



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:21 PM UTC

PDB ID : 9F9D / pdb_00009f9d
Title : Laser excitation effects on BR: Dark dataset recorded at SwissFEL
Authors : Bertrand, Q.; Weinert, T.; Standfuss, J.
Deposited on : 2024-05-07
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

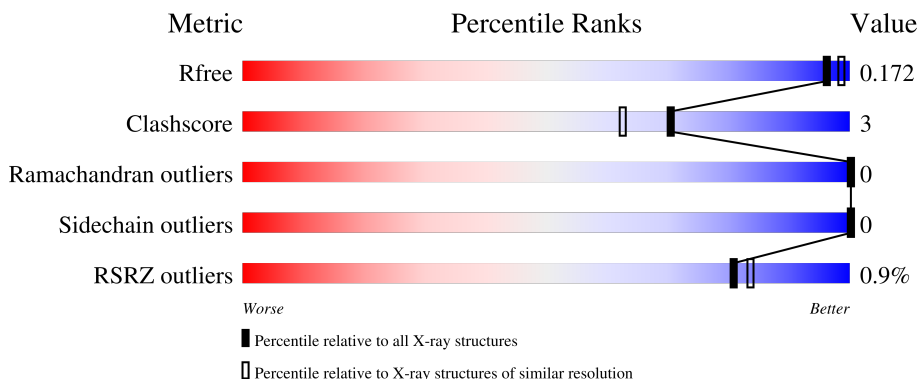
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

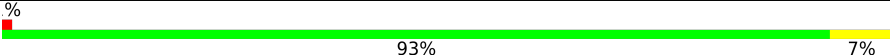
The reported resolution of this entry is 1.70 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4321 atoms, of which 2153 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.

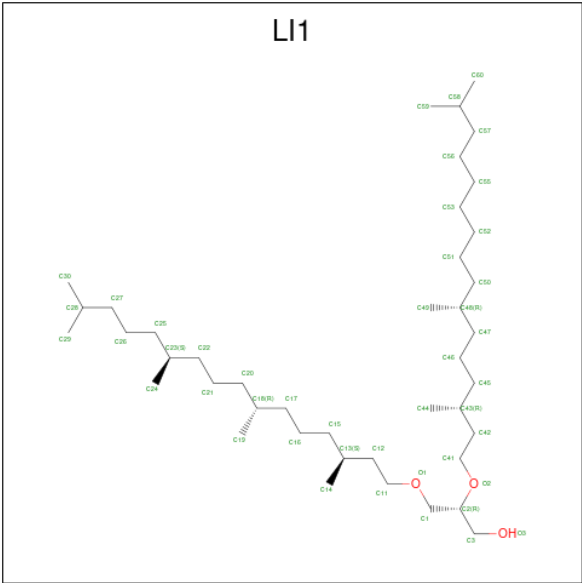
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	231	Total	C	H	N	O	S	1713	9	0
			3731	1233	1888	285	316	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	-	expression tag	UNP P02945

- Molecule 2 is 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (CCD ID: LI1) (formula: C₄₂H₈₆O₃).



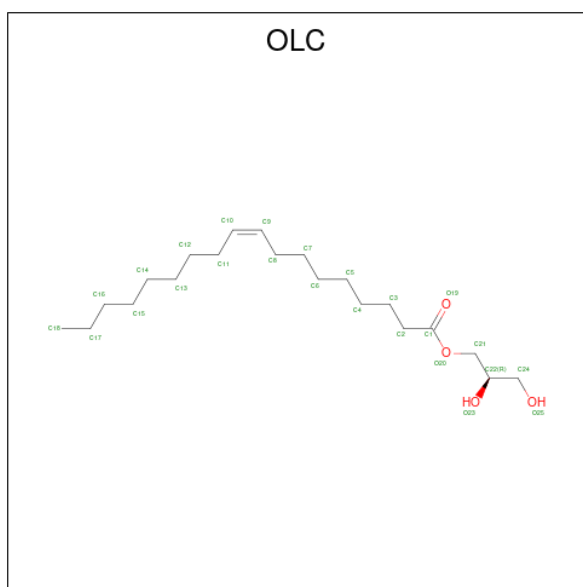
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C		0	0
			6	6			
2	A	1	Total	C	H	0	0
			19	14	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	A	1	Total C H 16 12 4	0	0
2	A	1	Total C H 19 13 6	0	0
2	A	1	Total C H 17 13 4	0	0
2	A	1	Total C H 16 10 6	0	0
2	A	1	Total C H 19 13 6	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C H 19 13 6	0	0
2	A	1	Total C 6 6	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



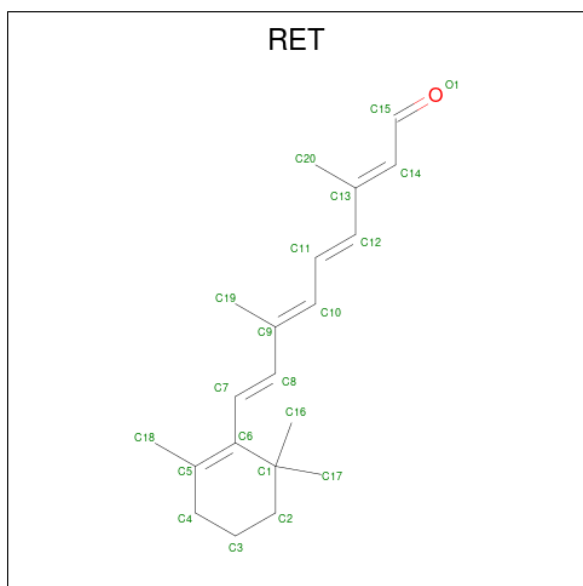
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 65 21 40 4	40	0

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

- Molecule 4 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest" by depositor).



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

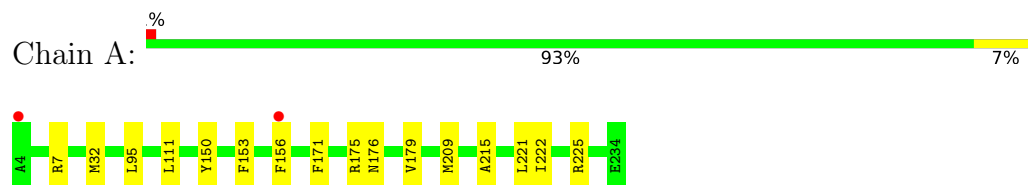
- Molecule 5 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	51	Total	O			0	0
			51	51				

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: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	62.95Å 62.95Å 111.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.02 – 1.70 16.02 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (16.02-1.70) 99.8 (16.02-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.138 , 0.172 0.138 , 0.172	Depositor DCC
R_{free} test set	2004 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 125.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4321	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LI1, RET, OLC

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	0.99	1/1897 (0.1%)	0.78	1/2591 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	ALA	CA-CB	6.37	1.64	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	MET	CG-SD-CE	-6.62	86.33	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ARG	Sidechain

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	1843	1888	1889	11	0
2	A	129	37	208	3	0
3	A	125	200	198	2	0
4	A	20	28	27	2	0
5	A	51	0	0	1	0
All	All	2168	2153	2322	15	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (15) 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:32:MET:O	5:A:401:HOH:O	1.90	0.88
1:A:95[B]:LEU:HD11	3:A:310:OLC:H11A	1.65	0.78
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.25	0.72
1:A:95[B]:LEU:HD11	3:A:310:OLC:C11	2.32	0.59
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.38	0.59
4:A:318:RET:H161	4:A:318:RET:H8	1.92	0.52
1:A:150:TYR:HB2	2:A:316:LI1:H531	1.92	0.51
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.71	0.50
2:A:314:LI1:C58	2:A:315:LI1:H571	2.44	0.48
4:A:318:RET:H7	4:A:318:RET:H181	1.80	0.44
1:A:221:LEU:O	1:A:225[A]:ARG:HG3	2.17	0.44
1:A:222:ILE:HG23	1:A:225[A]:ARG:NH2	2.34	0.42
1:A:111:LEU:HD11	1:A:156:PHE:CZ	2.56	0.41
1:A:175[B]:ARG:NH1	1:A:176:ASN:OD1	2.53	0.41
2:A:315:LI1:H561	2:A:315:LI1:H592	1.73	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/231 (103%)	236 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/184 (103%)	190 (100%)	0	100	100

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

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](#)

18 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
2	LI1	A	317	-	5,5,44	0.75	0	4,4,51	0.54	0
2	LI1	A	312	-	9,9,44	0.78	0	8,8,51	0.67	0
2	LI1	A	302	-	13,13,44	0.78	0	14,14,51	0.68	0
2	LI1	A	313	-	12,12,44	0.82	0	11,11,51	0.77	0
4	RET	A	318	1	20,20,21	1.66	2 (10%)	27,27,28	1.25	3 (11%)
2	LI1	A	301	-	5,5,44	0.72	0	4,4,51	0.57	0
3	OLC	A	307	-	24,24,24	1.02	1 (4%)	25,25,25	1.20	2 (8%)
2	LI1	A	315	-	12,12,44	0.75	0	12,12,51	0.86	0
2	LI1	A	306	-	12,12,44	0.68	0	12,12,51	1.00	0
3	OLC	A	308	-	24,24,24	0.97	1 (4%)	25,25,25	1.30	3 (12%)
3	OLC	A	309	-	24,24,24	1.11	1 (4%)	25,25,25	1.43	3 (12%)
3	OLC	A	310	-	24,24,24	1.08	1 (4%)	25,25,25	1.21	2 (8%)
2	LI1	A	305	-	12,12,44	0.76	0	11,11,51	0.79	0
2	LI1	A	303	-	7,7,44	0.83	0	6,6,51	0.55	0
2	LI1	A	316	-	12,12,44	0.83	0	11,11,51	0.76	0
3	OLC	A	311	-	24,24,24	1.06	1 (4%)	25,25,25	1.15	1 (4%)
2	LI1	A	314	-	7,7,44	0.78	0	6,6,51	0.57	0
2	LI1	A	304	-	11,11,44	0.82	0	10,10,51	0.64	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
2	LI1	A	317	-	-	3/3/3/49	-
2	LI1	A	312	-	-	6/7/7/49	-
2	LI1	A	302	-	-	4/12/12/49	-
2	LI1	A	313	-	-	4/10/10/49	-
4	RET	A	318	1	-	1/13/30/31	0/1/1/1
2	LI1	A	301	-	-	0/3/3/49	-
3	OLC	A	307	-	-	4/24/24/24	-
2	LI1	A	315	-	-	5/10/10/49	-
2	LI1	A	306	-	-	6/10/10/49	-
3	OLC	A	308	-	-	4/24/24/24	-
3	OLC	A	309	-	-	16/24/24/24	-
3	OLC	A	310	-	-	11/24/24/24	-
2	LI1	A	305	-	-	3/10/10/49	-
2	LI1	A	303	-	-	5/5/5/49	-
2	LI1	A	316	-	-	5/10/10/49	-
3	OLC	A	311	-	-	11/24/24/24	-
2	LI1	A	314	-	-	3/5/5/49	-
2	LI1	A	304	-	-	5/9/9/49	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	318	RET	C15-C14	-4.71	1.32	1.49
4	A	318	RET	C14-C13	4.57	1.36	1.33
3	A	309	OLC	O20-C1	3.10	1.42	1.33
3	A	310	OLC	O20-C1	2.85	1.41	1.33
3	A	311	OLC	O20-C1	2.84	1.41	1.33
3	A	308	OLC	O20-C1	2.79	1.41	1.33
3	A	307	OLC	O20-C1	2.33	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	310	OLC	C8-C9-C10	4.04	155.08	124.83
3	A	311	OLC	C8-C9-C10	3.96	154.50	124.83
3	A	309	OLC	C8-C9-C10	3.86	153.74	124.83
3	A	308	OLC	C8-C9-C10	3.83	153.51	124.83
4	A	318	RET	C7-C8-C9	3.70	131.71	126.23
3	A	309	OLC	O20-C1-C2	3.63	122.91	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	307	OLC	C8-C9-C10	3.62	151.96	124.83
3	A	310	OLC	O20-C1-C2	2.80	120.37	111.83
4	A	318	RET	C8-C7-C6	2.66	134.10	127.00
3	A	308	OLC	O20-C1-C2	2.35	119.02	111.83
3	A	309	OLC	O20-C1-O19	-2.10	118.38	123.63
3	A	308	OLC	C4-C3-C2	-2.06	105.57	113.13
4	A	318	RET	C2-C3-C4	2.05	115.78	111.28
3	A	307	OLC	O20-C1-C2	2.02	118.00	111.83

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	309	OLC	O20-C21-C22-C24
3	A	311	OLC	O20-C21-C22-C24
3	A	311	OLC	O20-C21-C22-O23
3	A	310	OLC	O19-C1-O20-C21
3	A	310	OLC	C2-C1-O20-C21
3	A	311	OLC	C2-C1-O20-C21
3	A	309	OLC	O20-C21-C22-O23
3	A	311	OLC	O19-C1-O20-C21
3	A	310	OLC	C1-C2-C3-C4
3	A	309	OLC	C1-C2-C3-C4
2	A	304	LI1	C53-C55-C56-C57
3	A	309	OLC	C21-C22-C24-O25
2	A	302	LI1	C56-C57-C58-C60
2	A	312	LI1	C46-C47-C48-C50
2	A	312	LI1	C47-C48-C50-C51
3	A	309	OLC	C3-C4-C5-C6
3	A	310	OLC	C12-C13-C14-C15
2	A	313	LI1	C50-C51-C52-C53
2	A	305	LI1	C53-C55-C56-C57
2	A	316	LI1	C50-C51-C52-C53
3	A	307	OLC	C12-C13-C14-C15
2	A	303	LI1	C53-C55-C56-C57
3	A	309	OLC	C4-C5-C6-C7
2	A	315	LI1	C46-C47-C48-C50
2	A	313	LI1	C51-C52-C53-C55
2	A	304	LI1	C50-C51-C52-C53
2	A	317	LI1	C55-C56-C57-C58
2	A	306	LI1	C56-C57-C58-C60
3	A	309	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	A	314	LI1	C52-C53-C55-C56
2	A	303	LI1	C51-C52-C53-C55
2	A	315	LI1	C52-C53-C55-C56
2	A	313	LI1	C52-C53-C55-C56
3	A	309	OLC	C11-C12-C13-C14
3	A	310	OLC	C3-C4-C5-C6
2	A	302	LI1	C51-C52-C53-C55
3	A	311	OLC	C3-C4-C5-C6
3	A	309	OLC	C13-C14-C15-C16
2	A	305	LI1	C48-C50-C51-C52
2	A	303	LI1	C52-C53-C55-C56
3	A	310	OLC	C6-C7-C8-C9
2	A	306	LI1	C53-C55-C56-C57
3	A	310	OLC	C13-C14-C15-C16
4	A	318	RET	C12-C13-C14-C15
2	A	303	LI1	C50-C51-C52-C53
2	A	316	LI1	C52-C53-C55-C56
2	A	314	LI1	C55-C56-C57-C58
2	A	315	LI1	C56-C57-C58-C60
2	A	312	LI1	C52-C53-C55-C56
2	A	306	LI1	C46-C47-C48-C50
2	A	312	LI1	C45-C46-C47-C48
2	A	316	LI1	C45-C46-C47-C48
2	A	313	LI1	C45-C46-C47-C48
2	A	304	LI1	C52-C53-C55-C56
2	A	302	LI1	C56-C57-C58-C59
2	A	306	LI1	C56-C57-C58-C59
2	A	317	LI1	C52-C53-C55-C56
2	A	317	LI1	C53-C55-C56-C57
3	A	311	OLC	C2-C3-C4-C5
2	A	315	LI1	C56-C57-C58-C59
3	A	310	OLC	C11-C12-C13-C14
3	A	309	OLC	C7-C8-C9-C10
2	A	316	LI1	C47-C48-C50-C51
2	A	312	LI1	C50-C51-C52-C53
3	A	311	OLC	C12-C13-C14-C15
2	A	303	LI1	C55-C56-C57-C58
3	A	310	OLC	C2-C3-C4-C5
2	A	304	LI1	C51-C52-C53-C55
2	A	305	LI1	C56-C57-C58-C59
3	A	307	OLC	C11-C12-C13-C14
3	A	308	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	A	309	OLC	C12-C13-C14-C15
3	A	309	OLC	C15-C16-C17-C18
3	A	307	OLC	C14-C15-C16-C17
3	A	307	OLC	C3-C4-C5-C6
2	A	306	LI1	C47-C48-C50-C51
2	A	315	LI1	C47-C48-C50-C51
2	A	316	LI1	C53-C55-C56-C57
3	A	308	OLC	C9-C10-C11-C12
3	A	308	OLC	C12-C13-C14-C15
3	A	309	OLC	C2-C1-O20-C21
3	A	311	OLC	C7-C8-C9-C10
2	A	314	LI1	C50-C51-C52-C53
2	A	312	LI1	C51-C52-C53-C55
3	A	310	OLC	C7-C8-C9-C10
3	A	308	OLC	C3-C4-C5-C6
2	A	304	LI1	C47-C48-C50-C51
2	A	302	LI1	C50-C51-C52-C53
3	A	309	OLC	C2-C3-C4-C5
3	A	311	OLC	C9-C10-C11-C12
3	A	309	OLC	O19-C1-O20-C21
3	A	311	OLC	O20-C1-C2-C3
2	A	306	LI1	C52-C53-C55-C56
3	A	311	OLC	O19-C1-C2-C3
3	A	309	OLC	O23-C22-C24-O25
3	A	310	OLC	O20-C1-C2-C3

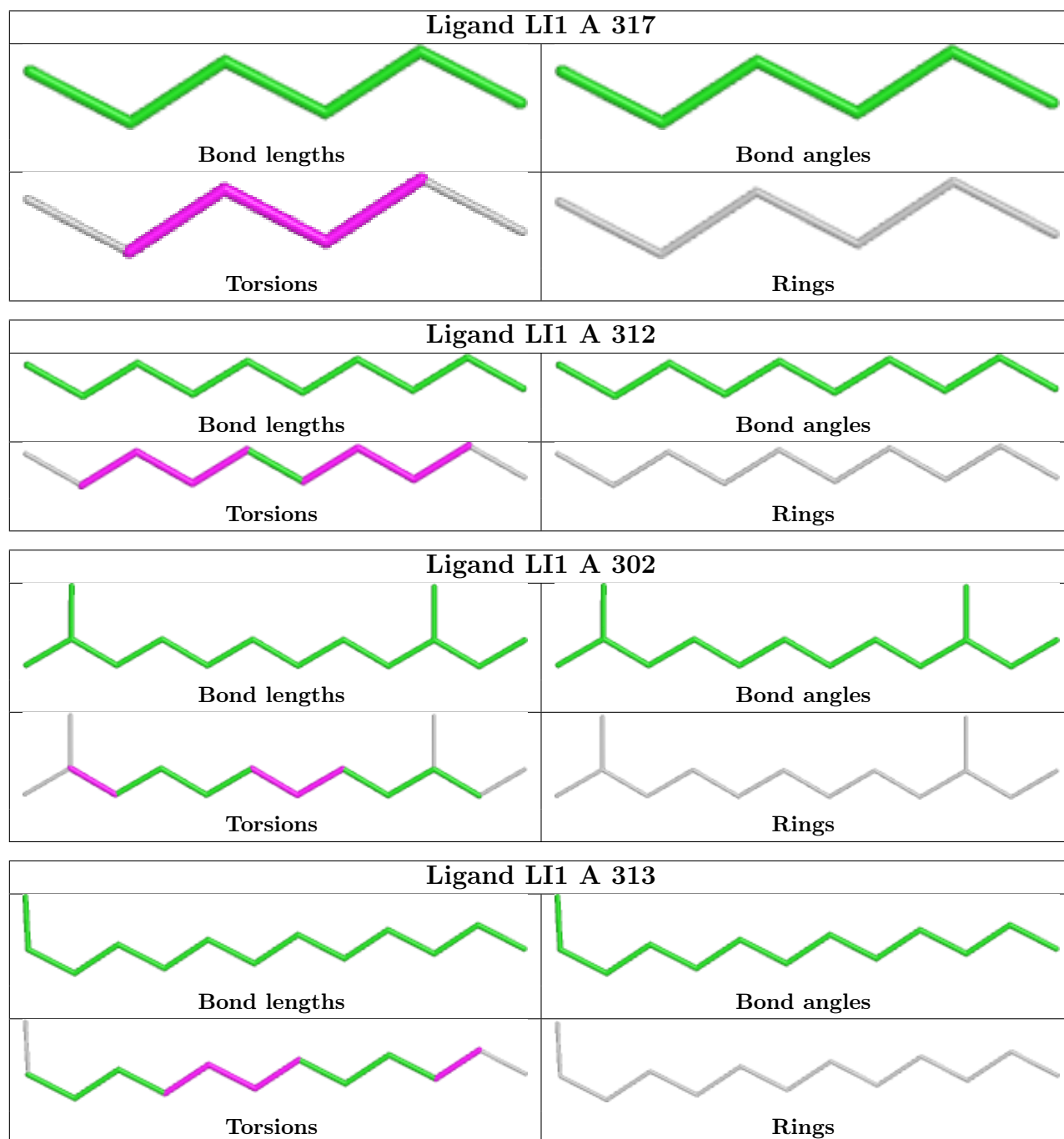
There are no ring outliers.

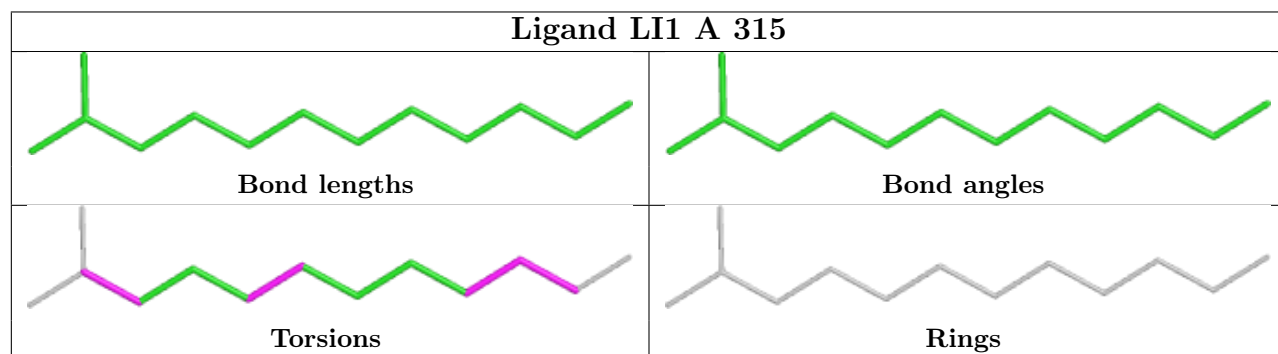
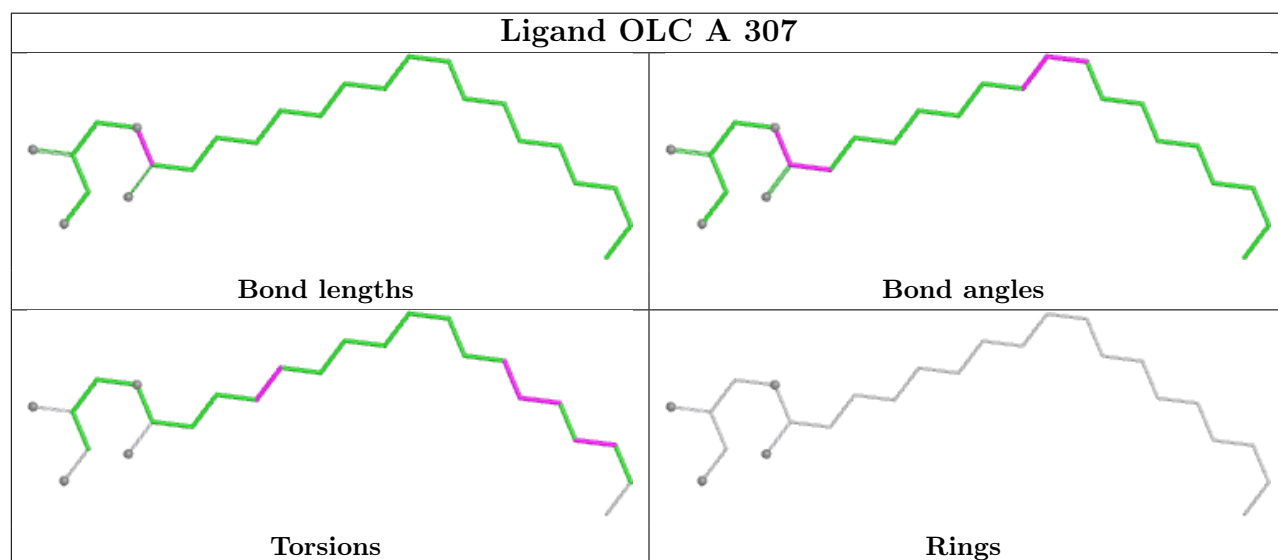
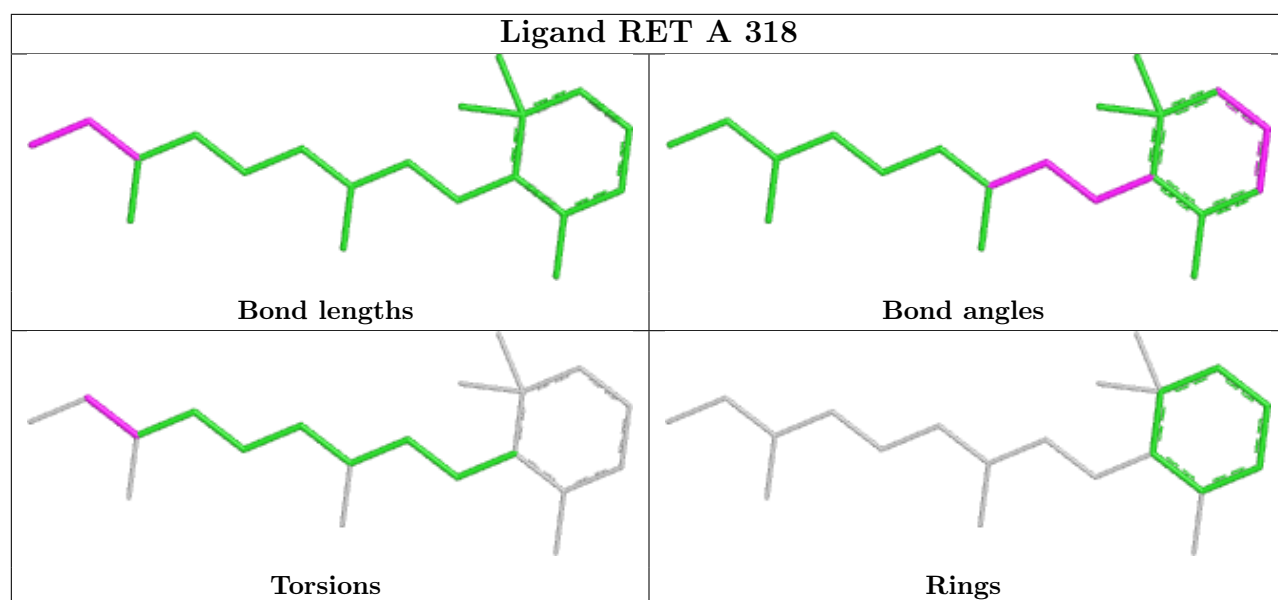
5 monomers are involved in 7 short contacts:

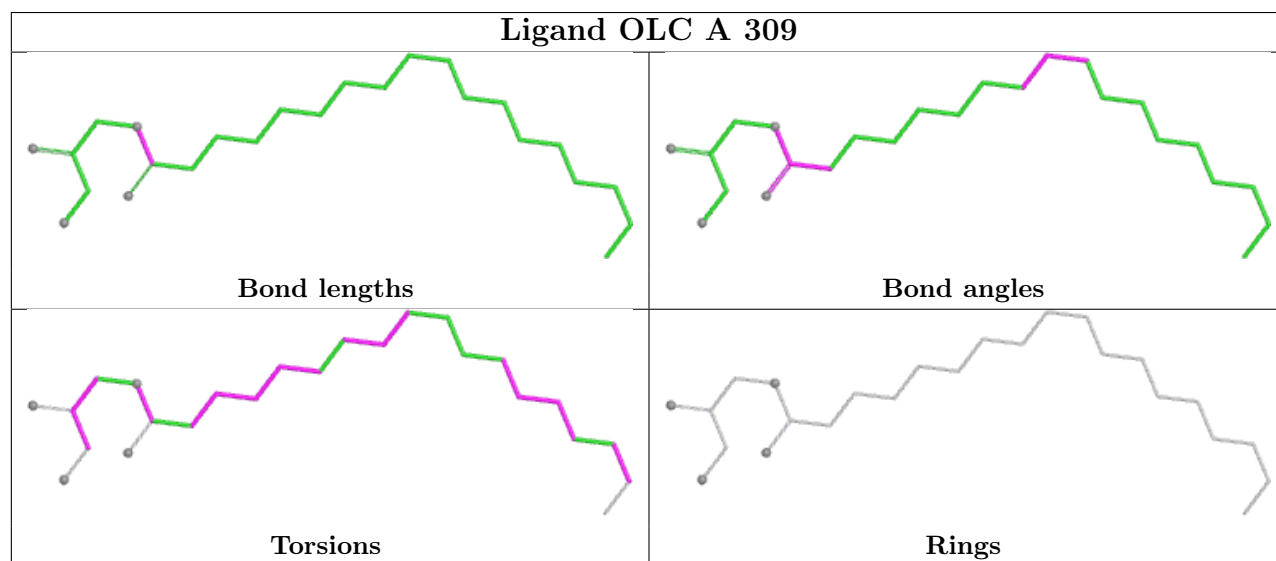
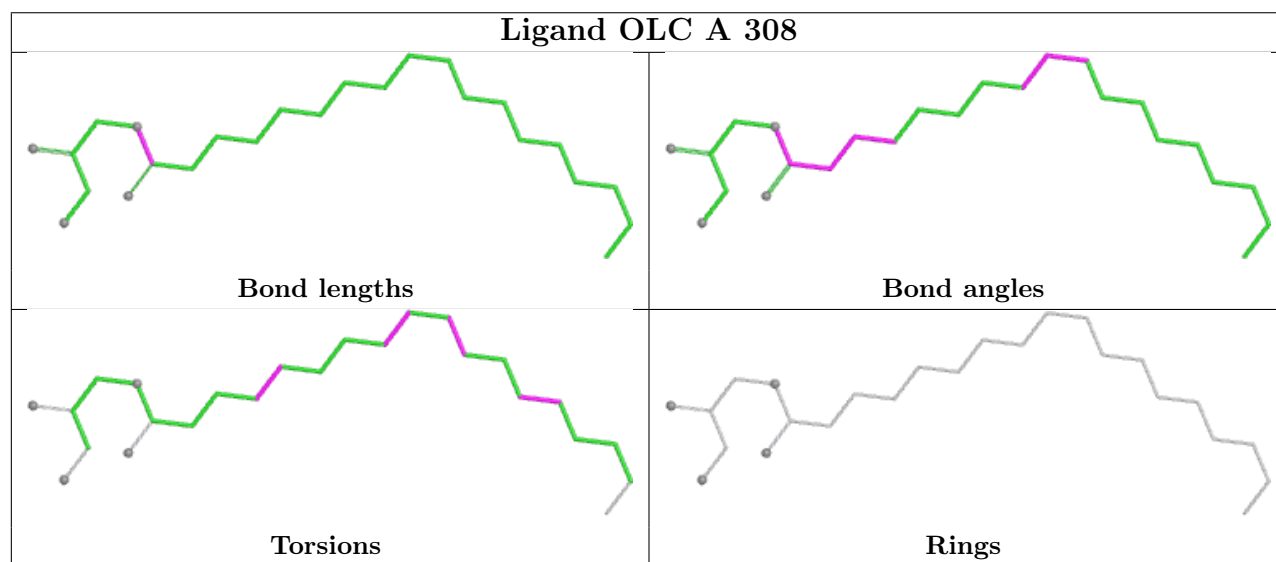
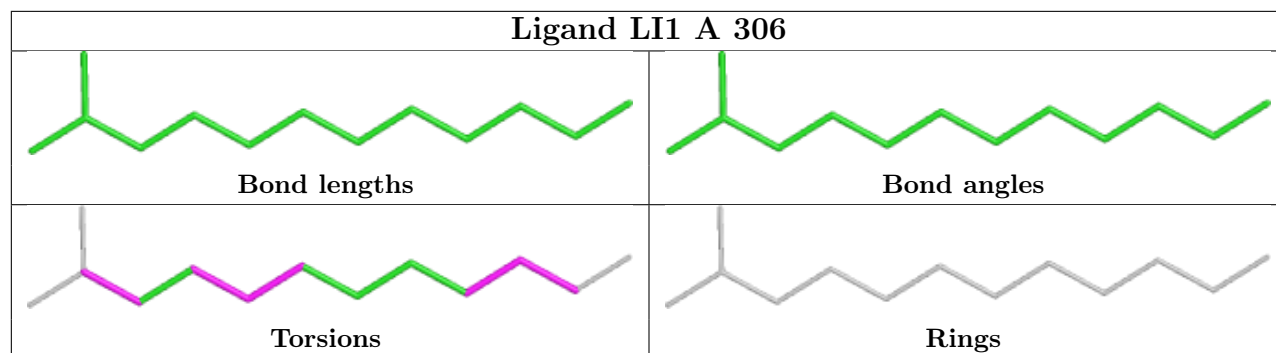
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	318	RET	2	0
2	A	315	LI1	2	0
3	A	310	OLC	2	0
2	A	316	LI1	1	0
2	A	314	LI1	1	0

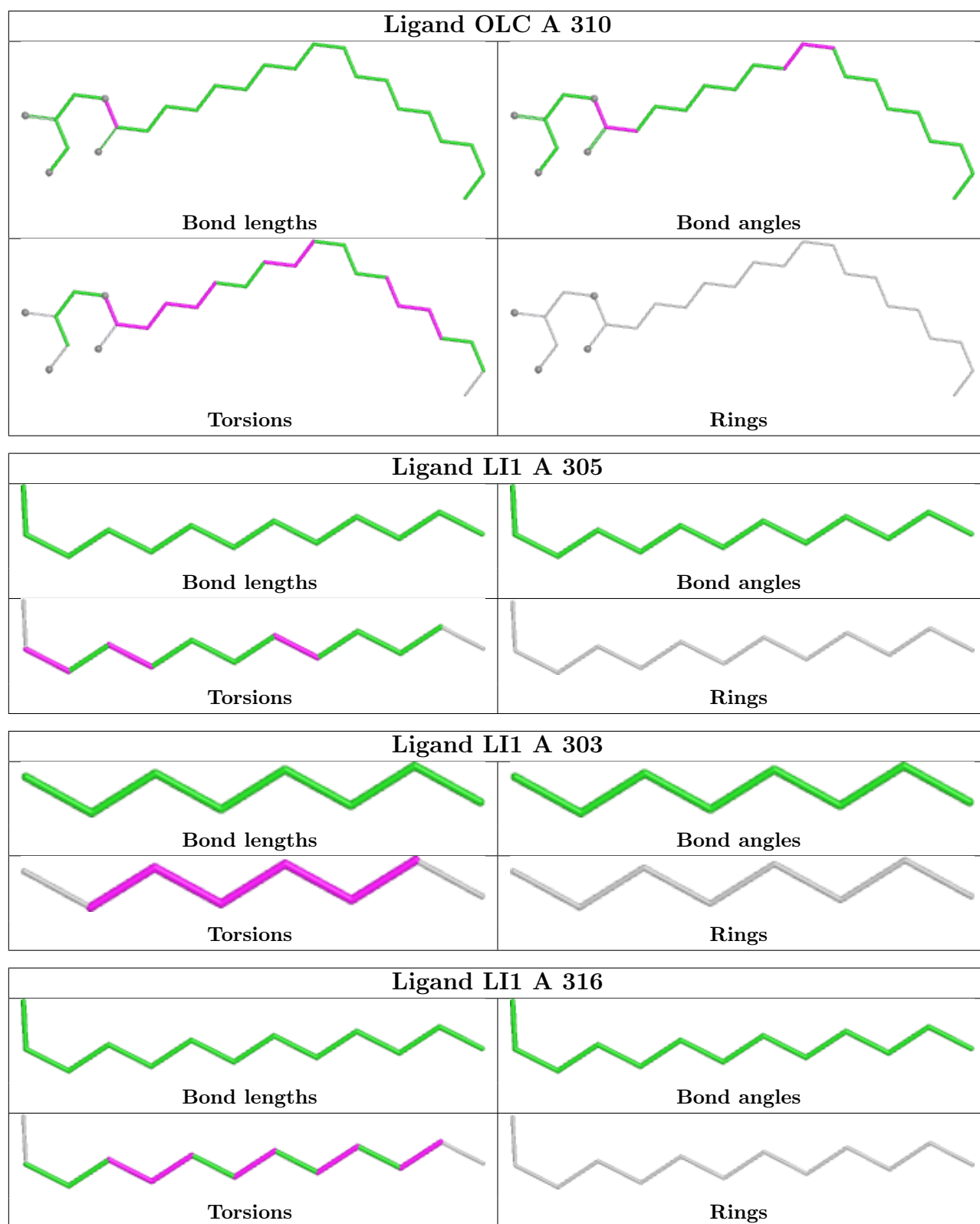
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

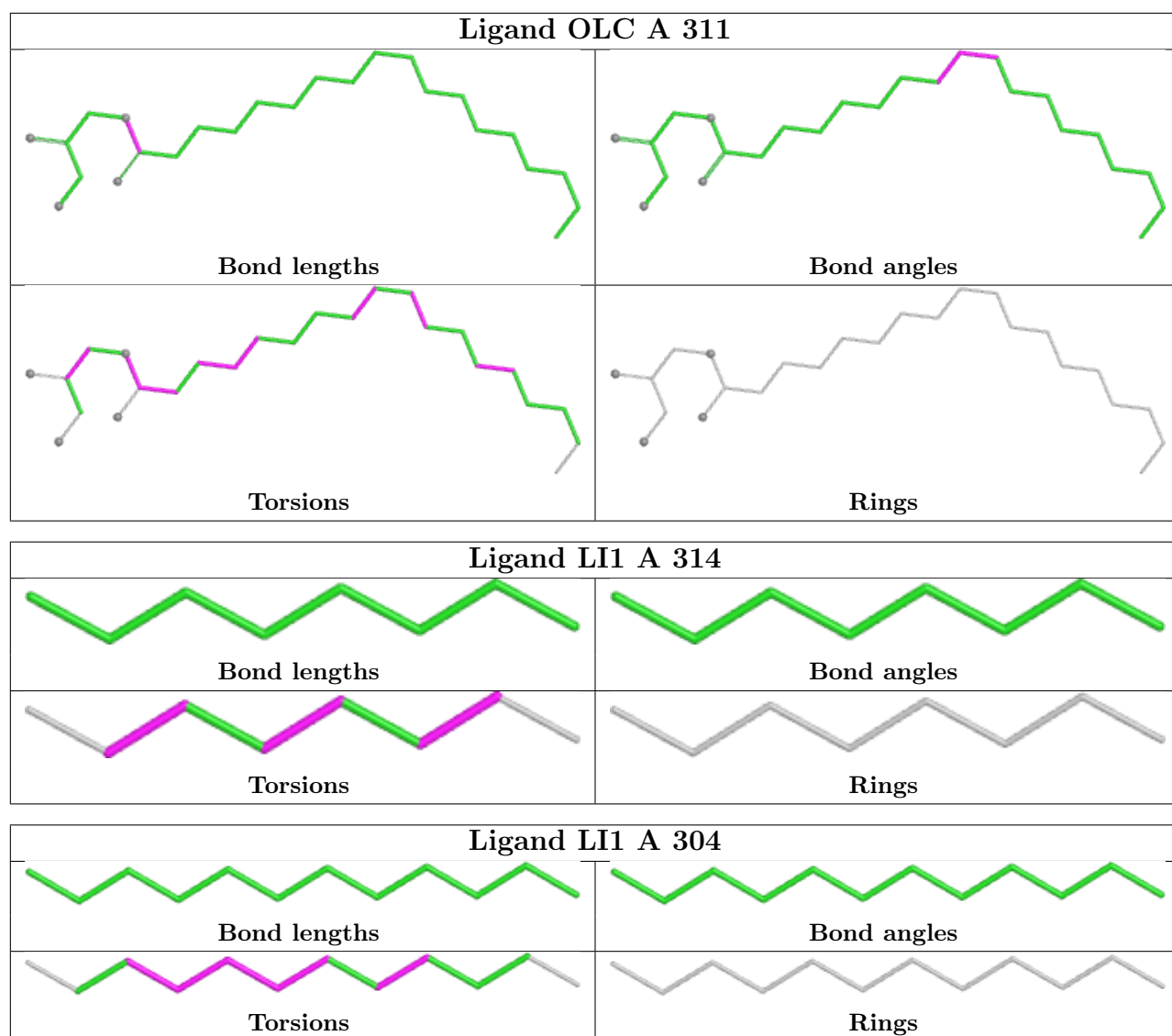
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/231 (100%)	-0.36	2 (0%) 81 83	9, 16, 37, 87	9 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ALA	2.8
1	A	156	PHE	2.4

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

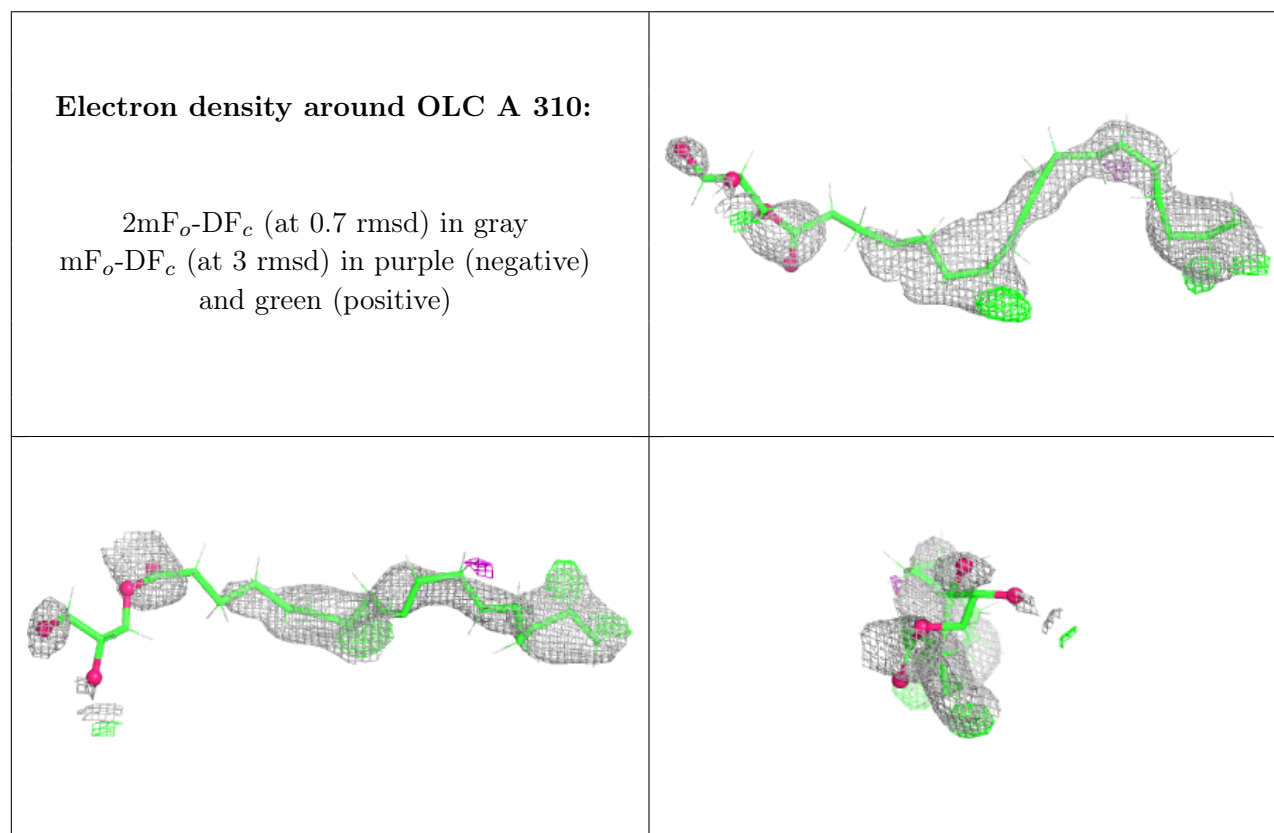
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLC	A	310	25/25	0.66	0.13	63,89,126,144	40
3	OLC	A	309	25/25	0.68	0.13	58,85,109,132	40
2	LI1	A	313	13/45	0.69	0.12	58,79,99,99	0
3	OLC	A	311	25/25	0.72	0.13	60,97,133,135	40
2	LI1	A	316	13/45	0.75	0.12	63,76,95,95	0

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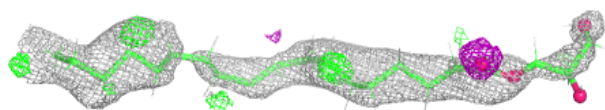
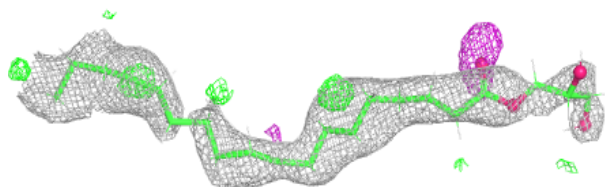
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LI1	A	314	8/45	0.75	0.12	56,74,84,90	0
2	LI1	A	301	6/45	0.78	0.12	49,57,59,71	0
2	LI1	A	315	13/45	0.78	0.09	71,80,92,100	0
2	LI1	A	312	10/45	0.79	0.09	58,82,102,102	0
2	LI1	A	306	13/45	0.81	0.11	60,82,120,120	0
2	LI1	A	317	6/45	0.82	0.08	62,72,81,83	0
2	LI1	A	303	8/45	0.83	0.11	58,62,66,69	0
2	LI1	A	304	12/45	0.83	0.10	49,64,76,76	0
2	LI1	A	302	14/45	0.84	0.09	57,73,98,103	0
2	LI1	A	305	13/45	0.86	0.08	65,74,93,93	0
3	OLC	A	307	25/25	0.87	0.11	44,67,86,96	40
3	OLC	A	308	25/25	0.89	0.08	42,72,97,113	40
4	RET	A	318	20/21	0.95	0.06	21,29,38,45	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.

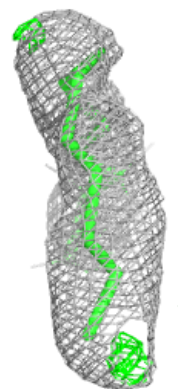
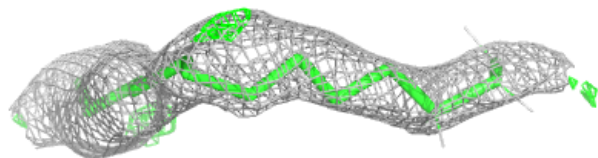
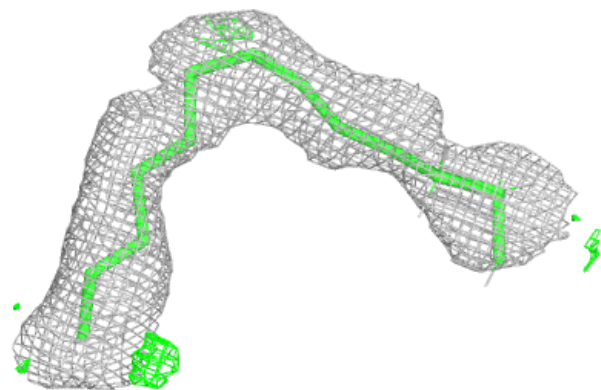


Electron density around OLC A 309:

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

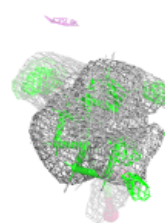
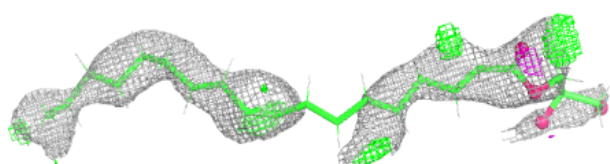
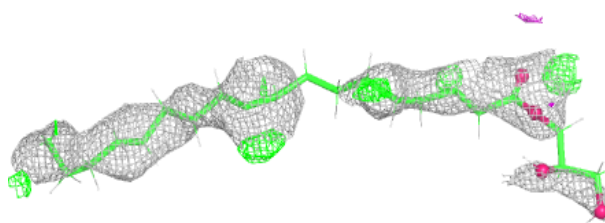
**Electron density around LI1 A 313:**

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

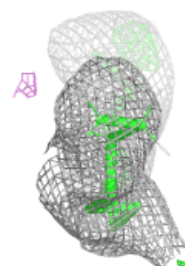
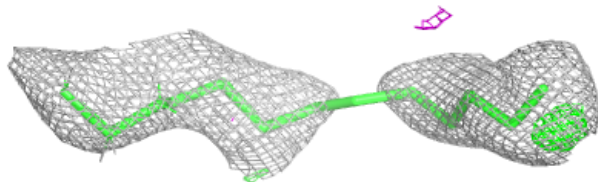
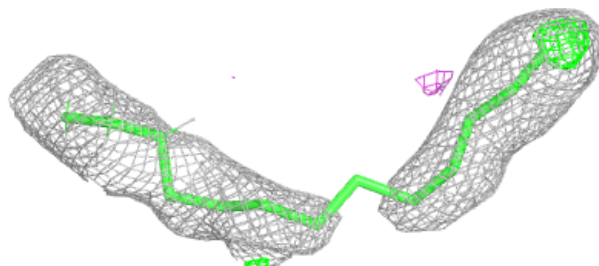


Electron density around OLC A 311:

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

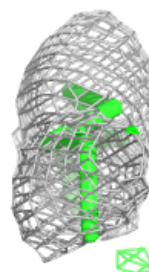
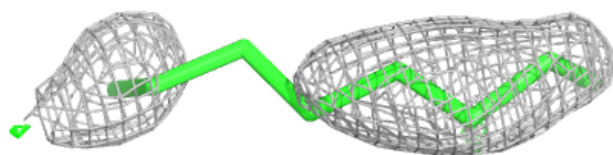
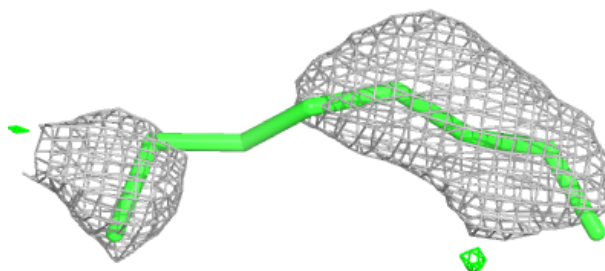
**Electron density around LI1 A 316:**

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

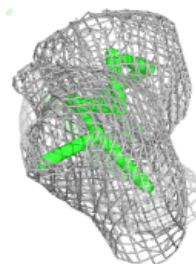
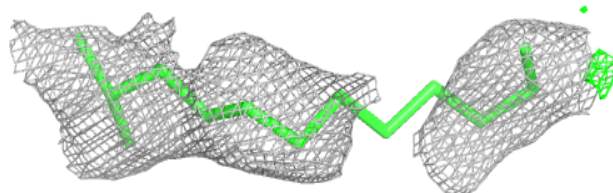
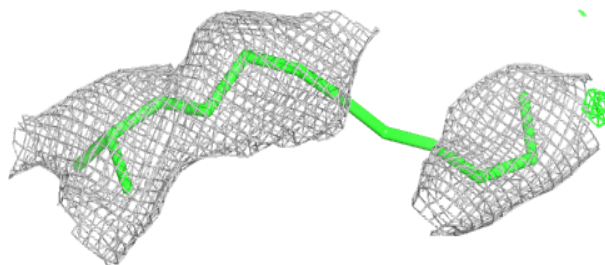


Electron density around LI1 A 314:

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

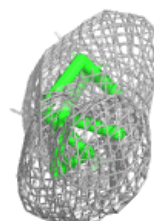
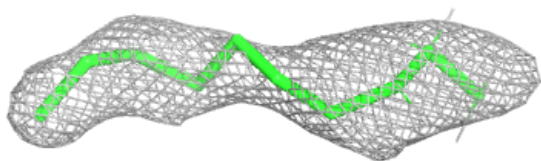
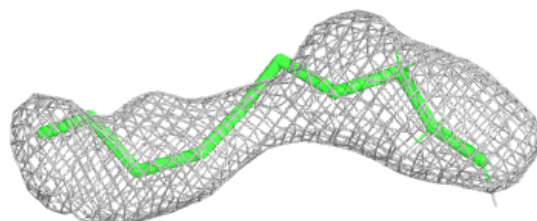
**Electron density around LI1 A 315:**

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

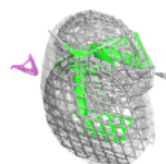
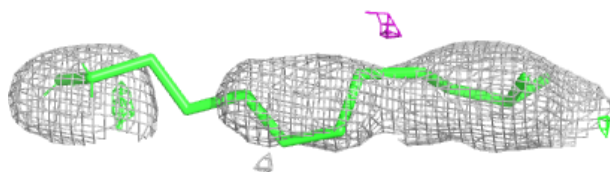
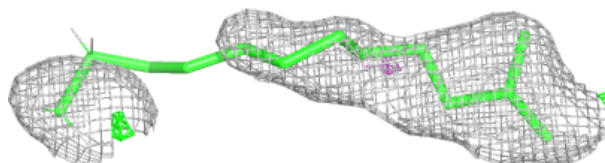


Electron density around LI1 A 312:

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

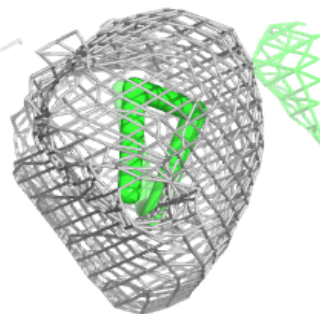
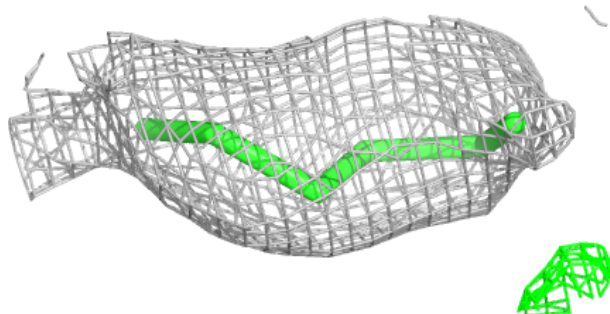
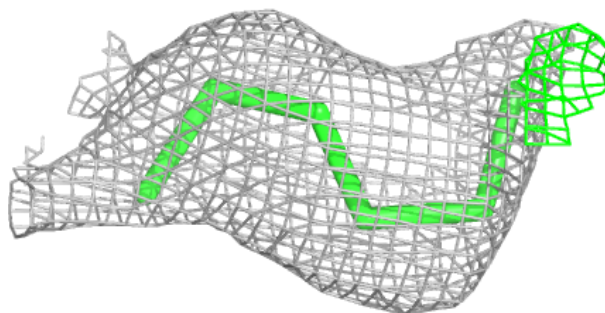
**Electron density around LI1 A 306:**

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

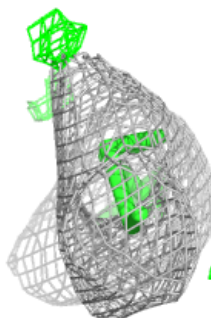
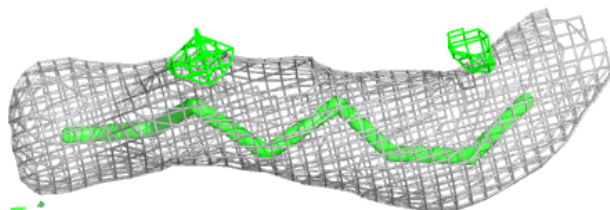
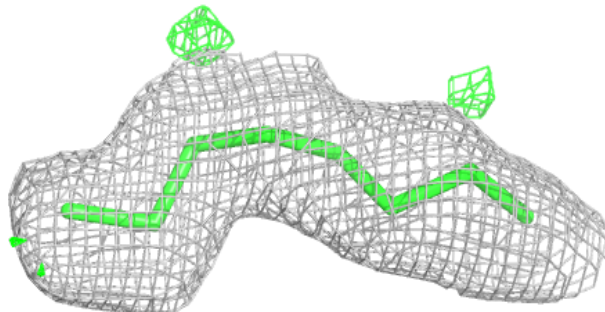


Electron density around LI1 A 317:

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

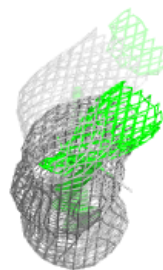
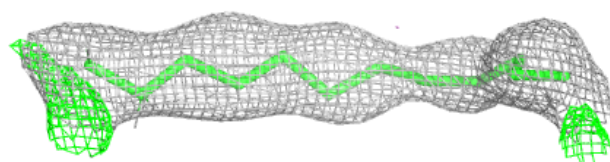
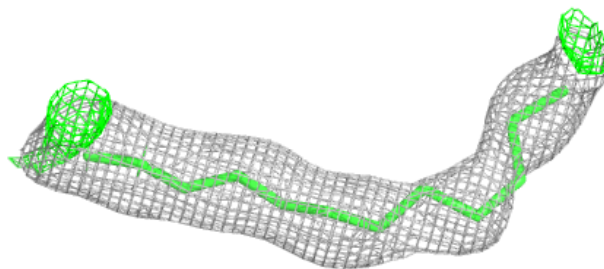
**Electron density around LI1 A 303:**

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

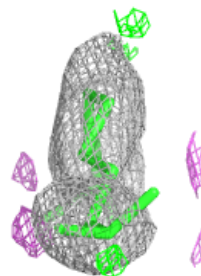
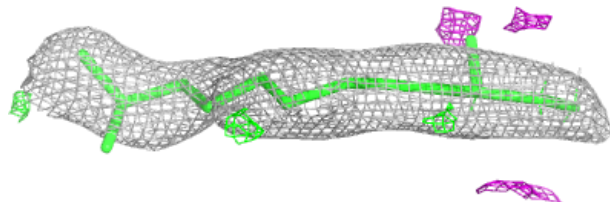
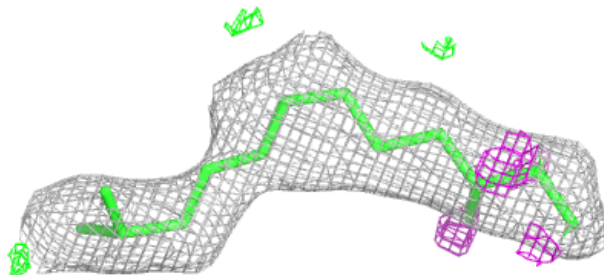


Electron density around LI1 A 304:

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

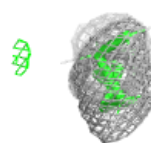
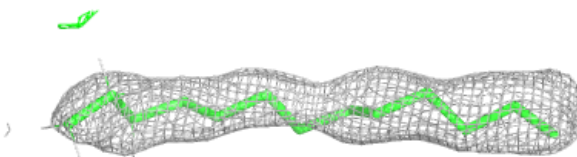
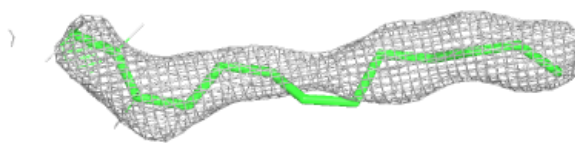
**Electron density around LI1 A 302:**

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

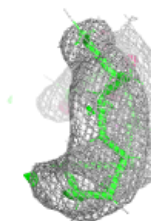
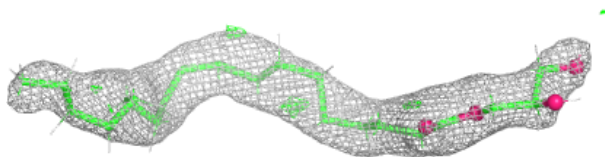
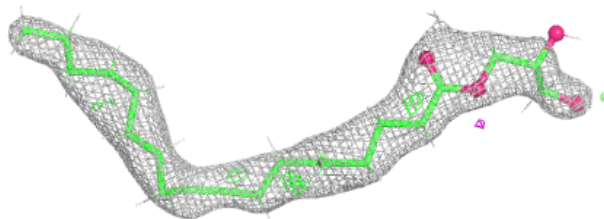


Electron density around LI1 A 305:

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

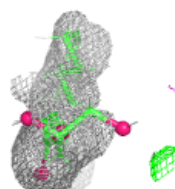
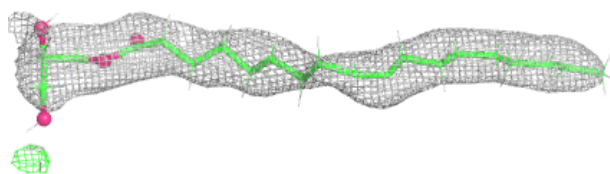
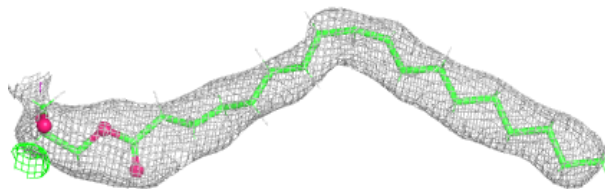
**Electron density around OLC A 307:**

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

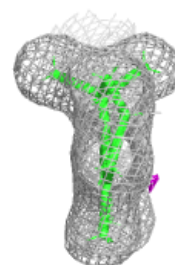
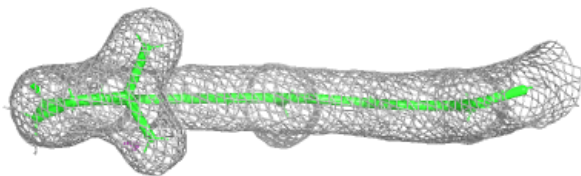
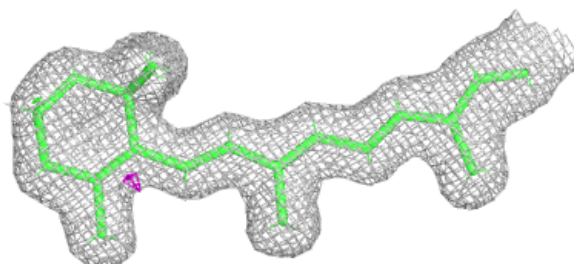


Electron density around OLC A 308:

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

**Electron density around RET A 318:**

$2mF_o-DF_c$ (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.