



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:41 AM UTC

PDB ID : 6YT4 / pdb_00006yt4
Title : Crystal structure of the N112A mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0
Authors : Kovalev, K.; Maliar, N.; Astashkin, R.; Gordeliy, V.
Deposited on : 2020-04-23
Resolution : 2.40 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

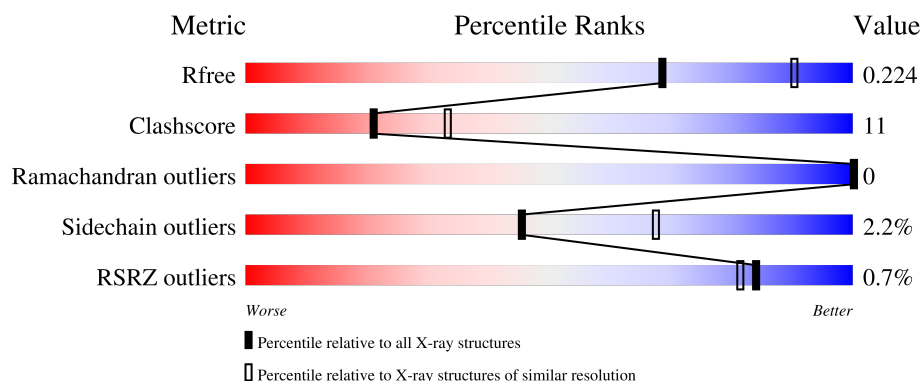
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	288	
1	B	288	
1	C	288	
1	D	288	
1	E	288	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11860 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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	2	0
			2154	1437	327	381	9			
1	B	269	Total	C	N	O	S	0	2	0
			2153	1436	327	381	9			
1	D	270	Total	C	N	O	S	0	2	0
			2160	1440	329	382	9			
1	E	273	Total	C	N	O	S	0	2	0
			2179	1452	333	385	9			
1	C	268	Total	C	N	O	S	0	2	0
			2145	1431	325	380	9			

There are 45 discrepancies between the modelled and reference sequences:

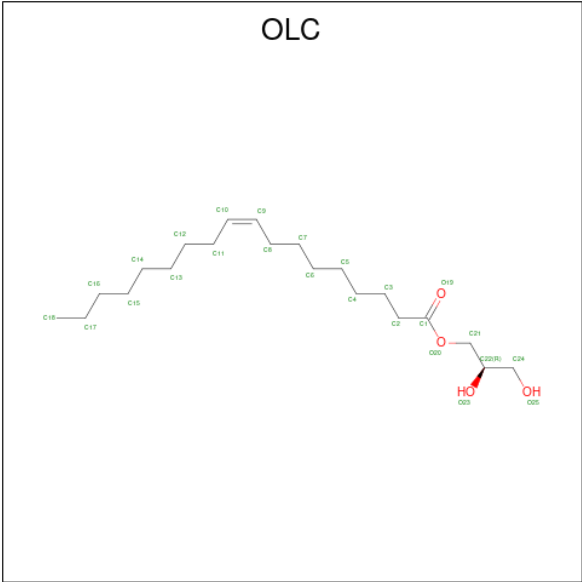
Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	ASN	engineered mutation	UNP N0DKS8
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	112	ALA	ASN	engineered mutation	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
D	112	ALA	ASN	engineered mutation	UNP N0DKS8

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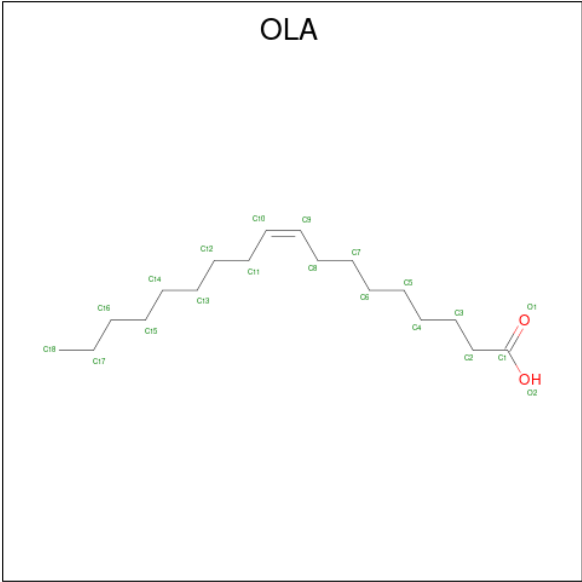
Chain	Residue	Modelled	Actual	Comment	Reference
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	112	ALA	ASN	engineered mutation	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8
C	112	ALA	ASN	engineered mutation	UNP N0DKS8
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



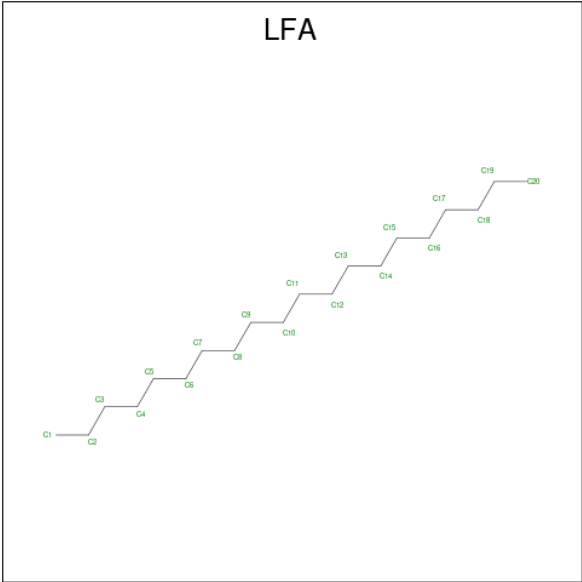
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	8	4		
2	B	1	Total	C	O	0	0
			13	10	3		
2	D	1	Total	C	O	0	0
			15	12	3		
2	E	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			11	8	3		

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	15	2		
3	A	1	Total	C	O	0	0
			16	14	2		
3	A	1	Total	C	O	0	0
			10	8	2		
3	A	1	Total	C	O	0	0
			13	11	2		
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			14	12	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			16	14	2		
3	B	1	Total	C	O	0	0
			12	10	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			20	18	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			20	18	2		
3	E	1	Total	C	O	0	0
			12	10	2		
3	E	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



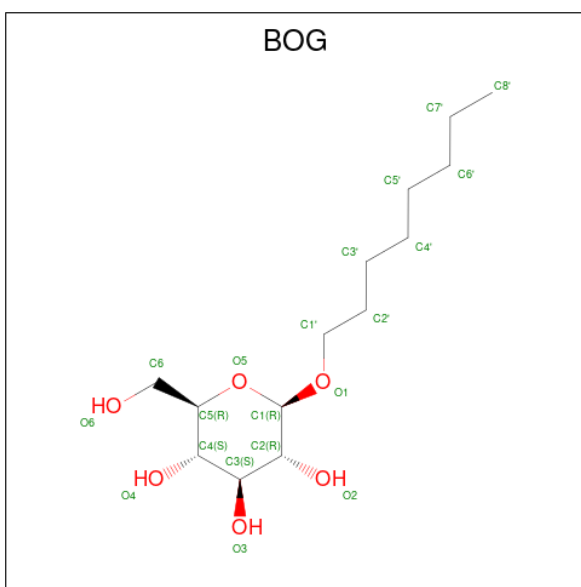
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 20 20	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 8 8	0	0
4	B	1	Total C 19 19	0	0
4	B	1	Total C 11 11	0	0
4	B	1	Total C 20 20	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 20 20	0	0
4	D	1	Total C 20 20	0	0
4	D	1	Total C 18 18	0	0
4	D	1	Total C 10 10	0	0
4	D	1	Total C 15 15	0	0
4	D	1	Total C 7 7	0	0

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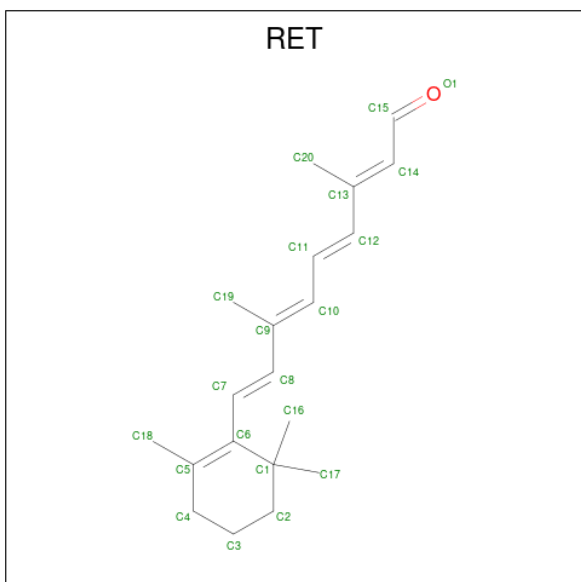
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C 8 8	0	0
4	D	1	Total C 7 7	0	0
4	E	1	Total C 5 5	0	0
4	E	1	Total C 20 20	0	0
4	E	1	Total C 19 19	0	0
4	E	1	Total C 18 18	0	0
4	E	1	Total C 5 5	0	0
4	E	1	Total C 5 5	0	0
4	E	1	Total C 8 8	0	0
4	C	1	Total C 16 16	0	0
4	C	1	Total C 15 15	0	0
4	C	1	Total C 3 3	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 5 5	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		
5	D	1	Total	C	O	0	0
			20	14	6		
5	E	1	Total	C	O	0	0
			20	14	6		
5	C	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 20 20	0	0
6	B	1	Total C 20 20	0	0
6	D	1	Total C 20 20	0	0
6	E	1	Total C 20 20	0	0
6	C	1	Total C 20 20	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	D	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0

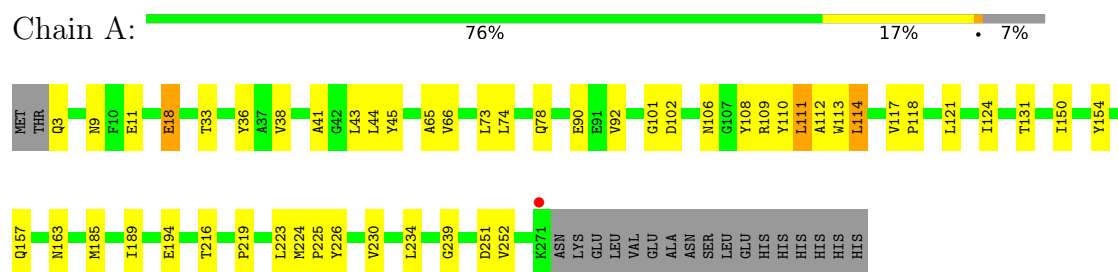
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	56	Total O 56 56	0	0
8	B	67	Total O 67 67	0	0
8	D	54	Total O 54 54	0	0
8	E	56	Total O 56 56	0	0
8	C	53	Total O 53 53	0	0

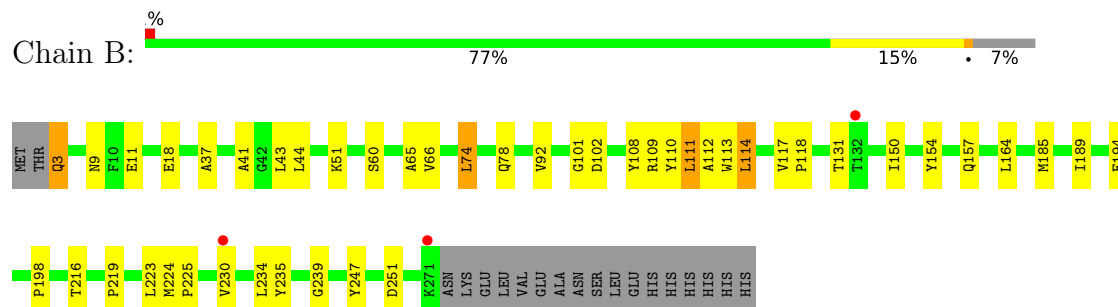
3 Residue-property plots [i](#)

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.

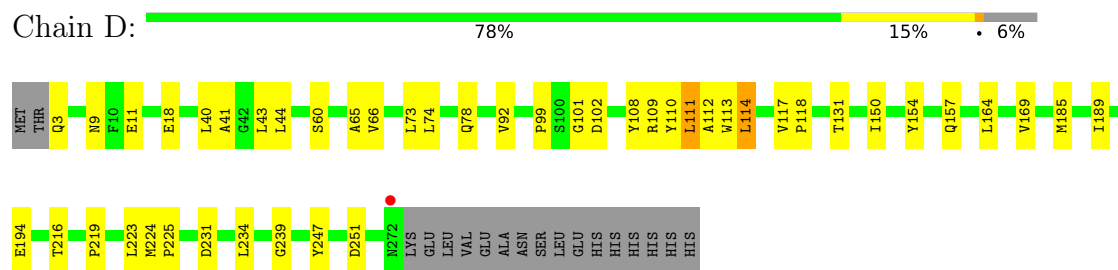
• Molecule 1: Sodium pumping rhodopsin



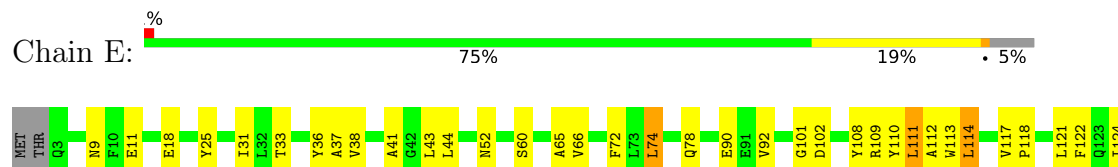
• Molecule 1: Sodium pumping rhodopsin

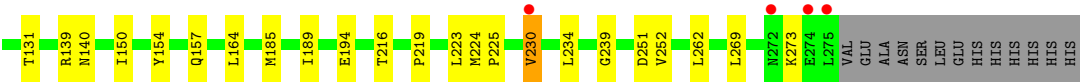


• Molecule 1: Sodium pumping rhodopsin



• Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.84Å 239.70Å 134.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.40) 93.8 (20.00-2.40)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.186 , 0.217 0.198 , 0.224	Depositor DCC
R_{free} test set	3771 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11860	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 5.98% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.93	0/2212	1.50	0/3008
1	B	0.93	0/2211	1.52	0/3007
1	C	0.93	0/2203	1.50	0/2997
1	D	0.93	0/2218	1.51	0/3016
1	E	0.93	0/2237	1.52	0/3041
All	All	0.93	0/11081	1.51	0/15069

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2154	0	2133	49	0
1	B	2153	0	2131	46	0
1	C	2145	0	2120	43	0
1	D	2160	0	2140	51	0
1	E	2179	0	2157	61	0
2	A	12	0	13	0	0
2	B	13	0	14	0	0
2	C	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	18	0	0
2	E	10	0	9	0	0
3	A	61	0	76	6	0
3	B	46	0	55	2	0
3	C	4	0	0	2	0
3	D	24	0	33	2	0
3	E	54	0	74	4	0
4	A	33	0	63	0	0
4	B	85	0	170	8	0
4	C	45	0	82	1	0
4	D	85	0	158	6	0
4	E	80	0	150	12	0
5	A	20	0	28	1	0
5	B	20	0	28	2	0
5	C	20	0	28	0	0
5	D	20	0	28	2	0
5	E	20	0	28	4	0
6	A	20	0	27	3	0
6	B	20	0	27	4	0
6	C	20	0	27	4	0
6	D	20	0	27	4	0
6	E	20	0	27	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	56	0	0	2	0
8	B	67	0	0	5	0
8	C	53	0	0	4	0
8	D	54	0	0	3	0
8	E	56	0	0	5	0
All	All	11860	0	11881	259	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 11.

All (259) 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)
4:D:401:LFA:C1	3:C:1401:OLA:C2	1.79	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:403:OLA:C2	4:E:406:LFA:H11	1.05	1.52
3:D:406:OLA:C2	4:E:402:LFA:H11	1.38	1.49
3:E:403:OLA:C2	4:E:406:LFA:C1	1.86	1.49
3:A:311:OLA:C3	4:B:304:LFA:H201	1.56	1.35
3:A:311:OLA:C3	4:B:304:LFA:C20	2.11	1.28
1:B:3:GLN:HE21	1:B:3:GLN:HA	1.13	1.13
3:D:406:OLA:C2	4:E:402:LFA:C1	2.29	1.08
1:E:74[B]:LEU:HG	1:E:112:ALA:HB2	1.34	1.08
4:D:401:LFA:H12	3:C:1401:OLA:C2	1.87	1.03
1:C:74[B]:LEU:HG	1:C:112:ALA:HB2	1.38	1.02
1:D:74[B]:LEU:HG	1:D:112:ALA:HB2	1.40	1.01
1:A:74[B]:LEU:HG	1:A:112:ALA:HB2	1.43	0.98
3:B:308:OLA:C2	4:B:312:LFA:H201	1.99	0.93
6:E:414:RET:H8	6:E:414:RET:H161	1.49	0.93
6:C:1409:RET:H161	6:C:1409:RET:H8	1.49	0.93
1:B:74[B]:LEU:HG	1:B:112:ALA:HB2	1.49	0.93
6:A:310:RET:H8	6:A:310:RET:H161	1.50	0.92
1:E:74[B]:LEU:HG	1:E:112:ALA:CB	2.00	0.91
6:B:311:RET:H8	6:B:311:RET:H161	1.52	0.88
1:C:99:PRO:HG2	8:C:1549:HOH:O	1.72	0.88
6:D:412:RET:H8	6:D:412:RET:H161	1.52	0.88
1:E:109[B]:ARG:NH1	1:E:251:ASP:OD2	2.07	0.86
1:B:109[B]:ARG:NH2	1:B:251:ASP:OD2	2.08	0.86
1:D:109[B]:ARG:NH1	1:D:251:ASP:OD2	2.08	0.85
3:B:308:OLA:C2	4:B:312:LFA:C20	2.55	0.85
3:E:407:OLA:C10	4:E:409:LFA:C16	2.56	0.84
3:A:311:OLA:C3	4:B:304:LFA:H203	2.09	0.82
1:C:18:GLU:OE1	8:C:1501:HOH:O	1.98	0.81
3:E:403:OLA:C2	4:E:406:LFA:H12	2.05	0.80
1:C:109[A]:ARG:NH1	1:C:251:ASP:OD2	2.15	0.80
1:B:3:GLN:HA	1:B:3:GLN:NE2	1.92	0.78
1:D:109[A]:ARG:NH1	1:D:251:ASP:OD2	2.19	0.76
1:B:198:PRO:HD2	8:B:459:HOH:O	1.85	0.76
1:A:109[A]:ARG:NH1	8:A:401:HOH:O	2.02	0.76
1:E:273:LYS:O	8:E:501:HOH:O	2.03	0.75
1:E:230:VAL:HG12	5:E:412:BOG:H2'2	1.67	0.75
1:D:18:GLU:OE1	8:D:501:HOH:O	2.04	0.75
1:A:109[B]:ARG:NH2	1:A:251:ASP:OD2	2.20	0.74
1:D:109[B]:ARG:HD2	8:D:530:HOH:O	1.88	0.72
1:C:60:SER:OG	8:C:1502:HOH:O	2.07	0.71
1:E:18:GLU:OE1	8:E:502:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HG3	8:A:435:HOH:O	1.92	0.68
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.75	0.68
1:E:74[B]:LEU:CG	1:E:112:ALA:HB2	2.19	0.67
1:C:106:ASN:O	1:C:109[B]:ARG:HG3	1.93	0.67
1:A:163:ASN:HD21	3:A:308:OLA:H21	1.58	0.67
1:B:234:LEU:O	1:B:239:GLY:HA3	1.95	0.66
1:D:234:LEU:O	1:D:239:GLY:HA3	1.96	0.66
1:C:234:LEU:O	1:C:239:GLY:HA3	1.96	0.66
1:A:234:LEU:O	1:A:239:GLY:HA3	1.96	0.66
1:E:234:LEU:O	1:E:239:GLY:HA3	1.96	0.65
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.77	0.65
6:D:412:RET:H161	6:D:412:RET:C8	2.27	0.65
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.79	0.65
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.78	0.65
1:E:109[A]:ARG:NH1	1:E:251:ASP:OD2	2.24	0.65
6:E:414:RET:H161	6:E:414:RET:C8	2.25	0.64
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.78	0.64
1:C:74[B]:LEU:HG	1:C:112:ALA:CB	2.21	0.64
1:B:164:LEU:HD21	5:B:310:BOG:H2'1	1.78	0.64
1:D:60:SER:OG	8:D:502:HOH:O	2.15	0.64
1:B:18:GLU:OE1	8:B:401:HOH:O	2.15	0.64
6:C:1409:RET:H161	6:C:1409:RET:C8	2.26	0.64
1:D:74[B]:LEU:HG	1:D:112:ALA:CB	2.22	0.64
1:B:109[B]:ARG:HD2	8:B:426:HOH:O	1.98	0.63
1:E:60:SER:OG	8:E:503:HOH:O	2.15	0.63
1:B:74[B]:LEU:HG	1:B:112:ALA:CB	2.26	0.62
1:C:111:LEU:O	1:C:114:LEU:HB2	1.99	0.62
1:E:139:ARG:HH11	4:E:408:LFA:H12	1.65	0.61
1:D:111:LEU:O	1:D:114:LEU:HB2	2.00	0.61
1:E:74[A]:LEU:HD13	1:E:74[A]:LEU:O	2.01	0.61
1:E:52:ASN:O	1:E:273:LYS:HG2	2.01	0.61
1:E:111:LEU:O	1:E:114:LEU:HB2	2.01	0.61
1:A:74[A]:LEU:C	1:A:74[A]:LEU:HD13	2.25	0.60
1:A:111:LEU:O	1:A:114:LEU:HB2	2.02	0.60
1:C:131:THR:HG21	1:C:194:GLU:OE1	2.02	0.60
1:C:74[A]:LEU:C	1:C:74[A]:LEU:HD13	2.27	0.60
1:B:111:LEU:O	1:B:114:LEU:HB2	2.01	0.59
1:D:164:LEU:HD21	5:D:408:BOG:H2'1	1.84	0.59
1:E:109[B]:ARG:HD2	8:E:524:HOH:O	2.02	0.59
1:D:74[A]:LEU:HD21	1:D:108:TYR:C	2.28	0.59
1:A:74[B]:LEU:HG	1:A:112:ALA:CB	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74[A]:LEU:HD21	1:D:108:TYR:HB3	1.85	0.58
1:C:74[A]:LEU:HD21	1:C:108:TYR:C	2.28	0.58
4:B:304:LFA:H182	4:B:312:LFA:H191	1.84	0.58
3:A:302:OLA:H22	1:E:122:PHE:HE2	1.68	0.58
1:E:230:VAL:HG12	5:E:412:BOG:C2'	2.33	0.58
1:D:131:THR:HG21	1:D:194:GLU:OE1	2.03	0.57
1:A:131:THR:HG21	1:A:194:GLU:OE1	2.04	0.57
1:C:74[A]:LEU:HD21	1:C:108:TYR:HB3	1.87	0.57
1:E:131:THR:HG21	1:E:194:GLU:OE1	2.04	0.57
1:E:230:VAL:HG12	5:E:412:BOG:C1'	2.36	0.56
1:A:74[A]:LEU:HD21	1:A:108:TYR:HB3	1.86	0.56
1:A:74[A]:LEU:HD21	1:A:108:TYR:C	2.30	0.56
1:B:109[B]:ARG:NH2	1:B:247:TYR:HB3	2.21	0.56
1:B:131:THR:HG21	1:B:194:GLU:OE1	2.05	0.55
6:B:311:RET:H161	6:B:311:RET:C8	2.27	0.55
1:E:74[A]:LEU:HD13	1:E:74[A]:LEU:C	2.31	0.55
1:D:74[A]:LEU:HD13	1:D:74[A]:LEU:C	2.32	0.55
1:C:216:THR:O	1:C:219:PRO:HG2	2.08	0.54
1:D:216:THR:O	1:D:219:PRO:HG2	2.07	0.54
1:E:185:MET:O	1:E:189:ILE:HG12	2.08	0.54
1:D:185:MET:O	1:D:189:ILE:HG12	2.08	0.54
1:A:185:MET:O	1:A:189:ILE:HG12	2.08	0.54
1:E:216:THR:O	1:E:219:PRO:HG2	2.08	0.54
1:C:185:MET:O	1:C:189:ILE:HG12	2.08	0.53
1:A:44:LEU:HD21	1:E:43:LEU:HD11	1.90	0.53
6:A:310:RET:H161	6:A:310:RET:C8	2.26	0.53
1:B:60:SER:OG	8:B:402:HOH:O	2.18	0.53
1:B:216:THR:O	1:B:219:PRO:HG2	2.08	0.53
1:A:78:GLN:HA	1:A:78:GLN:OE1	2.08	0.53
1:D:78:GLN:HA	1:D:78:GLN:OE1	2.09	0.53
1:E:78:GLN:OE1	1:E:78:GLN:HA	2.09	0.53
1:B:224:MET:N	1:B:225:PRO:HD2	2.24	0.53
1:B:185:MET:O	1:B:189:ILE:HG12	2.08	0.53
1:A:41:ALA:HB1	1:E:66:VAL:HG13	1.91	0.52
1:B:74[A]:LEU:HD21	1:B:108:TYR:C	2.34	0.52
1:B:74[A]:LEU:HD13	1:B:74[A]:LEU:O	2.09	0.52
1:D:223:LEU:HD11	4:D:407:LFA:H13	1.91	0.52
1:E:224:MET:N	1:E:225:PRO:HD2	2.25	0.52
1:A:224:MET:N	1:A:225:PRO:HD2	2.24	0.52
1:C:78:GLN:OE1	1:C:78:GLN:HA	2.10	0.52
1:D:224:MET:N	1:D:225:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74[A]:LEU:HD21	1:E:108:TYR:C	2.35	0.52
1:C:113:TRP:CD1	6:C:1409:RET:H14	2.45	0.52
1:C:224:MET:N	1:C:225:PRO:HD2	2.25	0.52
1:A:216:THR:O	1:A:219:PRO:HG2	2.11	0.51
1:B:74[A]:LEU:HD21	1:B:108:TYR:O	2.11	0.51
1:B:78:GLN:OE1	1:B:78:GLN:HA	2.10	0.51
1:D:66:VAL:HG13	1:E:41:ALA:HB1	1.93	0.51
1:E:74[A]:LEU:HD21	1:E:108:TYR:O	2.11	0.51
1:A:113:TRP:CD1	6:A:310:RET:H14	2.45	0.50
1:B:74[A]:LEU:HD13	1:B:74[A]:LEU:C	2.36	0.50
1:D:44:LEU:HD21	1:C:43:LEU:HD11	1.93	0.50
1:E:113:TRP:CD1	6:E:414:RET:H14	2.46	0.50
1:B:74[B]:LEU:CG	1:B:112:ALA:HB2	2.33	0.50
4:D:402:LFA:H21	4:C:1404:LFA:H52	1.93	0.50
1:D:113:TRP:CD1	6:D:412:RET:H14	2.47	0.50
1:D:231:ASP:H	5:D:408:BOG:HO6	1.54	0.50
1:B:113:TRP:CD1	6:B:311:RET:H14	2.47	0.50
1:D:43:LEU:HD11	1:E:44:LEU:HD21	1.94	0.49
1:A:109[A]:ARG:O	1:A:112:ALA:HB3	2.13	0.49
1:A:45:TYR:CE1	3:A:302:OLA:H41	2.48	0.48
1:A:109[B]:ARG:O	1:A:112:ALA:HB3	2.13	0.48
1:E:273:LYS:HD2	1:E:273:LYS:N	2.28	0.48
1:E:140:ASN:HD22	4:E:401:LFA:C7	2.27	0.48
1:D:223:LEU:C	1:D:225:PRO:HD2	2.38	0.48
1:E:72:PHE:HZ	4:E:406:LFA:H13	1.79	0.48
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.14	0.48
1:A:44:LEU:CD2	1:E:43:LEU:HD11	2.43	0.47
1:A:154:TYR:O	1:A:157:GLN:HG3	2.14	0.47
1:D:43:LEU:HD11	1:E:44:LEU:CD2	2.44	0.47
1:E:154:TYR:O	1:E:157:GLN:HG3	2.14	0.47
1:B:223:LEU:C	1:B:225:PRO:HD2	2.39	0.47
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.14	0.47
1:E:223:LEU:C	1:E:225:PRO:HD2	2.40	0.47
1:A:74[A]:LEU:HD13	1:A:74[A]:LEU:O	2.14	0.47
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.14	0.47
1:A:223:LEU:C	1:A:225:PRO:HD2	2.39	0.47
1:E:110:TYR:O	1:E:113:TRP:HB2	2.15	0.47
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.76	0.47
1:B:109[A]:ARG:O	1:B:112:ALA:HB3	2.15	0.47
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.15	0.47
1:C:110:TYR:O	1:C:113:TRP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ALA:HB1	1:E:44:LEU:HD21	1.96	0.47
1:D:109[B]:ARG:NH1	1:D:247:TYR:HB3	2.29	0.47
1:D:109[A]:ARG:O	1:D:112:ALA:HB3	2.15	0.46
1:D:154:TYR:O	1:D:157:GLN:HG3	2.15	0.46
1:B:109[B]:ARG:O	1:B:112:ALA:HB3	2.15	0.46
1:D:110:TYR:O	1:D:113:TRP:HB2	2.16	0.46
1:B:110:TYR:O	1:B:113:TRP:HB2	2.15	0.46
1:D:109[B]:ARG:O	1:D:112:ALA:HB3	2.15	0.46
1:C:109[A]:ARG:O	1:C:112:ALA:HB3	2.15	0.46
1:C:154:TYR:O	1:C:157:GLN:HG3	2.15	0.46
1:A:110:TYR:O	1:A:113:TRP:HB2	2.15	0.46
1:E:110:TYR:HA	1:E:113:TRP:CE3	2.51	0.46
1:A:3:GLN:HG2	8:B:406:HOH:O	2.14	0.46
1:A:110:TYR:HA	1:A:113:TRP:CE3	2.51	0.46
1:D:110:TYR:HA	1:D:113:TRP:CE3	2.51	0.46
1:E:109[A]:ARG:O	1:E:112:ALA:HB3	2.15	0.46
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.17	0.45
1:A:65:ALA:HB1	1:B:44:LEU:HD21	1.99	0.45
1:B:3:GLN:HE21	1:B:3:GLN:CA	2.01	0.45
1:C:114:LEU:HD13	1:C:150:ILE:HG21	1.99	0.45
1:A:114:LEU:O	1:A:118:PRO:HG2	2.16	0.45
1:C:74[A]:LEU:HD13	1:C:74[A]:LEU:O	2.17	0.45
1:D:114:LEU:O	1:D:118:PRO:HG2	2.16	0.45
1:E:74[A]:LEU:C	1:E:74[A]:LEU:CD1	2.89	0.45
1:B:154:TYR:O	1:B:157:GLN:HG3	2.16	0.45
1:C:223:LEU:C	1:C:225:PRO:HD2	2.41	0.45
1:E:139:ARG:NH1	4:E:408:LFA:H12	2.30	0.45
1:B:65:ALA:HB1	1:C:44:LEU:HD21	1.99	0.45
1:B:101:GLY:O	1:B:102:ASP:HB2	2.16	0.45
1:B:110:TYR:HA	1:B:113:TRP:CE3	2.52	0.45
1:E:31:ILE:HD12	1:E:31:ILE:HA	1.87	0.44
4:B:312:LFA:H182	4:D:401:LFA:H22	1.98	0.44
1:D:114:LEU:HD13	1:D:150:ILE:HG21	1.99	0.44
1:C:110:TYR:HA	1:C:113:TRP:CE3	2.52	0.44
1:D:41:ALA:HB1	1:C:66:VAL:HG13	1.99	0.44
1:D:99:PRO:HG3	1:E:90:GLU:CD	2.42	0.44
1:C:114:LEU:O	1:C:118:PRO:HG2	2.17	0.44
1:A:74[B]:LEU:HD13	1:A:74[B]:LEU:HA	1.79	0.44
4:B:303:LFA:H92	1:C:260:VAL:HG11	2.00	0.44
1:A:44:LEU:HD21	1:E:65:ALA:HB1	2.00	0.44
1:E:164:LEU:HD21	5:E:412:BOG:H2'1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.76	0.44
1:E:140:ASN:ND2	4:E:401:LFA:C7	2.81	0.44
1:A:66:VAL:HG13	1:B:41:ALA:HB1	2.00	0.44
1:E:109[B]:ARG:O	1:E:112:ALA:HB3	2.15	0.44
1:A:74[A]:LEU:HG	1:A:112:ALA:HB2	1.99	0.44
1:D:40:LEU:HD23	1:C:73:LEU:HD11	2.00	0.43
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.99	0.43
1:B:114:LEU:HD13	1:B:150:ILE:HG21	2.00	0.43
1:C:31:ILE:HD12	1:C:31:ILE:HA	1.86	0.43
1:D:44:LEU:CD2	1:C:43:LEU:HD11	2.47	0.43
1:D:101:GLY:O	1:D:102:ASP:HB2	2.18	0.43
4:E:402:LFA:H41	4:E:406:LFA:H32	2.00	0.43
1:B:74[B]:LEU:HD13	1:B:74[B]:LEU:HA	1.88	0.43
1:E:38:VAL:HG11	1:E:252:VAL:HG22	2.01	0.43
1:E:101:GLY:O	1:E:102:ASP:HB2	2.19	0.43
1:A:73:LEU:HD12	1:B:37:ALA:HA	2.01	0.43
1:A:101:GLY:O	1:A:102:ASP:HB2	2.19	0.43
1:B:66:VAL:HG13	1:C:41:ALA:HB1	2.00	0.43
1:D:169:VAL:HG11	4:D:403:LFA:H82	2.00	0.42
1:A:18:GLU:H	1:A:18:GLU:HG2	1.54	0.42
1:D:3:GLN:HG2	8:E:513:HOH:O	2.18	0.42
1:A:226:TYR:HE1	5:A:309:BOG:H5	1.83	0.42
1:B:43:LEU:HD11	1:C:44:LEU:HD21	2.01	0.42
1:E:114:LEU:O	1:E:118:PRO:HG2	2.19	0.42
1:B:114:LEU:O	1:B:118:PRO:HG2	2.20	0.42
1:E:33:THR:HA	1:E:36:TYR:CE2	2.55	0.42
6:B:311:RET:H181	6:B:311:RET:H7	1.82	0.42
1:D:102:ASP:OD2	1:E:25:TYR:OH	2.38	0.42
1:D:74[B]:LEU:HA	1:D:74[B]:LEU:HD13	1.80	0.41
1:D:73:LEU:HD12	1:E:37:ALA:HA	2.01	0.41
1:C:101:GLY:O	1:C:102:ASP:HB2	2.21	0.41
6:C:1409:RET:H7	6:C:1409:RET:H181	1.83	0.41
1:A:74[A]:LEU:C	1:A:74[A]:LEU:CD1	2.93	0.41
1:A:114:LEU:HD13	1:A:150:ILE:HG21	2.03	0.41
1:B:235:TYR:CD1	5:B:310:BOG:H61	2.55	0.41
1:C:60:SER:CB	8:C:1502:HOH:O	2.67	0.41
6:D:412:RET:H181	6:D:412:RET:H7	1.85	0.41
1:C:121:LEU:O	1:C:124:ILE:HG22	2.21	0.41
1:A:38:VAL:HG11	1:A:252:VAL:HG22	2.03	0.40
1:A:121:LEU:O	1:A:124:ILE:HG22	2.21	0.40
1:E:121:LEU:O	1:E:124:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74[A]:LEU:HG	1:D:112:ALA:CB	2.51	0.40
6:E:414:RET:H181	6:E:414:RET:H7	1.83	0.40
1:C:74[A]:LEU:HG	1:C:112:ALA:CB	2.51	0.40
1:D:74[A]:LEU:CD2	1:D:108:TYR:HB3	2.51	0.40
1:A:33:THR:HA	1:A:36:TYR:CE2	2.56	0.40
1:A:43:LEU:HD11	1:B:44:LEU:HD21	2.02	0.40
1:D:74[A]:LEU:HG	1:D:112:ALA:HB2	2.04	0.40
1:E:262:LEU:HD23	1:E:262:LEU:HA	1.93	0.40
1:C:38:VAL:HG11	1:C:252:VAL:HG22	2.04	0.40
1:A:106:ASN:O	1:A:109[A]:ARG:HB2	2.22	0.40
1:A:111:LEU:HA	1:A:111:LEU:HD12	1.78	0.40
1:C:33:THR:HA	1:C:36:TYR:CE2	2.56	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	269/288 (93%)	263 (98%)	6 (2%)	0	100	100
1	B	269/288 (93%)	262 (97%)	7 (3%)	0	100	100
1	C	268/288 (93%)	262 (98%)	6 (2%)	0	100	100
1	D	270/288 (94%)	261 (97%)	9 (3%)	0	100	100
1	E	273/288 (95%)	265 (97%)	8 (3%)	0	100	100
All	All	1349/1440 (94%)	1313 (97%)	36 (3%)	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	227/247 (92%)	222 (98%)	5 (2%)	45	67
1	B	227/247 (92%)	219 (96%)	8 (4%)	32	53
1	C	226/247 (92%)	222 (98%)	4 (2%)	51	73
1	D	228/247 (92%)	225 (99%)	3 (1%)	61	80
1	E	229/247 (93%)	222 (97%)	7 (3%)	35	57
All	All	1137/1235 (92%)	1110 (98%)	27 (2%)	45	65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	92	VAL
1	A	111	LEU
1	A	114	LEU
1	A	230	VAL
1	B	3	GLN
1	B	51	LYS
1	B	74[A]	LEU
1	B	74[B]	LEU
1	B	92	VAL
1	B	111	LEU
1	B	114	LEU
1	B	230	VAL
1	D	92	VAL
1	D	111	LEU
1	D	114	LEU
1	E	74[A]	LEU
1	E	74[B]	LEU
1	E	92	VAL
1	E	111	LEU
1	E	114	LEU
1	E	230	VAL
1	E	269	LEU

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Mol	Chain	Res	Type
1	C	92	VAL
1	C	111	LEU
1	C	114	LEU
1	C	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	B	3	GLN
1	B	81	ASN
1	C	3	GLN
1	C	7	ASN
1	C	141	GLN

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](#)

Of 64 ligands modelled in this entry, 5 are monoatomic - leaving 59 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLA	A	311	-	4,4,19	1.02	0	4,4,19	0.72	0
3	OLA	A	304	-	15,15,19	0.59	0	15,15,19	0.54	0
3	OLA	B	308	-	3,3,19	0.92	0	3,3,19	0.77	0
6	RET	A	310	1	20,20,21	1.49	3 (15%)	27,27,28	1.04	2 (7%)
6	RET	D	412	1	20,20,21	1.56	3 (15%)	27,27,28	1.03	2 (7%)
4	LFA	B	306	-	5,5,19	0.12	0	4,4,18	0.10	0
4	LFA	B	307	-	8,8,19	0.11	0	7,7,18	0.11	0
4	LFA	D	407	-	6,6,19	0.12	0	5,5,18	0.08	0
3	OLA	D	409	-	19,19,19	0.54	0	19,19,19	0.48	0
4	LFA	A	305	-	4,4,19	0.13	0	3,3,18	0.22	0
4	LFA	D	403	-	9,9,19	0.11	0	8,8,18	0.08	0
6	RET	C	1409	1	20,20,21	1.48	3 (15%)	27,27,28	1.04	1 (3%)
4	LFA	D	404	-	14,14,19	0.07	0	13,13,18	0.07	0
3	OLA	D	406	-	3,3,19	0.93	0	3,3,19	0.81	0
2	OLC	A	301	-	11,11,24	1.34	1 (9%)	12,12,25	1.15	2 (16%)
4	LFA	D	411	-	6,6,19	0.12	0	5,5,18	0.13	0
2	OLC	C	1402	-	10,10,24	1.46	1 (10%)	10,10,25	1.21	1 (10%)
5	BOG	B	310	-	20,20,20	0.59	1 (5%)	25,25,25	0.53	0
4	LFA	E	410	-	4,4,19	0.15	0	3,3,18	0.21	0
3	OLA	C	1401	-	3,3,19	0.90	0	3,3,19	0.81	0
4	LFA	E	402	-	19,19,19	0.07	0	18,18,18	0.04	0
4	LFA	D	401	-	19,19,19	0.10	0	18,18,18	0.05	0
4	LFA	E	406	-	18,18,19	0.06	0	17,17,18	0.07	0
5	BOG	C	1408	-	20,20,20	0.60	1 (5%)	25,25,25	0.59	0
4	LFA	C	1405	-	2,2,19	0.03	0	1,1,18	0.17	0
3	OLA	B	313	-	11,11,19	0.68	0	11,11,19	0.61	0
4	LFA	B	312	-	19,19,19	0.08	0	18,18,18	0.04	0
3	OLA	B	309	-	15,15,19	0.59	0	15,15,19	0.53	0
4	LFA	B	302	-	18,18,19	0.09	0	17,17,18	0.07	0
3	OLA	B	305	-	13,13,19	0.62	0	13,13,19	0.56	0
4	LFA	E	413	-	7,7,19	0.10	0	6,6,18	0.13	0
4	LFA	B	303	-	10,10,19	0.10	0	9,9,18	0.10	0
3	OLA	E	403	-	3,3,19	0.92	0	3,3,19	0.77	0
5	BOG	E	412	-	20,20,20	0.63	1 (5%)	25,25,25	0.52	0
4	LFA	D	402	-	17,17,19	0.07	0	16,16,18	0.06	0
2	OLC	D	405	-	14,14,24	1.23	1 (7%)	15,15,25	1.00	1 (6%)
4	LFA	E	408	-	17,17,19	0.07	0	16,16,18	0.07	0
5	BOG	D	408	-	20,20,20	0.60	1 (5%)	25,25,25	0.60	0
6	RET	B	311	1	20,20,21	1.55	3 (15%)	27,27,28	1.08	2 (7%)
4	LFA	B	304	-	19,19,19	0.09	0	18,18,18	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LFA	C	1406	-	5,5,19	0.10	0	4,4,18	0.12	0
3	OLA	E	411	-	17,17,19	0.56	0	17,17,19	0.50	0
4	LFA	D	410	-	7,7,19	0.09	0	6,6,18	0.12	0
4	LFA	C	1403	-	15,15,19	0.10	0	14,14,18	0.08	0
2	OLC	E	404	-	9,9,24	1.43	1 (11%)	10,10,25	1.41	2 (20%)
4	LFA	E	401	-	4,4,19	0.16	0	3,3,18	0.24	0
3	OLA	A	302	-	16,16,19	0.57	0	16,16,19	0.55	0
4	LFA	E	409	-	4,4,19	0.13	0	3,3,18	0.23	0
3	OLA	A	308	-	12,12,19	0.64	0	12,12,19	0.61	0
3	OLA	E	405	-	19,19,19	0.52	0	19,19,19	0.47	0
4	LFA	A	306	-	7,7,19	0.12	0	6,6,18	0.13	0
5	BOG	A	309	-	20,20,20	0.65	1 (5%)	25,25,25	0.60	0
6	RET	E	414	1	20,20,21	1.51	3 (15%)	27,27,28	1.04	2 (7%)
4	LFA	A	303	-	19,19,19	0.08	0	18,18,18	0.04	0
3	OLA	E	407	-	11,11,19	0.65	0	11,11,19	0.65	0
2	OLC	B	301	-	12,12,24	1.31	1 (8%)	13,13,25	1.06	2 (15%)
4	LFA	C	1404	-	14,14,19	0.09	0	13,13,18	0.06	0
3	OLA	A	307	-	9,9,19	0.73	0	9,9,19	0.68	0
4	LFA	C	1407	-	4,4,19	0.13	0	3,3,18	0.23	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	OLA	A	311	-	-	0/2/2/17	-
3	OLA	A	304	-	-	4/13/13/17	-
6	RET	A	310	1	-	0/13/30/31	0/1/1/1
6	RET	D	412	1	-	1/13/30/31	0/1/1/1
4	LFA	B	306	-	-	0/3/3/17	-
4	LFA	B	307	-	-	0/6/6/17	-
4	LFA	D	407	-	-	1/4/4/17	-
3	OLA	D	409	-	-	11/17/17/17	-
4	LFA	A	305	-	-	0/2/2/17	-
4	LFA	D	403	-	-	5/7/7/17	-
6	RET	C	1409	1	-	0/13/30/31	0/1/1/1
4	LFA	D	404	-	-	6/12/12/17	-
2	OLC	A	301	-	-	2/11/11/24	-
4	LFA	D	411	-	-	3/4/4/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	1402	-	-	1/9/9/24	-
5	BOG	B	310	-	-	8/11/31/31	0/1/1/1
4	LFA	E	410	-	-	1/2/2/17	-
4	LFA	E	402	-	-	7/17/17/17	-
4	LFA	D	401	-	-	7/17/17/17	-
4	LFA	E	406	-	-	9/16/16/17	-
5	BOG	C	1408	-	-	5/11/31/31	0/1/1/1
3	OLA	B	313	-	-	3/9/9/17	-
4	LFA	B	312	-	-	11/17/17/17	-
3	OLA	B	309	-	-	5/13/13/17	-
4	LFA	B	302	-	-	4/16/16/17	-
3	OLA	B	305	-	-	8/11/11/17	-
4	LFA	E	413	-	-	4/5/5/17	-
4	LFA	B	303	-	-	3/8/8/17	-
5	BOG	E	412	-	-	5/11/31/31	0/1/1/1
4	LFA	D	402	-	-	7/15/15/17	-
2	OLC	D	405	-	-	8/13/13/24	-
4	LFA	E	408	-	-	6/15/15/17	-
5	BOG	D	408	-	-	5/11/31/31	0/1/1/1
6	RET	B	311	1	-	0/13/30/31	0/1/1/1
4	LFA	B	304	-	-	10/17/17/17	-
4	LFA	C	1406	-	-	1/3/3/17	-
3	OLA	E	411	-	-	11/15/15/17	-
4	LFA	D	410	-	-	1/5/5/17	-
4	LFA	C	1403	-	-	9/13/13/17	-
2	OLC	E	404	-	-	2/9/9/24	-
4	LFA	E	401	-	-	0/2/2/17	-
3	OLA	A	302	-	-	10/14/14/17	-
4	LFA	E	409	-	-	1/2/2/17	-
3	OLA	A	308	-	-	7/10/10/17	-
3	OLA	E	405	-	-	8/17/17/17	-
4	LFA	A	306	-	-	5/5/5/17	-
5	BOG	A	309	-	-	5/11/31/31	0/1/1/1
6	RET	E	414	1	-	1/13/30/31	0/1/1/1
4	LFA	A	303	-	-	9/17/17/17	-
3	OLA	E	407	-	-	8/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	301	-	-	2/11/11/24	-
4	LFA	C	1404	-	-	5/12/12/17	-
3	OLA	A	307	-	-	5/7/7/17	-
4	LFA	C	1407	-	-	0/2/2/17	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	405	OLC	O20-C1	4.43	1.46	1.33
6	B	311	RET	C14-C13	4.43	1.36	1.33
2	C	1402	OLC	O20-C1	4.41	1.46	1.33
2	B	301	OLC	O20-C1	4.29	1.45	1.33
6	D	412	RET	C14-C13	4.24	1.36	1.33
2	A	301	OLC	O20-C1	4.21	1.45	1.33
6	E	414	RET	C14-C13	4.17	1.36	1.33
2	E	404	OLC	O20-C1	4.13	1.45	1.33
6	C	1409	RET	C14-C13	4.00	1.36	1.33
6	A	310	RET	C14-C13	3.85	1.36	1.33
6	D	412	RET	C8-C9	-2.73	1.40	1.46
6	A	310	RET	C10-C9	2.58	1.41	1.35
6	E	414	RET	C8-C9	-2.57	1.40	1.46
6	A	310	RET	C8-C9	-2.56	1.40	1.46
6	C	1409	RET	C10-C9	2.53	1.41	1.35
6	B	311	RET	C8-C9	-2.53	1.40	1.46
6	C	1409	RET	C8-C9	-2.51	1.40	1.46
6	D	412	RET	C10-C9	2.49	1.41	1.35
6	E	414	RET	C10-C9	2.43	1.41	1.35
5	A	309	BOG	O1-C1	2.42	1.44	1.40
5	E	412	BOG	O1-C1	2.31	1.44	1.40
6	B	311	RET	C10-C9	2.27	1.41	1.35
5	C	1408	BOG	O1-C1	2.18	1.43	1.40
5	B	310	BOG	O1-C1	2.17	1.43	1.40
5	D	408	BOG	O1-C1	2.17	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	311	RET	C19-C9-C10	-3.44	117.24	122.82
2	E	404	OLC	O20-C1-C2	3.44	121.58	111.15
6	E	414	RET	C19-C9-C10	-3.25	117.55	122.82
6	C	1409	RET	C19-C9-C10	-3.23	117.58	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	310	RET	C19-C9-C10	-3.19	117.65	122.82
6	D	412	RET	C19-C9-C10	-3.15	117.72	122.82
2	D	405	OLC	O20-C1-C2	2.80	120.37	111.83
2	A	301	OLC	O20-C1-C2	2.79	120.33	111.83
2	B	301	OLC	O20-C1-C2	2.73	120.17	111.83
2	C	1402	OLC	O20-C1-C2	2.72	120.12	111.83
2	E	404	OLC	O20-C1-O19	-2.41	117.59	123.63
2	A	301	OLC	O20-C1-O19	-2.36	117.72	123.63
2	B	301	OLC	O20-C1-O19	-2.26	117.97	123.63
6	D	412	RET	C19-C9-C8	2.11	121.31	118.09
6	B	311	RET	C19-C9-C8	2.06	121.24	118.09
6	E	414	RET	C19-C9-C8	2.03	121.20	118.09
6	A	310	RET	C19-C9-C8	2.01	121.15	118.09

There are no chirality outliers.

All (240) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	308	OLA	C11-C10-C9-C8
5	B	310	BOG	C4-C5-C6-O6
2	D	405	OLC	O19-C1-O20-C21
2	D	405	OLC	C2-C1-O20-C21
5	E	412	BOG	O5-C5-C6-O6
5	B	310	BOG	O5-C5-C6-O6
3	E	407	OLA	C6-C7-C8-C9
5	E	412	BOG	C4-C5-C6-O6
3	B	305	OLA	C11-C10-C9-C8
2	A	301	OLC	C2-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
3	B	305	OLA	C1-C2-C3-C4
3	E	411	OLA	C1-C2-C3-C4
2	A	301	OLC	O19-C1-O20-C21
2	E	404	OLC	O20-C21-C22-O23
5	A	309	BOG	O1-C1'-C2'-C3'
2	B	301	OLC	O19-C1-O20-C21
2	E	404	OLC	O20-C21-C22-C24
3	E	411	OLA	C11-C10-C9-C8
3	A	302	OLA	C1-C2-C3-C4
3	E	411	OLA	C5-C6-C7-C8
4	B	304	LFA	C4-C5-C6-C7
3	D	409	OLA	C4-C5-C6-C7
4	A	306	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	B	304	LFA	C14-C15-C16-C17
4	E	402	LFA	C5-C6-C7-C8
4	B	302	LFA	C12-C13-C14-C15
4	D	403	LFA	C2-C3-C4-C5
5	A	309	BOG	C1'-C2'-C3'-C4'
3	A	302	OLA	C11-C12-C13-C14
3	A	307	OLA	C2-C3-C4-C5
3	E	407	OLA	C3-C4-C5-C6
4	B	304	LFA	C2-C3-C4-C5
4	D	402	LFA	C7-C8-C9-C10
4	D	411	LFA	C4-C5-C6-C7
4	C	1403	LFA	C4-C5-C6-C7
4	C	1403	LFA	C5-C6-C7-C8
5	D	408	BOG	O5-C5-C6-O6
3	E	407	OLA	C2-C3-C4-C5
4	B	312	LFA	C7-C8-C9-C10
4	E	402	LFA	C4-C5-C6-C7
4	E	408	LFA	C11-C12-C13-C14
4	B	312	LFA	C10-C11-C12-C13
5	D	408	BOG	C4-C5-C6-O6
4	D	404	LFA	C4-C5-C6-C7
4	B	312	LFA	C14-C15-C16-C17
4	C	1404	LFA	C3-C4-C5-C6
3	B	313	OLA	C1-C2-C3-C4
4	A	303	LFA	C2-C3-C4-C5
3	E	411	OLA	C2-C3-C4-C5
4	E	406	LFA	C5-C6-C7-C8
4	D	401	LFA	C16-C17-C18-C19
3	B	305	OLA	C4-C5-C6-C7
4	E	413	LFA	C14-C15-C16-C17
4	E	413	LFA	C15-C16-C17-C18
2	D	405	OLC	C3-C4-C5-C6
3	E	411	OLA	C12-C13-C14-C15
4	D	401	LFA	C11-C10-C9-C8
4	A	303	LFA	C13-C14-C15-C16
3	E	405	OLA	C6-C7-C8-C9
3	A	307	OLA	C1-C2-C3-C4
2	D	405	OLC	C2-C3-C4-C5
3	D	409	OLA	C5-C6-C7-C8
4	D	401	LFA	C7-C8-C9-C10
4	C	1403	LFA	C2-C3-C4-C5
3	B	305	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	B	304	LFA	C15-C16-C17-C18
4	D	402	LFA	C11-C12-C13-C14
4	C	1404	LFA	C11-C10-C9-C8
4	E	406	LFA	C11-C12-C13-C14
5	C	1408	BOG	C3'-C4'-C5'-C6'
3	E	411	OLA	C3-C4-C5-C6
3	A	304	OLA	C1-C2-C3-C4
3	A	302	OLA	C4-C5-C6-C7
4	B	304	LFA	C10-C11-C12-C13
4	C	1404	LFA	C4-C5-C6-C7
4	D	411	LFA	C3-C4-C5-C6
5	B	310	BOG	C1'-C2'-C3'-C4'
4	C	1404	LFA	C5-C6-C7-C8
4	A	306	LFA	C5-C6-C7-C8
3	E	405	OLA	C1-C2-C3-C4
5	D	408	BOG	C1'-C2'-C3'-C4'
3	A	302	OLA	C3-C4-C5-C6
4	C	1403	LFA	C10-C11-C12-C13
3	E	405	OLA	C13-C14-C15-C16
4	C	1403	LFA	C3-C4-C5-C6
4	B	304	LFA	C3-C4-C5-C6
4	A	303	LFA	C14-C15-C16-C17
4	E	402	LFA	C11-C10-C9-C8
3	A	302	OLA	C11-C10-C9-C8
4	D	404	LFA	C6-C7-C8-C9
3	B	313	OLA	C4-C5-C6-C7
3	E	411	OLA	C4-C5-C6-C7
4	D	401	LFA	C15-C16-C17-C18
5	C	1408	BOG	C2'-C3'-C4'-C5'
4	B	312	LFA	C11-C12-C13-C14
5	A	309	BOG	C4-C5-C6-O6
4	B	302	LFA	C4-C5-C6-C7
5	E	412	BOG	C3'-C4'-C5'-C6'
4	B	302	LFA	C7-C8-C9-C10
3	D	409	OLA	C12-C13-C14-C15
4	E	408	LFA	C4-C5-C6-C7
4	E	406	LFA	C7-C8-C9-C10
4	A	306	LFA	C6-C7-C8-C9
3	B	313	OLA	C2-C3-C4-C5
6	D	412	RET	C12-C13-C14-C15
4	B	304	LFA	C11-C12-C13-C14
4	C	1403	LFA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	D	402	LFA	C4-C5-C6-C7
4	B	312	LFA	C16-C17-C18-C19
4	B	304	LFA	C1-C2-C3-C4
4	D	411	LFA	C5-C6-C7-C8
5	C	1408	BOG	C5'-C6'-C7'-C8'
3	B	305	OLA	C6-C7-C8-C9
4	A	306	LFA	C3-C4-C5-C6
4	E	406	LFA	C12-C13-C14-C15
4	B	312	LFA	C1-C2-C3-C4
3	E	407	OLA	C1-C2-C3-C4
4	E	408	LFA	C1-C2-C3-C4
3	E	407	OLA	C4-C5-C6-C7
4	A	303	LFA	C16-C17-C18-C19
5	B	310	BOG	C4'-C5'-C6'-C7'
3	A	307	OLA	C3-C4-C5-C6
5	B	310	BOG	C5'-C6'-C7'-C8'
4	E	410	LFA	C17-C18-C19-C20
4	D	404	LFA	C1-C2-C3-C4
3	B	309	OLA	C1-C2-C3-C4
4	D	402	LFA	C15-C16-C17-C18
4	E	406	LFA	C1-C2-C3-C4
3	D	409	OLA	C2-C3-C4-C5
2	C	1402	OLC	C2-C3-C4-C5
4	B	303	LFA	C4-C5-C6-C7
3	E	411	OLA	C13-C14-C15-C16
3	A	302	OLA	C5-C6-C7-C8
5	D	408	BOG	C4'-C5'-C6'-C7'
3	D	409	OLA	C13-C14-C15-C16
4	B	303	LFA	C3-C4-C5-C6
5	A	309	BOG	O5-C5-C6-O6
3	E	411	OLA	C11-C12-C13-C14
2	D	405	OLC	C4-C5-C6-C7
4	D	402	LFA	C14-C15-C16-C17
5	B	310	BOG	C3'-C4'-C5'-C6'
4	B	312	LFA	C11-C10-C9-C8
4	E	413	LFA	C13-C14-C15-C16
3	A	308	OLA	C3-C4-C5-C6
4	D	403	LFA	C1-C2-C3-C4
4	A	306	LFA	C7-C8-C9-C10
4	E	402	LFA	C3-C4-C5-C6
4	C	1403	LFA	C6-C7-C8-C9
4	E	402	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	B	309	OLA	C4-C5-C6-C7
3	D	409	OLA	C6-C7-C8-C9
3	E	407	OLA	C7-C8-C9-C10
4	B	312	LFA	C5-C6-C7-C8
5	E	412	BOG	C5'-C6'-C7'-C8'
5	B	310	BOG	O5-C1-O1-C1'
4	D	407	LFA	C3-C4-C5-C6
4	E	413	LFA	C16-C17-C18-C19
3	E	405	OLA	C14-C15-C16-C17
4	D	410	LFA	C4-C5-C6-C7
5	B	310	BOG	C2'-C3'-C4'-C5'
4	B	304	LFA	C11-C10-C9-C8
3	E	405	OLA	C5-C6-C7-C8
3	A	302	OLA	C10-C11-C12-C13
4	B	312	LFA	C13-C14-C15-C16
5	A	309	BOG	C5'-C6'-C7'-C8'
4	D	402	LFA	C3-C4-C5-C6
3	A	308	OLA	C2-C3-C4-C5
4	B	312	LFA	C6-C7-C8-C9
4	B	302	LFA	C11-C10-C9-C8
4	D	401	LFA	C17-C18-C19-C20
4	A	303	LFA	C12-C13-C14-C15
4	E	409	LFA	C17-C18-C19-C20
4	E	408	LFA	C7-C8-C9-C10
4	C	1403	LFA	C13-C14-C15-C16
4	D	401	LFA	C11-C12-C13-C14
4	A	303	LFA	C9-C10-C11-C12
4	B	303	LFA	C2-C3-C4-C5
4	C	1403	LFA	C7-C8-C9-C10
4	E	402	LFA	C17-C18-C19-C20
4	E	402	LFA	C7-C8-C9-C10
4	D	404	LFA	C11-C10-C9-C8
4	D	401	LFA	C6-C7-C8-C9
3	D	409	OLA	C9-C10-C11-C12
2	D	405	OLC	C6-C7-C8-C9
4	E	406	LFA	C10-C11-C12-C13
4	D	403	LFA	C3-C4-C5-C6
2	D	405	OLC	C5-C6-C7-C8
4	D	403	LFA	C7-C8-C9-C10
4	D	402	LFA	C1-C2-C3-C4
4	E	406	LFA	C3-C4-C5-C6
3	A	304	OLA	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	305	OLA	C2-C3-C4-C5
3	E	407	OLA	O2-C1-C2-C3
4	D	404	LFA	C9-C10-C11-C12
2	D	405	OLC	C1-C2-C3-C4
4	C	1404	LFA	C7-C8-C9-C10
3	A	308	OLA	O2-C1-C2-C3
4	B	312	LFA	C17-C18-C19-C20
3	A	302	OLA	O1-C1-C2-C3
3	A	304	OLA	O1-C1-C2-C3
3	A	308	OLA	C4-C5-C6-C7
5	C	1408	BOG	O5-C1-O1-C1'
3	D	409	OLA	O1-C1-C2-C3
4	D	403	LFA	C4-C5-C6-C7
5	D	408	BOG	C5'-C6'-C7'-C8'
4	E	406	LFA	C16-C17-C18-C19
5	C	1408	BOG	C1'-C2'-C3'-C4'
3	E	407	OLA	O1-C1-C2-C3
3	E	405	OLA	C11-C12-C13-C14
3	D	409	OLA	C3-C4-C5-C6
3	A	308	OLA	O1-C1-C2-C3
3	A	302	OLA	C12-C13-C14-C15
3	D	409	OLA	O2-C1-C2-C3
4	E	408	LFA	C14-C15-C16-C17
3	A	302	OLA	O2-C1-C2-C3
4	A	303	LFA	C17-C18-C19-C20
3	B	305	OLA	O2-C1-C2-C3
3	B	309	OLA	O2-C1-C2-C3
3	D	409	OLA	C7-C8-C9-C10
3	E	411	OLA	C9-C10-C11-C12
5	E	412	BOG	C1'-C2'-C3'-C4'
3	B	305	OLA	O1-C1-C2-C3
4	A	303	LFA	C7-C8-C9-C10
4	D	404	LFA	C11-C12-C13-C14
4	E	406	LFA	C13-C14-C15-C16
4	A	303	LFA	C3-C4-C5-C6
4	E	408	LFA	C12-C13-C14-C15
6	E	414	RET	C12-C13-C14-C15
3	A	307	OLA	O2-C1-C2-C3
3	B	309	OLA	O1-C1-C2-C3
3	A	307	OLA	O1-C1-C2-C3
3	A	308	OLA	C7-C8-C9-C10
3	B	309	OLA	C9-C10-C11-C12

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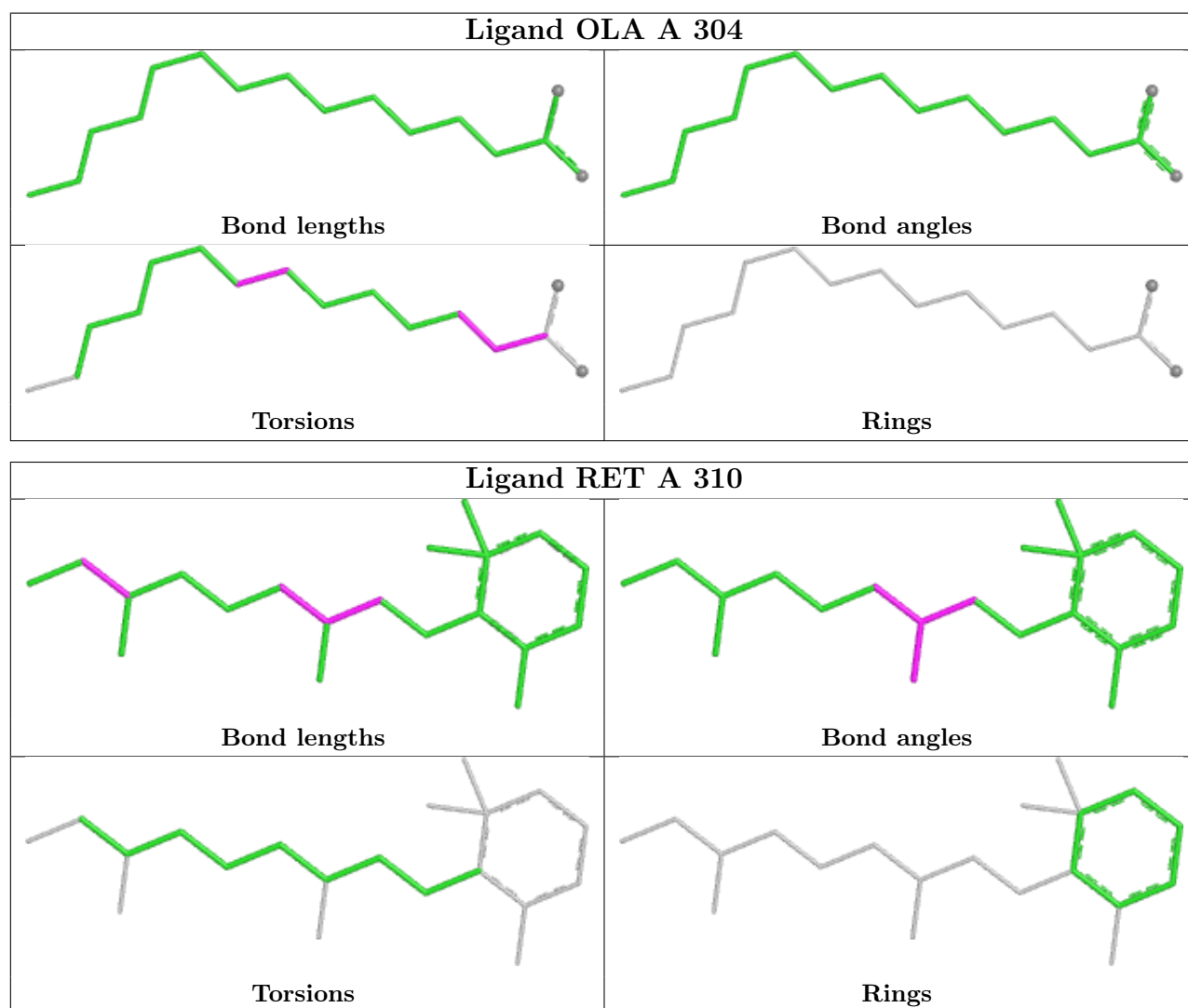
Mol	Chain	Res	Type	Atoms
3	E	405	OLA	C7-C8-C9-C10
3	A	304	OLA	C6-C7-C8-C9
4	B	304	LFA	C9-C10-C11-C12
4	C	1406	LFA	C3-C4-C5-C6
3	E	411	OLA	O2-C1-C2-C3
3	E	405	OLA	C12-C13-C14-C15

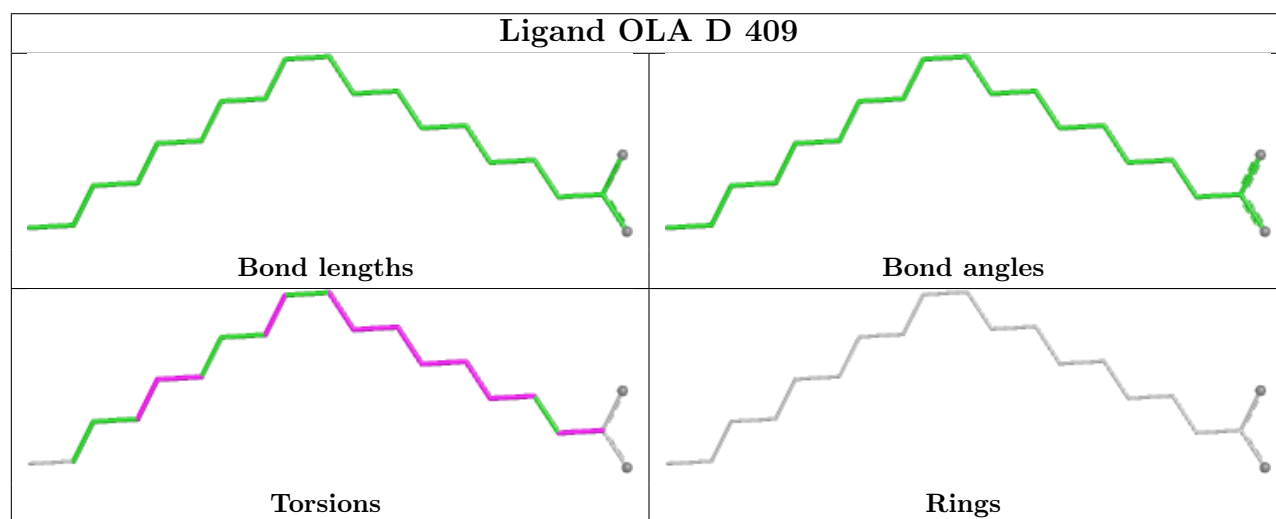
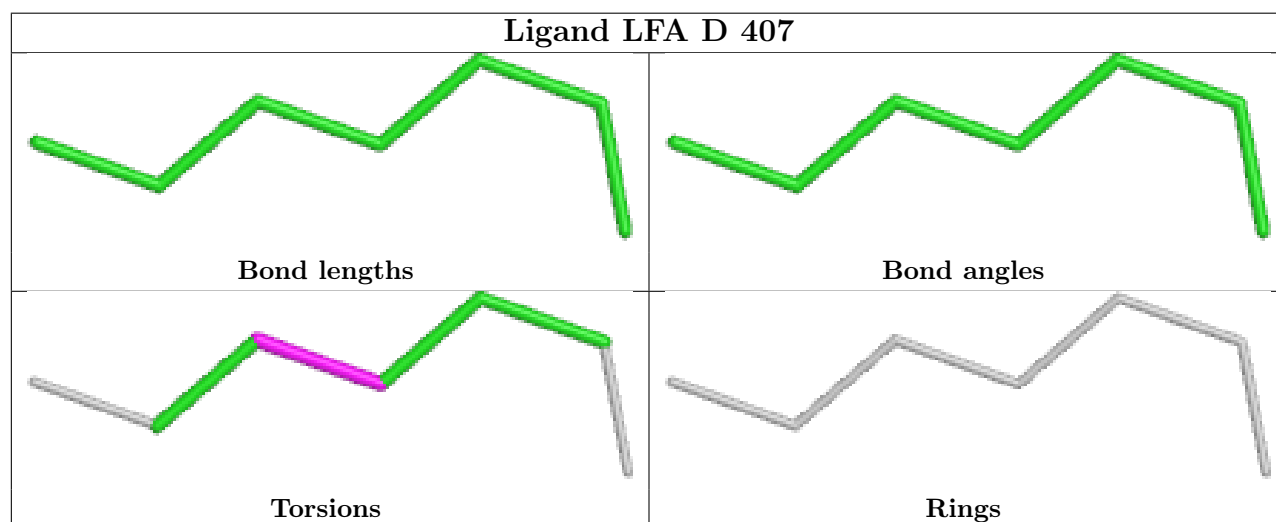
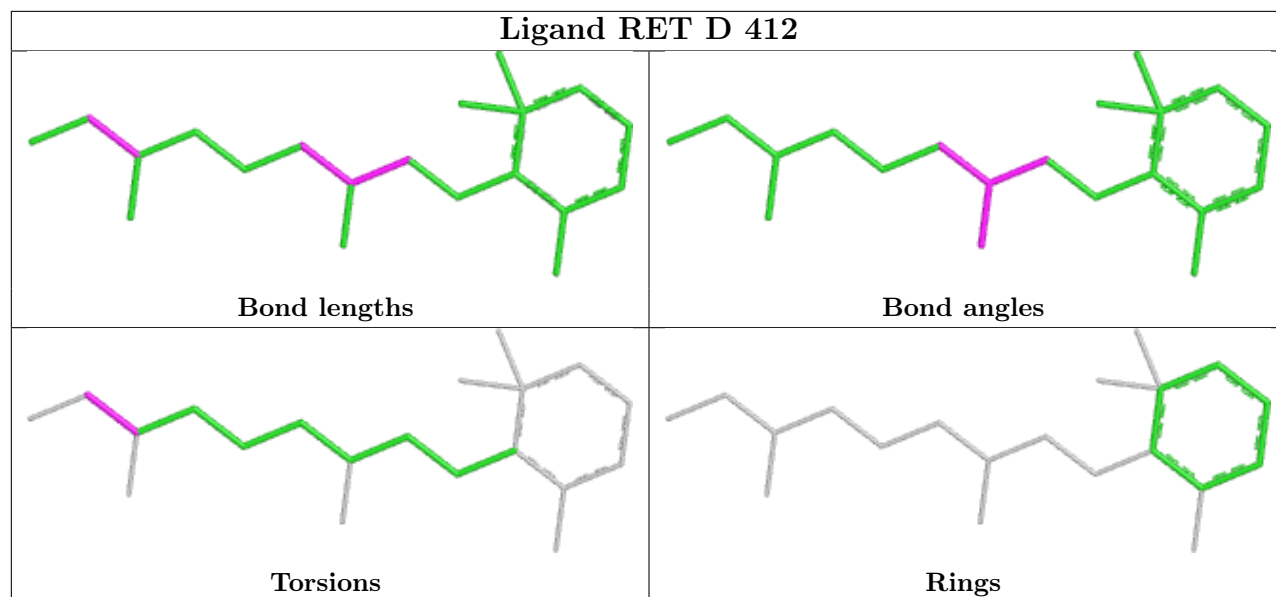
There are no ring outliers.

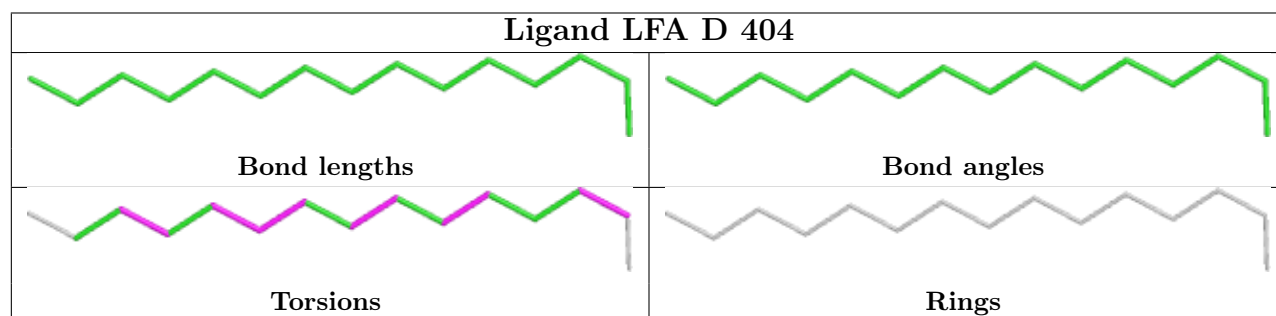
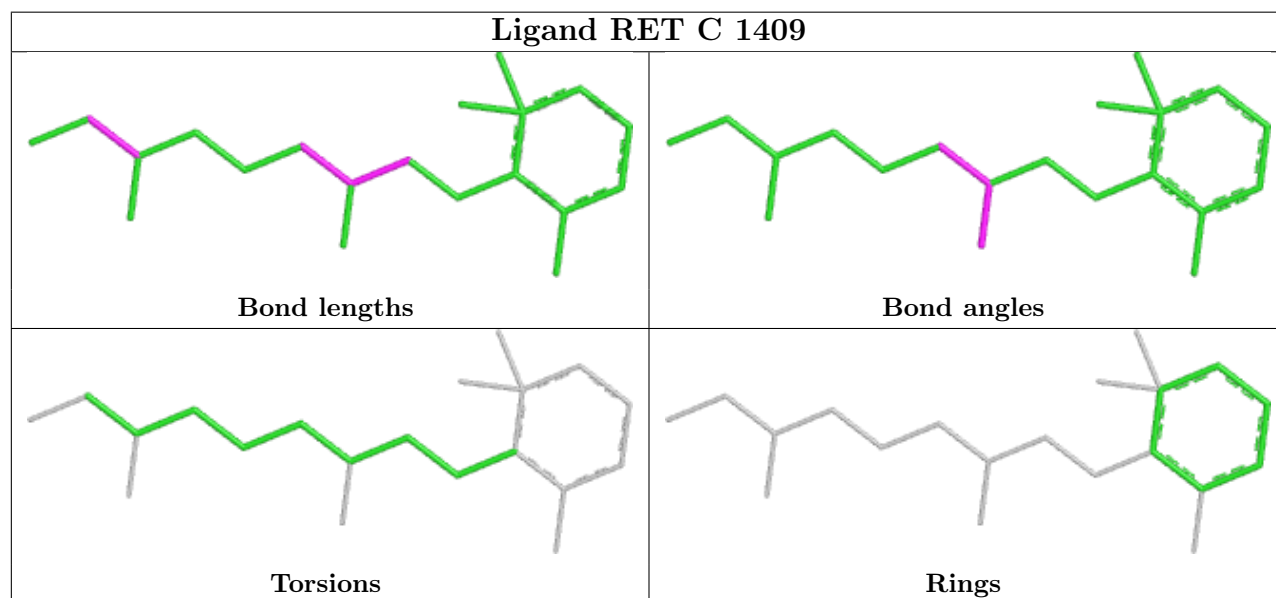
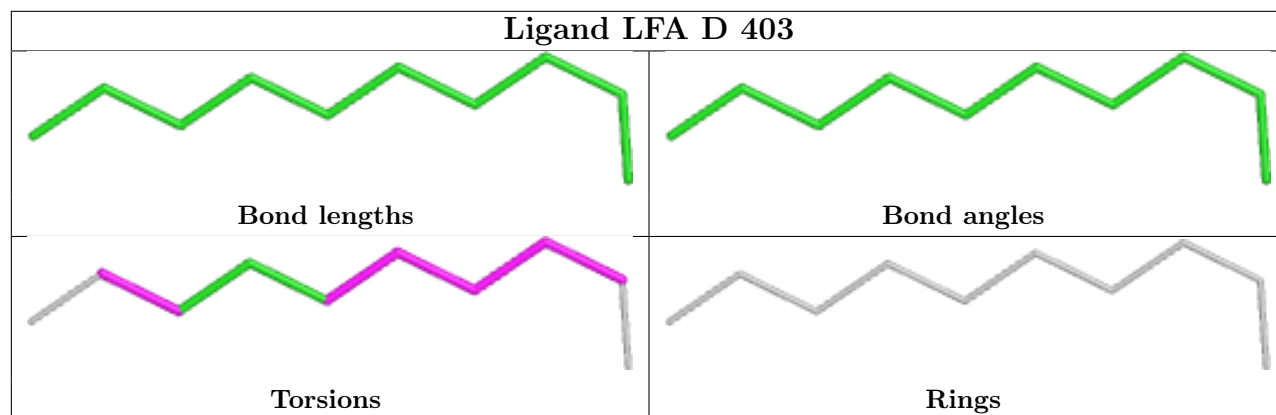
30 monomers are involved in 56 short contacts:

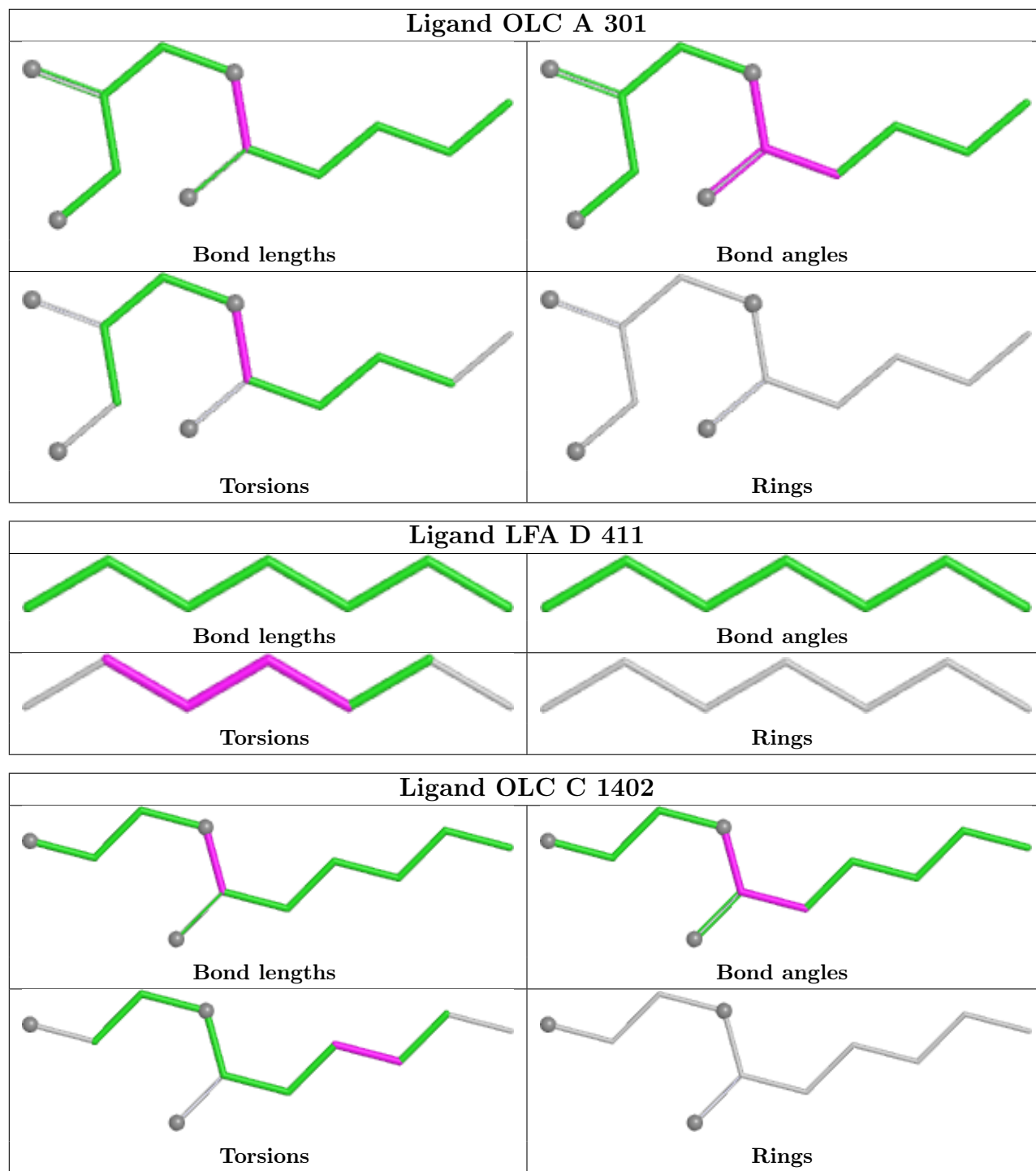
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	311	OLA	3	0
3	B	308	OLA	2	0
6	A	310	RET	3	0
6	D	412	RET	4	0
4	D	407	LFA	1	0
4	D	403	LFA	1	0
6	C	1409	RET	4	0
3	D	406	OLA	2	0
5	B	310	BOG	2	0
3	C	1401	OLA	2	0
4	E	402	LFA	3	0
4	D	401	LFA	3	0
4	E	406	LFA	5	0
4	B	312	LFA	4	0
4	B	303	LFA	1	0
3	E	403	OLA	3	0
5	E	412	BOG	4	0
4	D	402	LFA	1	0
4	E	408	LFA	2	0
5	D	408	BOG	2	0
6	B	311	RET	4	0
4	B	304	LFA	4	0
4	E	401	LFA	2	0
3	A	302	OLA	2	0
4	E	409	LFA	1	0
3	A	308	OLA	1	0
5	A	309	BOG	1	0
6	E	414	RET	4	0
3	E	407	OLA	1	0
4	C	1404	LFA	1	0

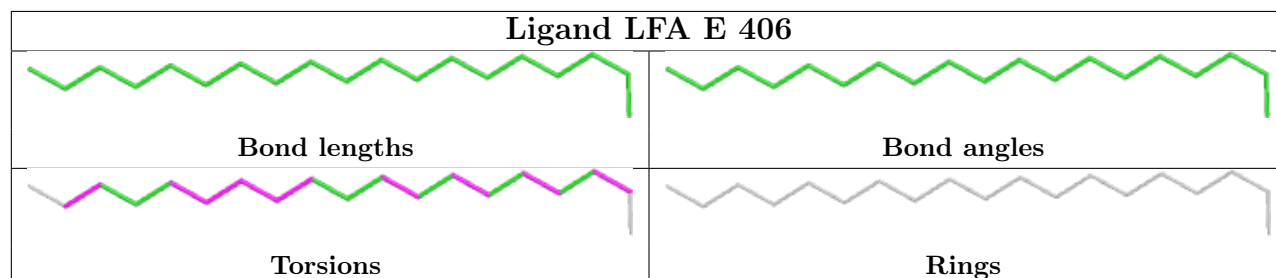
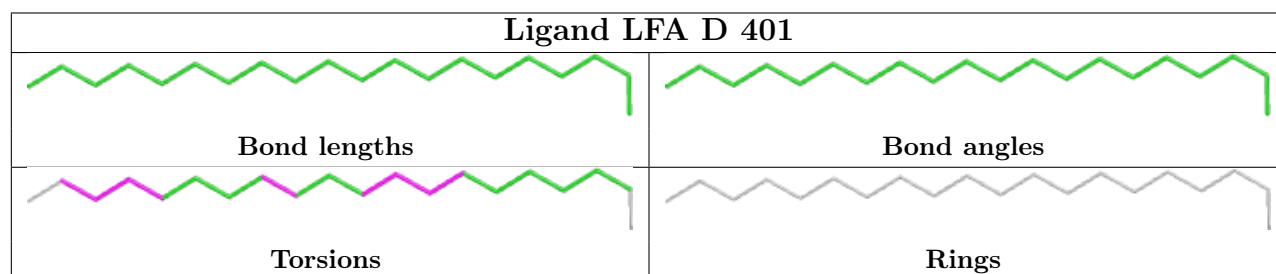
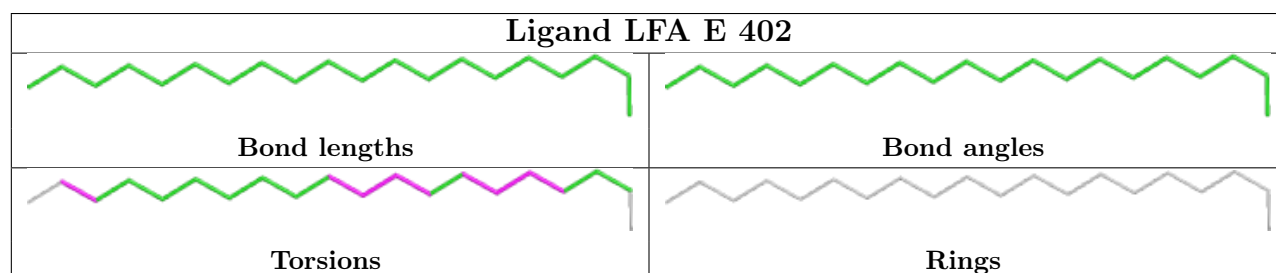
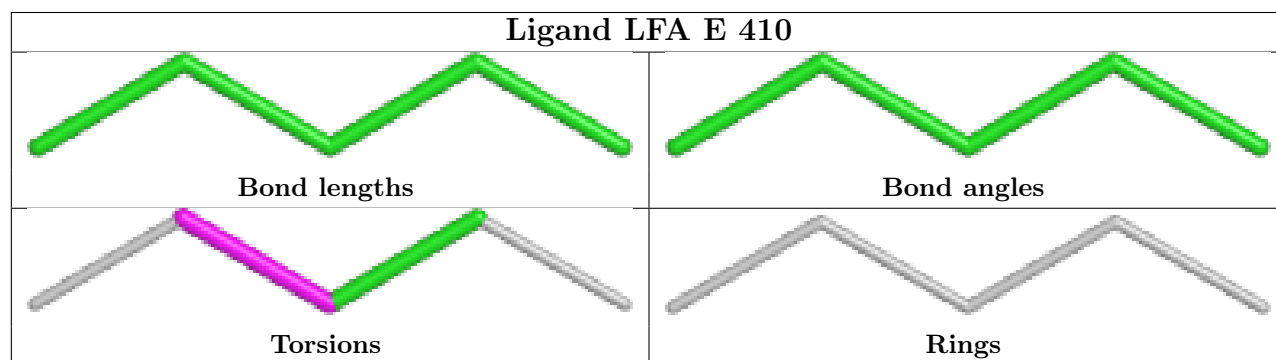
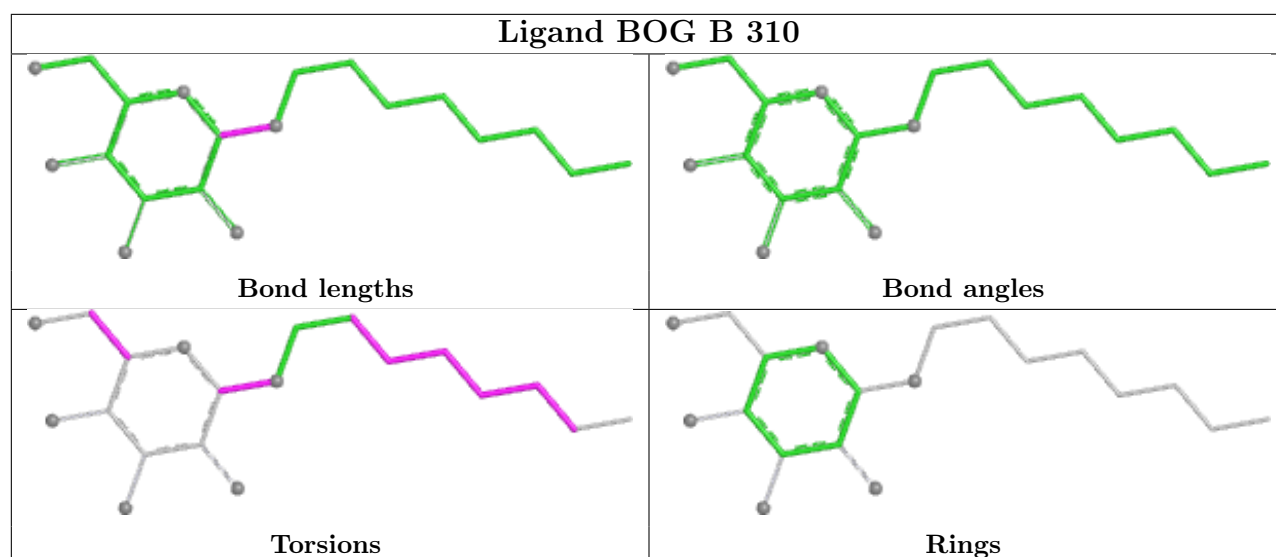
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

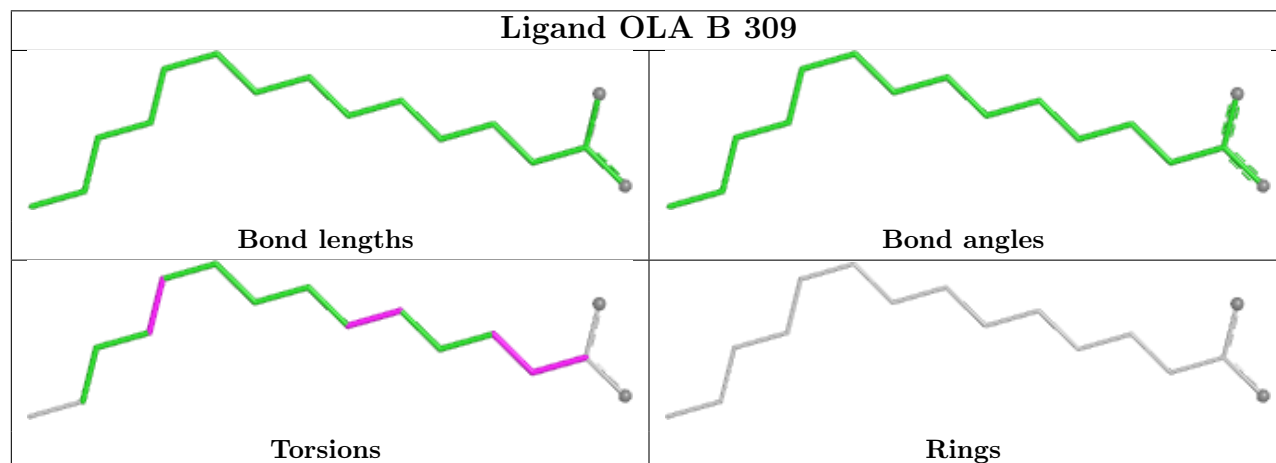
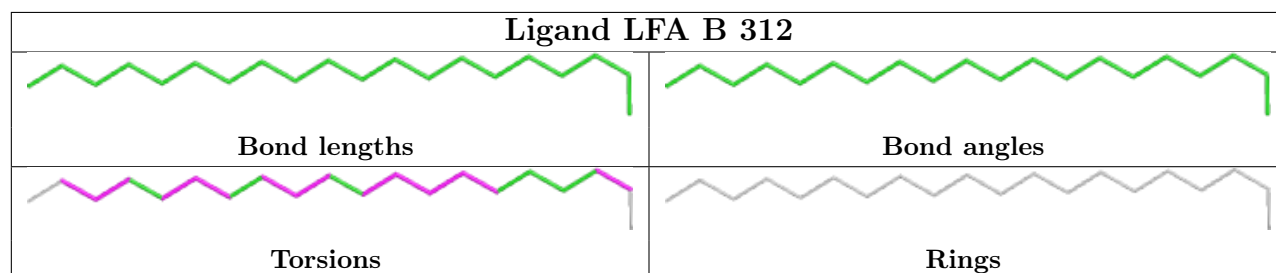
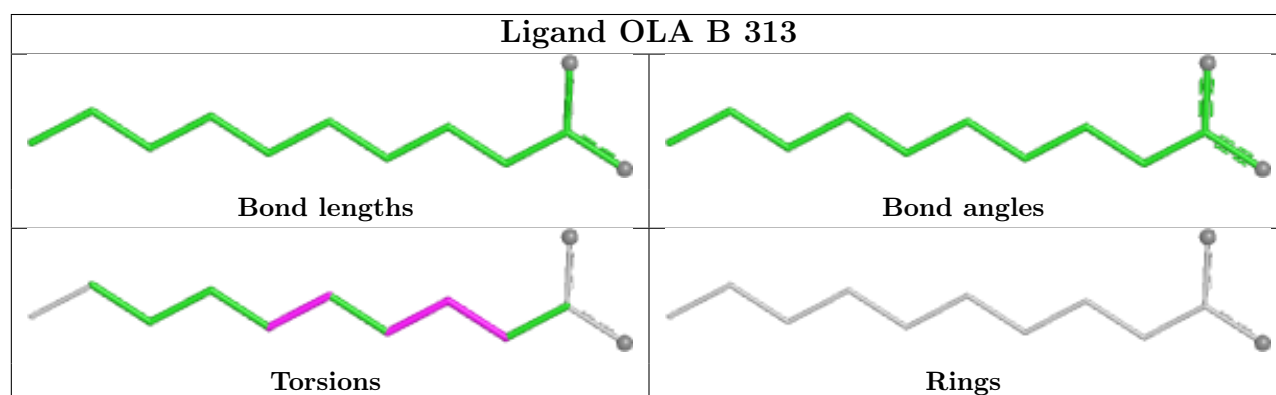
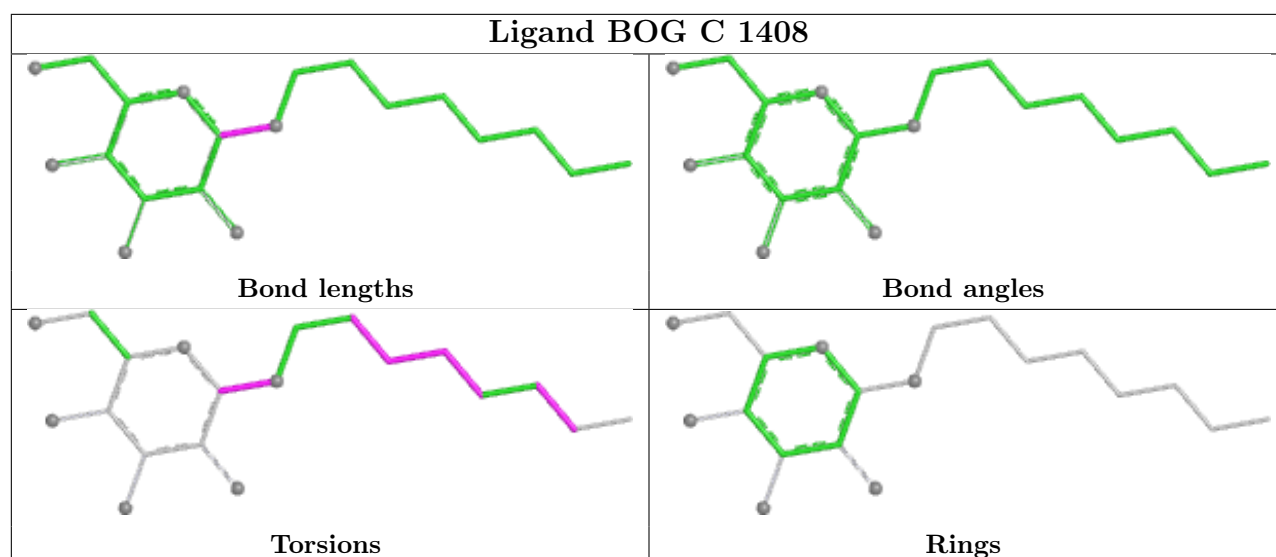


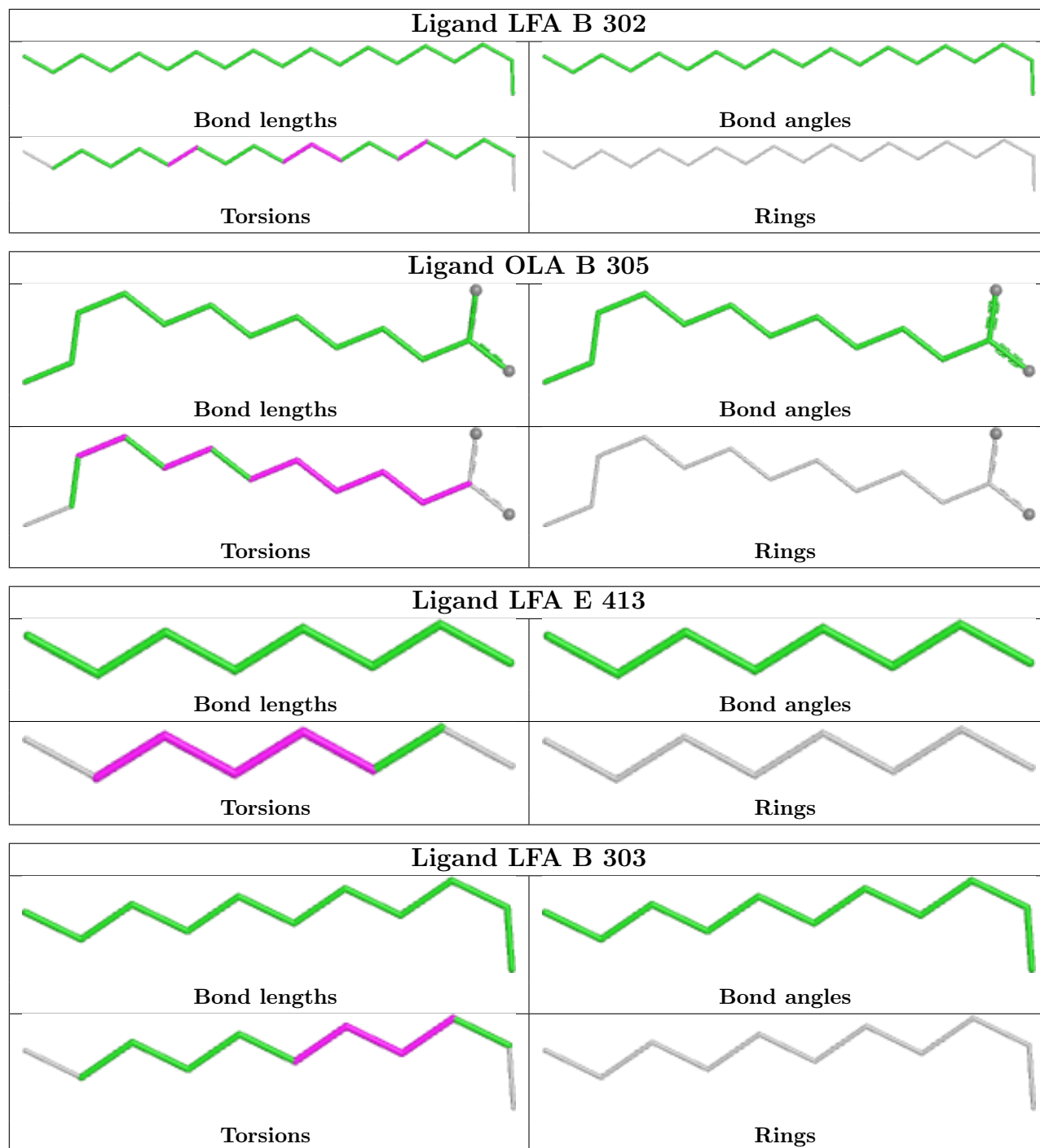


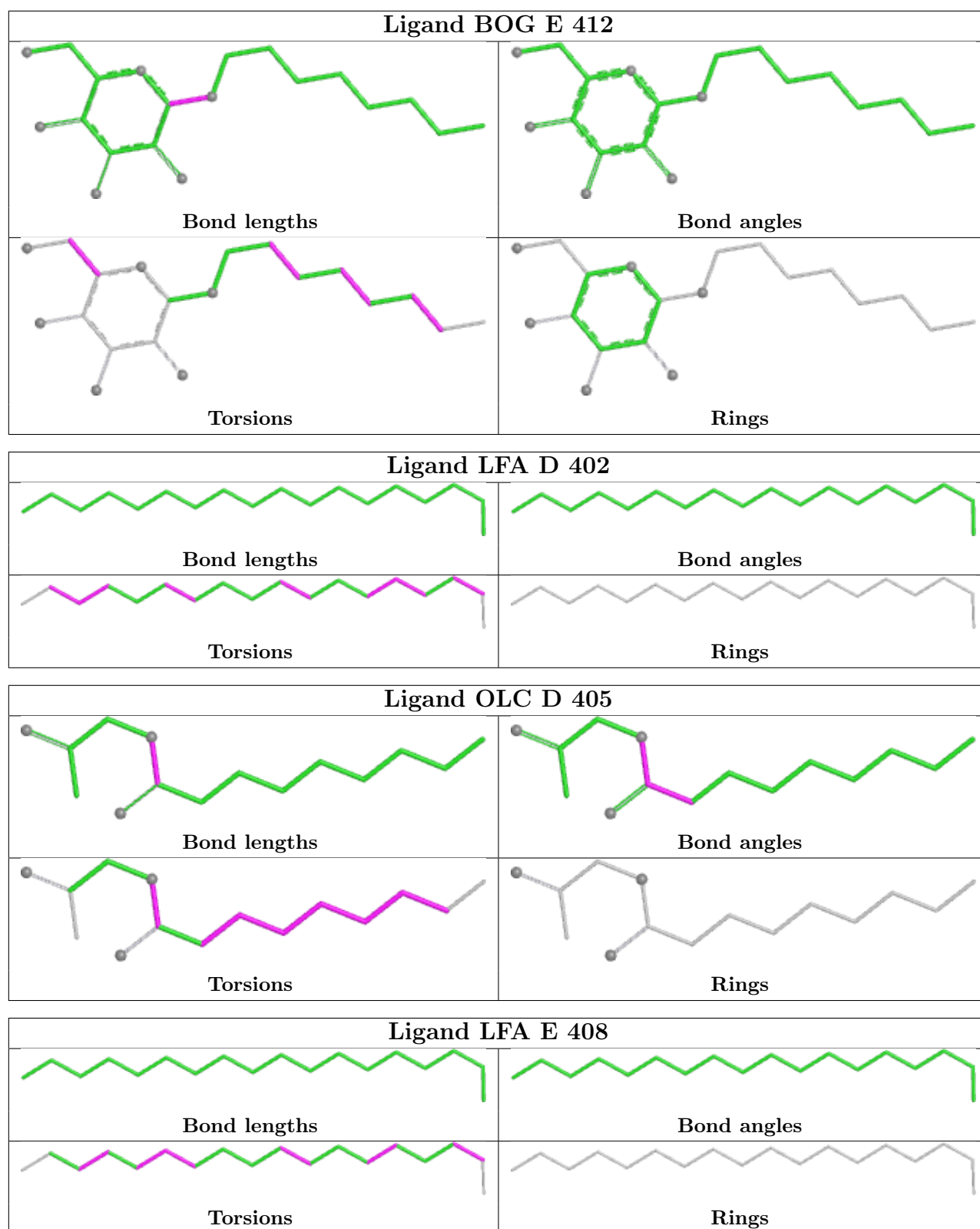


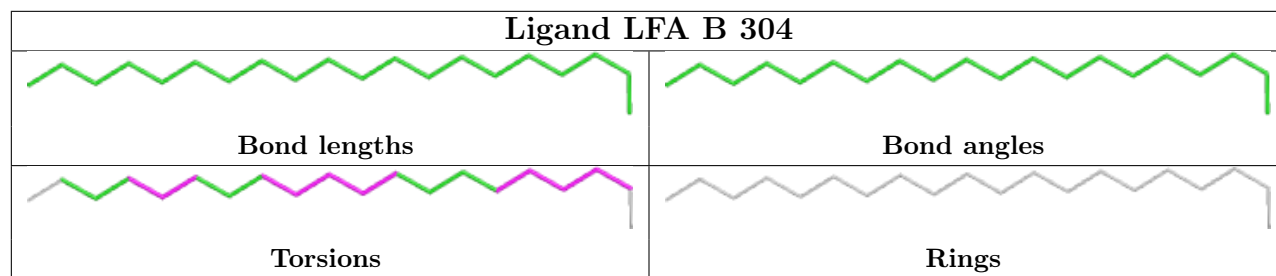
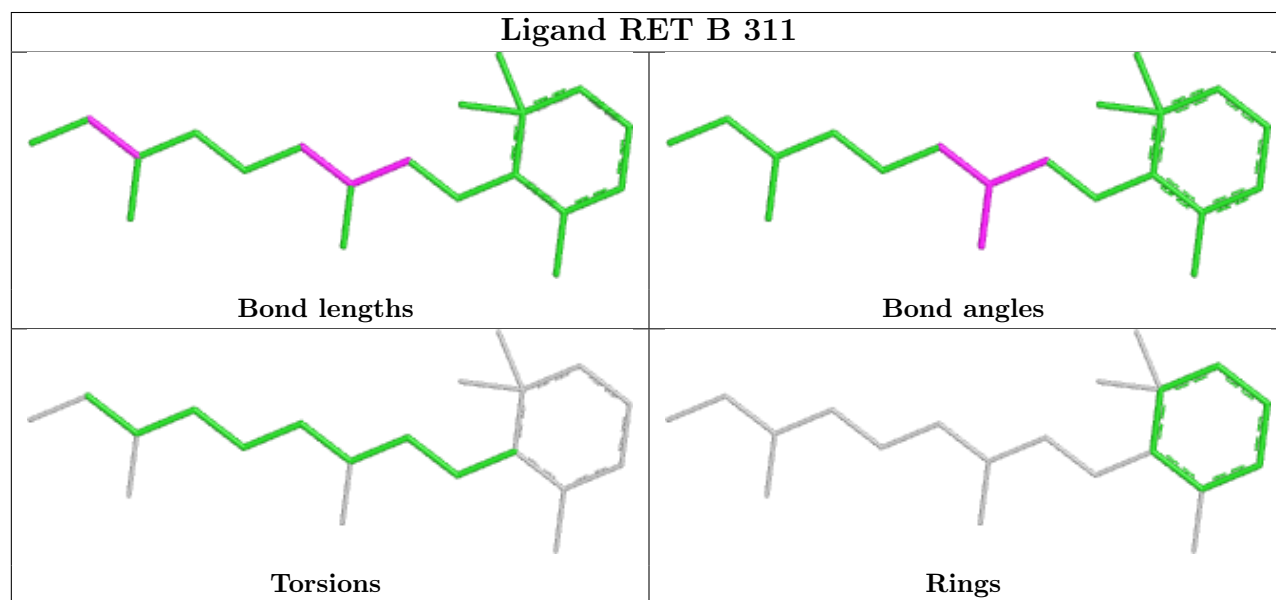
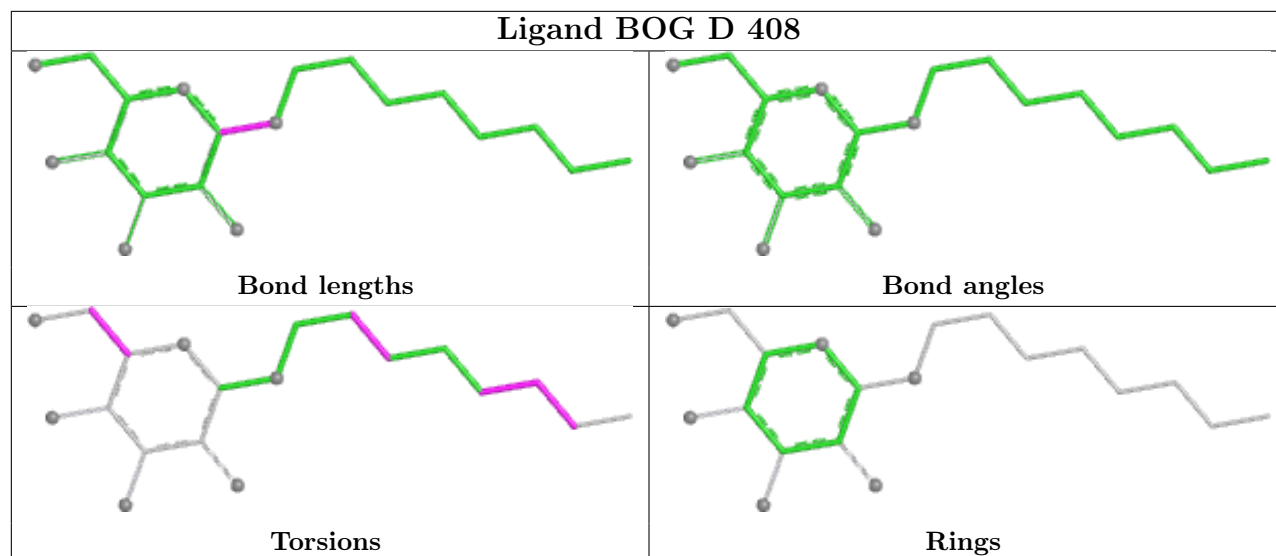


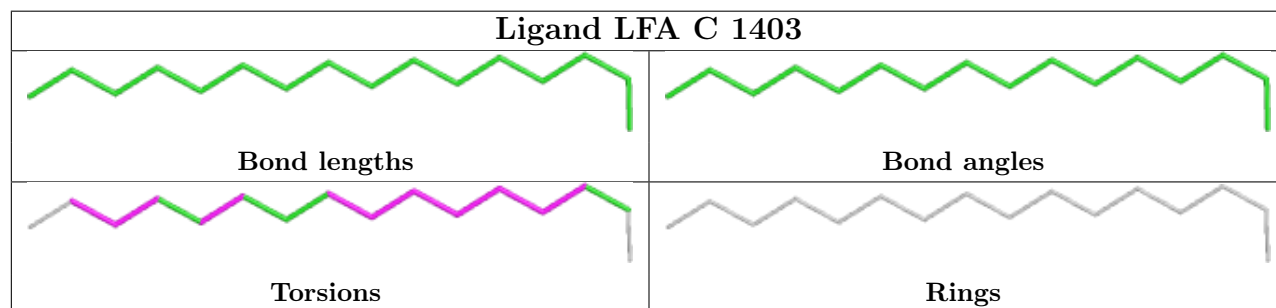
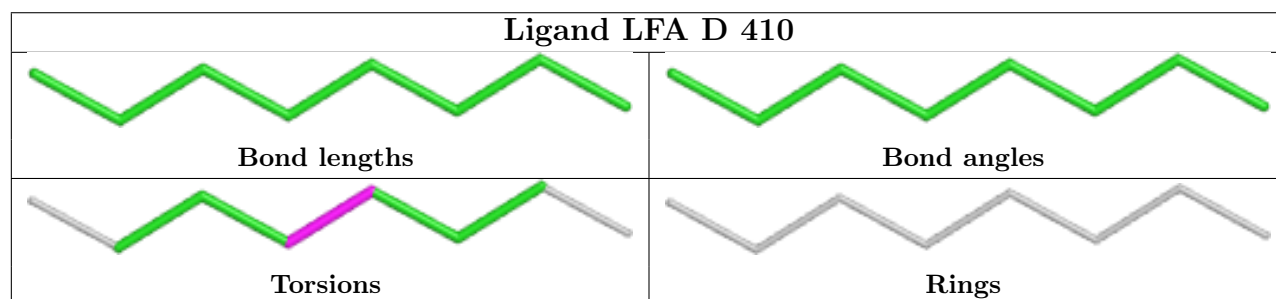
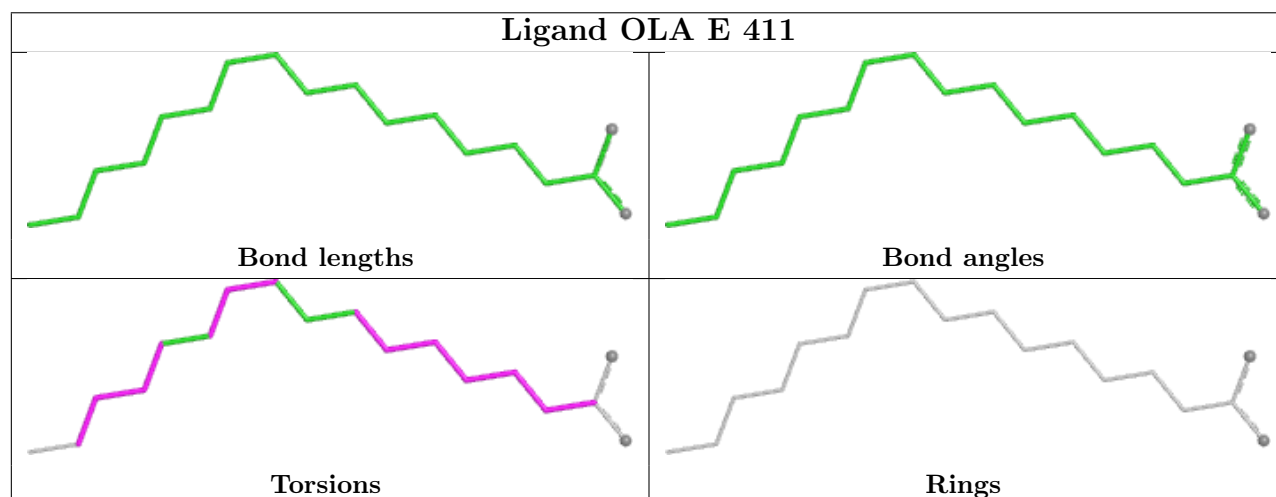
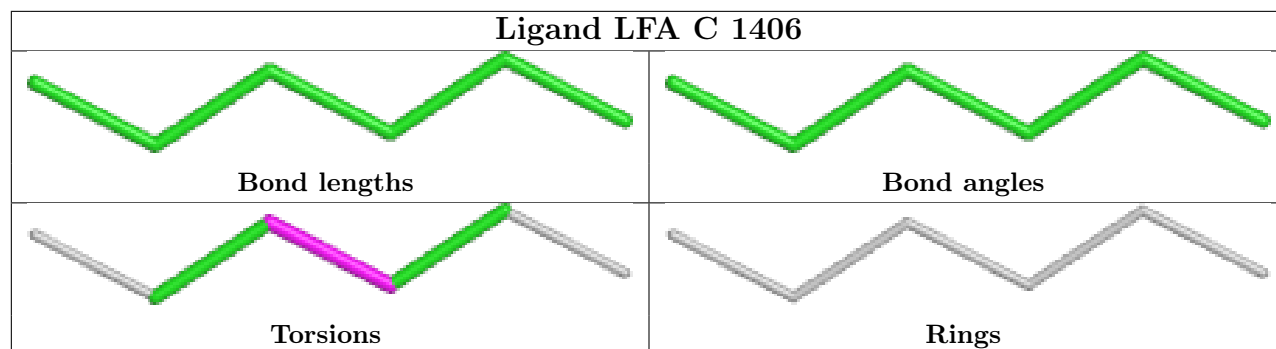


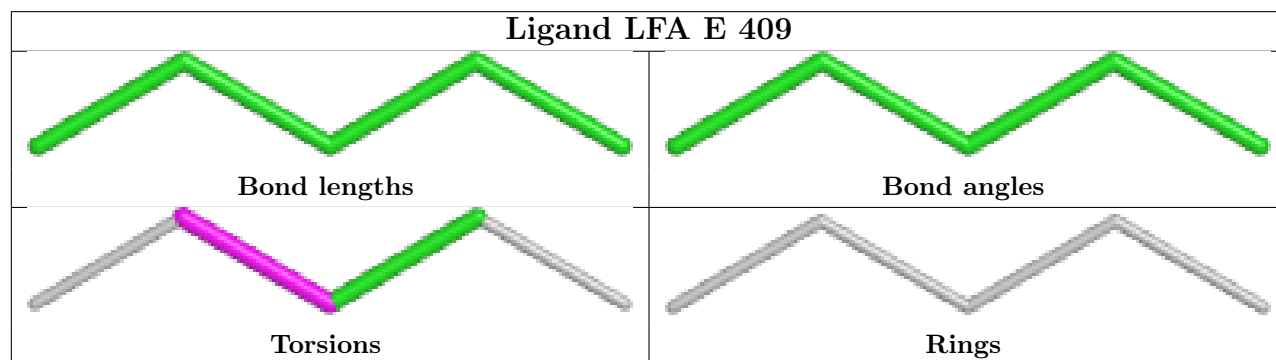
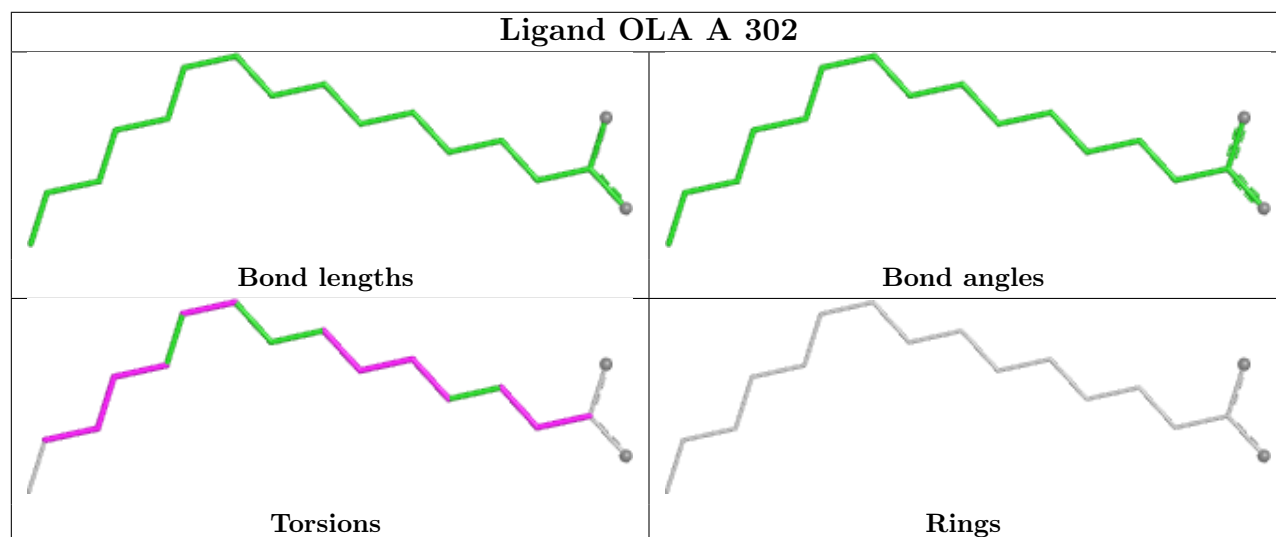
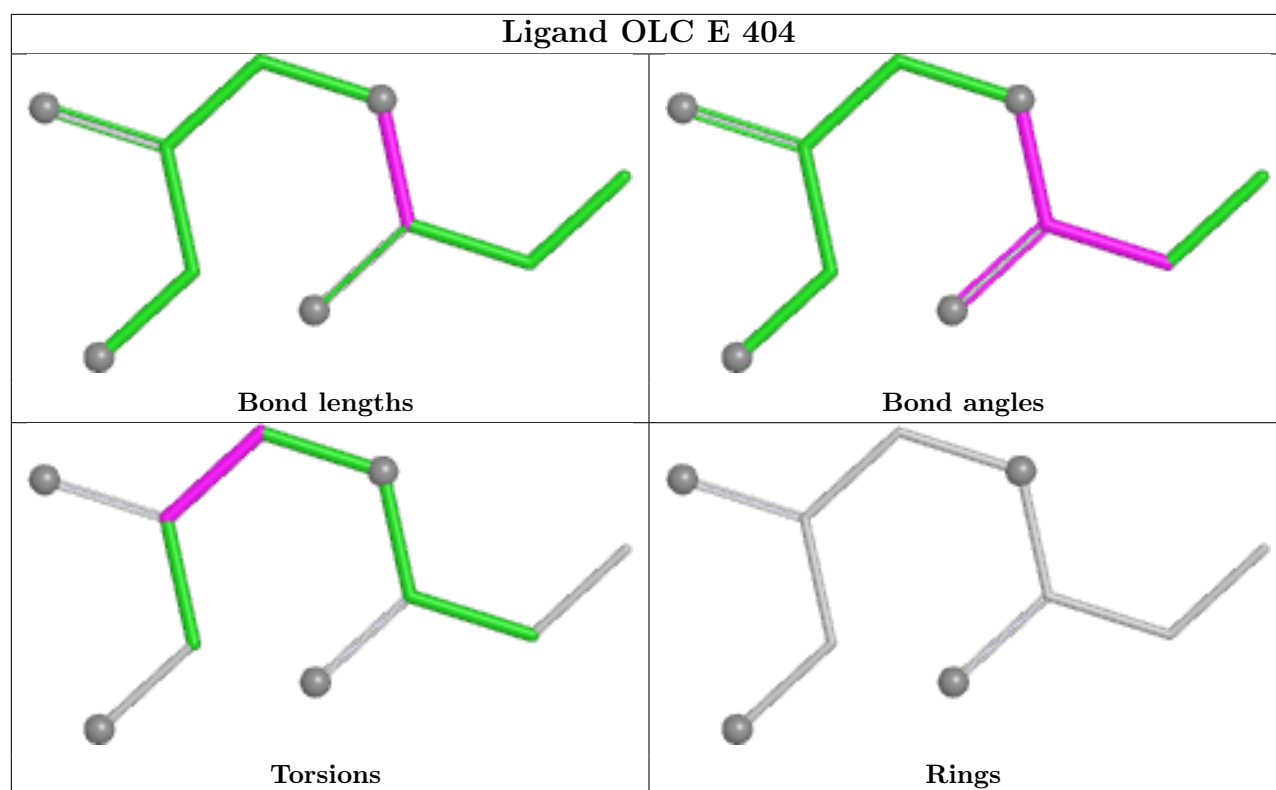


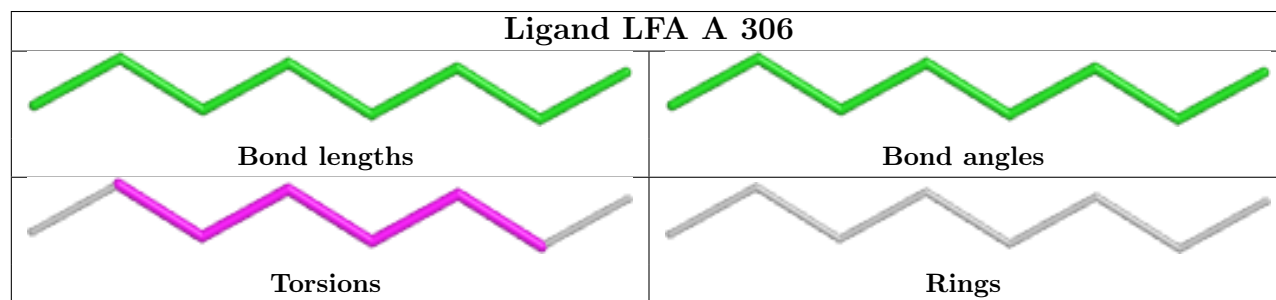
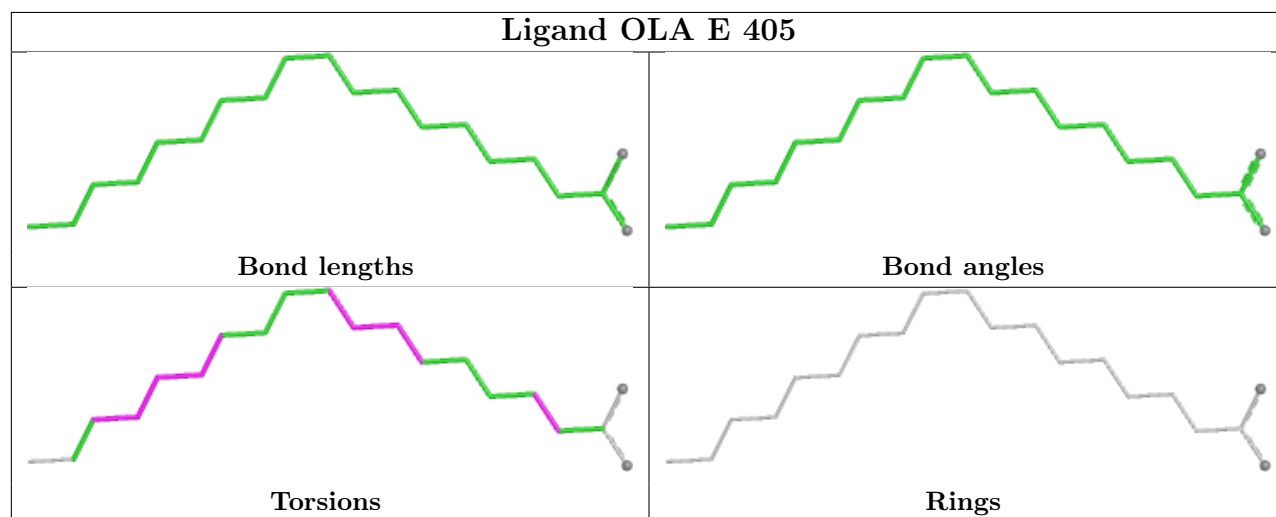
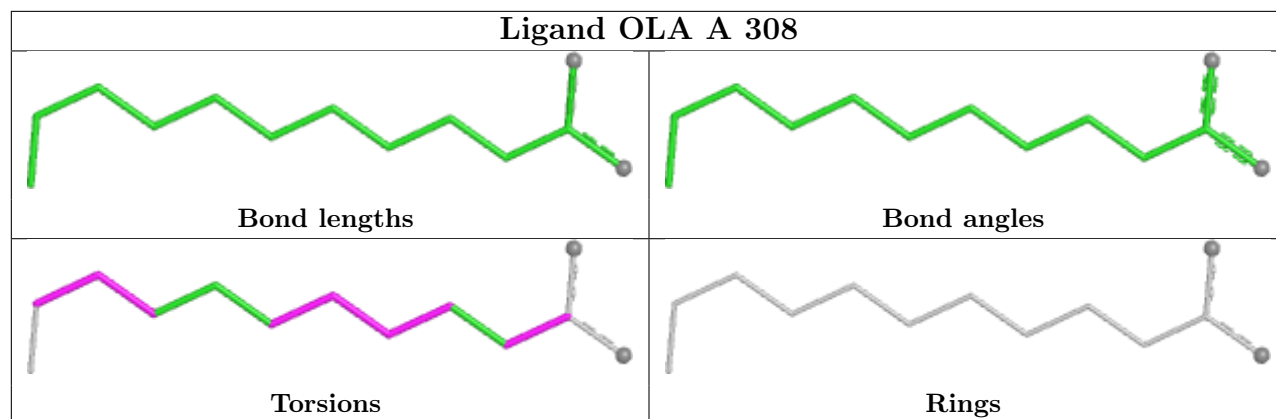


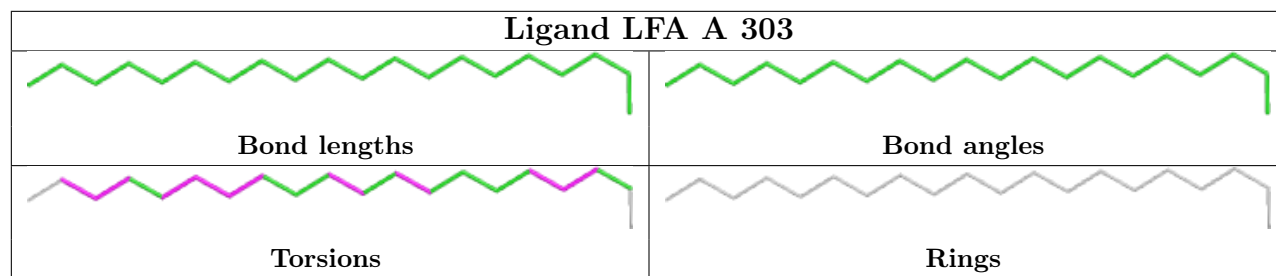
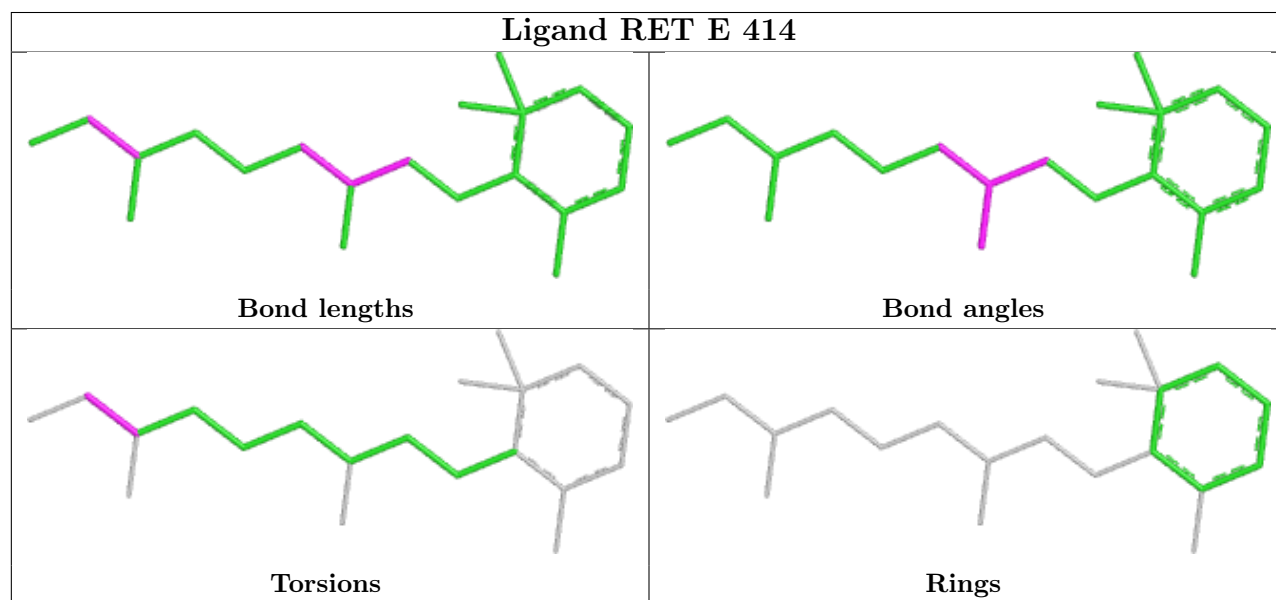
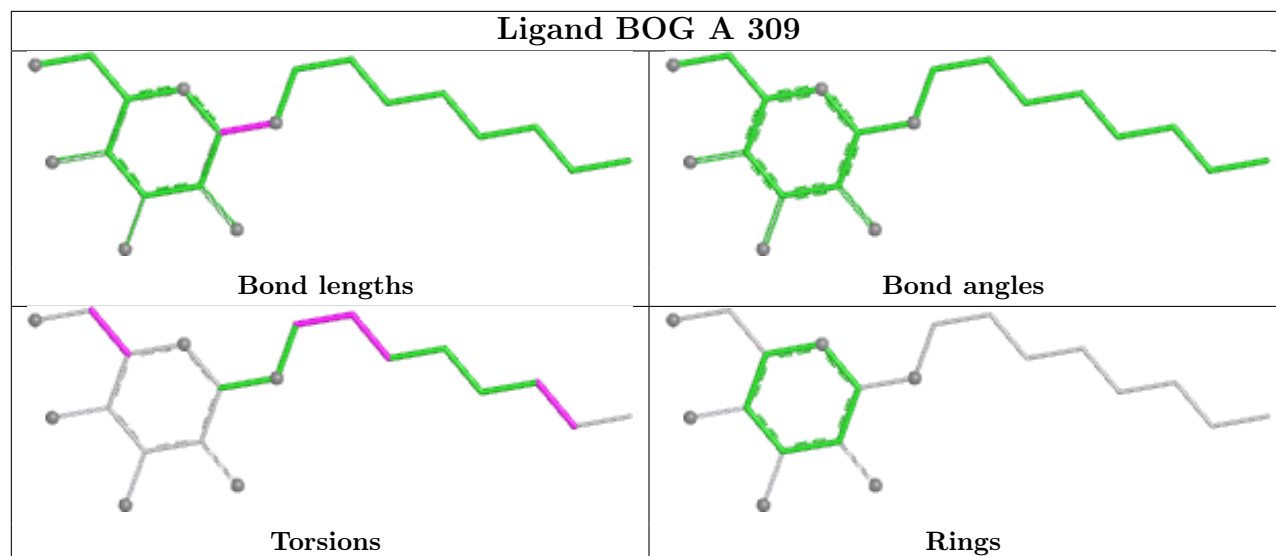


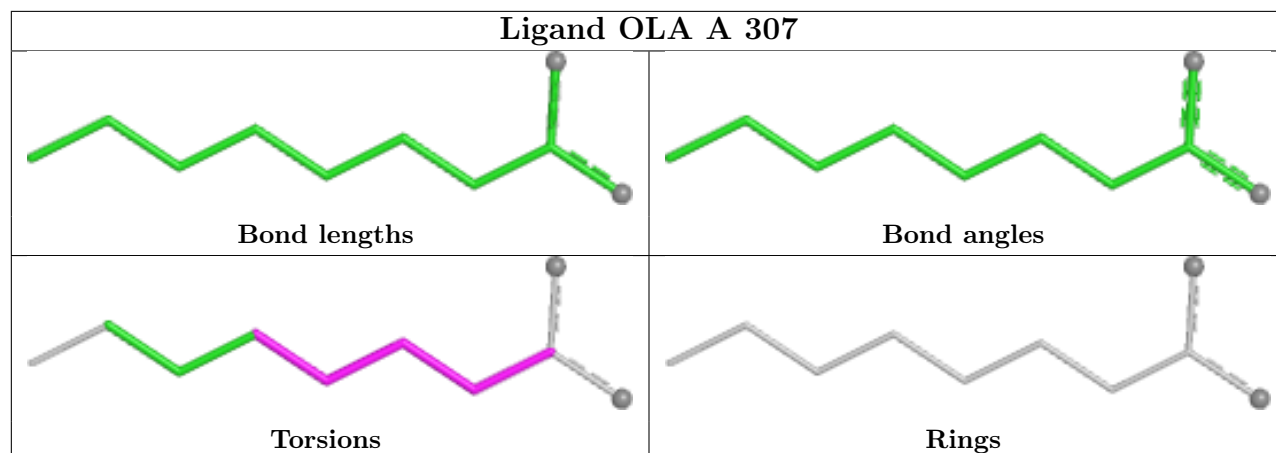
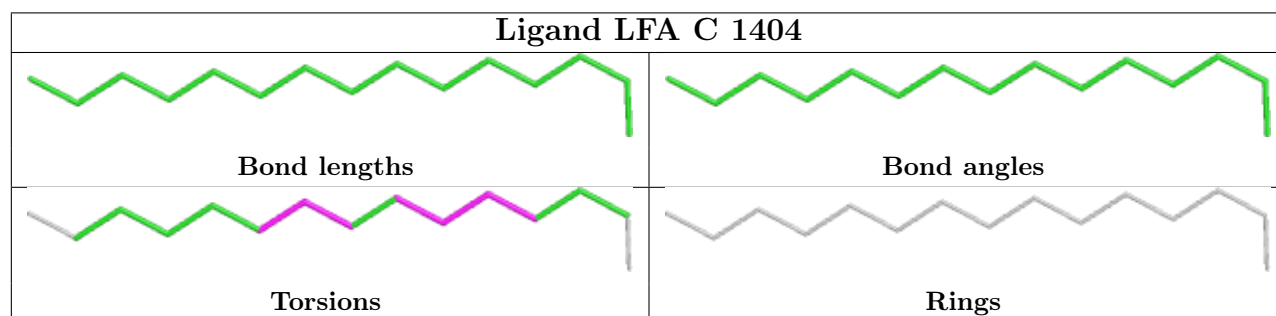
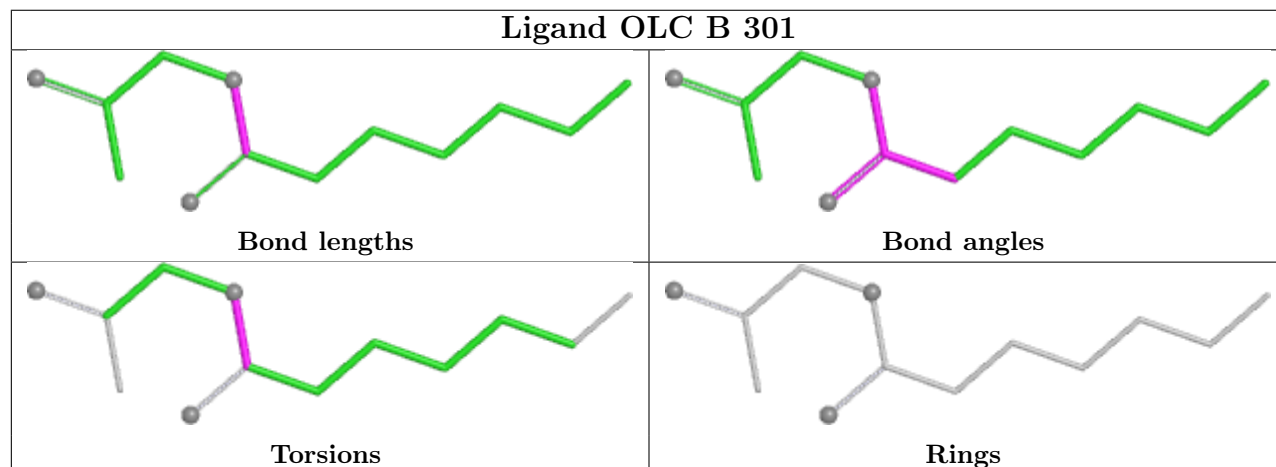
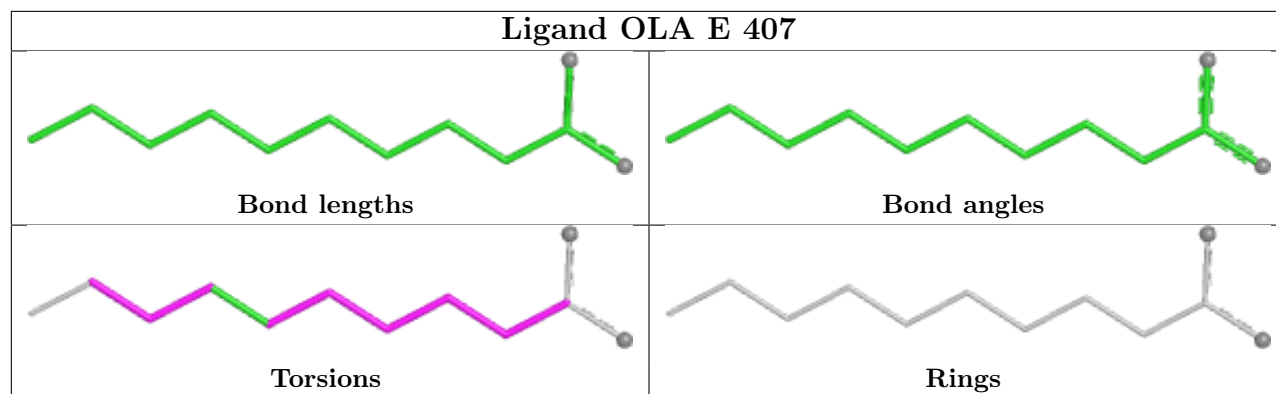












5.7 Other polymers [i](#)

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	269/288 (93%)	-0.25	1 (0%) 88 86	19, 40, 59, 82	2 (0%)
1	B	269/288 (93%)	-0.20	3 (1%) 78 74	18, 41, 60, 86	2 (0%)
1	C	268/288 (93%)	-0.13	1 (0%) 88 86	20, 43, 64, 89	2 (0%)
1	D	270/288 (93%)	-0.17	1 (0%) 88 86	19, 42, 62, 91	2 (0%)
1	E	273/288 (94%)	-0.15	4 (1%) 72 68	20, 43, 67, 130	2 (0%)
All	All	1349/1440 (93%)	-0.18	10 (0%) 84 81	18, 42, 63, 130	10 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	LYS	3.7
1	E	272	ASN	3.6
1	B	271	LYS	3.5
1	B	230	VAL	3.1
1	E	275	LEU	3.0
1	D	272	ASN	2.6
1	C	198	PRO	2.5
1	E	274	GLU	2.5
1	B	132	THR	2.4
1	E	230	VAL	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLA	D	409	20/20	0.67	0.20	65,80,103,103	0
4	LFA	D	411	7/20	0.67	0.21	56,62,64,69	0
5	BOG	E	412	20/20	0.67	0.20	69,102,129,136	0
4	LFA	D	403	10/20	0.68	0.26	59,65,69,72	0
4	LFA	B	307	9/20	0.69	0.23	58,67,80,84	0
5	BOG	B	310	20/20	0.73	0.17	65,99,114,118	0
5	BOG	A	309	20/20	0.73	0.19	66,93,122,127	0
4	LFA	E	410	5/20	0.74	0.30	57,63,72,73	0
3	OLA	A	307	10/20	0.76	0.16	65,76,82,85	0
4	LFA	E	413	8/20	0.76	0.20	62,69,79,84	0
4	LFA	C	1406	6/20	0.76	0.25	58,61,68,72	0
4	LFA	B	303	11/20	0.77	0.16	52,59,70,71	0
4	LFA	E	402	20/20	0.77	0.15	54,67,83,87	0
4	LFA	E	406	19/20	0.77	0.15	51,69,76,82	0
4	LFA	D	404	15/20	0.78	0.20	65,74,88,89	0
4	LFA	E	401	5/20	0.78	0.22	48,54,59,63	0
4	LFA	C	1405	3/20	0.79	0.28	54,54,57,59	0
3	OLA	A	308	13/20	0.79	0.17	55,65,84,93	0
2	OLC	D	405	15/25	0.79	0.15	61,74,78,80	0
4	LFA	B	312	20/20	0.79	0.14	56,68,77,77	0
5	BOG	D	408	20/20	0.79	0.15	65,81,109,120	0
4	LFA	D	401	20/20	0.79	0.13	54,65,76,77	0
4	LFA	B	304	20/20	0.81	0.13	61,73,76,78	0
4	LFA	A	306	8/20	0.81	0.15	55,64,76,77	0
2	OLC	B	301	13/25	0.81	0.16	63,68,78,83	0
3	OLA	E	403	4/20	0.82	0.14	50,77,81,82	0
3	OLA	B	308	4/20	0.82	0.14	62,78,80,92	0
2	OLC	C	1402	11/25	0.82	0.14	57,67,70,73	0
5	BOG	C	1408	20/20	0.82	0.16	71,94,116,116	0
4	LFA	C	1407	5/20	0.83	0.23	47,61,63,64	0
3	OLA	B	309	16/20	0.83	0.15	64,76,84,88	0
4	LFA	C	1403	16/20	0.83	0.15	50,54,61,62	0
4	LFA	D	410	8/20	0.84	0.15	55,63,73,74	0
4	LFA	B	302	19/20	0.84	0.16	47,62,70,79	0
3	OLA	B	305	14/20	0.84	0.15	72,79,88,89	0
4	LFA	C	1404	15/20	0.84	0.16	57,71,87,89	0
4	LFA	A	303	20/20	0.84	0.15	60,73,90,94	0

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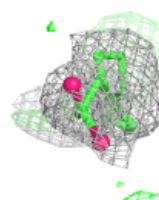
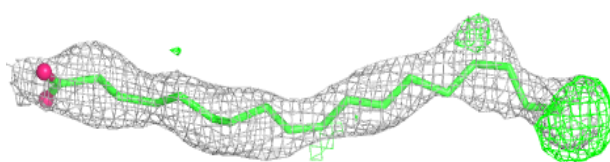
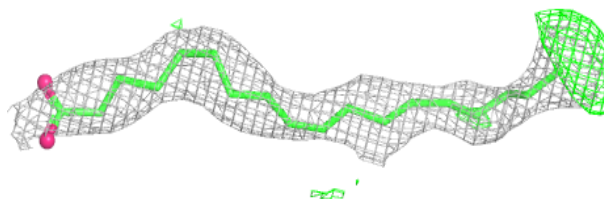
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	A	301	12/25	0.84	0.13	58,66,74,78	0
2	OLC	E	404	10/25	0.85	0.15	64,72,78,82	0
3	OLA	A	304	16/20	0.85	0.16	59,79,88,89	0
4	LFA	D	402	18/20	0.85	0.13	46,56,66,69	0
3	OLA	E	411	18/20	0.85	0.16	58,74,92,100	0
4	LFA	E	408	18/20	0.85	0.14	62,72,81,83	0
4	LFA	E	409	5/20	0.85	0.20	60,63,65,69	0
3	OLA	A	311	5/20	0.85	0.14	65,73,82,93	0
4	LFA	D	407	7/20	0.85	0.20	59,62,67,68	0
4	LFA	A	305	5/20	0.85	0.24	59,59,69,70	0
3	OLA	E	405	20/20	0.87	0.14	51,58,87,98	0
3	OLA	D	406	4/20	0.88	0.12	67,78,81,96	0
3	OLA	C	1401	4/20	0.89	0.10	52,73,75,86	0
4	LFA	B	306	6/20	0.89	0.20	50,64,71,74	0
3	OLA	E	407	12/20	0.89	0.13	72,79,85,86	0
3	OLA	B	313	12/20	0.89	0.12	64,73,84,88	0
3	OLA	A	302	17/20	0.90	0.11	45,54,70,72	0
6	RET	B	311	20/21	0.93	0.10	34,39,42,44	0
6	RET	D	412	20/21	0.93	0.10	36,43,46,47	0
6	RET	A	310	20/21	0.94	0.09	34,44,49,49	0
6	RET	E	414	20/21	0.94	0.10	39,44,48,52	0
6	RET	C	1409	20/21	0.94	0.10	38,42,51,52	0
7	NA	A	312	1/1	0.97	0.10	32,32,32,32	0
7	NA	B	314	1/1	0.98	0.05	33,33,33,33	0
7	NA	E	415	1/1	0.98	0.03	36,36,36,36	0
7	NA	D	413	1/1	0.99	0.08	31,31,31,31	0
7	NA	C	1410	1/1	0.99	0.08	33,33,33,33	0

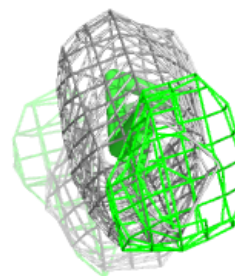
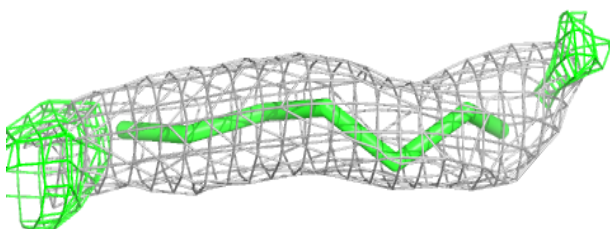
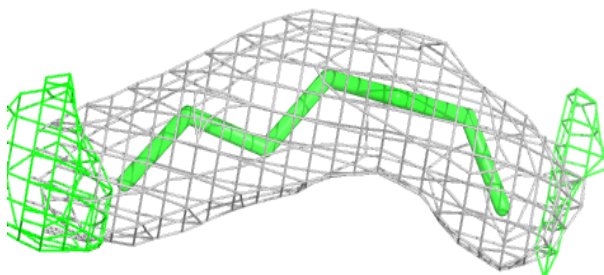
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA D 409:

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

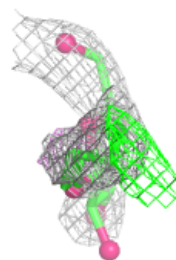
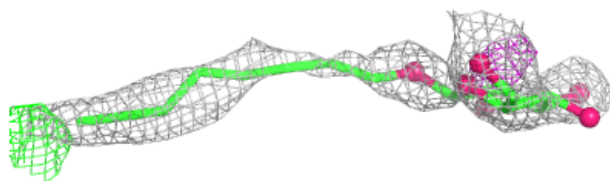
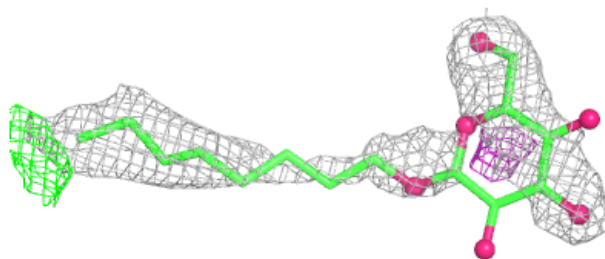
**Electron density around LFA D 411:**

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

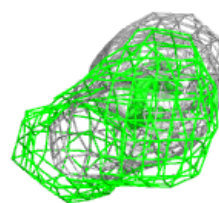
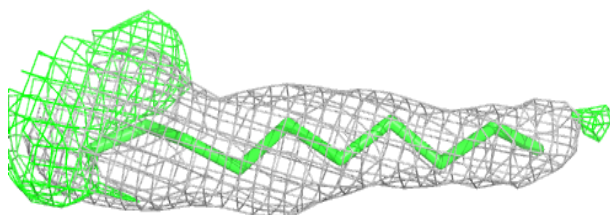
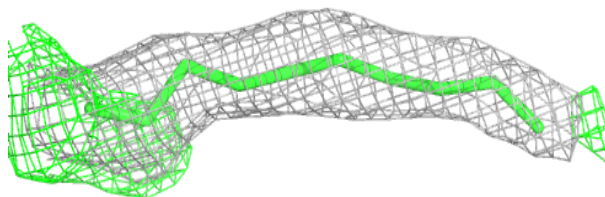


Electron density around BOG E 412:

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

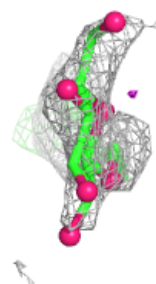
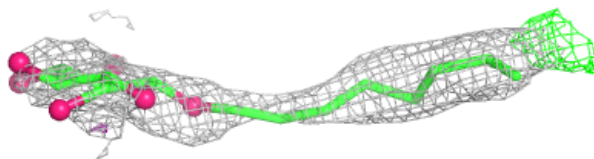
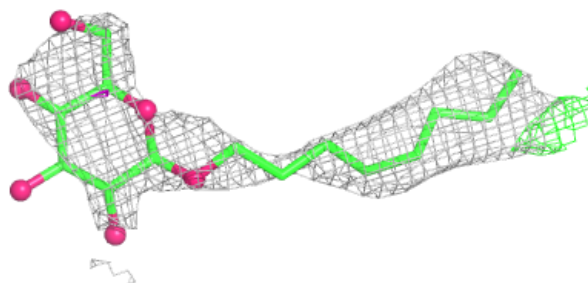
**Electron density around LFA D 403:**

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

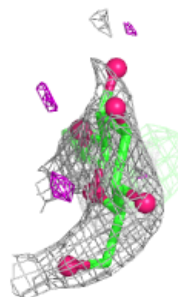
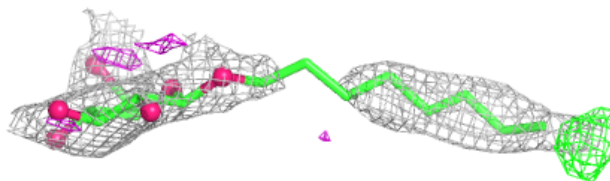
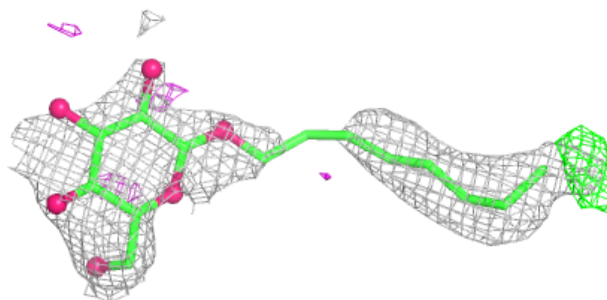


Electron density around BOG B 310:

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

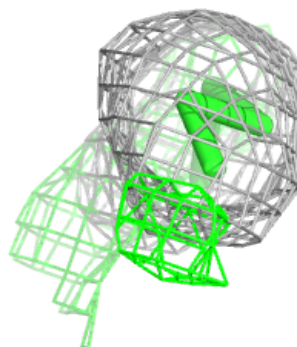
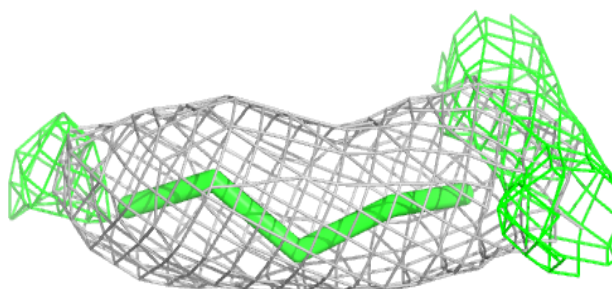
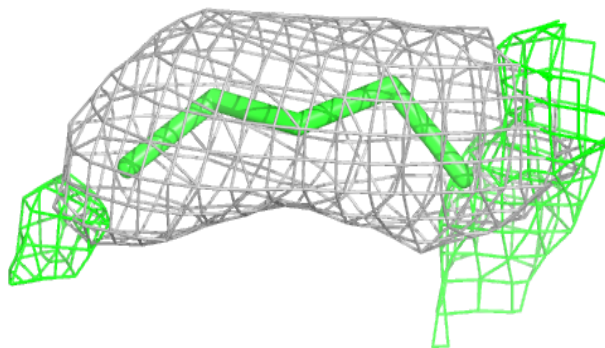
**Electron density around BOG A 309:**

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

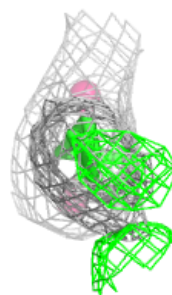
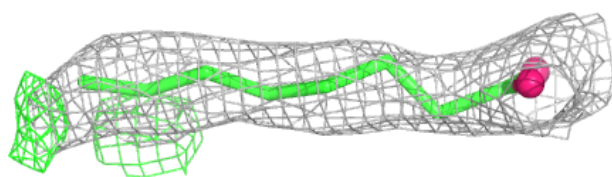
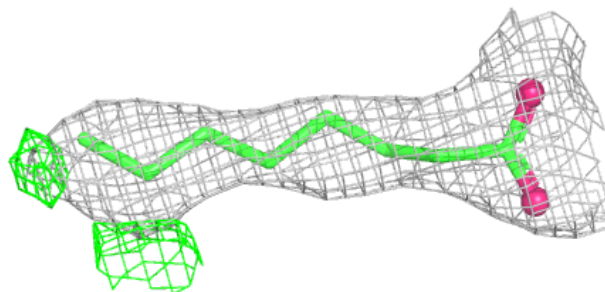


Electron density around LFA E 410:

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

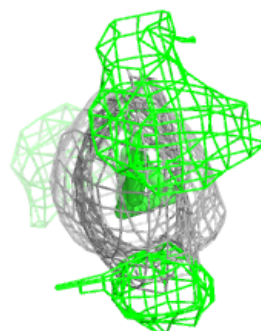
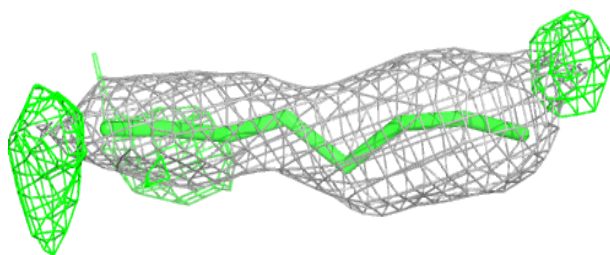
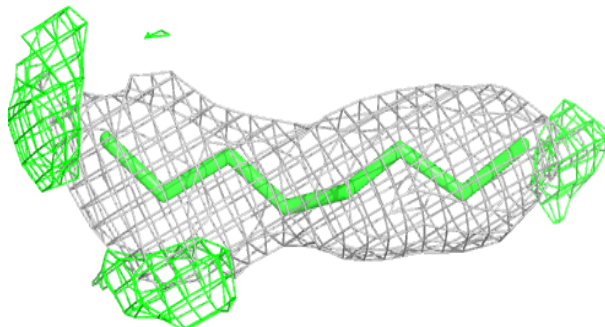
**Electron density around OLA A 307:**

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

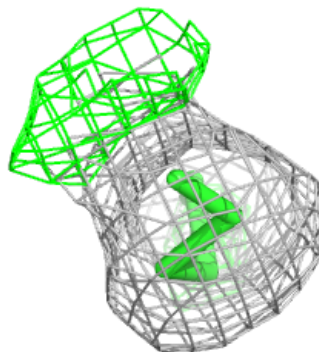
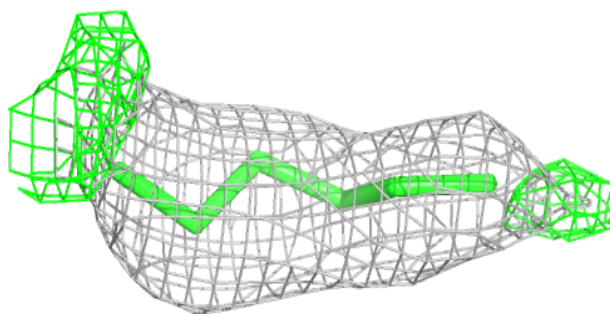
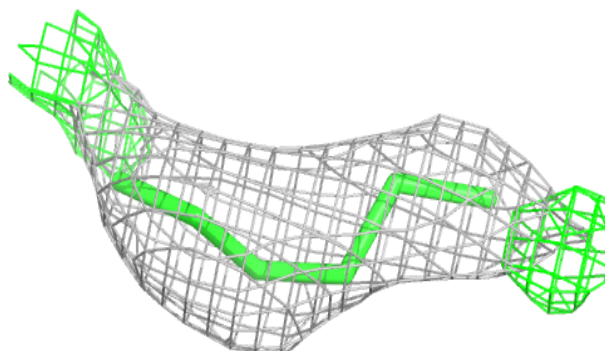


Electron density around LFA E 413:

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

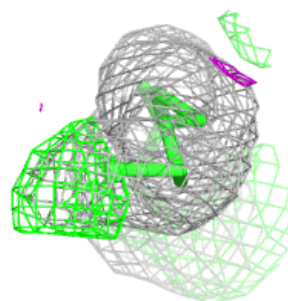
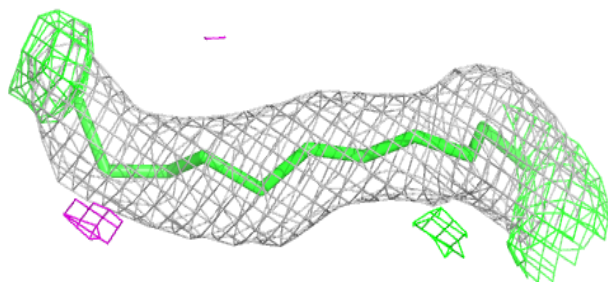
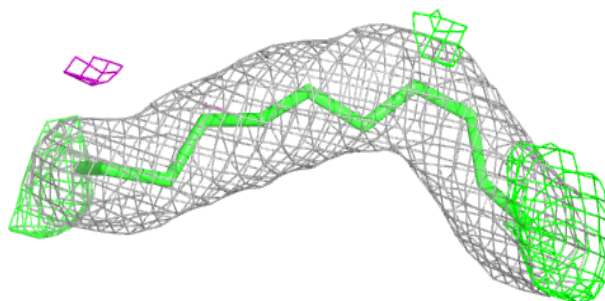
**Electron density around LFA C 1406:**

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

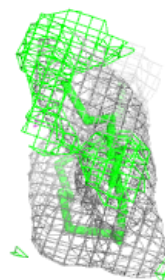
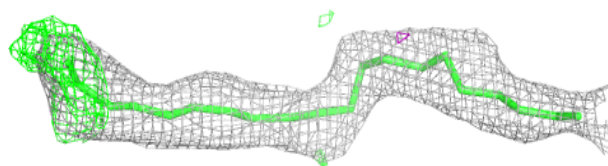
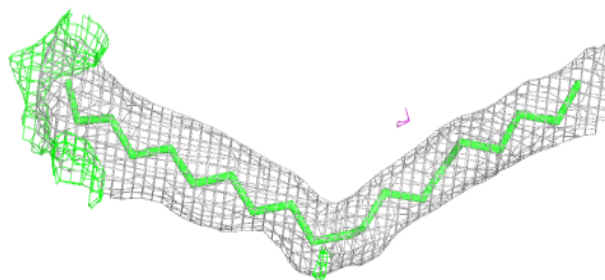


Electron density around LFA B 303:

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

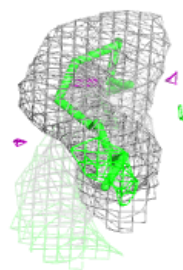
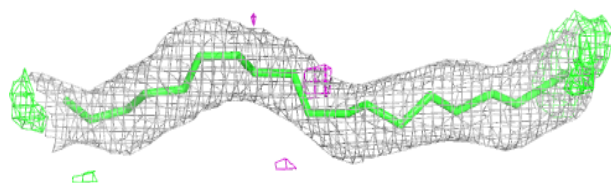
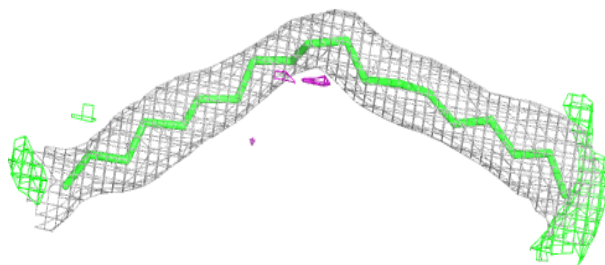
**Electron density around LFA E 402:**

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

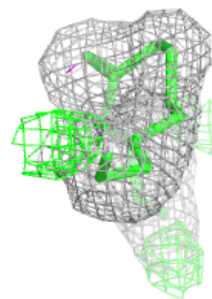
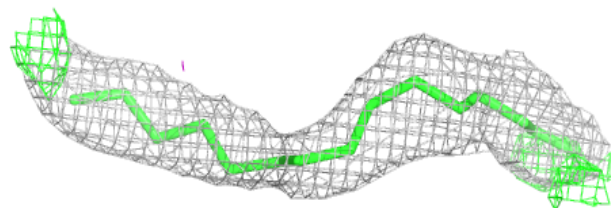
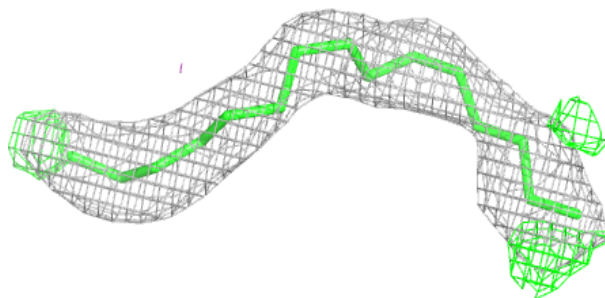


Electron density around LFA E 406:

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

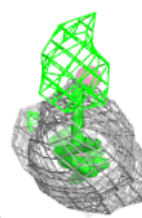
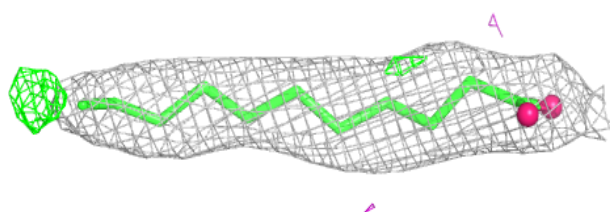
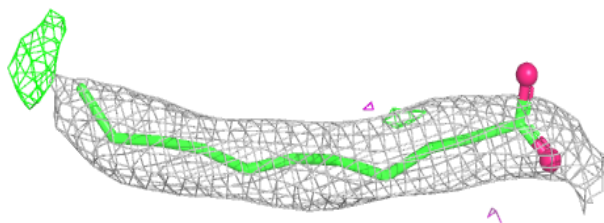
**Electron density around LFA D 404:**

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

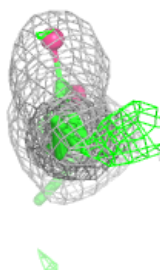
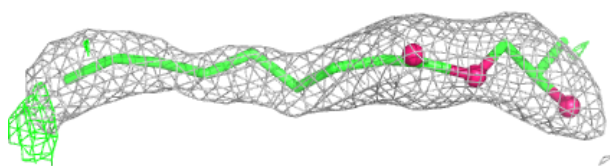
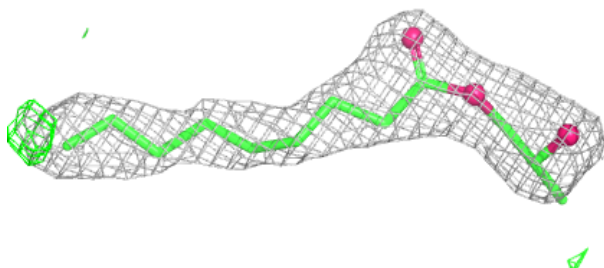


Electron density around OLA A 308:

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

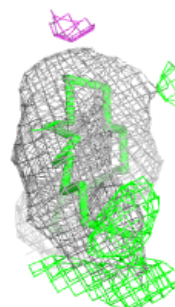
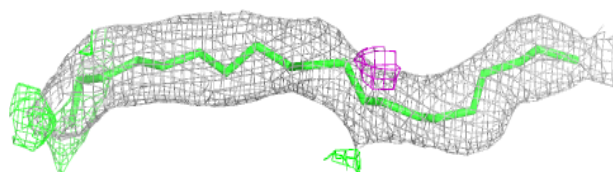
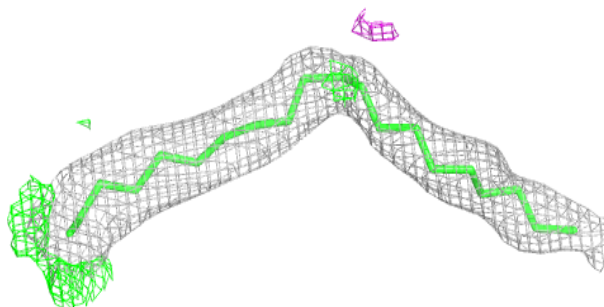
**Electron density around OLC D 405:**

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

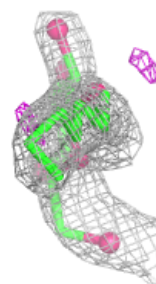
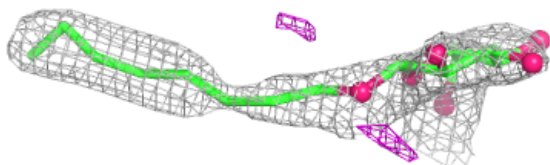
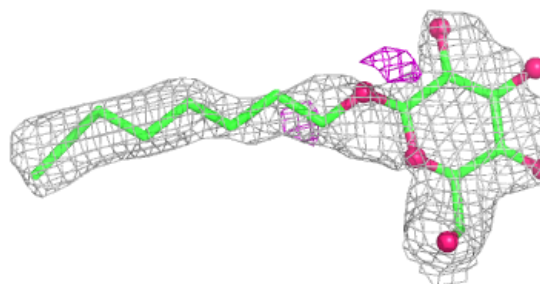


Electron density around LFA B 312:

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

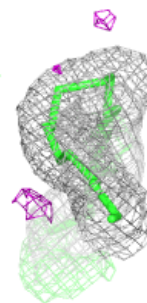
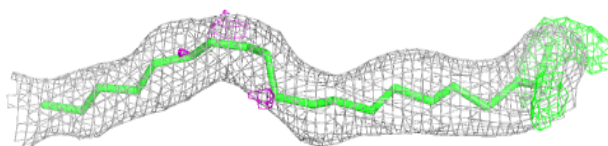
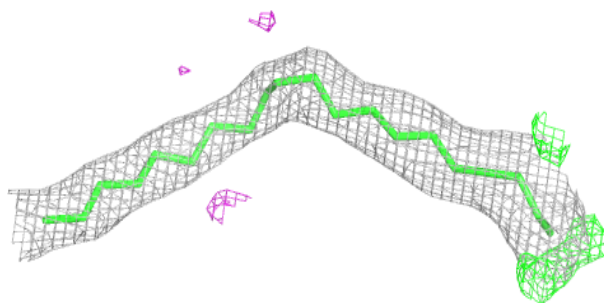
**Electron density around BOG D 408:**

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

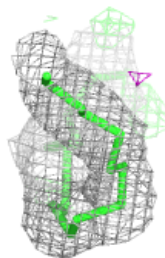
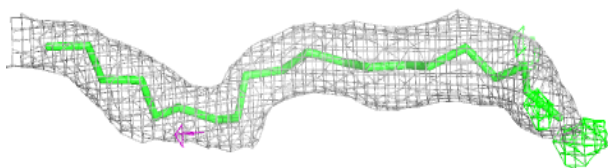
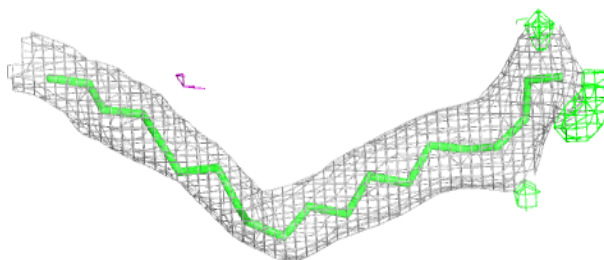


Electron density around LFA D 401:

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

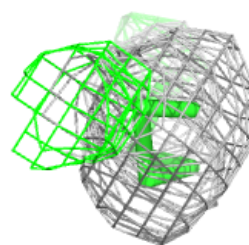
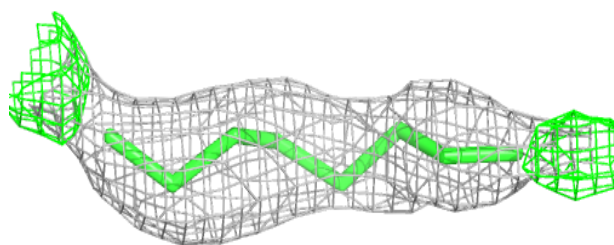
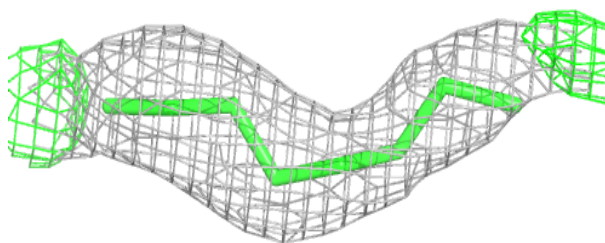
**Electron density around LFA B 304:**

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

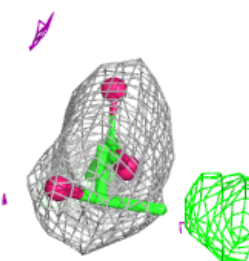
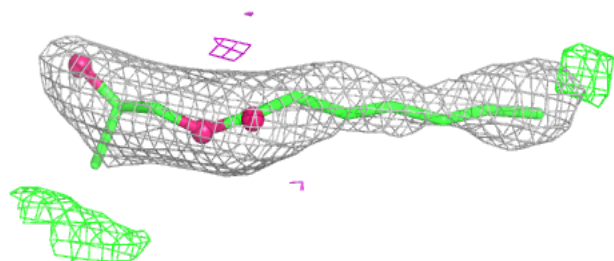
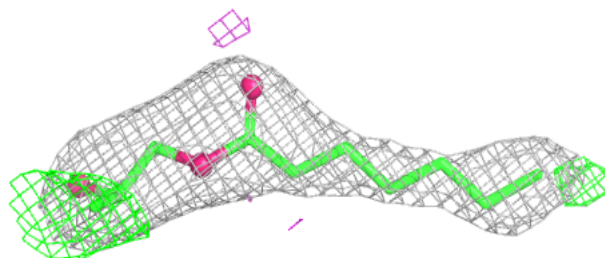


Electron density around LFA A 306:

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

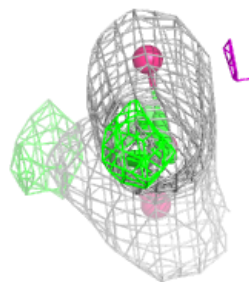
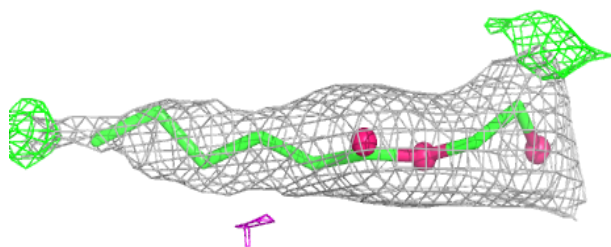
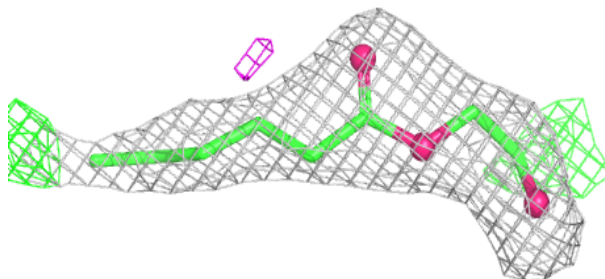
**Electron density around OLC B 301:**

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

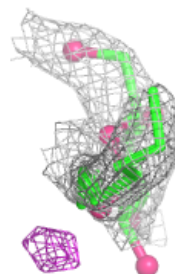
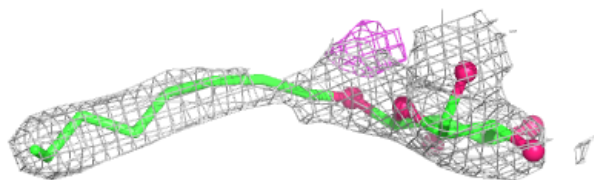
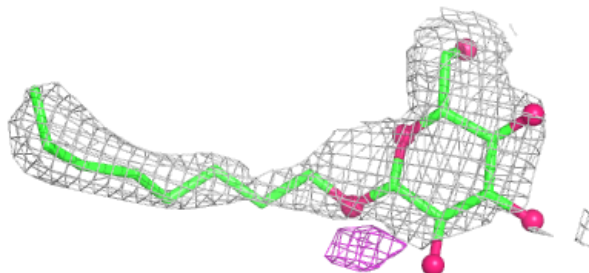


Electron density around OLC C 1402:

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

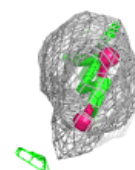
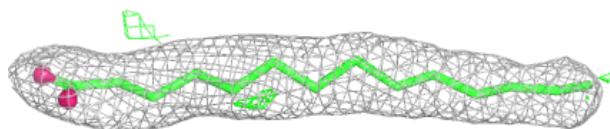
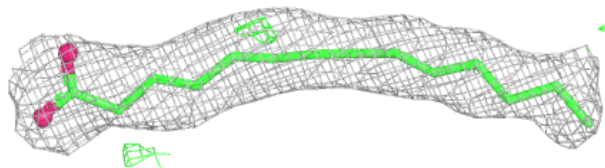
**Electron density around BOG C 1408:**

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

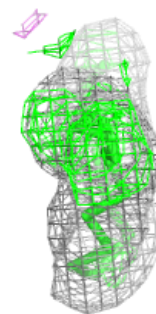
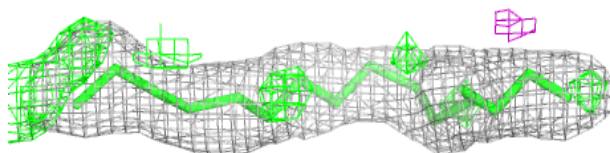
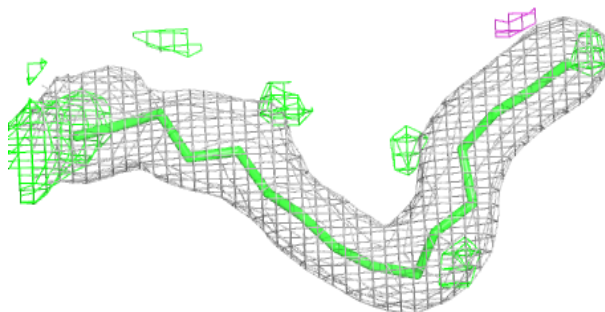


Electron density around OLA B 309:

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

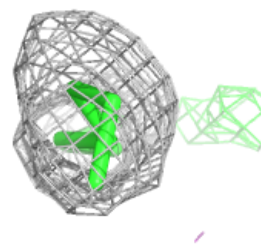
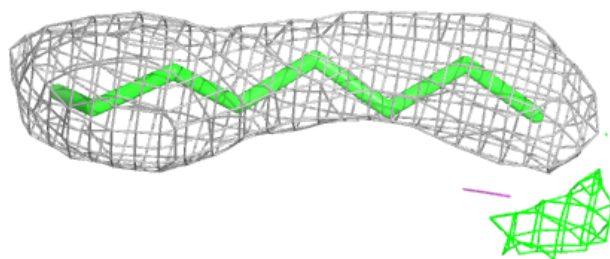
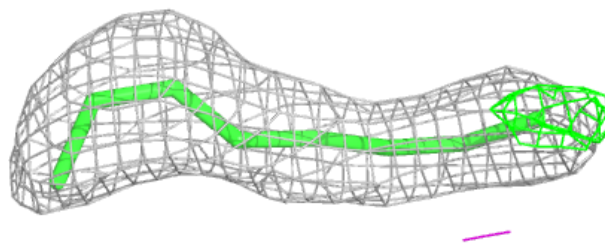
**Electron density around LFA C 1403:**

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

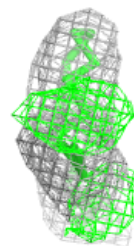
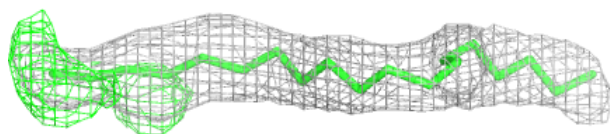
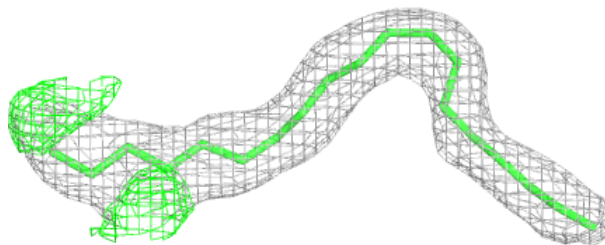


Electron density around LFA D 410:

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

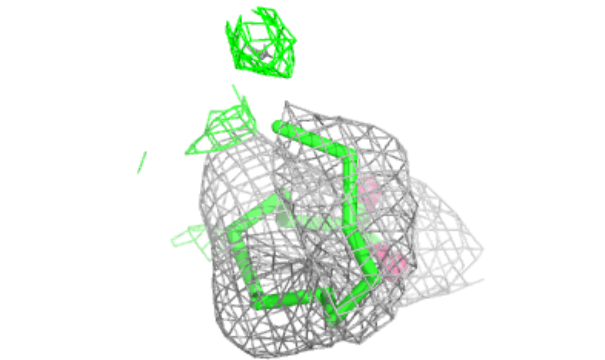
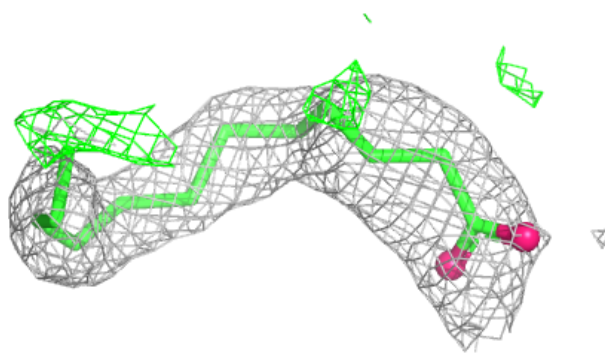
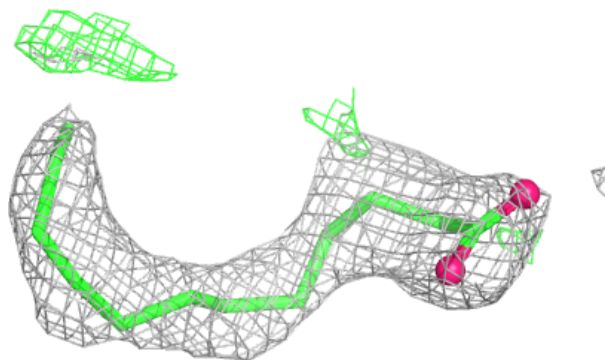
**Electron density around LFA B 302:**

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

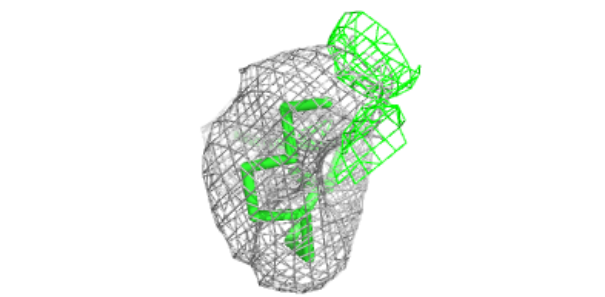
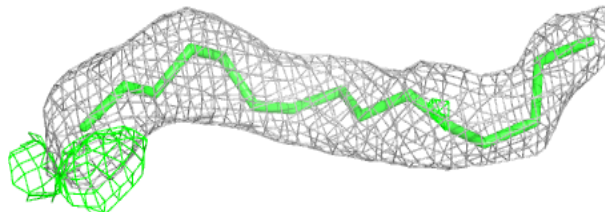
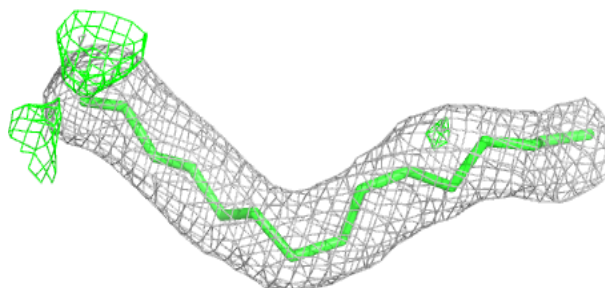


Electron density around OLA B 305:

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

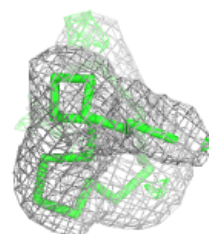
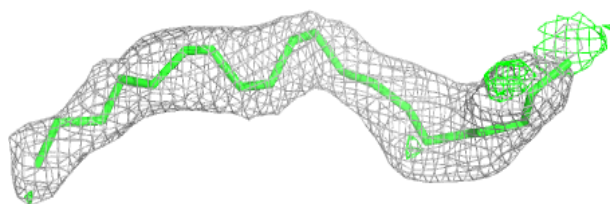
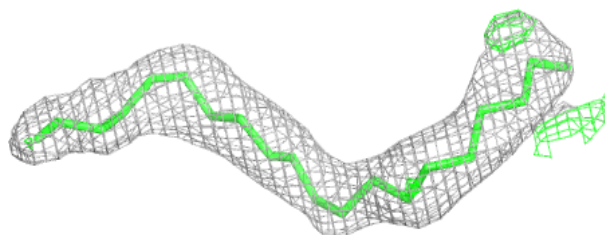
**Electron density around LFA C 1404:**

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

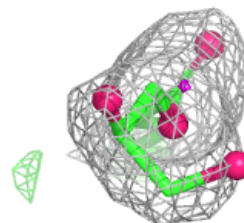
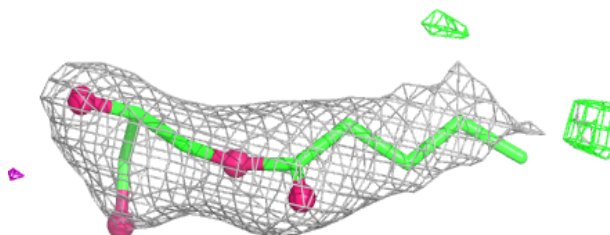
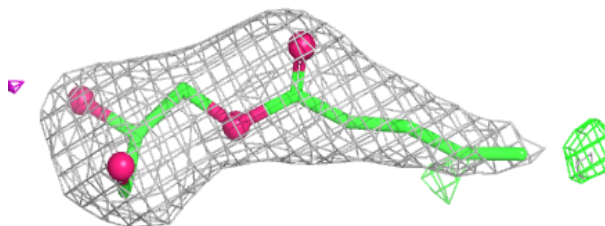


Electron density around LFA A 303:

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

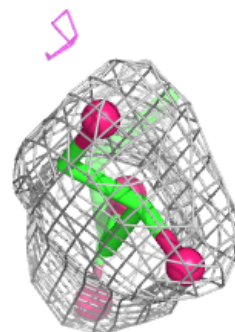
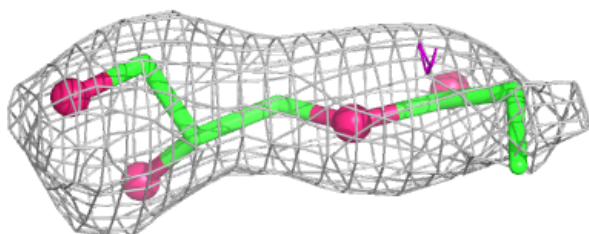
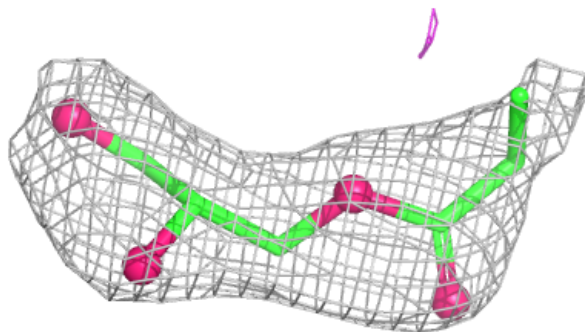
**Electron density around OLC A 301:**

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



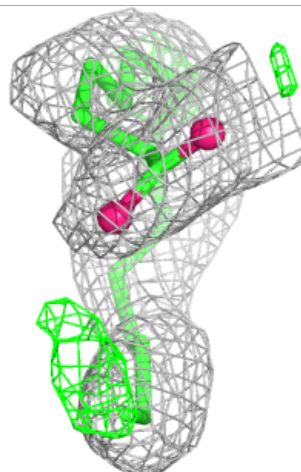
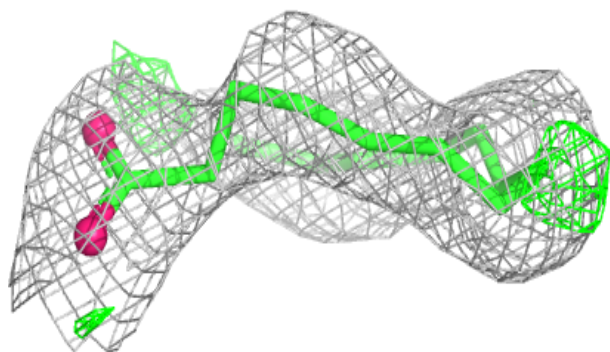
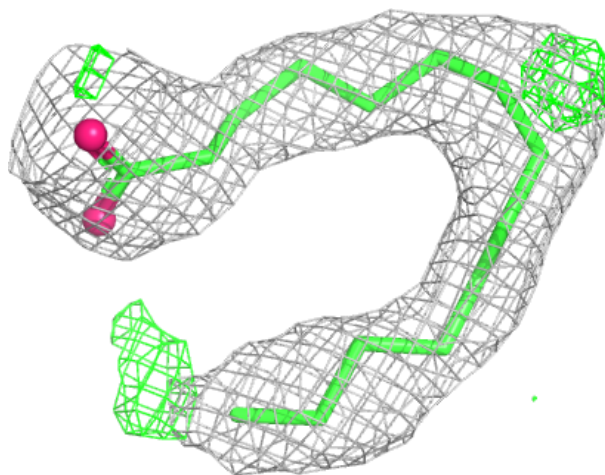
Electron density around OLC E 404:

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



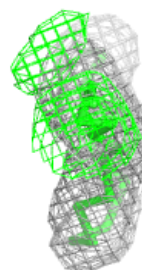
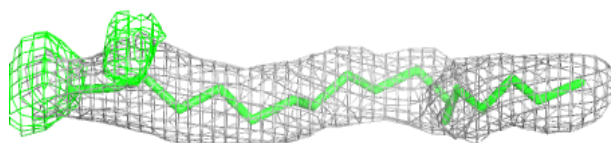
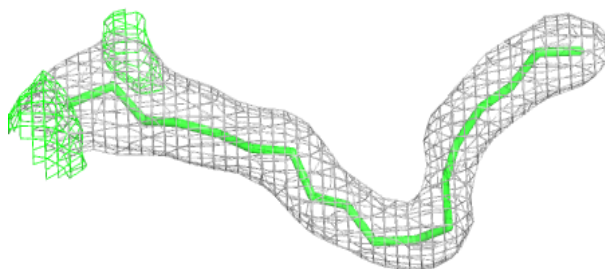
Electron density around OLA A 304:

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

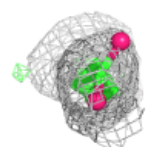
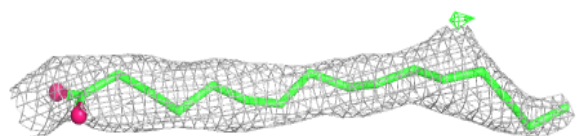
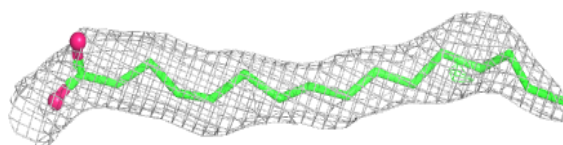


Electron density around LFA D 402:

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

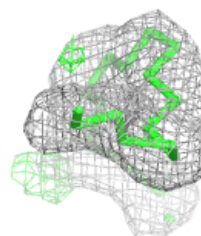
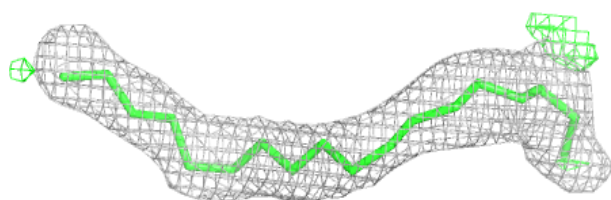
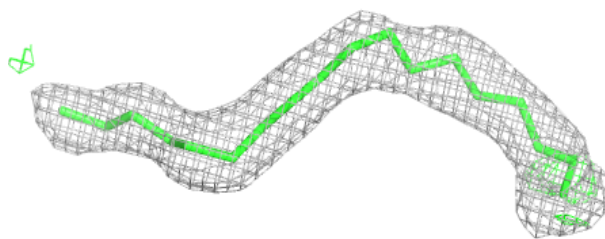
**Electron density around OLA E 411:**

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

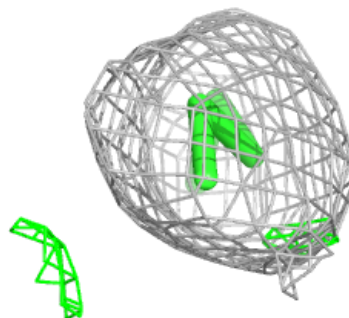
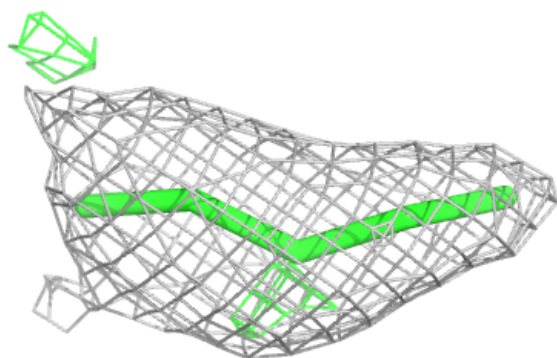
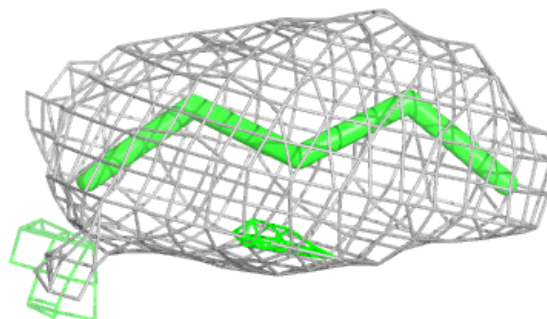


Electron density around LFA E 408:

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

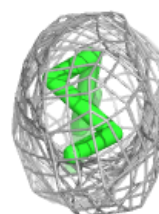
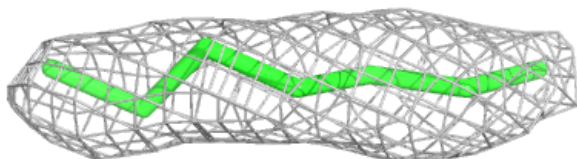
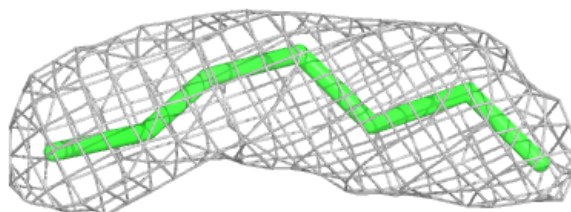
**Electron density around LFA E 409:**

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

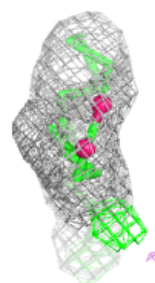
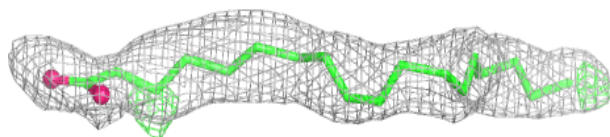
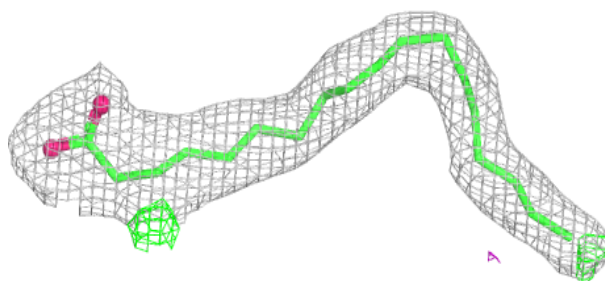


Electron density around LFA D 407:

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

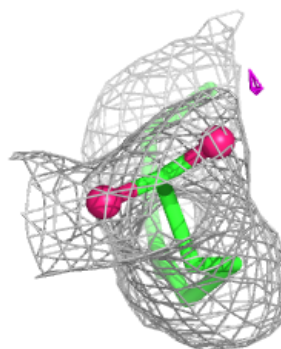
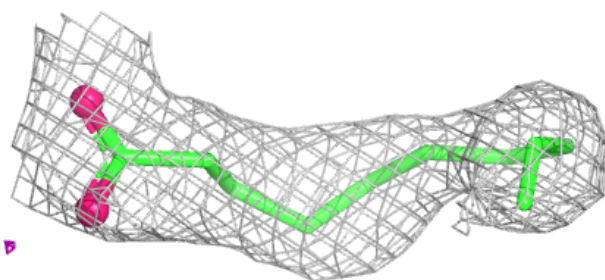
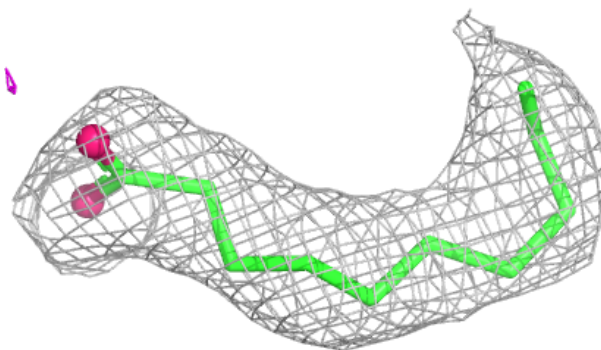
**Electron density around OLA E 405:**

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

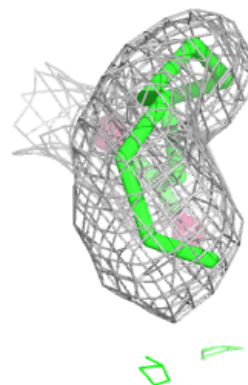
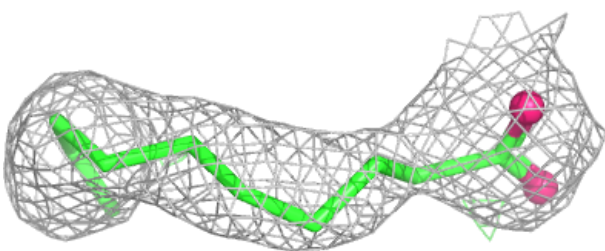
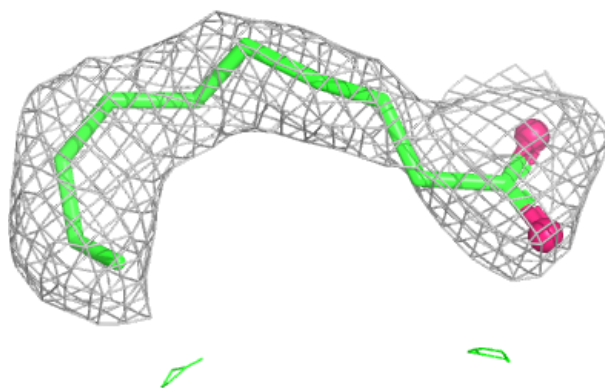


Electron density around OLA E 407:

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

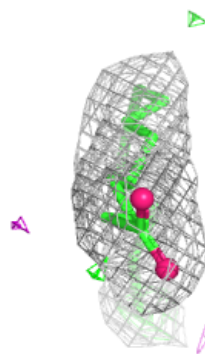
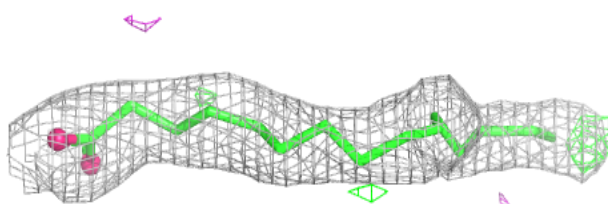
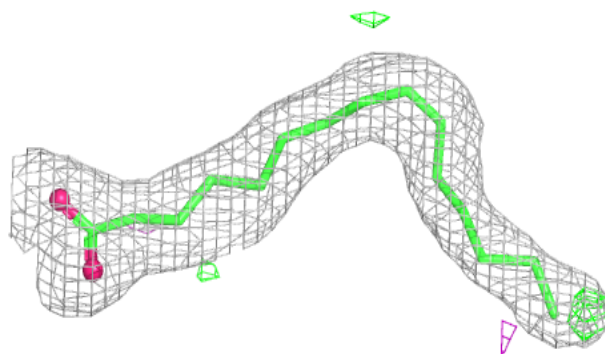
**Electron density around OLA B 313:**

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

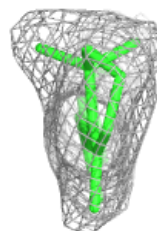
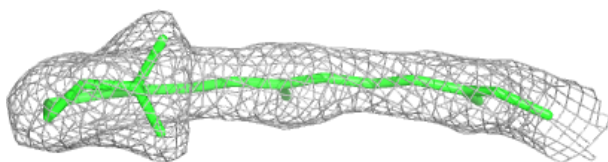
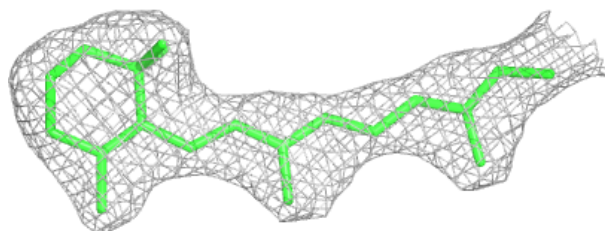


Electron density around OLA A 302:

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

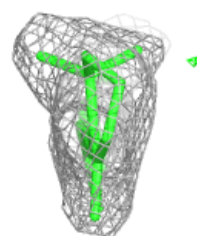
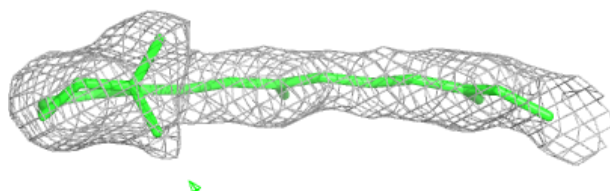
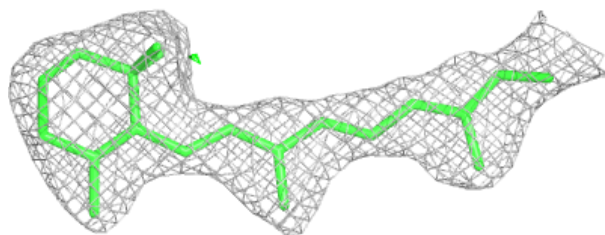
**Electron density around RET B 311:**

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

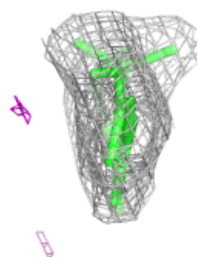
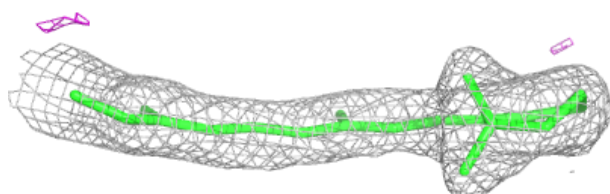
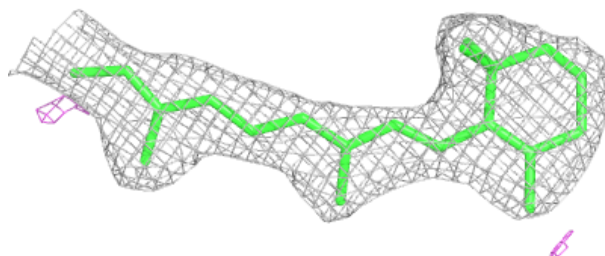


Electron density around RET D 412:

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

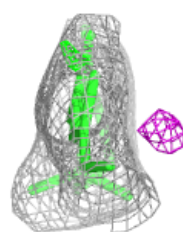
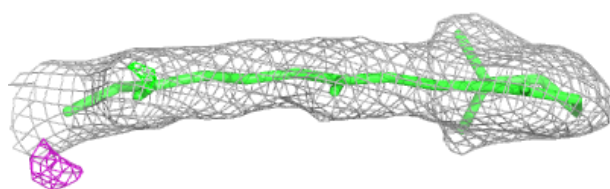
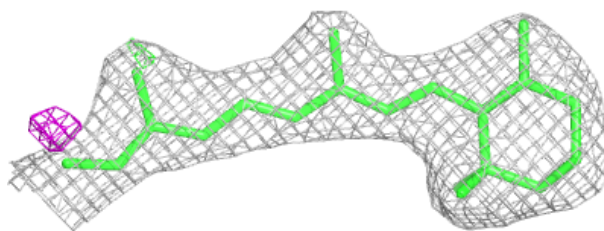
**Electron density around RET A 310:**

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

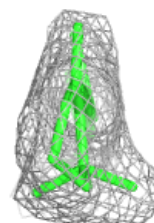
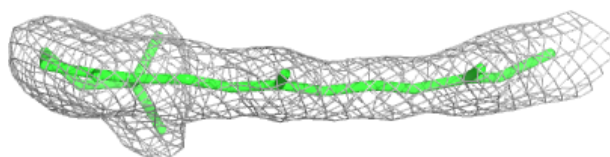
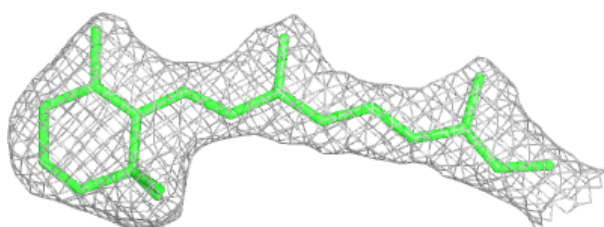


Electron density around RET E 414:

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

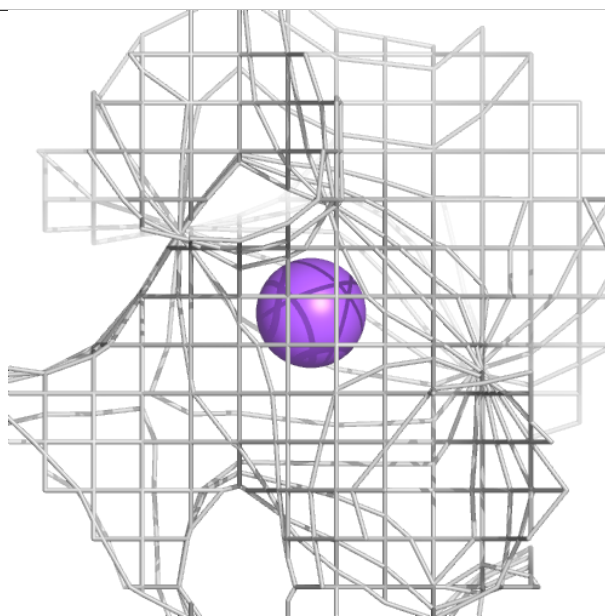
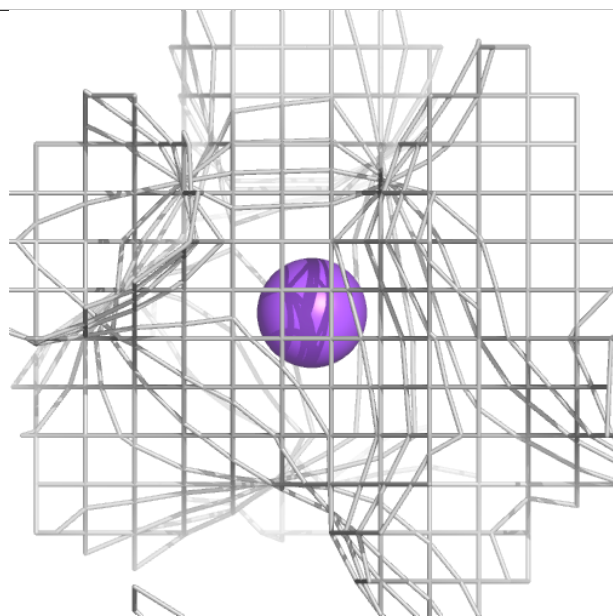
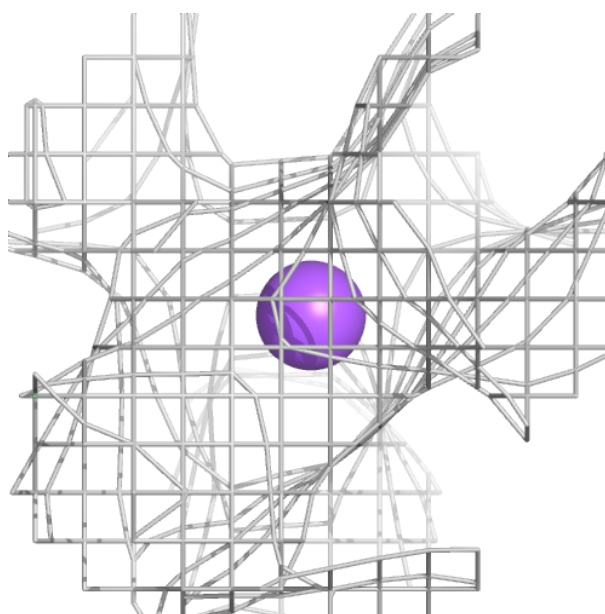
**Electron density around RET C 1409:**

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



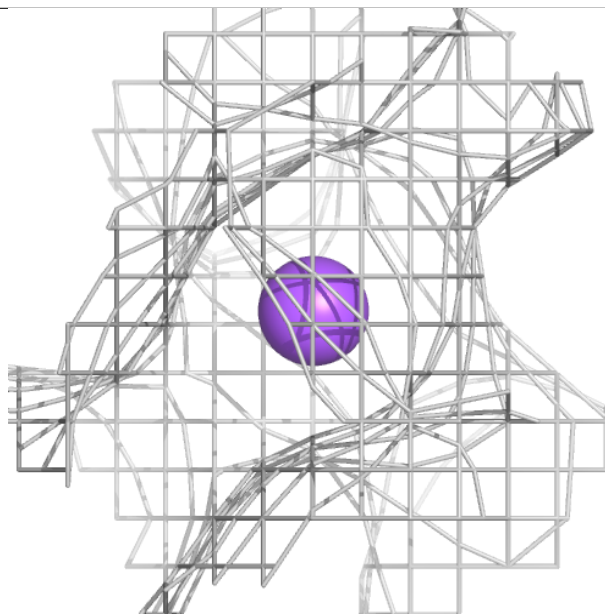
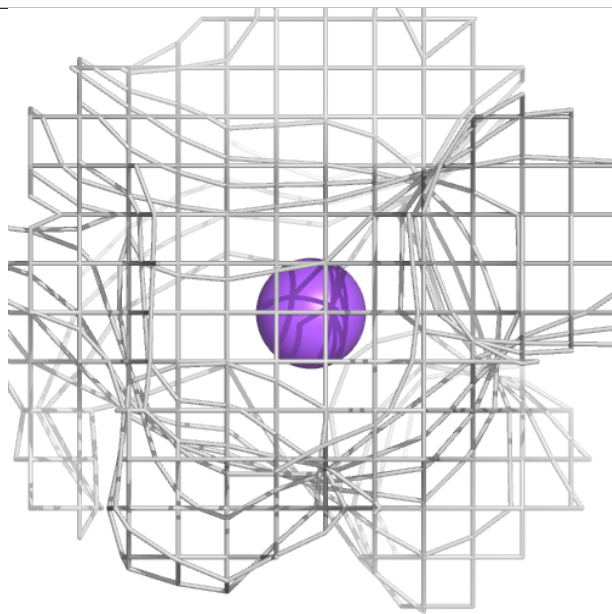
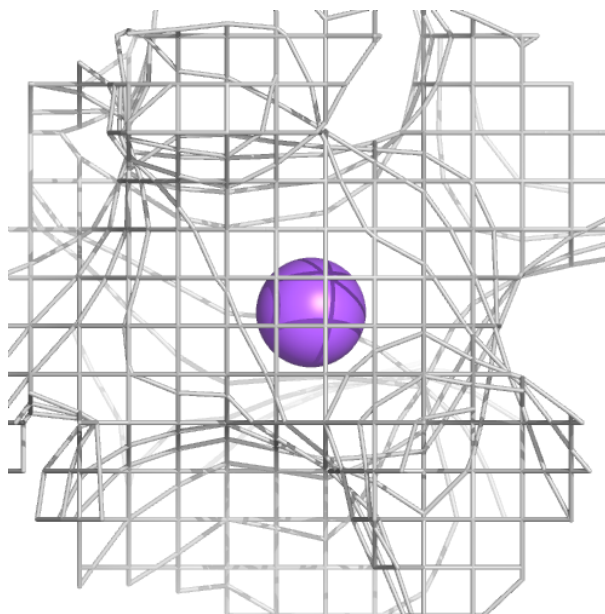
Electron density around NA A 312:

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



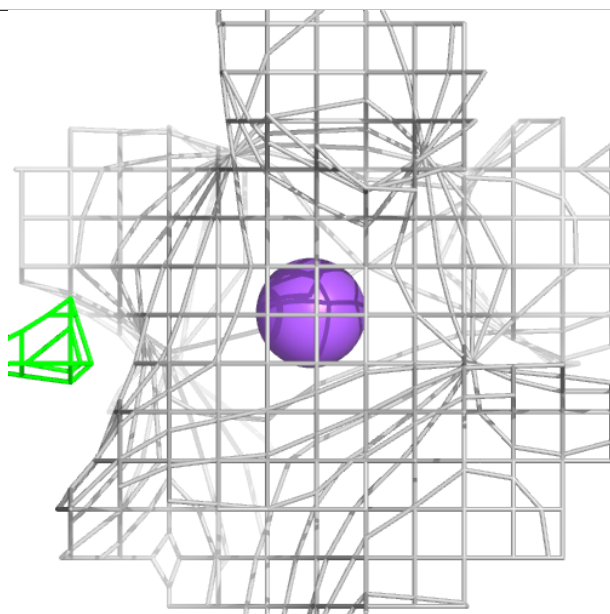
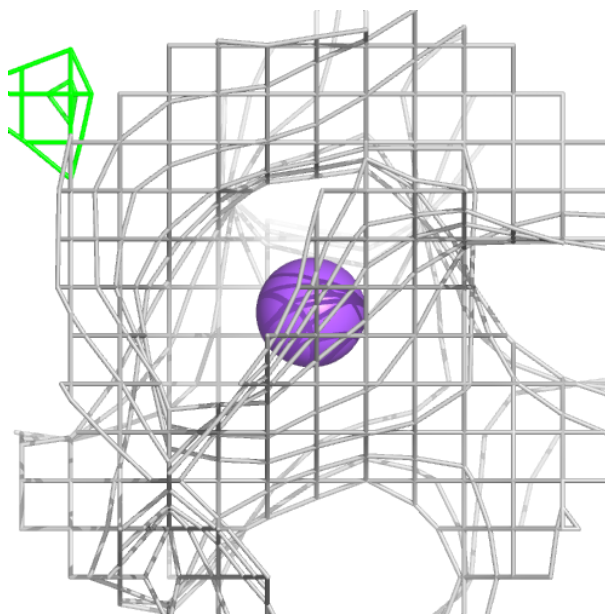
Electron density around NA B 314:

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



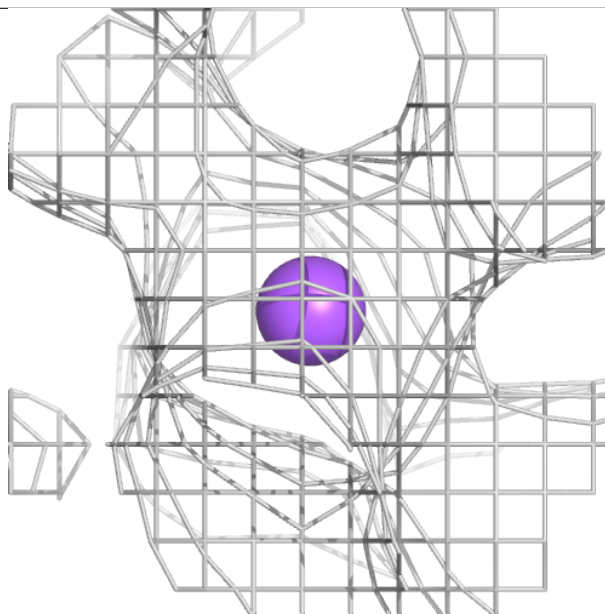
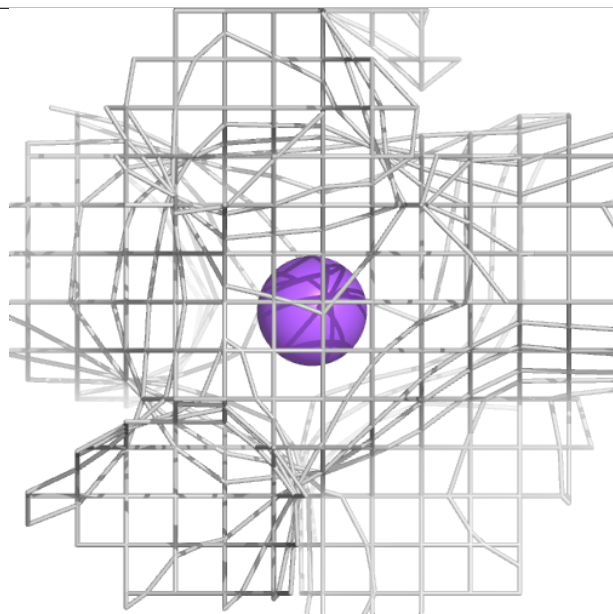
Electron density around NA E 415:

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



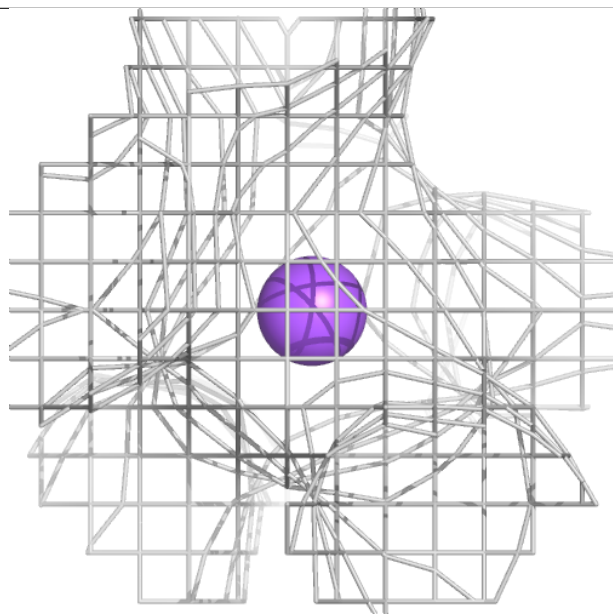
Electron density around NA D 413:

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



Electron density around NA C 1410:

$2mF_o-DF_c$ (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.