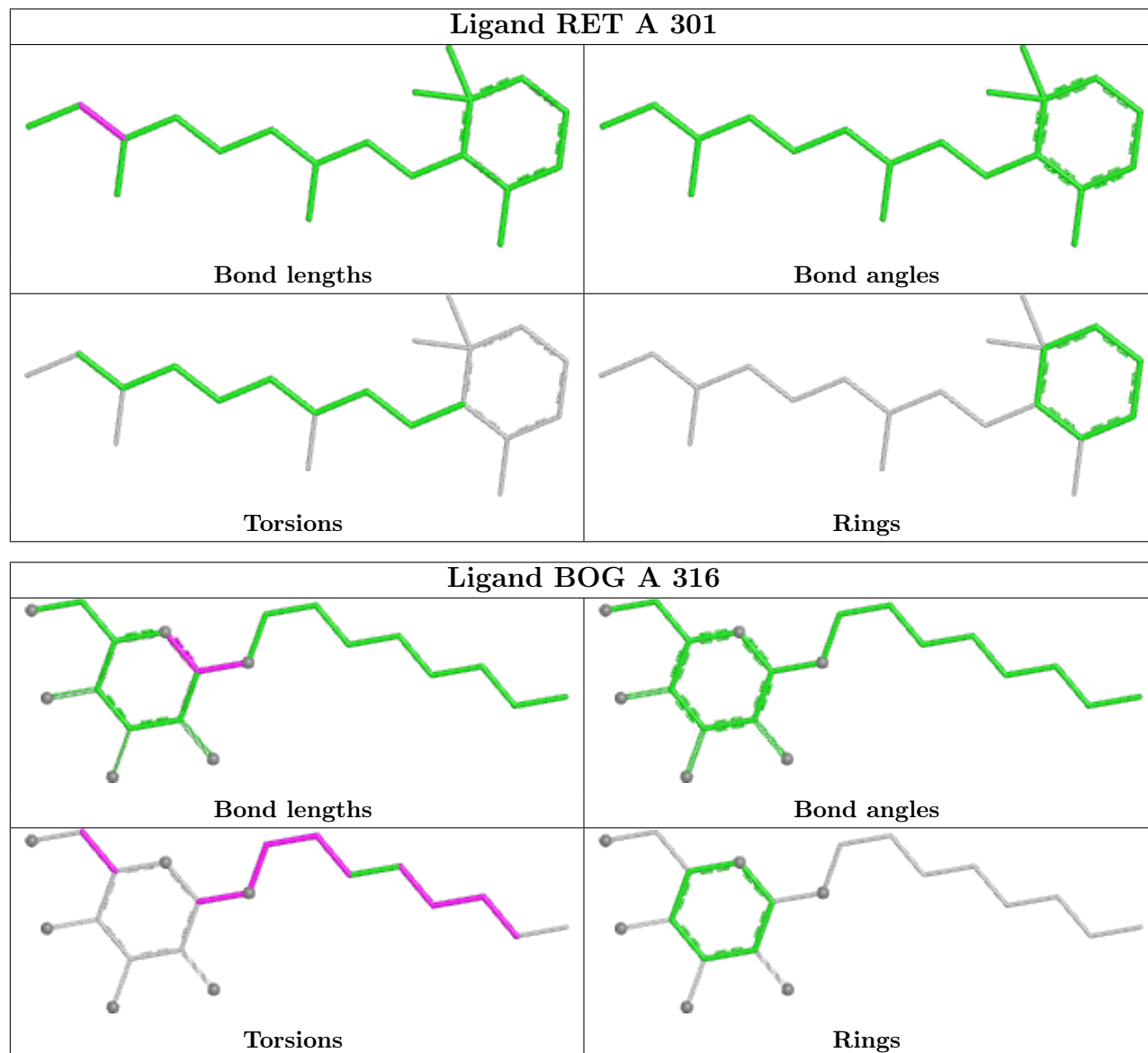
There are no ring outliers.

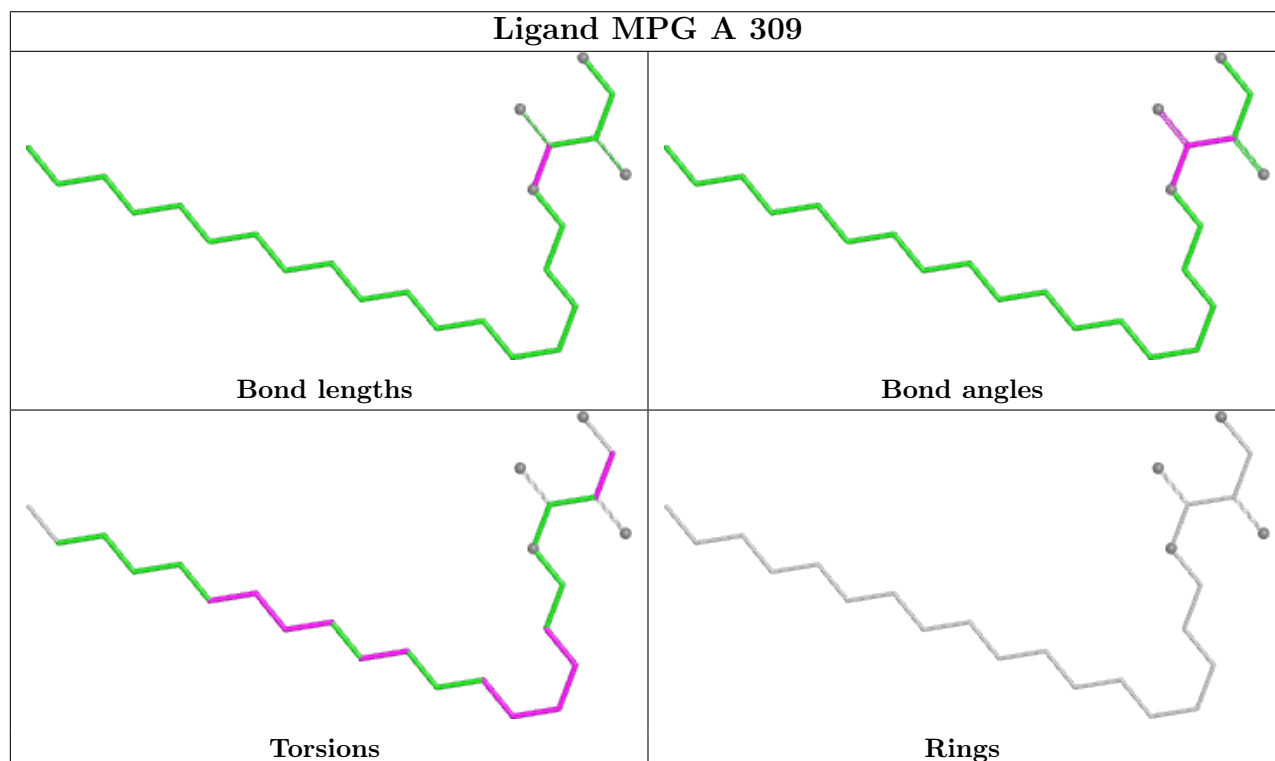
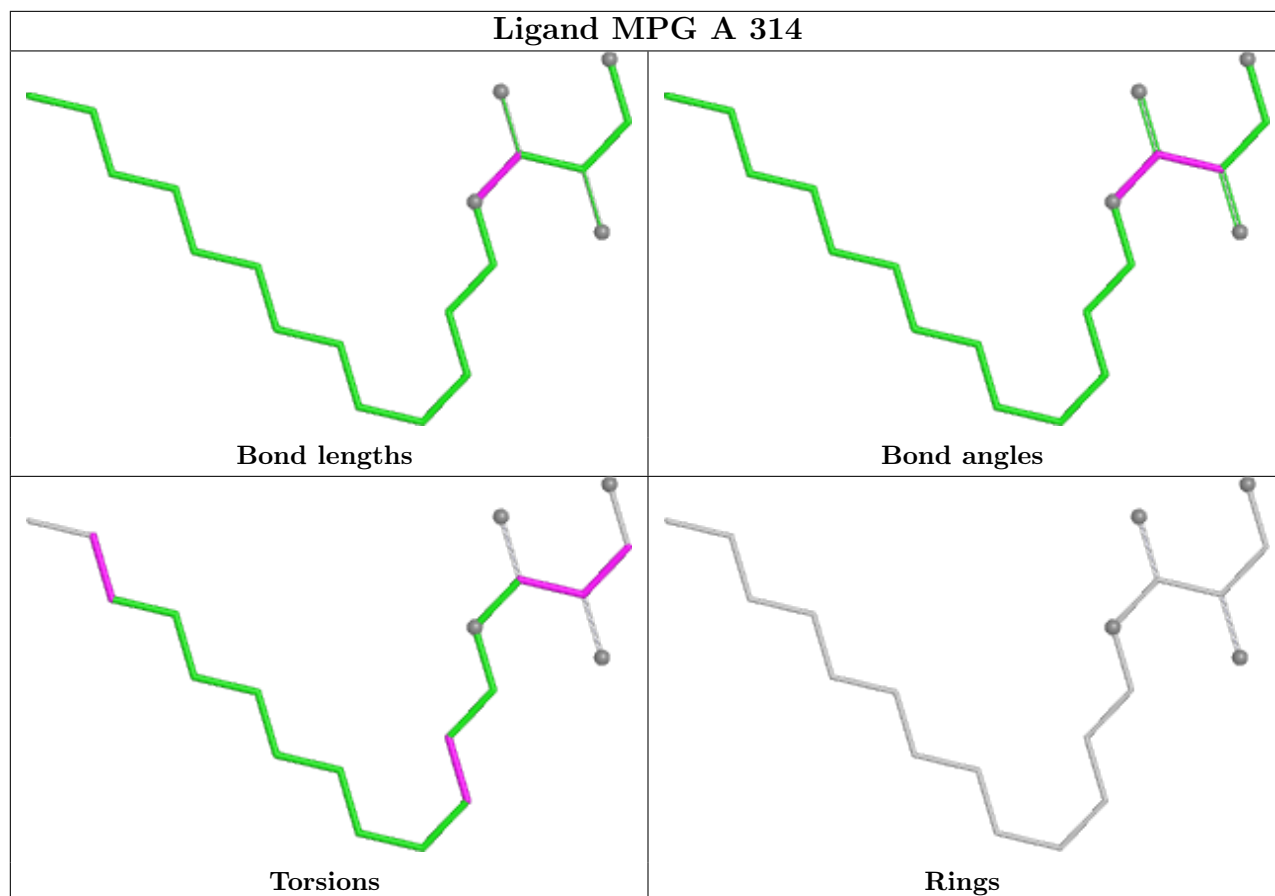
3 monomers are involved in 6 short contacts:

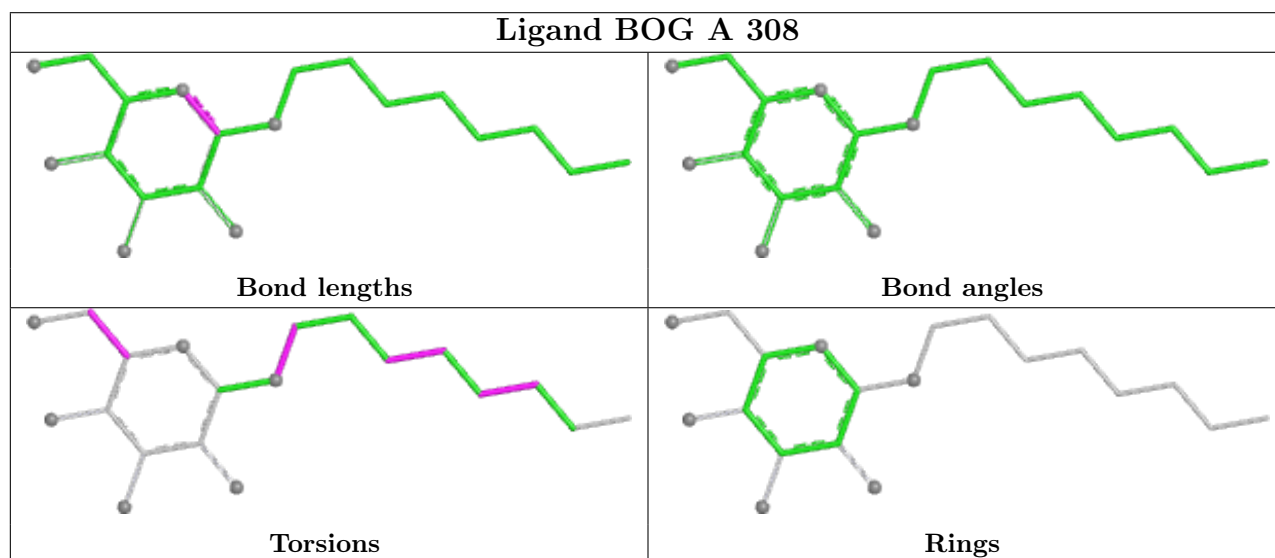
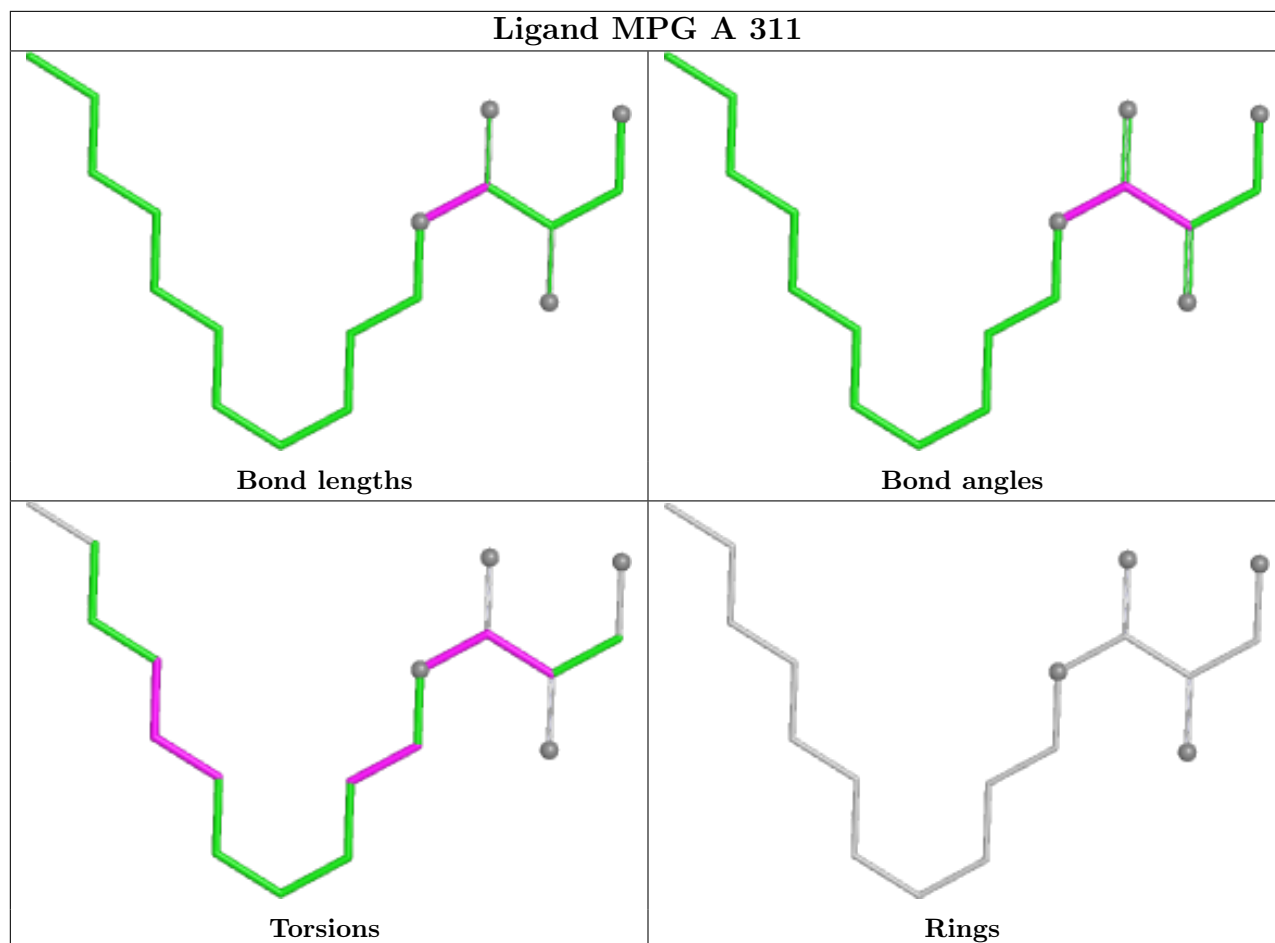
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	4	0
4	A	305	BOG	1	0
4	A	304	BOG	1	0

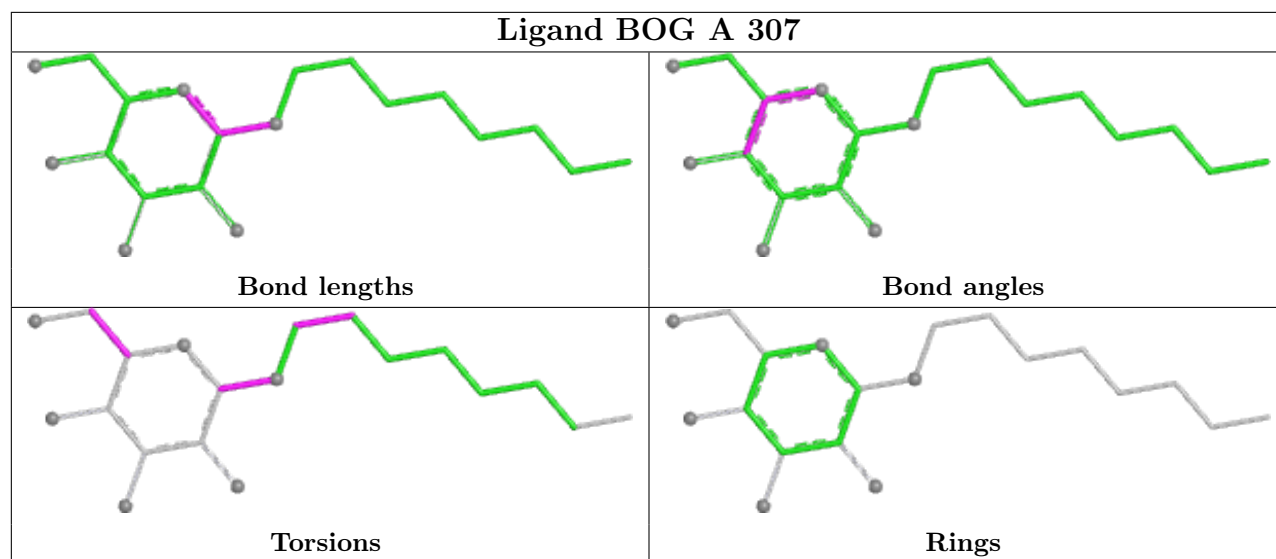
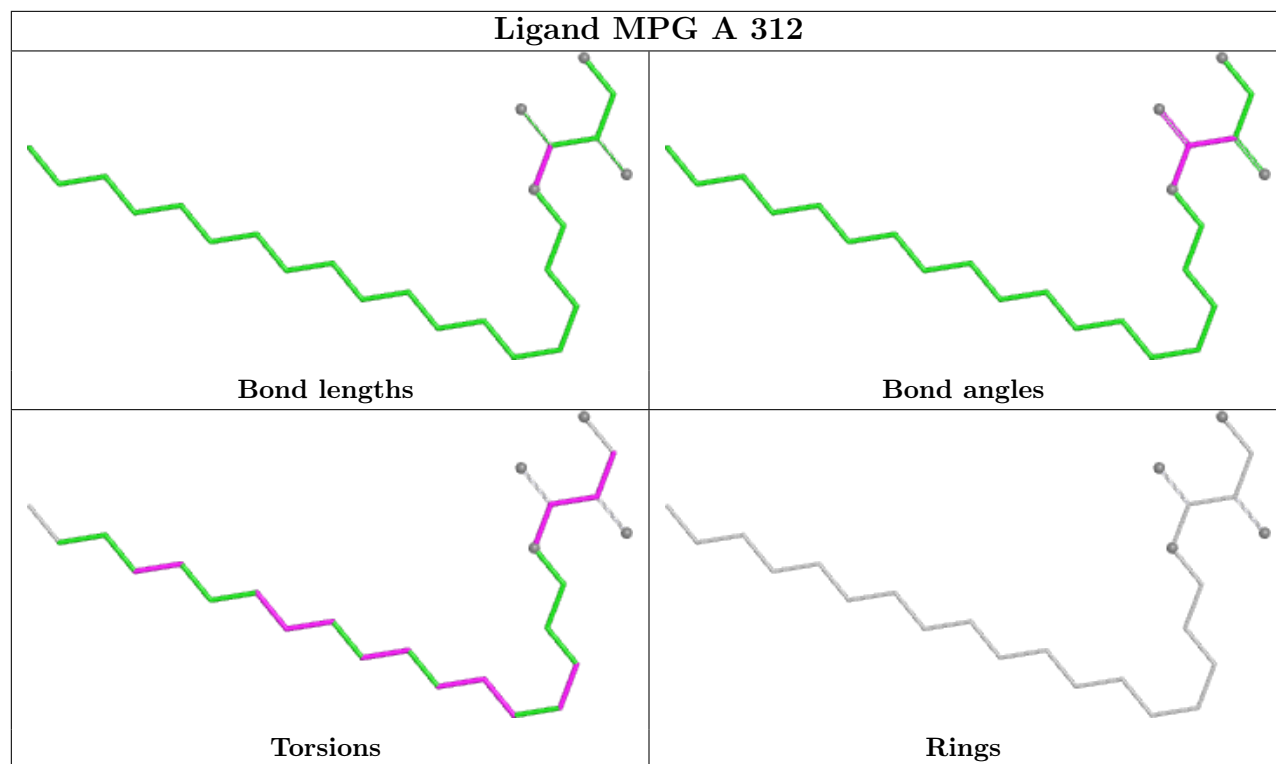
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

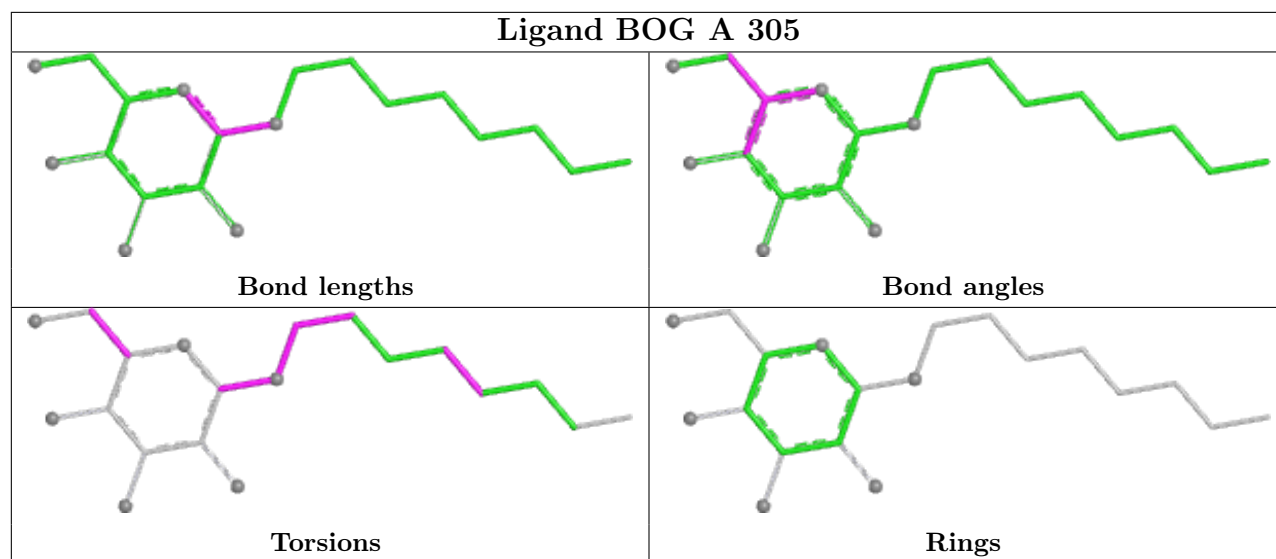
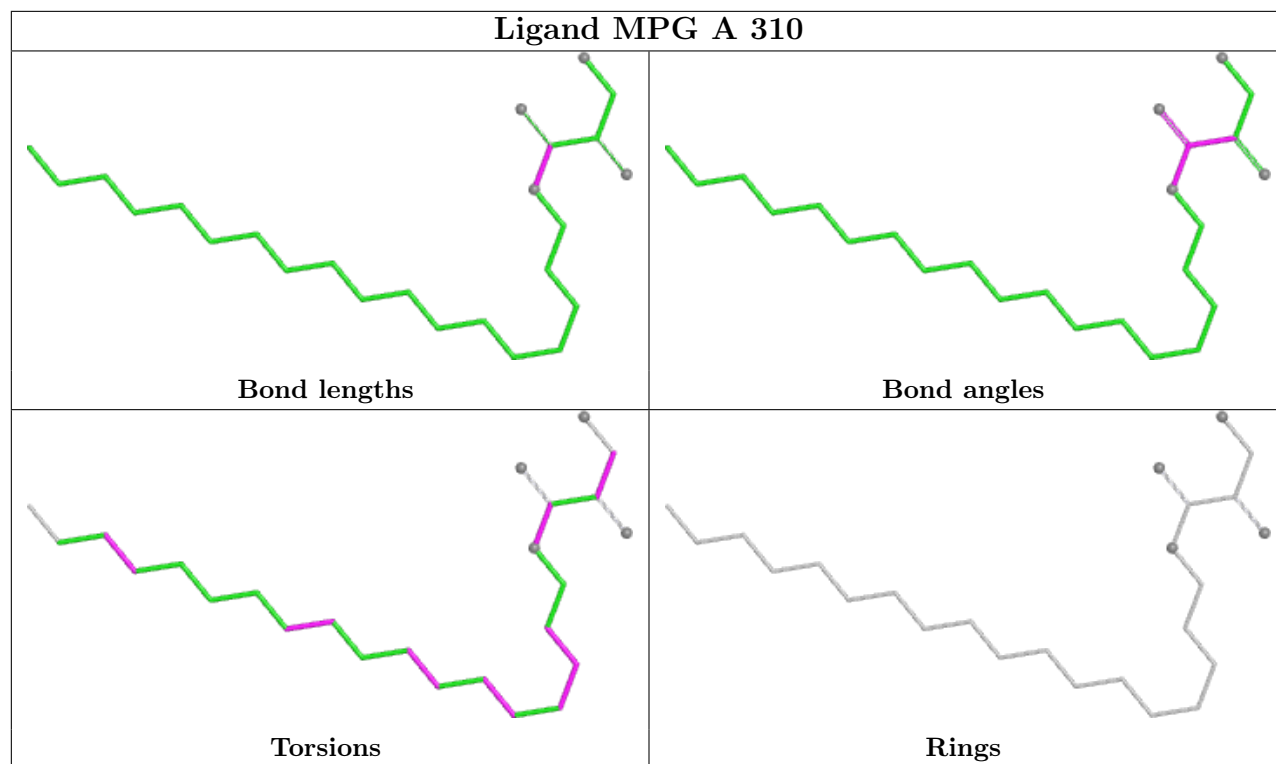
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

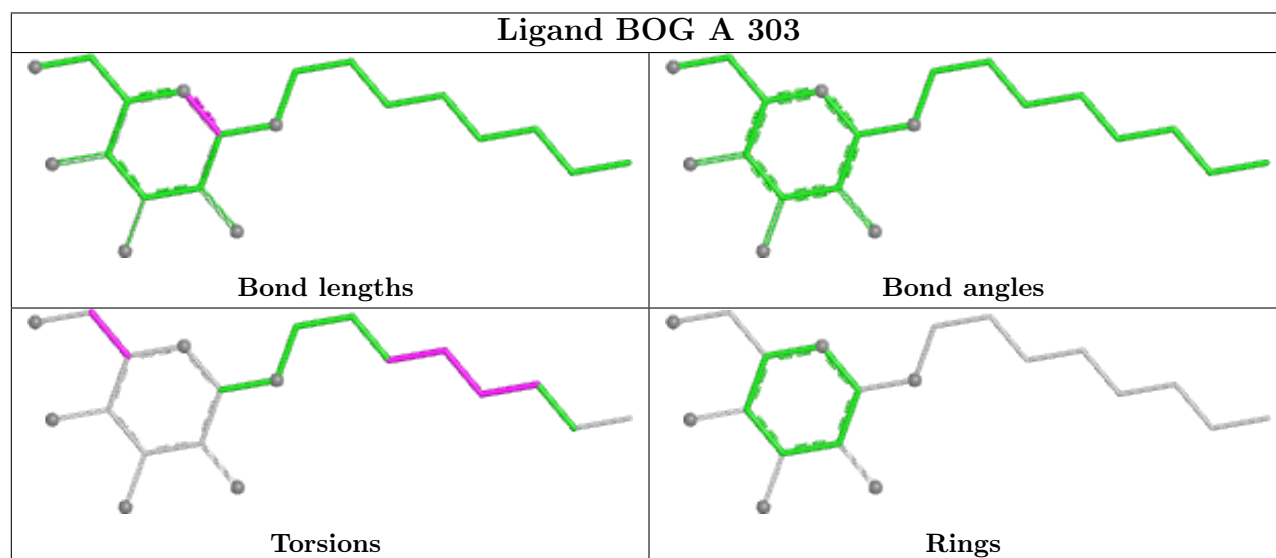
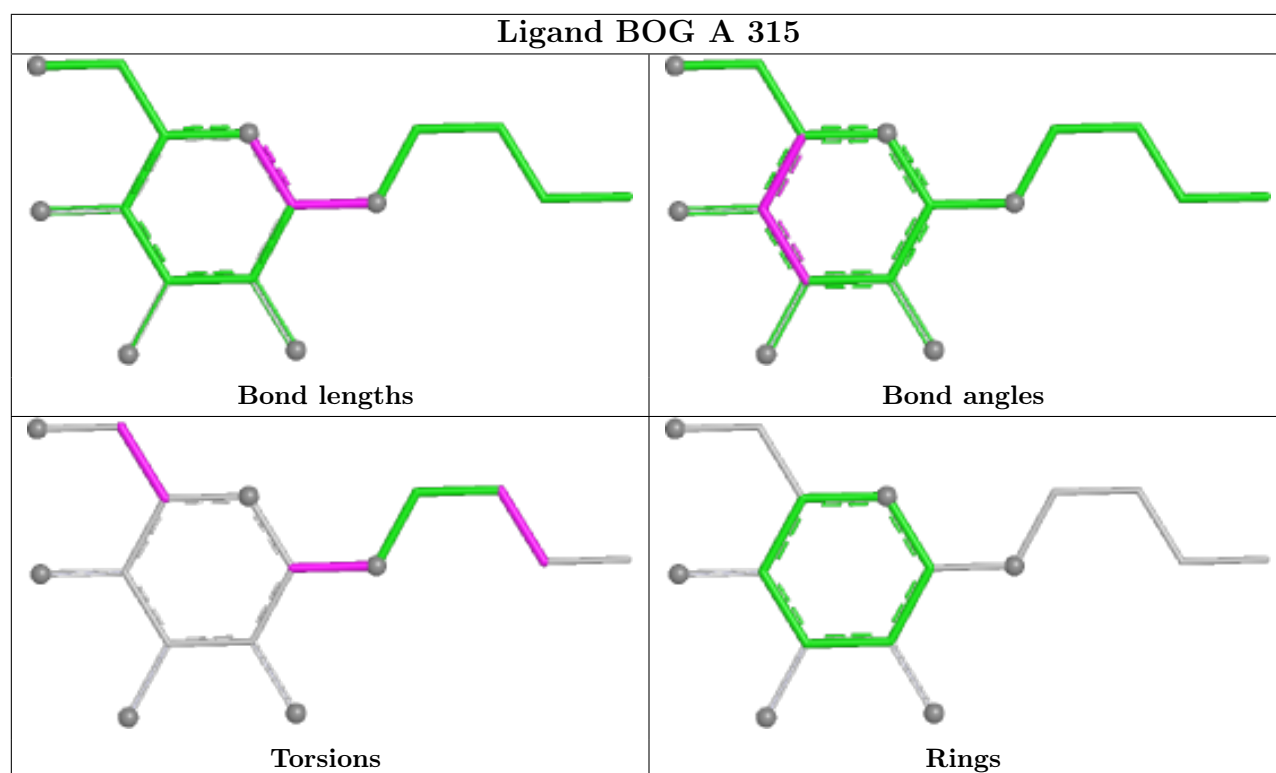


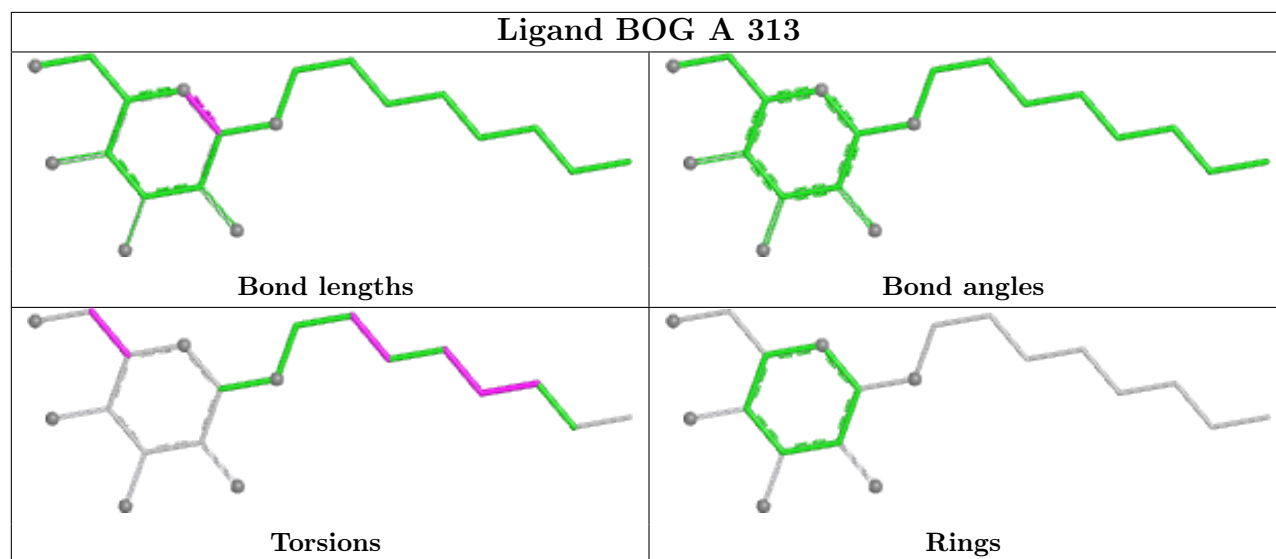
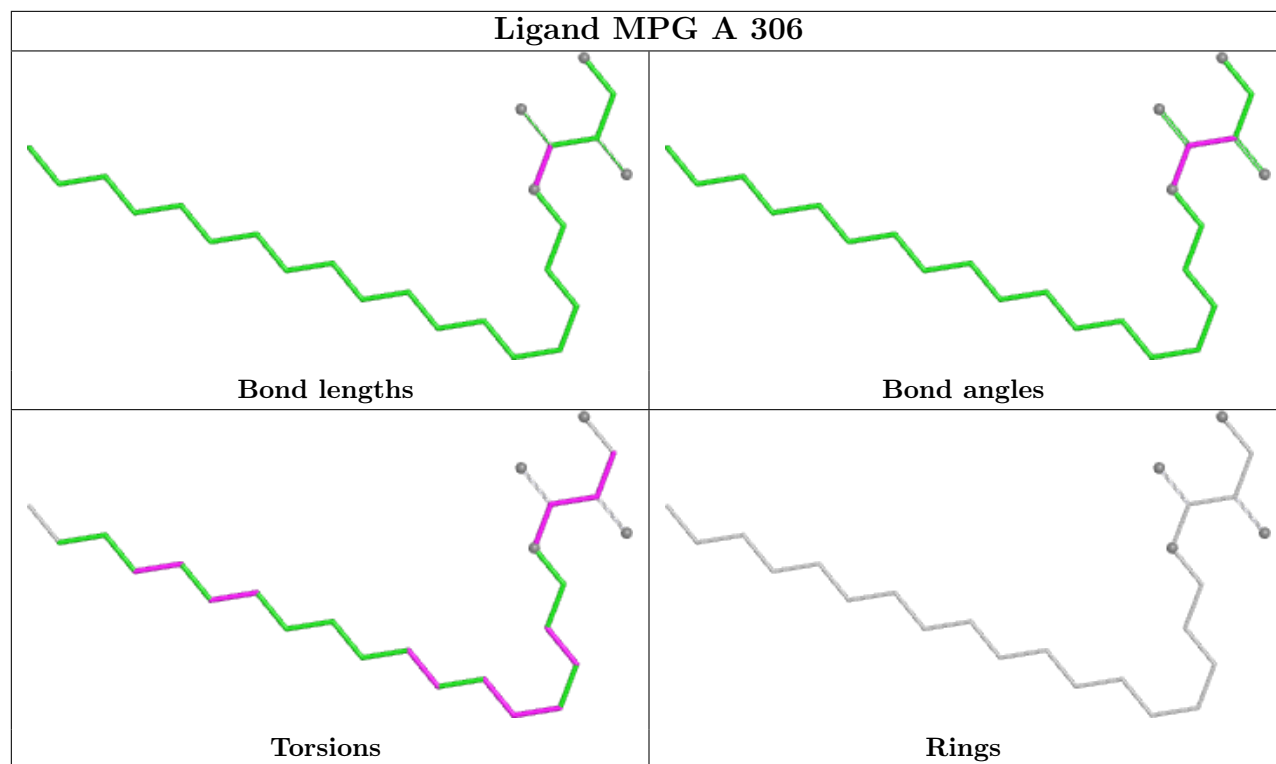




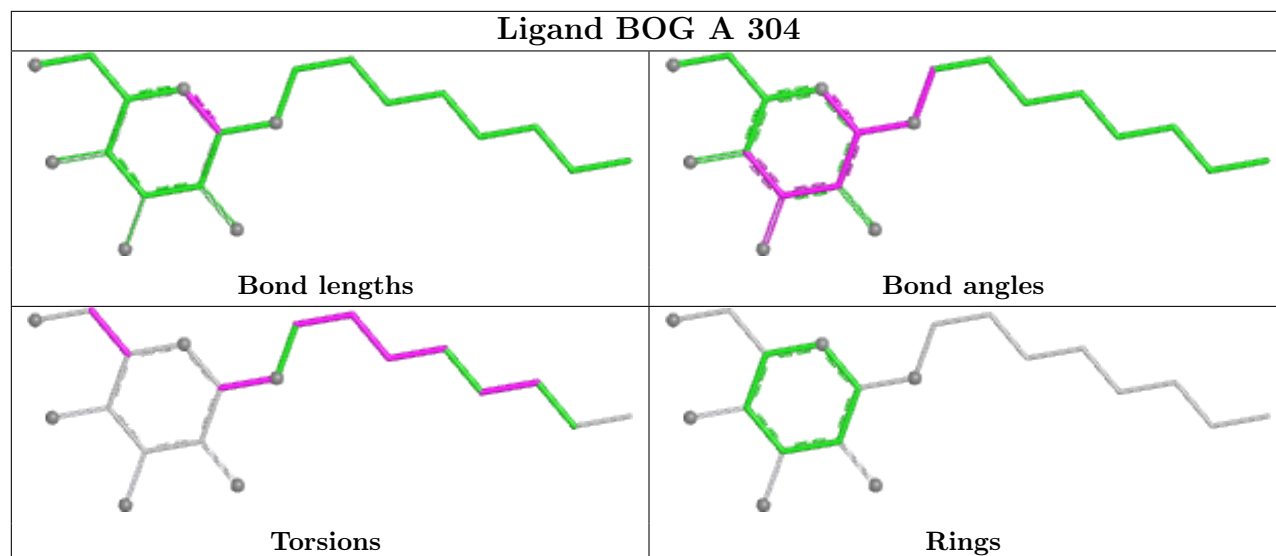












## 5.7 Other polymers [i](#)

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	219/249 (87%)	-0.36	9 (4%) 37 35	21, 39, 98, 156	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	5.2
1	A	32	GLY	3.1
1	A	217	ALA	2.9
1	A	27	ARG	2.4
1	A	96	ARG	2.3
1	A	31	SER	2.3
1	A	28	ASP	2.2
1	A	1	MET	2.1
1	A	29	ALA	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](#)

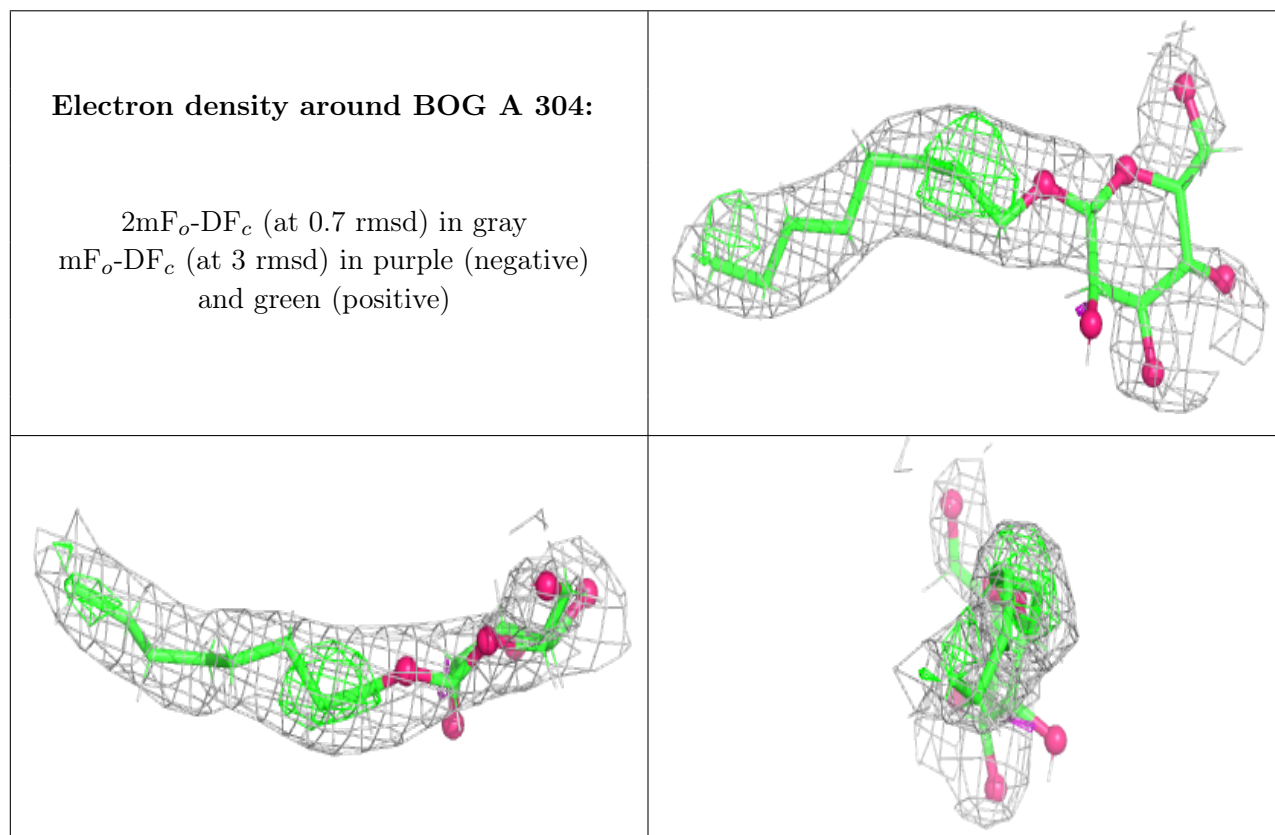
There are no monosaccharides in this entry.

### 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.

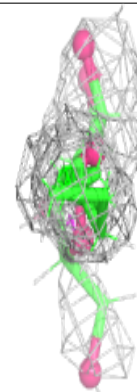
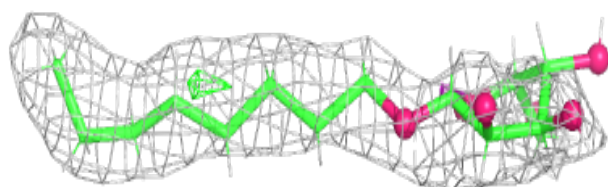
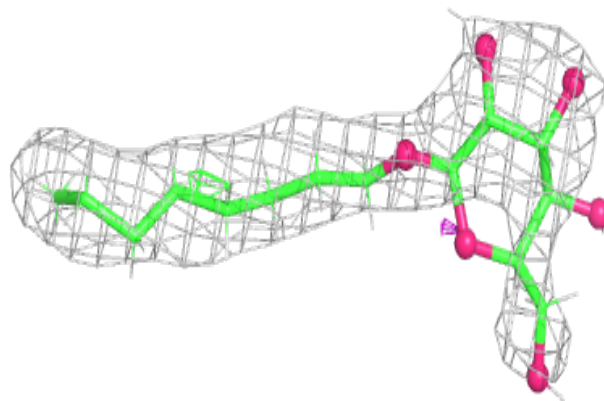
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BOG	A	304	20/20	0.31	0.35	79,106,130,149	0
4	BOG	A	303	20/20	0.39	0.32	63,122,170,191	0
4	BOG	A	305	20/20	0.42	0.45	110,143,172,188	0
4	BOG	A	313	20/20	0.47	0.41	129,156,177,179	0
4	BOG	A	316	20/20	0.48	0.41	106,136,188,226	0
5	MPG	A	314	20/25	0.48	0.39	88,125,136,140	0
4	BOG	A	315	16/20	0.51	0.34	104,130,165,166	0
5	MPG	A	312	25/25	0.53	0.41	94,117,146,175	0
4	BOG	A	307	20/20	0.54	0.31	109,134,159,164	0
5	MPG	A	309	25/25	0.55	0.36	82,110,133,139	0
4	BOG	A	308	20/20	0.61	0.31	108,136,155,176	0
5	MPG	A	310	25/25	0.61	0.26	89,114,140,151	0
5	MPG	A	306	25/25	0.63	0.24	72,105,127,137	0
5	MPG	A	311	18/25	0.78	0.31	72,99,132,140	0
3	CL	A	302	1/1	0.95	0.08	49,49,49,49	0
2	RET	A	301	20/21	0.97	0.12	18,23,27,30	0
3	CL	A	317	1/1	0.97	0.18	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.

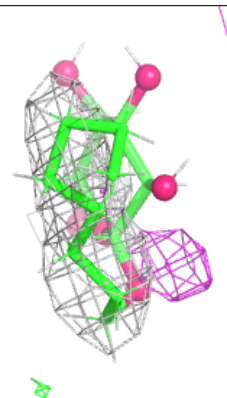
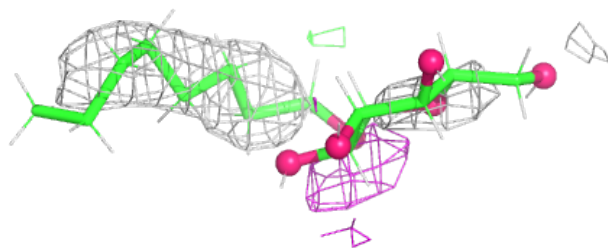
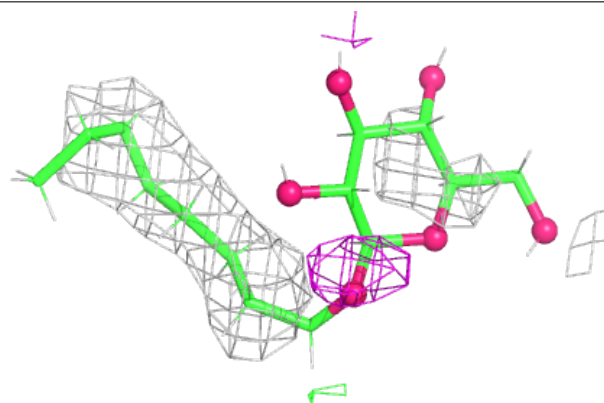


**Electron density around BOG A 303:**

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

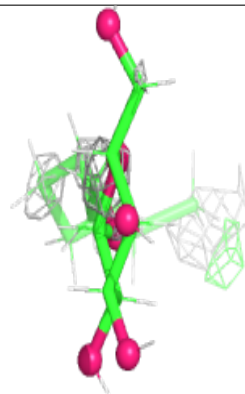
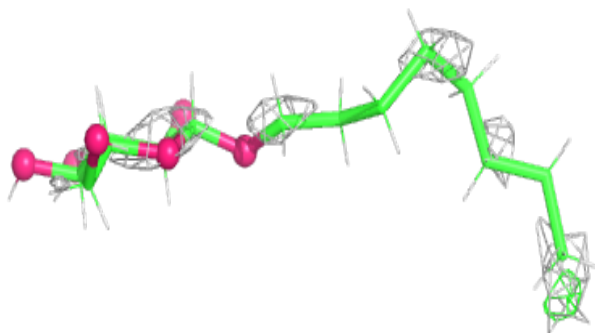
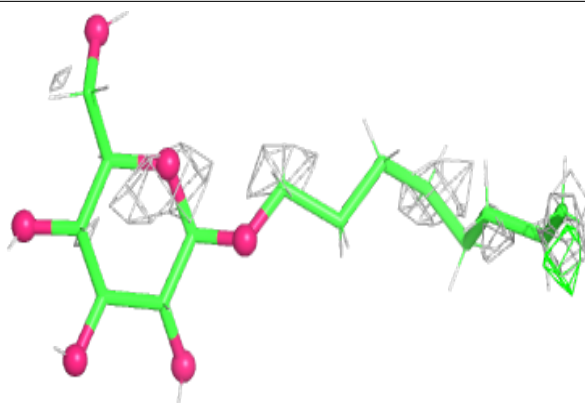
**Electron density around BOG A 305:**

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

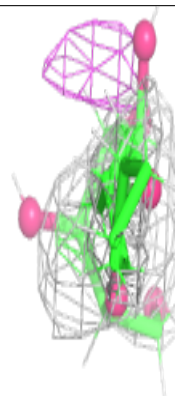
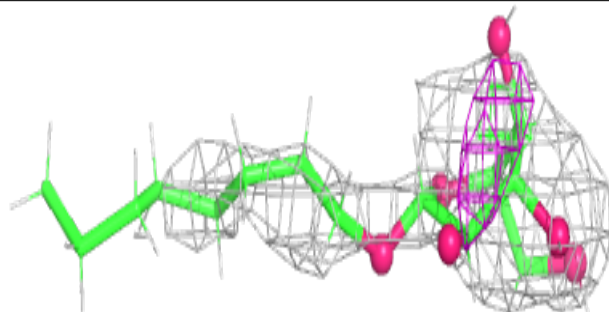
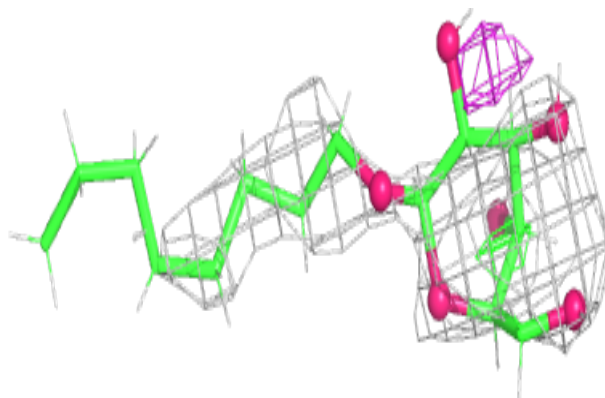


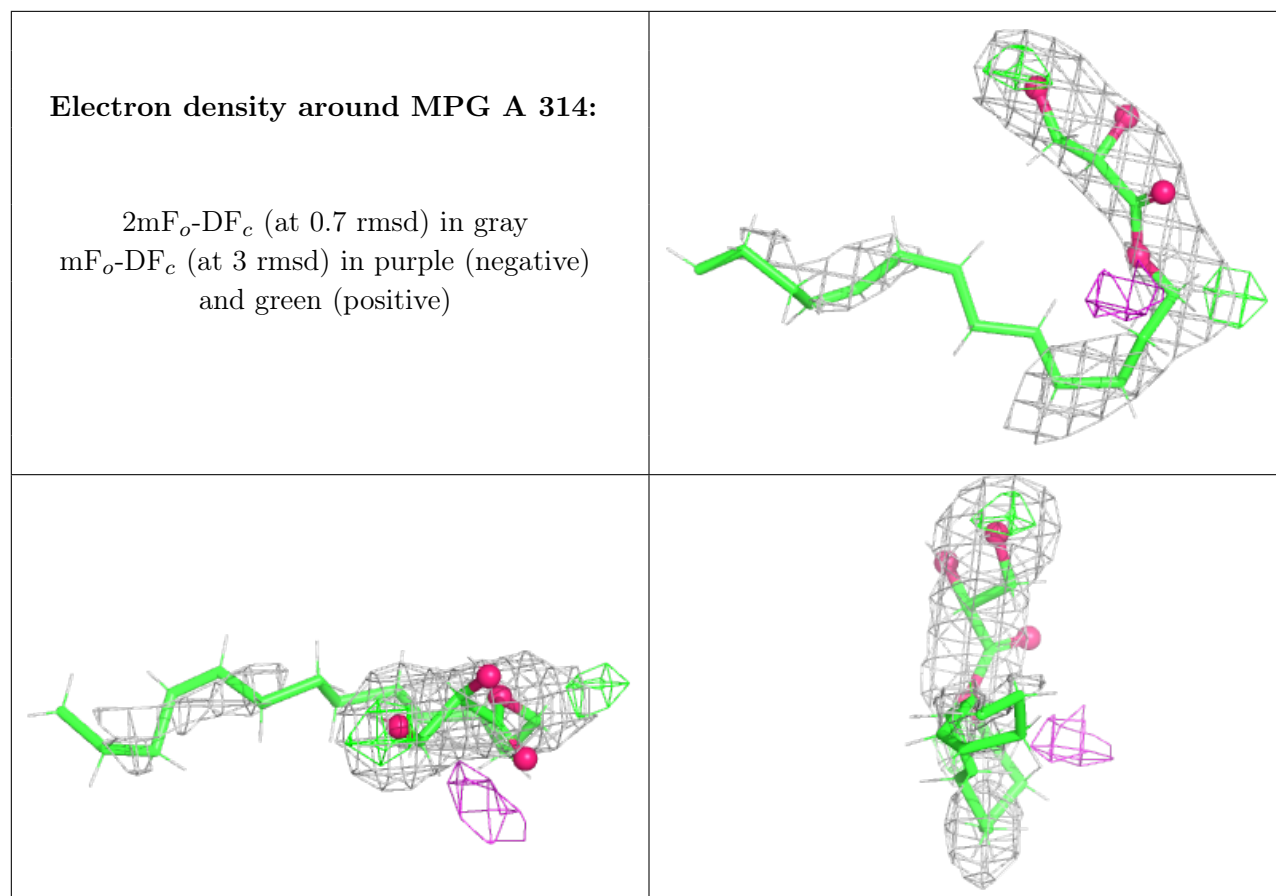
**Electron density around BOG A 313:**

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

**Electron density around BOG A 316:**

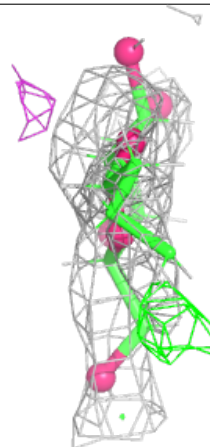
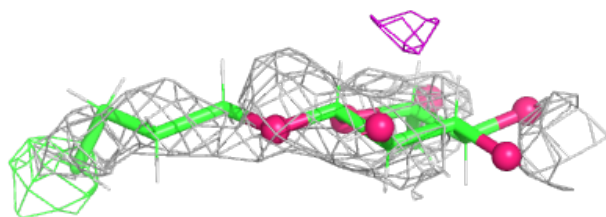
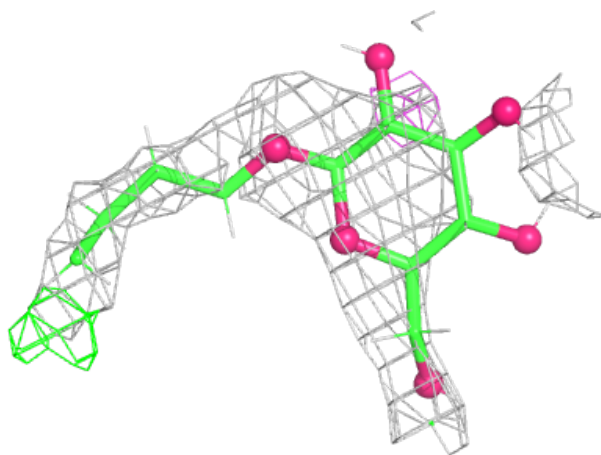
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





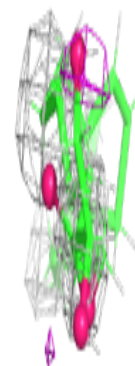
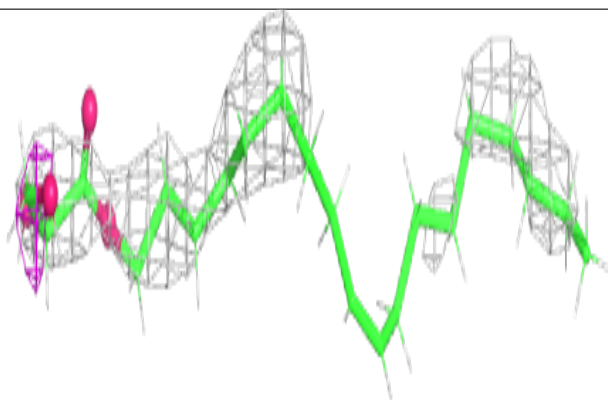
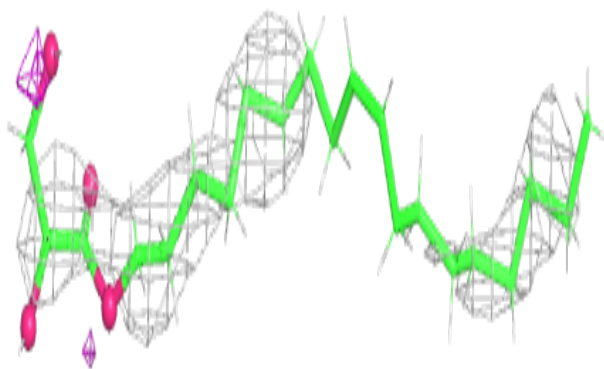
**Electron density around BOG A 315:**

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

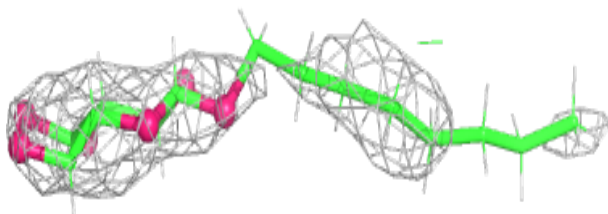
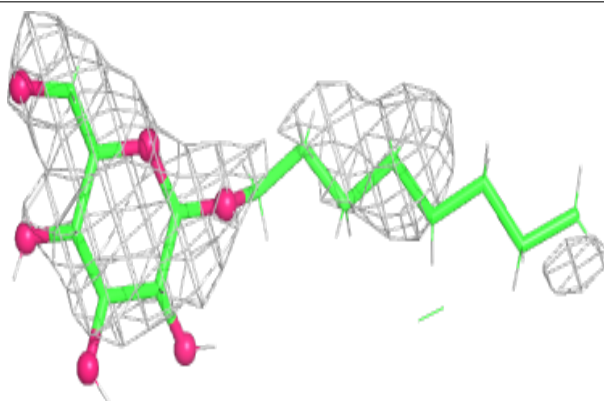


**Electron density around MPG A 312:**

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

**Electron density around BOG A 307:**

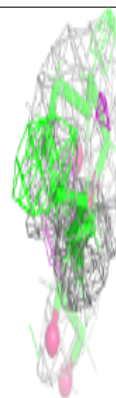
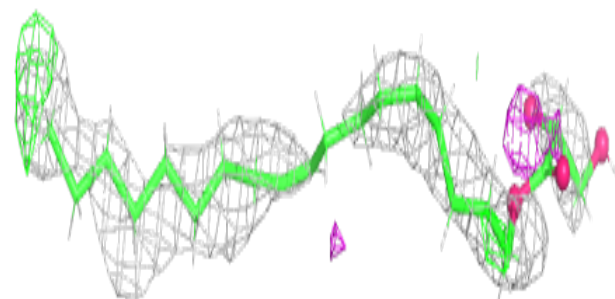
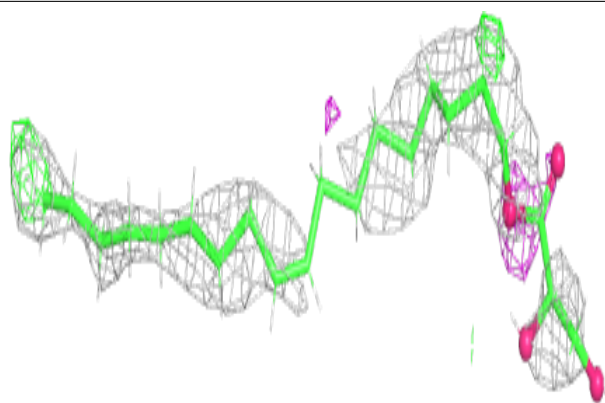
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



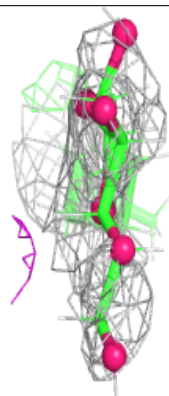
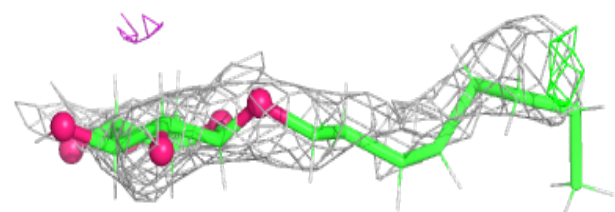
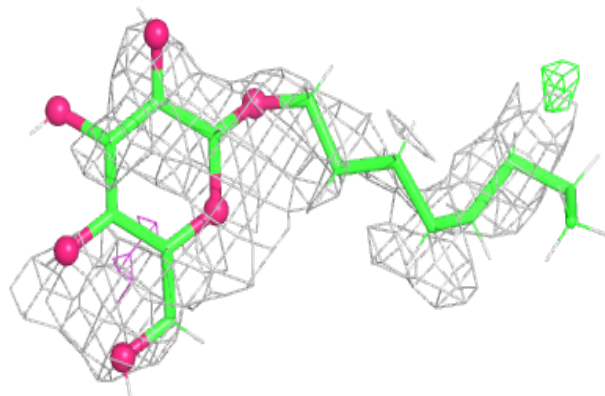


**Electron density around MPG A 309:**

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

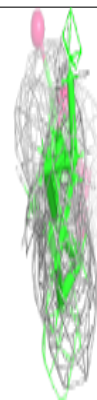
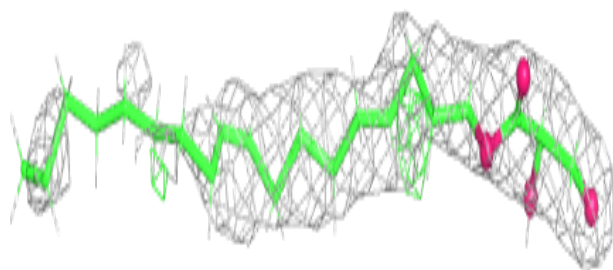
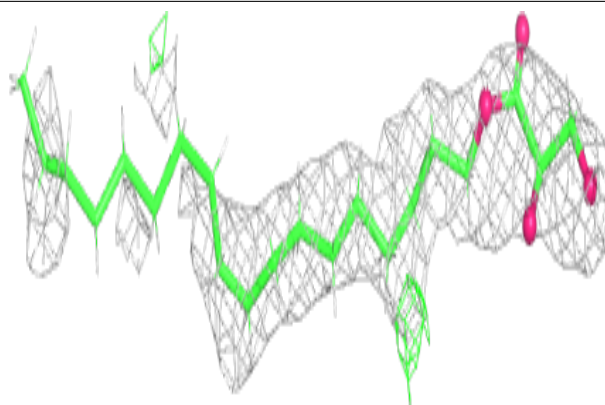
**Electron density around BOG A 308:**

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

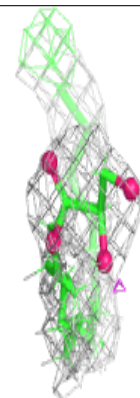
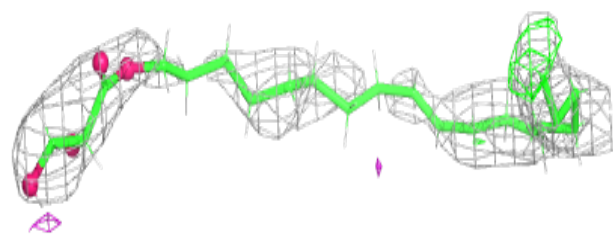
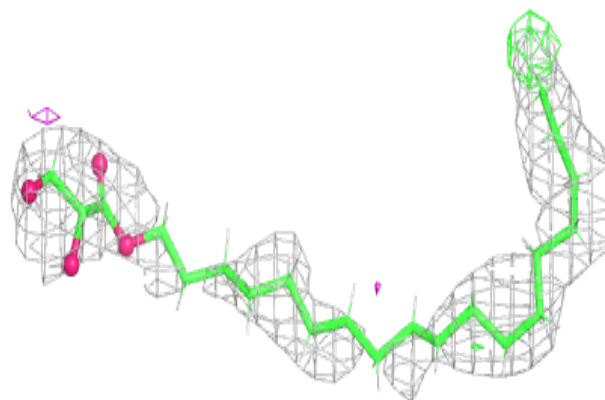


**Electron density around MPG A 310:**

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

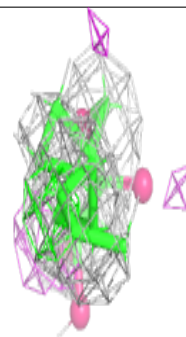
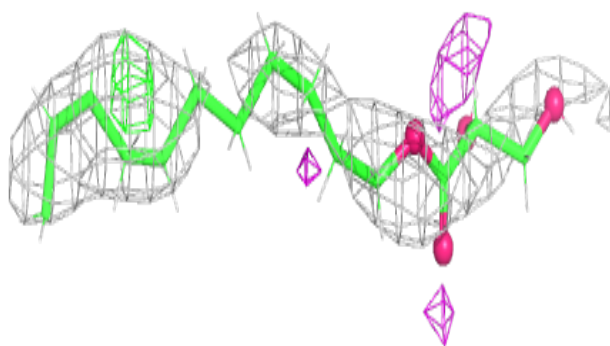
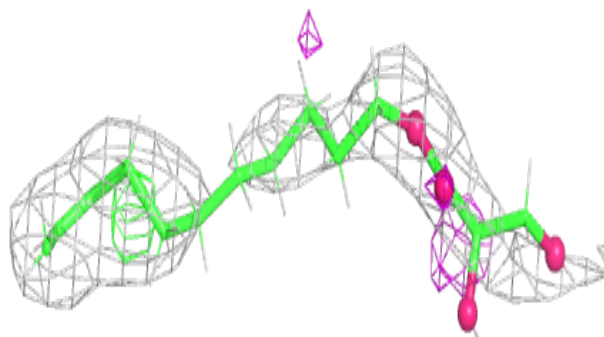
**Electron density around MPG A 306:**

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

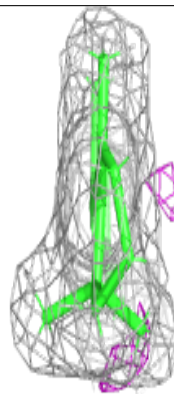
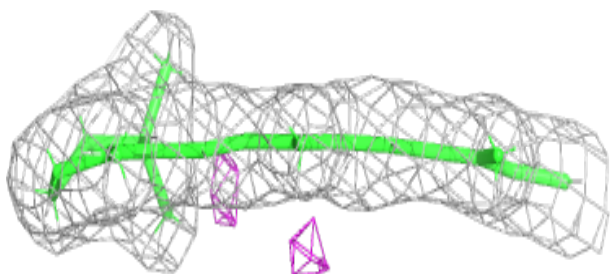
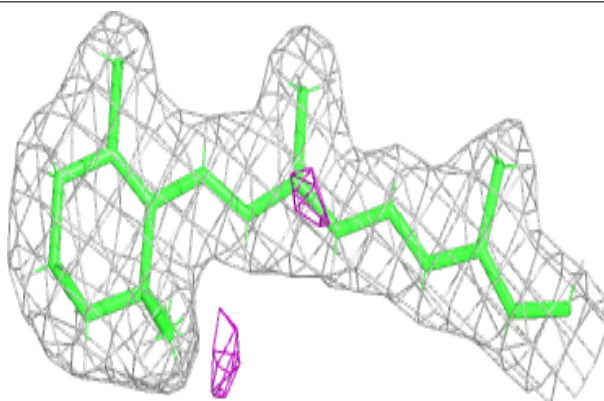


**Electron density around MPG A 311:**

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

**Electron density around RET 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 [i](#)

There are no such residues in this entry.