



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:57 PM BST

PDB ID : 4HYJ  
Title : Crystal structure of Exiguobacterium sibiricum rhodopsin  
Authors : Gushchin, I.; Chervakov, P.; Kuzmichev, P.; Popov, A.; Round, E.; Borshchevskiy, V.; Dolgikh, D.; Kirpichnikov, M.; Petrovskaya, L.; Chupin, V.; Arseniev, A.; Gordeliy, V.  
Deposited on : 2012-11-13  
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](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 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 : 2.13.1  
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) : 2.13.1

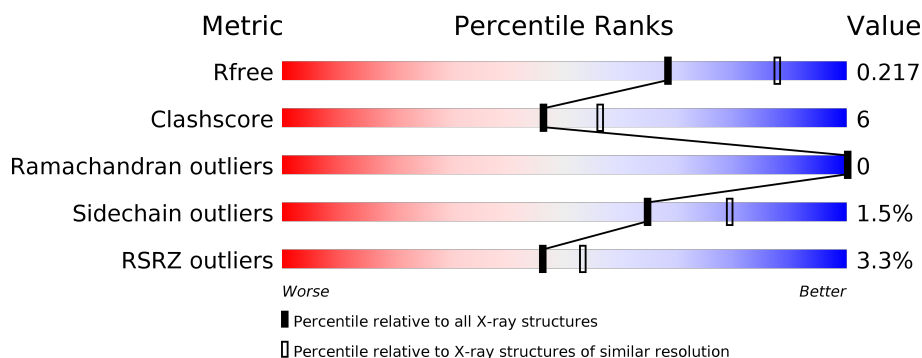
# 1 Overall quality at a glance

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  $\geq 3$ , 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	258	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
1	B	258	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3875 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.

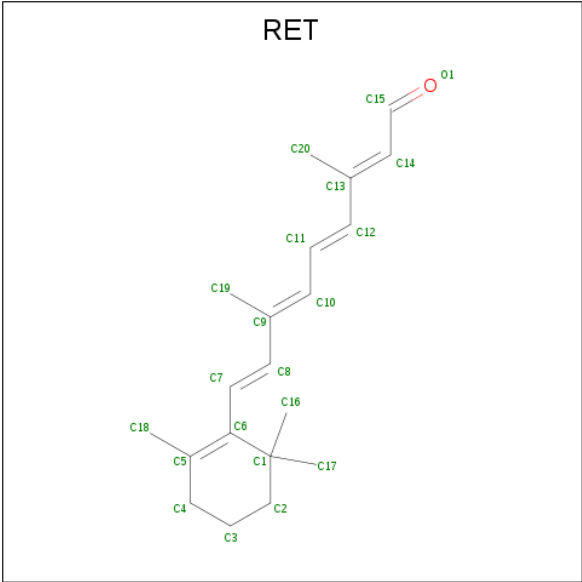
- Molecule 1 is a protein called Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1799	1218	272	303	6			
1	B	224	Total	C	N	O	S	0	1	0
			1700	1150	260	283	7			

There are 12 discrepancies between the modelled and reference sequences:

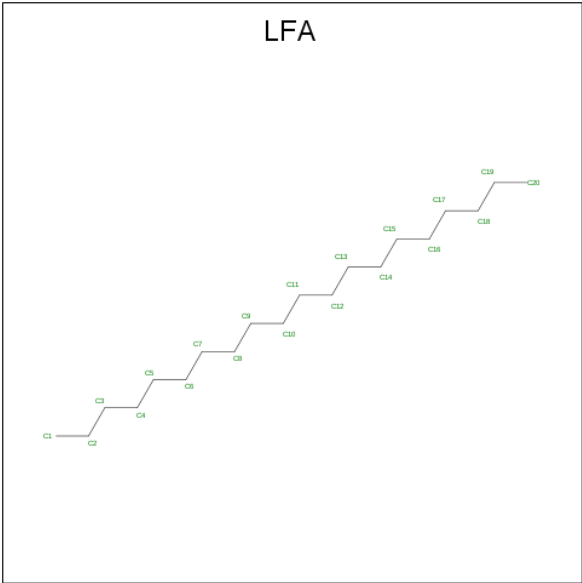
Chain	Residue	Modelled	Actual	Comment	Reference
A	253	HIS	-	EXPRESSION TAG	UNP B1YFV8
A	254	HIS	-	EXPRESSION TAG	UNP B1YFV8
A	255	HIS	-	EXPRESSION TAG	UNP B1YFV8
A	256	HIS	-	EXPRESSION TAG	UNP B1YFV8
A	257	HIS	-	EXPRESSION TAG	UNP B1YFV8
A	258	HIS	-	EXPRESSION TAG	UNP B1YFV8
B	253	HIS	-	EXPRESSION TAG	UNP B1YFV8
B	254	HIS	-	EXPRESSION TAG	UNP B1YFV8
B	255	HIS	-	EXPRESSION TAG	UNP B1YFV8
B	256	HIS	-	EXPRESSION TAG	UNP B1YFV8
B	257	HIS	-	EXPRESSION TAG	UNP B1YFV8
B	258	HIS	-	EXPRESSION TAG	UNP B1YFV8

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	B	1	Total C 20 20	0	0

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 9 9	0	0
3	A	1	Total C 10 10	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 18 18	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 6 6	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 8 8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 8 8	0	0

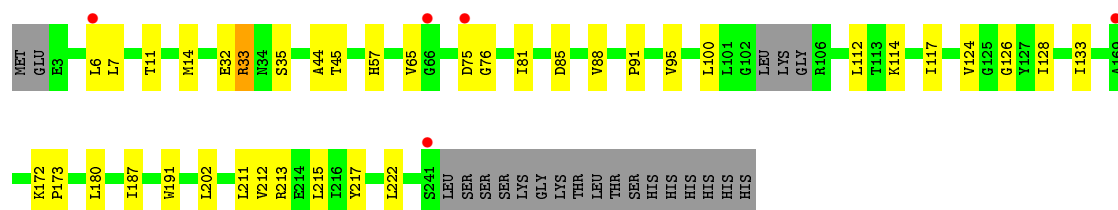
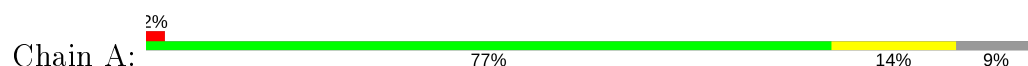
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	21	Total O 21 21	0	0

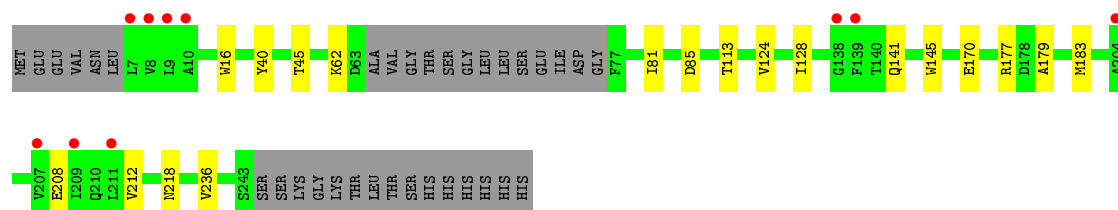
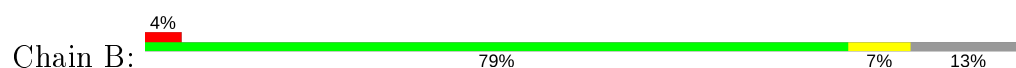
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Rhodopsin



#### • Molecule 1: Rhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.10 Å 96.10 Å 124.38 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.17 – 2.30 69.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (69.17-2.30) 97.5 (69.17-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.175 , 0.215 0.177 , 0.217	Depositor DCC
$R_{free}$ test set	1498 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, RET

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	0.39	0/1846	0.52	0/2524
1	B	0.40	0/1747	0.53	0/2387
All	All	0.39	0/3593	0.52	0/4911

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	1799	0	1805	29	0
1	B	1700	0	1700	16	0
2	A	20	0	27	3	0
2	B	20	0	27	3	0
3	A	129	0	246	7	0
3	B	174	0	330	7	0
4	A	12	0	0	0	0
4	B	21	0	0	0	0
All	All	3875	0	4135	50	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 6.

All (50) 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)
2:B:301:RET:H161	2:B:301:RET:H8	1.62	0.80
1:A:114:LYS:HG2	3:A:306:LFA:H41	1.70	0.73
2:A:301:RET:H161	2:A:301:RET:H8	1.71	0.72
1:A:75:ASP:OD2	1:A:76:GLY:N	2.29	0.65
1:A:7:LEU:O	1:A:11:THR:HG23	1.97	0.64
3:A:304:LFA:H151	1:B:81:ILE:HG23	1.81	0.62
1:A:91:PRO:O	1:A:95:VAL:HG23	2.00	0.62
3:B:305:LFA:H41	3:B:319:LFA:H22	1.84	0.59
1:A:88:VAL:HG11	3:A:305:LFA:H21	1.85	0.58
1:A:117:ILE:HD11	1:B:128:ILE:HD11	1.84	0.58
1:B:179:ALA:C	1:B:183:MET:HE2	2.28	0.54
1:A:45:THR:HG21	3:A:304:LFA:H82	1.89	0.52
1:A:11:THR:HG21	1:A:211:LEU:HB3	1.90	0.51
1:B:124:VAL:O	1:B:128:ILE:HG12	2.10	0.51
3:B:316:LFA:H41	3:B:318:LFA:H32	1.91	0.51
1:A:14:MET:HG3	1:A:215:LEU:HD22	1.93	0.51
1:B:179:ALA:O	1:B:183:MET:HE2	2.12	0.50
1:B:40:TYR:HB3	1:B:236:VAL:HB	1.94	0.50
1:B:16:TRP:CD2	3:B:318:LFA:H52	2.46	0.50
1:A:95:VAL:HG21	3:B:302:LFA:H92	1.94	0.49
1:A:95:VAL:HG22	1:A:112:LEU:HD11	1.96	0.48
1:A:100:LEU:HB2	1:A:180:LEU:HD21	1.96	0.48
1:A:117:ILE:HD11	1:B:128:ILE:CD1	2.44	0.47
2:A:301:RET:H181	2:A:301:RET:H7	1.59	0.47
1:B:141:GLN:HG2	1:B:145:TRP:NE1	2.29	0.47
1:A:124:VAL:O	1:A:128:ILE:HG12	2.14	0.47
1:A:128:ILE:HD12	1:B:113:THR:HG23	1.96	0.47
1:A:212:VAL:HG21	3:A:308:LFA:H81	1.96	0.46
1:A:88:VAL:O	1:A:91:PRO:HD2	2.16	0.45
1:A:124:VAL:HG21	3:A:311:LFA:H42	1.98	0.45
1:B:45:THR:HG23	3:B:303:LFA:H12	1.98	0.45
1:B:85:ASP:C	1:B:85:ASP:OD2	2.55	0.45
1:A:117:ILE:CD1	1:B:128:ILE:HD11	2.48	0.44
1:A:133:ILE:HD11	1:A:202:LEU:HD13	1.99	0.44
1:A:126:GLY:HA3	2:A:301:RET:H163	2.00	0.43
2:B:301:RET:H181	2:B:301:RET:H7	1.76	0.43
3:B:307:LFA:H22	3:B:308:LFA:H21	2.00	0.43
3:A:304:LFA:H71	3:A:304:LFA:H42	1.71	0.43
1:A:57:HIS:CD2	1:A:81:ILE:HG22	2.53	0.43
1:B:16:TRP:CE3	3:B:318:LFA:H52	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HD2	1:A:217:TYR:CZ	2.54	0.42
1:B:170:GLU:CD	1:B:177:ARG:HE	2.23	0.42
1:A:32:GLU:O	1:A:35:SER:HB3	2.19	0.42
1:A:187:ILE:O	1:A:191:TRP:HB2	2.19	0.42
1:A:33:ARG:HG3	1:A:44:ALA:HB3	2.02	0.42
1:B:208:GLU:O	1:B:212:VAL:HG13	2.20	0.41
1:A:172:LYS:HD3	1:A:173:PRO:HD2	2.02	0.41
1:A:85:ASP:OD2	1:A:85:ASP:C	2.58	0.41
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.92	0.40
2:B:301:RET:H191	2:B:301:RET:H11	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/258 (90%)	227 (98%)	5 (2%)	0	100	100
1	B	221/258 (86%)	218 (99%)	3 (1%)	0	100	100
All	All	453/516 (88%)	445 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/213 (82%)	171 (98%)	3 (2%)	60	76
1	B	161/213 (76%)	159 (99%)	2 (1%)	71	84
All	All	335/426 (79%)	330 (98%)	5 (2%)	65	79

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

Mol	Chain	Res	Type
1	A	6	LEU
1	A	33	ARG
1	A	65	VAL
1	B	62	LYS
1	B	218	ASN

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	B	316	-	5,5,19	0.24	0	4,4,18	0.38	0
3	LFA	B	302	-	13,13,19	0.20	0	12,12,18	0.79	0
3	LFA	A	311	-	9,9,19	0.27	0	8,8,18	0.43	0
3	LFA	A	310	-	9,9,19	0.28	0	8,8,18	0.42	0
3	LFA	B	306	-	7,7,19	0.26	0	6,6,18	0.48	0
3	LFA	B	307	-	9,9,19	0.31	0	8,8,18	0.39	0
2	RET	A	301	1	20,20,21	0.80	0	27,27,28	3.66	15 (55%)
3	LFA	A	313	-	5,5,19	0.30	0	4,4,18	0.26	0
3	LFA	A	307	-	13,13,19	0.29	0	12,12,18	0.48	0
3	LFA	B	313	-	7,7,19	0.28	0	6,6,18	0.41	0
3	LFA	B	310	-	7,7,19	0.26	0	6,6,18	0.41	0
3	LFA	B	318	-	11,11,19	0.25	0	10,10,18	0.50	0
3	LFA	B	317	-	5,5,19	0.24	0	4,4,18	0.42	0
3	LFA	B	312	-	7,7,19	0.27	0	6,6,18	0.48	0
3	LFA	A	308	-	9,9,19	0.30	0	8,8,18	0.39	0
3	LFA	B	305	-	11,11,19	0.29	0	10,10,18	0.45	0
3	LFA	B	311	-	7,7,19	0.26	0	6,6,18	0.48	0
3	LFA	B	309	-	13,13,19	0.30	0	12,12,18	0.49	0
3	LFA	B	308	-	11,11,19	0.28	0	10,10,18	0.64	0
3	LFA	B	315	-	7,7,19	0.28	0	6,6,18	0.35	0
3	LFA	B	319	-	7,7,19	0.31	0	6,6,18	0.39	0
3	LFA	B	314	-	9,9,19	0.26	0	8,8,18	0.55	0
3	LFA	A	309	-	7,7,19	0.31	0	6,6,18	0.37	0
3	LFA	A	304	-	17,17,19	0.27	0	16,16,18	0.60	0
3	LFA	A	302	-	8,8,19	0.28	0	7,7,18	0.51	0
3	LFA	A	303	-	9,9,19	0.27	0	8,8,18	0.48	0
3	LFA	A	306	-	13,13,19	0.25	0	12,12,18	0.55	0
3	LFA	B	303	-	11,11,19	0.29	0	10,10,18	0.45	0
3	LFA	A	312	-	5,5,19	0.26	0	4,4,18	0.37	0
3	LFA	A	305	-	13,13,19	0.30	0	12,12,18	0.67	0
3	LFA	B	304	-	9,9,19	0.27	0	8,8,18	0.51	0
2	RET	B	301	1	20,20,21	0.76	0	27,27,28	3.79	12 (44%)

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
3	LFA	B	316	-	-	0/3/3/17	-
3	LFA	B	302	-	-	5/11/11/17	-
3	LFA	A	311	-	-	3/7/7/17	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	310	-	-	0/7/7/17	-
3	LFA	B	306	-	-	0/5/5/17	-
3	LFA	B	307	-	-	4/7/7/17	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	LFA	A	313	-	-	1/3/3/17	-
3	LFA	A	307	-	-	5/11/11/17	-
3	LFA	B	313	-	-	0/5/5/17	-
3	LFA	B	310	-	-	1/5/5/17	-
3	LFA	B	318	-	-	4/9/9/17	-
3	LFA	B	317	-	-	0/3/3/17	-
3	LFA	B	312	-	-	0/5/5/17	-
3	LFA	A	308	-	-	2/7/7/17	-
3	LFA	B	305	-	-	2/9/9/17	-
3	LFA	B	311	-	-	2/5/5/17	-
3	LFA	B	309	-	-	4/11/11/17	-
3	LFA	B	308	-	-	0/9/9/17	-
3	LFA	B	315	-	-	3/5/5/17	-
3	LFA	B	319	-	-	2/5/5/17	-
3	LFA	B	314	-	-	2/7/7/17	-
3	LFA	A	309	-	-	0/5/5/17	-
3	LFA	A	304	-	-	6/15/15/17	-
3	LFA	A	302	-	-	1/6/6/17	-
3	LFA	A	303	-	-	3/7/7/17	-
3	LFA	A	306	-	-	3/11/11/17	-
3	LFA	B	303	-	-	2/9/9/17	-
3	LFA	A	312	-	-	1/3/3/17	-
3	LFA	A	305	-	-	1/11/11/17	-
3	LFA	B	304	-	-	3/7/7/17	-
2	RET	B	301	1	-	3/13/30/31	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C17-C1-C6	-11.05	92.38	110.30
2	A	301	RET	C17-C1-C6	-10.00	94.08	110.30
2	B	301	RET	C16-C1-C6	8.55	124.16	110.30
2	A	301	RET	C16-C1-C6	8.01	123.28	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C17-C1-C16	-7.06	86.86	108.53
2	A	301	RET	C17-C1-C16	-6.68	88.03	108.53
2	A	301	RET	C17-C1-C2	-5.35	87.52	108.91
2	B	301	RET	C17-C1-C2	-5.16	88.26	108.91
2	B	301	RET	C1-C6-C5	-5.11	115.42	122.61
2	A	301	RET	C1-C6-C5	-4.49	116.29	122.61
2	A	301	RET	C1-C6-C7	4.05	127.24	115.78
2	B	301	RET	C1-C6-C7	3.91	126.85	115.78
2	A	301	RET	C3-C2-C1	-3.80	101.00	114.60
2	A	301	RET	C18-C5-C6	-3.74	120.33	124.53
2	B	301	RET	C11-C10-C9	-3.37	122.50	127.31
2	B	301	RET	C3-C2-C1	-3.34	102.67	114.60
2	B	301	RET	C18-C5-C6	-3.33	120.79	124.53
2	A	301	RET	C16-C1-C2	3.14	121.48	108.91
2	A	301	RET	C2-C1-C6	3.09	115.23	110.48
2	B	301	RET	C2-C1-C6	3.08	115.22	110.48
2	A	301	RET	C11-C10-C9	-2.94	123.11	127.31
2	B	301	RET	C16-C1-C2	2.91	120.56	108.91
2	A	301	RET	C7-C8-C9	-2.28	122.79	126.23
2	A	301	RET	C7-C6-C5	-2.21	116.11	121.46
2	A	301	RET	C10-C11-C12	-2.18	116.41	123.22
2	B	301	RET	C20-C13-C12	2.11	121.41	118.08
2	A	301	RET	C20-C13-C12	2.04	121.29	118.08

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	RET	C7-C8-C9-C19
3	B	302	LFA	C6-C7-C8-C9
3	B	304	LFA	C4-C5-C6-C7
3	B	307	LFA	C2-C3-C4-C5
3	B	319	LFA	C4-C5-C6-C7
3	B	314	LFA	C3-C4-C5-C6
3	A	306	LFA	C7-C8-C9-C10
3	B	302	LFA	C3-C4-C5-C6
3	A	311	LFA	C6-C7-C8-C9
3	A	307	LFA	C9-C10-C11-C12
3	B	305	LFA	C4-C5-C6-C7
3	B	304	LFA	C3-C4-C5-C6
3	B	318	LFA	C6-C7-C8-C9
3	B	302	LFA	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	309	LFA	C2-C3-C4-C5
3	A	304	LFA	C10-C11-C12-C13
3	A	304	LFA	C2-C3-C4-C5
3	B	318	LFA	C7-C8-C9-C10
3	A	305	LFA	C3-C4-C5-C6
3	A	311	LFA	C5-C6-C7-C8
3	A	306	LFA	C11-C10-C9-C8
3	A	307	LFA	C11-C10-C9-C8
3	B	305	LFA	C3-C4-C5-C6
3	A	302	LFA	C6-C7-C8-C9
3	A	308	LFA	C6-C7-C8-C9
3	A	304	LFA	C11-C10-C9-C8
3	B	309	LFA	C6-C7-C8-C9
3	A	307	LFA	C11-C12-C13-C14
3	B	311	LFA	C3-C4-C5-C6
3	B	315	LFA	C1-C2-C3-C4
3	A	304	LFA	C7-C8-C9-C10
3	B	303	LFA	C3-C4-C5-C6
3	A	313	LFA	C1-C2-C3-C4
3	B	318	LFA	C11-C10-C9-C8
3	A	308	LFA	C5-C6-C7-C8
3	A	307	LFA	C3-C4-C5-C6
3	A	307	LFA	C7-C8-C9-C10
3	A	306	LFA	C10-C11-C12-C13
3	B	310	LFA	C4-C5-C6-C7
3	A	304	LFA	C1-C2-C3-C4
3	B	302	LFA	C2-C3-C4-C5
3	A	303	LFA	C4-C5-C6-C7
3	B	314	LFA	C5-C6-C7-C8
3	A	304	LFA	C4-C5-C6-C7
3	B	319	LFA	C2-C3-C4-C5
3	B	304	LFA	C7-C8-C9-C10
3	B	307	LFA	C4-C5-C6-C7
3	B	315	LFA	C2-C3-C4-C5
3	A	312	LFA	C3-C4-C5-C6
3	B	307	LFA	C6-C7-C8-C9
3	B	311	LFA	C2-C3-C4-C5
3	B	318	LFA	C5-C6-C7-C8
3	B	309	LFA	C7-C8-C9-C10
2	B	301	RET	C7-C8-C9-C10
3	B	309	LFA	C9-C10-C11-C12
3	B	303	LFA	C1-C2-C3-C4

*Continued on next page...*

*Continued from previous page...*

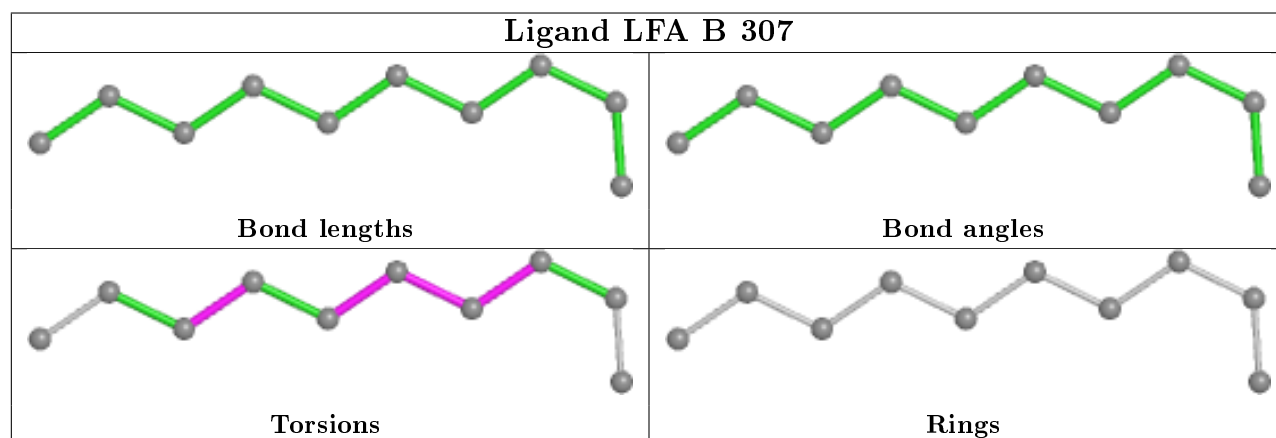
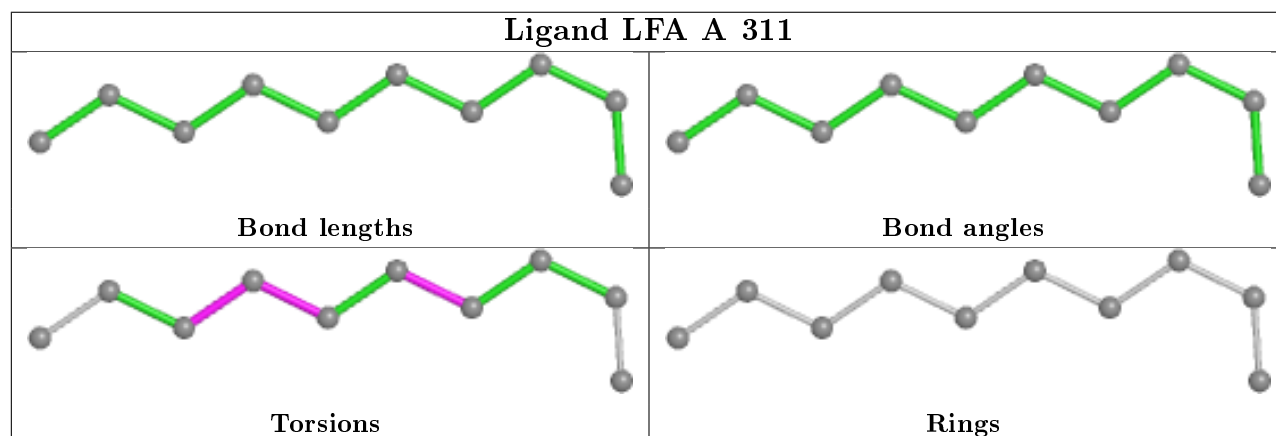
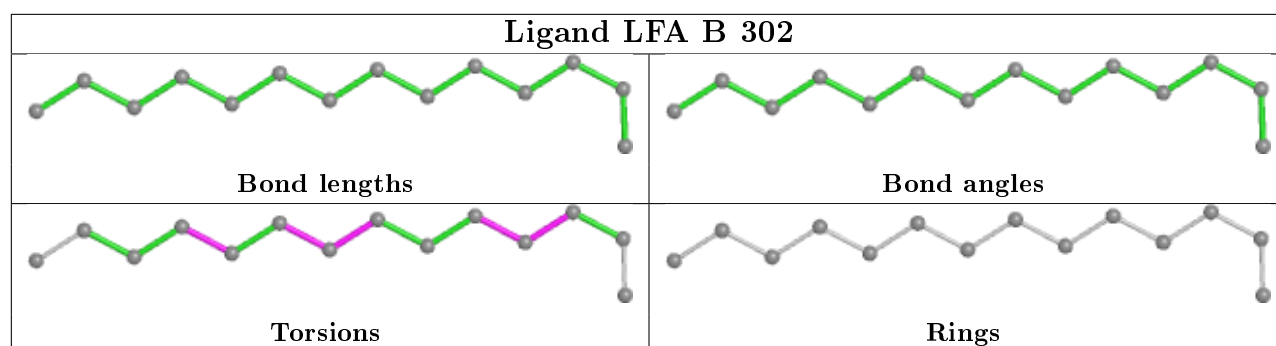
Mol	Chain	Res	Type	Atoms
3	B	302	LFA	C9-C10-C11-C12
3	B	315	LFA	C5-C6-C7-C8
3	A	303	LFA	C2-C3-C4-C5
3	A	311	LFA	C3-C4-C5-C6
2	B	301	RET	C5-C6-C7-C8
3	B	307	LFA	C3-C4-C5-C6
3	A	303	LFA	C1-C2-C3-C4

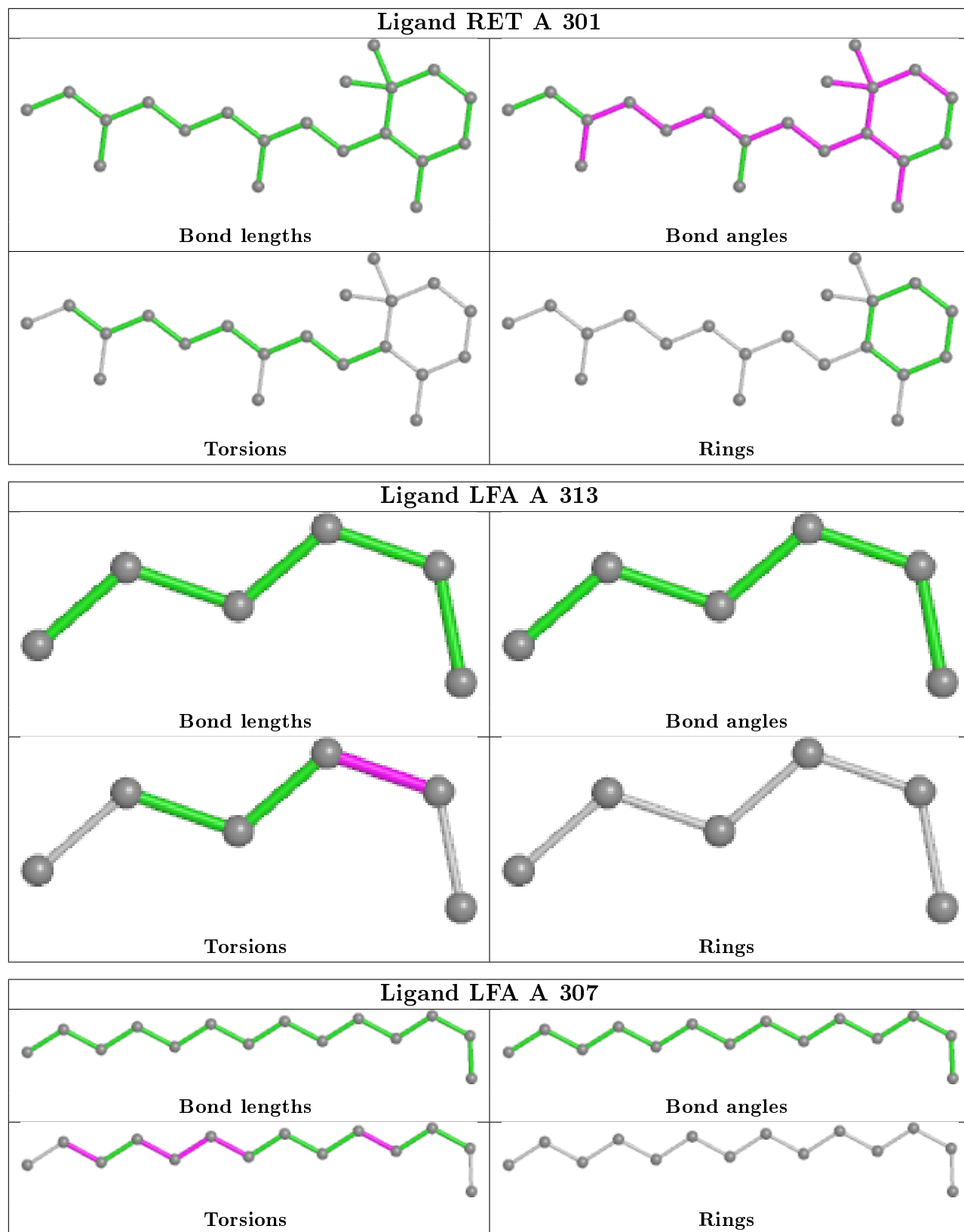
There are no ring outliers.

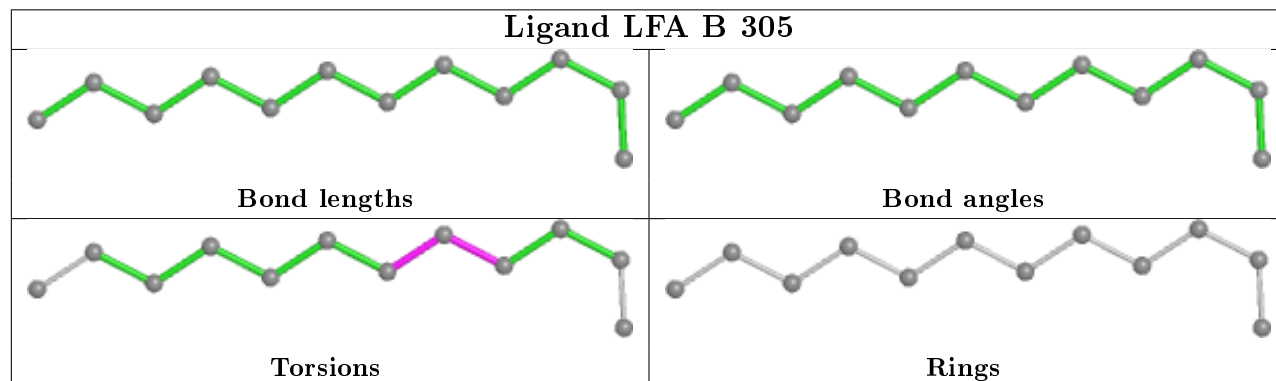
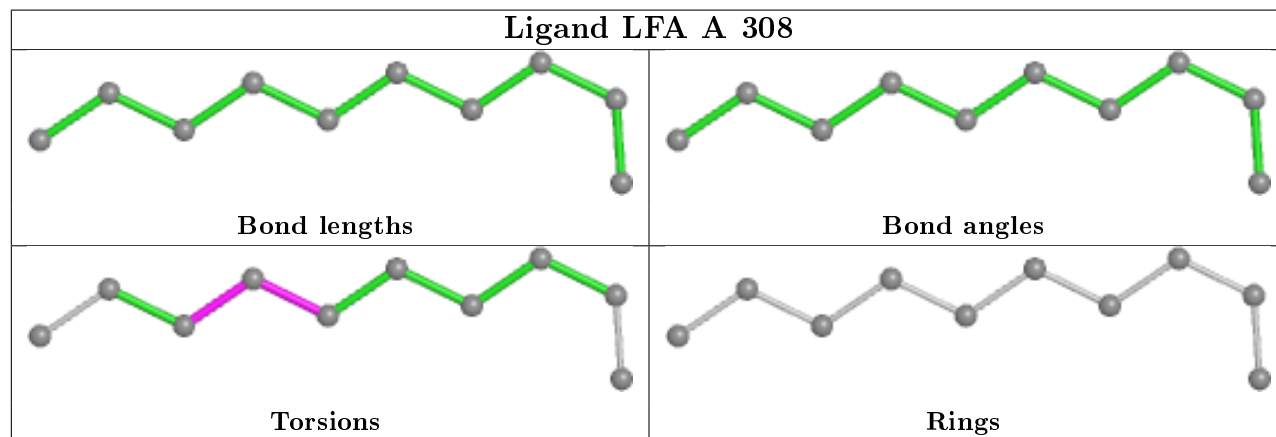
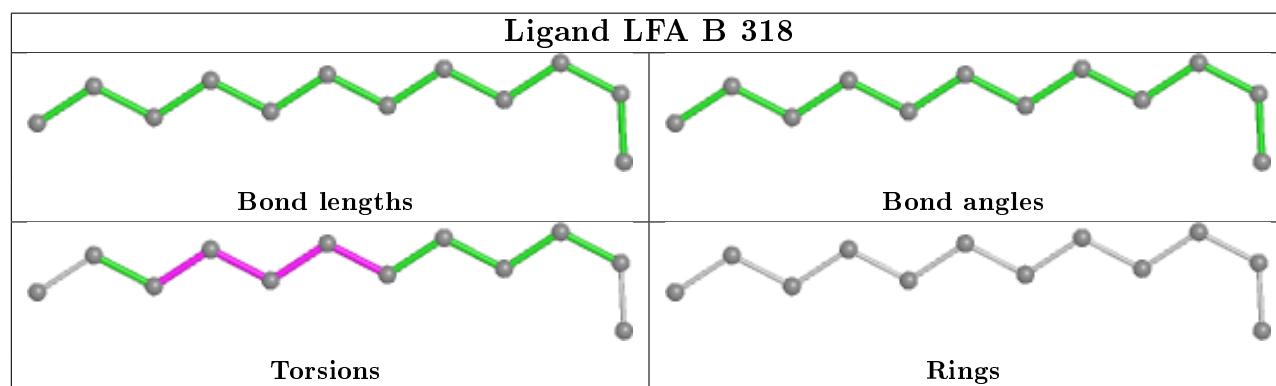
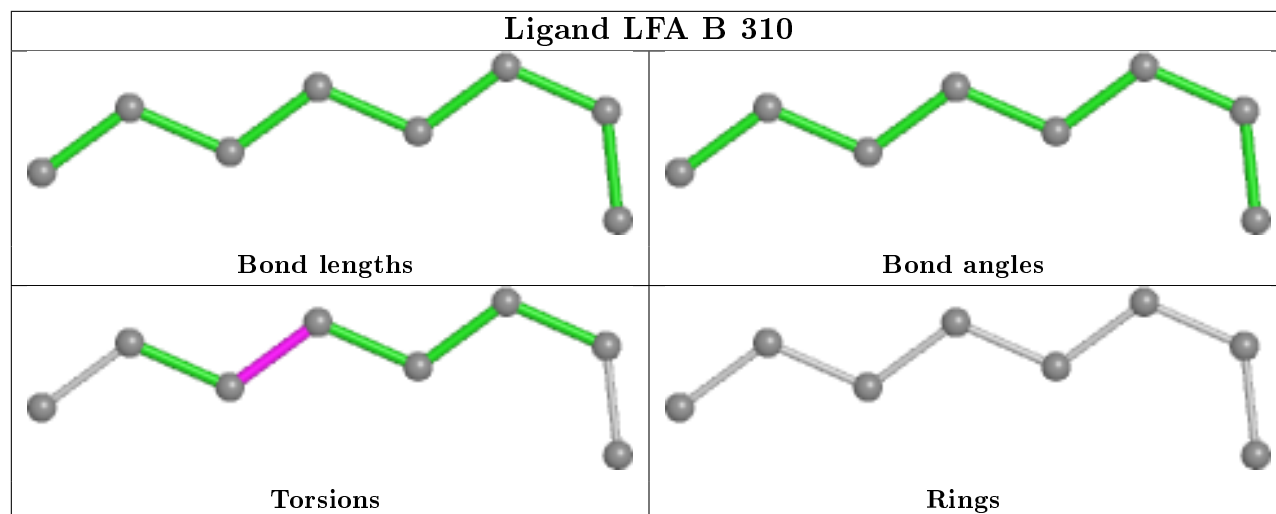
15 monomers are involved in 20 short contacts:

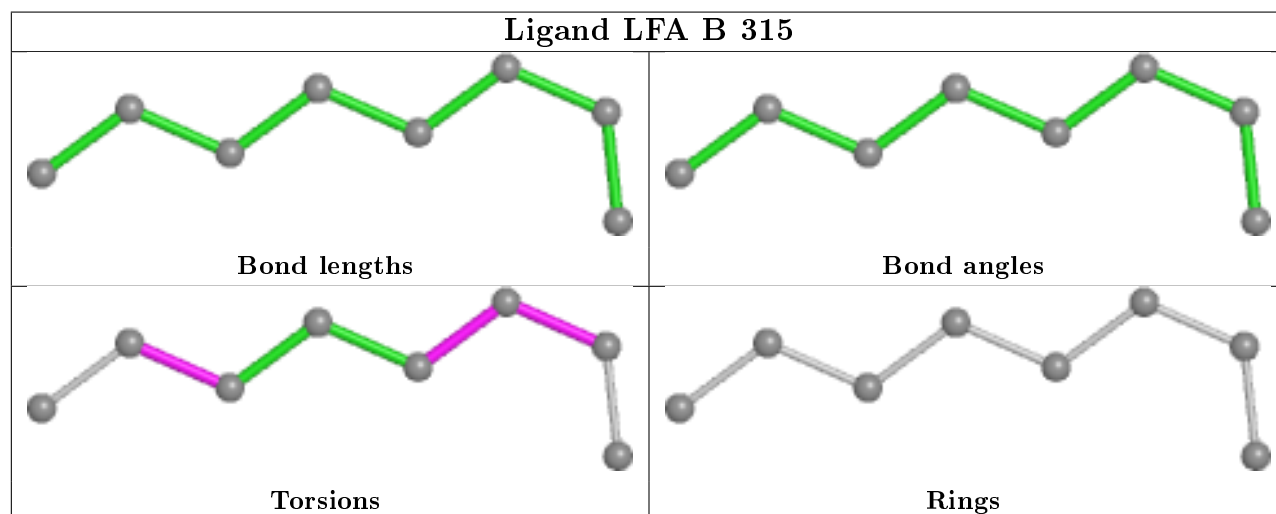
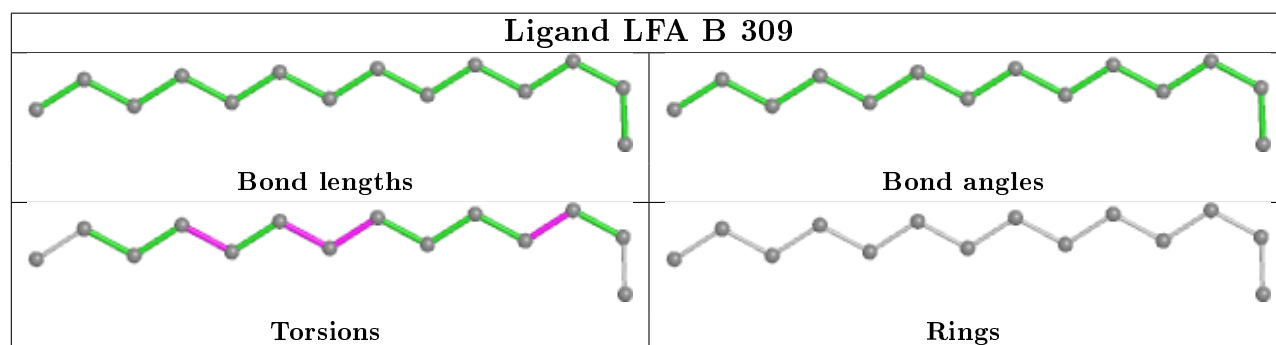
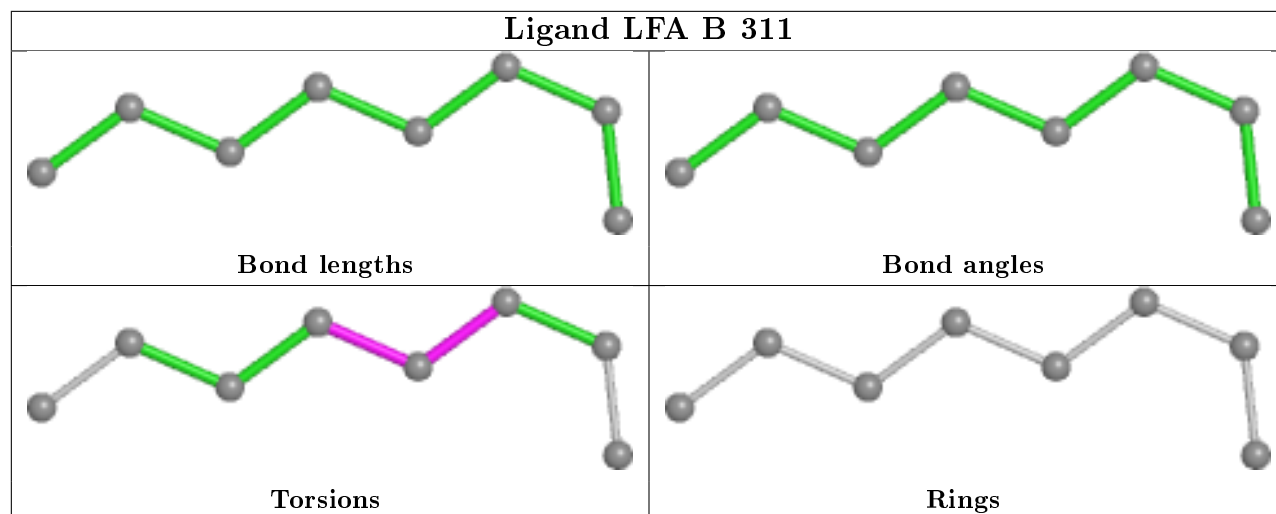
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	316	LFA	1	0
3	B	302	LFA	1	0
3	A	311	LFA	1	0
3	B	307	LFA	1	0
2	A	301	RET	3	0
3	B	318	LFA	3	0
3	A	308	LFA	1	0
3	B	305	LFA	1	0
3	B	308	LFA	1	0
3	B	319	LFA	1	0
3	A	304	LFA	3	0
3	A	306	LFA	1	0
3	B	303	LFA	1	0
3	A	305	LFA	1	0
2	B	301	RET	3	0

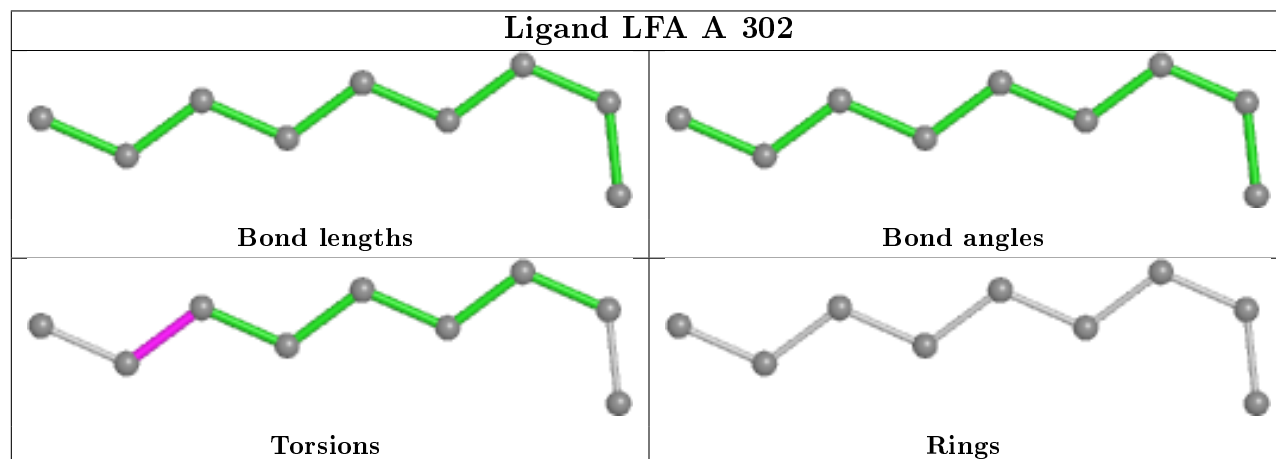
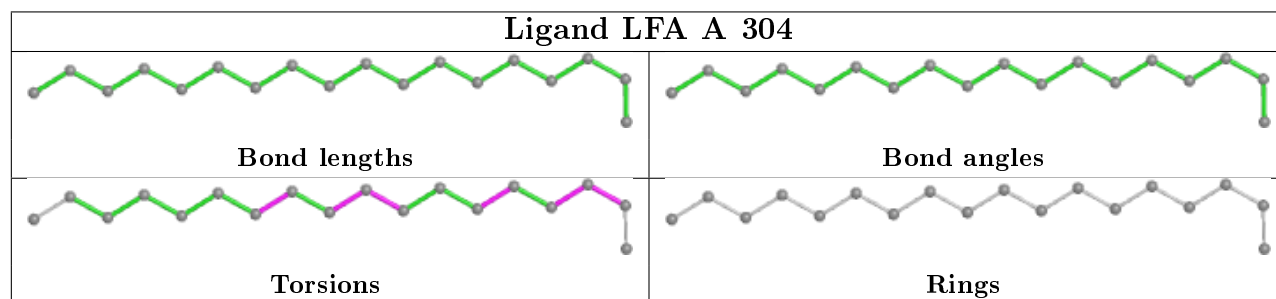
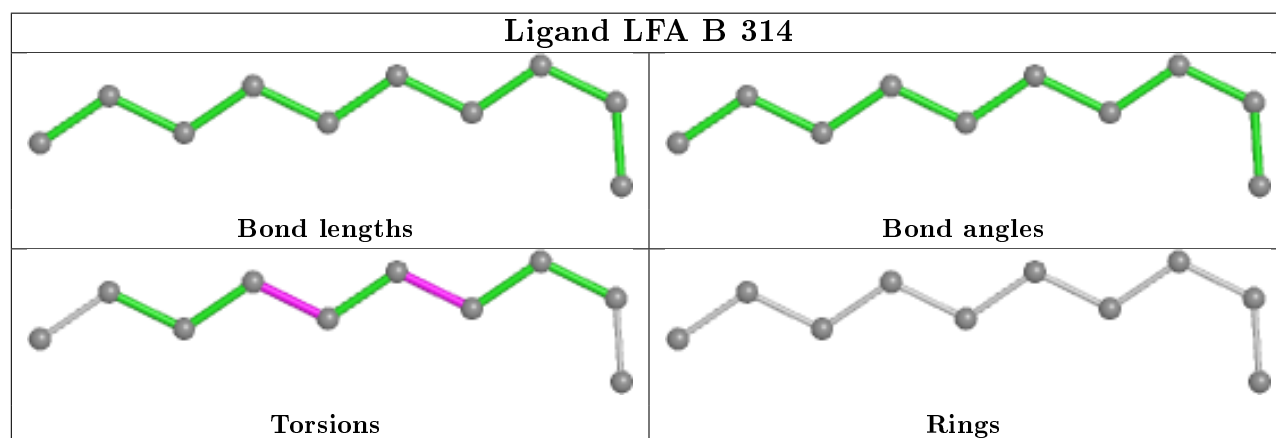
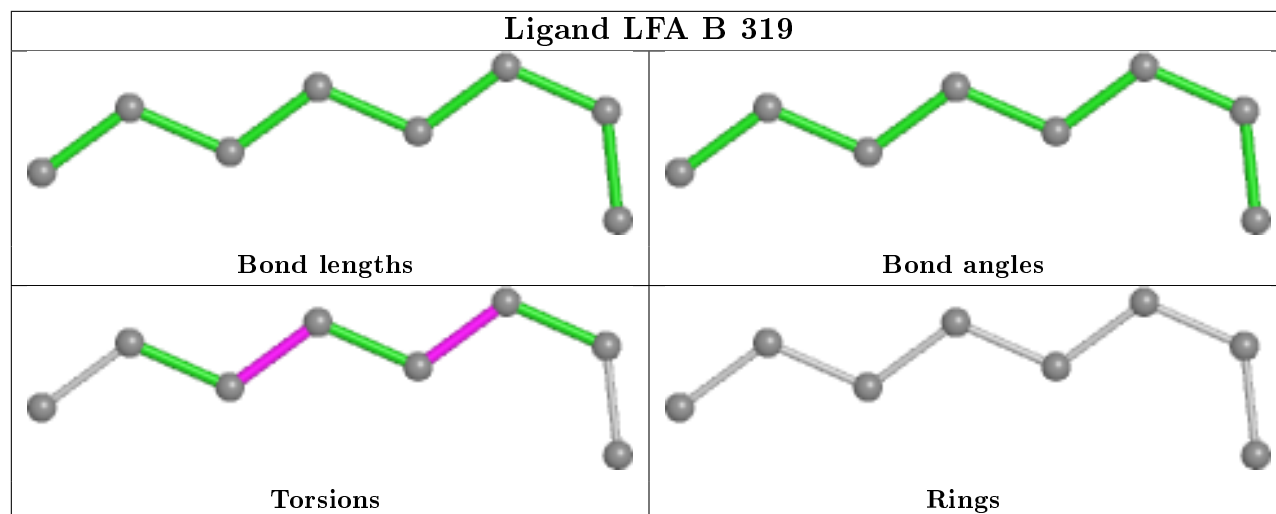
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

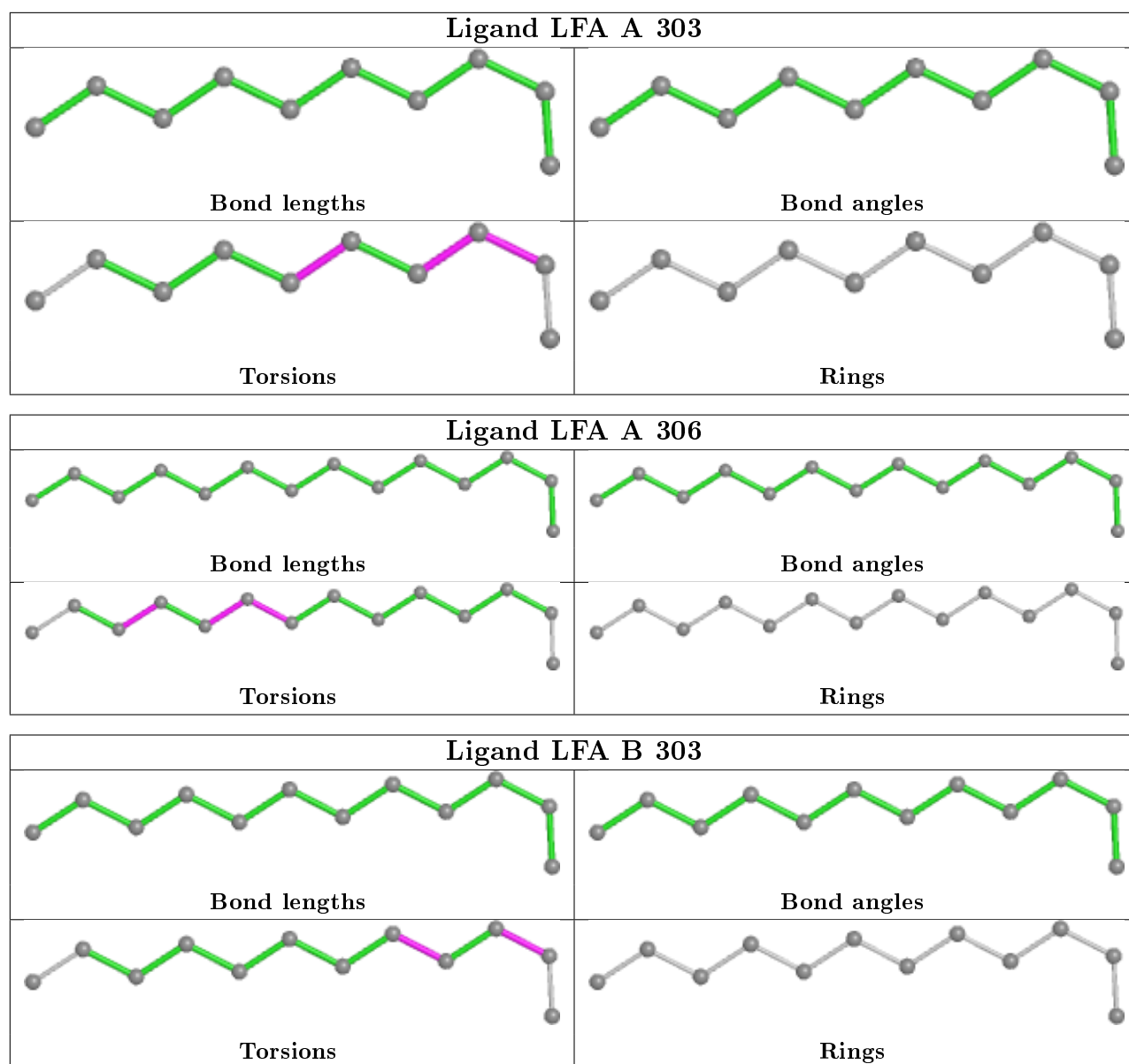


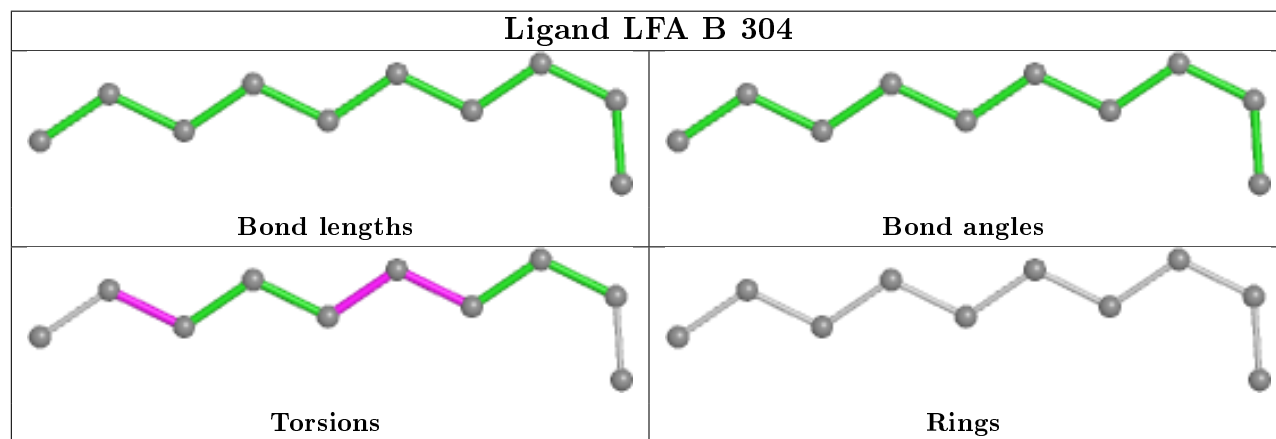
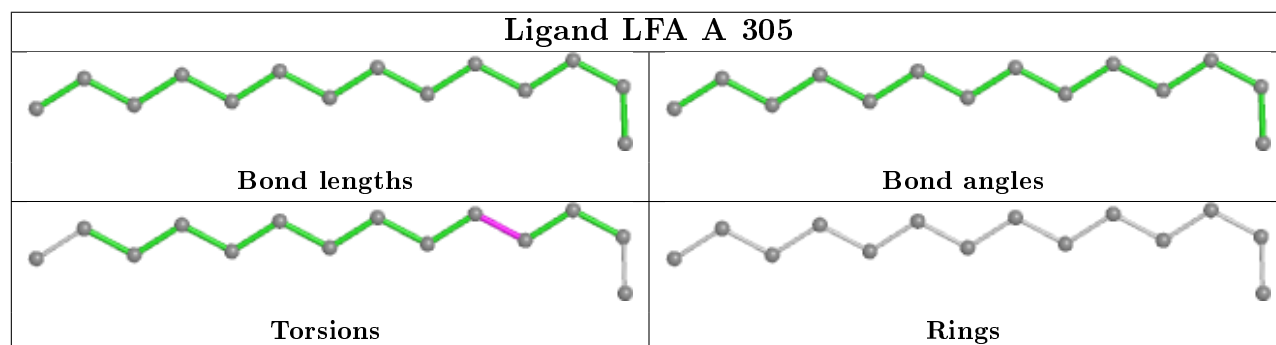
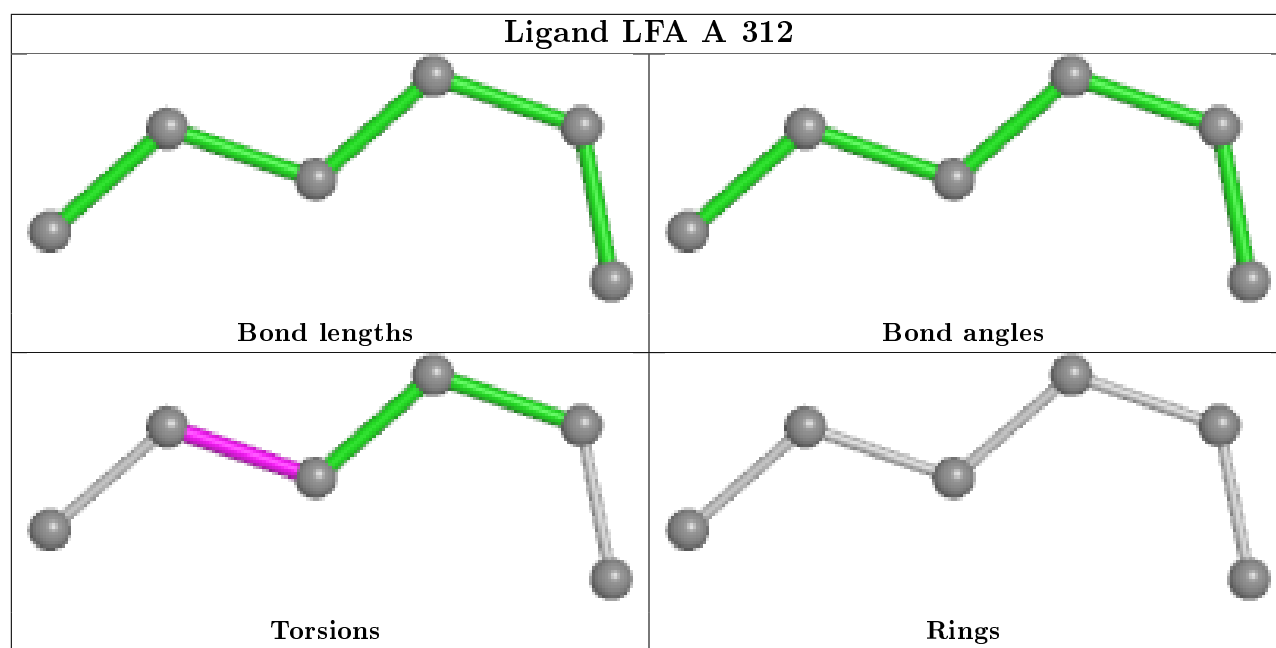


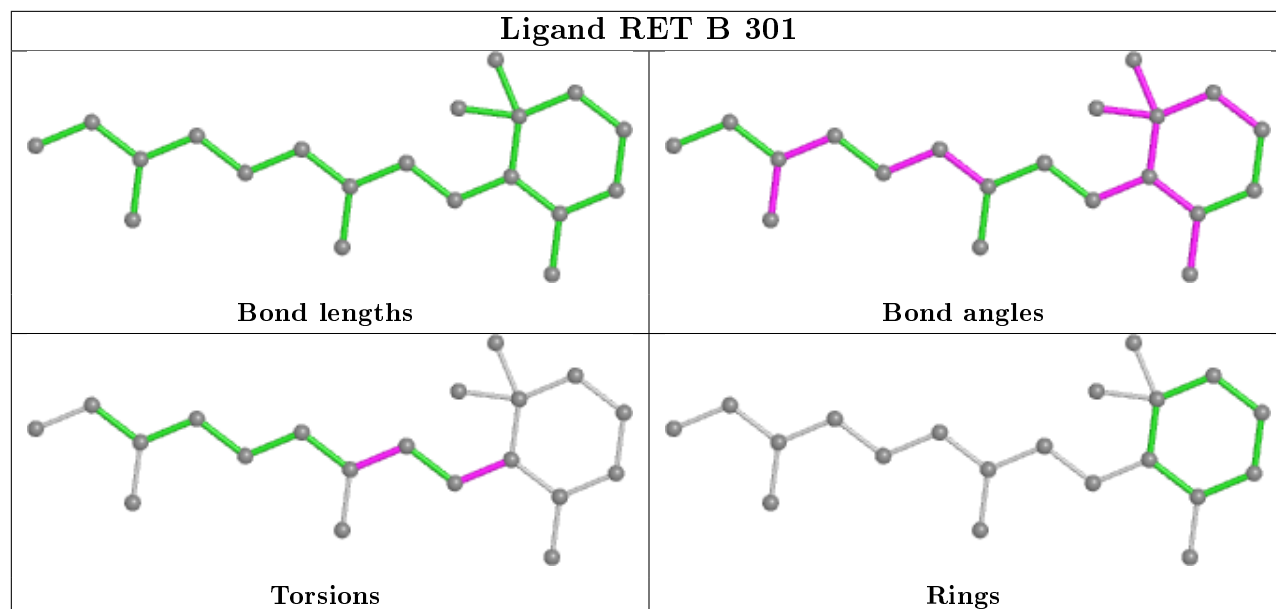












## 5.7 Other polymers [i](#)

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	236/258 (91%)	-0.04	5 (2%) 63 70	17, 35, 69, 101	3 (1%)
1	B	224/258 (86%)	0.06	10 (4%) 33 40	17, 31, 70, 98	2 (0%)
All	All	460/516 (89%)	0.01	15 (3%) 46 53	17, 32, 70, 101	5 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	4.4
1	B	204	ALA	4.3
1	B	209	ILE	3.9
1	B	8	VAL	3.7
1	B	10	ALA	3.7
1	A	169	ALA	2.7
1	A	6	LEU	2.7
1	B	138	GLY	2.6
1	A	241	SER	2.5
1	A	66	GLY	2.5
1	B	7	LEU	2.5
1	B	139	PHE	2.5
1	B	211	LEU	2.2
1	B	207	VAL	2.1
1	A	75	ASP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

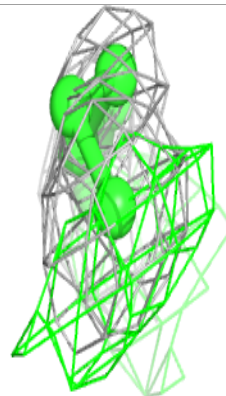
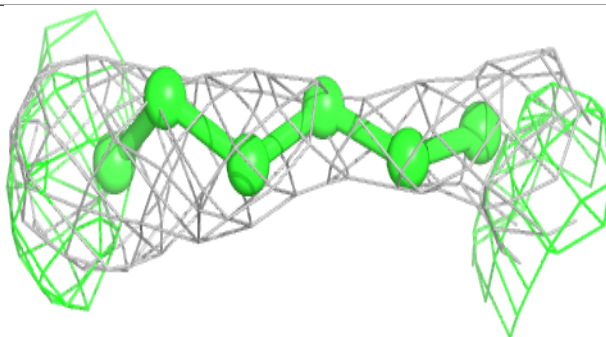
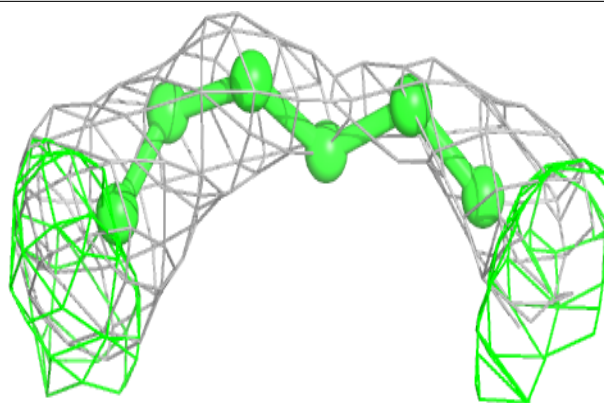
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	LFA	A	313	6/20	0.36	0.33	62,70,73,74	0
3	LFA	B	319	8/20	0.43	0.37	49,66,76,78	0
3	LFA	B	316	6/20	0.54	0.23	83,87,88,88	0
3	LFA	B	305	12/20	0.59	0.22	58,62,71,72	0
3	LFA	A	310	10/20	0.60	0.26	64,68,72,72	0
3	LFA	B	317	6/20	0.64	0.29	71,74,76,79	0
3	LFA	B	313	8/20	0.65	0.22	65,70,72,74	0
3	LFA	B	304	10/20	0.68	0.20	46,60,74,74	0
3	LFA	A	309	8/20	0.70	0.23	49,55,61,61	0
3	LFA	A	307	14/20	0.72	0.22	62,67,79,81	0
3	LFA	B	309	14/20	0.75	0.21	30,41,71,76	0
3	LFA	A	312	6/20	0.75	0.26	62,63,65,65	0
3	LFA	B	306	8/20	0.75	0.29	59,63,73,76	0
3	LFA	A	304	18/20	0.79	0.18	31,60,73,75	0
3	LFA	A	302	9/20	0.79	0.11	63,68,71,73	0
3	LFA	B	307	10/20	0.80	0.14	44,47,56,57	0
3	LFA	A	308	10/20	0.80	0.15	43,60,68,73	0
3	LFA	B	314	10/20	0.81	0.22	41,61,72,72	0
3	LFA	B	308	12/20	0.82	0.17	23,34,55,57	0
3	LFA	A	303	10/20	0.82	0.24	44,53,77,77	0
3	LFA	B	312	8/20	0.84	0.16	57,69,71,73	0
3	LFA	A	305	14/20	0.86	0.24	33,42,53,53	0
3	LFA	B	303	12/20	0.87	0.21	37,45,59,60	0
3	LFA	B	318	12/20	0.88	0.31	49,59,76,78	0
3	LFA	A	311	10/20	0.89	0.20	41,50,53,55	0
3	LFA	B	311	8/20	0.89	0.15	42,46,57,61	0
3	LFA	B	315	8/20	0.90	0.20	38,43,47,49	0
3	LFA	A	306	14/20	0.91	0.19	41,49,55,57	0
3	LFA	B	310	8/20	0.92	0.10	49,53,55,55	0
2	RET	A	301	20/21	0.95	0.13	10,21,29,30	0
2	RET	B	301	20/21	0.95	0.10	16,21,26,27	0
3	LFA	B	302	14/20	0.96	0.16	23,45,58,59	0

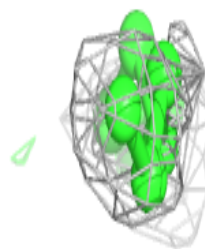
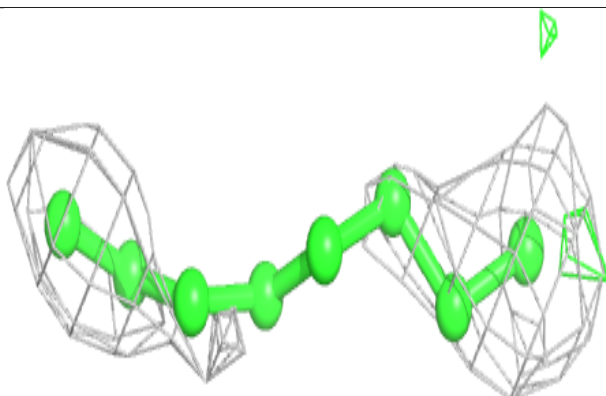
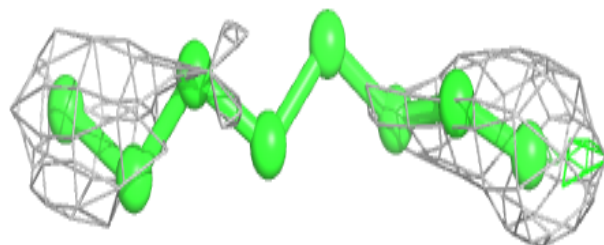
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LFA 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)

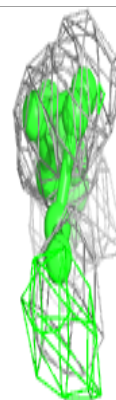
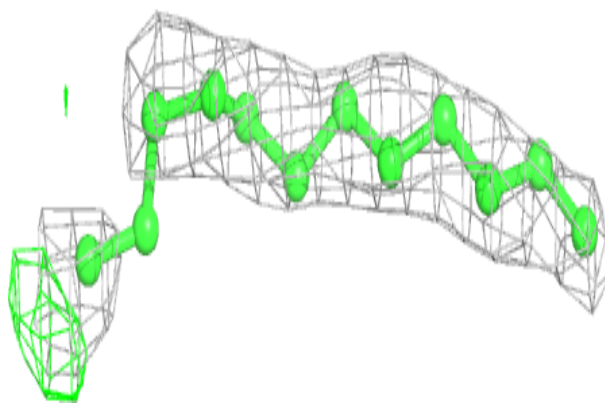
**Electron density around LFA B 319:**

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

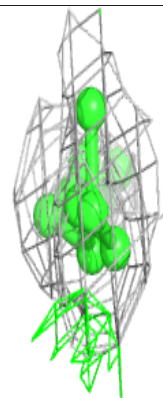
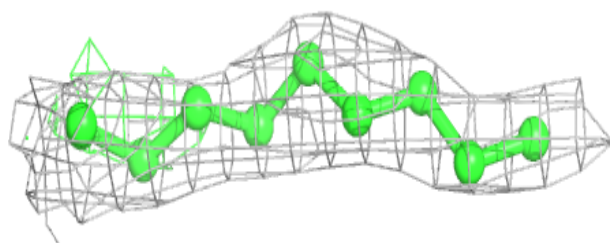
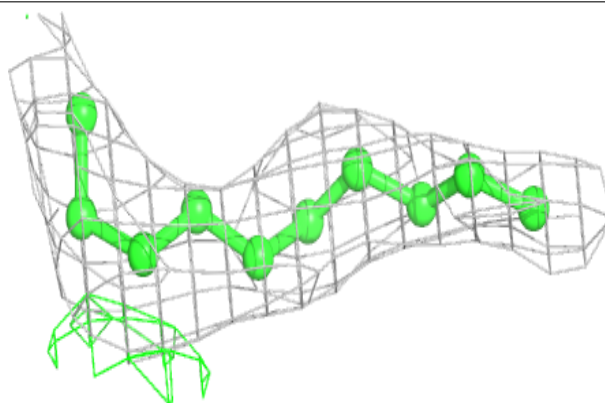


**Electron density around LFA B 305:**

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

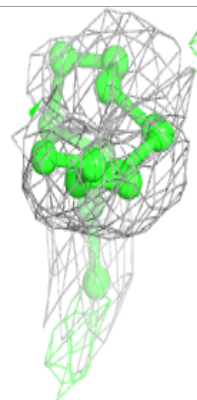
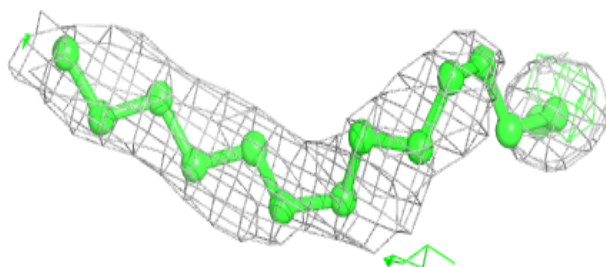
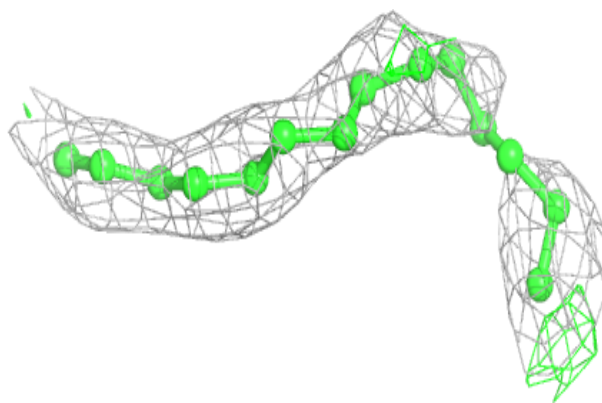
**Electron density around LFA B 304:**

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

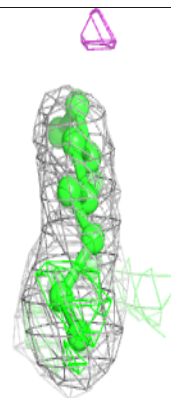
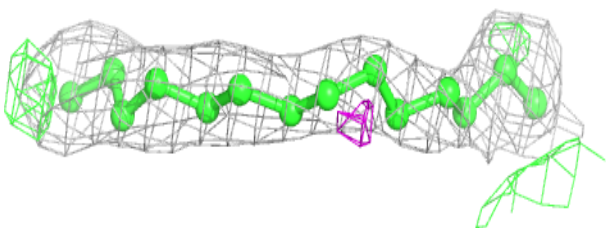
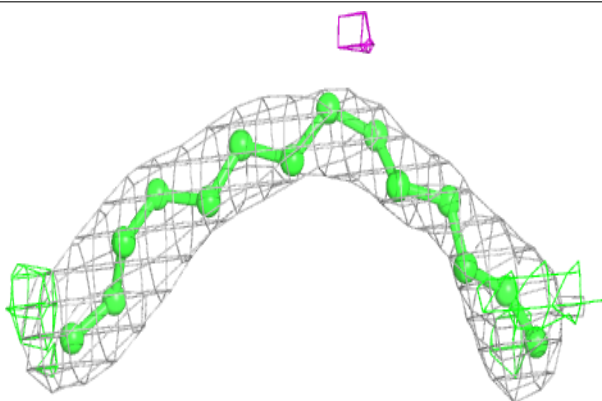


**Electron density around LFA A 307:**

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

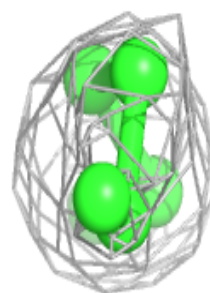
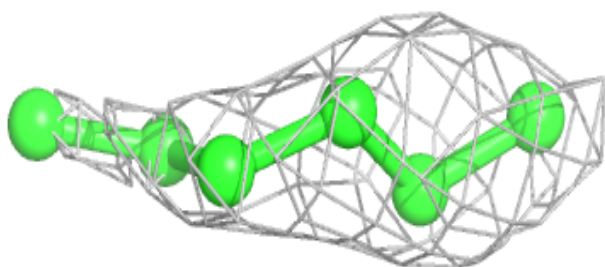
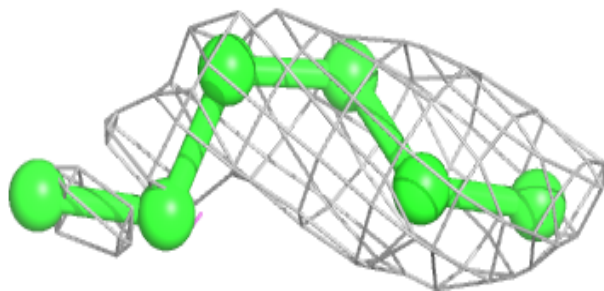
**Electron density around LFA B 309:**

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

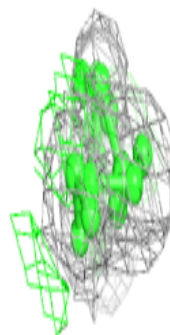
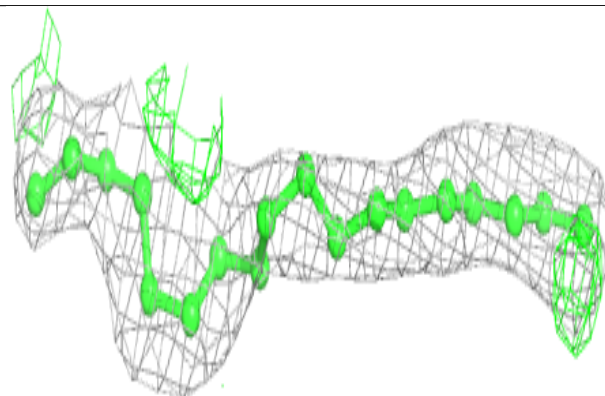
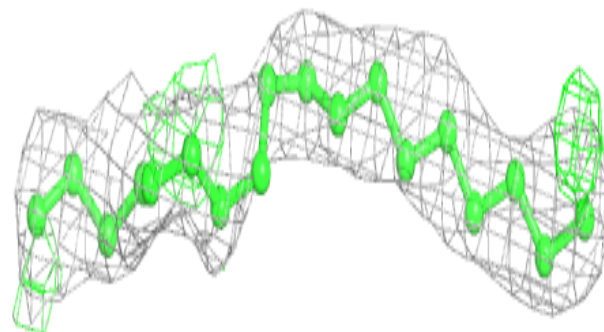


**Electron density around LFA A 312:**

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

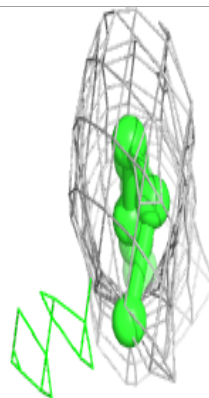
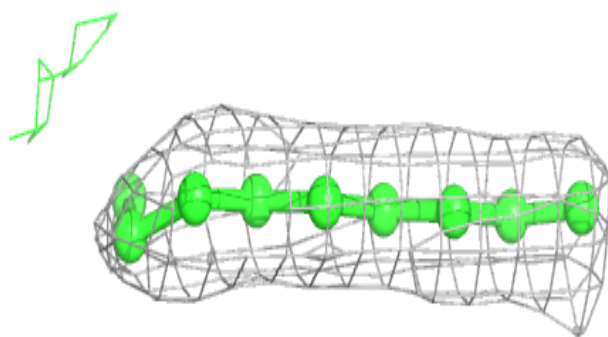
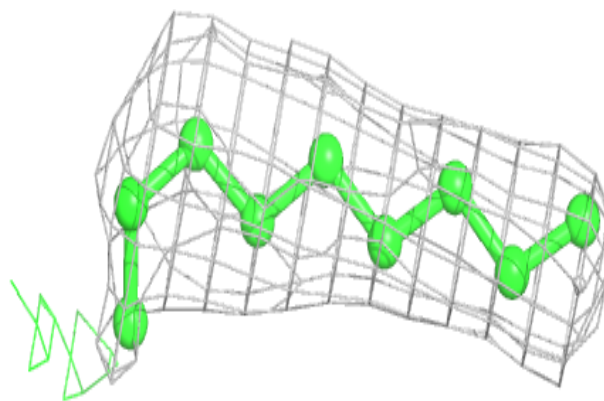
**Electron density around LFA A 304:**

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

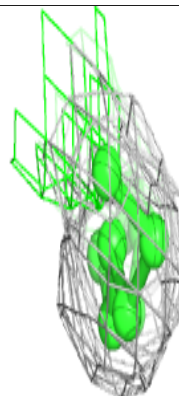
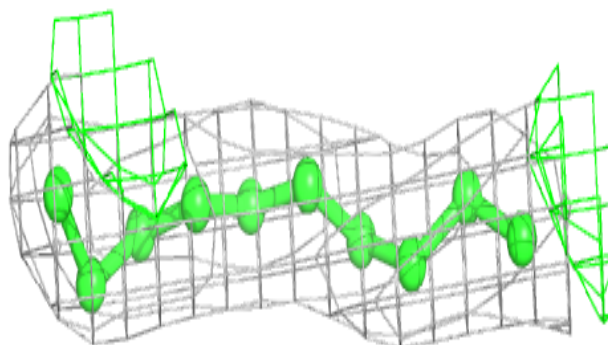
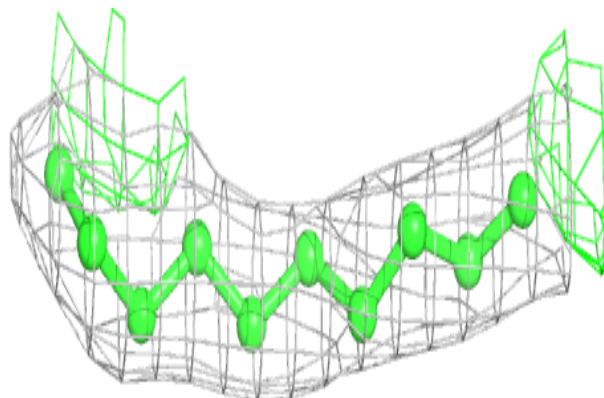


**Electron density around LFA A 302:**

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

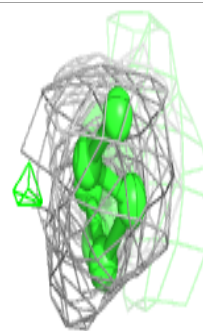
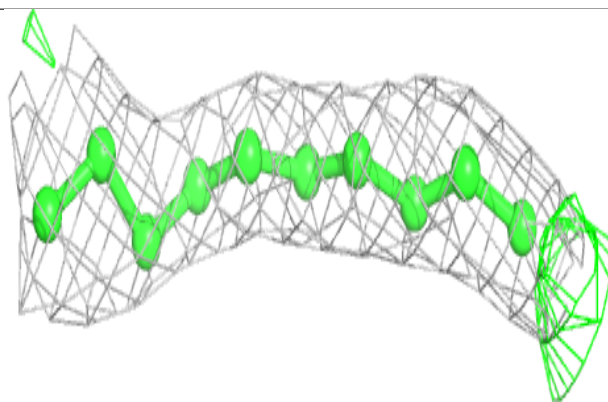
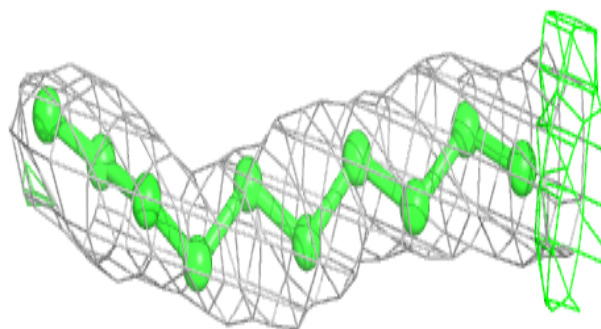
**Electron density around LFA B 307:**

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

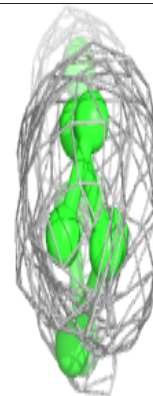
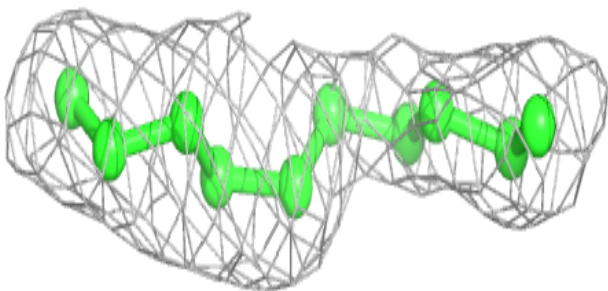
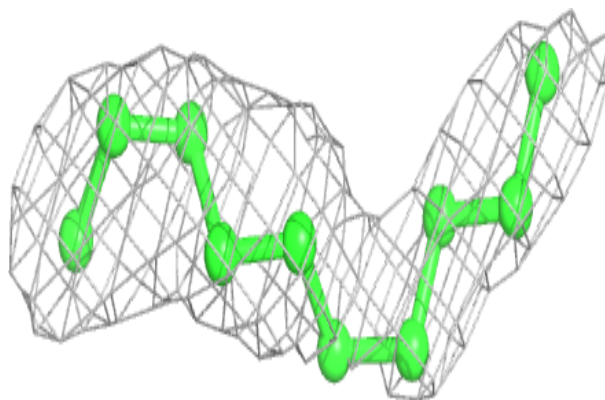


**Electron density around LFA A 308:**

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

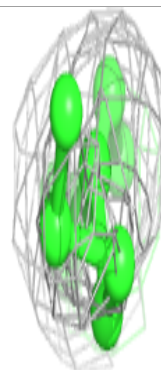
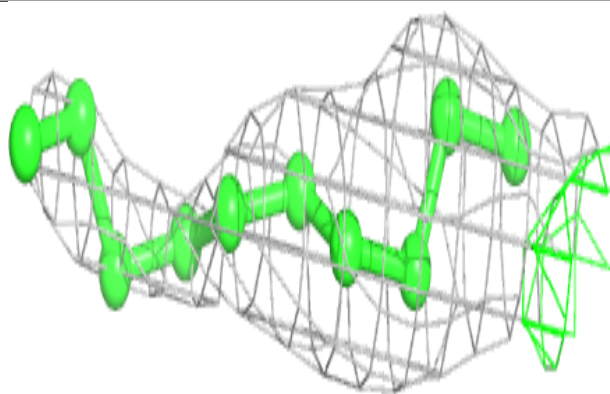
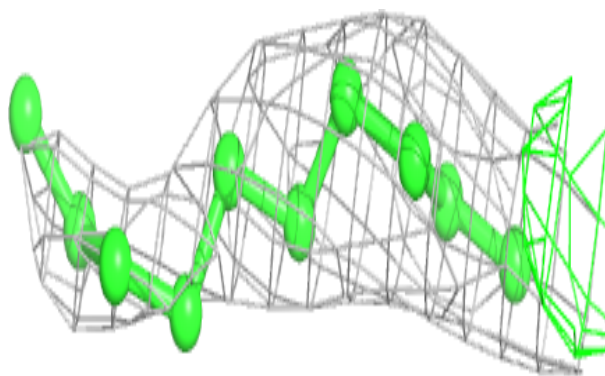
**Electron density around LFA B 314:**

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

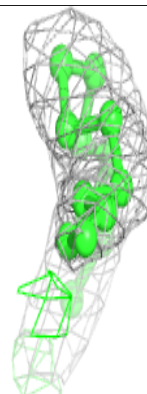
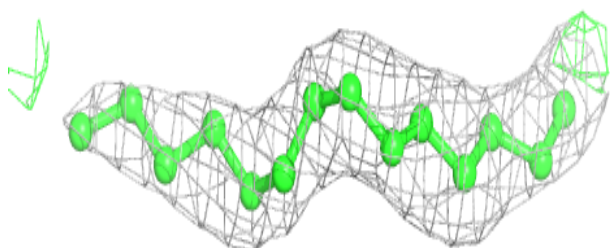
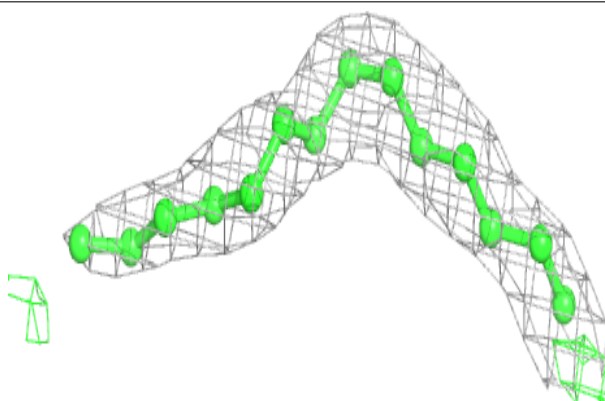


**Electron density around LFA A 303:**

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

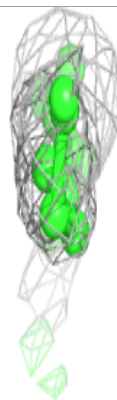
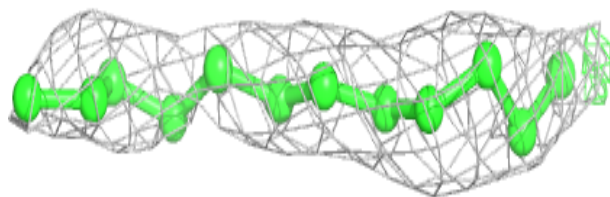
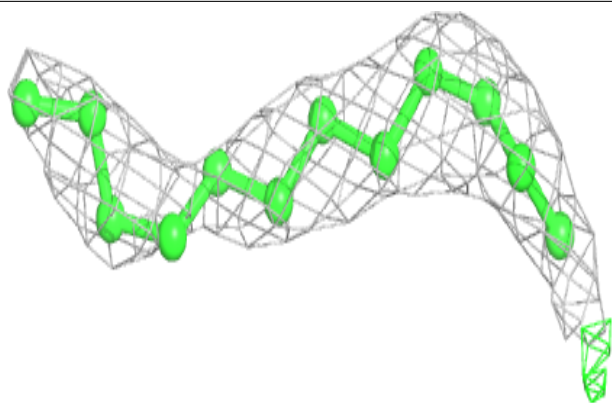
**Electron density around LFA A 305:**

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

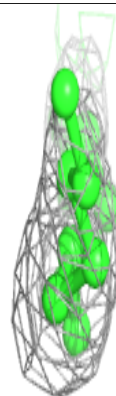
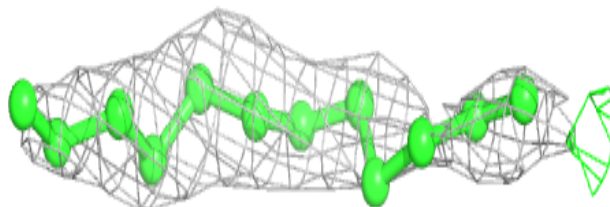
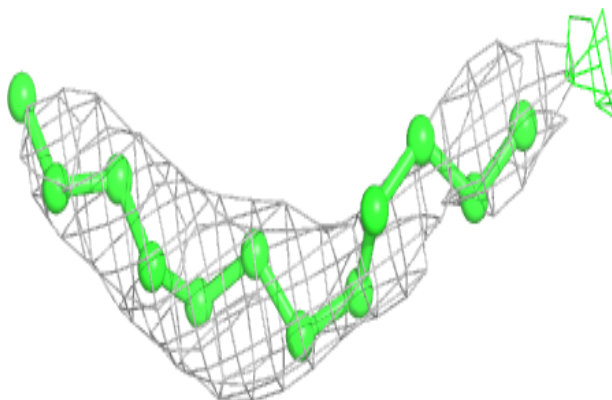


**Electron density around LFA B 303:**

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

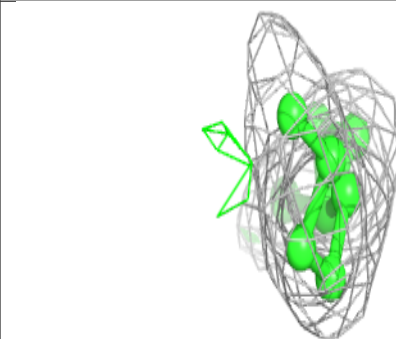
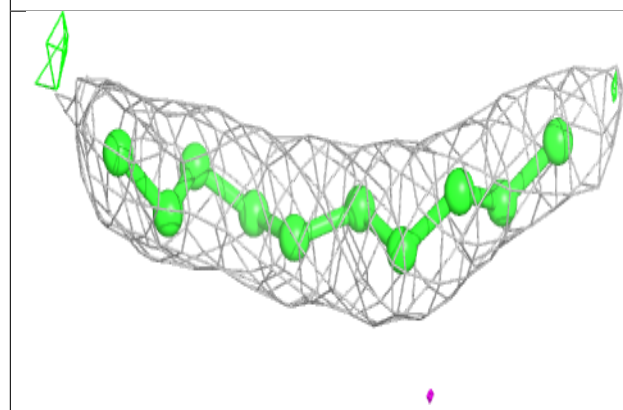
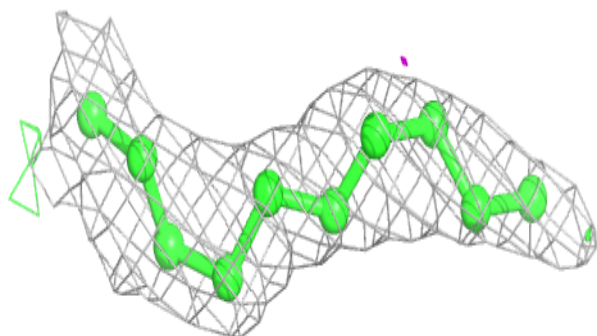
**Electron density around LFA B 318:**

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

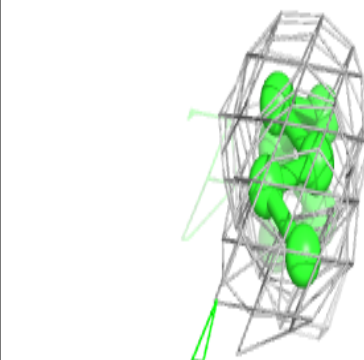
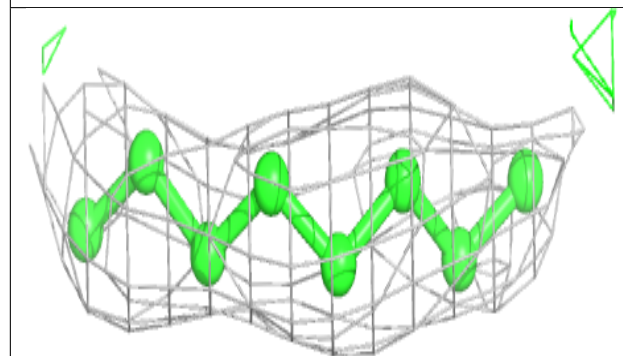
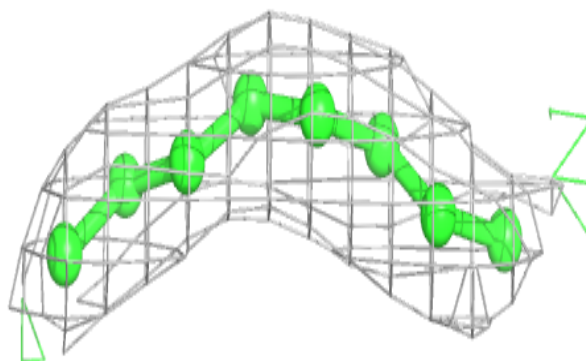


**Electron density around LFA A 311:**

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

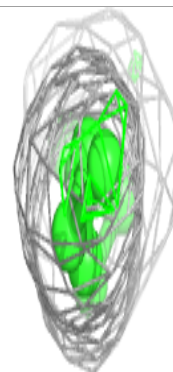
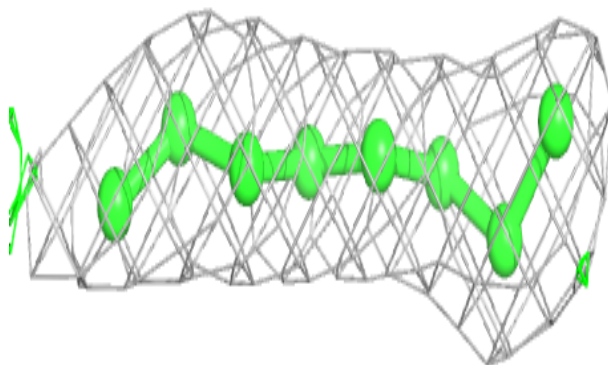
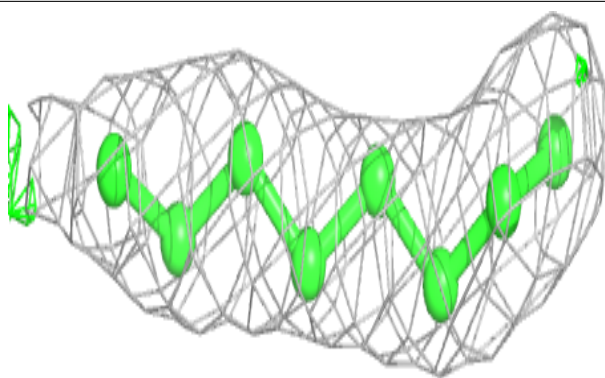
**Electron density around LFA B 311:**

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

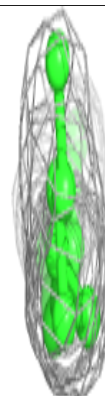
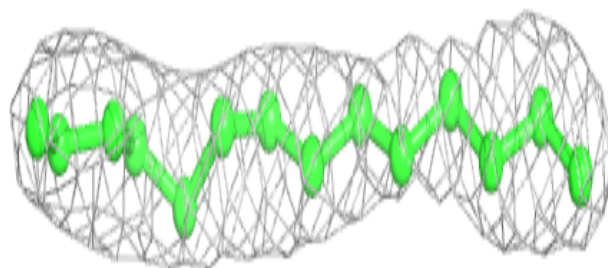
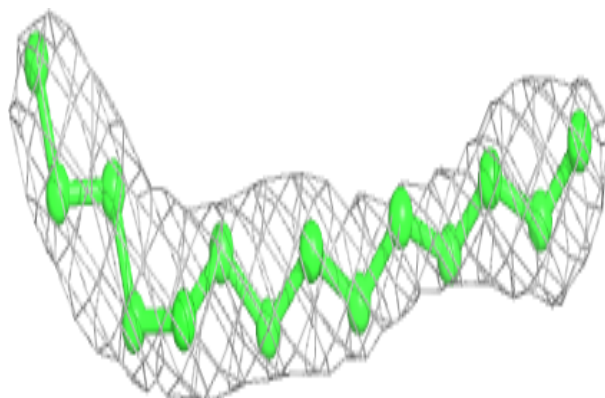


**Electron density around LFA B 315:**

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

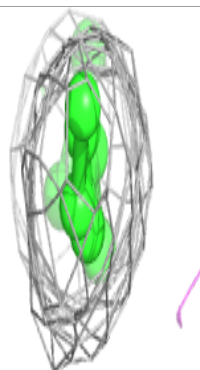
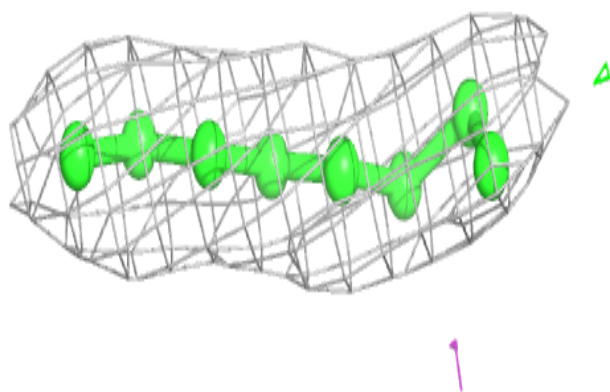
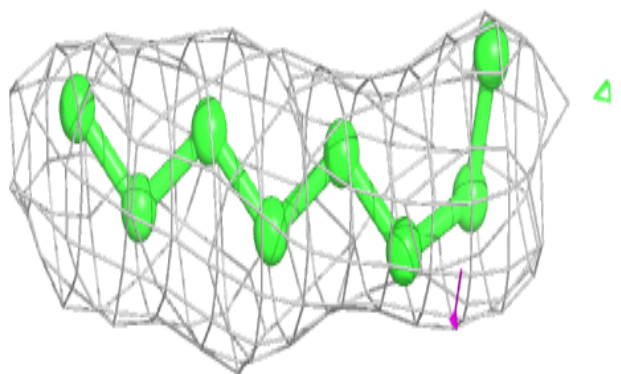
**Electron density around LFA A 306:**

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

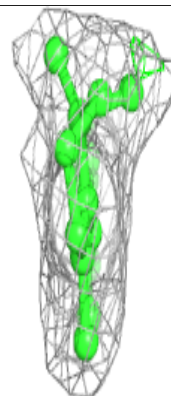
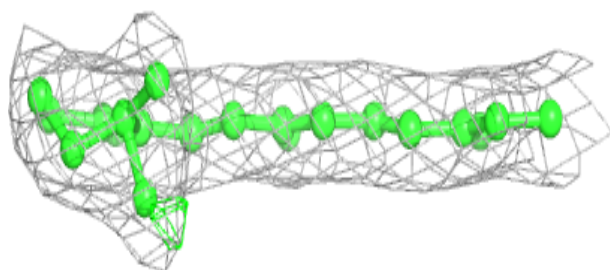
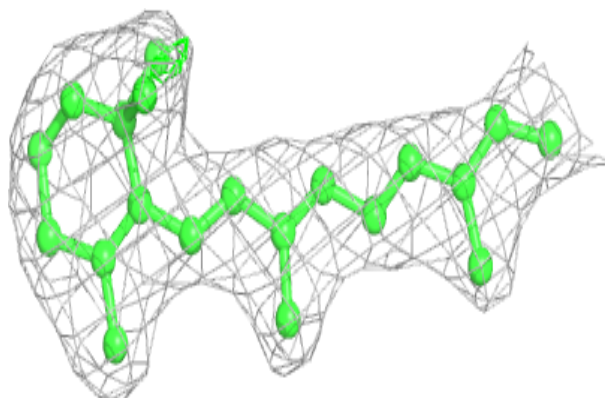


**Electron density around LFA B 310:**

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

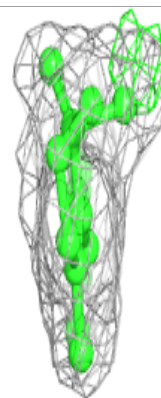
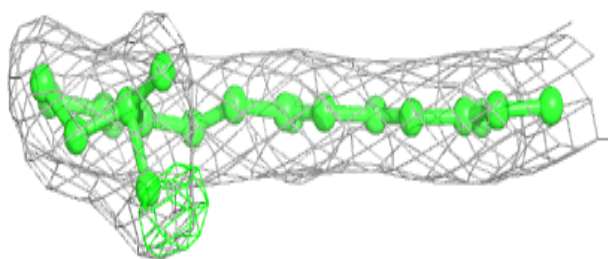
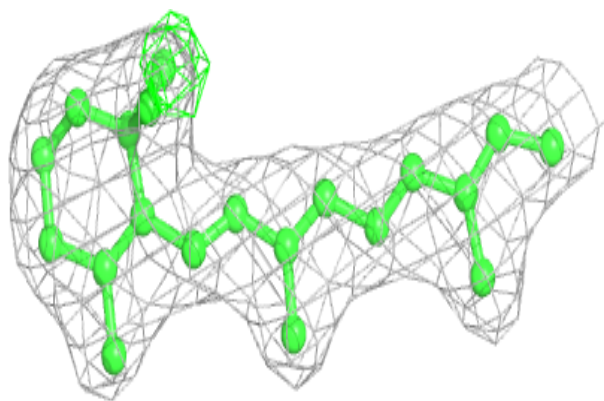
**Electron density around RET A 301:**

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

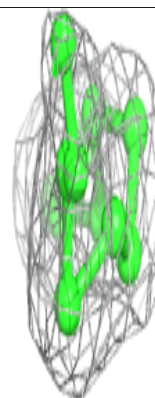
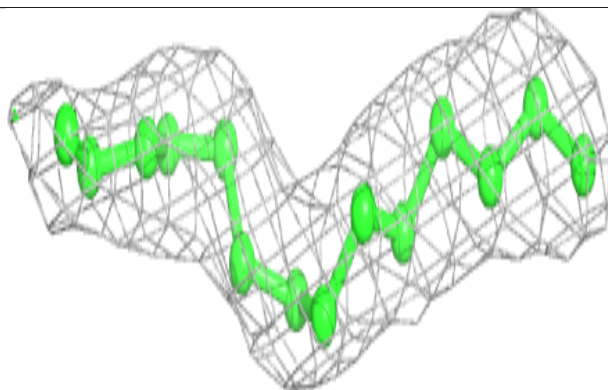
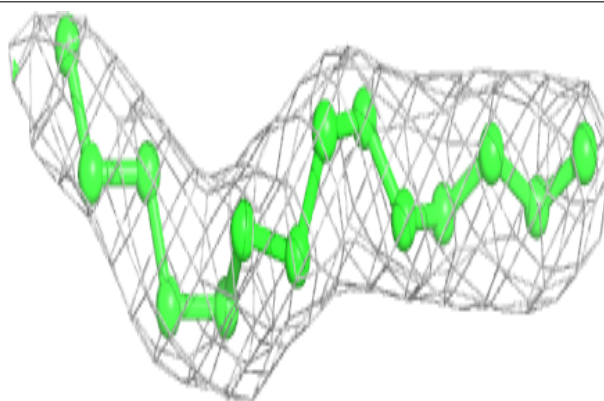


**Electron density around RET B 301:**

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

**Electron density around LFA B 302:**

$2mF_o-DF_c$  (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.