



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2025 – 12:16 pm GMT

PDB ID : 8RSO  
Title : Crystal structure of marine actinobacteria clade rhodopsin (MAR) in the ground state  
Authors : Bukhdruker, S.; Kovalev, K.; Astashkin, R.; Gordeliy, V.  
Deposited on : 2024-01-25  
Resolution : 1.25 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>.

---

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)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

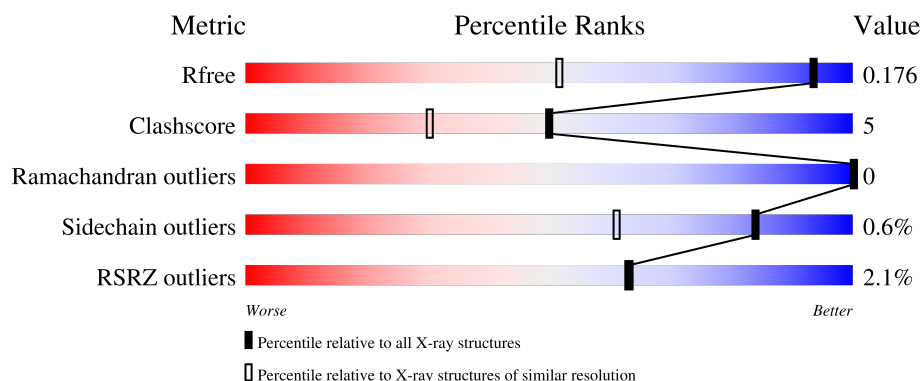
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.25 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))
$R_{free}$	164625	1447 (1.28-1.24)
Clashscore	180529	1571 (1.28-1.24)
Ramachandran outliers	177936	1538 (1.28-1.24)
Sidechain outliers	177891	1537 (1.28-1.24)
RSRZ outliers	164620	1447 (1.28-1.24)

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	220	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	220	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>

## 2 Entry composition (i)

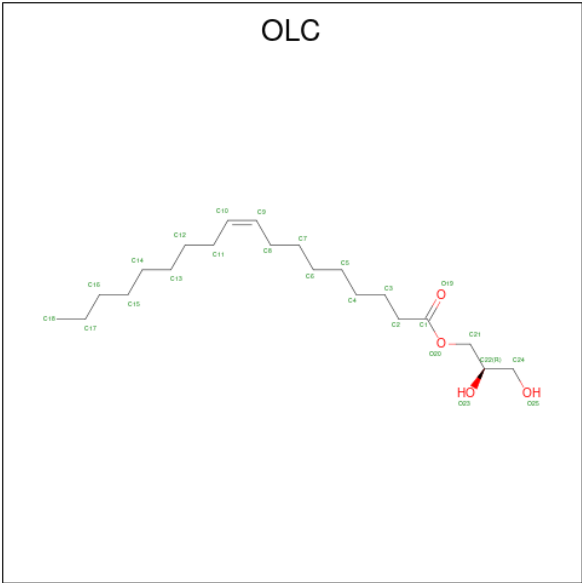
There are 7 unique types of molecules in this entry. The entry contains 3969 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Microbial rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	10	0
			1732	1129	283	307	13			
1	B	217	Total	C	N	O	S	0	14	1
			1774	1153	296	312	13			

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



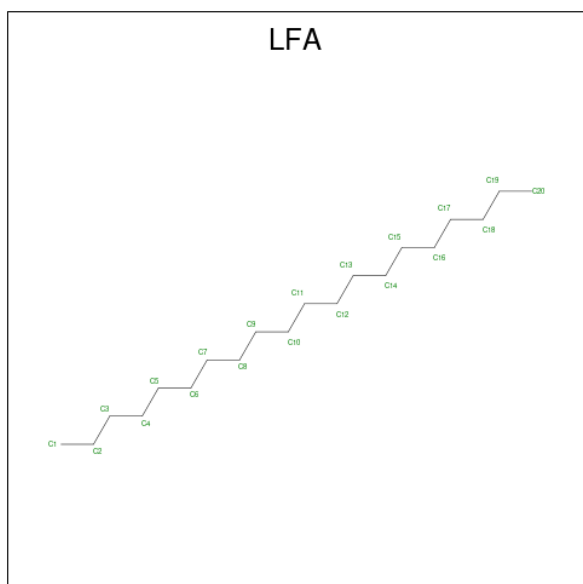
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			19	17	2		
2	A	1	Total	C	O	0	0
			15	11	4		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 15 15	0	0
2	A	1	Total C O 13 11 2	0	0
2	A	1	Total C O 9 7 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 12 10 2	0	0

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



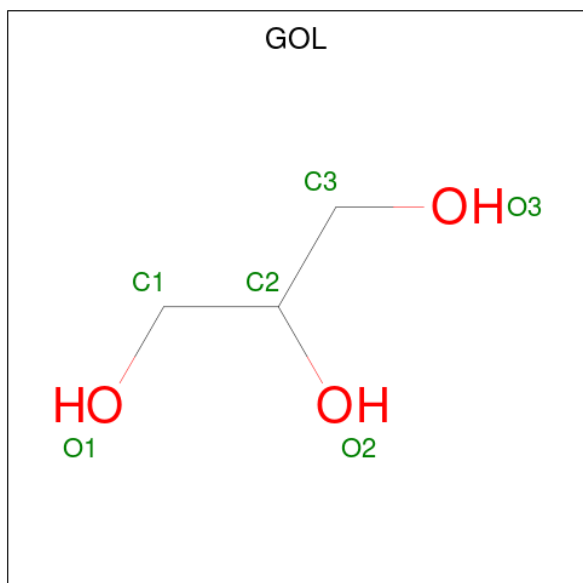
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 12 12	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 3 3	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 3 3	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 8 8	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 3 3	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 4 4	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



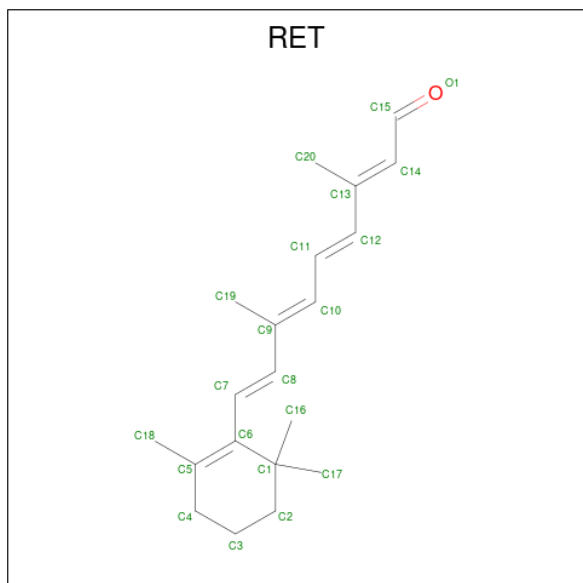
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

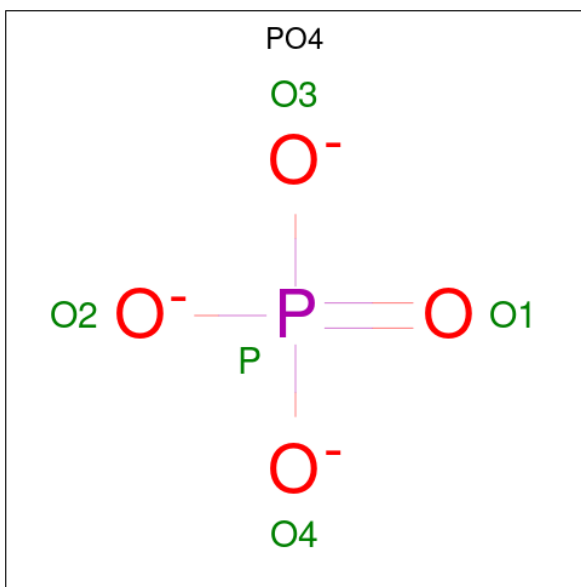
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 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
5	A	1	Total	C	0	0
			20	20		
5	B	1	Total	C	0	0
			20	20		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	64	Total	O	0	4
			68	68		
7	B	69	Total	O	0	3
			70	70		

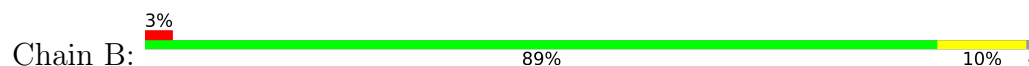
### 3 Residue-property plots [i](#)

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: Microbial rhodopsin



- Molecule 1: Microbial rhodopsin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.71Å 55.85Å 56.64Å 64.09° 81.52° 85.29°	Depositor
Resolution (Å)	47.23 – 1.25 47.23 – 1.25	Depositor EDS
% Data completeness (in resolution range)	74.8 (47.23-1.25) 75.7 (47.23-1.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.24Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.151 , 0.177 0.152 , 0.176	Depositor DCC
$R_{free}$ test set	117959 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, RET, LFA, OLC, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.52	0/1772	0.69	1/2413 (0.0%)
1	B	0.52	0/1813	0.70	0/2462
All	All	0.52	0/3585	0.70	1/4875 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASP	CB-CG-OD1	5.69	123.42	118.30

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	1732	0	1699	17	0
1	B	1774	0	1753	19	0
2	A	116	0	171	8	0
2	B	31	0	35	4	0
3	A	66	0	123	4	0
3	B	49	0	89	1	0
4	A	18	0	21	4	0
5	A	20	0	27	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	27	3	0
6	B	5	0	0	0	0
7	A	68	0	0	2	0
7	B	70	0	0	2	0
All	All	3969	0	3945	41	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 5.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:O	7:A:601[A]:HOH:O	2.05	0.74
1:A:25:ALA:O	7:A:601[B]:HOH:O	2.11	0.66
1:A:50[A]:TYR:CZ	1:B:75:LEU:HD11	2.36	0.60
1:B:25:ALA:HB1	3:B:506:LFA:H112	1.84	0.60
1:A:51:HIS:HE1	4:A:515:GOL:H12	1.66	0.60
4:A:515:GOL:H32	1:B:50:TYR:CD2	2.37	0.59
3:A:516:LFA:H13	1:B:75:LEU:HD13	1.85	0.59
1:A:51:HIS:CE1	4:A:515:GOL:H12	2.41	0.56
2:A:501:OLC:H21	2:A:512:OLC:H7A	1.86	0.56
1:A:194:ILE:HG21	2:A:501:OLC:H11	1.89	0.53
1:A:36:ARG:NH2	1:B:36:ARG:HH22	2.07	0.51
5:B:511:RET:H161	5:B:511:RET:H8	1.93	0.51
2:A:517:OLC:H3	1:B:39:TYR:CZ	2.47	0.50
1:A:173:PRO:HB3	5:A:520:RET:H183	1.95	0.48
1:B:126:TRP:CZ3	1:B:177:ILE:HD11	2.49	0.48
1:B:114:TYR:CZ	2:B:504:OLC:H2	2.48	0.47
1:A:177:ILE:O	1:A:180:VAL:HG22	2.17	0.45
1:B:217:GLU:N	7:B:608:HOH:O	2.50	0.45
1:A:80:MET:O	1:A:83:GLU:HG2	2.17	0.45
1:B:132:ALA:HB3	5:B:511:RET:H41	1.99	0.45
1:B:173:PRO:HB3	5:B:511:RET:H183	1.99	0.45
2:A:502:OLC:H15	2:A:502:OLC:H12	1.80	0.44
1:A:113:TYR:CZ	2:A:518:OLC:H2A	2.53	0.44
5:A:520:RET:H171	5:A:520:RET:H8	1.99	0.44
4:A:519:GOL:O2	1:B:36:ARG:NH1	2.51	0.44
1:A:104:ALA:O	1:A:135[A]:THR:HG21	2.18	0.43
1:A:168:GLY:HA2	2:A:501:OLC:H5A	1.99	0.43
2:B:503:OLC:H4	2:B:504:OLC:H7	2.00	0.43
1:B:40[A]:ILE:HG22	1:B:83:GLU:HB3	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ALA:HA	2:B:504:OLC:H5A	2.01	0.42
1:A:135[B]:THR:HG22	3:A:510:LFA:H182	2.01	0.42
1:B:129:PHE:CZ	1:B:133[A]:MET:HG3	2.54	0.42
1:A:134:ALA:HB2	3:A:504:LFA:H141	2.01	0.42
2:A:503:OLC:C17	3:A:516:LFA:H51	2.50	0.42
5:A:520:RET:H181	5:A:520:RET:H7	1.75	0.42
1:B:28:ARG:HD2	7:B:612:HOH:O	2.19	0.41
1:B:114:TYR:HB2	2:B:503:OLC:H3A	2.02	0.41
1:B:205:VAL:O	1:B:209[A]:GLN:HG2	2.20	0.41
1:A:113:TYR:CE1	2:A:518:OLC:H2A	2.56	0.41
1:B:80:MET:O	1:B:83:GLU:HG2	2.20	0.41
1:A:9:PHE:O	1:A:13[B]:THR:HG23	2.20	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	224/220 (102%)	224 (100%)	0	0	100	100
1	B	229/220 (104%)	228 (100%)	1 (0%)	0	100	100
All	All	453/440 (103%)	452 (100%)	1 (0%)	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	169/173 (98%)	168 (99%)	1 (1%)	84	61
1	B	173/173 (100%)	172 (99%)	1 (1%)	84	61
All	All	342/346 (99%)	340 (99%)	2 (1%)	84	61

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	B	180	VAL

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

31 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	A	506	-	6,6,19	0.10	0	5,5,18	0.30	0
3	LFA	A	509	-	2,2,19	0.06	0	0,1,18	-	-
2	OLC	B	503	-	6,6,24	0.48	0	6,6,25	0.43	0
3	LFA	A	504	-	11,11,19	0.11	0	10,10,18	0.18	0
2	OLC	B	504	-	11,11,24	0.35	0	11,11,25	0.40	0
3	LFA	A	505	-	6,6,19	0.13	0	5,5,18	0.09	0
2	OLC	A	502	-	19,19,24	0.34	0	19,19,25	0.35	0
4	GOL	A	511	-	5,5,5	1.09	1 (20%)	5,5,5	0.85	0
3	LFA	A	507	-	5,5,19	0.11	0	4,4,18	0.12	0
3	LFA	A	516	-	7,7,19	0.09	0	6,6,18	0.12	0
4	GOL	A	515	-	5,5,5	0.89	0	5,5,5	1.03	0
2	OLC	A	503	-	18,18,24	0.35	0	18,18,25	0.39	0
3	LFA	B	506	-	11,11,19	0.14	0	10,10,18	0.15	0
3	LFA	A	514	-	12,12,19	0.10	0	11,11,18	0.19	0
3	LFA	B	502	-	2,2,19	0.01	0	0,1,18	-	-
5	RET	B	511	1	20,20,21	1.10	1 (5%)	27,27,28	0.91	1 (3%)
2	OLC	A	512	-	14,14,24	0.29	0	15,15,25	0.34	0
2	OLC	A	518	-	8,8,24	0.29	0	8,8,25	0.13	0
3	LFA	B	507	-	10,10,19	0.10	0	9,9,18	0.15	0
3	LFA	B	509	-	3,3,19	0.25	0	2,2,18	0.37	0
3	LFA	A	508	-	2,2,19	0.02	0	0,1,18	-	-
2	OLC	A	501	-	24,24,24	0.28	0	25,25,25	0.35	0
2	OLC	B	505	-	11,11,24	0.37	0	11,11,25	0.18	0
3	LFA	B	508	-	11,11,19	0.13	0	10,10,18	0.31	0
6	PO4	B	510	-	4,4,4	0.82	0	6,6,6	0.33	0
4	GOL	A	519	-	5,5,5	1.55	1 (20%)	5,5,5	1.25	0
5	RET	A	520	1	20,20,21	0.79	1 (5%)	27,27,28	1.01	1 (3%)
2	OLC	A	517	-	12,12,24	0.37	0	12,12,25	0.45	0
3	LFA	B	501	-	6,6,19	0.10	0	5,5,18	0.12	0
2	OLC	A	513	-	14,14,24	0.30	0	13,13,25	0.23	0
3	LFA	A	510	-	6,6,19	0.13	0	5,5,18	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	506	-	-	0/4/4/17	-
2	OLC	B	503	-	-	1/4/4/24	-
3	LFA	A	504	-	-	2/9/9/17	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	504	-	-	3/9/9/24	-
3	LFA	A	505	-	-	1/4/4/17	-
2	OLC	A	502	-	-	4/17/17/24	-
4	GOL	A	511	-	-	2/4/4/4	-
3	LFA	A	507	-	-	0/3/3/17	-
3	LFA	A	516	-	-	0/5/5/17	-
4	GOL	A	515	-	-	4/4/4/4	-
2	OLC	A	503	-	-	4/16/16/24	-
3	LFA	B	506	-	-	3/9/9/17	-
3	LFA	A	514	-	-	1/10/10/17	-
5	RET	B	511	1	-	1/13/30/31	0/1/1/1
2	OLC	A	512	-	-	1/14/14/24	-
2	OLC	A	518	-	-	1/7/7/24	-
3	LFA	B	507	-	-	2/8/8/17	-
3	LFA	B	509	-	-	0/1/1/17	-
2	OLC	A	501	-	-	2/24/24/24	-
2	OLC	B	505	-	-	1/10/10/24	-
3	LFA	B	508	-	-	0/9/9/17	-
4	GOL	A	519	-	-	2/4/4/4	-
5	RET	A	520	1	-	0/13/30/31	0/1/1/1
2	OLC	A	517	-	-	1/10/10/24	-
3	LFA	B	501	-	-	0/4/4/17	-
2	OLC	A	513	-	-	2/12/12/24	-
3	LFA	A	510	-	-	2/4/4/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	511	RET	C14-C13	3.97	1.36	1.33
4	A	519	GOL	O2-C2	-2.38	1.36	1.43
5	A	520	RET	C14-C13	2.26	1.35	1.33
4	A	511	GOL	O2-C2	-2.26	1.36	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	520	RET	C18-C5-C6	-2.53	121.69	124.53
5	B	511	RET	C17-C1-C6	2.42	114.23	110.30

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	GOL	O1-C1-C2-C3
4	A	519	GOL	C1-C2-C3-O3
3	A	505	LFA	C16-C17-C18-C19
4	A	515	GOL	C1-C2-C3-O3
3	B	507	LFA	C15-C16-C17-C18
2	B	503	OLC	C1-C2-C3-C4
4	A	511	GOL	O1-C1-C2-O2
3	A	510	LFA	C15-C16-C17-C18
3	B	506	LFA	C3-C4-C5-C6
3	B	507	LFA	C14-C15-C16-C17
5	B	511	RET	C12-C13-C14-C15
3	A	504	LFA	C11-C12-C13-C14
2	A	502	OLC	C12-C13-C14-C15
3	A	510	LFA	C17-C18-C19-C20
2	A	503	OLC	C10-C11-C12-C13
4	A	515	GOL	O1-C1-C2-O2
4	A	519	GOL	O2-C2-C3-O3
3	B	506	LFA	C6-C7-C8-C9
2	B	504	OLC	C2-C3-C4-C5
3	A	504	LFA	C12-C13-C14-C15
2	A	503	OLC	C7-C8-C9-C10
3	B	506	LFA	C11-C10-C9-C8
2	A	517	OLC	C7-C8-C9-C10
2	A	502	OLC	O19-C1-C2-C3
2	B	504	OLC	O19-C1-C2-C3
2	B	504	OLC	O20-C1-C2-C3
3	A	514	LFA	C15-C16-C17-C18
2	A	501	OLC	C9-C10-C11-C12
2	A	513	OLC	C9-C10-C11-C12
2	A	502	OLC	O20-C1-C2-C3
2	A	503	OLC	O20-C1-C2-C3
4	A	515	GOL	O2-C2-C3-O3
2	A	502	OLC	C10-C11-C12-C13
2	A	501	OLC	C7-C8-C9-C10
2	A	512	OLC	C5-C6-C7-C8
2	A	503	OLC	O19-C1-C2-C3
2	A	513	OLC	C7-C8-C9-C10
2	B	505	OLC	C5-C6-C7-C8
4	A	515	GOL	O1-C1-C2-C3
2	A	518	OLC	C1-C2-C3-C4

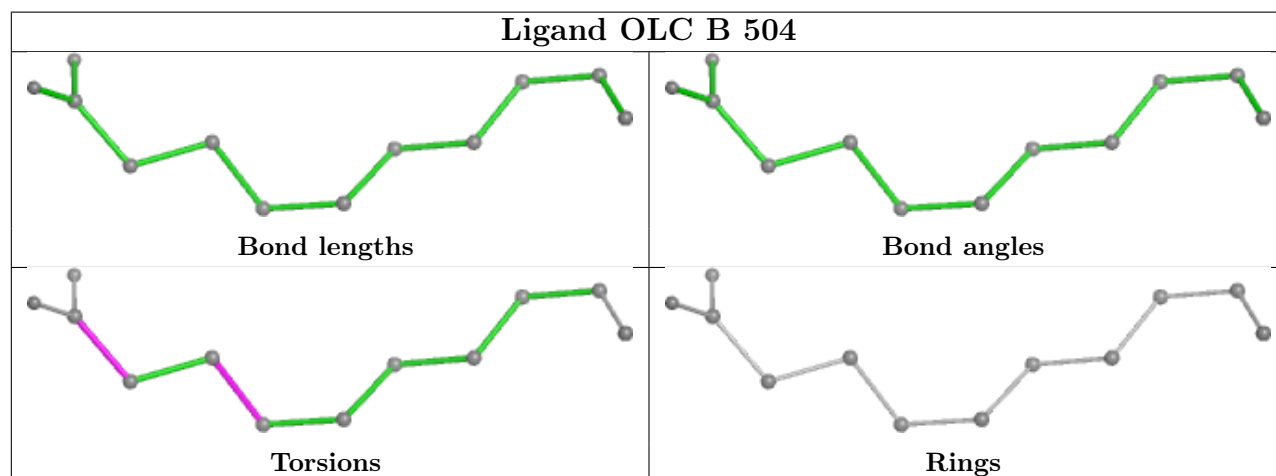
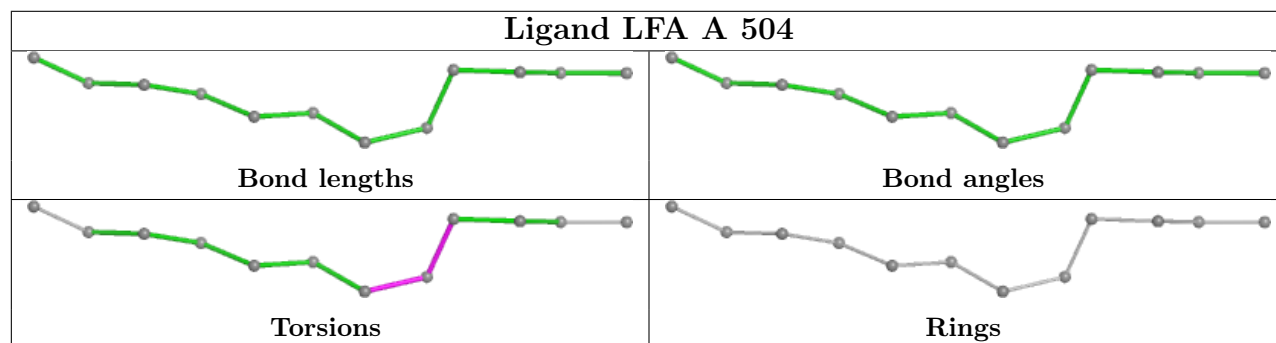
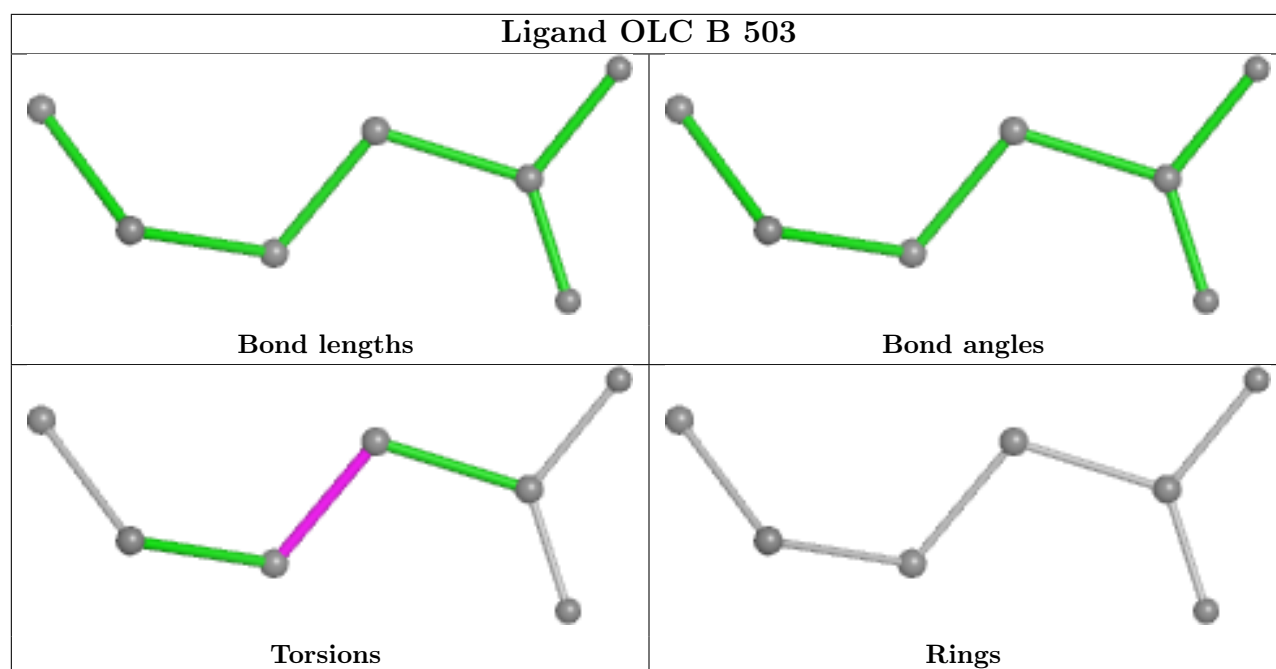
There are no ring outliers.

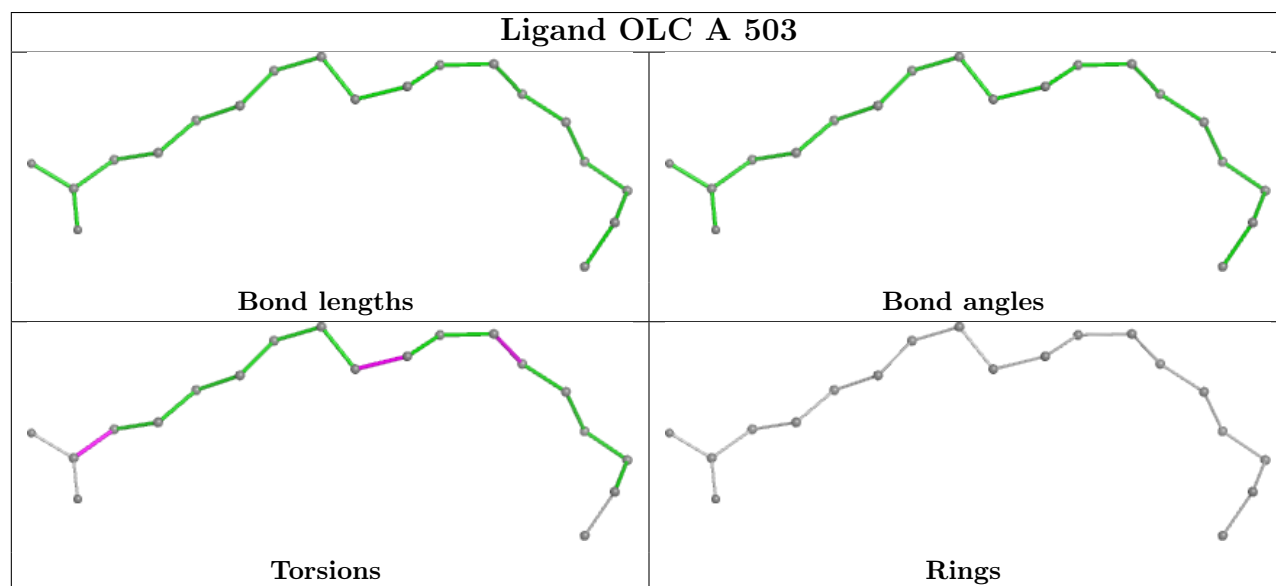
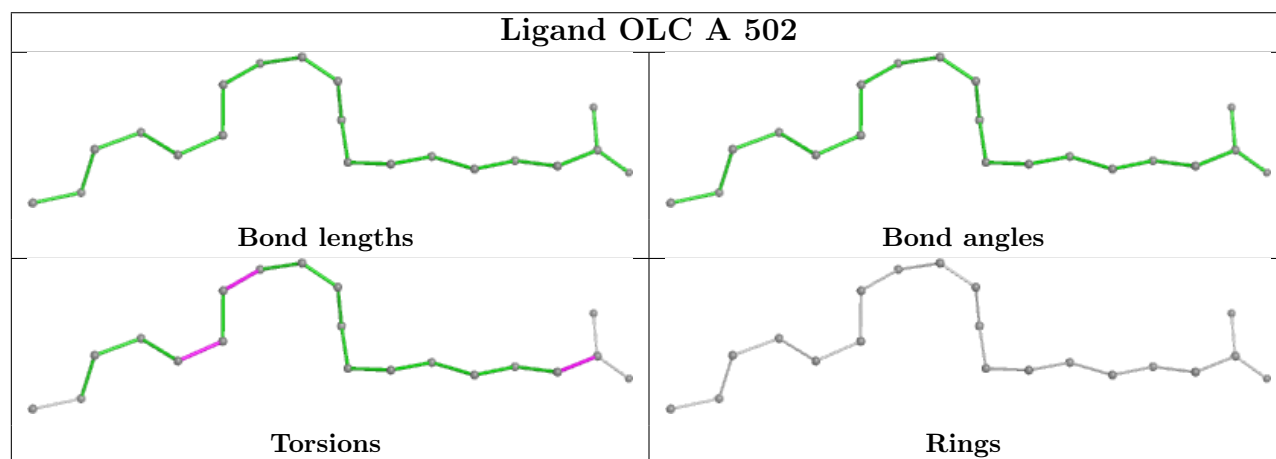
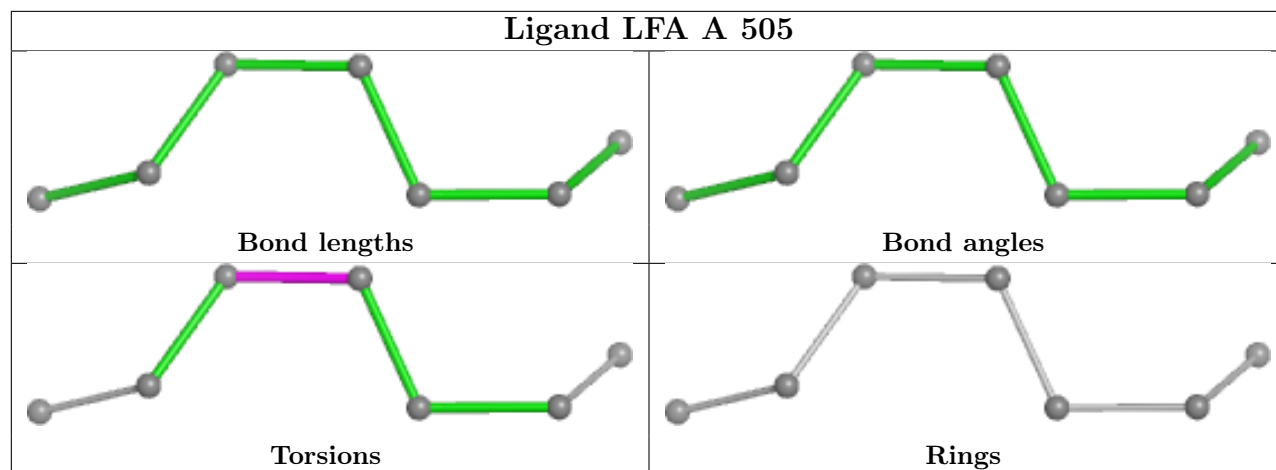


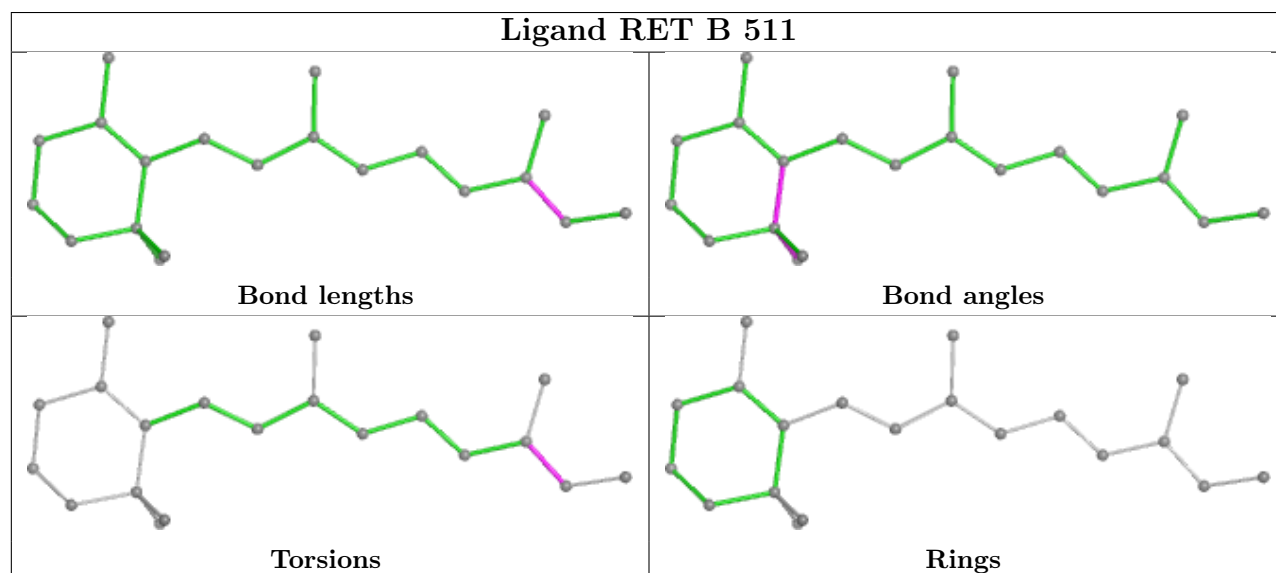
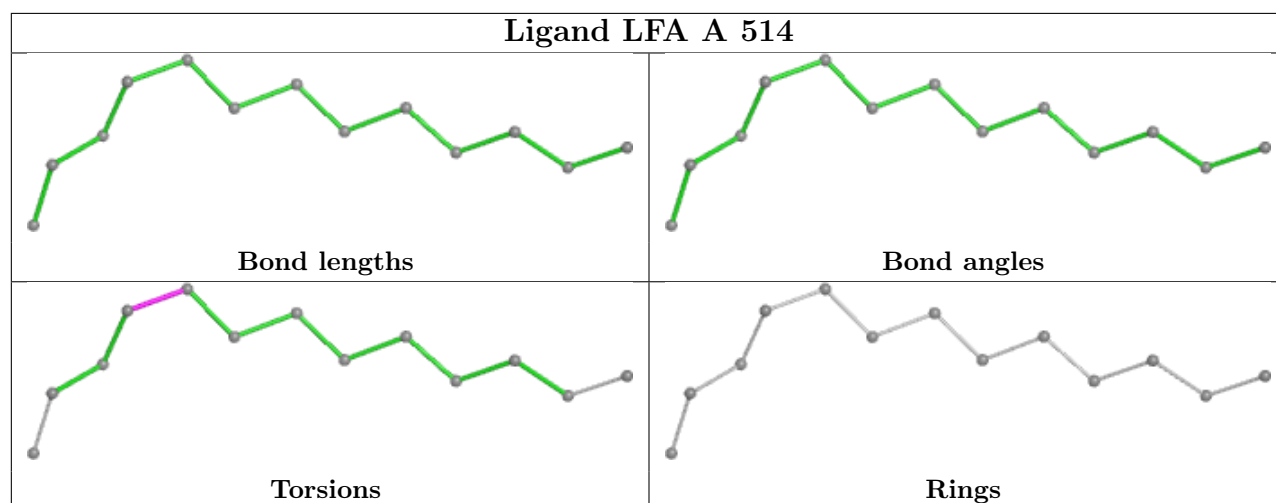
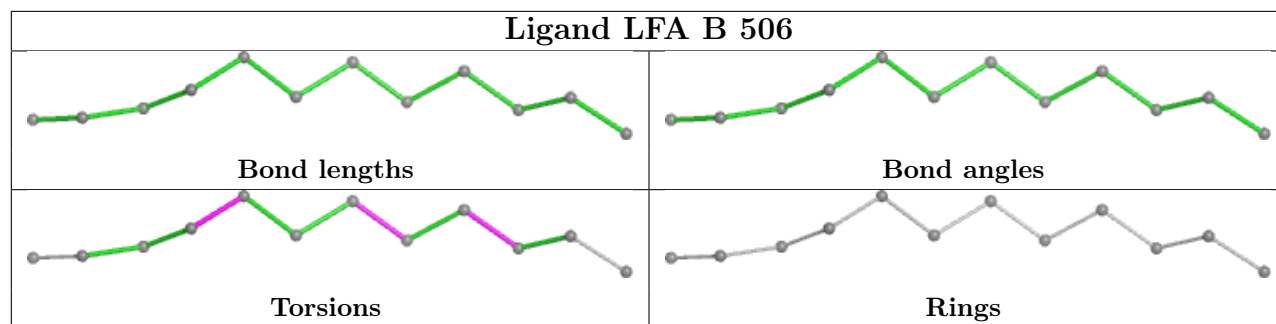
16 monomers are involved in 26 short contacts:

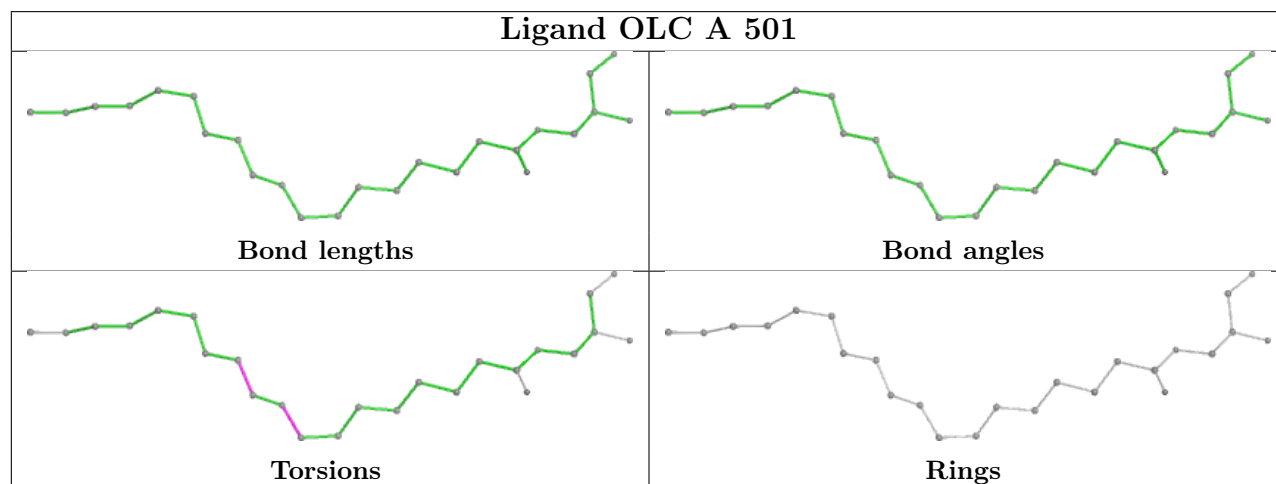
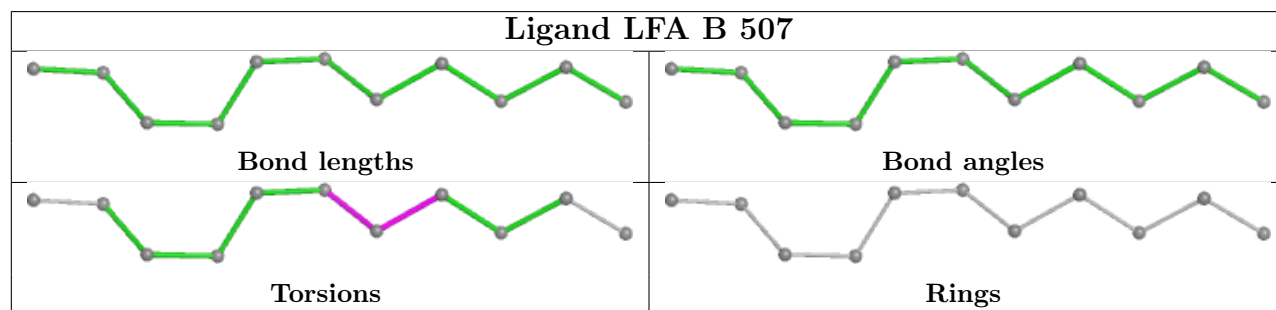
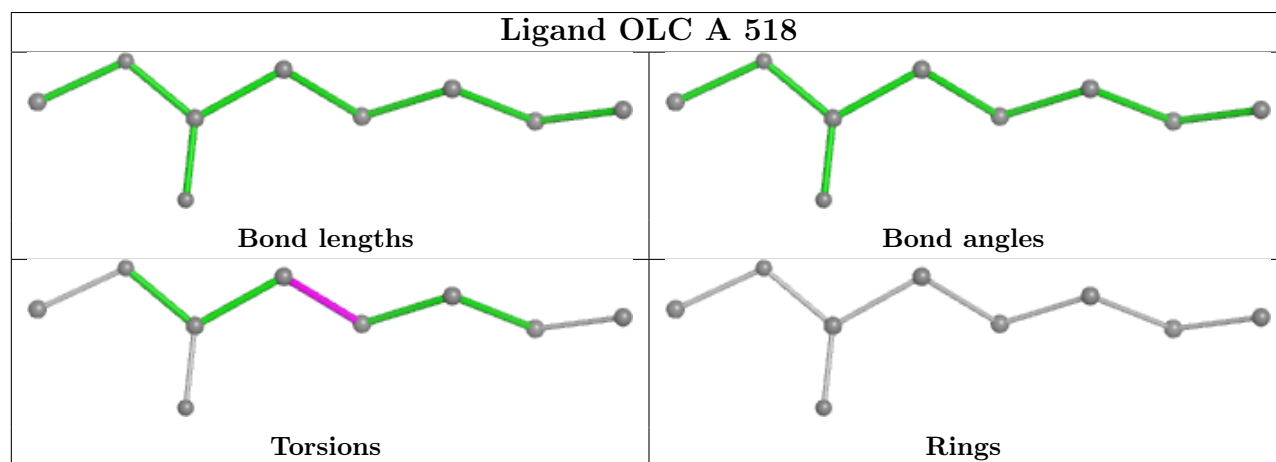
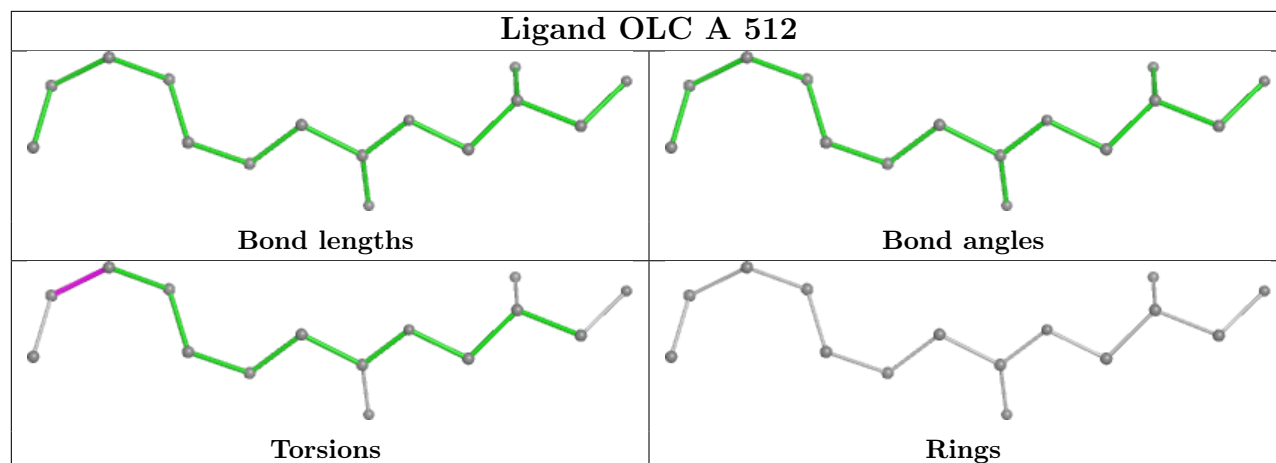
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	OLC	2	0
3	A	504	LFA	1	0
2	B	504	OLC	3	0
2	A	502	OLC	1	0
3	A	516	LFA	2	0
4	A	515	GOL	3	0
2	A	503	OLC	1	0
3	B	506	LFA	1	0
5	B	511	RET	3	0
2	A	512	OLC	1	0
2	A	518	OLC	2	0
2	A	501	OLC	3	0
4	A	519	GOL	1	0
5	A	520	RET	3	0
2	A	517	OLC	1	0
3	A	510	LFA	1	0

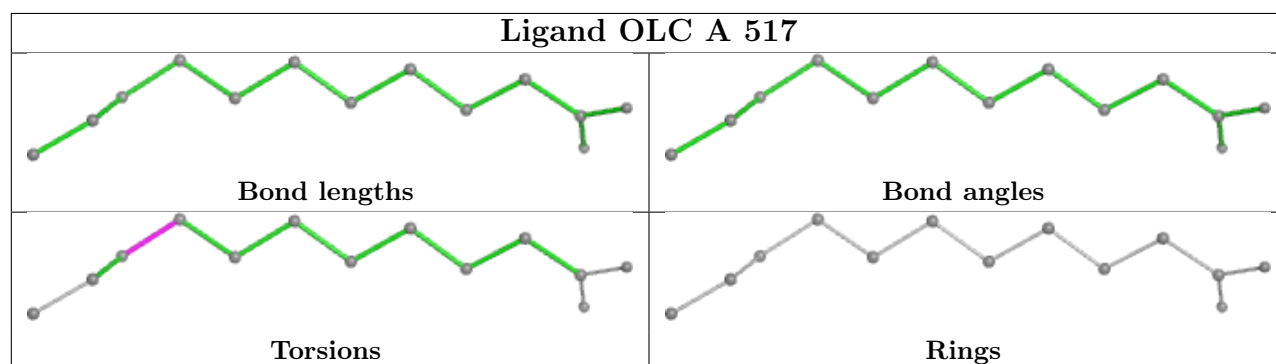
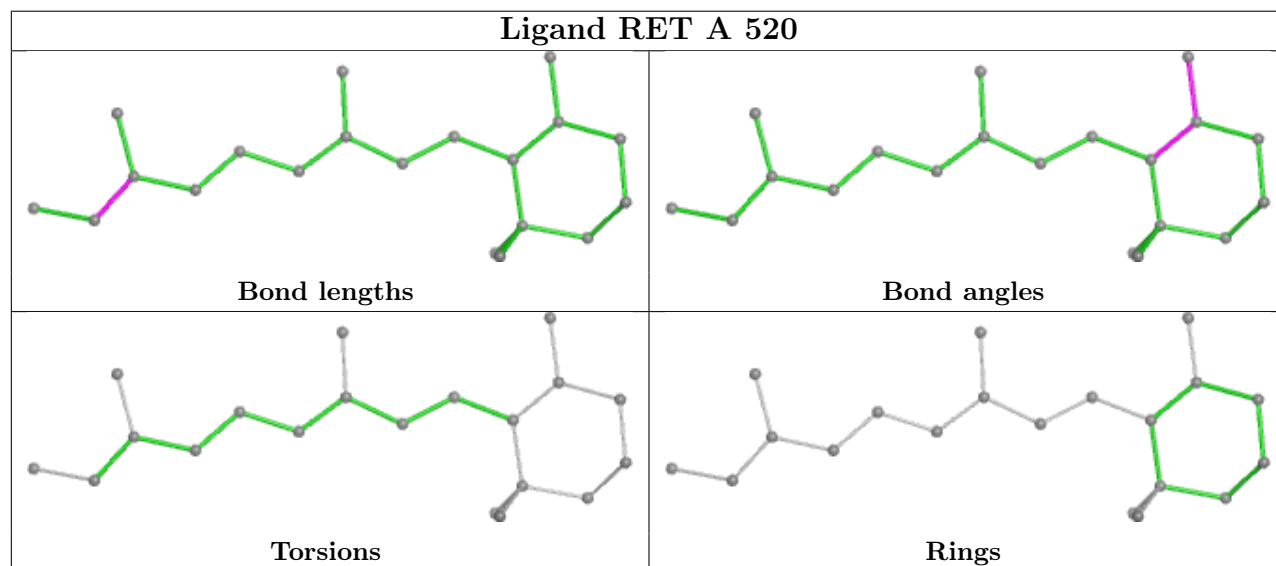
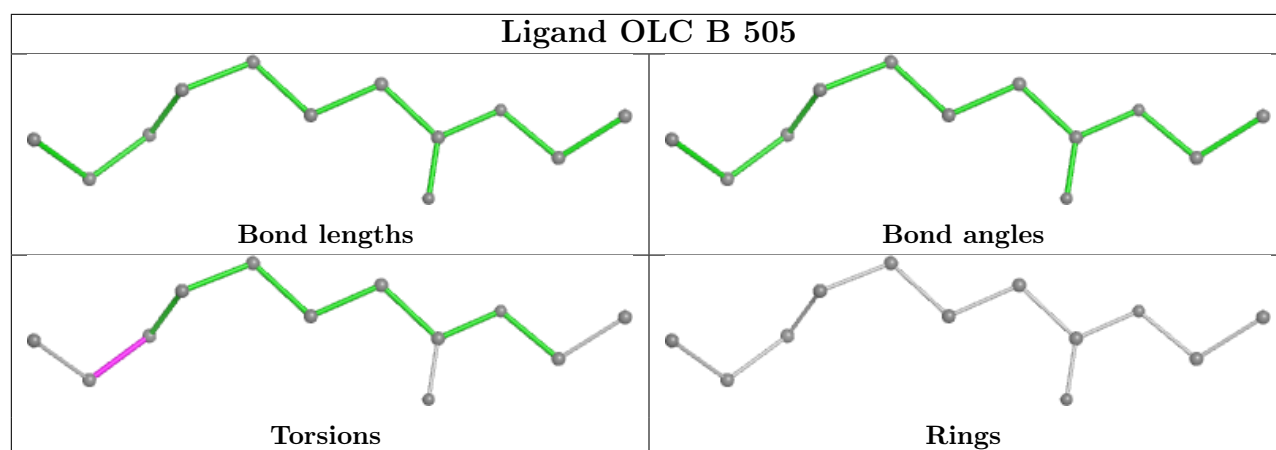
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

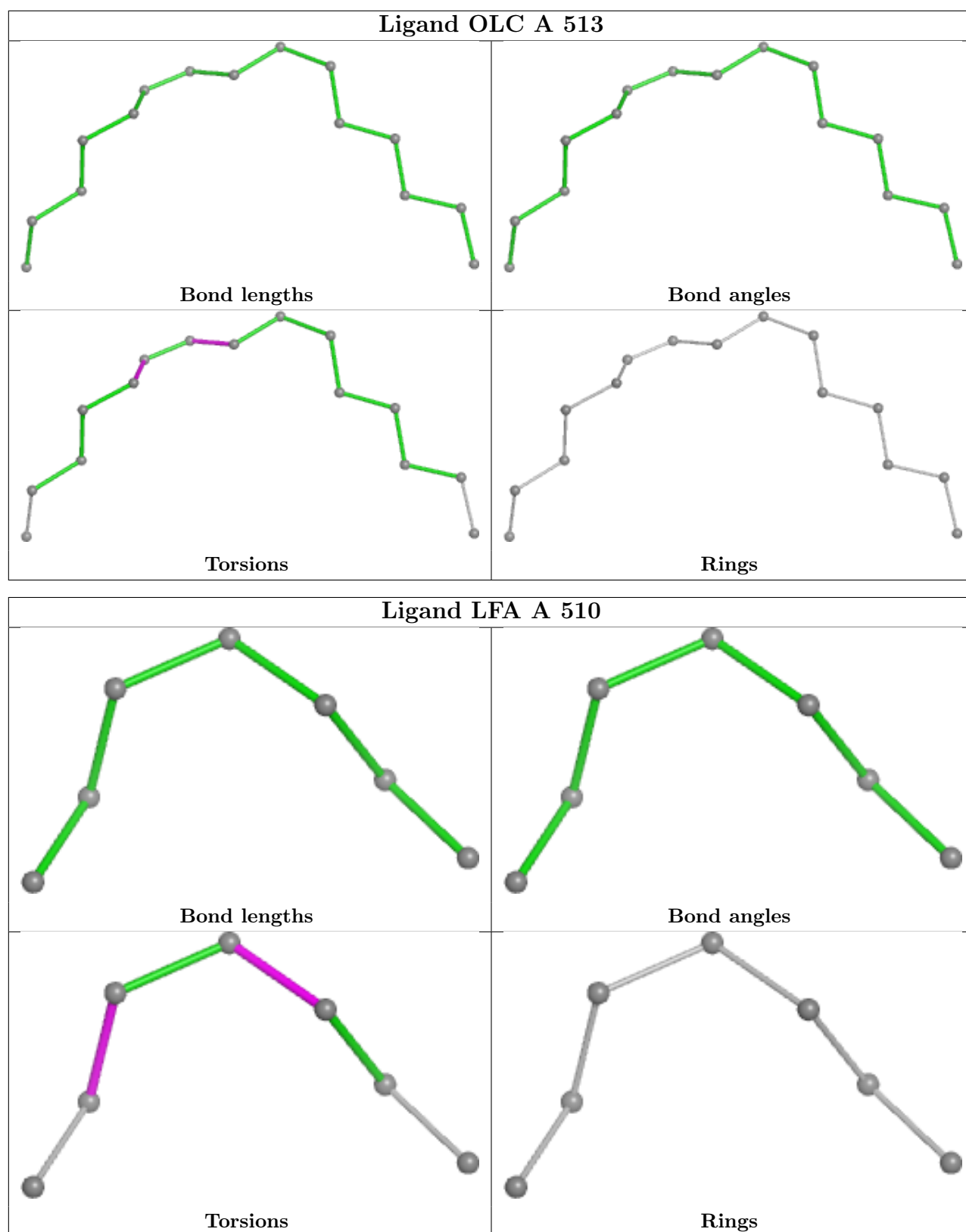












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	216/220 (98%)	0.19	3 (1%) 73 72	8, 21, 36, 45	10 (4%)
1	B	217/220 (98%)	0.25	6 (2%) 55 55	8, 21, 40, 45	14 (6%)
All	All	433/440 (98%)	0.22	9 (2%) 63 63	8, 21, 38, 45	24 (5%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	THR	3.3
1	B	63	SER	3.1
1	B	180	VAL	2.6
1	A	10[A]	MET	2.6
1	B	184	PHE	2.4
1	B	216	GLY	2.3
1	A	25	ALA	2.2
1	B	145	ALA	2.1
1	A	216	GLY	2.1

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

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

### 6.3 Carbohydrates [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,

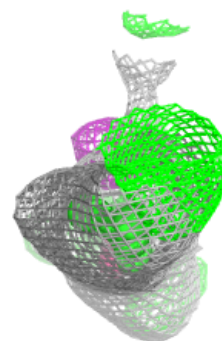
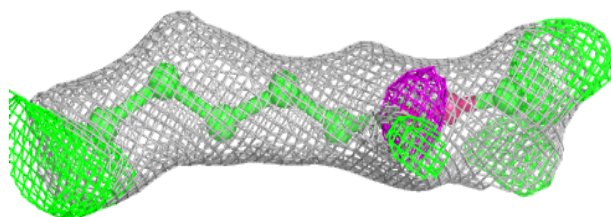
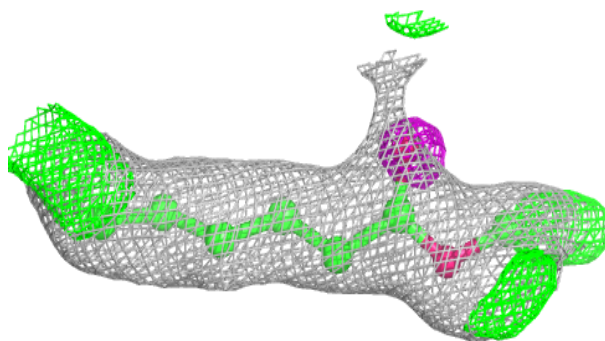
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OLC	A	518	9/25	0.69	0.16	38,41,44,46	0
2	OLC	A	512	15/25	0.77	0.15	39,45,54,54	0
2	OLC	A	502	20/25	0.78	0.15	44,46,53,53	0
2	OLC	B	503	7/25	0.78	0.14	45,47,50,51	0
3	LFA	A	506	7/20	0.78	0.18	38,39,40,40	0
3	LFA	B	508	12/20	0.78	0.15	43,45,45,46	0
3	LFA	B	509	4/20	0.78	0.19	39,40,41,41	0
4	GOL	A	519	6/6	0.78	0.13	42,45,46,47	0
3	LFA	B	502	3/20	0.79	0.17	44,44,44,44	0
2	OLC	B	504	12/25	0.80	0.14	45,47,53,53	0
3	LFA	A	505	7/20	0.80	0.13	38,41,44,44	0
2	OLC	A	517	13/25	0.80	0.14	38,41,46,46	0
3	LFA	A	516	8/20	0.80	0.15	40,42,42,43	0
3	LFA	A	514	13/20	0.81	0.13	41,43,44,44	0
2	OLC	A	503	19/25	0.81	0.14	41,43,53,54	0
4	GOL	A	515	6/6	0.81	0.14	46,47,48,48	0
2	OLC	A	501	25/25	0.81	0.15	41,44,46,48	0
6	PO4	B	510	5/5	0.81	0.11	56,58,58,59	0
2	OLC	B	505	12/25	0.82	0.14	40,42,47,49	0
3	LFA	A	510	7/20	0.83	0.14	42,42,44,44	0
3	LFA	A	509	3/20	0.84	0.17	36,36,36,37	0
3	LFA	B	506	12/20	0.84	0.15	38,39,42,43	0
4	GOL	A	511	6/6	0.84	0.12	47,47,48,50	0
2	OLC	A	513	15/25	0.86	0.12	36,41,43,44	0
3	LFA	A	508	3/20	0.86	0.13	37,37,38,39	0
3	LFA	A	507	6/20	0.87	0.11	40,40,41,41	0
3	LFA	A	504	12/20	0.87	0.15	39,41,42,43	0
3	LFA	B	507	11/20	0.87	0.11	44,44,46,46	0
3	LFA	B	501	7/20	0.93	0.10	39,40,40,41	0
5	RET	A	520	20/21	0.95	0.06	14,16,17,18	0
5	RET	B	511	20/21	0.96	0.07	14,16,17,18	0

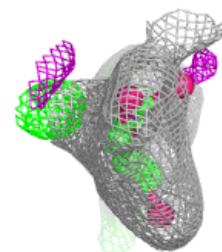
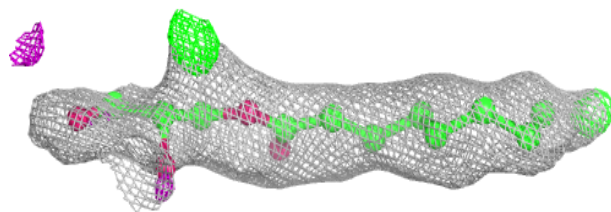
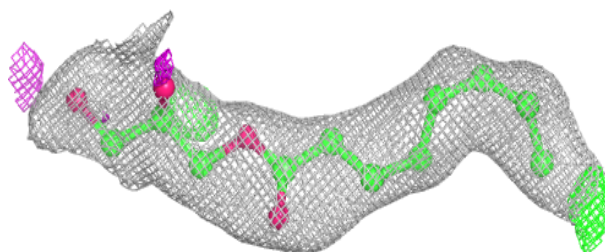
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC A 518:**

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

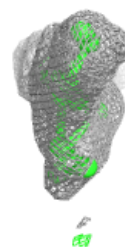
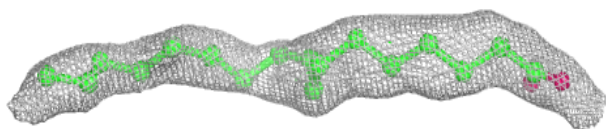
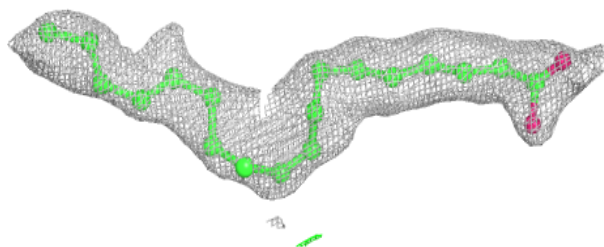
**Electron density around OLC A 512:**

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

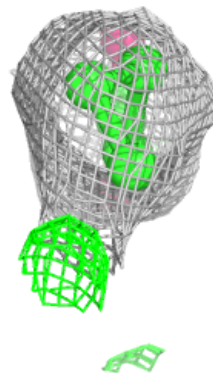
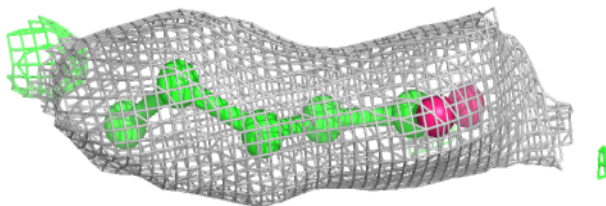
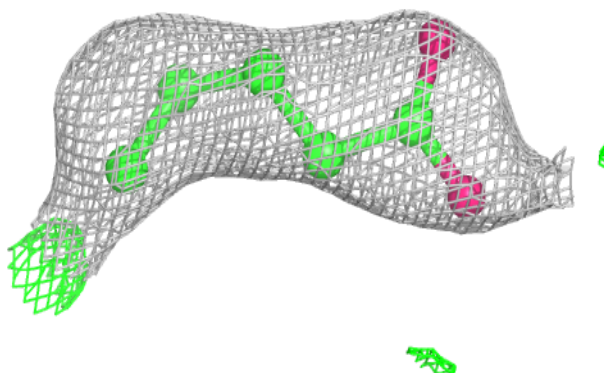


**Electron density around OLC A 502:**

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

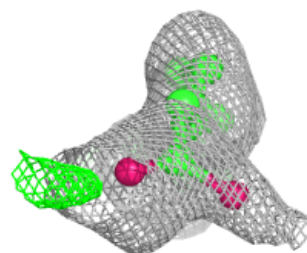
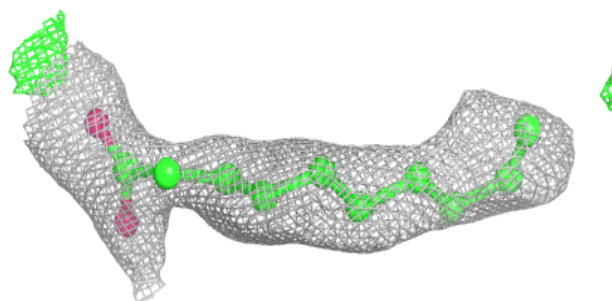
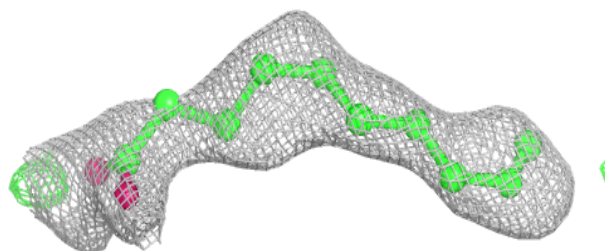
**Electron density around OLC B 503:**

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

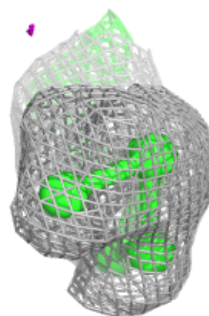
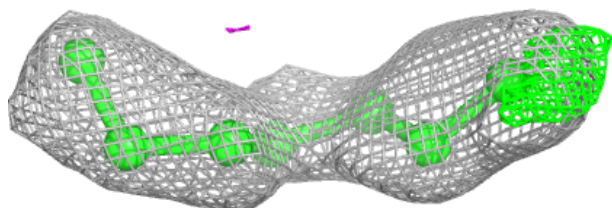
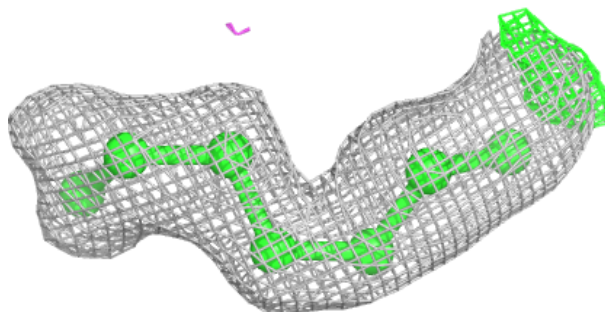


**Electron density around OLC B 504:**

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

**Electron density around LFA A 505:**

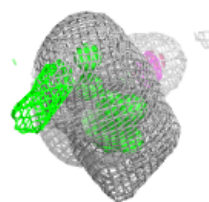
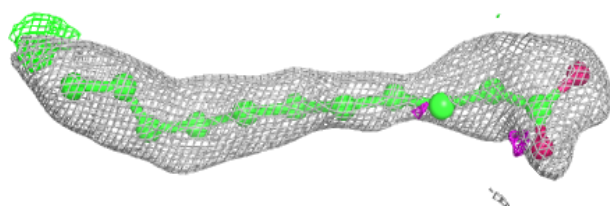
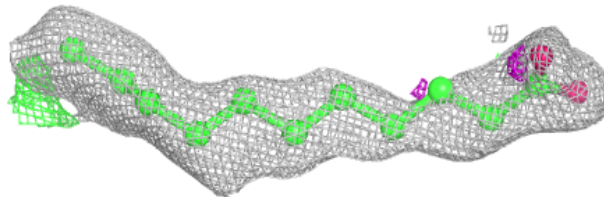
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



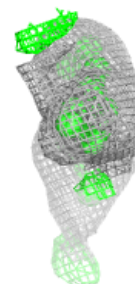
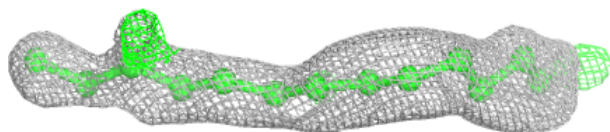
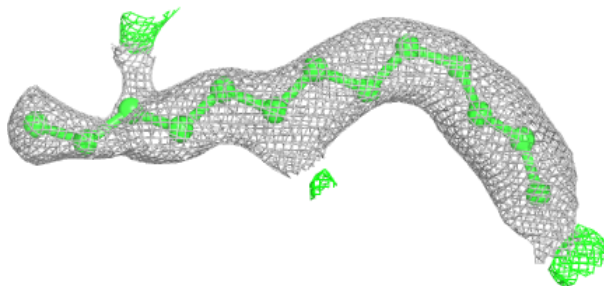


**Electron density around OLC A 517:**

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

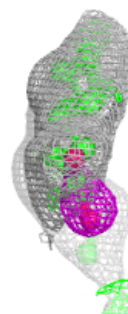
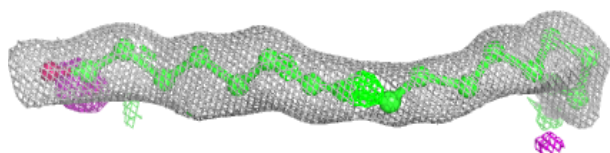
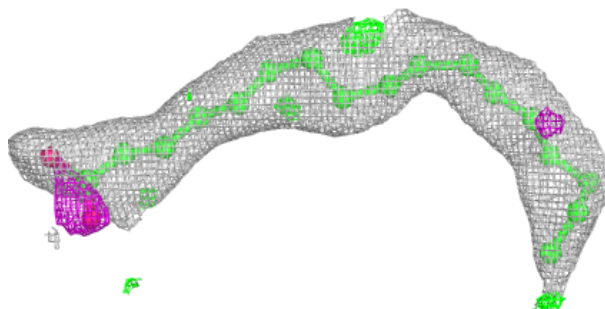
**Electron density around LFA A 514:**

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

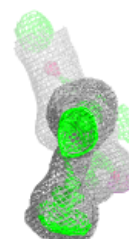
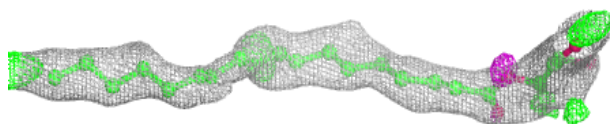
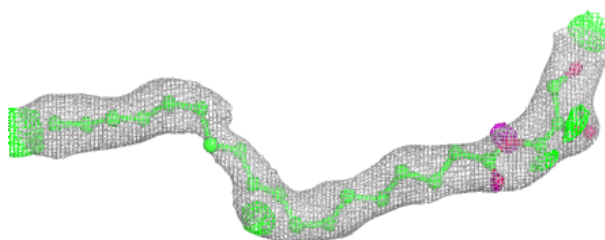


**Electron density around OLC A 503:**

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

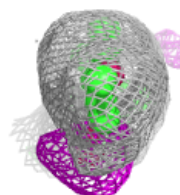
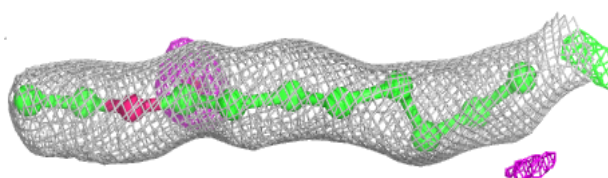
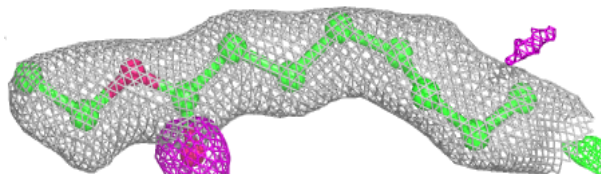
**Electron density around OLC A 501:**

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

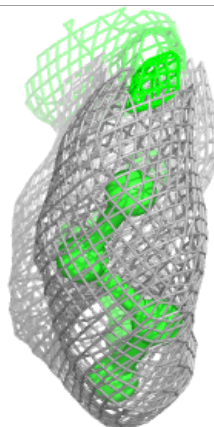
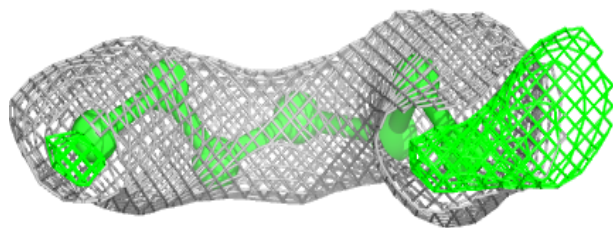
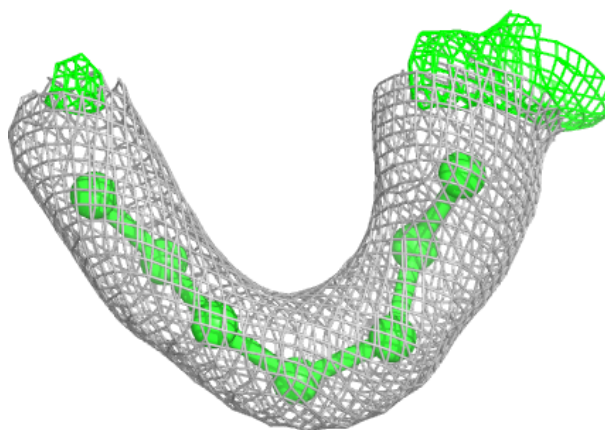


**Electron density around OLC B 505:**

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

**Electron density around LFA A 510:**

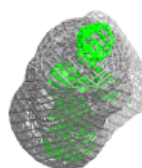
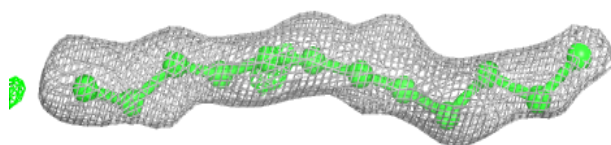
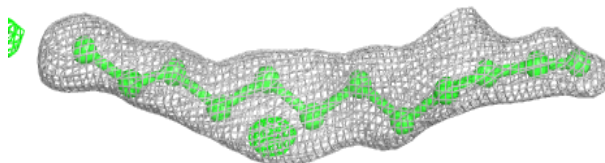
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



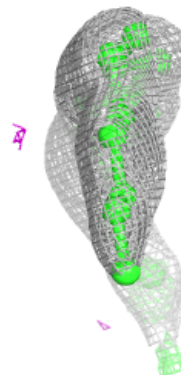
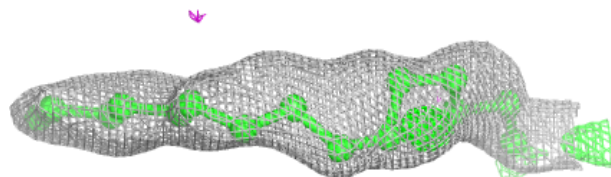
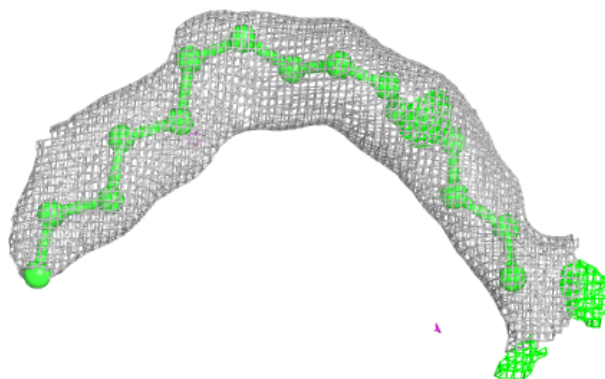


**Electron density around LFA B 506:**

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

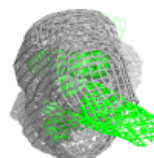
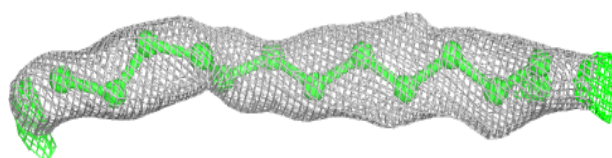
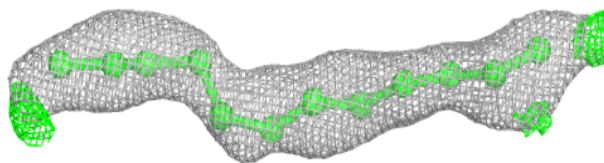
**Electron density around OLC A 513:**

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

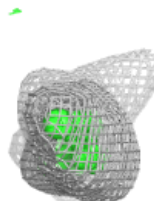
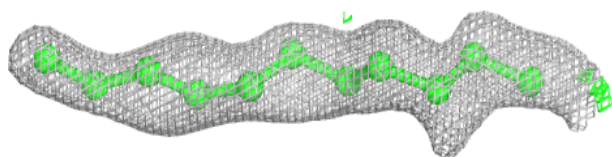
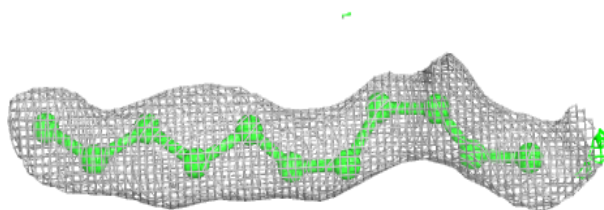


**Electron density around LFA A 504:**

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

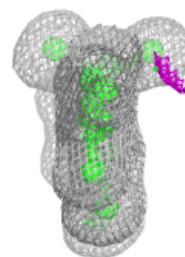
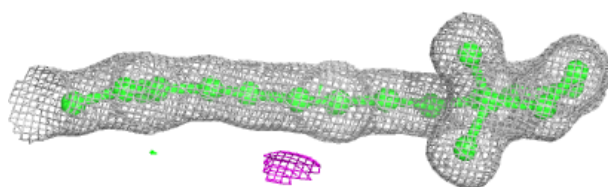
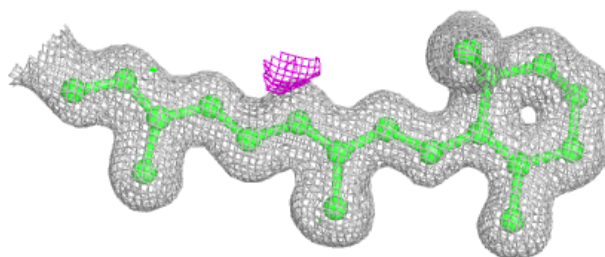
**Electron density around LFA B 507:**

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

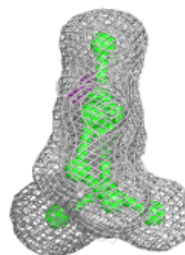
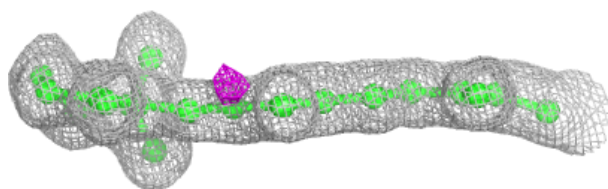
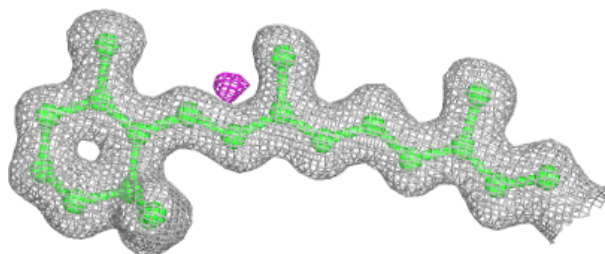


**Electron density around RET A 520:**

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

**Electron density around RET B 511:**

$2mF_o-DF_c$  (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.