



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 6YC0 / pdb_00006yc0
Title : Crystal structure of the steady-state-SMX activated state of the light-driven sodium pump KR2 in the pentameric form at room temperature, pH 8.0
Authors : Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on : 2020-03-18
Resolution : 2.70 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

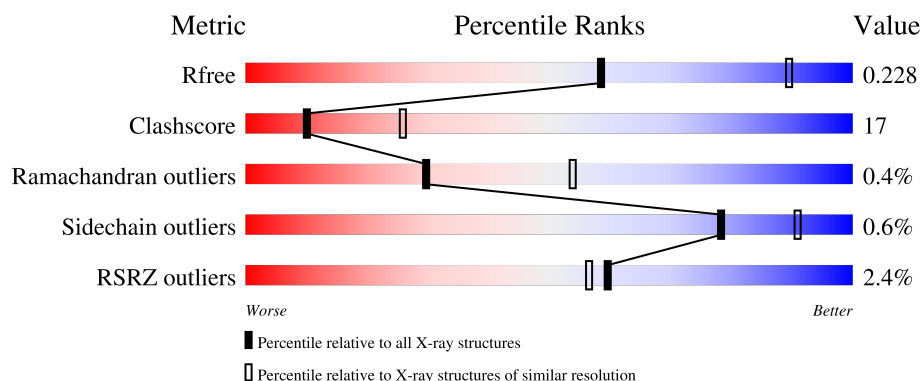
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	273	4% 76% 22% .
1	B	273	% 73% 25% .
1	C	273	% 74% 24% .
1	D	273	3% 74% 24% .
1	E	273	2% 74% 24% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LFA	A	309	-	-	-	X

2 Entry composition [i](#)

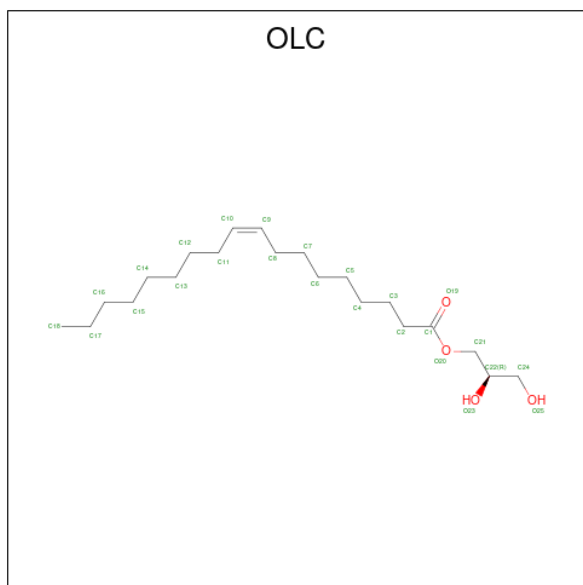
There are 8 unique types of molecules in this entry. The entry contains 13442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	41	0
			2477	1653	375	438	11			
1	B	269	Total	C	N	O	S	0	41	0
			2475	1651	375	438	11			
1	C	269	Total	C	N	O	S	0	41	0
			2472	1650	375	436	11			
1	D	269	Total	C	N	O	S	0	41	0
			2475	1651	375	438	11			
1	E	269	Total	C	N	O	S	0	41	0
			2475	1652	376	436	11			

- Molecule 2 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
2	A	1	Total	C	0	0
			9	9		

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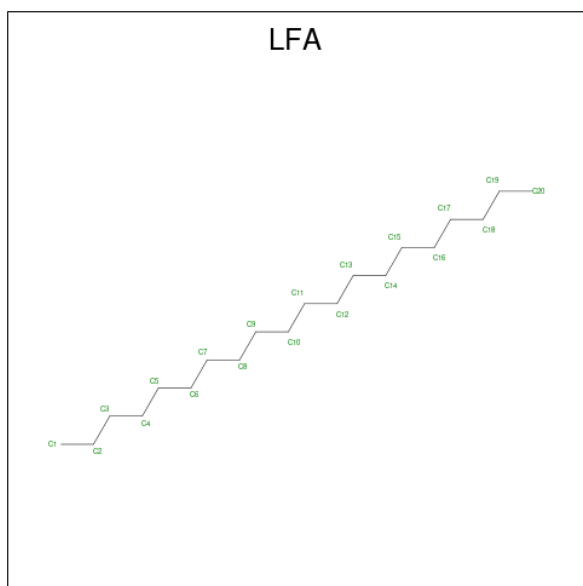
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 17 15 2	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C O 13 9 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	A	1	Total C O 19 17 2	0	0
2	A	1	Total C O 20 18 2	0	0
2	A	1	Total C O 18 16 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C O 12 10 2	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 19 17 2	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C O 12 10 2	0	0
2	C	1	Total C O 17 15 2	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 16 13 3	0	0
2	D	1	Total C 5 5	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 14 10 4	0	0
2	D	1	Total C O 20 18 2	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

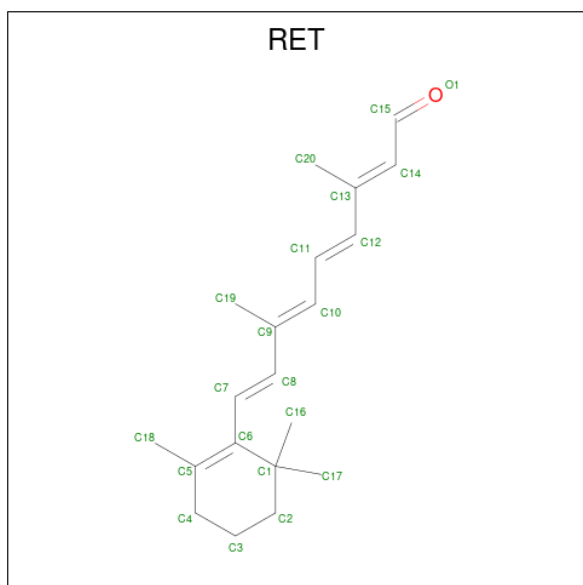
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0
4	B	2	Total Na 2 2	0	0
4	C	2	Total Na 2 2	0	0

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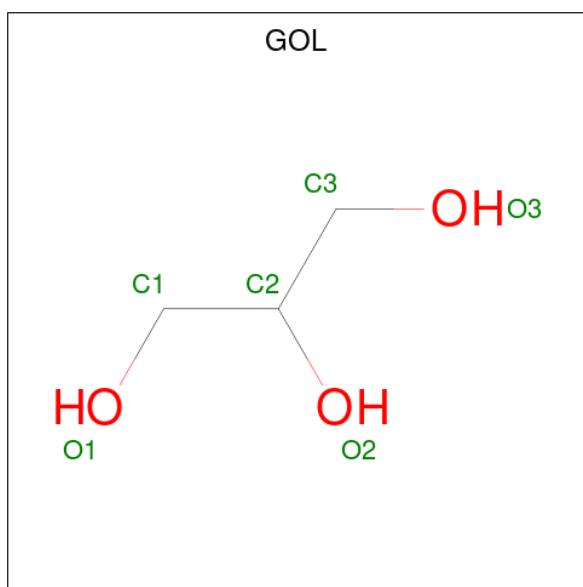
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Na	0	0
			2	2		
4	E	2	Total	Na	0	0
			2	2		

- Molecule 5 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



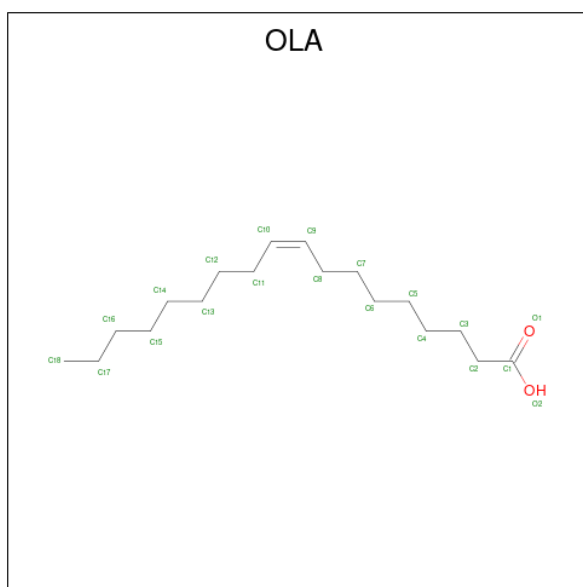
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			20	20		
5	B	1	Total	C	0	0
			20	20		
5	C	1	Total	C	0	0
			20	20		
5	D	1	Total	C	0	0
			20	20		
5	E	1	Total	C	0	0
			20	20		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			17	15	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			18	16	2		
7	C	1	Total	C	O	0	0
			18	16	2		
7	D	1	Total	C	O	0	0
			7	5	2		
7	E	1	Total	C	O	0	0
			20	18	2		
7	E	1	Total	C	O	0	0
			17	15	2		
7	E	1	Total	C	O	0	0
			15	13	2		
7	E	1	Total	C	O	0	0
			6	4	2		

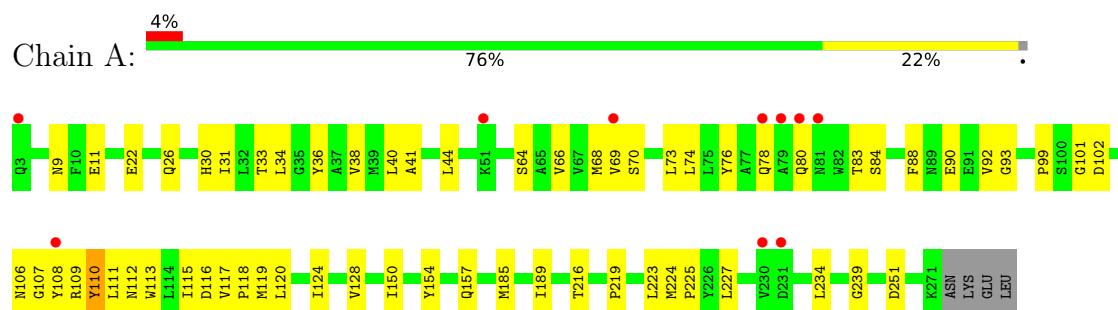
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	41	Total	O	0	0
			41	41		
8	B	52	Total	O	0	0
			52	52		
8	C	46	Total	O	0	0
			46	46		
8	D	46	Total	O	0	0
			46	46		
8	E	42	Total	O	0	0
			42	42		

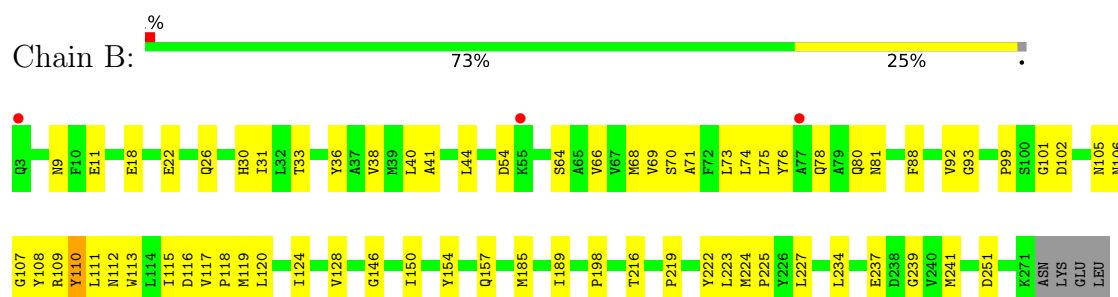
3 Residue-property plots [i](#)

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.

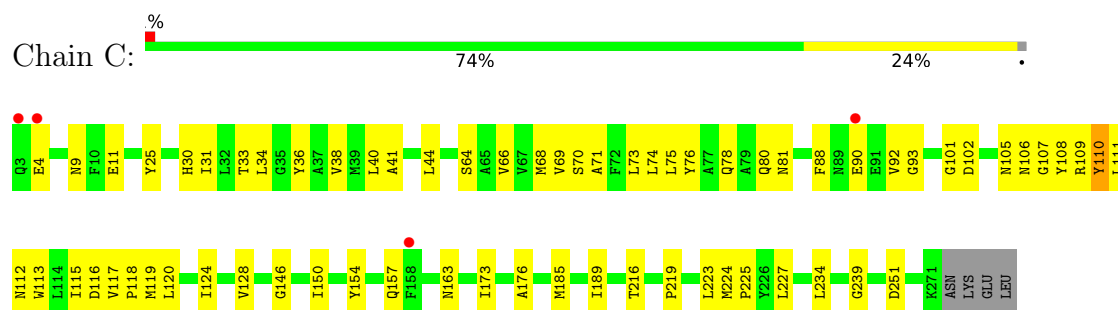
• Molecule 1: Sodium pumping rhodopsin



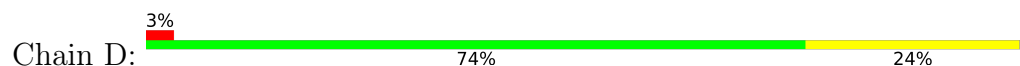
• Molecule 1: Sodium pumping rhodopsin

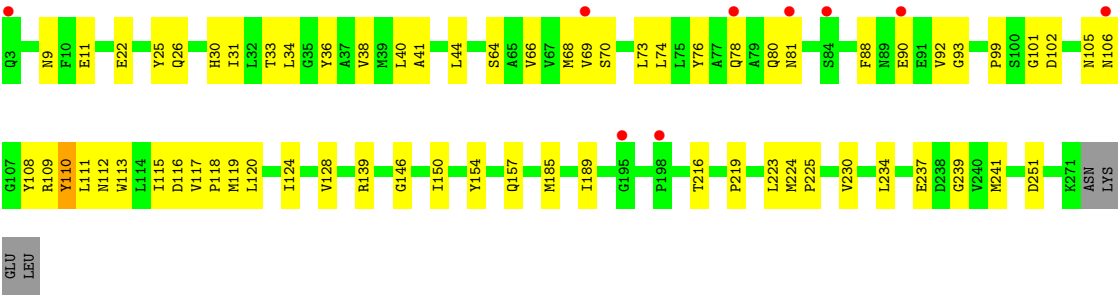


• Molecule 1: Sodium pumping rhodopsin

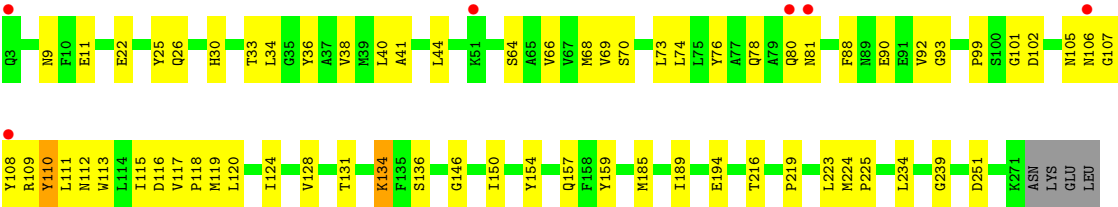
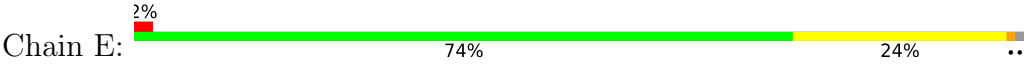


• Molecule 1: Sodium pumping rhodopsin





● 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	135.21Å 240.34Å 138.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.70 50.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.01-2.70) 100.0 (50.01-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.192 , 0.220 0.200 , 0.228	Depositor DCC
R_{free} test set	3862 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 100.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13442	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: NA, RET, OLA, LFA, OLC, GOL

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	0.95	0/2546	1.51	0/3467
1	B	0.95	0/2544	1.51	0/3465
1	C	0.95	0/2541	1.52	0/3461
1	D	0.95	0/2544	1.52	0/3465
1	E	0.95	0/2544	1.51	0/3464
All	All	0.95	0/12719	1.51	0/17322

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	2477	0	2436	101	0
1	B	2475	0	2432	103	1
1	C	2472	0	2429	107	0
1	D	2475	0	2431	107	0
1	E	2475	0	2438	105	1
2	A	118	0	163	6	0
2	B	33	0	40	1	0
2	C	129	0	169	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	62	0	85	1	0
2	E	59	0	84	1	0
3	A	40	0	74	0	0
3	B	25	0	47	0	0
3	C	32	0	64	1	0
3	D	72	0	145	3	0
3	E	31	0	58	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	20	0	27	7	0
5	B	20	0	27	8	0
5	C	20	0	27	7	0
5	D	20	0	27	6	0
5	E	20	0	27	8	0
6	A	4	0	4	0	0
6	B	4	0	4	0	0
6	C	4	0	3	0	0
7	B	35	0	50	0	0
7	C	18	0	26	1	0
7	D	7	0	6	0	0
7	E	58	0	81	4	0
8	A	41	0	0	2	0
8	B	52	0	0	4	0
8	C	46	0	0	2	0
8	D	46	0	0	2	0
8	E	42	0	0	3	0
All	All	13442	0	13404	461	1

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 17.

All (461) 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:B:146:GLY:O	1:B:150[B]:ILE:CD1	1.79	1.30
1:B:146:GLY:O	1:B:150[B]:ILE:HD12	1.54	1.05
1:B:146:GLY:O	1:B:150[B]:ILE:HD13	1.55	1.04
5:B:308:RET:H161	5:B:308:RET:H8	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:315:RET:H161	5:A:315:RET:H8	1.44	0.99
5:D:311:RET:H161	5:D:311:RET:H8	1.41	0.98
5:C:314:RET:H8	5:C:314:RET:H161	1.43	0.98
5:E:414:RET:H8	5:E:414:RET:H161	1.44	0.98
1:D:112[B]:ASN:O	1:D:115[B]:ILE:HG22	1.64	0.97
3:E:409:LFA:H141	3:E:410:LFA:H201	1.48	0.92
1:A:119[B]:MET:HE2	1:A:119[B]:MET:HA	1.51	0.90
1:C:113[A]:TRP:CD1	5:C:314:RET:H14	2.07	0.90
1:B:113[A]:TRP:CD1	5:B:308:RET:H14	2.07	0.90
1:B:119[B]:MET:HE2	1:B:119[B]:MET:HA	1.51	0.90
1:D:113[A]:TRP:CD1	5:D:311:RET:H14	2.06	0.89
1:E:113[A]:TRP:CD1	5:E:414:RET:H14	2.07	0.89
1:E:117[B]:VAL:HB	1:E:118[B]:PRO:HD3	1.55	0.88
1:A:113[A]:TRP:CD1	5:A:315:RET:H14	2.08	0.88
1:C:119[B]:MET:HE2	1:C:119[B]:MET:HA	1.52	0.88
1:A:117[B]:VAL:HB	1:A:118[B]:PRO:HD3	1.56	0.87
1:A:119[A]:MET:HE2	1:A:119[A]:MET:HA	1.54	0.87
1:B:117[B]:VAL:HB	1:B:118[B]:PRO:HD3	1.56	0.87
1:B:119[A]:MET:HE2	1:B:119[A]:MET:HA	1.56	0.87
1:E:119[B]:MET:HE2	1:E:119[B]:MET:HA	1.57	0.87
1:D:68[B]:MET:HE2	1:D:68[B]:MET:HA	1.57	0.86
1:C:30:HIS:HB3	1:D:111[B]:LEU:HD22	1.56	0.86
1:E:68[B]:MET:HA	1:E:68[B]:MET:HE2	1.58	0.86
1:B:68[B]:MET:HE2	1:B:68[B]:MET:HA	1.58	0.86
1:D:119[A]:MET:HE2	1:D:119[A]:MET:HA	1.57	0.85
1:C:68[B]:MET:HE2	1:C:68[B]:MET:HA	1.56	0.85
1:A:68[B]:MET:HE2	1:A:68[B]:MET:HA	1.58	0.85
1:E:119[A]:MET:HA	1:E:119[A]:MET:HE2	1.58	0.85
1:C:117[B]:VAL:HB	1:C:118[B]:PRO:HD3	1.58	0.84
1:C:119[A]:MET:HE2	1:C:119[A]:MET:HA	1.58	0.83
1:D:119[B]:MET:HA	1:D:119[B]:MET:HE2	1.59	0.82
1:A:68[A]:MET:HA	1:A:68[A]:MET:HE2	1.62	0.80
1:E:78[A]:GLN:HE22	1:E:106[A]:ASN:HA	1.47	0.80
1:B:68[A]:MET:HE2	1:B:68[A]:MET:HA	1.64	0.80
1:C:30:HIS:CB	1:D:111[B]:LEU:HD22	2.12	0.80
1:D:30:HIS:HB3	1:E:111[A]:LEU:CD1	2.12	0.79
1:C:30:HIS:HB3	1:D:111[B]:LEU:CD2	2.13	0.79
1:D:68[A]:MET:HE2	1:D:68[A]:MET:HA	1.65	0.78
1:A:111[A]:LEU:CD1	1:E:30:HIS:HB3	2.12	0.78
1:C:163:ASN:HD22	2:C:307:OLC:H24A	1.48	0.78
1:D:78[A]:GLN:HE22	1:D:106[A]:ASN:HA	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78[A]:GLN:HE22	1:B:106[A]:ASN:HA	1.50	0.76
1:C:68[A]:MET:HA	1:C:68[A]:MET:HE2	1.66	0.76
1:C:116[B]:ASP:O	1:C:120[B]:LEU:HG	1.85	0.76
1:C:4:GLU:CG	8:C:445:HOH:O	2.34	0.76
1:E:68[A]:MET:HE2	1:E:68[A]:MET:HA	1.67	0.75
1:A:106[A]:ASN:O	1:A:110[A]:TYR:HD1	1.69	0.75
1:C:30:HIS:CB	1:D:111[B]:LEU:CD2	2.64	0.75
1:D:70[B]:SER:OG	1:D:115[B]:ILE:HG21	1.86	0.74
1:D:117[A]:VAL:HB	1:D:118[A]:PRO:HD3	1.71	0.73
1:C:90:GLU:OE1	1:D:99:PRO:HG3	1.90	0.72
1:C:106[A]:ASN:O	1:C:110[A]:TYR:HD1	1.71	0.72
1:C:113[A]:TRP:HD1	5:C:314:RET:H14	1.55	0.72
1:A:30:HIS:HB3	1:B:111[A]:LEU:CD1	2.20	0.72
1:B:113[A]:TRP:HD1	5:B:308:RET:H14	1.54	0.72
5:D:311:RET:H161	5:D:311:RET:C8	2.20	0.72
1:A:117[A]:VAL:HB	1:A:118[A]:PRO:HD3	1.72	0.71
1:D:74[B]:LEU:HD21	1:D:108[B]:TYR:HB3	1.72	0.71
1:E:78[A]:GLN:NE2	1:E:106[A]:ASN:HA	2.04	0.71
1:E:117[A]:VAL:HB	1:E:118[A]:PRO:HD3	1.73	0.70
1:E:113[A]:TRP:HD1	5:E:414:RET:H14	1.55	0.70
1:B:30:HIS:HB3	1:C:111[A]:LEU:CD1	2.22	0.69
5:C:314:RET:H161	5:C:314:RET:C8	2.21	0.69
1:D:106[A]:ASN:O	1:D:110[A]:TYR:HD1	1.76	0.68
1:B:78[A]:GLN:NE2	1:B:106[A]:ASN:HA	2.09	0.68
1:D:80[B]:GLN:NE2	8:D:406:HOH:O	2.27	0.68
1:B:117[A]:VAL:HB	1:B:118[A]:PRO:HD3	1.75	0.68
1:D:78[A]:GLN:NE2	1:D:106[A]:ASN:HA	2.07	0.68
1:B:76[B]:TYR:O	1:B:80[B]:GLN:HG2	1.93	0.67
1:D:40:LEU:HD23	1:E:73[A]:LEU:HD11	1.76	0.67
1:A:74[B]:LEU:HB2	1:A:112[B]:ASN:HD22	1.60	0.67
1:D:113[A]:TRP:HD1	5:D:311:RET:H14	1.55	0.67
1:E:106[A]:ASN:O	1:E:110[A]:TYR:HD1	1.78	0.67
1:A:110[B]:TYR:O	1:A:113[B]:TRP:N	2.23	0.66
1:C:117[A]:VAL:HB	1:C:118[A]:PRO:HD3	1.75	0.66
1:A:119[B]:MET:HE2	1:A:119[B]:MET:CA	2.24	0.66
1:C:110[B]:TYR:O	1:C:113[B]:TRP:N	2.23	0.66
1:A:116[B]:ASP:O	1:A:120[B]:LEU:HG	1.95	0.66
1:A:113[A]:TRP:HD1	5:A:315:RET:H14	1.55	0.66
1:D:139:ARG:NH2	3:D:306:LFA:C20	2.58	0.66
1:A:76[B]:TYR:O	1:A:80[B]:GLN:HG2	1.96	0.65
1:C:76[B]:TYR:O	1:C:80[B]:GLN:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:O	1:D:239:GLY:HA3	1.97	0.65
1:C:78[A]:GLN:HE22	1:C:106[A]:ASN:HA	1.62	0.65
1:D:70[B]:SER:OG	1:D:115[B]:ILE:CG2	2.45	0.64
1:A:111[A]:LEU:HD12	1:E:30:HIS:HB3	1.78	0.64
1:B:234:LEU:O	1:B:239:GLY:HA3	1.98	0.64
1:E:78[A]:GLN:OE1	1:E:78[A]:GLN:HA	1.97	0.64
1:A:234:LEU:O	1:A:239:GLY:HA3	1.98	0.64
1:C:234:LEU:O	1:C:239:GLY:HA3	1.98	0.64
1:A:119[A]:MET:HE2	1:A:119[A]:MET:CA	2.27	0.64
1:B:105[B]:ASN:OD1	1:B:107[B]:GLY:N	2.30	0.64
1:A:74[B]:LEU:HD23	1:A:112[B]:ASN:ND2	2.13	0.63
1:D:117[B]:VAL:HB	1:D:118[B]:PRO:HD3	1.79	0.63
1:E:234:LEU:O	1:E:239:GLY:HA3	1.97	0.63
1:D:30:HIS:HB3	1:E:111[A]:LEU:HD11	1.78	0.63
1:D:78[A]:GLN:HA	1:D:78[A]:GLN:OE1	1.96	0.63
1:B:150[B]:ILE:HD12	1:B:150[B]:ILE:H	1.64	0.62
2:C:302:OLC:H11	3:C:310:LFA:H111	1.81	0.62
1:C:40:LEU:HD23	1:D:73[A]:LEU:HD11	1.80	0.62
1:C:119[B]:MET:HE2	1:C:119[B]:MET:CA	2.25	0.62
1:E:74[B]:LEU:HD21	1:E:108[B]:TYR:HB3	1.81	0.62
1:B:40:LEU:HD23	1:C:73[A]:LEU:HD11	1.82	0.62
1:C:163:ASN:HD22	2:C:307:OLC:C24	2.12	0.62
1:C:30:HIS:HB2	1:D:111[B]:LEU:CD2	2.29	0.62
1:E:76[B]:TYR:O	1:E:80[B]:GLN:HG2	2.00	0.62
1:B:78[A]:GLN:HA	1:B:78[A]:GLN:OE1	1.99	0.61
1:A:68[B]:MET:HE2	1:A:68[B]:MET:CA	2.30	0.61
5:A:315:RET:H161	5:A:315:RET:C8	2.22	0.61
1:B:119[B]:MET:HE2	1:B:119[B]:MET:CA	2.29	0.61
1:D:68[B]:MET:HE2	1:D:68[B]:MET:CA	2.30	0.61
1:B:106[A]:ASN:O	1:B:110[A]:TYR:HD1	1.83	0.61
1:B:78[B]:GLN:OE1	1:B:78[B]:GLN:HA	1.98	0.61
1:C:78[B]:GLN:HA	1:C:78[B]:GLN:OE1	2.01	0.60
1:E:119[B]:MET:HE2	1:E:119[B]:MET:CA	2.29	0.60
1:C:33:THR:HG22	1:D:74[A]:LEU:CD1	2.30	0.60
1:C:68[B]:MET:HE2	1:C:68[B]:MET:CA	2.30	0.60
1:E:119[A]:MET:HE2	1:E:119[A]:MET:CA	2.31	0.60
1:C:223:LEU:C	1:C:225:PRO:HD2	2.27	0.59
1:B:54:ASP:HB3	8:B:449:HOH:O	2.01	0.59
1:C:34:LEU:HD11	1:D:115[A]:ILE:HG21	1.83	0.59
1:D:74[B]:LEU:HD21	1:D:108[B]:TYR:C	2.27	0.59
1:D:90:GLU:OE1	1:E:99:PRO:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:C	1:A:225:PRO:HD2	2.27	0.59
1:C:78[A]:GLN:OE1	1:C:78[A]:GLN:HA	2.02	0.59
1:D:44:LEU:HD22	1:E:69[A]:VAL:HG21	1.83	0.59
1:E:26:GLN:OE1	8:E:504:HOH:O	2.16	0.59
1:A:115[A]:ILE:HG22	2:A:313:OLC:H16A	1.85	0.59
1:D:33:THR:HG22	1:E:74[A]:LEU:CD1	2.33	0.59
1:C:34:LEU:HD11	1:D:115[A]:ILE:CG2	2.32	0.59
1:B:110[B]:TYR:HA	1:B:113[B]:TRP:CE3	2.38	0.59
5:B:308:RET:H161	5:B:308:RET:C8	2.22	0.59
1:D:40:LEU:CD2	1:E:73[A]:LEU:HD11	2.32	0.59
1:D:36:TYR:CD2	1:D:76[B]:TYR:HA	2.38	0.59
1:D:64:SER:O	1:D:68[B]:MET:HG2	2.02	0.58
1:D:223:LEU:C	1:D:225:PRO:HD2	2.27	0.58
1:E:36:TYR:CD2	1:E:76[B]:TYR:HA	2.38	0.58
1:E:78[B]:GLN:OE1	1:E:78[B]:GLN:HA	2.03	0.58
1:A:68[A]:MET:HE2	1:A:68[A]:MET:CA	2.34	0.58
1:C:74[B]:LEU:HB2	1:C:112[B]:ASN:ND2	2.18	0.58
1:C:40:LEU:CD2	1:D:73[A]:LEU:HD11	2.33	0.58
1:B:223:LEU:C	1:B:225:PRO:HD2	2.29	0.57
1:C:119[A]:MET:HE2	1:C:119[A]:MET:CA	2.31	0.57
1:E:64:SER:O	1:E:68[B]:MET:HG2	2.04	0.57
1:B:64:SER:O	1:B:68[B]:MET:HG2	2.04	0.57
1:E:113[A]:TRP:NE1	8:E:510:HOH:O	2.35	0.57
1:A:64:SER:O	1:A:68[A]:MET:HG2	2.04	0.57
1:A:110[B]:TYR:HA	1:A:113[B]:TRP:CE3	2.40	0.57
1:E:223:LEU:C	1:E:225:PRO:HD2	2.29	0.57
1:C:163:ASN:ND2	2:C:307:OLC:H24A	2.16	0.57
1:B:68[B]:MET:HE2	1:B:68[B]:MET:CA	2.31	0.57
1:B:64:SER:O	1:B:68[A]:MET:HG2	2.04	0.57
1:A:83[B]:THR:HG21	8:A:430:HOH:O	2.05	0.57
1:A:73[A]:LEU:HD11	1:E:40:LEU:HD23	1.87	0.56
1:C:64:SER:O	1:C:68[A]:MET:HG2	2.05	0.56
1:A:74[A]:LEU:CD1	1:E:33:THR:HG22	2.36	0.56
1:B:36:TYR:CD2	1:B:76[B]:TYR:HA	2.41	0.56
1:D:64:SER:O	1:D:68[A]:MET:HG2	2.04	0.56
1:A:106[A]:ASN:O	1:A:110[A]:TYR:CD1	2.54	0.56
1:C:78[A]:GLN:NE2	1:C:106[A]:ASN:HA	2.21	0.56
1:E:110[B]:TYR:HA	1:E:113[B]:TRP:CE3	2.41	0.56
1:A:109[A]:ARG:NH1	1:A:251:ASP:OD2	2.38	0.55
1:B:74[B]:LEU:HD21	1:B:108[B]:TYR:HB3	1.88	0.55
1:B:116[B]:ASP:O	1:B:120[B]:LEU:HG	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74[B]:LEU:C	1:C:74[B]:LEU:HD13	2.31	0.55
1:E:64:SER:O	1:E:68[A]:MET:HG2	2.04	0.55
1:B:30:HIS:HB3	1:C:111[A]:LEU:HD12	1.88	0.55
1:E:74[B]:LEU:C	1:E:74[B]:LEU:HD13	2.32	0.55
1:C:64:SER:O	1:C:68[B]:MET:HG2	2.05	0.55
1:C:74[B]:LEU:HD21	1:C:108[B]:TYR:HB3	1.88	0.55
1:A:64:SER:O	1:A:68[B]:MET:HG2	2.05	0.55
1:C:109[A]:ARG:NH1	1:C:251:ASP:OD2	2.40	0.55
5:E:414:RET:H161	5:E:414:RET:C8	2.23	0.55
1:A:154:TYR:O	1:A:157:GLN:HG3	2.07	0.55
1:C:117[B]:VAL:HB	1:C:118[B]:PRO:CD	2.35	0.55
1:D:30:HIS:HB3	1:E:111[A]:LEU:HD12	1.89	0.54
1:A:40:LEU:HD23	1:B:73[A]:LEU:HD11	1.90	0.54
1:D:68[A]:MET:HE2	1:D:68[A]:MET:CA	2.37	0.54
1:D:154:TYR:O	1:D:157:GLN:HG3	2.07	0.54
1:D:74[B]:LEU:CD2	1:D:108[B]:TYR:HB3	2.37	0.54
1:D:119[A]:MET:HE2	1:D:119[A]:MET:CA	2.35	0.54
1:E:68[B]:MET:HE2	1:E:68[B]:MET:CA	2.32	0.54
1:E:109[A]:ARG:NH1	1:E:251:ASP:OD2	2.40	0.54
1:A:78[A]:GLN:HE22	1:A:106[A]:ASN:HA	1.73	0.54
1:E:68[A]:MET:HE2	1:E:68[A]:MET:CA	2.37	0.54
1:B:109[A]:ARG:NH1	1:B:251:ASP:OD2	2.40	0.54
1:C:90:GLU:CD	1:D:99:PRO:HG3	2.32	0.54
1:E:154:TYR:O	1:E:157:GLN:HG3	2.08	0.54
2:C:303:OLC:H12	1:D:115[B]:ILE:HG13	1.90	0.54
1:B:74[B]:LEU:HB2	1:B:112[B]:ASN:HD22	1.73	0.54
1:D:110[B]:TYR:O	1:D:113[B]:TRP:HB2	2.07	0.54
1:E:74[B]:LEU:HB2	1:E:112[B]:ASN:ND2	2.23	0.54
1:A:117[B]:VAL:HB	1:A:118[B]:PRO:CD	2.34	0.54
1:B:33:THR:HG22	1:C:74[A]:LEU:CD1	2.37	0.54
1:D:109[A]:ARG:NH1	1:D:251:ASP:OD2	2.41	0.54
1:A:70[A]:SER:O	1:A:74[A]:LEU:HD23	2.07	0.54
1:B:154:TYR:O	1:B:157:GLN:HG3	2.07	0.54
1:D:119[B]:MET:HE2	1:D:119[B]:MET:CA	2.34	0.54
1:A:30:HIS:HB3	1:B:111[A]:LEU:HD12	1.89	0.53
1:B:111[B]:LEU:HD13	1:B:154:TYR:CD1	2.43	0.53
1:C:106[A]:ASN:O	1:C:110[A]:TYR:CD1	2.56	0.53
1:C:154:TYR:O	1:C:157:GLN:HG3	2.08	0.53
1:D:74[B]:LEU:HD13	1:D:74[B]:LEU:C	2.34	0.53
1:C:44:LEU:HD22	1:D:69[A]:VAL:HG21	1.90	0.53
1:D:110[B]:TYR:HA	1:D:113[B]:TRP:CE3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68[A]:MET:HE2	1:C:68[A]:MET:CA	2.37	0.53
1:E:81[A]:ASN:HD21	1:E:105[A]:ASN:H	1.56	0.53
1:B:44:LEU:HD22	1:C:69[A]:VAL:HG21	1.91	0.53
1:D:81[A]:ASN:HD21	1:D:105[A]:ASN:H	1.56	0.53
1:C:110[B]:TYR:HA	1:C:113[B]:TRP:CE3	2.44	0.53
1:A:36:TYR:CD2	1:A:76[B]:TYR:HA	2.44	0.52
1:A:115[A]:ILE:HG21	1:E:34:LEU:HD11	1.91	0.52
2:A:302:OLC:H14	1:B:115[A]:ILE:HG22	1.90	0.52
1:B:68[A]:MET:HE2	1:B:68[A]:MET:CA	2.36	0.52
1:B:40:LEU:CD2	1:C:73[A]:LEU:HD11	2.39	0.52
1:B:115[B]:ILE:O	1:B:119[B]:MET:HG2	2.09	0.52
1:D:33:THR:HG22	1:E:74[A]:LEU:HD13	1.92	0.52
1:A:111[A]:LEU:HD11	1:E:30:HIS:HB3	1.90	0.52
1:D:30:HIS:CB	1:E:111[A]:LEU:HD11	2.40	0.52
1:D:70[A]:SER:HB2	1:D:115[A]:ILE:HD11	1.92	0.52
1:D:139:ARG:NH2	3:D:306:LFA:H202	2.23	0.52
3:E:409:LFA:C14	3:E:410:LFA:H201	2.31	0.52
1:C:111[B]:LEU:HD13	1:C:154:TYR:CE1	2.44	0.52
1:A:74[B]:LEU:HD13	1:A:74[B]:LEU:C	2.35	0.52
1:C:76[A]:TYR:O	1:C:80[A]:GLN:HG2	2.10	0.52
1:C:38:VAL:HG22	1:D:115[B]:ILE:HD12	1.91	0.52
1:C:111[B]:LEU:HD13	1:C:154:TYR:CD1	2.44	0.52
1:D:44:LEU:HD22	1:E:69[A]:VAL:CG2	2.40	0.52
1:D:116[B]:ASP:O	1:D:120[B]:LEU:HG	2.10	0.52
1:B:110[B]:TYR:O	1:B:113[B]:TRP:N	2.37	0.52
1:C:117[B]:VAL:CB	1:C:118[B]:PRO:HD3	2.37	0.52
1:D:76[A]:TYR:CZ	1:D:80[A]:GLN:NE2	2.76	0.52
1:A:111[B]:LEU:HD13	1:A:154:TYR:CD1	2.45	0.51
1:A:119[B]:MET:HA	1:A:119[B]:MET:CE	2.31	0.51
1:B:119[A]:MET:HE2	1:B:119[A]:MET:CA	2.34	0.51
1:B:150[B]:ILE:HD12	1:B:150[B]:ILE:N	2.24	0.51
1:B:74[B]:LEU:HB2	1:B:112[B]:ASN:ND2	2.26	0.51
1:A:44:LEU:HD22	1:B:69[A]:VAL:HG21	1.91	0.51
1:C:115[A]:ILE:HG22	2:C:301:OLC:H13A	1.93	0.51
1:D:106[A]:ASN:O	1:D:110[A]:TYR:CD1	2.62	0.51
1:A:69[A]:VAL:HG21	1:E:44:LEU:HD22	1.91	0.51
1:B:117[B]:VAL:CB	1:B:118[B]:PRO:HD3	2.36	0.51
1:D:224:MET:N	1:D:225:PRO:HD2	2.26	0.51
1:B:33:THR:HG22	1:C:74[A]:LEU:HD13	1.92	0.51
1:B:74[B]:LEU:C	1:B:74[B]:LEU:HD13	2.36	0.51
1:E:119[B]:MET:HA	1:E:119[B]:MET:CE	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74[B]:LEU:HB2	1:C:112[B]:ASN:HD22	1.76	0.51
1:A:33:THR:HG22	1:B:74[A]:LEU:CD1	2.41	0.51
1:A:117[B]:VAL:HG21	1:A:150[B]:ILE:HD11	1.93	0.51
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.11	0.51
1:B:38:VAL:HG22	1:C:115[B]:ILE:HD11	1.93	0.50
1:B:119[B]:MET:HA	1:B:119[B]:MET:CE	2.33	0.50
1:C:33:THR:HG22	1:D:74[A]:LEU:HD13	1.92	0.50
1:B:224:MET:N	1:B:225:PRO:HD2	2.26	0.50
1:D:76[B]:TYR:O	1:D:80[B]:GLN:HG2	2.11	0.50
1:A:78[A]:GLN:OE1	1:A:78[A]:GLN:HA	2.10	0.50
1:A:74[B]:LEU:HB2	1:A:112[B]:ASN:ND2	2.25	0.50
1:A:111[A]:LEU:CD1	1:E:30:HIS:CB	2.88	0.50
1:E:115[B]:ILE:O	1:E:119[B]:MET:HG2	2.12	0.50
1:C:115[B]:ILE:O	1:C:119[B]:MET:HG2	2.10	0.50
1:E:117[B]:VAL:HB	1:E:118[B]:PRO:CD	2.34	0.50
1:A:111[B]:LEU:HD13	1:A:154:TYR:CE1	2.47	0.50
1:B:110[B]:TYR:O	1:B:113[B]:TRP:HB2	2.12	0.50
1:C:224:MET:N	1:C:225:PRO:HD2	2.27	0.50
1:E:111[B]:LEU:HD13	1:E:154:TYR:CD1	2.47	0.50
1:A:74[A]:LEU:HD13	1:E:33:THR:HG22	1.94	0.49
1:B:111[B]:LEU:HD13	1:B:154:TYR:CE1	2.46	0.49
5:C:314:RET:H8	5:C:314:RET:C16	2.26	0.49
1:A:115[A]:ILE:CG2	1:E:34:LEU:HD11	2.42	0.49
1:A:224:MET:N	1:A:225:PRO:HD2	2.27	0.49
1:C:113[A]:TRP:NE1	8:C:409:HOH:O	2.37	0.49
1:A:78[B]:GLN:HA	1:A:78[B]:GLN:OE1	2.12	0.49
1:E:70[A]:SER:O	1:E:74[A]:LEU:HD23	2.12	0.49
1:A:99:PRO:HG3	1:E:90:GLU:OE1	2.12	0.49
1:A:117[B]:VAL:CB	1:A:118[B]:PRO:HD3	2.36	0.49
1:C:68[B]:MET:HA	1:C:68[B]:MET:CE	2.36	0.49
1:E:117[B]:VAL:CB	1:E:118[B]:PRO:HD3	2.35	0.49
1:E:224:MET:N	1:E:225:PRO:HD2	2.27	0.49
1:E:111[B]:LEU:HD13	1:E:154:TYR:CE1	2.47	0.49
1:D:25:TYR:OH	1:E:102:ASP:OD2	2.31	0.49
1:E:74[B]:LEU:HB2	1:E:112[B]:ASN:HD22	1.77	0.49
5:E:414:RET:H8	5:E:414:RET:C16	2.28	0.49
1:A:90:GLU:OE1	1:B:99:PRO:HG3	2.12	0.48
1:B:18:GLU:OE1	8:B:404:HOH:O	2.20	0.48
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.95	0.48
1:C:81[A]:ASN:HD21	1:C:105[A]:ASN:H	1.61	0.48
1:A:33:THR:HG22	1:B:74[A]:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81[A]:ASN:HD21	1:B:105[A]:ASN:H	1.60	0.48
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.13	0.48
1:E:113[A]:TRP:CG	5:E:414:RET:H12	2.49	0.48
1:C:36:TYR:CD2	1:C:76[B]:TYR:HA	2.47	0.48
1:C:71[B]:ALA:O	1:C:75[B]:LEU:HG	2.13	0.48
1:C:185:MET:O	1:C:189:ILE:HG12	2.14	0.48
1:C:117[B]:VAL:HG21	1:C:150[B]:ILE:HD11	1.96	0.48
1:D:185:MET:O	1:D:189:ILE:HG12	2.14	0.48
1:A:115[A]:ILE:HG22	2:A:313:OLC:H14	1.96	0.47
1:C:90:GLU:OE1	1:D:99:PRO:CG	2.61	0.47
1:D:216:THR:O	1:D:219:PRO:HG2	2.14	0.47
1:C:74[B]:LEU:HD13	1:C:74[B]:LEU:O	2.14	0.47
1:C:119[B]:MET:HA	1:C:119[B]:MET:CE	2.32	0.47
1:D:90:GLU:CD	1:E:99:PRO:HG3	2.38	0.47
1:D:113[A]:TRP:CG	5:D:311:RET:H12	2.49	0.47
1:D:113[B]:TRP:C	1:D:115[B]:ILE:H	2.21	0.47
1:E:109[B]:ARG:NH1	1:E:251:ASP:OD2	2.46	0.47
7:E:402:OLA:C15	7:E:413:OLA:C4	2.92	0.47
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.15	0.47
1:A:33:THR:HA	1:A:36:TYR:CE2	2.50	0.47
1:A:73[A]:LEU:HD11	1:E:40:LEU:CD2	2.44	0.47
1:A:113[A]:TRP:CG	5:A:315:RET:H12	2.49	0.47
1:B:33:THR:HA	1:B:36:TYR:CE2	2.50	0.47
1:B:68[B]:MET:HA	1:B:68[B]:MET:CE	2.38	0.47
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.97	0.47
1:A:74[B]:LEU:HD21	1:A:108[B]:TYR:HB3	1.97	0.47
1:A:30:HIS:HB3	1:B:111[A]:LEU:HD11	1.94	0.47
1:A:40:LEU:CD2	1:B:73[A]:LEU:HD11	2.45	0.47
1:A:84[A]:SER:HB2	8:A:405:HOH:O	2.12	0.47
1:B:113[A]:TRP:CG	5:B:308:RET:H12	2.49	0.47
1:D:30:HIS:CB	1:E:111[A]:LEU:CD1	2.91	0.47
1:A:111[A]:LEU:HD11	1:E:30:HIS:CB	2.44	0.47
1:B:109[B]:ARG:NH1	1:B:251:ASP:OD2	2.48	0.47
1:C:113[A]:TRP:CG	5:C:314:RET:H12	2.50	0.47
1:B:30:HIS:CE1	1:C:107[A]:GLY:HA3	2.50	0.47
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.14	0.47
1:B:185:MET:O	1:B:189:ILE:HG12	2.15	0.47
1:E:185:MET:O	1:E:189:ILE:HG12	2.14	0.47
1:A:34:LEU:HD11	1:B:115[A]:ILE:HG21	1.97	0.46
1:A:102:ASP:OD2	1:E:25:TYR:OH	2.33	0.46
1:B:216:THR:O	1:B:219:PRO:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:HIS:CB	1:D:111[B]:LEU:HD23	2.43	0.46
1:C:109[B]:ARG:NH1	1:C:251:ASP:OD2	2.47	0.46
1:A:115[B]:ILE:O	1:A:119[B]:MET:HG2	2.15	0.46
1:C:110[B]:TYR:O	1:C:113[B]:TRP:HB2	2.15	0.46
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.15	0.46
1:A:109[B]:ARG:NH1	1:A:251:ASP:OD2	2.47	0.46
1:A:227:LEU:HB2	1:A:234:LEU:HD12	1.96	0.46
1:B:119[A]:MET:HA	1:B:119[A]:MET:CE	2.38	0.46
1:A:185:MET:O	1:A:189:ILE:HG12	2.15	0.46
1:D:33:THR:HA	1:D:36:TYR:CE2	2.51	0.46
1:E:216:THR:O	1:E:219:PRO:HG2	2.16	0.46
1:E:33:THR:HA	1:E:36:TYR:CE2	2.50	0.46
1:C:30:HIS:HB2	1:D:111[B]:LEU:HD22	1.92	0.46
1:E:194:GLU:O	8:E:505:HOH:O	2.21	0.46
1:B:117[B]:VAL:HB	1:B:118[B]:PRO:CD	2.36	0.45
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.98	0.45
1:D:41:ALA:HB1	1:E:66:VAL:HG13	1.98	0.45
2:A:313:OLC:H16	2:A:314:OLC:H15A	1.98	0.45
1:A:44:LEU:HD22	1:B:69[A]:VAL:CG2	2.47	0.45
1:A:99:PRO:HG3	1:E:90:GLU:CD	2.42	0.45
2:C:303:OLC:H13	2:C:315:OLC:H4A	1.98	0.45
1:E:159:TYR:CE1	2:E:407:OLC:H24A	2.51	0.45
1:B:31:ILE:HD12	1:B:31:ILE:HA	1.86	0.45
1:C:30:HIS:HB3	1:D:111[B]:LEU:HD23	1.96	0.45
1:C:36:TYR:HB3	1:C:75[B]:LEU:HB2	1.98	0.45
1:A:115[B]:ILE:HD11	1:E:38:VAL:HG22	1.99	0.45
1:C:31:ILE:HD12	1:C:31:ILE:HA	1.87	0.45
1:D:38:VAL:HG22	1:E:115[B]:ILE:HD11	1.99	0.45
1:B:44:LEU:HD22	1:C:69[A]:VAL:CG2	2.47	0.45
1:A:119[A]:MET:HA	1:A:119[A]:MET:CE	2.35	0.45
1:A:216:THR:O	1:A:219:PRO:HG2	2.17	0.45
1:A:110[B]:TYR:O	1:A:113[B]:TRP:HB2	2.17	0.44
1:A:38:VAL:HG22	1:B:115[B]:ILE:HD11	1.98	0.44
1:D:78[B]:GLN:OE1	1:D:78[B]:GLN:HA	2.17	0.44
1:C:216:THR:O	1:C:219:PRO:HG2	2.17	0.44
1:C:33:THR:HA	1:C:36:TYR:CE2	2.51	0.44
1:C:70[A]:SER:O	1:C:74[A]:LEU:HD23	2.18	0.44
1:C:146:GLY:O	1:C:150[A]:ILE:HG12	2.18	0.44
1:D:31:ILE:HD12	1:D:31:ILE:HA	1.87	0.44
1:B:113[B]:TRP:CD1	5:B:308:RET:H14	2.53	0.44
1:C:44:LEU:HD22	1:D:69[A]:VAL:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLY:O	1:B:150[A]:ILE:HG12	2.18	0.44
1:D:109[B]:ARG:NH1	1:D:251:ASP:OD2	2.46	0.44
1:A:69[A]:VAL:CG2	1:E:44:LEU:HD22	2.48	0.43
7:E:402:OLA:H42	7:E:403:OLA:H42	2.00	0.43
1:A:113[B]:TRP:CD1	5:A:315:RET:H14	2.52	0.43
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.53	0.43
1:B:222:TYR:HA	8:B:420:HOH:O	2.18	0.43
2:C:303:OLC:H8A	2:C:303:OLC:H11	1.71	0.43
1:C:38:VAL:HG22	1:D:115[B]:ILE:CD1	2.48	0.43
1:E:34:LEU:O	1:E:38:VAL:HG23	2.19	0.43
1:D:80[B]:GLN:CD	8:D:406:HOH:O	2.57	0.43
1:D:146:GLY:O	1:D:150[A]:ILE:HG12	2.19	0.43
1:E:146:GLY:O	1:E:150[A]:ILE:HG12	2.18	0.43
1:A:30:HIS:CB	1:B:111[A]:LEU:CD1	2.95	0.43
1:A:70[A]:SER:O	1:A:74[A]:LEU:CD2	2.66	0.43
1:B:124:ILE:O	1:B:128:VAL:HG22	2.19	0.43
2:B:301:OLC:H11	2:B:301:OLC:H8	1.77	0.43
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.54	0.43
1:E:124:ILE:O	1:E:128:VAL:HG22	2.19	0.43
1:D:70[A]:SER:CB	1:D:115[A]:ILE:HD11	2.49	0.43
1:D:30:HIS:C	1:E:111[A]:LEU:HD12	2.43	0.42
2:A:316:OLC:H11	2:A:316:OLC:H8	1.83	0.42
1:B:115[B]:ILE:HG21	8:B:408:HOH:O	2.17	0.42
1:C:116[B]:ASP:O	1:C:120[B]:LEU:CG	2.61	0.42
1:D:22:GLU:O	1:D:26:GLN:HG2	2.18	0.42
1:D:34:LEU:O	1:D:38:VAL:HG23	2.19	0.42
1:E:106[A]:ASN:O	1:E:110[A]:TYR:CD1	2.66	0.42
1:A:31:ILE:HD12	1:A:31:ILE:HA	1.83	0.42
1:B:30:HIS:HB3	1:C:111[A]:LEU:HD11	2.00	0.42
1:C:124:ILE:O	1:C:128:VAL:HG22	2.19	0.42
7:C:312:OLA:H42	7:E:403:OLA:H21	2.02	0.42
1:D:30:HIS:CE1	1:E:107[A]:GLY:HA3	2.54	0.42
1:A:30:HIS:CB	1:B:111[A]:LEU:HD11	2.50	0.42
5:B:308:RET:H11	5:B:308:RET:H191	1.91	0.42
5:B:308:RET:H181	5:B:308:RET:H7	1.81	0.42
1:E:74[B]:LEU:HD13	1:E:74[B]:LEU:O	2.19	0.42
1:A:101:GLY:O	1:A:102:ASP:HB2	2.20	0.42
1:A:111[A]:LEU:HD12	1:E:30:HIS:C	2.45	0.42
1:B:101:GLY:O	1:B:102:ASP:HB2	2.19	0.42
1:C:88:PHE:CZ	1:C:93:GLY:HA2	2.54	0.42
1:D:34:LEU:HD11	1:E:115[A]:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:GLU:O	1:E:26:GLN:HG2	2.20	0.42
1:D:237:GLU:O	1:D:241:MET:HG3	2.20	0.42
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.55	0.42
1:A:117[B]:VAL:CG2	1:A:150[B]:ILE:HD11	2.49	0.42
1:A:124:ILE:O	1:A:128:VAL:HG22	2.20	0.42
1:B:30:HIS:C	1:C:111[A]:LEU:HD12	2.45	0.42
5:C:314:RET:H181	5:C:314:RET:H7	1.81	0.42
1:D:88:PHE:CZ	1:D:93:GLY:HA2	2.54	0.42
1:E:146:GLY:O	1:E:150[B]:ILE:HG13	2.20	0.42
1:A:34:LEU:O	1:A:38:VAL:HG23	2.21	0.41
1:C:101:GLY:O	1:C:102:ASP:HB2	2.21	0.41
1:D:101:GLY:O	1:D:102:ASP:HB2	2.19	0.41
7:E:401:OLA:C18	7:E:413:OLA:C4	2.98	0.41
5:E:414:RET:H181	5:E:414:RET:H7	1.81	0.41
1:B:41:ALA:HB1	1:C:66:VAL:HG13	2.02	0.41
1:E:113[B]:TRP:CD1	5:E:414:RET:H14	2.55	0.41
1:B:227:LEU:HB2	1:B:234:LEU:HD12	2.01	0.41
5:D:311:RET:H7	5:D:311:RET:H181	1.81	0.41
1:C:80[B]:GLN:OE1	1:C:80[B]:GLN:HA	2.20	0.41
3:D:305:LFA:H203	3:D:307:LFA:H11	2.02	0.41
2:D:312:OLC:H13	2:D:312:OLC:H10	1.85	0.41
1:E:110[B]:TYR:O	1:E:113[B]:TRP:HB2	2.20	0.41
1:C:227:LEU:HB2	1:C:234:LEU:HD12	2.03	0.41
1:E:76[A]:TYR:O	1:E:80[A]:GLN:HG2	2.21	0.41
1:E:134:LYS:HD3	1:E:136:SER:OG	2.20	0.41
1:A:107[A]:GLY:HA3	1:E:30:HIS:CE1	2.55	0.41
1:B:22:GLU:O	1:B:26:GLN:HG2	2.20	0.41
1:B:74[B]:LEU:HD13	1:B:74[B]:LEU:O	2.21	0.41
1:C:34:LEU:O	1:C:38:VAL:HG23	2.21	0.41
1:E:101:GLY:O	1:E:102:ASP:HB2	2.21	0.41
1:A:22:GLU:O	1:A:26:GLN:HG2	2.21	0.41
1:A:30:HIS:C	1:B:111[A]:LEU:HD12	2.45	0.41
2:A:302:OLC:H11	2:A:302:OLC:H8A	1.75	0.41
1:C:25:TYR:OH	1:D:102:ASP:OD2	2.39	0.41
1:D:34:LEU:HD11	1:E:115[A]:ILE:CG2	2.50	0.41
1:E:116[B]:ASP:O	1:E:120[B]:LEU:HG	2.21	0.41
1:B:71[A]:ALA:O	1:B:75[A]:LEU:HG	2.21	0.41
1:B:80[A]:GLN:OE1	1:B:80[A]:GLN:HA	2.20	0.41
1:D:124:ILE:O	1:D:128:VAL:HG22	2.21	0.41
1:D:30:HIS:O	1:E:111[A]:LEU:HD12	2.21	0.40
1:D:110[B]:TYR:O	1:D:113[B]:TRP:N	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:CE1	1:B:107[A]:GLY:HA3	2.57	0.40
1:B:70[A]:SER:O	1:B:74[A]:LEU:HD23	2.21	0.40
1:C:173:ILE:O	1:C:176:ALA:HB3	2.22	0.40
5:A:315:RET:H11	5:A:315:RET:H191	1.91	0.40
1:B:237:GLU:O	1:B:241:MET:HG3	2.22	0.40
1:D:90:GLU:OE1	1:E:99:PRO:CG	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:CB	1:E:131:THR:O[8_445]	2.11	0.09

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	308/273 (113%)	285 (92%)	21 (7%)	2 (1%)	21	44
1	B	308/273 (113%)	284 (92%)	22 (7%)	2 (1%)	21	44
1	C	308/273 (113%)	286 (93%)	20 (6%)	2 (1%)	21	44
1	D	308/273 (113%)	289 (94%)	17 (6%)	2 (1%)	21	44
1	E	308/273 (113%)	286 (93%)	20 (6%)	2 (1%)	21	44
All	All	1540/1365 (113%)	1430 (93%)	100 (6%)	10 (1%)	30	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110[A]	TYR
1	A	110[B]	TYR
1	C	110[A]	TYR

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Mol	Chain	Res	Type
1	C	110[B]	TYR
1	B	110[A]	TYR
1	B	110[B]	TYR
1	E	110[A]	TYR
1	E	110[B]	TYR
1	D	110[A]	TYR
1	D	110[B]	TYR

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	262/234 (112%)	261 (100%)	1 (0%)	84	93
1	B	262/234 (112%)	261 (100%)	1 (0%)	84	93
1	C	261/234 (112%)	260 (100%)	1 (0%)	84	93
1	D	262/234 (112%)	260 (99%)	2 (1%)	73	88
1	E	262/234 (112%)	260 (99%)	2 (1%)	73	88
All	All	1309/1170 (112%)	1302 (100%)	7 (0%)	78	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	B	92	VAL
1	C	92	VAL
1	D	92	VAL
1	D	230	VAL
1	E	92	VAL
1	E	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	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 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 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	$\# Z > 2$
7	OLA	E	401	-	19,19,19	0.53	0	19,19,19	0.48	0
7	OLA	B	310	-	17,17,19	0.56	0	17,17,19	0.51	0
3	LFA	E	411	-	4,4,19	0.12	0	3,3,18	0.22	0
2	OLC	C	304	-	7,7,24	0.35	0	6,6,25	0.62	0
3	LFA	C	308	-	3,3,19	0.20	0	2,2,18	0.46	0
7	OLA	E	403	-	14,14,19	0.60	0	14,14,19	0.56	0
3	LFA	D	305	-	19,19,19	0.08	0	18,18,18	0.04	0
2	OLC	D	301	-	4,4,24	0.27	0	3,3,25	0.43	0
5	RET	A	315	1	20,20,21	1.62	3 (15%)	27,27,28	1.04	1 (3%)
5	RET	E	414	1	20,20,21	1.56	3 (15%)	27,27,28	1.02	1 (3%)
2	OLC	A	316	-	17,17,24	1.08	1 (5%)	17,17,25	0.90	1 (5%)
2	OLC	A	303	-	6,6,24	0.36	0	5,5,25	0.62	0
5	RET	D	311	1	20,20,21	1.65	3 (15%)	27,27,28	1.03	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	C	306	-	16,16,24	1.95	2 (12%)	16,16,25	0.96	1 (6%)
3	LFA	D	307	-	7,7,19	0.09	0	6,6,18	0.09	0
2	OLC	B	301	-	15,15,24	1.15	1 (6%)	15,15,25	0.92	1 (6%)
3	LFA	B	306	-	6,6,19	0.11	0	5,5,18	0.09	0
2	OLC	E	407	-	14,14,24	1.20	1 (7%)	15,15,25	1.03	2 (13%)
2	OLC	D	302	-	17,17,24	1.10	1 (5%)	18,18,25	1.03	1 (5%)
3	LFA	D	309	-	6,6,19	0.11	0	5,5,18	0.09	0
3	LFA	B	305	-	9,9,19	0.09	0	8,8,18	0.09	0
3	LFA	A	308	-	7,7,19	0.10	0	6,6,18	0.09	0
2	OLC	C	307	-	15,15,24	1.17	1 (6%)	16,16,25	1.02	1 (6%)
7	OLA	D	313	-	6,6,19	0.90	0	6,6,19	0.83	0
2	OLC	B	303	-	11,11,24	1.32	1 (9%)	11,11,25	1.04	1 (9%)
2	OLC	A	304	-	12,12,24	1.31	1 (8%)	13,13,25	1.11	1 (7%)
5	RET	B	308	1	20,20,21	1.60	3 (15%)	27,27,28	1.03	2 (7%)
2	OLC	D	304	-	13,13,24	1.25	1 (7%)	14,14,25	1.03	2 (14%)
3	LFA	D	308	-	16,16,19	0.08	0	15,15,18	0.06	0
3	LFA	B	304	-	7,7,19	0.10	0	6,6,18	0.08	0
7	OLA	E	402	-	16,16,19	0.57	0	16,16,19	0.52	0
3	LFA	A	306	-	6,6,19	0.10	0	5,5,18	0.09	0
2	OLC	A	305	-	14,14,24	1.21	1 (7%)	15,15,25	1.03	1 (6%)
2	OLC	A	313	-	18,18,24	1.09	1 (5%)	18,18,25	0.90	0
3	LFA	D	306	-	19,19,19	0.08	0	18,18,18	0.04	0
7	OLA	B	309	-	16,16,19	0.57	0	16,16,19	0.51	0
2	OLC	D	312	-	19,19,24	1.09	1 (5%)	19,19,25	0.93	1 (5%)
2	OLC	A	314	-	19,19,24	1.08	1 (5%)	19,19,25	0.92	1 (5%)
2	OLC	C	301	-	20,20,24	1.01	1 (5%)	21,21,25	0.94	1 (4%)
2	OLC	E	405	-	15,15,24	0.26	0	14,14,25	0.52	0
3	LFA	A	311	-	6,6,19	0.11	0	5,5,18	0.10	0
2	OLC	E	404	-	7,7,24	0.25	0	6,6,25	0.49	0
3	LFA	E	409	-	13,13,19	0.08	0	12,12,18	0.06	0
2	OLC	A	302	-	16,16,24	1.17	1 (6%)	16,16,25	0.91	0
2	OLC	C	305	-	11,11,24	1.33	1 (9%)	11,11,25	1.04	1 (9%)
6	GOL	C	313	-	3,3,5	0.31	0	2,2,5	0.20	0
7	OLA	E	413	-	5,5,19	0.96	0	5,5,19	0.89	0
2	OLC	E	406	-	19,19,24	1.05	1 (5%)	20,20,25	0.95	1 (5%)
6	GOL	B	311	-	3,3,5	0.32	0	2,2,5	0.20	0
3	LFA	C	310	-	19,19,19	0.09	0	18,18,18	0.04	0
2	OLC	B	302	-	4,4,24	0.26	0	3,3,25	0.42	0
3	LFA	E	408	-	7,7,19	0.10	0	6,6,18	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	317	-	3,3,5	0.31	0	2,2,5	0.21	0
2	OLC	C	302	-	19,19,24	1.05	1 (5%)	20,20,25	0.94	2 (10%)
3	LFA	C	309	-	7,7,19	0.10	0	6,6,18	0.09	0
7	OLA	C	312	-	17,17,19	0.55	0	17,17,19	0.51	0
2	OLC	A	301	-	8,8,24	0.33	0	7,7,25	0.57	0
3	LFA	E	410	-	3,3,19	0.21	0	2,2,18	0.46	0
2	OLC	C	315	-	15,15,24	1.18	1 (6%)	15,15,25	1.09	1 (6%)
3	LFA	A	309	-	3,3,19	0.22	0	2,2,18	0.46	0
3	LFA	A	310	-	5,5,19	0.12	0	4,4,18	0.11	0
5	RET	C	314	1	20,20,21	1.62	4 (20%)	27,27,28	1.02	1 (3%)
2	OLC	D	303	-	4,4,24	0.32	0	3,3,25	0.36	0
3	LFA	A	307	-	7,7,19	0.10	0	6,6,18	0.08	0
2	OLC	C	303	-	18,18,24	1.05	1 (5%)	18,18,25	0.84	1 (5%)

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
7	OLA	E	401	-	-	4/17/17/17	-
7	OLA	B	310	-	-	11/15/15/17	-
3	LFA	E	411	-	-	0/2/2/17	-
2	OLC	C	304	-	-	3/5/5/24	-
3	LFA	C	308	-	-	0/1/1/17	-
7	OLA	E	403	-	-	8/12/12/17	-
3	LFA	D	305	-	-	11/17/17/17	-
2	OLC	D	301	-	-	1/2/2/24	-
5	RET	A	315	1	-	0/13/30/31	0/1/1/1
5	RET	E	414	1	-	0/13/30/31	0/1/1/1
2	OLC	A	316	-	-	2/16/16/24	-
2	OLC	A	303	-	-	2/4/4/24	-
5	RET	D	311	1	-	0/13/30/31	0/1/1/1
2	OLC	C	306	-	-	8/14/14/24	-
3	LFA	D	307	-	-	4/5/5/17	-
2	OLC	B	301	-	-	2/14/14/24	-
3	LFA	B	306	-	-	2/4/4/17	-
2	OLC	E	407	-	-	4/14/14/24	-
2	OLC	D	302	-	-	6/17/17/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	D	309	-	-	2/4/4/17	-
3	LFA	B	305	-	-	0/7/7/17	-
3	LFA	A	308	-	-	2/5/5/17	-
2	OLC	C	307	-	-	7/15/15/24	-
7	OLA	D	313	-	-	2/4/4/17	-
2	OLC	B	303	-	-	3/10/10/24	-
2	OLC	A	304	-	-	3/12/12/24	-
5	RET	B	308	1	-	0/13/30/31	0/1/1/1
2	OLC	D	304	-	-	8/13/13/24	-
3	LFA	D	308	-	-	4/14/14/17	-
3	LFA	B	304	-	-	2/5/5/17	-
7	OLA	E	402	-	-	6/14/14/17	-
3	LFA	A	306	-	-	2/4/4/17	-
2	OLC	A	305	-	-	3/14/14/24	-
2	OLC	A	313	-	-	8/16/16/24	-
3	LFA	D	306	-	-	9/17/17/17	-
7	OLA	B	309	-	-	4/14/14/17	-
2	OLC	D	312	-	-	7/17/17/24	-
2	OLC	A	314	-	-	10/17/17/24	-
2	OLC	C	301	-	-	8/20/20/24	-
2	OLC	E	405	-	-	9/13/13/24	-
3	LFA	A	311	-	-	1/4/4/17	-
2	OLC	E	404	-	-	2/5/5/24	-
3	LFA	E	409	-	-	0/11/11/17	-
2	OLC	A	302	-	-	5/14/14/24	-
2	OLC	C	305	-	-	3/10/10/24	-
6	GOL	C	313	-	-	1/1/1/4	-
7	OLA	E	413	-	-	2/3/3/17	-
2	OLC	E	406	-	-	7/19/19/24	-
6	GOL	B	311	-	-	1/1/1/4	-
3	LFA	C	310	-	-	12/17/17/17	-
2	OLC	B	302	-	-	0/2/2/24	-
3	LFA	E	408	-	-	0/5/5/17	-
6	GOL	A	317	-	-	0/1/1/4	-
2	OLC	C	302	-	-	11/19/19/24	-
3	LFA	C	309	-	-	4/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLA	C	312	-	-	8/15/15/17	-
2	OLC	A	301	-	-	1/6/6/24	-
3	LFA	E	410	-	-	1/1/1/17	-
2	OLC	C	315	-	-	5/14/14/24	-
3	LFA	A	309	-	-	0/1/1/17	-
3	LFA	A	310	-	-	1/3/3/17	-
5	RET	C	314	1	-	0/13/30/31	0/1/1/1
2	OLC	D	303	-	-	0/2/2/24	-
3	LFA	A	307	-	-	1/5/5/17	-
2	OLC	C	303	-	-	5/17/17/24	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	306	OLC	O19-C1	7.29	1.45	1.22
5	D	311	RET	C14-C13	4.90	1.37	1.33
5	A	315	RET	C14-C13	4.75	1.37	1.33
5	B	308	RET	C14-C13	4.65	1.36	1.33
2	D	312	OLC	O20-C1	4.65	1.46	1.30
5	C	314	RET	C14-C13	4.61	1.36	1.33
2	A	314	OLC	O20-C1	4.58	1.46	1.30
2	A	302	OLC	O20-C1	4.55	1.45	1.30
2	A	313	OLC	O20-C1	4.49	1.45	1.30
5	E	414	RET	C14-C13	4.37	1.36	1.33
2	A	304	OLC	O20-C1	4.36	1.46	1.33
2	E	406	OLC	O20-C1	4.34	1.46	1.33
2	A	305	OLC	O20-C1	4.33	1.46	1.33
2	C	307	OLC	O20-C1	4.31	1.45	1.33
2	C	315	OLC	O20-C1	4.31	1.45	1.33
2	C	302	OLC	O20-C1	4.31	1.45	1.33
2	C	301	OLC	O20-C1	4.29	1.45	1.33
2	D	302	OLC	O20-C1	4.28	1.45	1.33
2	E	407	OLC	O20-C1	4.27	1.45	1.33
2	D	304	OLC	O20-C1	4.26	1.45	1.33
2	B	301	OLC	O20-C1	4.25	1.46	1.33
2	C	305	OLC	O20-C1	4.24	1.46	1.33
2	A	316	OLC	O20-C1	4.23	1.46	1.33
2	B	303	OLC	O20-C1	4.21	1.46	1.33
2	C	303	OLC	O20-C1	4.21	1.46	1.33
5	C	314	RET	C8-C9	-2.73	1.40	1.46
5	D	311	RET	C8-C9	-2.67	1.40	1.46
5	E	414	RET	C8-C9	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	315	RET	C8-C9	-2.62	1.40	1.46
5	B	308	RET	C8-C9	-2.62	1.40	1.46
2	C	306	OLC	O20-C1	-2.56	1.22	1.30
5	D	311	RET	C10-C9	2.42	1.41	1.35
5	B	308	RET	C10-C9	2.33	1.41	1.35
5	A	315	RET	C10-C9	2.33	1.41	1.35
5	E	414	RET	C10-C9	2.31	1.41	1.35
5	C	314	RET	C10-C9	2.25	1.41	1.35
5	C	314	RET	C20-C13	-2.02	1.46	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	315	RET	C19-C9-C10	-3.44	117.24	122.82
5	B	308	RET	C19-C9-C10	-3.39	117.32	122.82
5	E	414	RET	C19-C9-C10	-3.36	117.37	122.82
5	D	311	RET	C19-C9-C10	-3.34	117.40	122.82
5	C	314	RET	C19-C9-C10	-3.34	117.40	122.82
2	A	304	OLC	O20-C1-C2	2.89	120.64	111.83
2	C	301	OLC	O20-C1-C2	2.82	120.45	111.83
2	E	406	OLC	O20-C1-C2	2.82	120.44	111.83
2	D	302	OLC	O20-C1-C2	2.81	120.40	111.83
2	A	305	OLC	O20-C1-C2	2.81	120.39	111.83
2	E	407	OLC	O20-C1-C2	2.79	120.34	111.83
2	C	302	OLC	O20-C1-C2	2.78	120.33	111.83
2	C	307	OLC	O20-C1-C2	2.75	120.23	111.83
2	D	304	OLC	O20-C1-C2	2.68	120.02	111.83
2	C	315	OLC	O20-C1-C2	2.66	119.94	111.83
2	A	316	OLC	O20-C1-C2	2.20	120.47	112.14
2	B	303	OLC	O20-C1-C2	2.19	120.41	112.14
2	C	305	OLC	O20-C1-C2	2.18	120.38	112.14
2	B	301	OLC	O20-C1-C2	2.15	120.25	112.14
2	D	312	OLC	O20-C1-C2	2.13	120.74	114.00
2	A	314	OLC	O20-C1-C2	2.11	120.67	114.00
2	E	407	OLC	O20-C1-O19	-2.09	118.40	123.63
2	C	303	OLC	O20-C1-C2	2.07	119.95	112.14
2	D	304	OLC	O20-C1-O19	-2.06	118.48	123.63
2	C	306	OLC	O20-C1-C2	2.05	120.46	114.00
2	C	302	OLC	O20-C1-O19	-2.04	118.53	123.63
5	B	308	RET	C8-C9-C10	2.01	122.17	119.01
5	D	311	RET	C8-C9-C10	2.00	122.16	119.01

There are no chirality outliers.

All (238) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	305	OLC	C21-C22-C24-O25
2	C	307	OLC	C21-C22-C24-O25
2	C	307	OLC	O20-C21-C22-O23
3	E	410	LFA	C17-C18-C19-C20
7	E	402	OLA	C11-C10-C9-C8
2	B	303	OLC	C2-C1-O20-C21
2	D	304	OLC	O20-C21-C22-O23
2	E	407	OLC	O20-C21-C22-O23
3	C	310	LFA	C14-C15-C16-C17
2	B	303	OLC	O19-C1-O20-C21
7	B	309	OLA	C11-C10-C9-C8
7	B	310	OLA	C11-C10-C9-C8
7	C	312	OLA	C11-C10-C9-C8
2	D	304	OLC	O20-C21-C22-C24
2	E	406	OLC	C1-C2-C3-C4
2	D	304	OLC	C1-C2-C3-C4
2	D	312	OLC	C1-C2-C3-C4
2	E	406	OLC	C2-C1-O20-C21
7	E	403	OLA	C1-C2-C3-C4
7	E	403	OLA	C11-C10-C9-C8
2	A	304	OLC	C1-C2-C3-C4
7	E	403	OLA	C2-C3-C4-C5
3	C	310	LFA	C13-C14-C15-C16
3	D	305	LFA	C6-C7-C8-C9
3	D	305	LFA	C9-C10-C11-C12
2	A	305	OLC	O23-C22-C24-O25
2	E	406	OLC	C5-C6-C7-C8
3	C	310	LFA	C10-C11-C12-C13
2	A	313	OLC	C10-C11-C12-C13
2	A	314	OLC	C5-C6-C7-C8
7	B	310	OLA	C12-C13-C14-C15
7	E	402	OLA	C1-C2-C3-C4
3	D	308	LFA	C11-C12-C13-C14
2	E	406	OLC	O19-C1-O20-C21
2	D	302	OLC	C2-C1-O20-C21
2	C	305	OLC	C5-C6-C7-C8
3	A	308	LFA	C14-C15-C16-C17
2	C	306	OLC	C4-C5-C6-C7
7	B	310	OLA	C2-C3-C4-C5
2	C	303	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	D	305	LFA	C3-C4-C5-C6
7	E	401	OLA	C12-C13-C14-C15
3	D	306	LFA	C14-C15-C16-C17
2	E	405	OLC	C6-C7-C8-C9
3	B	306	LFA	C15-C16-C17-C18
3	D	308	LFA	C6-C7-C8-C9
2	A	314	OLC	C2-C3-C4-C5
3	C	310	LFA	C12-C13-C14-C15
2	C	306	OLC	C2-C3-C4-C5
2	D	302	OLC	O19-C1-O20-C21
7	C	312	OLA	C3-C4-C5-C6
7	B	310	OLA	C3-C4-C5-C6
7	E	401	OLA	C14-C15-C16-C17
2	A	302	OLC	C6-C7-C8-C9
2	C	306	OLC	C6-C7-C8-C9
3	D	306	LFA	C5-C6-C7-C8
2	A	302	OLC	C2-C3-C4-C5
2	A	313	OLC	C2-C3-C4-C5
2	E	405	OLC	C4-C5-C6-C7
3	D	305	LFA	C11-C12-C13-C14
2	C	301	OLC	C5-C6-C7-C8
2	C	301	OLC	C6-C7-C8-C9
2	C	306	OLC	C3-C4-C5-C6
2	D	304	OLC	C2-C3-C4-C5
3	D	306	LFA	C12-C13-C14-C15
2	C	307	OLC	O23-C22-C24-O25
2	C	302	OLC	C6-C7-C8-C9
2	C	306	OLC	C10-C11-C12-C13
7	E	402	OLA	C10-C11-C12-C13
3	D	305	LFA	C11-C10-C9-C8
7	C	312	OLA	C4-C5-C6-C7
2	D	304	OLC	C3-C4-C5-C6
3	C	309	LFA	C15-C16-C17-C18
7	E	401	OLA	C4-C5-C6-C7
3	A	310	LFA	C2-C3-C4-C5
2	A	314	OLC	C10-C11-C12-C13
7	B	310	OLA	C10-C11-C12-C13
2	E	404	OLC	C4-C5-C6-C7
2	C	315	OLC	C2-C3-C4-C5
2	C	301	OLC	C21-C22-C24-O25
3	D	306	LFA	C3-C4-C5-C6
7	B	309	OLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	D	306	LFA	C6-C7-C8-C9
3	C	309	LFA	C16-C17-C18-C19
3	D	305	LFA	C13-C14-C15-C16
2	C	303	OLC	C12-C13-C14-C15
7	E	402	OLA	C12-C13-C14-C15
2	B	303	OLC	C4-C5-C6-C7
2	D	312	OLC	C4-C5-C6-C7
7	D	313	OLA	C2-C3-C4-C5
2	D	302	OLC	C4-C5-C6-C7
2	C	306	OLC	C11-C12-C13-C14
3	D	305	LFA	C4-C5-C6-C7
2	C	301	OLC	C4-C5-C6-C7
2	C	307	OLC	C2-C1-O20-C21
2	C	315	OLC	C2-C1-O20-C21
2	C	302	OLC	O20-C21-C22-O23
3	D	306	LFA	C1-C2-C3-C4
3	D	309	LFA	C14-C15-C16-C17
3	D	308	LFA	C11-C10-C9-C8
2	C	307	OLC	O20-C21-C22-C24
2	E	405	OLC	C3-C4-C5-C6
2	C	305	OLC	C6-C7-C8-C9
2	D	312	OLC	C3-C4-C5-C6
3	A	311	LFA	C3-C4-C5-C6
3	B	304	LFA	C2-C3-C4-C5
3	A	307	LFA	C1-C2-C3-C4
3	D	309	LFA	C16-C17-C18-C19
2	C	307	OLC	C6-C7-C8-C9
2	E	405	OLC	C2-C3-C4-C5
3	B	304	LFA	C3-C4-C5-C6
3	C	310	LFA	C9-C10-C11-C12
3	C	310	LFA	C17-C18-C19-C20
2	C	302	OLC	C2-C3-C4-C5
2	C	303	OLC	C11-C12-C13-C14
7	E	403	OLA	C3-C4-C5-C6
2	E	405	OLC	C10-C11-C12-C13
2	E	405	OLC	C13-C14-C15-C16
3	D	305	LFA	C14-C15-C16-C17
3	C	310	LFA	C11-C10-C9-C8
2	E	407	OLC	O20-C21-C22-C24
3	A	306	LFA	C17-C18-C19-C20
2	C	302	OLC	C5-C6-C7-C8
2	C	304	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	C	309	LFA	C17-C18-C19-C20
2	C	302	OLC	C3-C4-C5-C6
3	D	306	LFA	C15-C16-C17-C18
2	C	304	OLC	C5-C6-C7-C8
3	D	307	LFA	C5-C6-C7-C8
3	D	307	LFA	C1-C2-C3-C4
2	C	307	OLC	O19-C1-O20-C21
2	C	315	OLC	O19-C1-O20-C21
2	D	302	OLC	C6-C7-C8-C9
7	C	312	OLA	C6-C7-C8-C9
3	D	306	LFA	C4-C5-C6-C7
7	E	403	OLA	C4-C5-C6-C7
2	A	302	OLC	C11-C12-C13-C14
3	D	305	LFA	C10-C11-C12-C13
3	B	306	LFA	C16-C17-C18-C19
2	A	313	OLC	C6-C7-C8-C9
2	C	302	OLC	O20-C21-C22-C24
2	D	301	OLC	C6-C7-C8-C9
2	A	305	OLC	C2-C3-C4-C5
7	B	309	OLA	C12-C13-C14-C15
2	E	405	OLC	C5-C6-C7-C8
2	E	407	OLC	C3-C4-C5-C6
2	B	301	OLC	C2-C3-C4-C5
3	D	308	LFA	C14-C15-C16-C17
2	C	302	OLC	C2-C1-O20-C21
2	C	315	OLC	C1-C2-C3-C4
2	C	301	OLC	O23-C22-C24-O25
3	A	306	LFA	C16-C17-C18-C19
2	C	302	OLC	O19-C1-O20-C21
2	A	316	OLC	C2-C3-C4-C5
3	D	305	LFA	C15-C16-C17-C18
2	A	314	OLC	C9-C10-C11-C12
7	E	401	OLA	C7-C8-C9-C10
2	A	313	OLC	C3-C4-C5-C6
2	D	302	OLC	O20-C21-C22-O23
2	C	303	OLC	C5-C6-C7-C8
3	C	309	LFA	C13-C14-C15-C16
2	C	302	OLC	C9-C10-C11-C12
7	C	312	OLA	C7-C8-C9-C10
3	C	310	LFA	C5-C6-C7-C8
3	C	310	LFA	C1-C2-C3-C4
2	A	303	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	314	OLC	C1-C2-C3-C4
7	B	310	OLA	C11-C12-C13-C14
2	C	302	OLC	C4-C5-C6-C7
2	D	312	OLC	C5-C6-C7-C8
7	B	310	OLA	C6-C7-C8-C9
7	C	312	OLA	C5-C6-C7-C8
2	D	304	OLC	C4-C5-C6-C7
7	C	312	OLA	C12-C13-C14-C15
3	C	310	LFA	C4-C5-C6-C7
2	C	301	OLC	C9-C10-C11-C12
2	D	312	OLC	C7-C8-C9-C10
7	B	310	OLA	O2-C1-C2-C3
7	B	310	OLA	C4-C5-C6-C7
2	E	405	OLC	C7-C8-C9-C10
2	B	301	OLC	C10-C11-C12-C13
7	B	310	OLA	O1-C1-C2-C3
2	D	312	OLC	C2-C3-C4-C5
2	A	313	OLC	C5-C6-C7-C8
2	A	314	OLC	C12-C13-C14-C15
3	A	308	LFA	C17-C18-C19-C20
7	E	402	OLA	O2-C1-C2-C3
7	D	313	OLA	C1-C2-C3-C4
2	E	404	OLC	C2-C3-C4-C5
2	E	406	OLC	C4-C5-C6-C7
2	A	302	OLC	O19-C1-C2-C3
7	E	403	OLA	O1-C1-C2-C3
2	C	306	OLC	C12-C13-C14-C15
3	C	310	LFA	C3-C4-C5-C6
2	A	316	OLC	C3-C4-C5-C6
3	D	305	LFA	C5-C6-C7-C8
3	C	310	LFA	C6-C7-C8-C9
2	A	302	OLC	O20-C1-C2-C3
7	E	402	OLA	O1-C1-C2-C3
7	C	312	OLA	C10-C11-C12-C13
2	D	304	OLC	O19-C1-O20-C21
6	B	311	GOL	O1-C1-C2-O2
2	D	302	OLC	C7-C8-C9-C10
7	E	403	OLA	O2-C1-C2-C3
3	D	307	LFA	C2-C3-C4-C5
2	C	305	OLC	C3-C4-C5-C6
7	B	309	OLA	C4-C5-C6-C7
2	A	314	OLC	O20-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	303	OLC	C9-C10-C11-C12
2	A	313	OLC	C9-C10-C11-C12
2	A	314	OLC	C7-C8-C9-C10
2	E	406	OLC	C9-C10-C11-C12
2	D	304	OLC	C2-C1-O20-C21
2	C	304	OLC	C7-C8-C9-C10
7	E	403	OLA	C7-C8-C9-C10
2	A	304	OLC	O19-C1-O20-C21
2	A	304	OLC	C2-C1-O20-C21
2	A	301	OLC	C9-C10-C11-C12
2	A	314	OLC	O19-C1-C2-C3
2	C	315	OLC	C6-C7-C8-C9
3	D	306	LFA	C7-C8-C9-C10
2	C	306	OLC	C7-C8-C9-C10
2	D	312	OLC	C9-C10-C11-C12
2	E	406	OLC	C7-C8-C9-C10
6	C	313	GOL	O2-C2-C3-O3
2	C	301	OLC	C7-C8-C9-C10
2	C	302	OLC	C7-C8-C9-C10
7	B	310	OLA	C9-C10-C11-C12
2	E	407	OLC	C5-C6-C7-C8
2	C	303	OLC	C3-C4-C5-C6
2	A	313	OLC	C12-C13-C14-C15
2	A	313	OLC	C14-C15-C16-C17
2	E	405	OLC	C11-C12-C13-C14
2	C	301	OLC	C3-C4-C5-C6
2	A	314	OLC	C13-C14-C15-C16
3	D	307	LFA	C4-C5-C6-C7
7	E	413	OLA	O2-C1-C2-C3
7	E	413	OLA	O1-C1-C2-C3

There are no ring outliers.

28 monomers are involved in 62 short contacts:

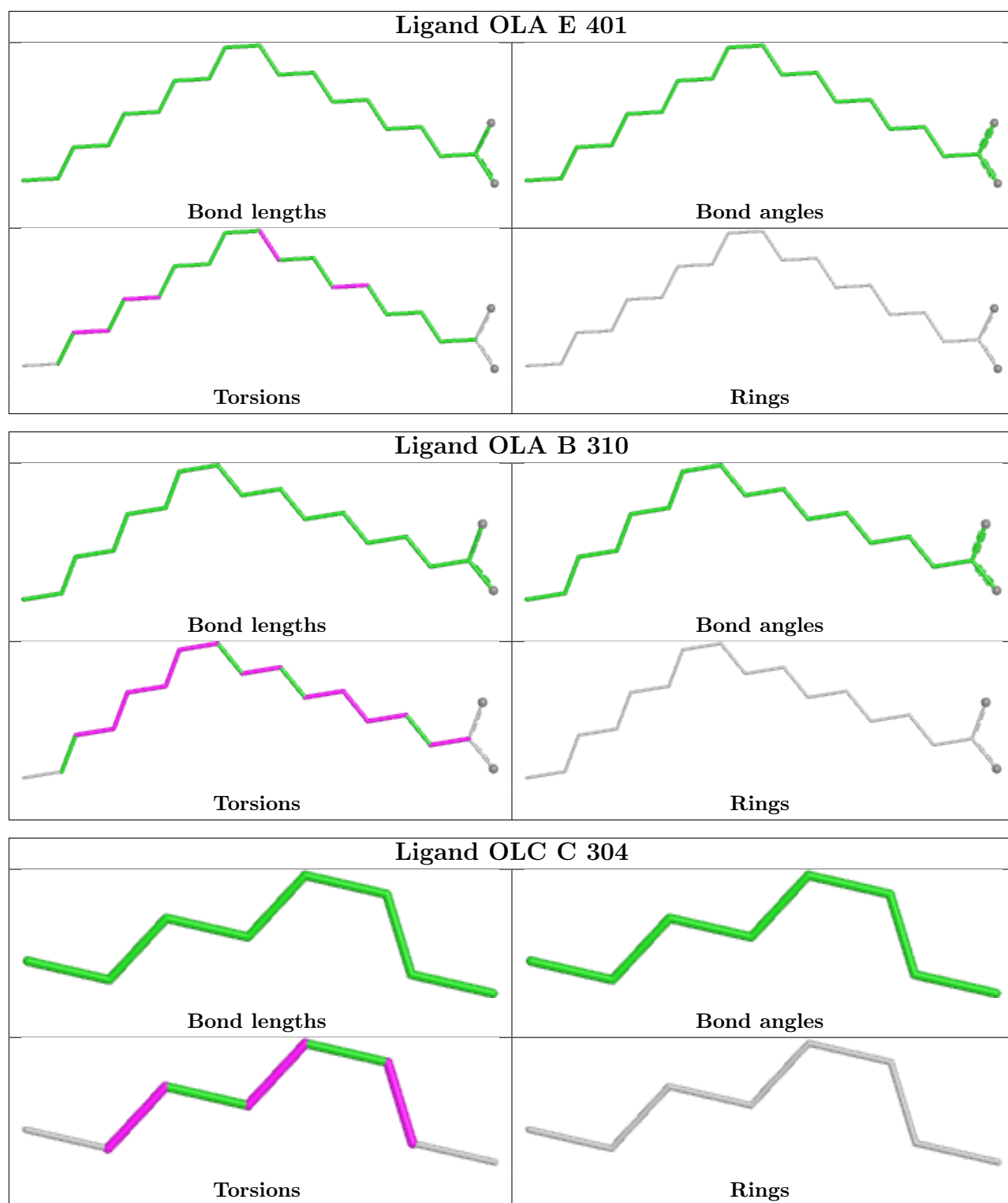
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	401	OLA	1	0
7	E	403	OLA	2	0
3	D	305	LFA	1	0
5	A	315	RET	7	0
5	E	414	RET	8	0
2	A	316	OLC	1	0
5	D	311	RET	6	0

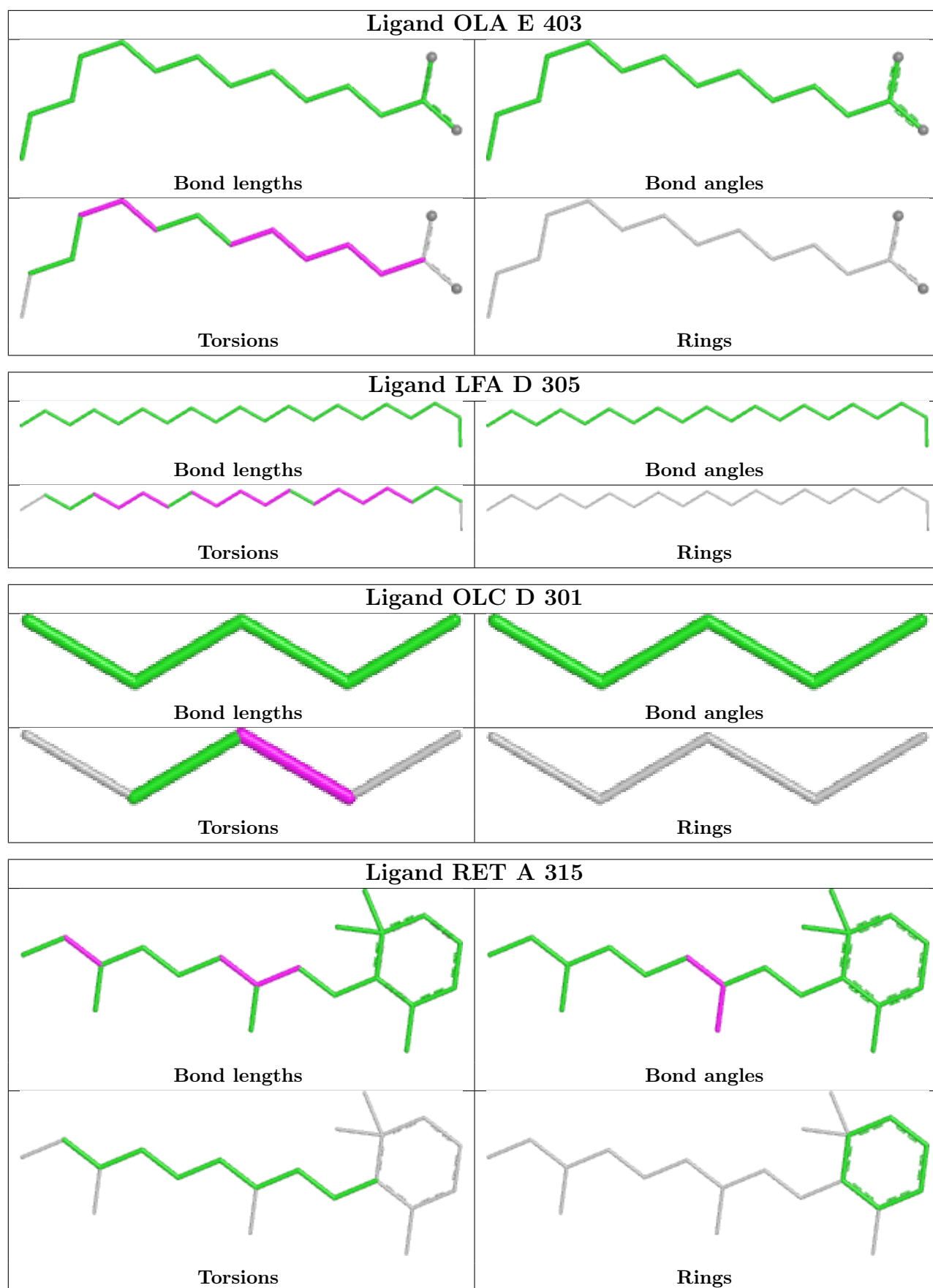
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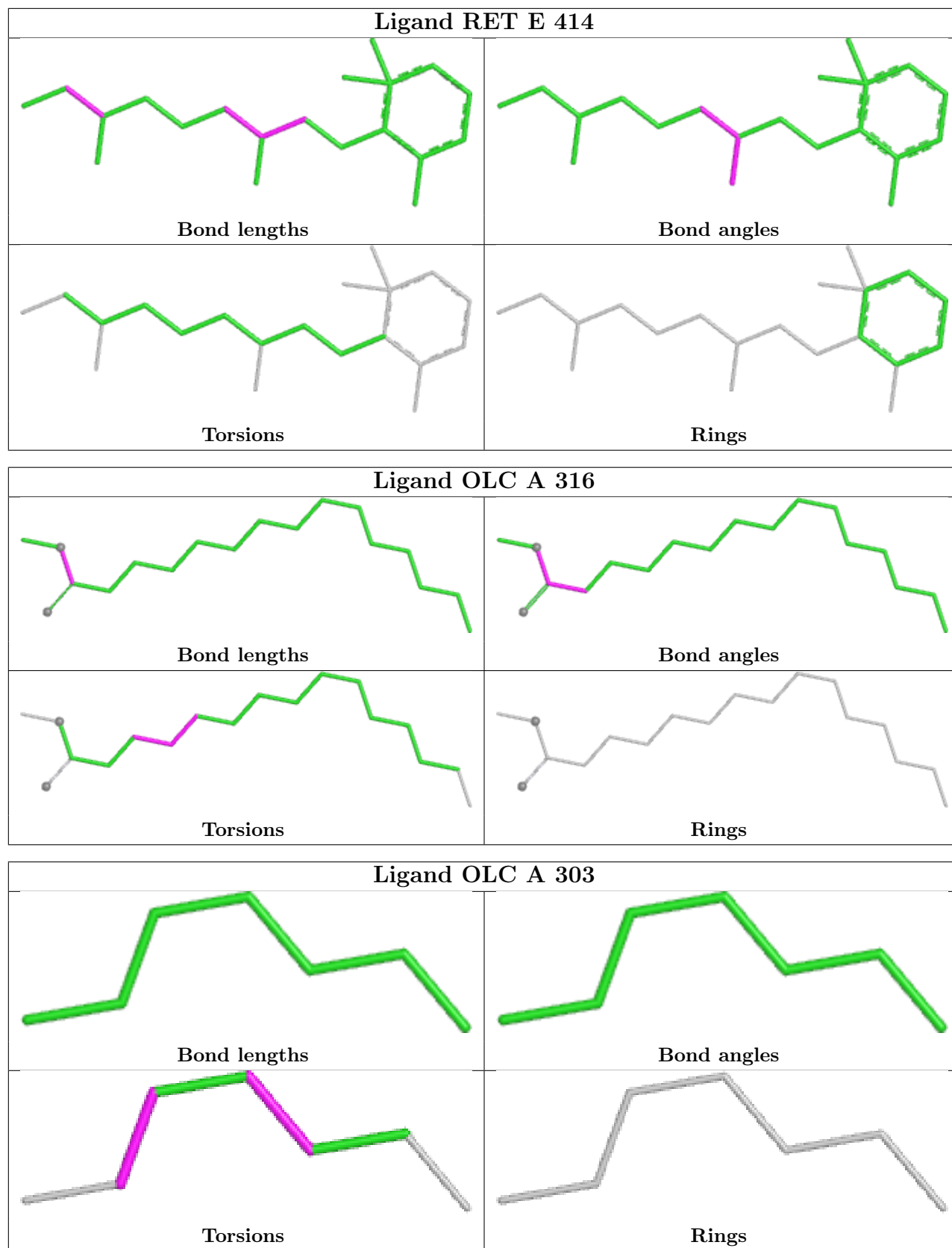
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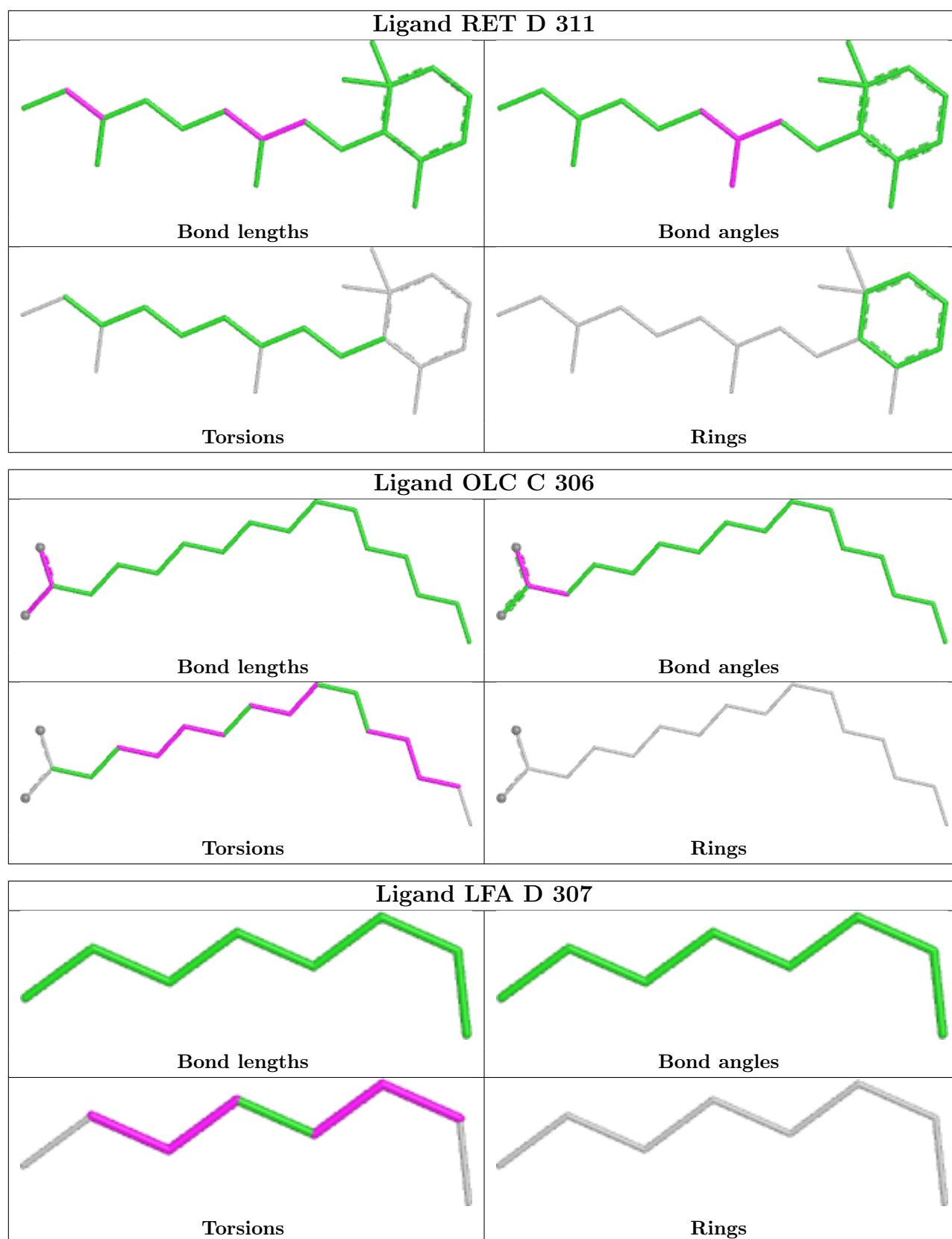
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	307	LFA	1	0
2	B	301	OLC	1	0
2	E	407	OLC	1	0
2	C	307	OLC	3	0
5	B	308	RET	8	0
7	E	402	OLA	2	0
2	A	313	OLC	3	0
3	D	306	LFA	2	0
2	D	312	OLC	1	0
2	A	314	OLC	1	0
2	C	301	OLC	1	0
3	E	409	LFA	2	0
2	A	302	OLC	2	0
7	E	413	OLA	2	0
3	C	310	LFA	1	0
2	C	302	OLC	1	0
7	C	312	OLA	1	0
3	E	410	LFA	2	0
2	C	315	OLC	1	0
5	C	314	RET	7	0
2	C	303	OLC	3	0

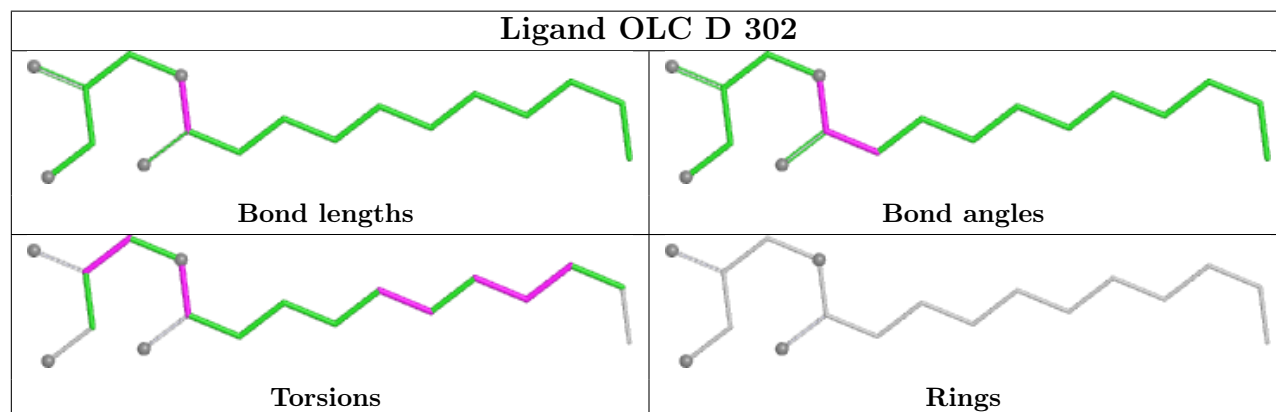
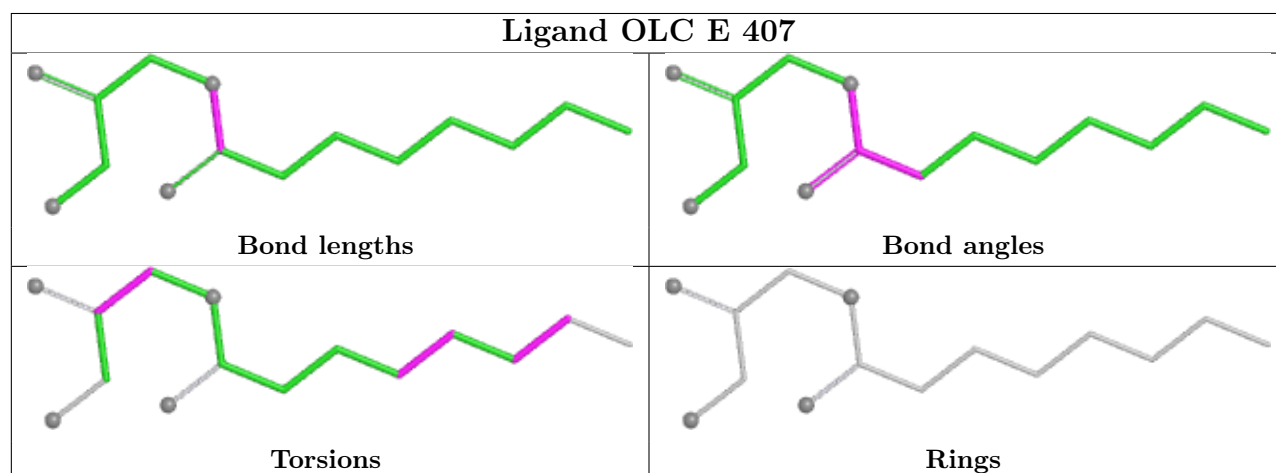
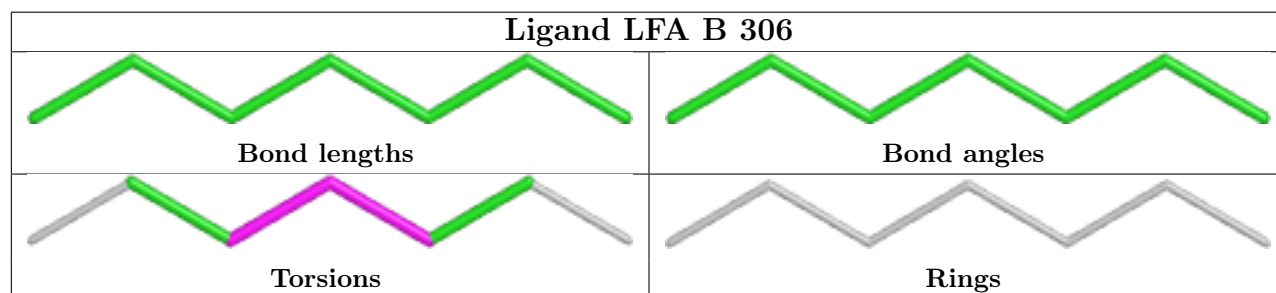
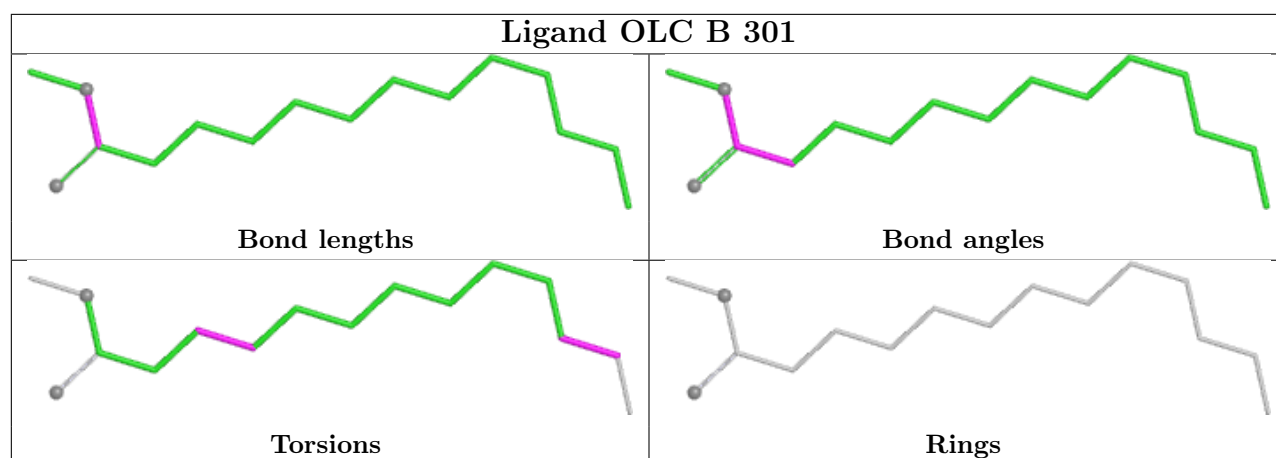
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

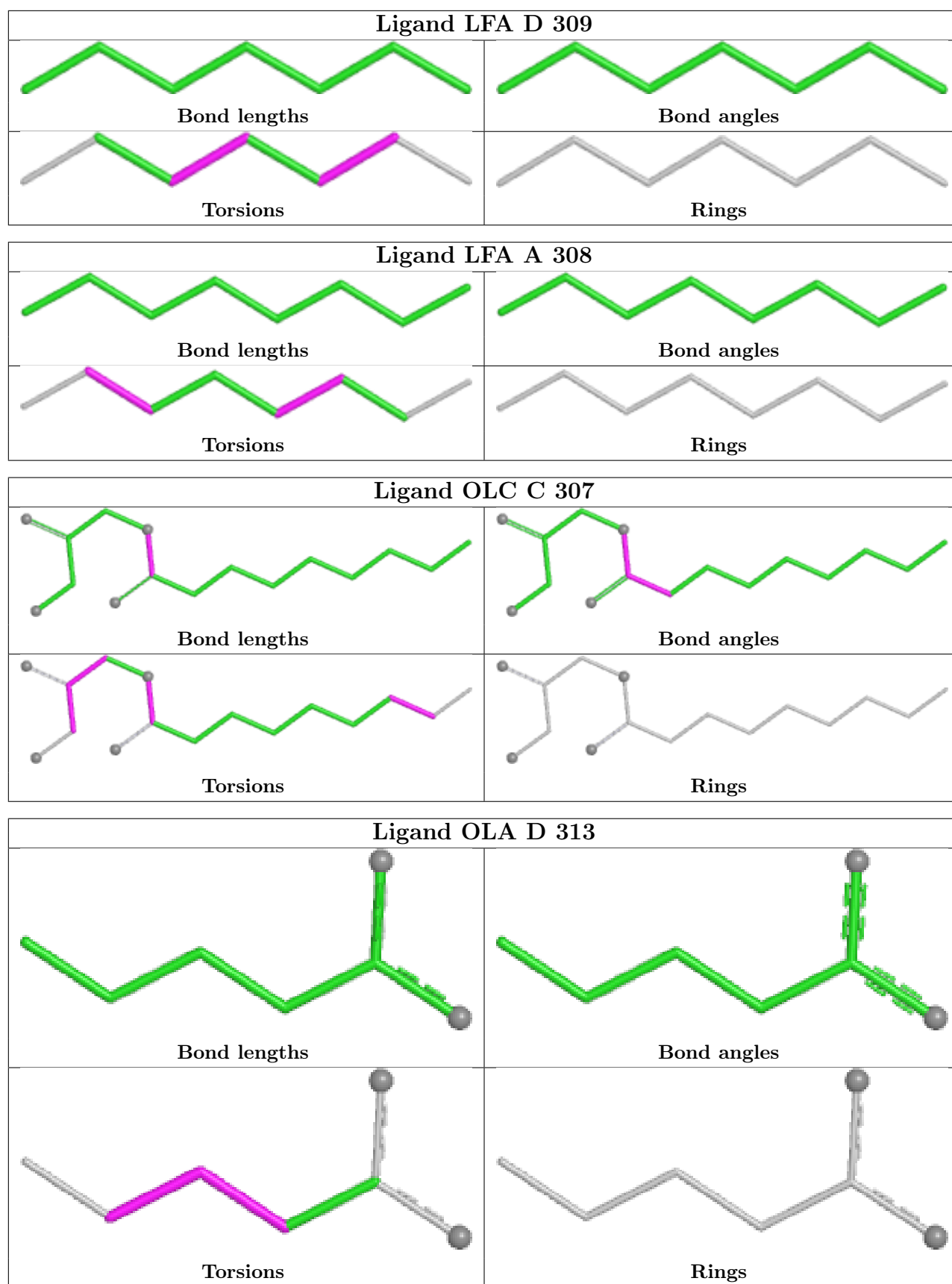


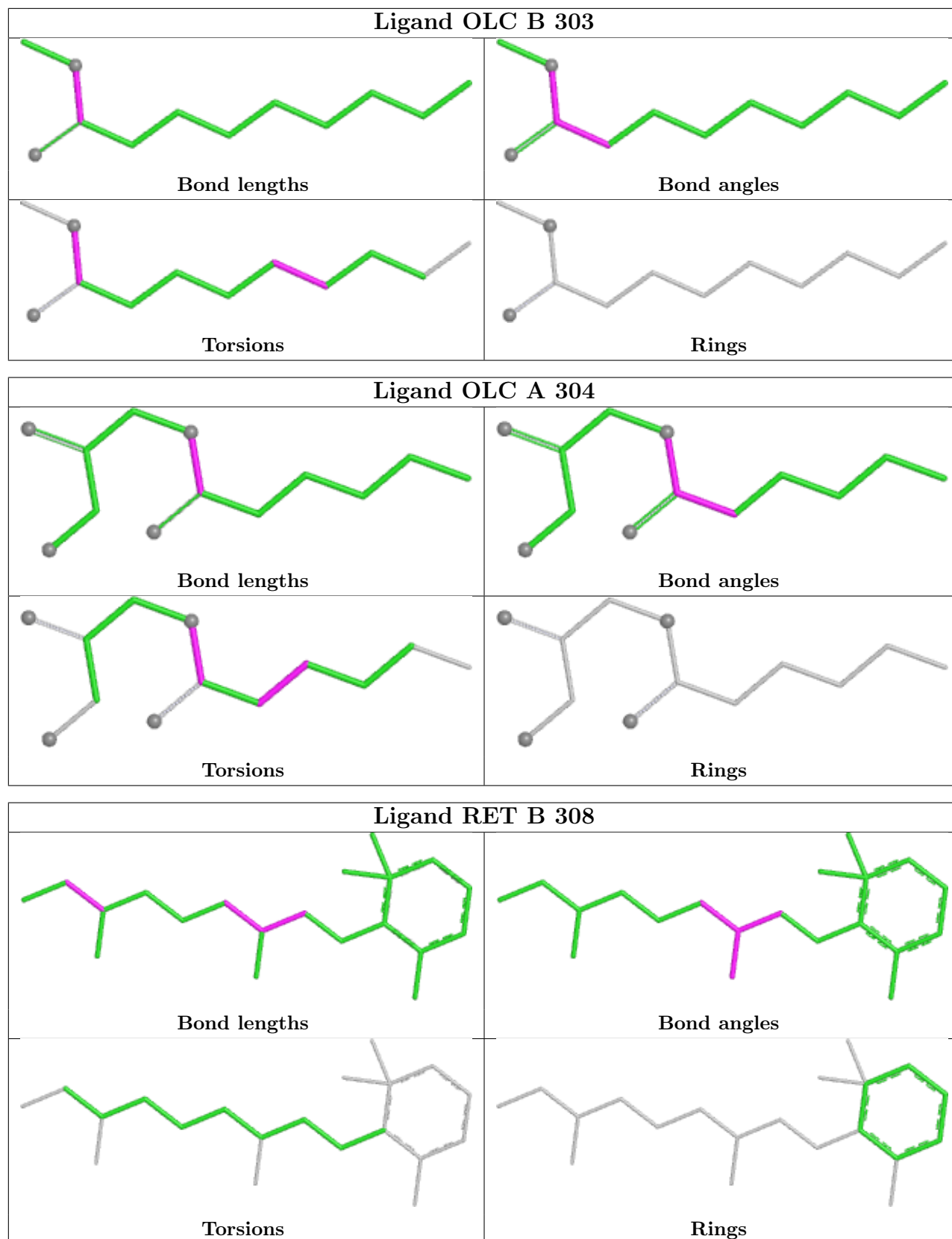


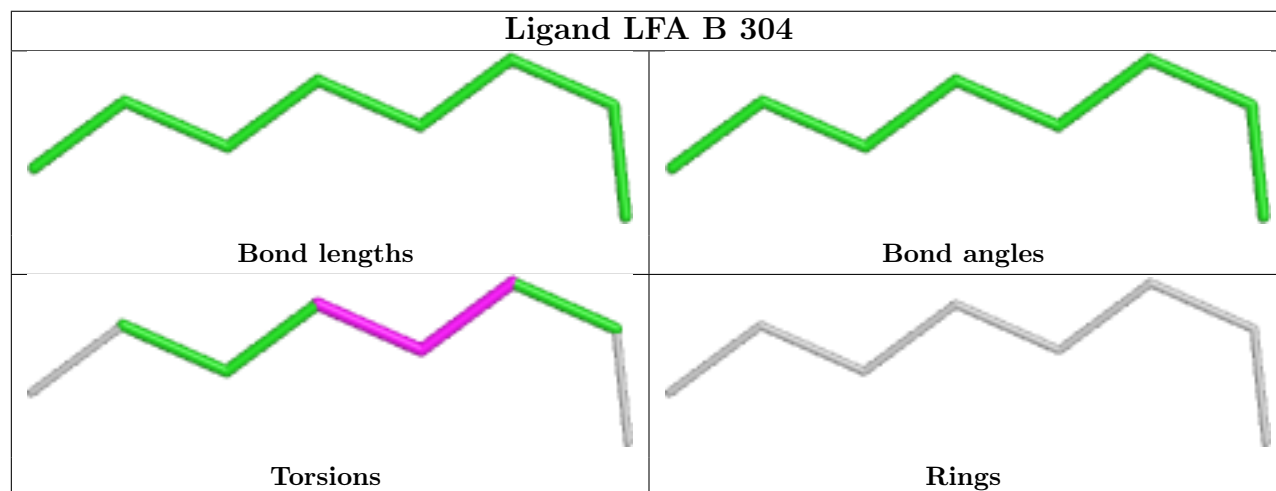
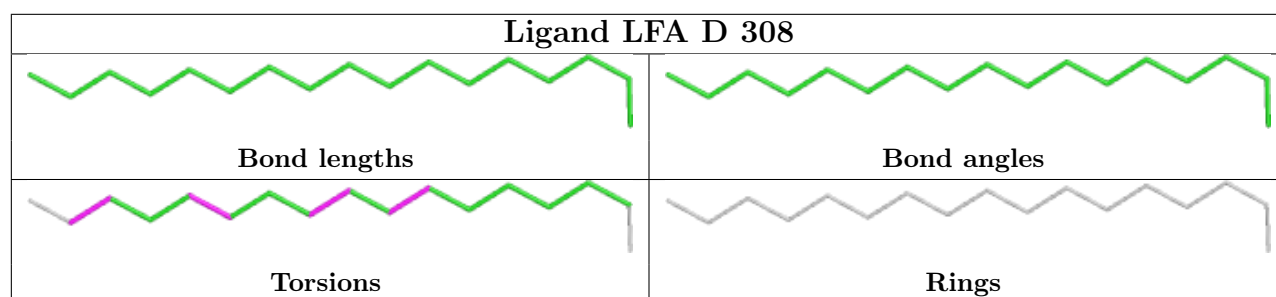
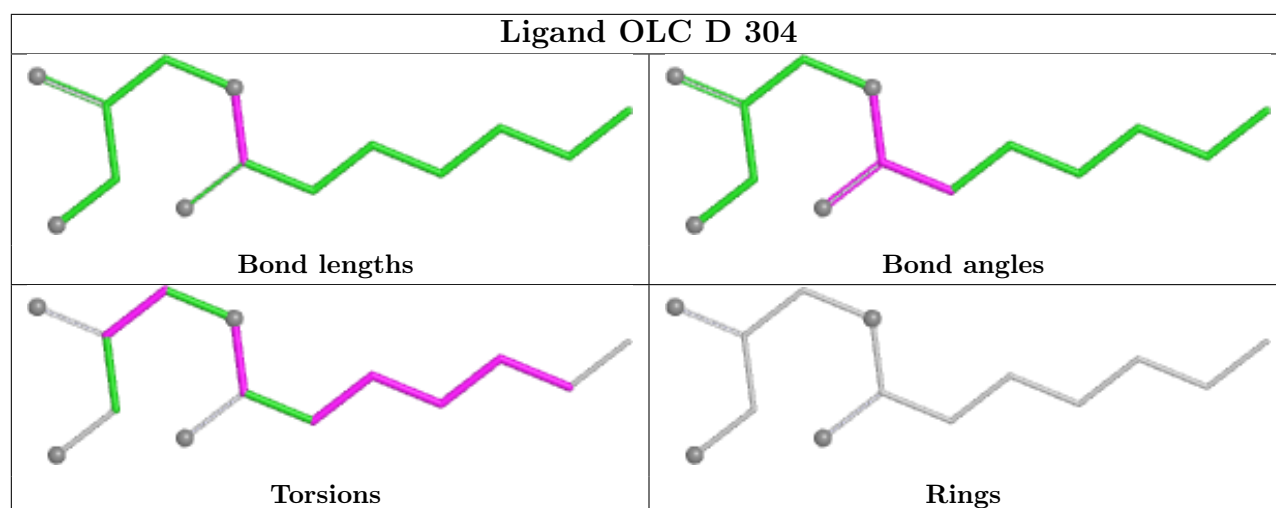


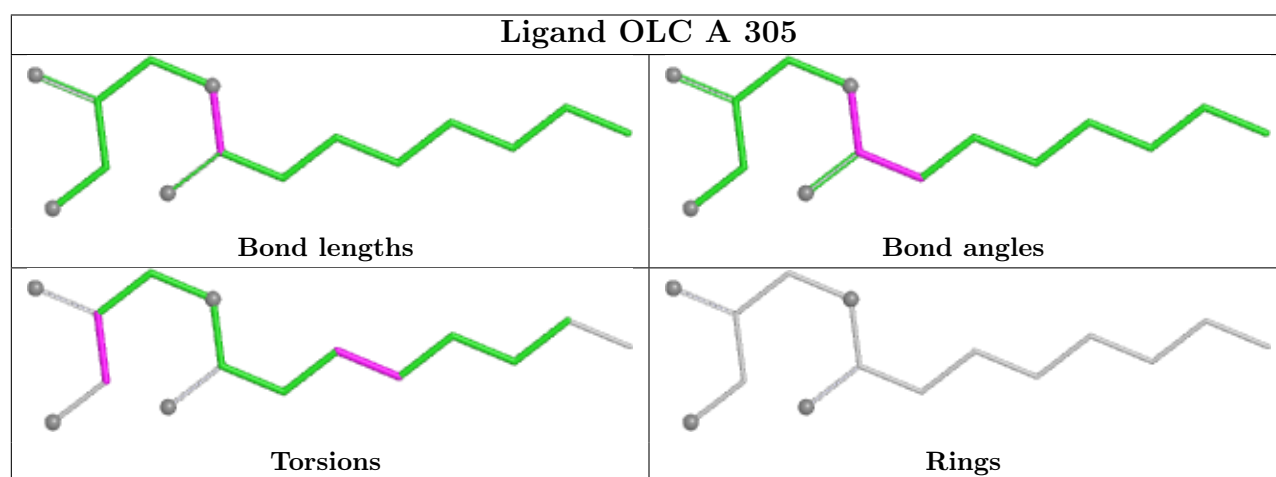
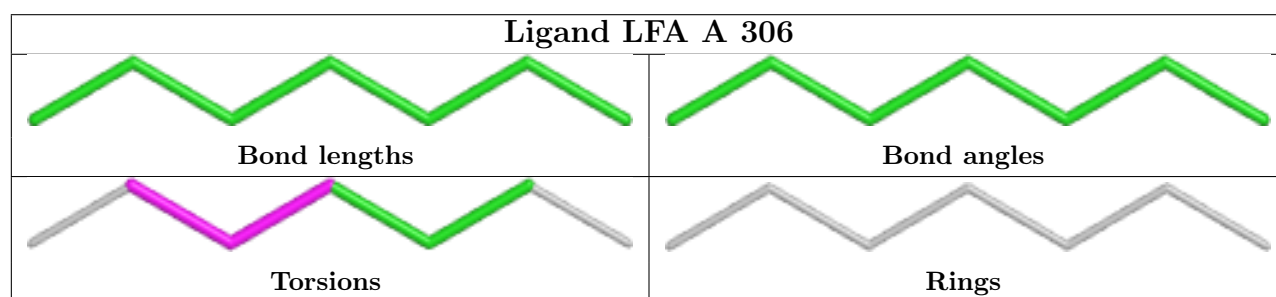
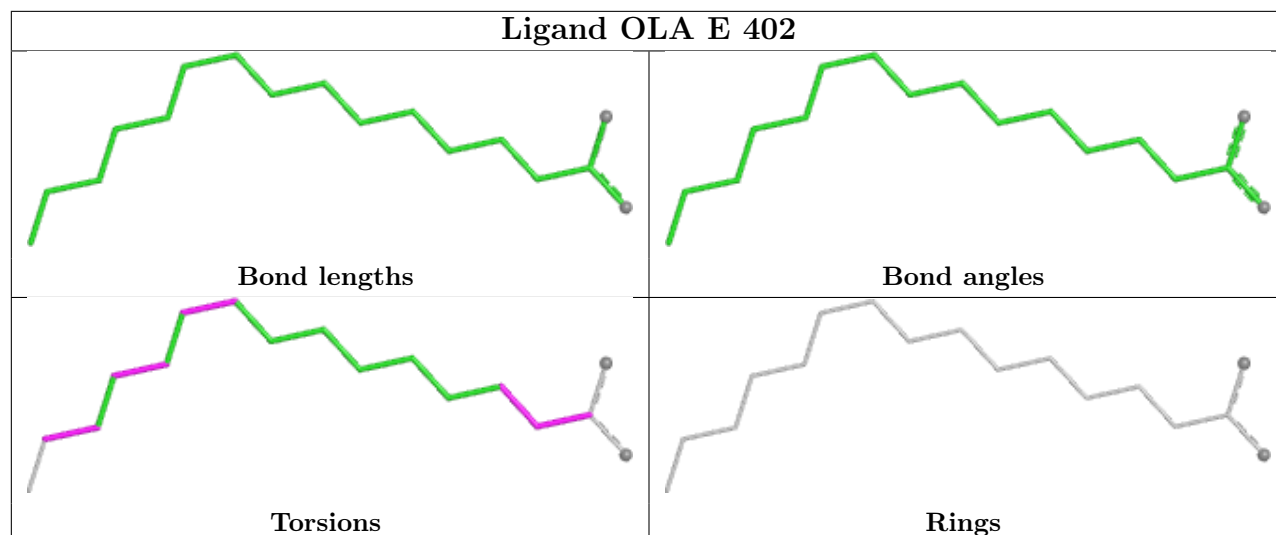


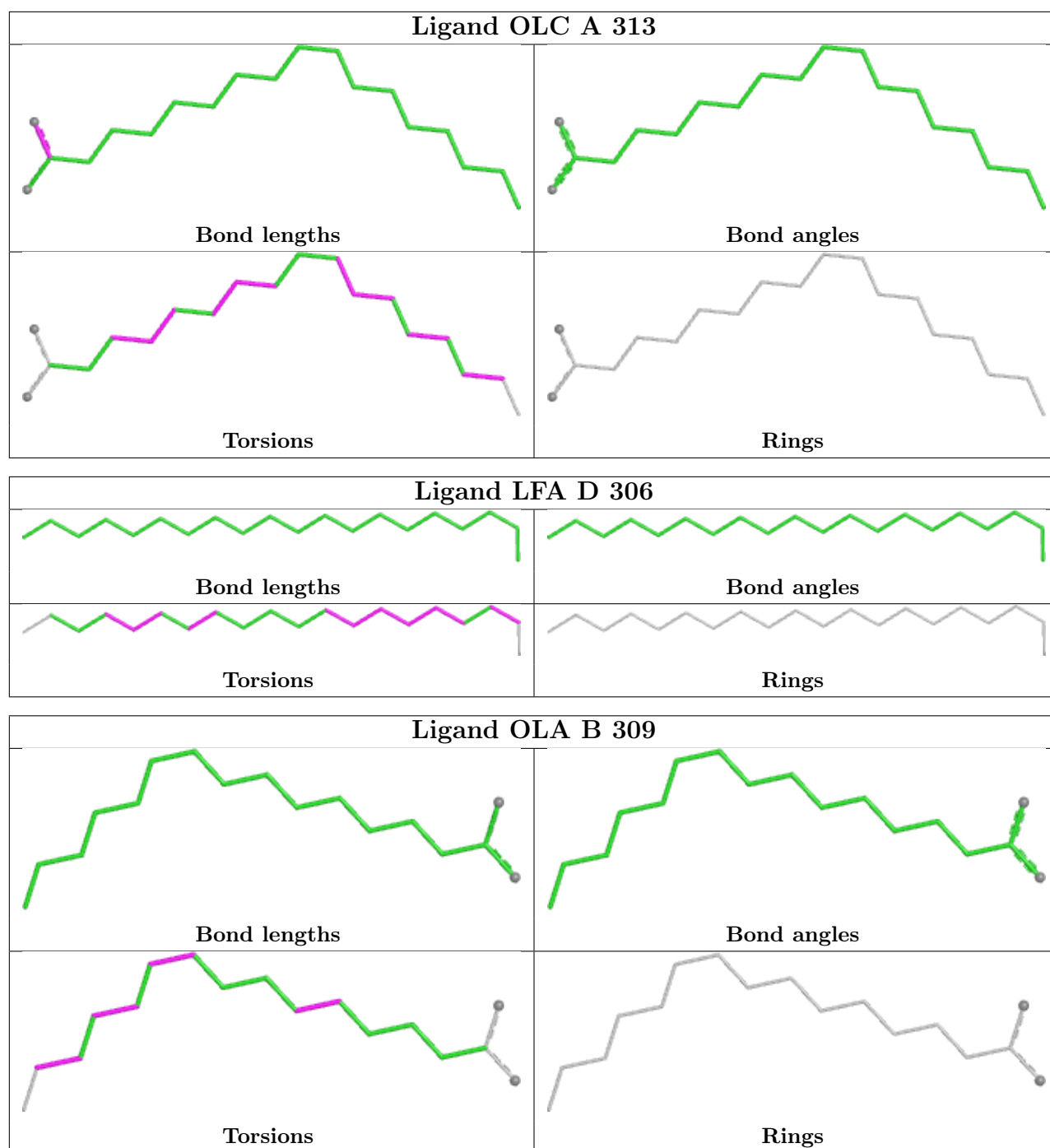


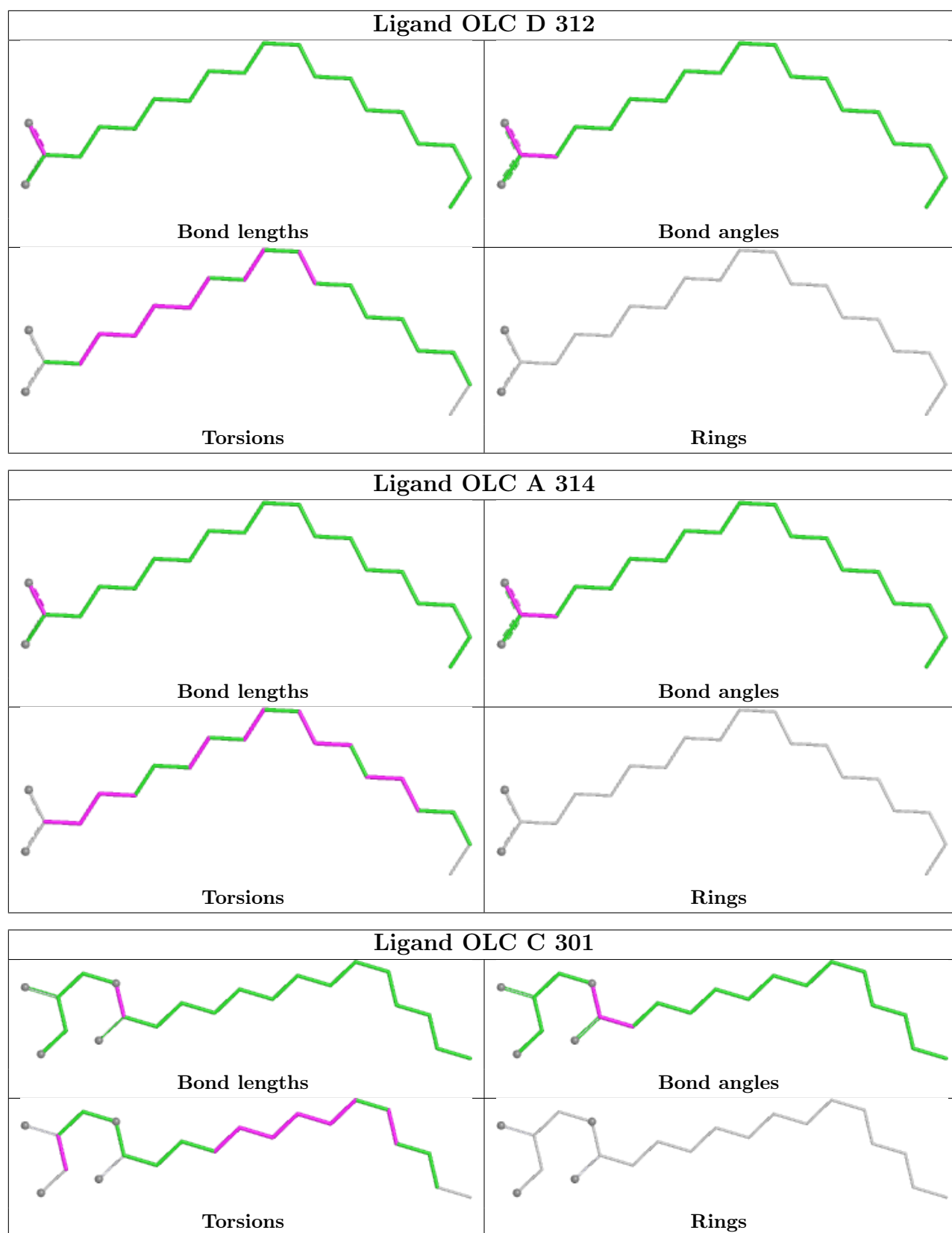


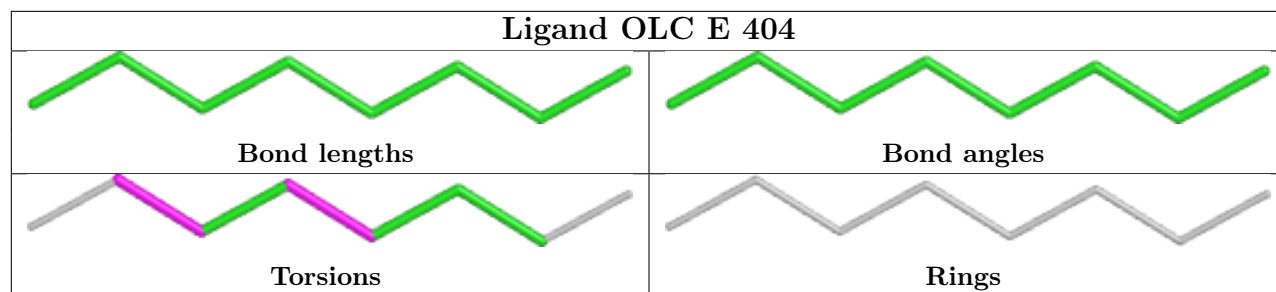
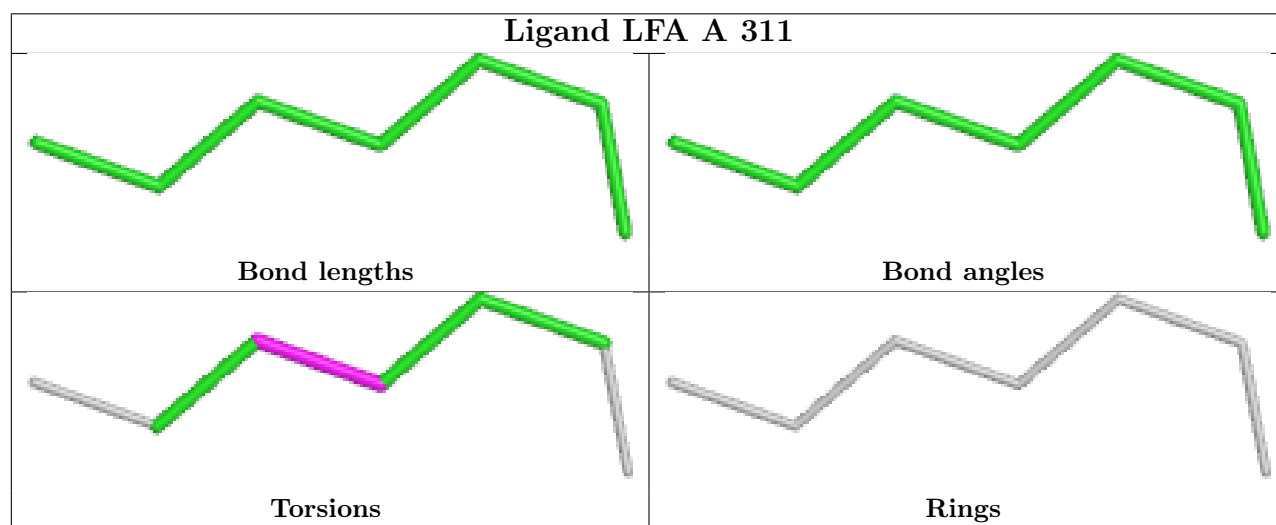
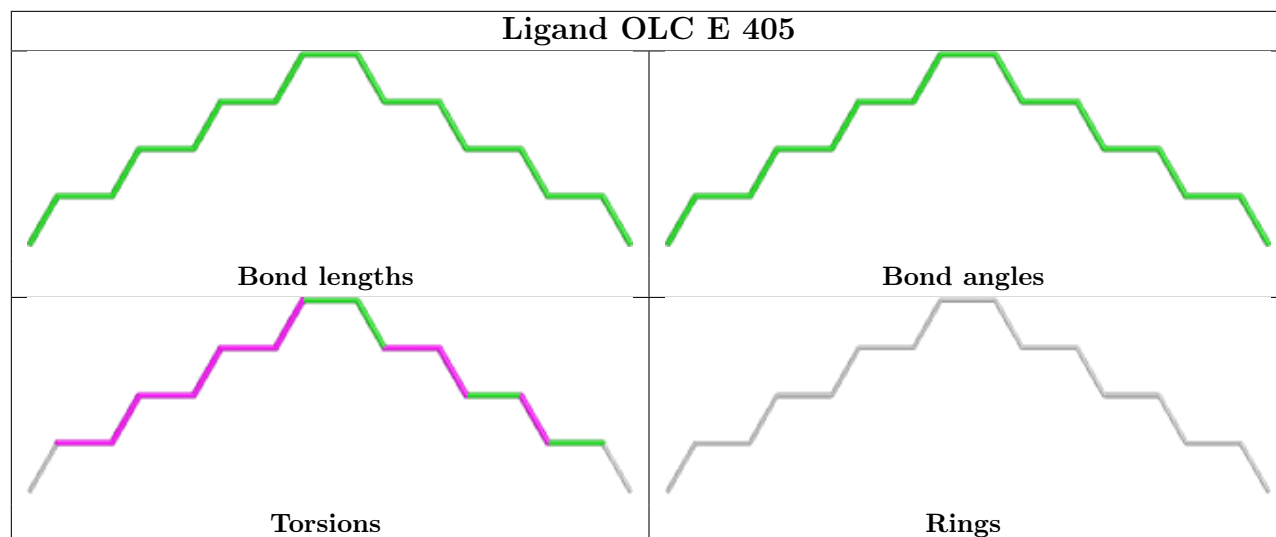


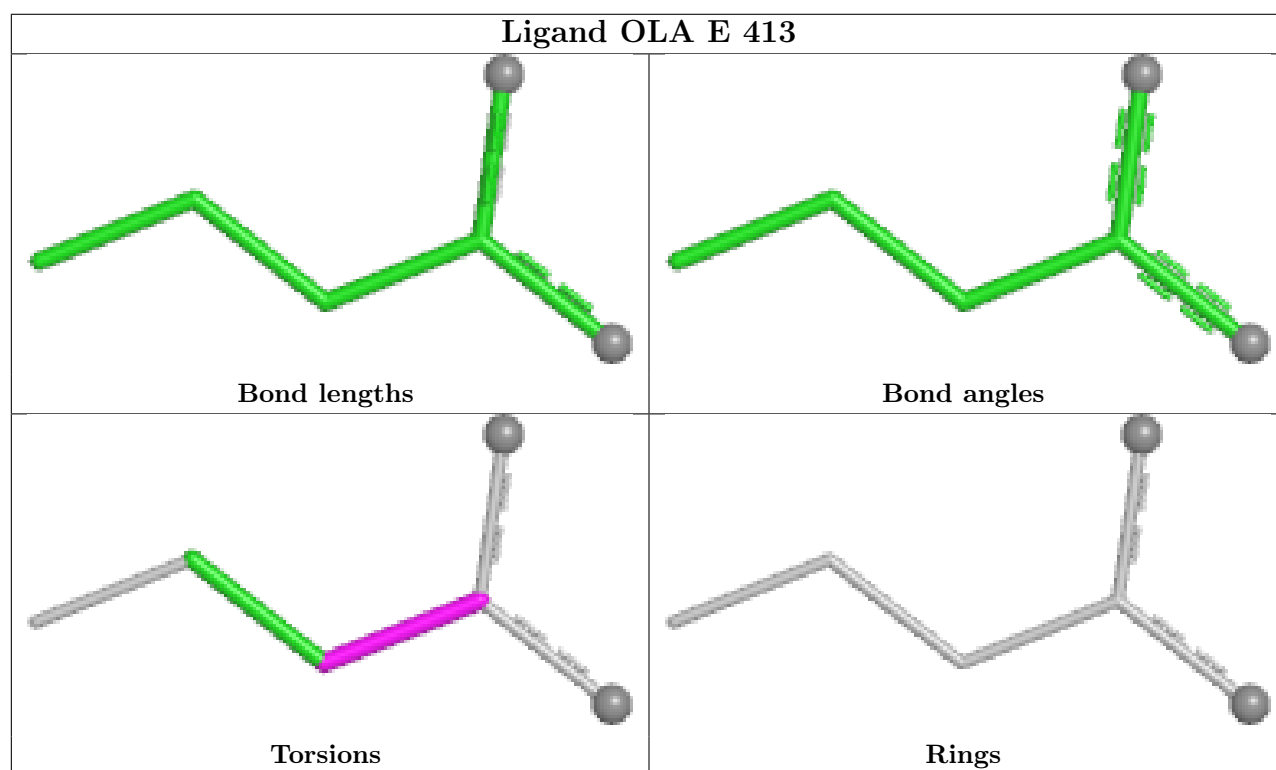
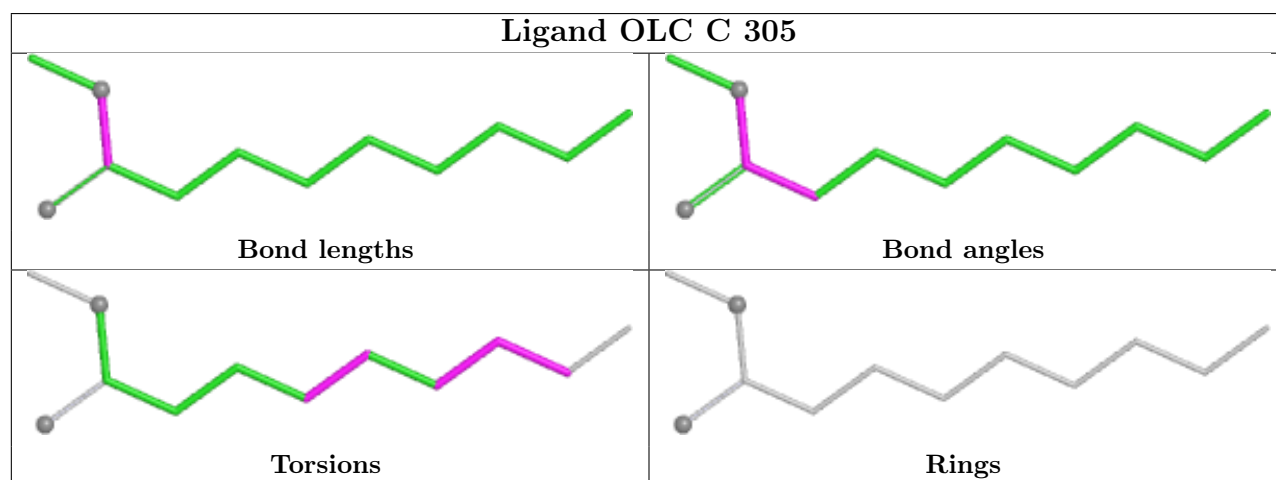
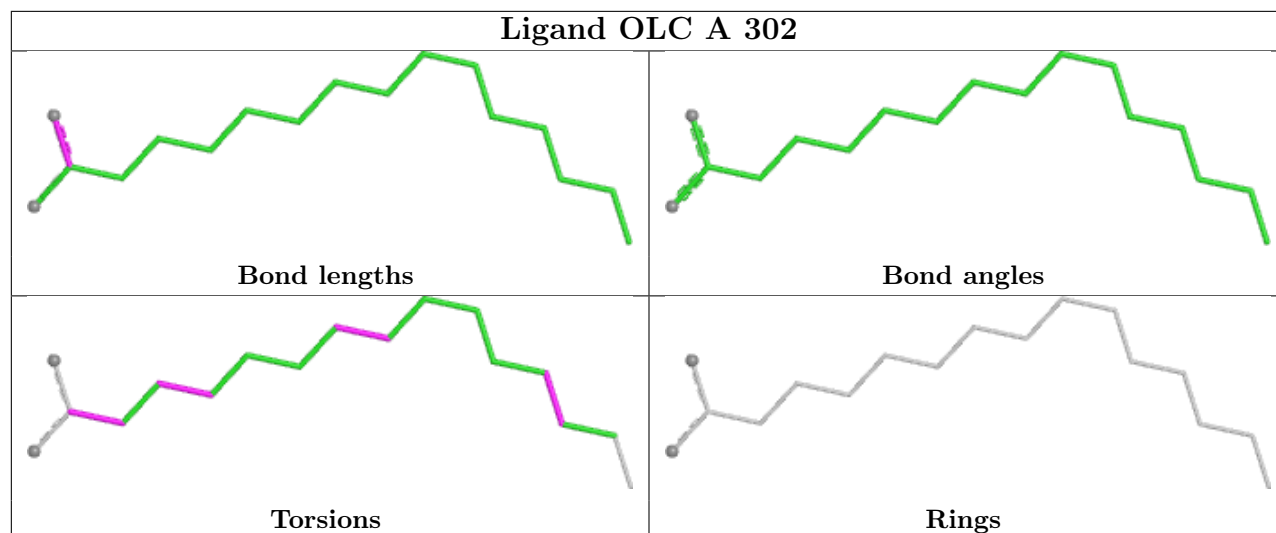


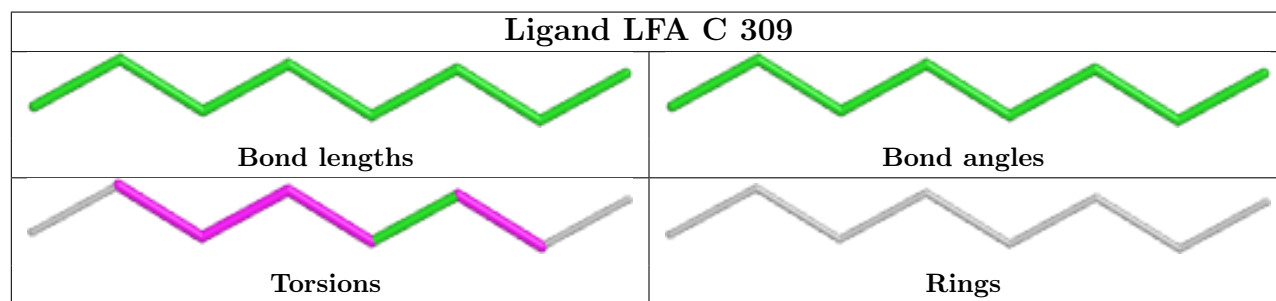
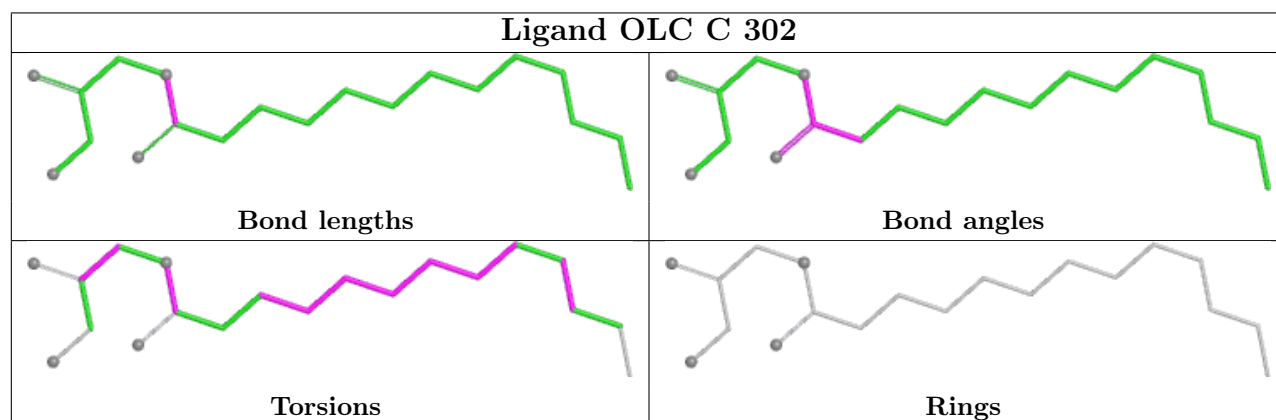
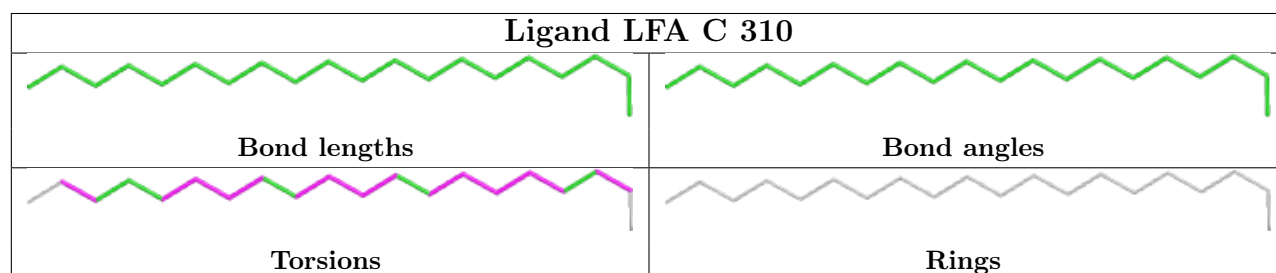
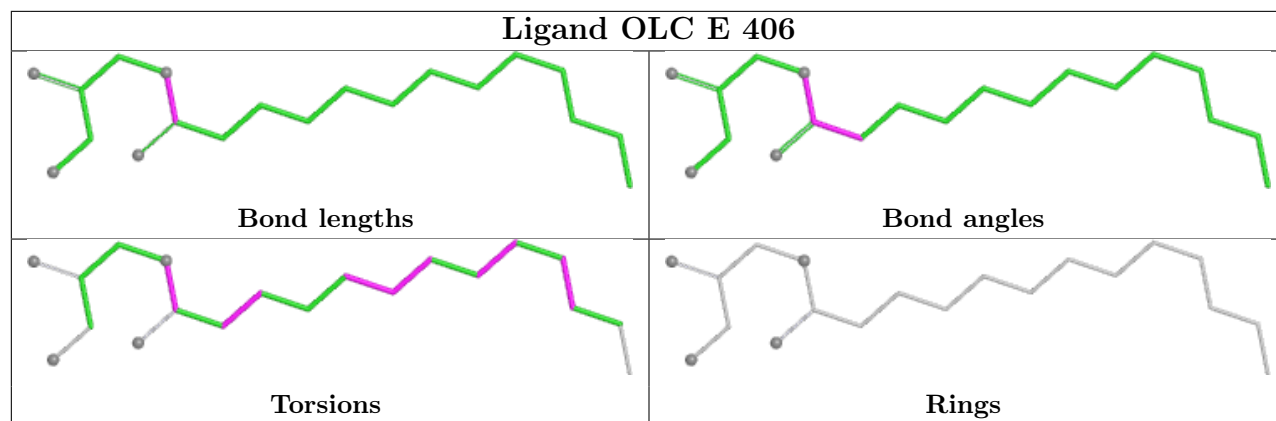


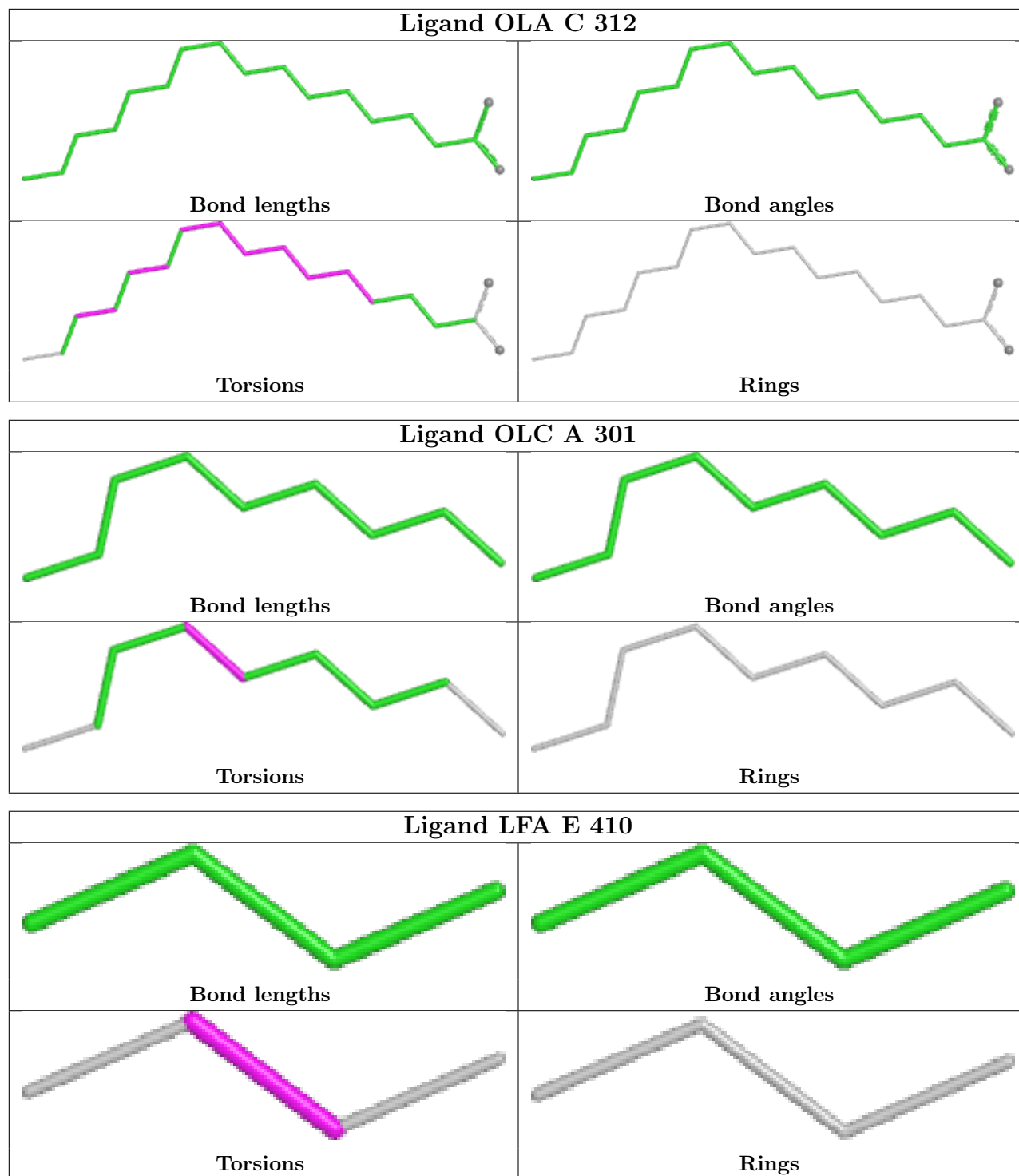


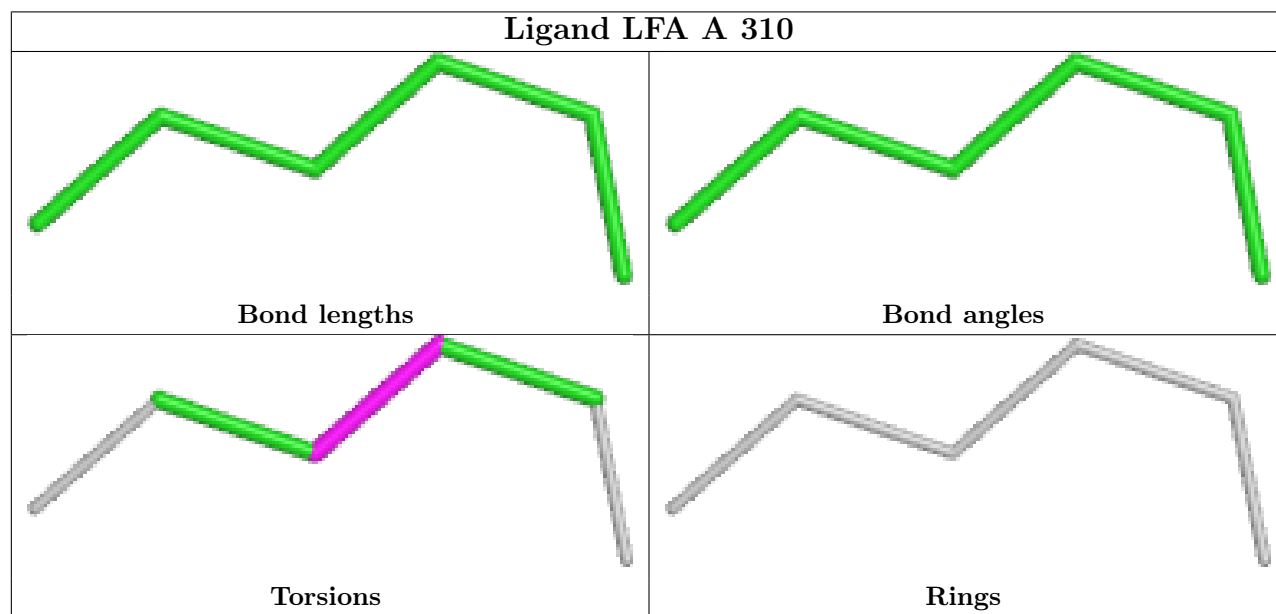
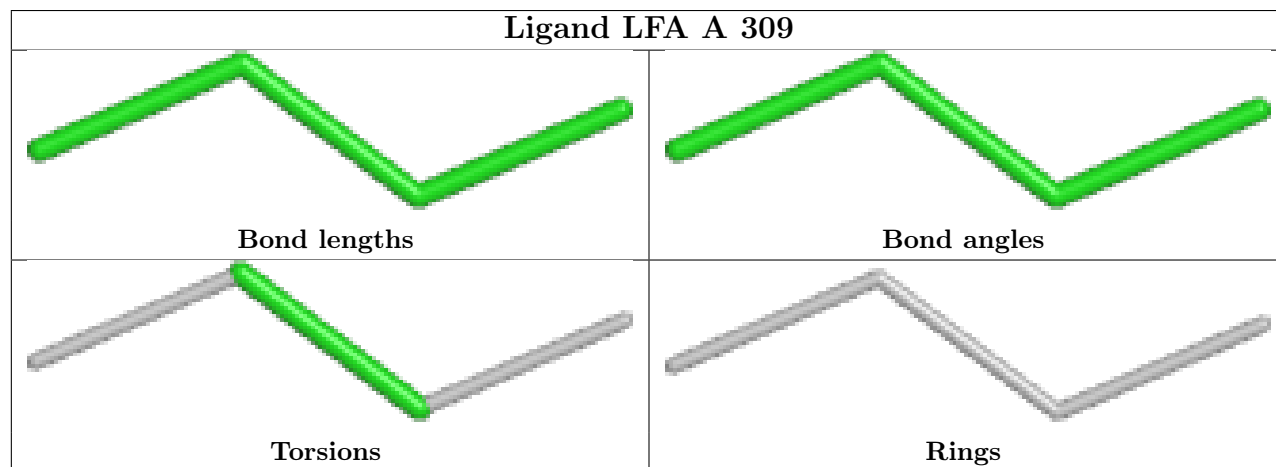
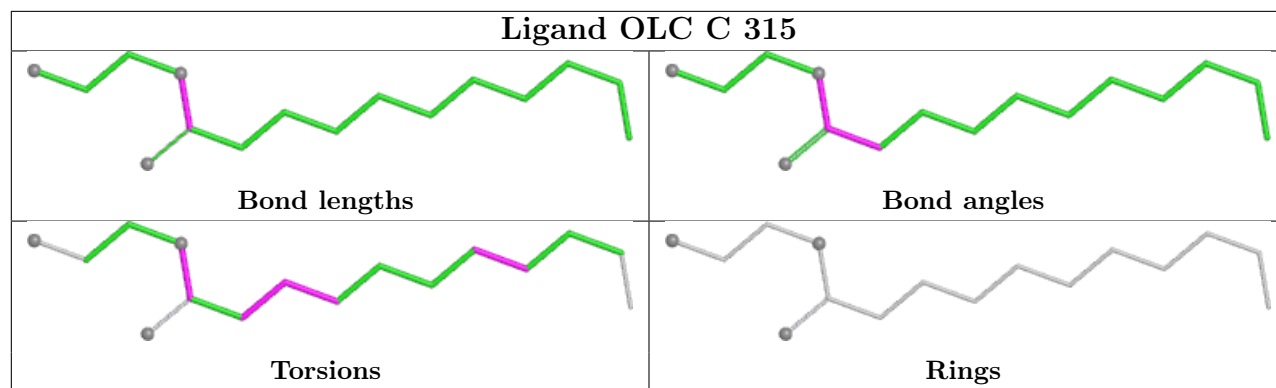


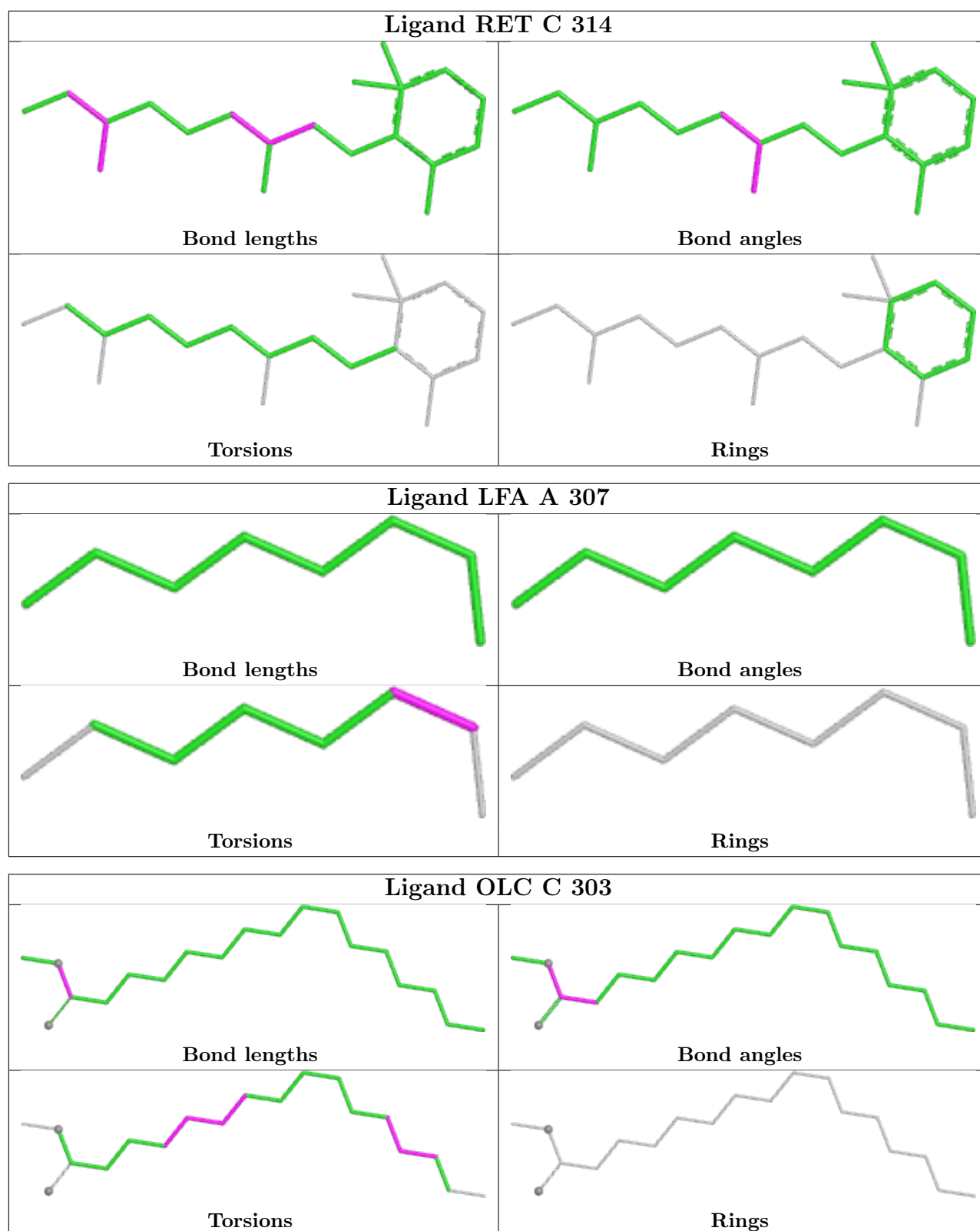












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	269/273 (98%)	0.20	10 (3%) 45 41	23, 59, 87, 125	41 (15%)
1	B	269/273 (98%)	0.12	3 (1%) 78 76	23, 59, 83, 126	41 (15%)
1	C	269/273 (98%)	0.09	4 (1%) 72 70	22, 60, 84, 134	41 (15%)
1	D	269/273 (98%)	0.20	9 (3%) 49 45	24, 62, 98, 125	41 (15%)
1	E	269/273 (98%)	0.23	6 (2%) 62 59	23, 60, 86, 115	41 (15%)
All	All	1345/1365 (98%)	0.17	32 (2%) 59 56	22, 60, 88, 134	205 (15%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	GLN	5.5
1	D	3	GLN	5.2
1	E	3	GLN	5.2
1	A	3	GLN	4.9
1	D	78[A]	GLN	4.7
1	D	106[A]	ASN	4.3
1	D	81[A]	ASN	4.1
1	A	81[A]	ASN	4.0
1	A	78[A]	GLN	3.8
1	B	3	GLN	3.7
1	E	81[A]	ASN	3.7
1	A	230	VAL	3.6
1	A	80[A]	GLN	3.4
1	E	108[A]	TYR	3.2
1	C	4	GLU	3.1
1	A	79[A]	ALA	3.0
1	E	106[A]	ASN	2.9
1	B	55	LYS	2.7
1	D	90	GLU	2.6
1	A	69[A]	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	77[A]	ALA	2.6
1	E	51	LYS	2.5
1	E	80[A]	GLN	2.5
1	A	108[A]	TYR	2.4
1	D	84[A]	SER	2.4
1	D	198	PRO	2.4
1	A	51	LYS	2.2
1	C	158	PHE	2.2
1	D	195	GLY	2.1
1	D	69[A]	VAL	2.0
1	A	231	ASP	2.0
1	C	90	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	LFA	A	309	4/20	0.61	0.45	83,96,103,109	0
2	OLC	D	301	5/25	0.78	0.30	72,77,91,93	0
3	LFA	A	311	7/20	0.79	0.31	85,94,109,111	0
2	OLC	C	304	8/25	0.80	0.27	82,99,105,116	0
3	LFA	E	410	4/20	0.80	0.38	96,102,102,104	0
3	LFA	A	306	7/20	0.81	0.34	90,99,135,148	0
2	OLC	D	302	18/25	0.83	0.18	105,124,138,142	0
2	OLC	B	301	16/25	0.84	0.21	86,114,146,180	0
2	OLC	C	305	12/25	0.84	0.18	96,113,138,142	0
2	OLC	D	303	5/25	0.85	0.32	74,81,104,106	0
3	LFA	C	310	20/20	0.85	0.23	94,118,154,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	E	407	15/25	0.85	0.16	87,106,125,128	0
2	OLC	B	303	12/25	0.86	0.17	85,95,110,120	0
3	LFA	D	306	20/20	0.86	0.28	108,127,151,154	0
3	LFA	A	308	8/20	0.86	0.28	82,109,119,127	0
6	GOL	C	313	4/6	0.86	0.20	83,101,103,106	0
2	OLC	E	405	16/25	0.87	0.26	82,120,134,147	0
2	OLC	C	307	16/25	0.87	0.16	93,117,134,146	0
2	OLC	B	302	5/25	0.87	0.38	66,77,80,81	0
2	OLC	A	303	7/25	0.87	0.25	85,105,109,109	0
2	OLC	C	306	17/25	0.87	0.18	72,118,149,161	0
7	OLA	B	310	18/20	0.87	0.22	65,110,130,143	0
7	OLA	E	403	15/20	0.87	0.19	102,141,235,249	0
3	LFA	A	307	8/20	0.88	0.22	80,104,118,120	0
6	GOL	A	317	4/6	0.88	0.16	100,103,110,113	0
6	GOL	B	311	4/6	0.88	0.22	101,103,108,129	0
2	OLC	A	304	13/25	0.88	0.16	96,113,120,121	0
2	OLC	A	301	9/25	0.88	0.20	67,90,105,107	0
7	OLA	C	312	18/20	0.88	0.18	85,101,121,122	0
7	OLA	E	401	20/20	0.88	0.21	87,122,136,141	0
3	LFA	D	307	8/20	0.88	0.31	103,115,137,143	0
3	LFA	C	309	8/20	0.89	0.32	92,121,129,134	0
7	OLA	E	402	17/20	0.89	0.19	87,107,133,140	0
2	OLC	E	406	20/25	0.89	0.17	96,119,140,142	0
2	OLC	D	304	14/25	0.90	0.14	81,99,105,118	0
3	LFA	D	305	20/20	0.90	0.23	91,116,137,141	0
7	OLA	B	309	17/20	0.90	0.19	78,102,127,129	0
3	LFA	B	304	8/20	0.90	0.24	87,102,111,113	0
3	LFA	B	305	10/20	0.90	0.25	77,131,150,153	0
3	LFA	E	409	14/20	0.90	0.22	103,130,147,154	0
3	LFA	B	306	7/20	0.90	0.34	102,115,138,139	0
2	OLC	C	302	20/25	0.90	0.19	94,109,122,122	0
7	OLA	E	413	6/20	0.90	0.17	118,121,129,131	0
3	LFA	E	408	8/20	0.91	0.25	95,110,131,144	0
2	OLC	A	316	18/25	0.91	0.22	71,121,150,155	0
2	OLC	A	305	15/25	0.91	0.12	81,109,120,121	0
3	LFA	E	411	5/20	0.91	0.24	94,94,118,120	0
3	LFA	A	310	6/20	0.91	0.21	73,94,107,114	0
2	OLC	A	314	20/25	0.91	0.25	83,121,153,157	0
3	LFA	D	309	7/20	0.91	0.23	80,104,121,124	0
3	LFA	C	308	4/20	0.92	0.24	93,94,95,97	0
2	OLC	C	315	16/25	0.92	0.21	88,110,125,128	0
2	OLC	E	404	8/25	0.92	0.20	85,121,128,128	0

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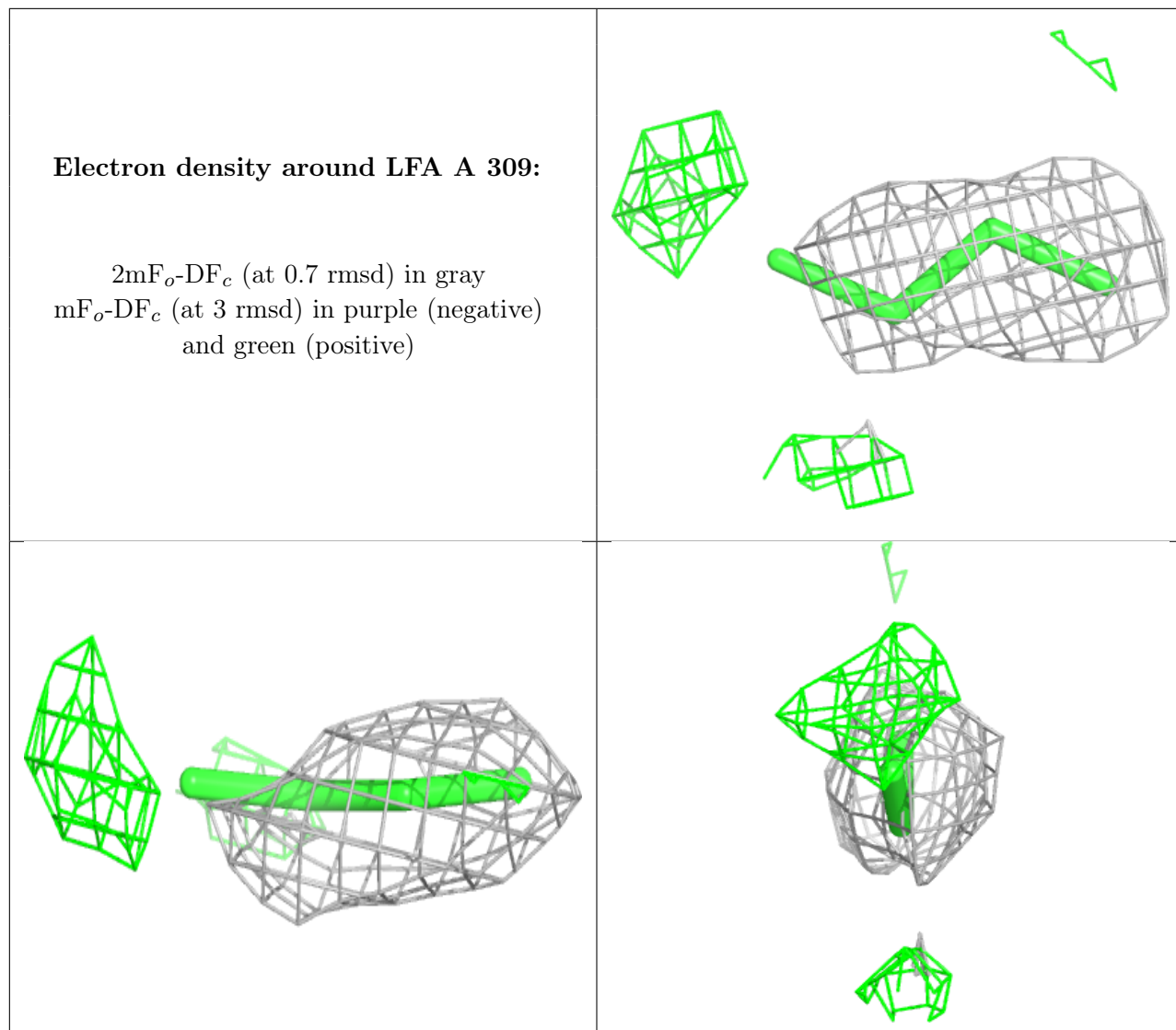
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	D	312	20/25	0.93	0.19	79,104,137,154	0
7	OLA	D	313	7/20	0.93	0.15	99,106,122,128	0
5	RET	E	414	20/21	0.94	0.14	41,65,80,84	0
3	LFA	D	308	17/20	0.94	0.19	66,79,94,97	0
2	OLC	C	303	19/25	0.94	0.16	70,81,99,103	0
5	RET	A	315	20/21	0.94	0.13	48,65,83,87	0
5	RET	B	308	20/21	0.94	0.14	52,68,78,82	0
5	RET	D	311	20/21	0.94	0.14	59,74,84,86	0
2	OLC	A	313	19/25	0.95	0.14	66,74,93,93	0
2	OLC	C	301	21/25	0.96	0.11	60,81,92,107	0
2	OLC	A	302	17/25	0.96	0.13	67,75,88,89	0
5	RET	C	314	20/21	0.96	0.11	53,67,79,84	0
4	NA	A	318	1/1	0.96	0.10	52,52,52,52	1
4	NA	D	310	1/1	0.97	0.13	46,46,46,46	0
4	NA	E	415	1/1	0.97	0.06	56,56,56,56	1
4	NA	C	316	1/1	0.97	0.07	71,71,71,71	1
4	NA	D	314	1/1	0.98	0.06	48,48,48,48	1
4	NA	C	311	1/1	0.98	0.14	49,49,49,49	0
4	NA	B	312	1/1	0.99	0.05	81,81,81,81	1
4	NA	A	312	1/1	0.99	0.06	52,52,52,52	0
4	NA	E	412	1/1	0.99	0.06	36,36,36,36	0
4	NA	B	307	1/1	0.99	0.05	55,55,55,55	0

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

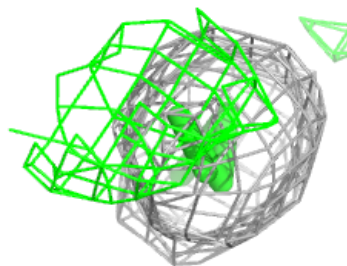
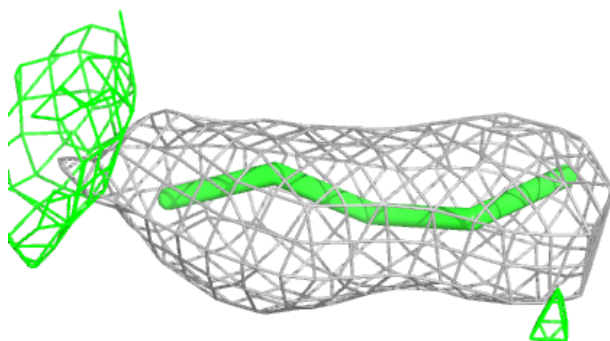
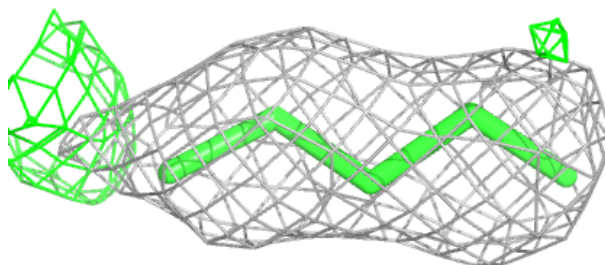
Electron density around LFA A 309:

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

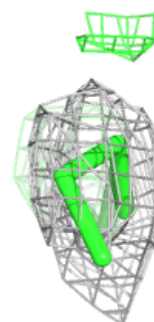
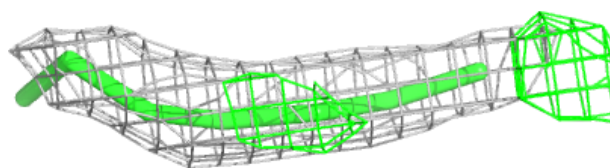
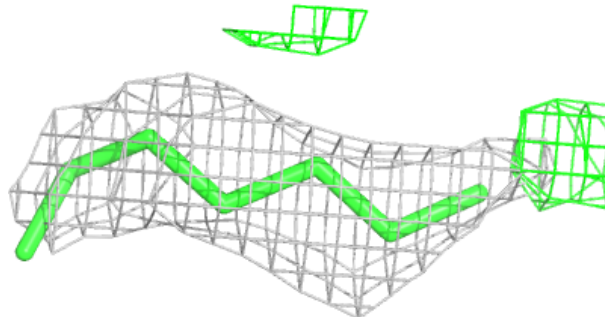


Electron density around OLC D 301:

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

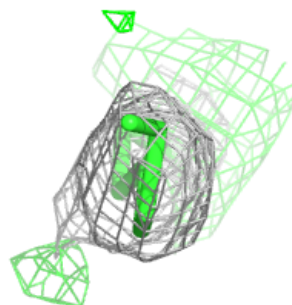
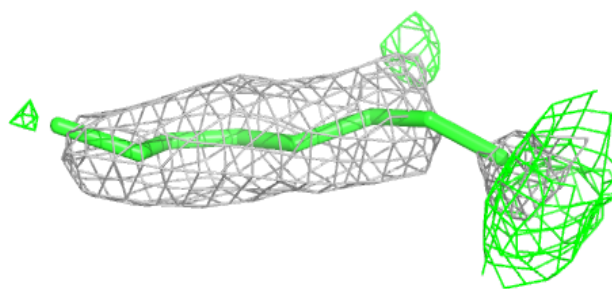
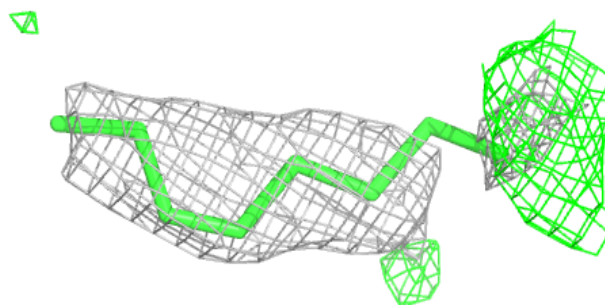
**Electron density around LFA A 311:**

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

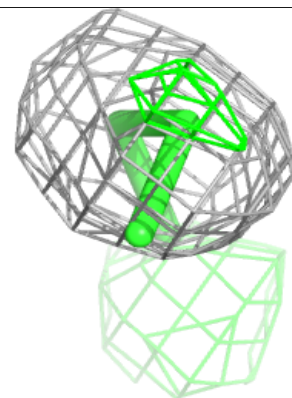
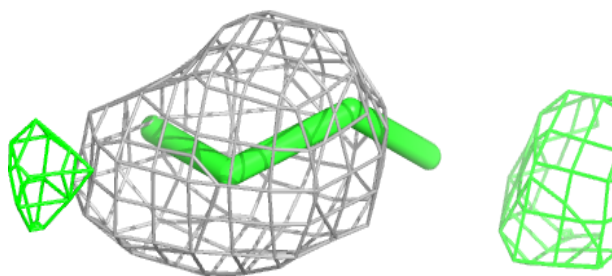
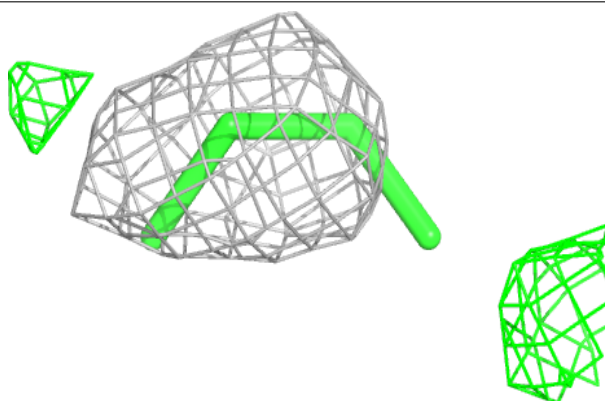


Electron density around OLC C 304:

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

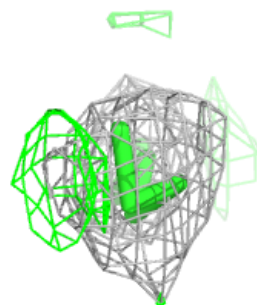
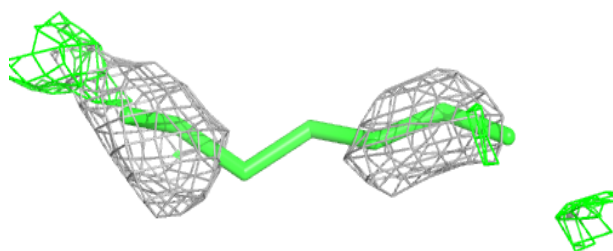
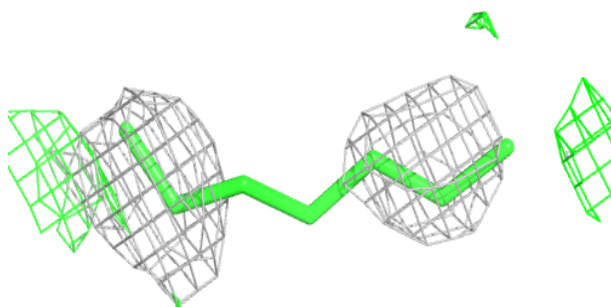
**Electron density around LFA E 410:**

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

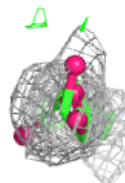
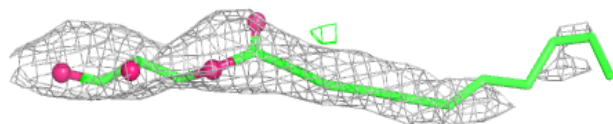
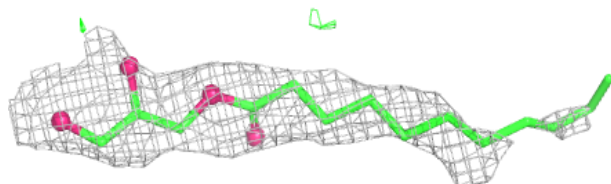


Electron density around LFA A 306:

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

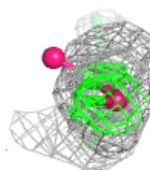
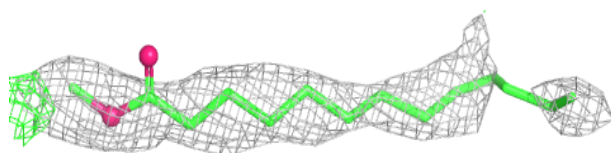
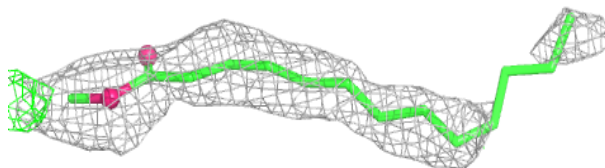
**Electron density around OLC D 302:**

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

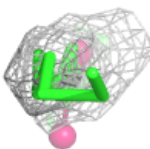
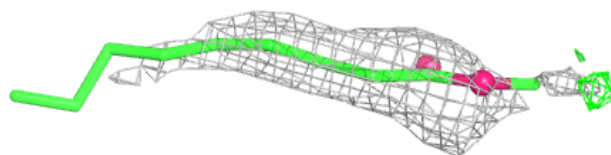
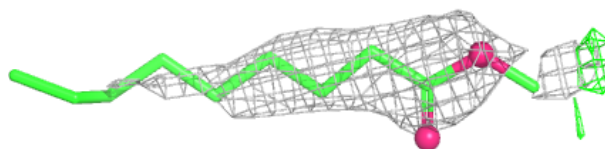


Electron density around OLC B 301:

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

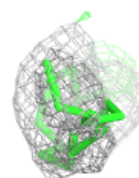
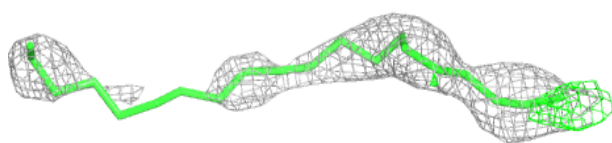
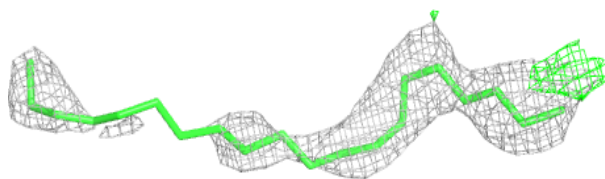
**Electron density around OLC C 305:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

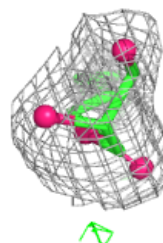
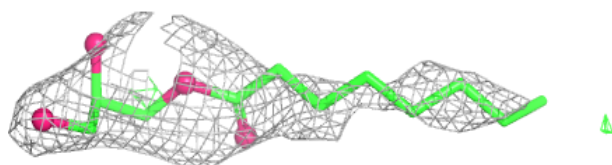
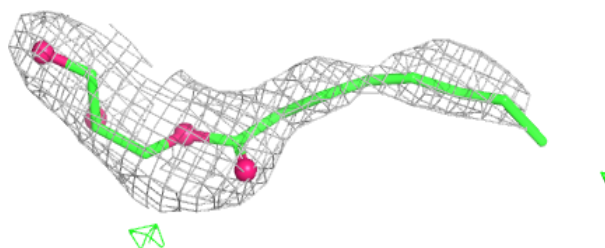


Electron density around LFA C 310:

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

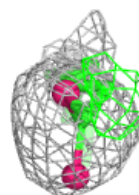
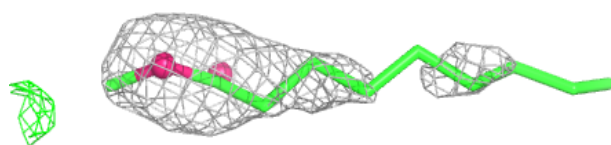
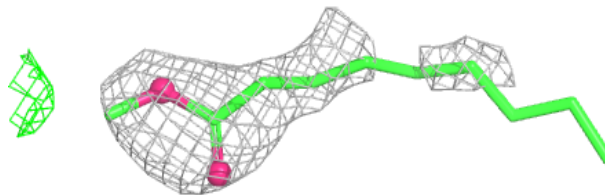
**Electron density around OLC E 407:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

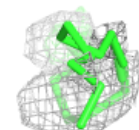
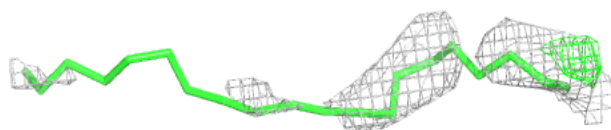
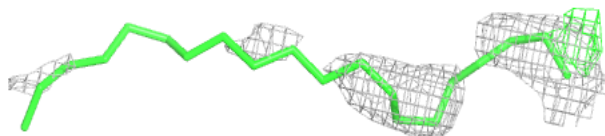


Electron density around OLC B 303:

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

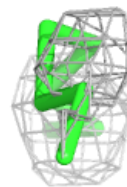
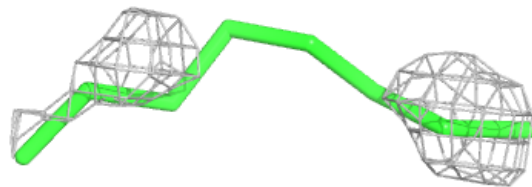
**Electron density around LFA D 306:**

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

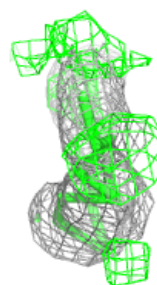
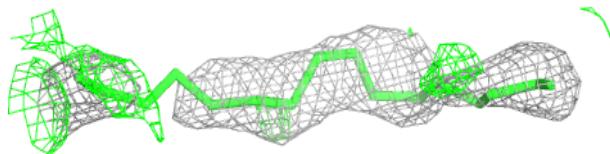
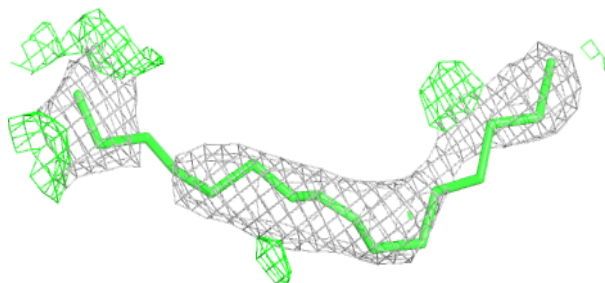


Electron density around LFA A 308:

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

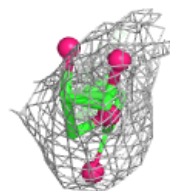
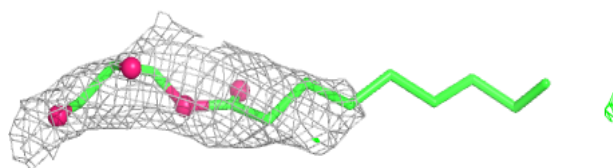
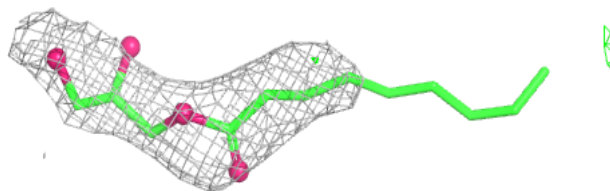
**Electron density around OLC E 405:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

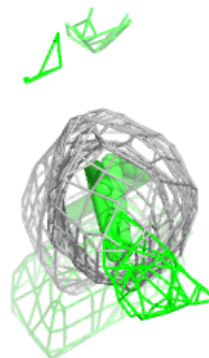
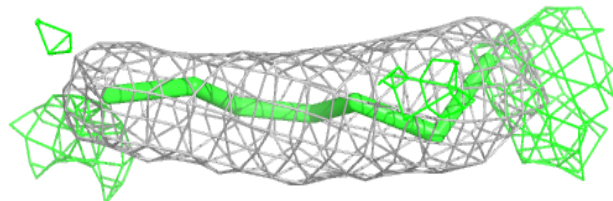
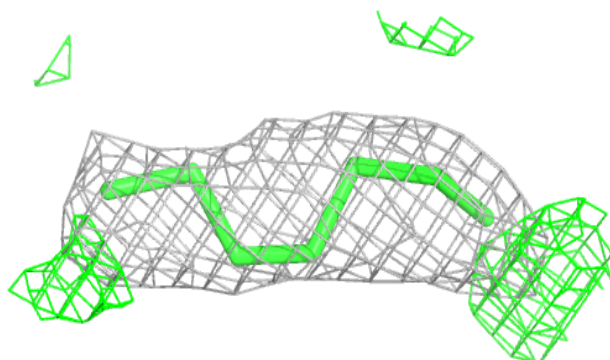


Electron density around OLC C 307:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

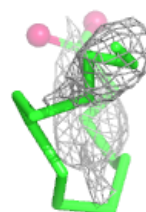
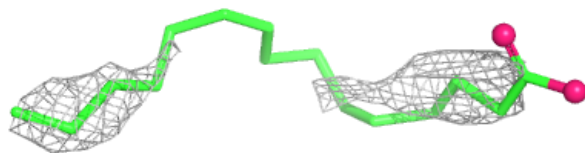
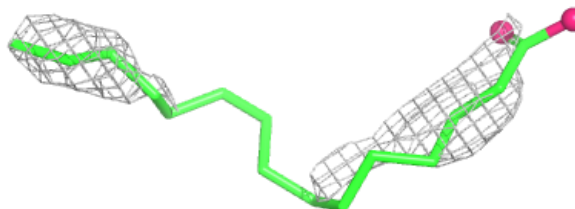
**Electron density around OLC A 303:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

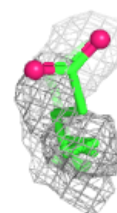
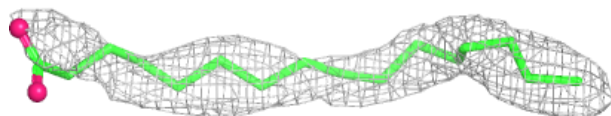
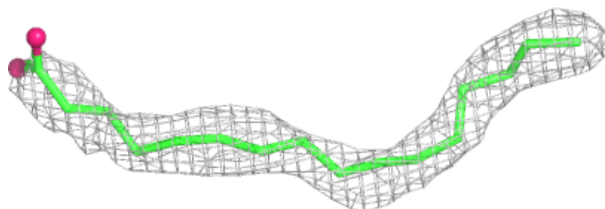


Electron density around OLC C 306:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

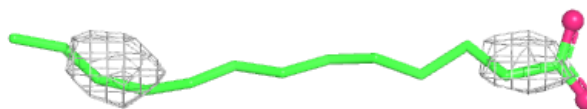
**Electron density around OLA B 310:**

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

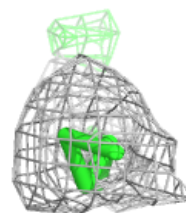
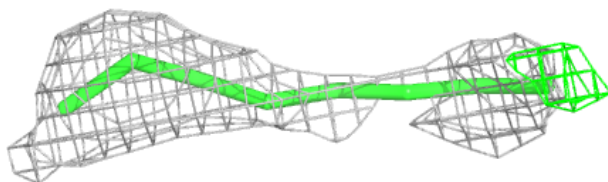
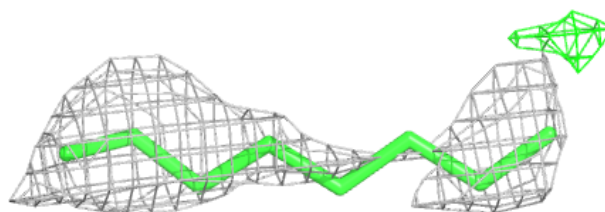


Electron density around OLA E 403:

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

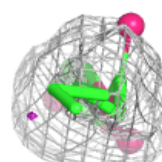
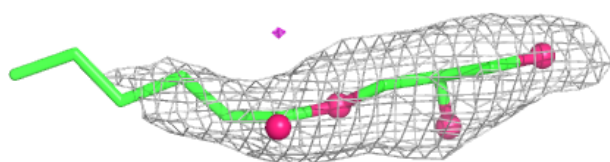
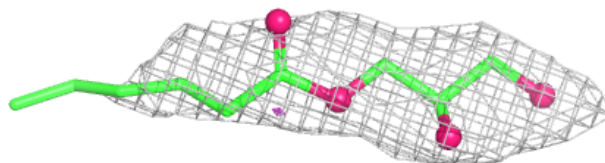
**Electron density around LFA A 307:**

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

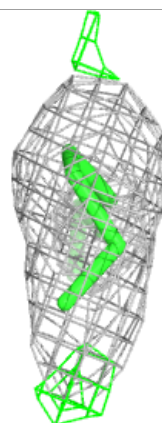
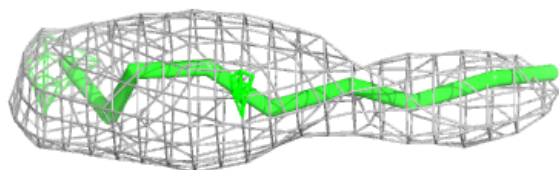
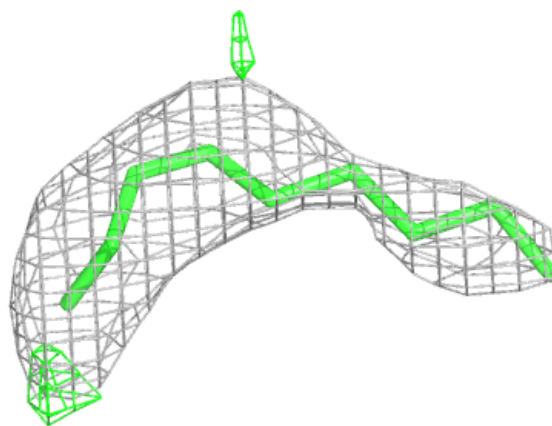


Electron density around OLC A 304:

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

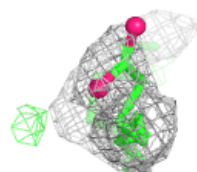
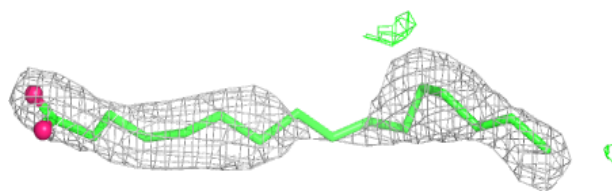
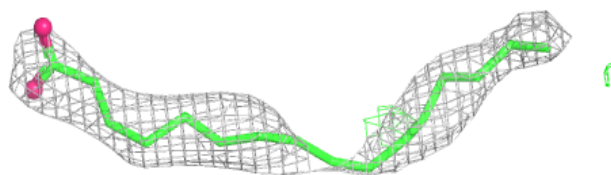
**Electron density around OLC A 301:**

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

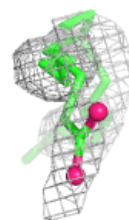
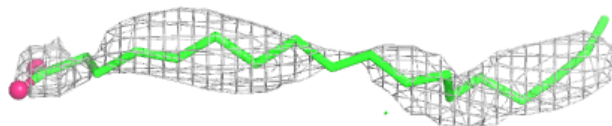
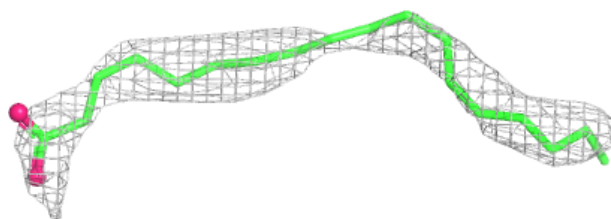


Electron density around OLA C 312:

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

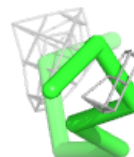
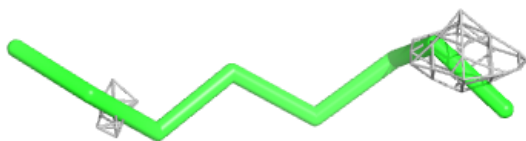
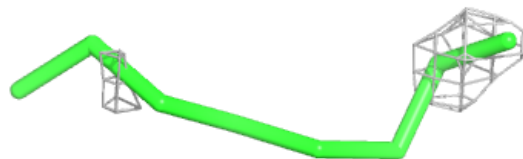
**Electron density around OLA E 401:**

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

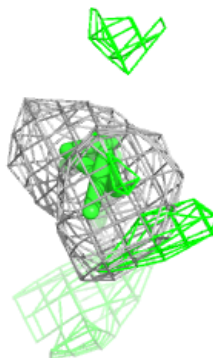
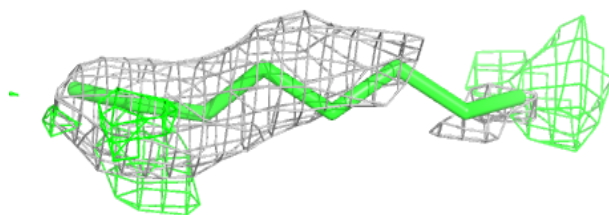
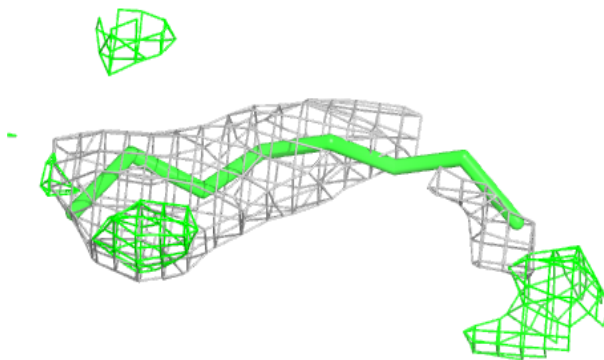


Electron density around LFA D 307:

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

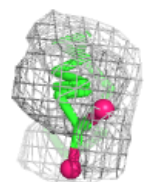
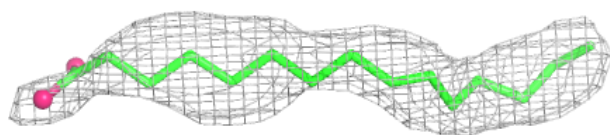
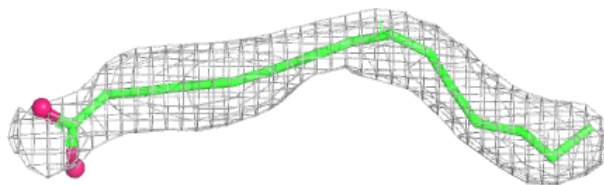
**Electron density around LFA C 309:**

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

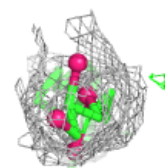
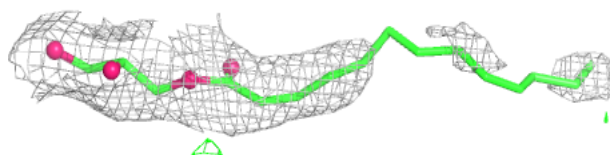
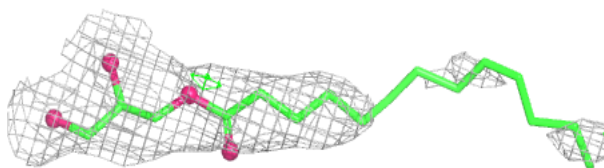


Electron density around OLA E 402:

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

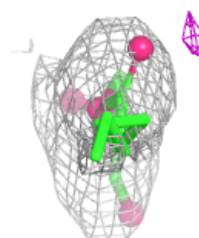
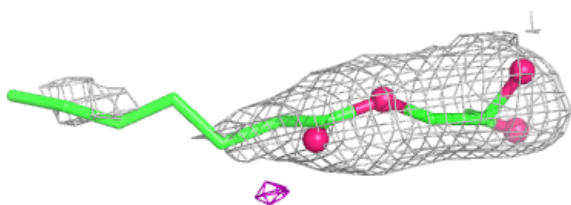
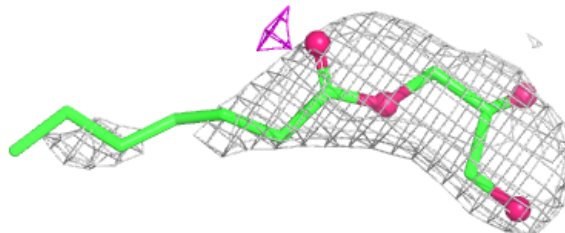
**Electron density around OLC E 406:**

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

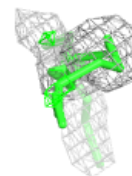
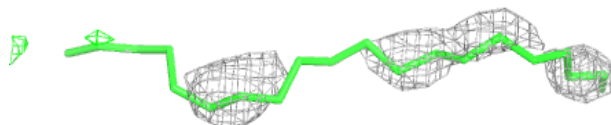
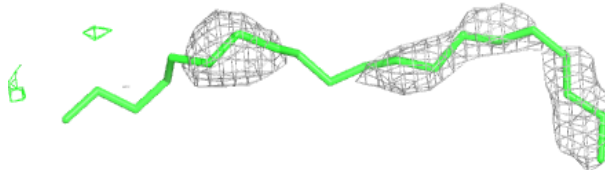


Electron density around OLC D 304:

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

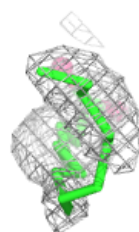
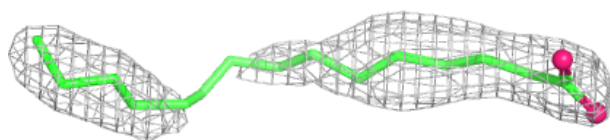
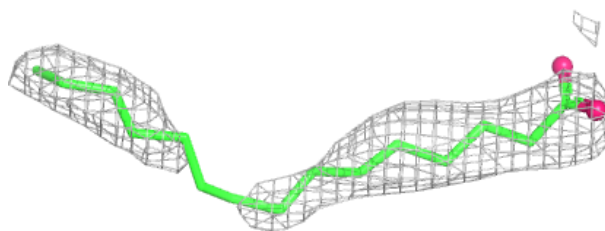
**Electron density around LFA D 305:**

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

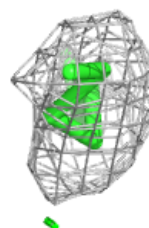
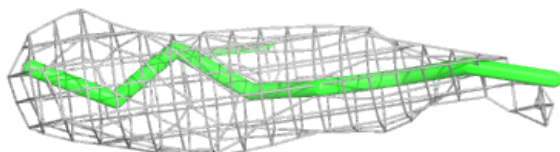
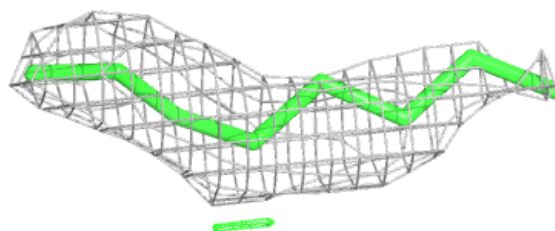


Electron density around OLA B 309:

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

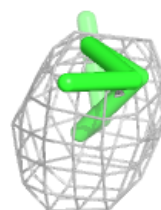
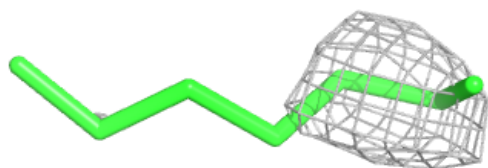
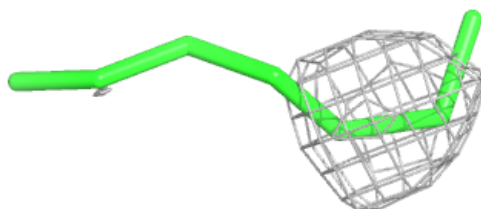
**Electron density around LFA B 304:**

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

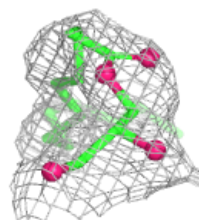
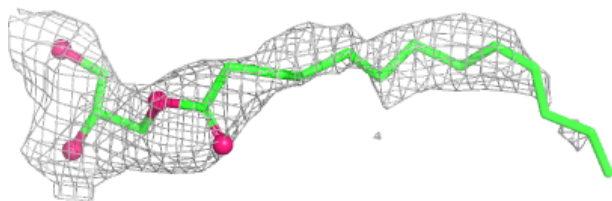


Electron density around LFA B 306:

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

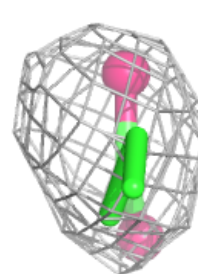
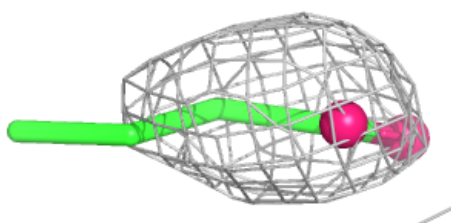
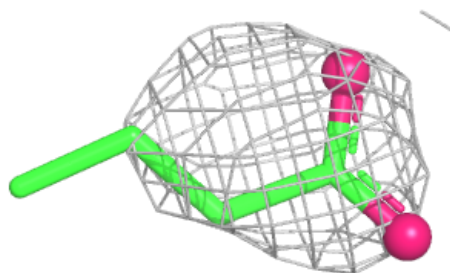
**Electron density around OLC C 302:**

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

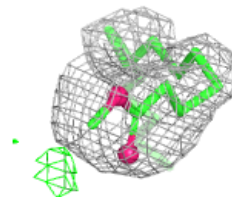
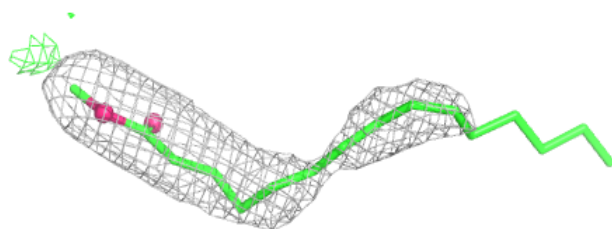
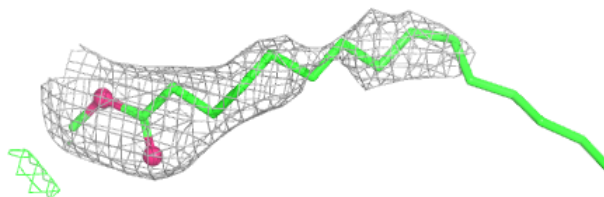


Electron density around OLA E 413:

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

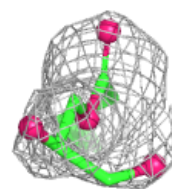
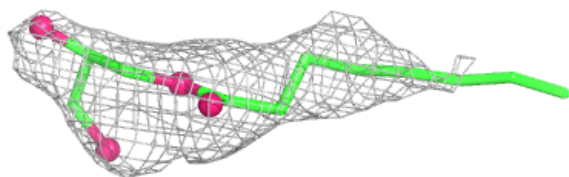
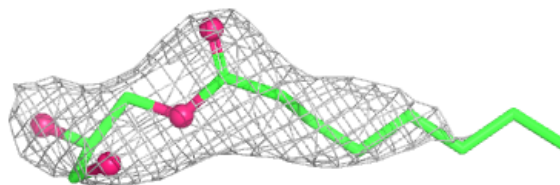
**Electron density around OLC A 316:**

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

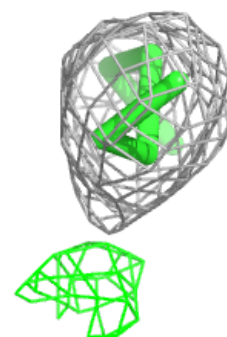
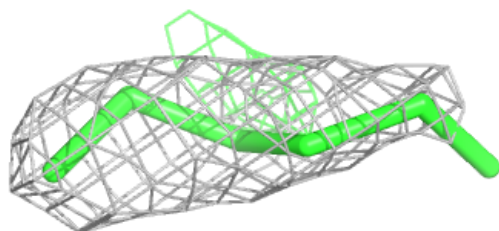
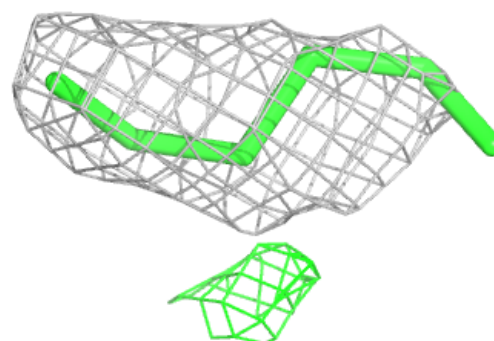


Electron density around OLC A 305:

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

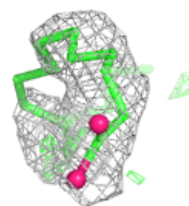
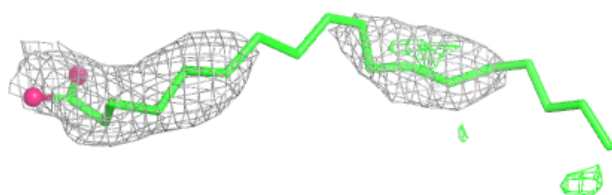
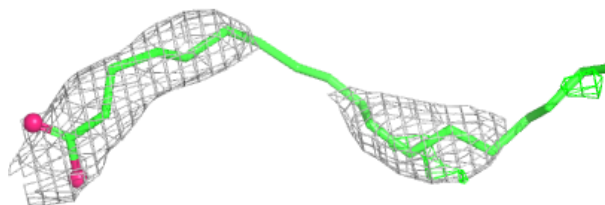
**Electron density around LFA A 310:**

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

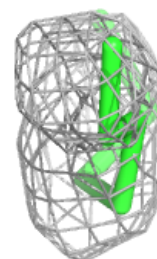
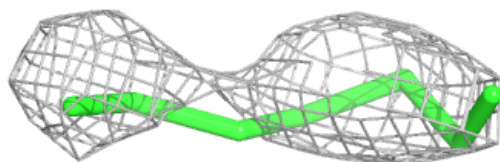


Electron density around OLC A 314:

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

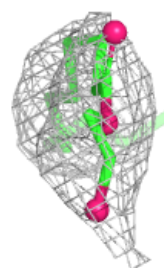
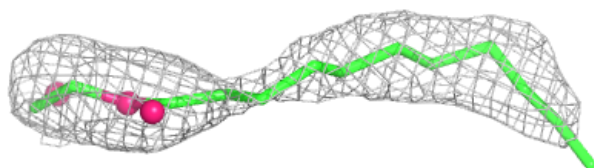
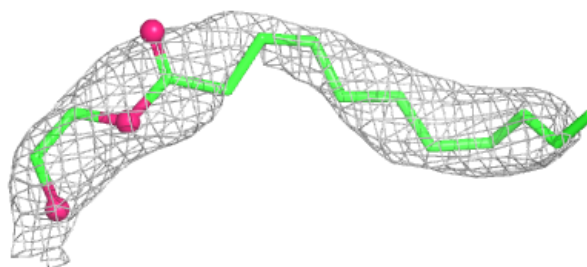
**Electron density around LFA D 309:**

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

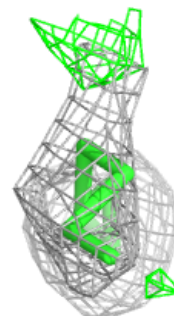
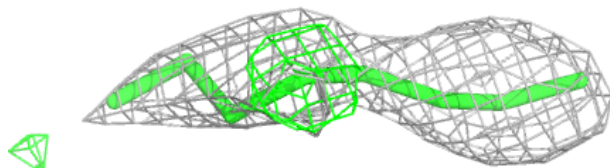
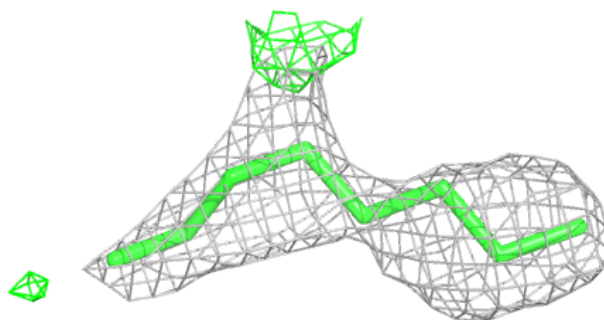


Electron density around OLC C 315:

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

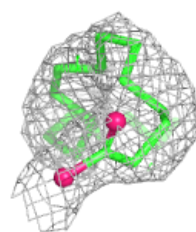
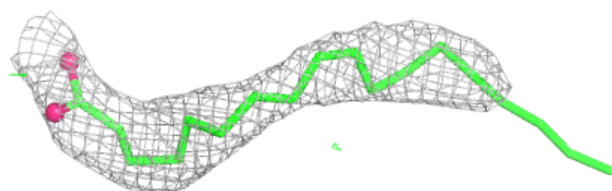
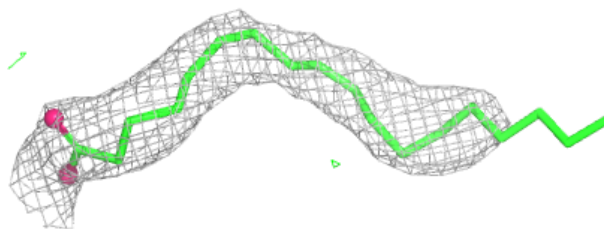
**Electron density around OLC E 404:**

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

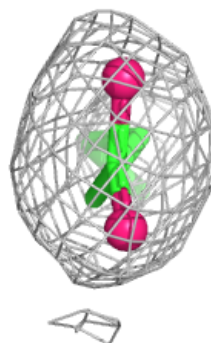
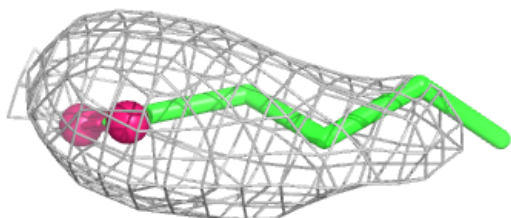
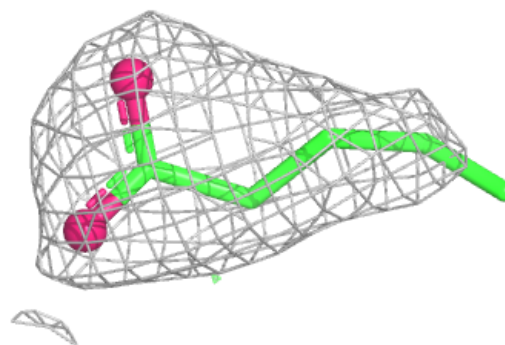


Electron density around OLC D 312:

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

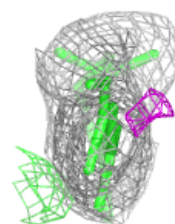
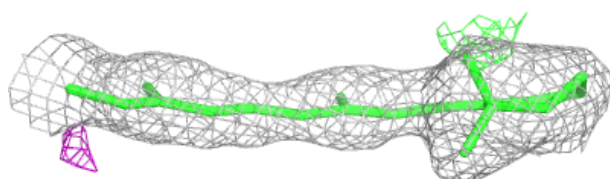
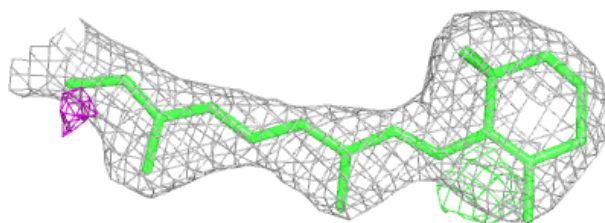
**Electron density around OLA D 313:**

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

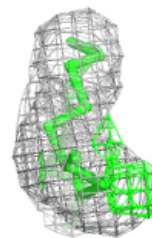
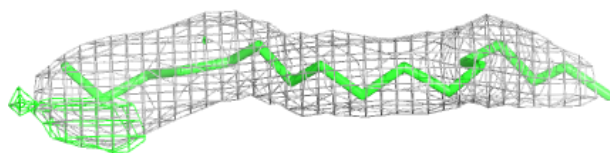
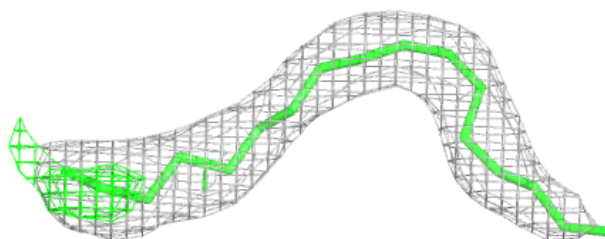


Electron density around RET E 414:

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

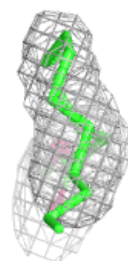
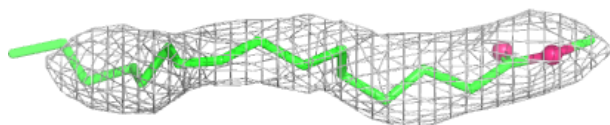
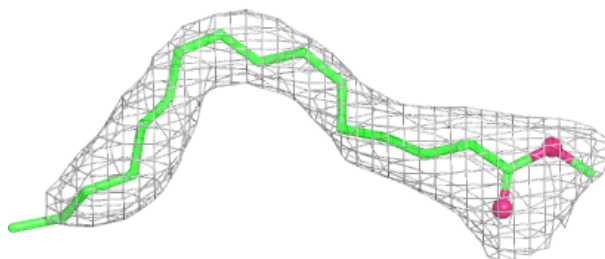
**Electron density around LFA D 308:**

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

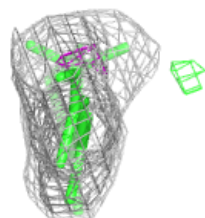
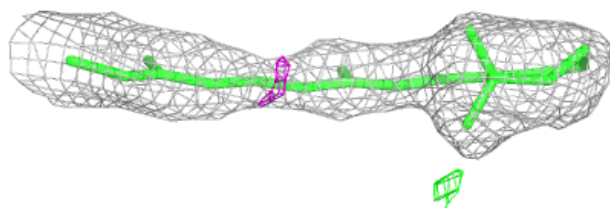
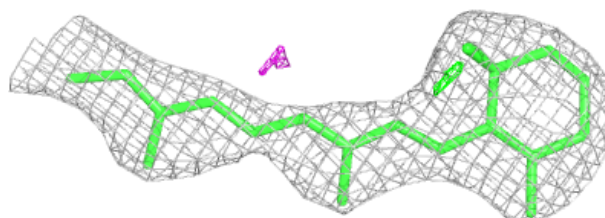


Electron density around OLC C 303:

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

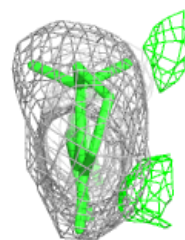
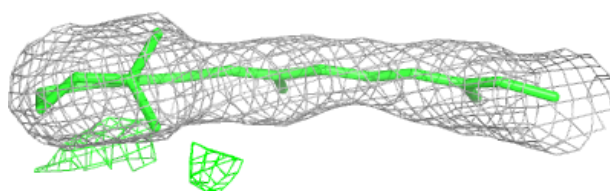
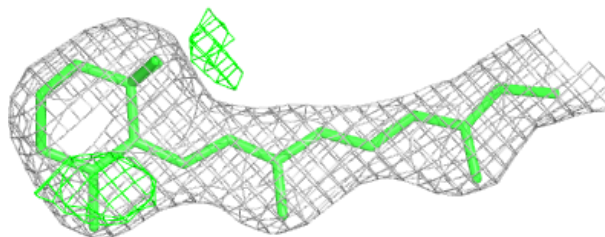
**Electron density around RET A 315:**

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

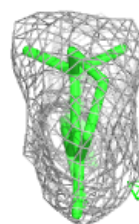
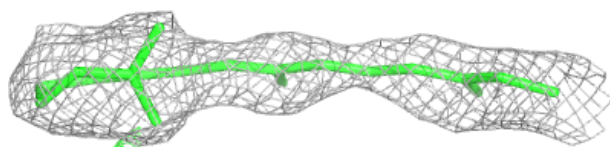
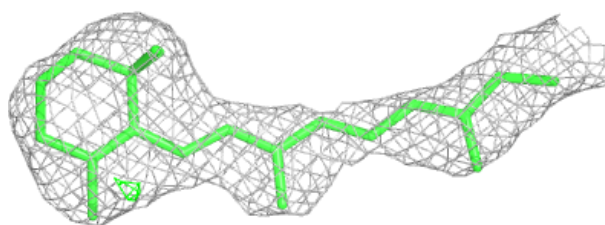


Electron density around RET B 308:

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

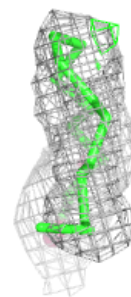
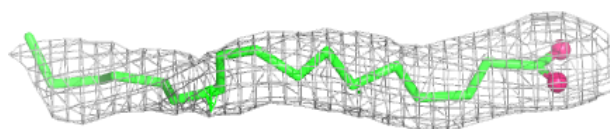
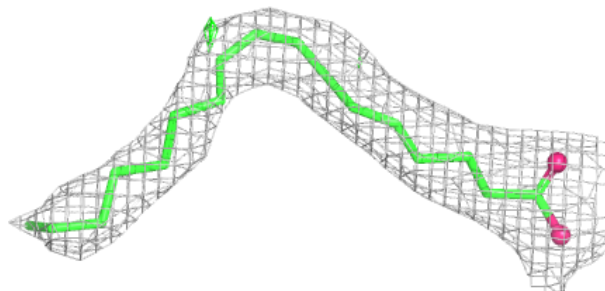
**Electron density around RET D 311:**

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

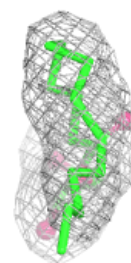
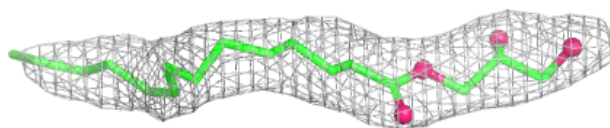
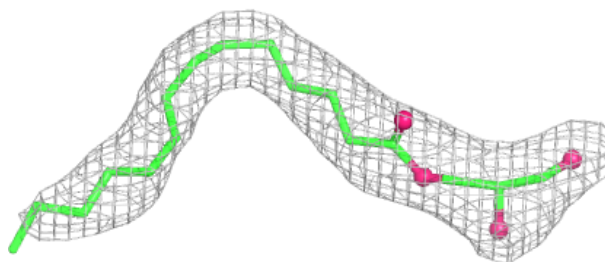


Electron density around OLC A 313:

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

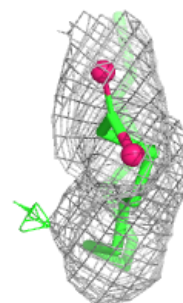
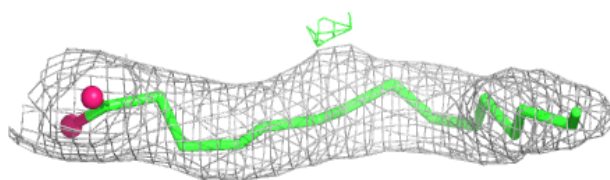
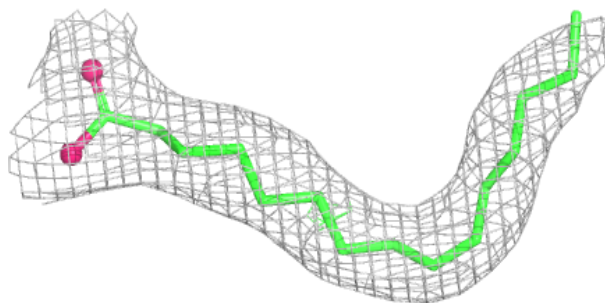
**Electron density around OLC C 301:**

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

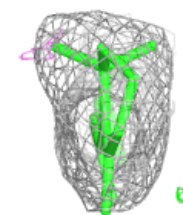
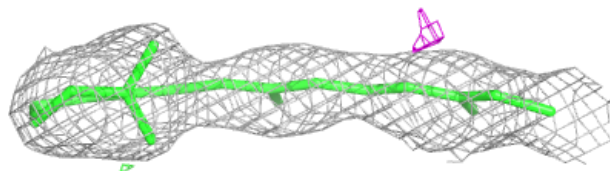
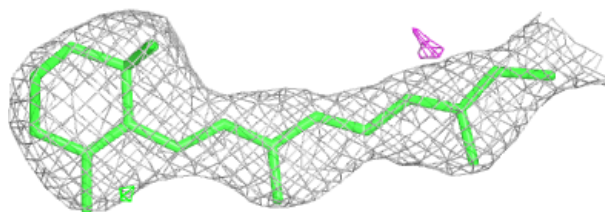


Electron density around OLC A 302:

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

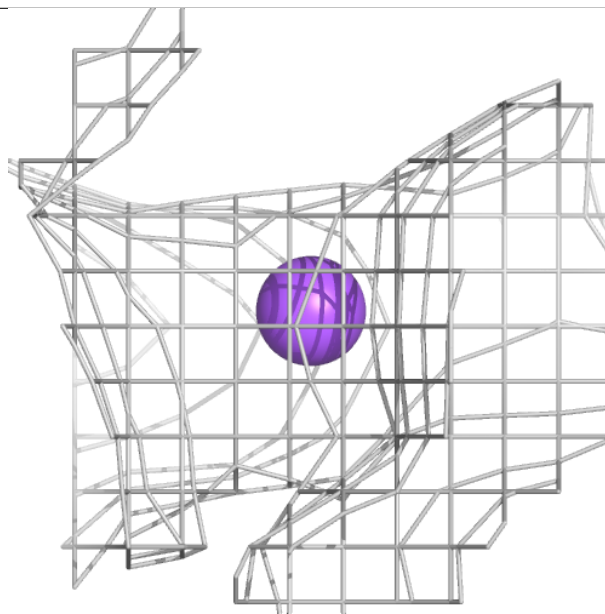
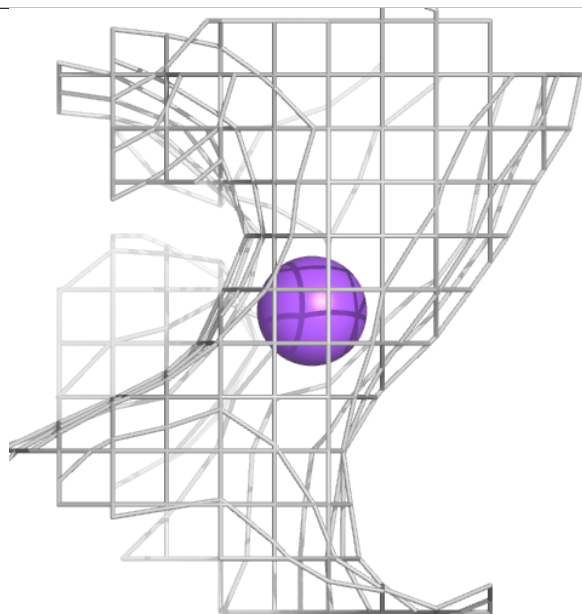
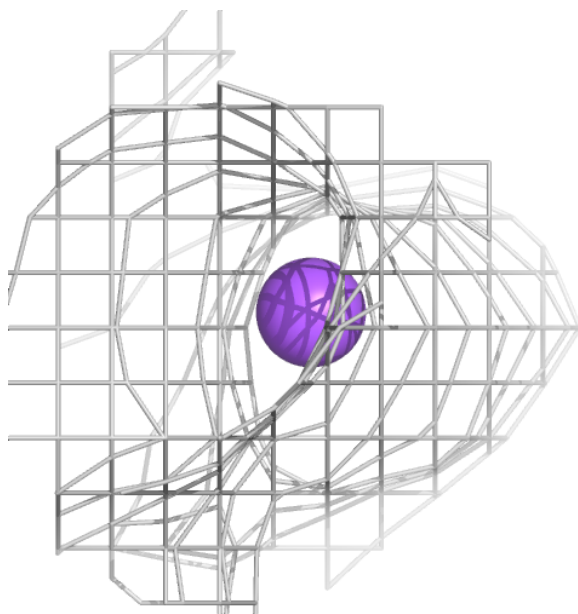
**Electron density around RET C 314:**

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



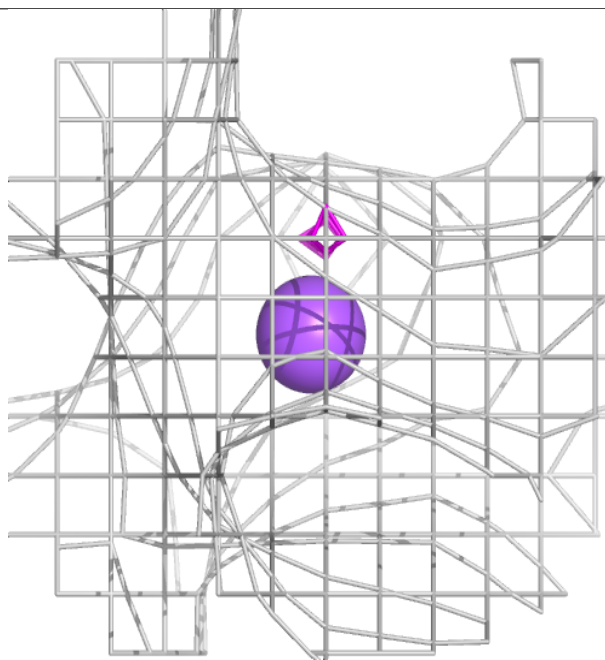
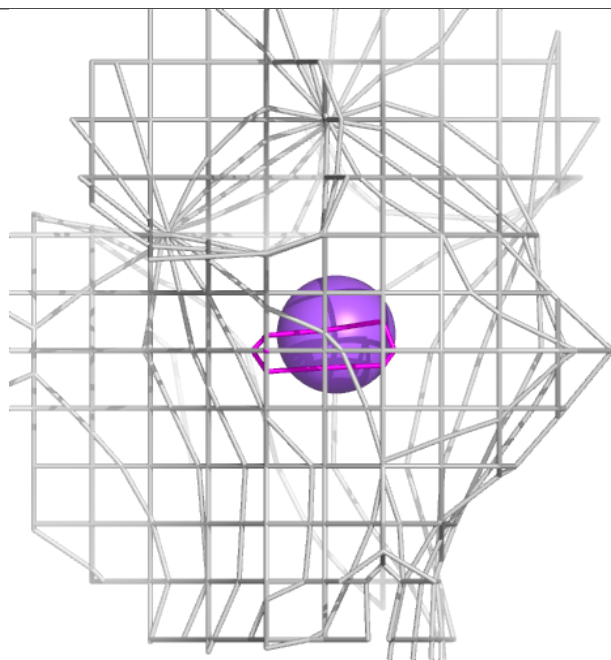
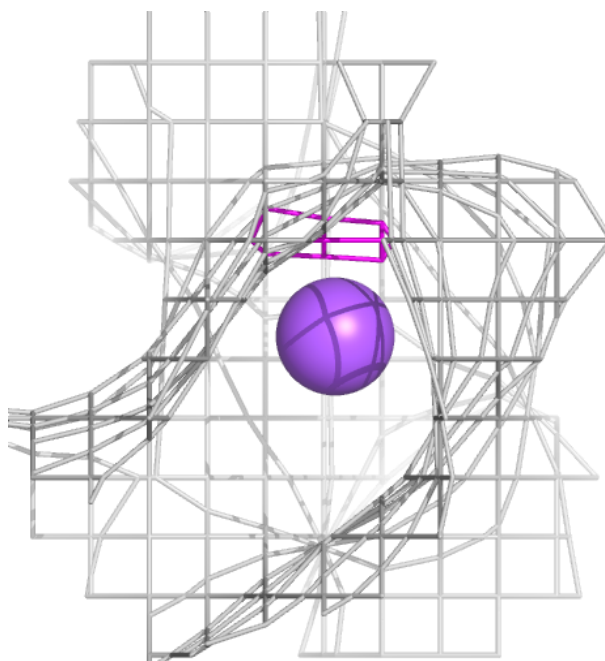
Electron density around NA A 318:

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



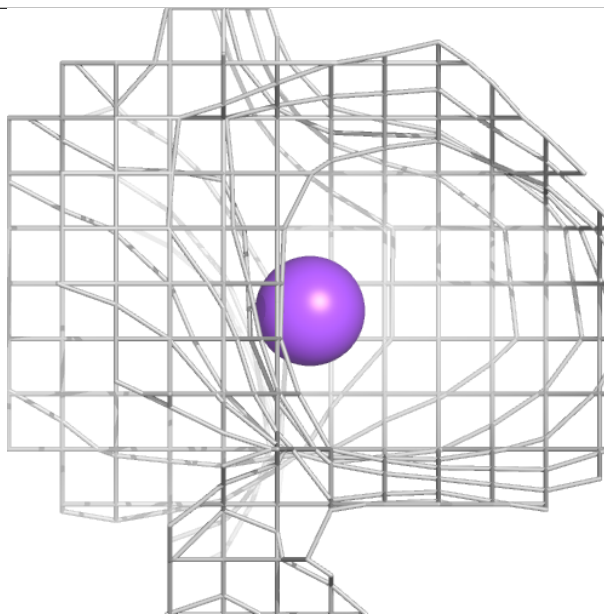
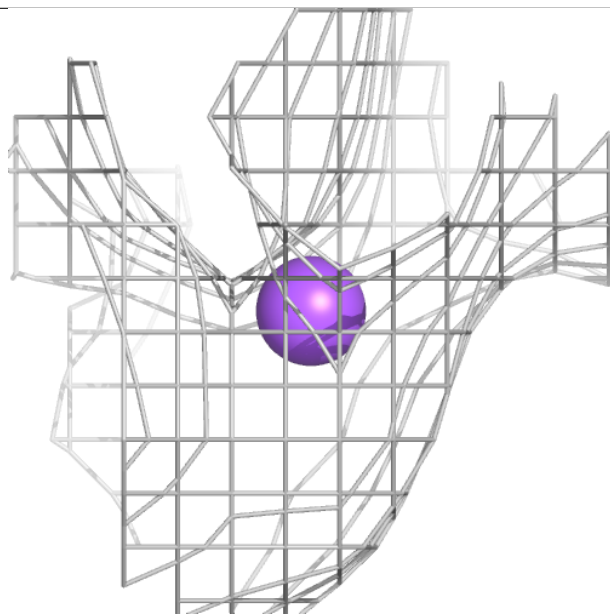
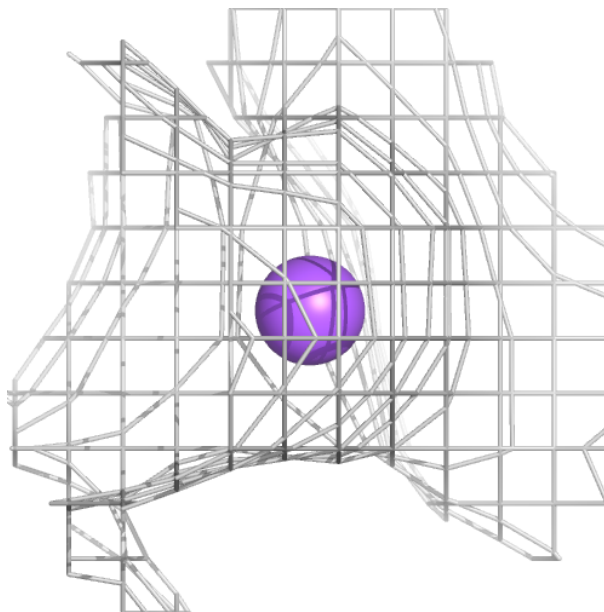
Electron density around NA D 310:

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



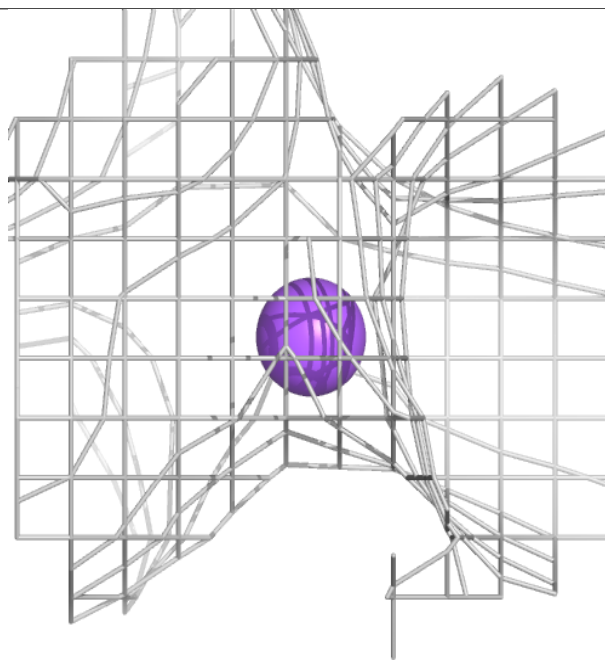
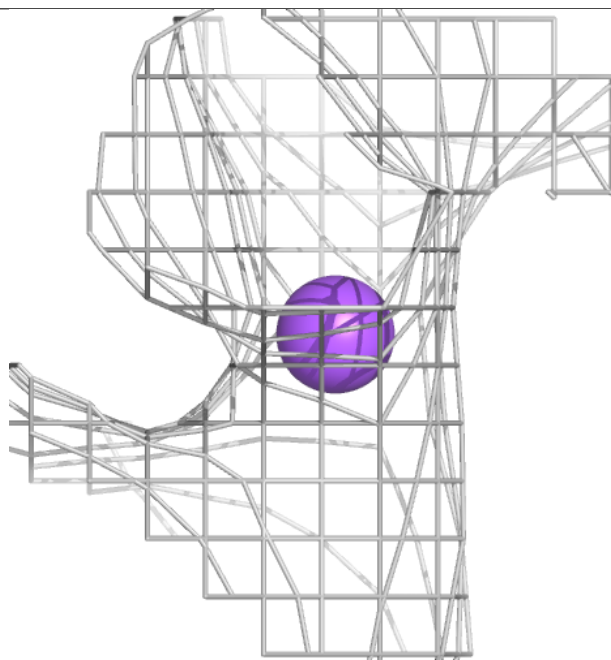
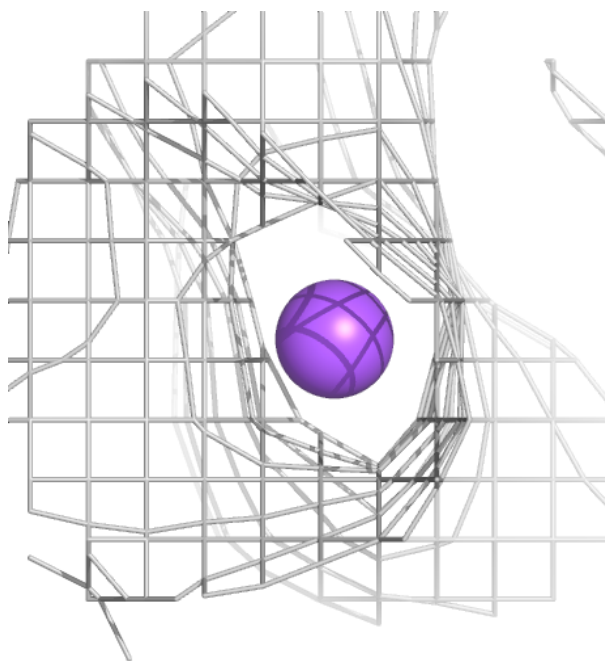
Electron density around NA E 415:

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



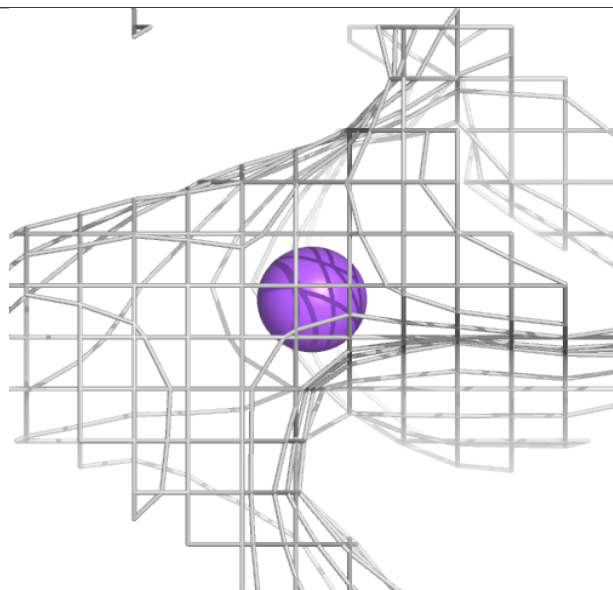
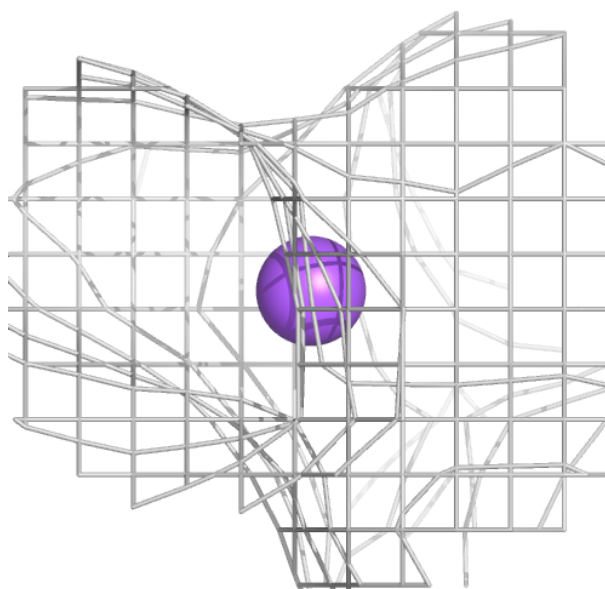
Electron density around NA C 316:

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



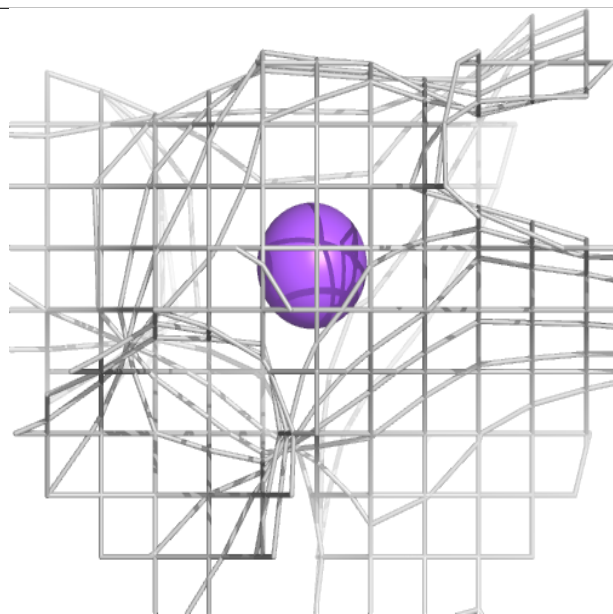
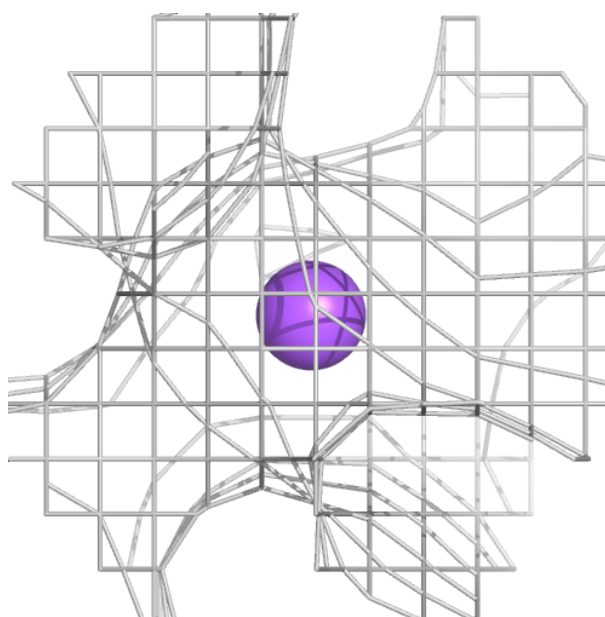
Electron density around NA D 314:

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



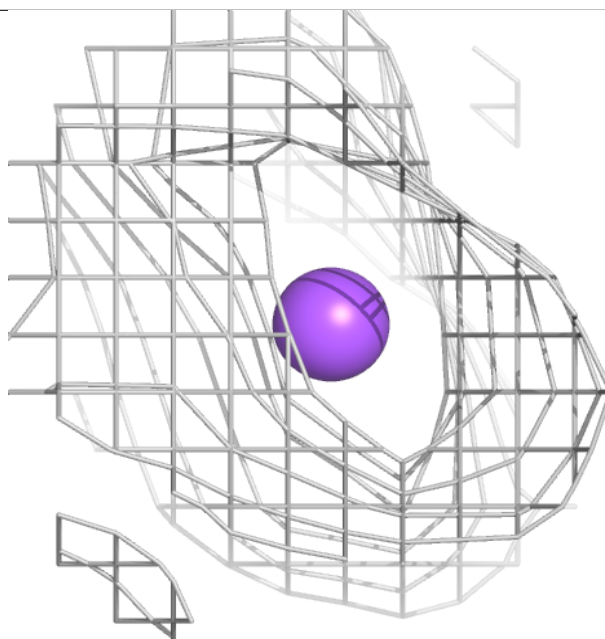
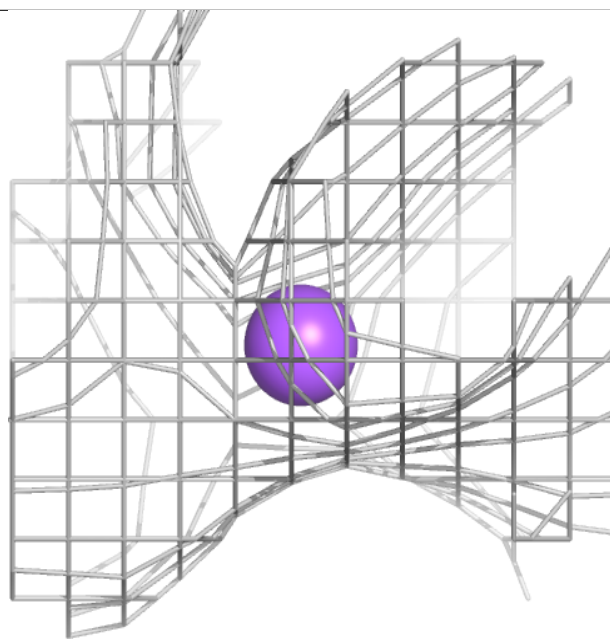
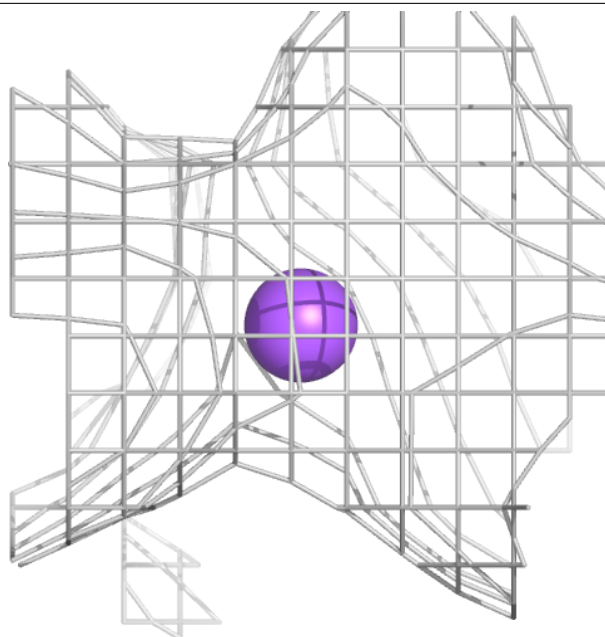
Electron density around NA C 311:

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



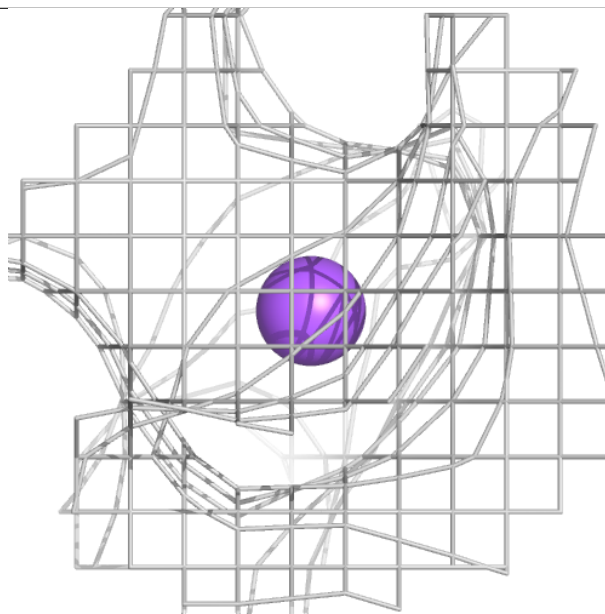
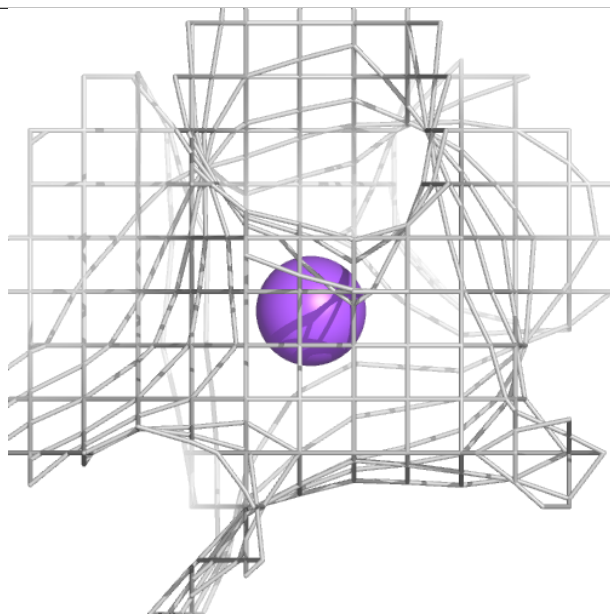
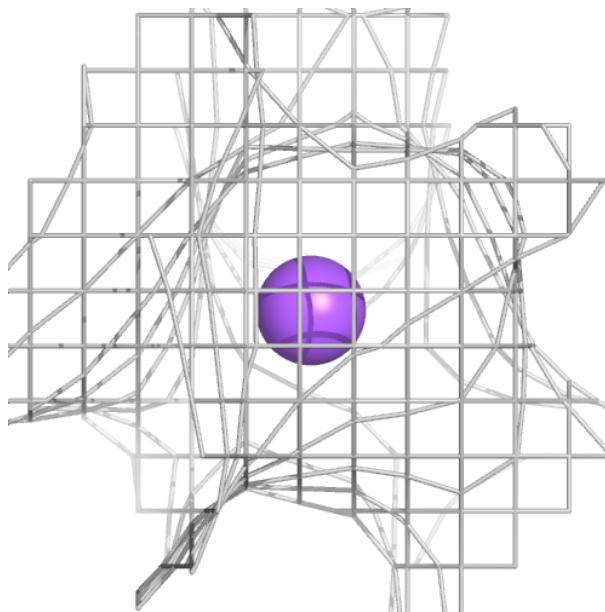
Electron density around NA B 312:

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



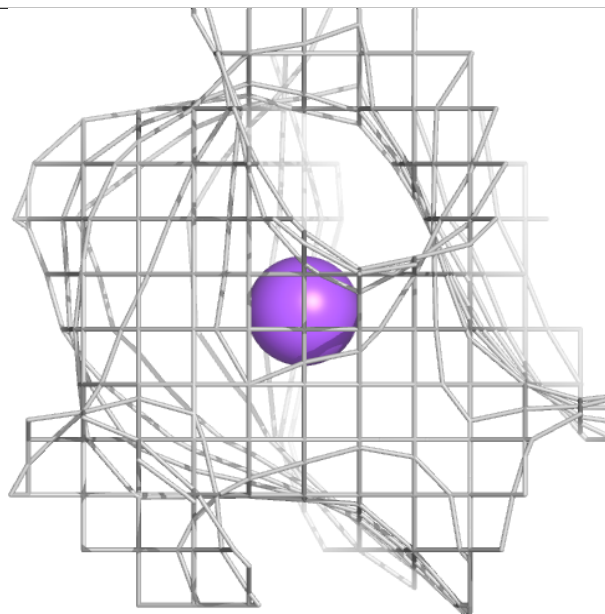
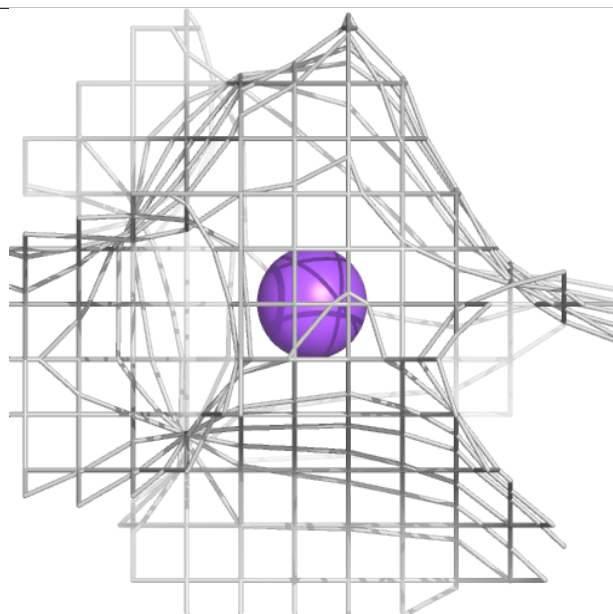
Electron density around NA A 312:

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



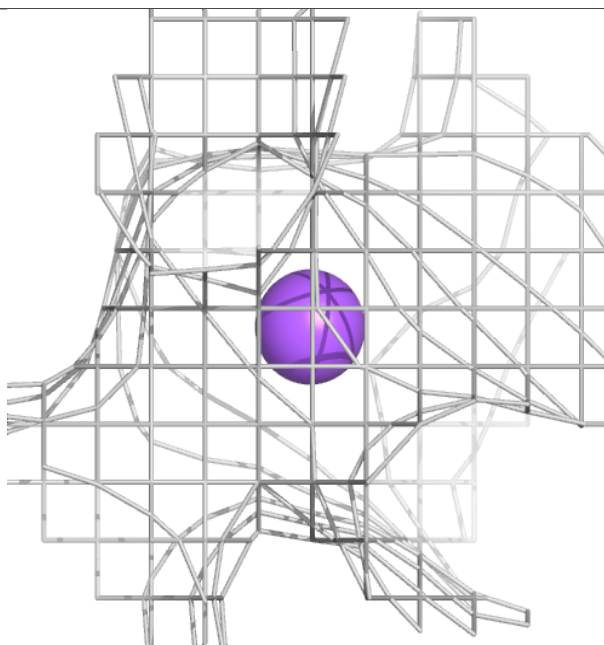
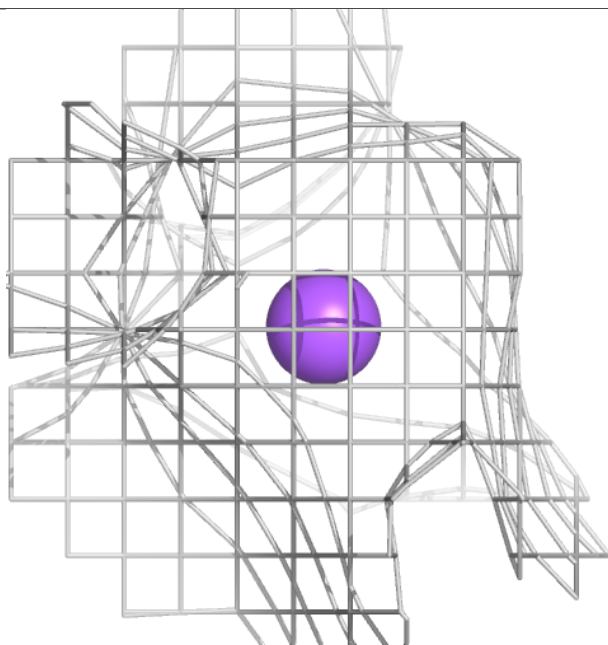
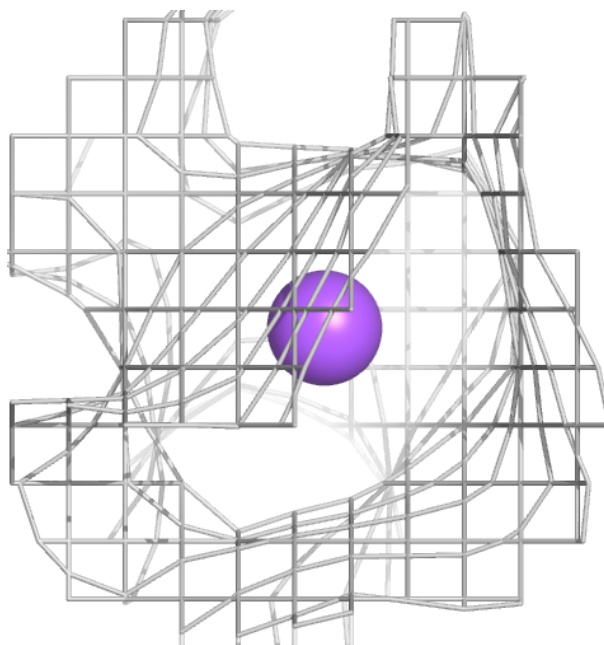
Electron density around NA E 412:

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



Electron density around NA B 307:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.