



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:15 AM UTC

PDB ID : 8XX8 / pdb_00008xx8
Title : Structure of Glycylhalorhodopsin from Salinarimonas soli
Authors : Suzuki, K.; Ishizuka, T.; Konno, M.; Inoue, K.; Murata, T.
Deposited on : 2024-01-17
Resolution : 2.63 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

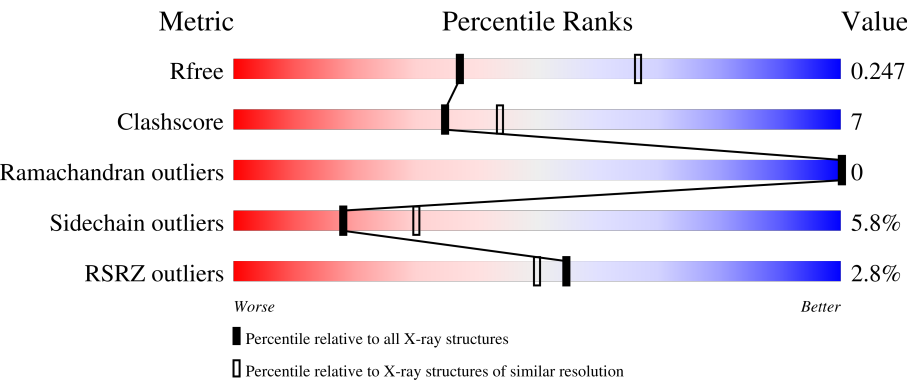
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	263	3% 76%19% . .
1	B	263	3% 79%15% . .
1	C	263	3% 78%17% . .
1	D	263	2% 78%17% . .
1	E	263	3% 78%17% . .

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Mol	Chain	Length	Quality of chain
1	F	263	3% 79% 15%

2 Entry composition [i](#)

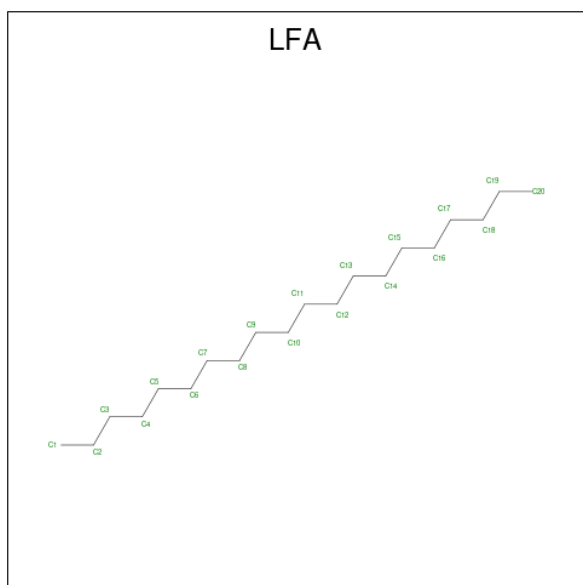
There are 6 unique types of molecules in this entry. The entry contains 12495 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1913	1253	321	333	6			
1	B	252	Total	C	N	O	S	0	2	0
			1927	1261	323	337	6			
1	D	254	Total	C	N	O	S	0	0	0
			1913	1254	319	334	6			
1	E	253	Total	C	N	O	S	0	0	0
			1917	1256	322	333	6			
1	F	253	Total	C	N	O	S	0	0	0
			1911	1254	318	333	6			
1	C	255	Total	C	N	O	S	0	0	0
			1924	1259	323	336	6			

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).

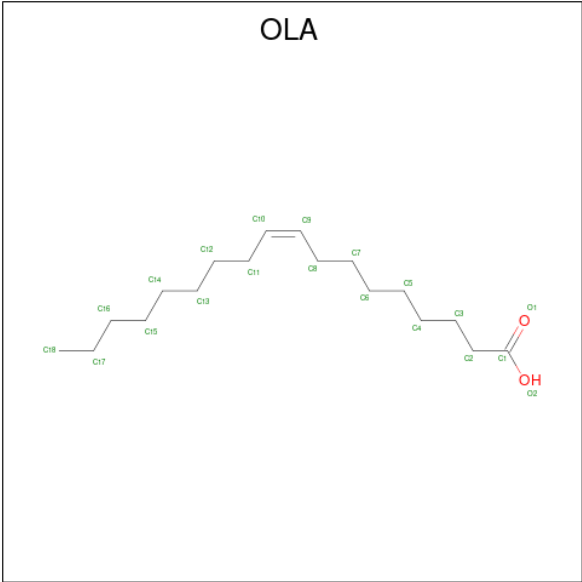


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	B	1	Total C 7 7	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 12 12	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 6 6	0	0
2	E	1	Total C 7 7	0	0
2	F	1	Total C 15 15	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C 11 11	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



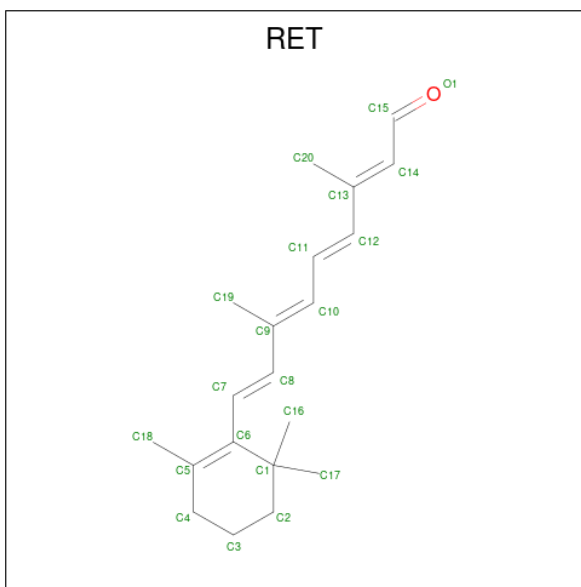
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	D	1	Total	C	O	0	0
			20	18	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			20	18	2		
4	D	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	F	1	Total	C	O	0	0
			20	18	2		
4	F	1	Total	C	O	0	0
			20	18	2		
4	F	1	Total	C	O	0	0
			20	18	2		
4	F	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest" by depositor).



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

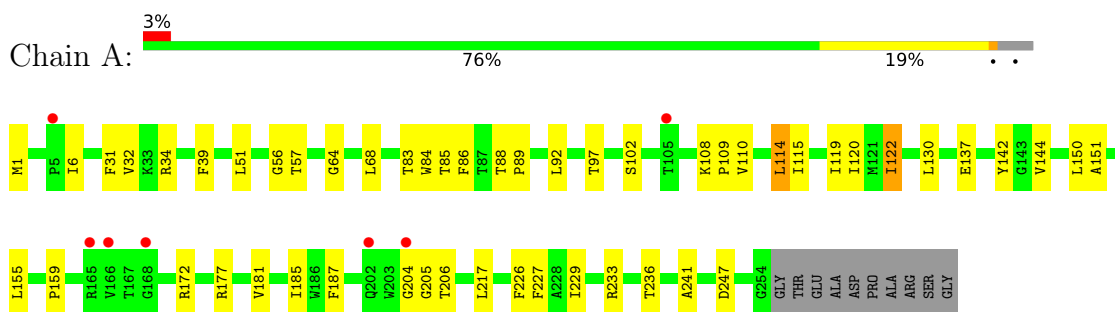
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	15	Total O 15 15	0	0
6	B	13	Total O 13 13	0	0
6	D	23	Total O 23 23	0	0
6	E	13	Total O 13 13	0	0
6	F	10	Total O 10 10	0	0
6	C	11	Total O 11 11	0	0

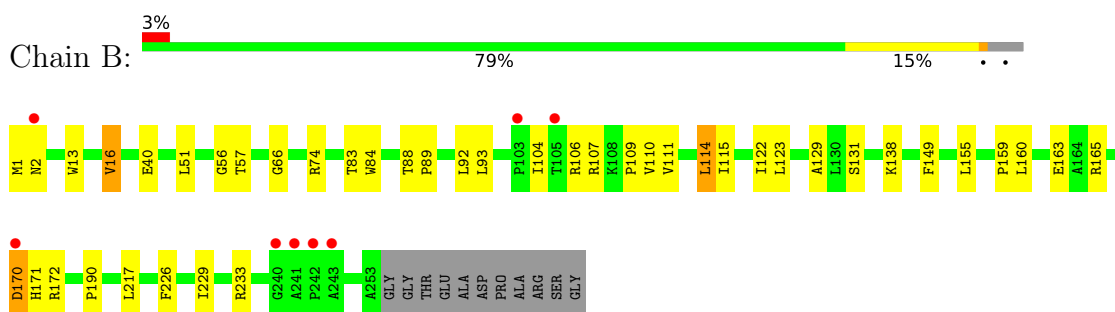
3 Residue-property plots [i](#)

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

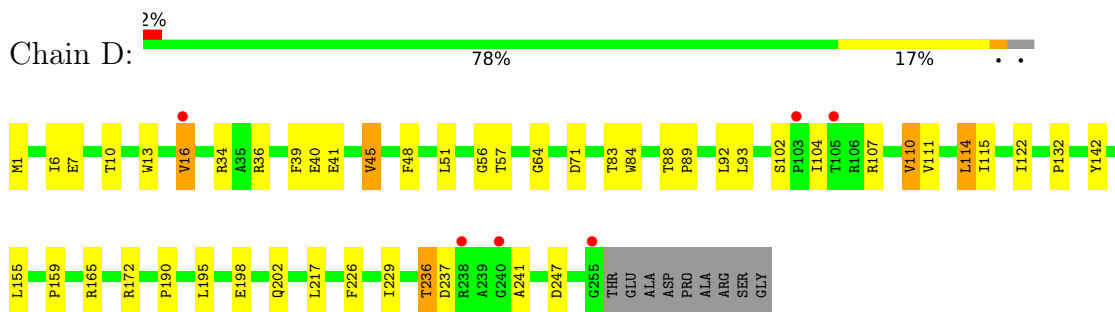
- Molecule 1: Rhodopsin



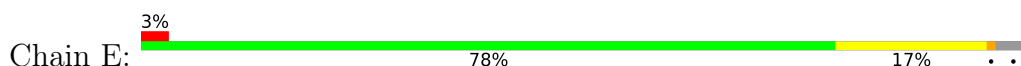
- Molecule 1: Rhodopsin

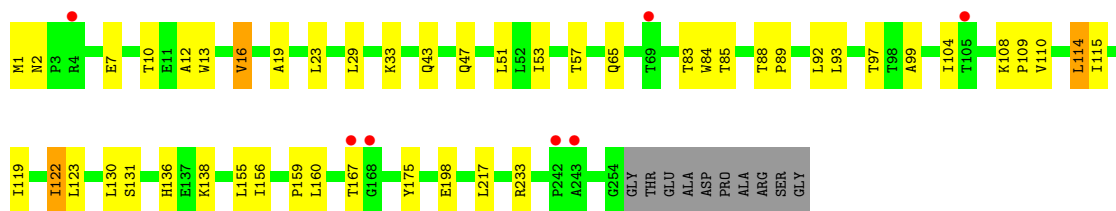


- Molecule 1: Rhodopsin

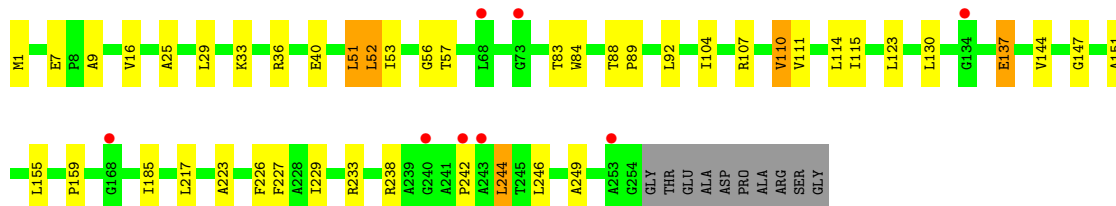
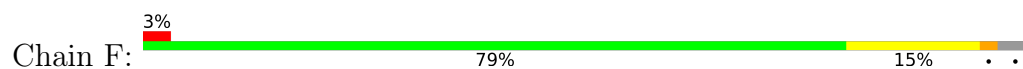


- Molecule 1: Rhodopsin

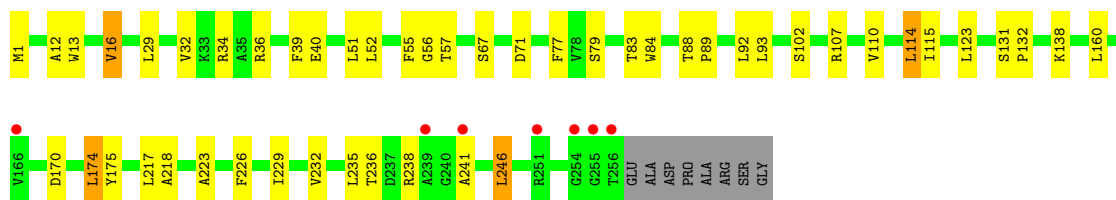
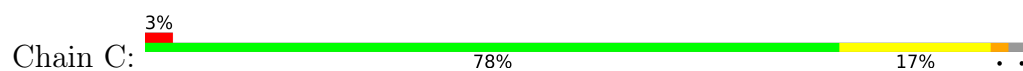




● Molecule 1: Rhodopsin



● Molecule 1: Rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.22Å 126.18Å 97.61Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	47.19 – 2.63 47.19 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.19-2.63) 91.0 (47.19-2.63)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.209 , 0.246 0.215 , 0.247	Depositor DCC
R_{free} test set	1981 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12495	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: CL, RET, LFA, OLA

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	0.10	0/1960	0.26	0/2679
1	B	0.11	0/1974	0.28	0/2697
1	C	0.11	0/1971	0.28	0/2694
1	D	0.11	0/1960	0.27	0/2679
1	E	0.11	0/1964	0.28	0/2683
1	F	0.11	0/1958	0.28	0/2676
All	All	0.11	0/11787	0.27	0/16108

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	1913	0	1957	36	0
1	B	1927	0	1972	27	0
1	C	1924	0	1966	30	0
1	D	1913	0	1952	33	0
1	E	1917	0	1968	31	0
1	F	1911	0	1953	30	0
2	A	8	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	13	1	0
2	D	33	0	59	4	0
2	E	7	0	13	4	0
2	F	44	0	84	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	180	0	297	21	0
4	B	80	0	132	4	0
4	C	140	0	231	10	0
4	D	60	0	99	7	0
4	E	140	0	231	10	0
4	F	80	0	132	6	0
5	A	20	0	27	1	0
5	B	20	0	27	3	0
5	C	20	0	27	1	0
5	D	20	0	27	1	0
5	E	20	0	27	2	0
5	F	20	0	27	1	0
6	A	15	0	0	1	0
6	B	13	0	0	1	0
6	C	11	0	0	1	0
6	D	23	0	0	1	0
6	E	13	0	0	2	0
6	F	10	0	0	1	0
All	All	12495	0	13236	192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (192) 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:D:236:THR:HG22	1:D:241:ALA:HB2	1.71	0.72
1:B:1:MET:N	6:B:401:HOH:O	2.22	0.72
1:C:1:MET:N	6:C:401:HOH:O	2.21	0.70
1:C:16:VAL:HG12	4:C:304:OLA:H132	1.73	0.70
1:B:56:GLY:HA3	4:B:305:OLA:H152	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MET:N	6:F:401:HOH:O	2.25	0.69
1:C:56:GLY:HA3	4:C:305:OLA:H141	1.74	0.69
1:E:1:MET:N	6:E:401:HOH:O	2.24	0.68
1:D:247:ASP:OD1	1:F:107:ARG:NH1	2.26	0.68
1:F:89:PRO:HB3	1:F:115:ILE:HG13	1.74	0.68
1:A:1:MET:N	6:A:401:HOH:O	2.27	0.68
1:B:74:ARG:NH2	1:B:129:ALA:O	2.26	0.67
1:F:56:GLY:HA3	4:F:307:OLA:H151	1.74	0.67
1:A:34:ARG:HH11	2:E:301:LFA:H22	1.60	0.67
4:D:308:OLA:H42	1:F:151:ALA:HB1	1.77	0.66
1:A:144:VAL:HG13	4:C:305:OLA:H182	1.77	0.66
1:D:34:ARG:HD2	2:D:303:LFA:H51	1.78	0.64
1:D:1:MET:N	6:D:401:HOH:O	2.24	0.64
1:A:92:LEU:HD13	1:A:114:LEU:HD22	1.79	0.64
1:F:53:ILE:HA	4:F:307:OLA:H142	1.80	0.63
1:E:29:LEU:HG	1:E:33:LYS:HE3	1.80	0.63
1:E:155:LEU:HA	1:E:159:PRO:HD2	1.80	0.62
1:D:41:GLU:OE2	1:F:107:ARG:NH2	2.32	0.62
1:A:206:THR:HB	4:A:308:OLA:H41	1.80	0.62
1:A:236:THR:HG22	1:A:241:ALA:HB2	1.81	0.61
1:F:104:ILE:HD13	1:F:111:VAL:HG21	1.83	0.61
1:B:66:GLY:HA2	4:B:305:OLA:H62	1.81	0.61
1:D:92:LEU:HD13	1:D:114:LEU:HD22	1.83	0.60
1:B:106:ARG:NE	1:B:163:GLU:OE1	2.34	0.60
1:F:223:ALA:HA	2:F:304:LFA:H12	1.84	0.60
4:A:310:OLA:H51	1:C:29:LEU:HD11	1.83	0.60
1:B:131:SER:O	1:B:138:LYS:NZ	2.34	0.60
1:F:226:PHE:HA	1:F:229:ILE:HG22	1.84	0.59
1:A:151:ALA:HB2	4:A:310:OLA:H9	1.84	0.59
1:D:71:ASP:HB2	1:E:2:ASN:ND2	2.17	0.59
1:E:84:TRP:HB3	1:E:122:ILE:HG12	1.85	0.59
1:A:206:THR:H	4:A:308:OLA:H22	1.67	0.58
1:C:89:PRO:HB3	1:C:115:ILE:HG13	1.83	0.58
1:A:34:ARG:HD2	2:E:301:LFA:H52	1.84	0.58
1:B:84:TRP:HB3	1:B:122:ILE:HG12	1.85	0.58
1:D:190:PRO:HG2	2:D:301:LFA:H51	1.85	0.58
1:F:185:ILE:HG12	4:F:309:OLA:H171	1.87	0.57
1:E:92:LEU:HD13	1:E:114:LEU:HD22	1.87	0.56
1:C:174:LEU:HD12	1:C:235:LEU:HD13	1.86	0.56
4:C:306:OLA:H82	4:C:308:OLA:H21	1.86	0.56
1:D:56:GLY:HA3	4:D:307:OLA:H142	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:HB	1:A:83:THR:HG21	1.86	0.56
1:F:244:LEU:HD21	1:F:249:ALA:HB2	1.88	0.56
4:E:309:OLA:H71	1:F:29:LEU:HD21	1.87	0.56
1:A:68:LEU:HD23	4:A:303:OLA:H21	1.88	0.55
1:F:155:LEU:HA	1:F:159:PRO:HD2	1.88	0.55
1:B:89:PRO:HB3	1:B:115:ILE:HG13	1.88	0.54
4:E:303:OLA:H10	1:F:52:LEU:HD21	1.89	0.54
4:D:308:OLA:H142	1:F:144:VAL:HA	1.90	0.54
1:E:19:ALA:HB2	4:E:308:OLA:H121	1.89	0.54
1:E:47:GLN:NE2	6:E:403:HOH:O	2.41	0.54
1:D:104:ILE:HD13	1:D:111:VAL:HG21	1.90	0.53
1:B:57:THR:HB	1:B:83:THR:HG21	1.90	0.53
1:B:226:PHE:HA	1:B:229:ILE:HG22	1.90	0.53
4:E:303:OLA:H71	4:E:309:OLA:H9	1.91	0.53
1:B:165:ARG:HG2	1:B:172:ARG:HG3	1.90	0.53
1:B:92:LEU:HD13	1:B:114:LEU:HD22	1.91	0.53
1:E:92:LEU:HB3	1:E:114:LEU:HD13	1.89	0.53
1:A:84:TRP:HB3	1:A:122:ILE:HG12	1.91	0.52
1:C:107:ARG:O	1:C:110:VAL:HG12	2.09	0.52
1:B:107:ARG:O	1:B:110:VAL:HG12	2.08	0.52
1:A:155:LEU:HA	1:A:159:PRO:HD2	1.91	0.52
1:D:190:PRO:HD3	5:D:309:RET:H7	1.90	0.52
1:C:57:THR:HB	1:C:83:THR:HG21	1.91	0.52
1:B:2:ASN:CG	1:C:132:PRO:HG3	2.35	0.51
1:D:34:ARG:HH11	2:D:303:LFA:H81	1.76	0.51
1:D:84:TRP:HB3	1:D:122:ILE:HG12	1.93	0.51
1:A:226:PHE:HA	1:A:229:ILE:HG22	1.92	0.51
1:C:92:LEU:HD13	1:C:114:LEU:HD22	1.93	0.51
1:D:48:PHE:HE2	4:D:308:OLA:H51	1.75	0.51
1:A:56:GLY:HA3	4:A:303:OLA:H131	1.92	0.50
1:D:132:PRO:HG3	1:E:2:ASN:ND2	2.26	0.50
1:D:142:TYR:HE2	2:D:302:LFA:H72	1.77	0.50
1:D:57:THR:HB	1:D:83:THR:HG21	1.93	0.50
1:D:89:PRO:HB3	1:D:115:ILE:HG13	1.92	0.50
1:C:52:LEU:HD11	4:C:305:OLA:H171	1.94	0.50
4:A:309:OLA:H21	4:A:310:OLA:H31	1.94	0.50
1:C:131:SER:O	1:C:138:LYS:NZ	2.44	0.50
1:D:13:TRP:O	1:D:16:VAL:HG12	2.12	0.50
1:D:36:ARG:HD3	1:D:40:GLU:OE1	2.12	0.50
1:E:136:HIS:NE2	2:E:301:LFA:H31	2.27	0.50
1:F:84:TRP:O	1:F:88:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LYS:HZ2	2:F:302:LFA:H32	1.76	0.49
1:F:9:ALA:HA	4:F:308:OLA:H32	1.95	0.49
4:A:309:OLA:C10	4:C:305:OLA:H181	2.42	0.49
1:E:57:THR:HB	1:E:83:THR:HG21	1.93	0.49
1:A:92:LEU:HB3	1:A:114:LEU:HD13	1.94	0.48
1:B:170[B]:ASP:OD1	1:B:171:HIS:ND1	2.43	0.48
1:D:36:ARG:NH1	1:D:237:ASP:OD2	2.46	0.48
1:E:43:GLN:NE2	1:E:97:THR:OG1	2.46	0.48
1:B:40:GLU:OE2	1:B:233:ARG:NH1	2.47	0.48
1:A:204:GLY:H	4:A:308:OLA:H62	1.78	0.48
1:B:2:ASN:CG	1:C:71:ASP:HB2	2.39	0.48
1:A:187:PHE:CE1	2:A:301:LFA:H32	2.49	0.48
1:E:88:THR:OG1	1:E:89:PRO:HD3	2.14	0.48
1:A:85:THR:HG23	1:A:119:ILE:HG23	1.96	0.48
1:D:88:THR:OG1	1:D:89:PRO:HD3	2.13	0.48
1:D:155:LEU:HA	1:D:159:PRO:HD2	1.96	0.48
4:A:309:OLA:H10	4:C:305:OLA:H181	1.96	0.48
1:B:104:ILE:HD13	1:B:111:VAL:HG21	1.95	0.48
1:B:84:TRP:NE1	5:B:307:RET:H14	2.30	0.47
4:D:308:OLA:H122	1:F:147:GLY:HA3	1.97	0.47
1:F:227:PHE:CD1	2:F:303:LFA:H71	2.49	0.47
1:C:92:LEU:HB3	1:C:114:LEU:HD13	1.96	0.47
1:F:107:ARG:O	1:F:110:VAL:HG12	2.15	0.47
1:D:195:LEU:HD22	1:D:202:GLN:HG3	1.97	0.46
1:D:165:ARG:HG2	1:D:172:ARG:HD2	1.97	0.46
1:E:136:HIS:CG	4:E:307:OLA:H62	2.51	0.46
1:F:25:ALA:HB2	1:F:51:LEU:HB3	1.98	0.46
1:B:56:GLY:HA3	4:B:305:OLA:H171	1.97	0.46
1:D:39:PHE:HA	1:D:102:SER:HB3	1.98	0.46
1:A:120:ILE:HG21	4:C:305:OLA:H183	1.97	0.46
1:A:233:ARG:HB3	4:E:307:OLA:H32	1.97	0.46
1:B:155:LEU:HA	1:B:159:PRO:HD2	1.98	0.46
1:E:12:ALA:HA	4:E:308:OLA:H71	1.98	0.46
1:E:99:ALA:O	1:E:167:THR:OG1	2.30	0.45
1:E:53:ILE:HD11	4:E:304:OLA:H141	1.98	0.45
1:F:57:THR:HB	1:F:83:THR:HG21	1.99	0.45
1:D:107:ARG:O	1:D:110:VAL:HG12	2.17	0.45
1:C:84:TRP:NE1	5:C:309:RET:H14	2.31	0.45
1:E:89:PRO:HB3	1:E:115:ILE:HG23	1.99	0.45
1:E:97:THR:HG22	1:E:104:ILE:HD11	1.98	0.45
1:B:13:TRP:O	1:B:16:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PHE:HD2	4:C:305:OLA:H161	1.82	0.45
1:A:32:VAL:HG11	4:B:303:OLA:H22	1.99	0.44
1:E:7:GLU:HG3	1:E:10:THR:H	1.81	0.44
1:C:12:ALA:O	1:C:16:VAL:HG13	2.17	0.44
1:B:88:THR:OG1	1:B:89:PRO:HD3	2.16	0.44
1:C:88:THR:OG1	1:C:89:PRO:HD3	2.17	0.44
1:A:88:THR:OG1	1:A:89:PRO:HD3	2.18	0.44
1:E:131:SER:O	1:E:138:LYS:NZ	2.51	0.44
1:C:79:SER:HB2	4:C:305:OLA:H51	2.00	0.44
1:C:39:PHE:HA	1:C:102:SER:HB3	1.99	0.44
1:A:39:PHE:HA	1:A:102:SER:HB3	1.99	0.43
4:A:311:OLA:H82	4:A:311:OLA:H111	1.82	0.43
1:E:85:THR:HG23	1:E:119:ILE:HG23	2.00	0.43
1:D:48:PHE:CE2	4:D:308:OLA:H51	2.53	0.43
4:E:303:OLA:H121	4:F:307:OLA:H182	2.01	0.43
1:C:236:THR:HB	1:C:241:ALA:HB2	2.00	0.43
1:D:6:ILE:HD11	1:D:64:GLY:HA2	2.01	0.43
1:D:41:GLU:O	1:D:45:VAL:HG13	2.19	0.43
1:D:226:PHE:HA	1:D:229:ILE:HG22	2.00	0.43
4:A:311:OLA:H112	4:A:311:OLA:H142	1.72	0.43
1:F:40:GLU:OE2	1:F:233:ARG:HD2	2.17	0.43
1:F:88:THR:OG1	1:F:89:PRO:HD3	2.19	0.43
1:E:136:HIS:NE2	2:E:301:LFA:H61	2.34	0.43
1:C:13:TRP:O	1:C:16:VAL:HG22	2.19	0.42
4:D:307:OLA:H61	4:D:307:OLA:H9	1.73	0.42
1:B:190:PRO:HD3	5:B:307:RET:H7	2.02	0.42
1:A:205:GLY:H	4:A:308:OLA:C1	2.32	0.42
4:A:309:OLA:H151	4:A:310:OLA:H171	2.00	0.42
1:B:84:TRP:CD1	5:B:307:RET:H14	2.54	0.42
1:E:84:TRP:NE1	5:E:310:RET:H14	2.34	0.42
1:A:177:ARG:NH2	1:A:227:PHE:O	2.52	0.42
1:F:36:ARG:HD2	1:F:242:PRO:O	2.20	0.42
1:D:195:LEU:HB3	1:D:202:GLN:HB2	2.02	0.42
1:A:31:PHE:HZ	4:E:307:OLA:H61	1.84	0.42
1:E:138:LYS:HE3	1:E:198:GLU:O	2.20	0.41
1:C:67:SER:HB3	1:C:77:PHE:CD1	2.55	0.41
1:A:97:THR:HG23	1:A:102:SER:HB2	2.02	0.41
4:A:304:OLA:H42	1:B:109:PRO:HB3	2.02	0.41
1:C:160:LEU:HB3	1:C:175:TYR:OH	2.21	0.41
1:E:130:LEU:O	1:F:1:MET:N	2.50	0.41
1:A:181:VAL:HG11	4:A:307:OLA:H9	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HD12	1:A:229:ILE:HA	1.95	0.41
1:D:7:GLU:HG3	1:D:10:THR:H	1.84	0.41
1:E:156:ILE:O	1:E:175:TYR:OH	2.33	0.41
1:F:137:GLU:H	1:F:137:GLU:CD	2.27	0.41
4:F:307:OLA:H72	4:F:307:OLA:H41	1.64	0.41
1:C:226:PHE:HA	1:C:229:ILE:HG22	2.03	0.41
1:A:6:ILE:HD11	1:A:64:GLY:HA2	2.01	0.41
1:E:13:TRP:O	1:E:16:VAL:HG22	2.21	0.41
4:A:309:OLA:H9	1:C:52:LEU:HD11	2.03	0.41
1:E:108:LYS:N	1:E:109:PRO:HD2	2.35	0.41
4:A:310:OLA:H22	1:C:32:VAL:HG12	2.02	0.41
1:F:84:TRP:NE1	5:F:310:RET:H14	2.36	0.41
1:A:84:TRP:NE1	5:A:312:RET:H14	2.36	0.41
4:A:311:OLA:H51	4:A:311:OLA:H22	1.71	0.40
1:E:84:TRP:CD1	5:E:310:RET:H14	2.56	0.40
1:C:218:ALA:HA	1:C:223:ALA:HB3	2.04	0.40
1:C:246:LEU:HD12	1:C:246:LEU:HA	1.93	0.40
1:A:108:LYS:N	1:A:109:PRO:HD2	2.36	0.40
1:C:36:ARG:HD3	1:C:40:GLU:OE1	2.22	0.40
1:A:86:PHE:C	1:A:89:PRO:HD2	2.47	0.40
1:A:142:TYR:HE2	4:A:311:OLA:H183	1.86	0.40
1:A:185:ILE:HG12	4:A:305:OLA:H171	2.03	0.40
1:B:149:PHE:CD2	2:B:301:LFA:H13	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/263 (95%)	247 (98%)	4 (2%)	0	100	100
1	B	252/263 (96%)	249 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	253/263 (96%)	250 (99%)	3 (1%)	0	100	100
1	D	252/263 (96%)	250 (99%)	2 (1%)	0	100	100
1	E	251/263 (95%)	250 (100%)	1 (0%)	0	100	100
1	F	251/263 (95%)	248 (99%)	3 (1%)	0	100	100
All	All	1510/1578 (96%)	1494 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/197 (96%)	179 (94%)	11 (6%)	18	30
1	B	193/197 (98%)	184 (95%)	9 (5%)	23	38
1	C	191/197 (97%)	179 (94%)	12 (6%)	16	27
1	D	189/197 (96%)	180 (95%)	9 (5%)	23	37
1	E	191/197 (97%)	179 (94%)	12 (6%)	16	27
1	F	189/197 (96%)	175 (93%)	14 (7%)	13	20
All	All	1143/1182 (97%)	1076 (94%)	67 (6%)	18	29

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	110	VAL
1	A	114	LEU
1	A	115	ILE
1	A	122	ILE
1	A	130	LEU
1	A	137	GLU
1	A	150	LEU
1	A	172	ARG

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Mol	Chain	Res	Type
1	A	217	LEU
1	A	247	ASP
1	B	16	VAL
1	B	51	LEU
1	B	93	LEU
1	B	114	LEU
1	B	123	LEU
1	B	160	LEU
1	B	170[A]	ASP
1	B	170[B]	ASP
1	B	217	LEU
1	D	16	VAL
1	D	45	VAL
1	D	51	LEU
1	D	93	LEU
1	D	110	VAL
1	D	114	LEU
1	D	198	GLU
1	D	217	LEU
1	D	236	THR
1	E	16	VAL
1	E	23	LEU
1	E	51	LEU
1	E	65	GLN
1	E	93	LEU
1	E	110	VAL
1	E	114	LEU
1	E	122	ILE
1	E	123	LEU
1	E	160	LEU
1	E	217	LEU
1	E	233	ARG
1	F	7	GLU
1	F	16	VAL
1	F	51	LEU
1	F	52	LEU
1	F	92	LEU
1	F	110	VAL
1	F	114	LEU
1	F	123	LEU
1	F	130	LEU
1	F	137	GLU

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Mol	Chain	Res	Type
1	F	217	LEU
1	F	238	ARG
1	F	244	LEU
1	F	246	LEU
1	C	16	VAL
1	C	34	ARG
1	C	51	LEU
1	C	93	LEU
1	C	114	LEU
1	C	123	LEU
1	C	170	ASP
1	C	174	LEU
1	C	217	LEU
1	C	232	VAL
1	C	238	ARG
1	C	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	197	ASN
1	D	43	GLN
1	D	47	GLN
1	E	2	ASN
1	E	47	GLN
1	E	75	GLN
1	F	197	ASN
1	C	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 57 ligands modelled in this entry, 6 are monoatomic - leaving 51 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	$\# Z > 2$
2	LFA	D	303	-	6,6,19	0.10	0	5,5,18	0.10	0
4	OLA	B	303	-	19,19,19	0.80	1 (5%)	19,19,19	0.82	0
4	OLA	C	302	-	19,19,19	0.81	1 (5%)	19,19,19	0.92	1 (5%)
4	OLA	C	303	-	19,19,19	0.82	1 (5%)	19,19,19	0.89	1 (5%)
4	OLA	B	305	-	19,19,19	0.80	1 (5%)	19,19,19	0.92	1 (5%)
4	OLA	D	307	-	19,19,19	0.80	1 (5%)	19,19,19	0.92	1 (5%)
4	OLA	C	305	-	19,19,19	0.80	1 (5%)	19,19,19	1.00	2 (10%)
2	LFA	A	301	-	7,7,19	0.11	0	6,6,18	0.13	0
4	OLA	A	307	-	19,19,19	0.82	1 (5%)	19,19,19	0.89	1 (5%)
5	RET	C	309	1	20,20,21	0.77	1 (5%)	27,27,28	0.38	0
5	RET	E	310	1	20,20,21	0.76	1 (5%)	27,27,28	0.36	0
4	OLA	A	309	-	19,19,19	0.82	1 (5%)	19,19,19	0.90	1 (5%)
4	OLA	F	308	-	19,19,19	0.80	1 (5%)	19,19,19	0.89	1 (5%)
4	OLA	A	310	-	19,19,19	0.83	1 (5%)	19,19,19	0.91	0
4	OLA	E	306	-	19,19,19	0.81	1 (5%)	19,19,19	0.91	1 (5%)
4	OLA	A	308	-	19,19,19	0.82	1 (5%)	19,19,19	0.90	1 (5%)
4	OLA	A	303	-	19,19,19	0.79	1 (5%)	19,19,19	0.93	1 (5%)
4	OLA	C	308	-	19,19,19	0.80	1 (5%)	19,19,19	0.90	1 (5%)
4	OLA	E	305	-	19,19,19	0.79	1 (5%)	19,19,19	0.96	1 (5%)
2	LFA	D	304	-	5,5,19	0.12	0	4,4,18	0.09	0
4	OLA	E	303	-	19,19,19	0.81	1 (5%)	19,19,19	0.93	0
4	OLA	A	311	-	19,19,19	0.81	1 (5%)	19,19,19	0.93	1 (5%)
4	OLA	B	304	-	19,19,19	0.79	1 (5%)	19,19,19	0.85	0
4	OLA	C	304	-	19,19,19	0.82	1 (5%)	19,19,19	0.90	1 (5%)
5	RET	A	312	1	20,20,21	0.77	1 (5%)	27,27,28	0.39	0
4	OLA	D	308	-	19,19,19	0.81	1 (5%)	19,19,19	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLA	C	307	-	19,19,19	0.82	1 (5%)	19,19,19	0.90	1 (5%)
2	LFA	F	304	-	10,10,19	0.10	0	9,9,18	0.12	0
2	LFA	D	301	-	7,7,19	0.10	0	6,6,18	0.16	0
4	OLA	F	309	-	19,19,19	0.78	1 (5%)	19,19,19	0.91	0
4	OLA	E	304	-	19,19,19	0.83	1 (5%)	19,19,19	0.86	1 (5%)
4	OLA	A	304	-	19,19,19	0.81	1 (5%)	19,19,19	0.86	0
4	OLA	A	306	-	19,19,19	0.80	1 (5%)	19,19,19	0.93	1 (5%)
2	LFA	B	301	-	6,6,19	0.11	0	5,5,18	0.10	0
2	LFA	F	302	-	6,6,19	0.11	0	5,5,18	0.11	0
2	LFA	F	303	-	10,10,19	0.12	0	9,9,18	0.11	0
4	OLA	F	306	-	19,19,19	0.80	1 (5%)	19,19,19	0.95	1 (5%)
4	OLA	F	307	-	19,19,19	0.79	1 (5%)	19,19,19	1.00	2 (10%)
4	OLA	E	309	-	19,19,19	0.82	1 (5%)	19,19,19	0.88	0
5	RET	D	309	1	20,20,21	0.75	1 (5%)	27,27,28	0.36	0
5	RET	F	310	1	20,20,21	0.78	1 (5%)	27,27,28	0.37	0
2	LFA	F	301	-	14,14,19	0.09	0	13,13,18	0.17	0
4	OLA	B	306	-	19,19,19	0.82	1 (5%)	19,19,19	0.89	0
4	OLA	E	308	-	19,19,19	0.80	1 (5%)	19,19,19	0.92	1 (5%)
4	OLA	D	306	-	19,19,19	0.81	1 (5%)	19,19,19	0.92	1 (5%)
4	OLA	C	306	-	19,19,19	0.82	1 (5%)	19,19,19	0.89	1 (5%)
2	LFA	E	301	-	6,6,19	0.11	0	5,5,18	0.05	0
5	RET	B	307	1	20,20,21	0.76	1 (5%)	27,27,28	0.36	0
2	LFA	D	302	-	11,11,19	0.09	0	10,10,18	0.07	0
4	OLA	A	305	-	19,19,19	0.81	1 (5%)	19,19,19	0.93	1 (5%)
4	OLA	E	307	-	19,19,19	0.78	1 (5%)	19,19,19	0.93	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	D	303	-	-	0/4/4/17	-
4	OLA	B	303	-	-	12/17/17/17	-
4	OLA	C	302	-	-	9/17/17/17	-
4	OLA	C	303	-	-	8/17/17/17	-
4	OLA	B	305	-	-	9/17/17/17	-
4	OLA	D	307	-	-	11/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	C	305	-	-	11/17/17/17	-
2	LFA	A	301	-	-	2/5/5/17	-
4	OLA	A	307	-	-	9/17/17/17	-
5	RET	C	309	1	-	4/13/30/31	0/1/1/1
5	RET	E	310	1	-	4/13/30/31	0/1/1/1
4	OLA	A	309	-	-	9/17/17/17	-
4	OLA	F	308	-	-	9/17/17/17	-
4	OLA	A	310	-	-	10/17/17/17	-
4	OLA	E	306	-	-	10/17/17/17	-
4	OLA	A	308	-	-	6/17/17/17	-
4	OLA	A	303	-	-	9/17/17/17	-
4	OLA	C	308	-	-	9/17/17/17	-
4	OLA	E	305	-	-	8/17/17/17	-
2	LFA	D	304	-	-	0/3/3/17	-
4	OLA	E	303	-	-	7/17/17/17	-
4	OLA	A	311	-	-	9/17/17/17	-
4	OLA	B	304	-	-	8/17/17/17	-
4	OLA	C	304	-	-	7/17/17/17	-
5	RET	A	312	1	-	4/13/30/31	0/1/1/1
4	OLA	D	308	-	-	9/17/17/17	-
4	OLA	C	307	-	-	8/17/17/17	-
2	LFA	F	304	-	-	2/8/8/17	-
2	LFA	D	301	-	-	1/5/5/17	-
4	OLA	F	309	-	-	7/17/17/17	-
4	OLA	E	304	-	-	10/17/17/17	-
4	OLA	A	304	-	-	11/17/17/17	-
4	OLA	A	306	-	-	8/17/17/17	-
2	LFA	B	301	-	-	0/4/4/17	-
2	LFA	F	302	-	-	0/4/4/17	-
2	LFA	F	303	-	-	1/8/8/17	-
4	OLA	F	306	-	-	8/17/17/17	-
4	OLA	F	307	-	-	10/17/17/17	-
4	OLA	E	309	-	-	7/17/17/17	-
5	RET	D	309	1	-	4/13/30/31	0/1/1/1
5	RET	F	310	1	-	4/13/30/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	F	301	-	-	0/12/12/17	-
4	OLA	B	306	-	-	6/17/17/17	-
4	OLA	E	308	-	-	12/17/17/17	-
4	OLA	D	306	-	-	8/17/17/17	-
4	OLA	C	306	-	-	9/17/17/17	-
2	LFA	E	301	-	-	0/4/4/17	-
5	RET	B	307	1	-	4/13/30/31	0/1/1/1
2	LFA	D	302	-	-	2/9/9/17	-
4	OLA	A	305	-	-	9/17/17/17	-
4	OLA	E	307	-	-	8/17/17/17	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	310	RET	C14-C13	3.15	1.35	1.33
5	C	309	RET	C14-C13	3.08	1.35	1.33
5	A	312	RET	C14-C13	3.07	1.35	1.33
5	B	307	RET	C14-C13	3.05	1.35	1.33
5	E	310	RET	C14-C13	3.02	1.35	1.33
5	D	309	RET	C14-C13	2.97	1.35	1.33
4	E	304	OLA	C10-C9	2.84	1.47	1.31
4	C	302	OLA	C10-C9	2.82	1.47	1.31
4	C	304	OLA	C10-C9	2.82	1.47	1.31
4	A	308	OLA	C10-C9	2.82	1.47	1.31
4	A	307	OLA	C10-C9	2.81	1.47	1.31
4	D	308	OLA	C10-C9	2.81	1.47	1.31
4	C	307	OLA	C10-C9	2.81	1.47	1.31
4	B	306	OLA	C10-C9	2.81	1.47	1.31
4	A	304	OLA	C10-C9	2.80	1.47	1.31
4	A	310	OLA	C10-C9	2.80	1.47	1.31
4	D	306	OLA	C10-C9	2.80	1.47	1.31
4	A	311	OLA	C10-C9	2.80	1.47	1.31
4	C	306	OLA	C10-C9	2.80	1.47	1.31
4	E	306	OLA	C10-C9	2.80	1.47	1.31
4	C	303	OLA	C10-C9	2.80	1.47	1.31
4	A	309	OLA	C10-C9	2.79	1.47	1.31
4	E	309	OLA	C10-C9	2.79	1.47	1.31
4	A	305	OLA	C10-C9	2.78	1.47	1.31
4	A	306	OLA	C10-C9	2.78	1.47	1.31
4	F	306	OLA	C10-C9	2.78	1.47	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	303	OLA	C10-C9	2.77	1.47	1.31
4	B	305	OLA	C10-C9	2.77	1.47	1.31
4	D	307	OLA	C10-C9	2.77	1.47	1.31
4	C	308	OLA	C10-C9	2.77	1.47	1.31
4	E	308	OLA	C10-C9	2.76	1.47	1.31
4	E	305	OLA	C10-C9	2.75	1.47	1.31
4	A	303	OLA	C10-C9	2.74	1.47	1.31
4	F	307	OLA	C10-C9	2.74	1.47	1.31
4	C	305	OLA	C10-C9	2.73	1.47	1.31
4	F	308	OLA	C10-C9	2.73	1.47	1.31
4	B	304	OLA	C10-C9	2.72	1.47	1.31
4	E	307	OLA	C10-C9	2.71	1.47	1.31
4	B	303	OLA	C10-C9	2.71	1.47	1.31
4	F	309	OLA	C10-C9	2.69	1.47	1.31

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	307	OLA	C3-C2-C1	-2.29	108.54	114.51
4	C	304	OLA	O2-C1-C2	2.19	120.93	114.00
4	D	308	OLA	O2-C1-C2	2.19	120.92	114.00
4	F	306	OLA	O2-C1-C2	2.16	120.83	114.00
4	C	302	OLA	O2-C1-C2	2.14	120.78	114.00
4	C	307	OLA	O2-C1-C2	2.13	120.73	114.00
4	E	306	OLA	O2-C1-C2	2.13	120.72	114.00
4	D	306	OLA	C3-C2-C1	-2.12	108.97	114.51
4	E	305	OLA	O2-C1-C2	2.12	120.71	114.00
4	A	308	OLA	O2-C1-C2	2.12	120.70	114.00
4	C	305	OLA	C3-C2-C1	-2.12	108.97	114.51
4	E	304	OLA	O2-C1-C2	2.12	120.70	114.00
4	A	309	OLA	O2-C1-C2	2.10	120.63	114.00
4	E	307	OLA	C3-C2-C1	-2.08	109.07	114.51
4	A	306	OLA	O2-C1-C2	2.07	120.54	114.00
4	A	307	OLA	O2-C1-C2	2.07	120.54	114.00
4	C	305	OLA	O2-C1-C2	2.06	120.52	114.00
4	E	308	OLA	O2-C1-C2	2.06	120.52	114.00
4	C	306	OLA	O2-C1-C2	2.06	120.50	114.00
4	A	305	OLA	C3-C2-C1	-2.05	109.15	114.51
4	F	307	OLA	O2-C1-C2	2.05	120.48	114.00
4	F	308	OLA	O2-C1-C2	2.04	120.45	114.00
4	D	307	OLA	O2-C1-C2	2.03	120.42	114.00
4	C	303	OLA	O2-C1-C2	2.02	120.39	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	305	OLA	O2-C1-C2	2.02	120.37	114.00
4	A	303	OLA	O2-C1-C2	2.01	120.35	114.00
4	A	311	OLA	C3-C2-C1	-2.01	109.27	114.51
4	C	308	OLA	O2-C1-C2	2.01	120.34	114.00
4	E	307	OLA	O2-C1-C2	2.01	120.34	114.00

There are no chirality outliers.

All (332) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	OLA	C11-C10-C9-C8
5	B	307	RET	C5-C6-C7-C8
5	D	309	RET	C5-C6-C7-C8
5	F	310	RET	C5-C6-C7-C8
4	A	309	OLA	C11-C10-C9-C8
4	A	310	OLA	C11-C10-C9-C8
4	B	304	OLA	C11-C10-C9-C8
4	D	306	OLA	C11-C10-C9-C8
4	E	303	OLA	C11-C10-C9-C8
4	E	307	OLA	C11-C10-C9-C8
4	E	309	OLA	C11-C10-C9-C8
4	F	306	OLA	C11-C10-C9-C8
4	C	303	OLA	C11-C10-C9-C8
4	F	309	OLA	C11-C10-C9-C8
4	C	306	OLA	C11-C10-C9-C8
4	A	311	OLA	C11-C12-C13-C14
4	F	309	OLA	C11-C12-C13-C14
4	C	308	OLA	C4-C5-C6-C7
5	A	312	RET	C7-C8-C9-C19
5	E	310	RET	C7-C8-C9-C19
5	F	310	RET	C7-C8-C9-C19
5	C	309	RET	C7-C8-C9-C19
5	A	312	RET	C7-C8-C9-C10
5	E	310	RET	C7-C8-C9-C10
5	F	310	RET	C7-C8-C9-C10
5	C	309	RET	C7-C8-C9-C10
4	A	308	OLA	C1-C2-C3-C4
4	A	307	OLA	C4-C5-C6-C7
4	B	306	OLA	C11-C10-C9-C8
4	E	304	OLA	C11-C10-C9-C8
4	D	307	OLA	C1-C2-C3-C4
4	C	304	OLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	303	OLA	C1-C2-C3-C4
4	C	308	OLA	C1-C2-C3-C4
4	A	304	OLA	C1-C2-C3-C4
4	A	305	OLA	C1-C2-C3-C4
4	A	307	OLA	C1-C2-C3-C4
4	B	305	OLA	C1-C2-C3-C4
4	D	308	OLA	C1-C2-C3-C4
4	E	305	OLA	C1-C2-C3-C4
4	E	308	OLA	C1-C2-C3-C4
4	F	307	OLA	C1-C2-C3-C4
4	F	309	OLA	C1-C2-C3-C4
4	C	307	OLA	C1-C2-C3-C4
4	A	309	OLA	C1-C2-C3-C4
4	A	311	OLA	C1-C2-C3-C4
4	E	304	OLA	C1-C2-C3-C4
4	E	306	OLA	C1-C2-C3-C4
4	E	307	OLA	C1-C2-C3-C4
4	F	308	OLA	C1-C2-C3-C4
4	C	302	OLA	C1-C2-C3-C4
4	C	305	OLA	C1-C2-C3-C4
4	B	303	OLA	C1-C2-C3-C4
4	D	306	OLA	C1-C2-C3-C4
4	A	305	OLA	C11-C10-C9-C8
4	A	307	OLA	C11-C10-C9-C8
4	B	303	OLA	C12-C13-C14-C15
5	B	307	RET	C7-C8-C9-C19
5	D	309	RET	C7-C8-C9-C19
5	B	307	RET	C7-C8-C9-C10
5	D	309	RET	C7-C8-C9-C10
4	F	308	OLA	C3-C4-C5-C6
4	C	303	OLA	C1-C2-C3-C4
4	E	309	OLA	C1-C2-C3-C4
4	D	306	OLA	C11-C12-C13-C14
4	E	306	OLA	C11-C12-C13-C14
4	C	305	OLA	C11-C12-C13-C14
4	C	308	OLA	C13-C14-C15-C16
4	E	305	OLA	C11-C10-C9-C8
4	C	304	OLA	C4-C5-C6-C7
4	F	308	OLA	C5-C6-C7-C8
4	B	304	OLA	C2-C3-C4-C5
4	F	306	OLA	C3-C4-C5-C6
4	D	307	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	A	309	OLA	C2-C3-C4-C5
4	C	302	OLA	C4-C5-C6-C7
4	F	308	OLA	C4-C5-C6-C7
4	F	309	OLA	C4-C5-C6-C7
4	E	303	OLA	C11-C12-C13-C14
4	E	309	OLA	C3-C4-C5-C6
4	B	304	OLA	C4-C5-C6-C7
4	C	306	OLA	C1-C2-C3-C4
5	A	312	RET	C5-C6-C7-C8
5	B	307	RET	C1-C6-C7-C8
5	E	310	RET	C5-C6-C7-C8
5	C	309	RET	C5-C6-C7-C8
4	E	306	OLA	C11-C10-C9-C8
4	A	303	OLA	C12-C13-C14-C15
4	C	308	OLA	C11-C12-C13-C14
4	E	305	OLA	C3-C4-C5-C6
4	C	307	OLA	C3-C4-C5-C6
4	E	309	OLA	C12-C13-C14-C15
4	A	309	OLA	C3-C4-C5-C6
4	B	306	OLA	C4-C5-C6-C7
4	B	303	OLA	C14-C15-C16-C17
4	F	307	OLA	C3-C4-C5-C6
4	C	306	OLA	C5-C6-C7-C8
4	A	307	OLA	C11-C12-C13-C14
4	F	308	OLA	C2-C3-C4-C5
4	F	307	OLA	C4-C5-C6-C7
4	B	303	OLA	C10-C11-C12-C13
4	A	309	OLA	C5-C6-C7-C8
4	D	307	OLA	C11-C12-C13-C14
4	C	305	OLA	C4-C5-C6-C7
4	E	309	OLA	C4-C5-C6-C7
4	A	304	OLA	C13-C14-C15-C16
4	F	306	OLA	C4-C5-C6-C7
4	A	305	OLA	C11-C12-C13-C14
4	A	308	OLA	C3-C4-C5-C6
4	C	307	OLA	C11-C12-C13-C14
4	B	304	OLA	C6-C7-C8-C9
4	D	306	OLA	C6-C7-C8-C9
4	A	311	OLA	C4-C5-C6-C7
4	A	305	OLA	C4-C5-C6-C7
4	E	308	OLA	C11-C10-C9-C8
4	C	305	OLA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	A	308	OLA	C4-C5-C6-C7
4	B	303	OLA	C3-C4-C5-C6
4	A	311	OLA	C14-C15-C16-C17
4	C	308	OLA	C12-C13-C14-C15
4	E	305	OLA	C4-C5-C6-C7
4	D	307	OLA	C14-C15-C16-C17
4	F	306	OLA	C1-C2-C3-C4
4	E	308	OLA	C11-C12-C13-C14
4	C	305	OLA	C12-C13-C14-C15
4	D	308	OLA	C3-C4-C5-C6
4	C	303	OLA	C12-C13-C14-C15
4	A	303	OLA	C11-C10-C9-C8
4	A	306	OLA	C11-C10-C9-C8
4	F	307	OLA	C11-C10-C9-C8
4	C	304	OLA	C11-C10-C9-C8
4	C	308	OLA	C11-C10-C9-C8
4	D	308	OLA	C5-C6-C7-C8
4	C	308	OLA	C10-C11-C12-C13
4	E	308	OLA	C5-C6-C7-C8
4	E	306	OLA	C4-C5-C6-C7
4	C	302	OLA	C5-C6-C7-C8
4	B	305	OLA	C3-C4-C5-C6
4	A	303	OLA	C4-C5-C6-C7
4	A	310	OLA	C10-C11-C12-C13
4	B	303	OLA	C13-C14-C15-C16
4	B	305	OLA	C11-C10-C9-C8
4	D	307	OLA	C11-C10-C9-C8
4	D	308	OLA	C11-C10-C9-C8
4	E	304	OLA	C4-C5-C6-C7
4	D	308	OLA	C12-C13-C14-C15
4	A	304	OLA	C4-C5-C6-C7
4	C	305	OLA	C14-C15-C16-C17
4	C	305	OLA	C3-C4-C5-C6
4	A	305	OLA	C2-C3-C4-C5
4	A	304	OLA	C3-C4-C5-C6
4	A	304	OLA	C11-C10-C9-C8
4	A	308	OLA	C11-C10-C9-C8
4	C	302	OLA	C11-C10-C9-C8
4	C	307	OLA	C11-C10-C9-C8
4	A	310	OLA	C13-C14-C15-C16
4	A	311	OLA	C12-C13-C14-C15
4	D	306	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	F	309	OLA	C15-C16-C17-C18
4	A	307	OLA	C12-C13-C14-C15
4	B	304	OLA	C1-C2-C3-C4
4	A	309	OLA	C12-C13-C14-C15
4	E	304	OLA	C14-C15-C16-C17
4	F	308	OLA	C12-C13-C14-C15
4	A	304	OLA	C5-C6-C7-C8
2	A	301	LFA	C3-C4-C5-C6
4	E	306	OLA	C5-C6-C7-C8
4	C	308	OLA	C3-C4-C5-C6
2	F	304	LFA	C6-C7-C8-C9
5	A	312	RET	C1-C6-C7-C8
5	D	309	RET	C1-C6-C7-C8
5	F	310	RET	C1-C6-C7-C8
4	A	304	OLA	C11-C12-C13-C14
4	A	310	OLA	C1-C2-C3-C4
4	F	308	OLA	C13-C14-C15-C16
4	E	309	OLA	C2-C3-C4-C5
4	E	308	OLA	C4-C5-C6-C7
4	F	306	OLA	C5-C6-C7-C8
4	C	303	OLA	C11-C12-C13-C14
4	A	306	OLA	C3-C4-C5-C6
4	E	307	OLA	C12-C13-C14-C15
4	A	311	OLA	C6-C7-C8-C9
4	D	307	OLA	C12-C13-C14-C15
4	B	304	OLA	C11-C12-C13-C14
4	E	304	OLA	C11-C12-C13-C14
4	A	307	OLA	C6-C7-C8-C9
4	C	303	OLA	C14-C15-C16-C17
4	D	307	OLA	C3-C4-C5-C6
4	A	309	OLA	C11-C12-C13-C14
4	C	306	OLA	C3-C4-C5-C6
4	F	307	OLA	C9-C10-C11-C12
4	A	308	OLA	C5-C6-C7-C8
4	C	304	OLA	C3-C4-C5-C6
4	A	309	OLA	C14-C15-C16-C17
5	E	310	RET	C1-C6-C7-C8
4	E	305	OLA	C9-C10-C11-C12
4	F	306	OLA	C9-C10-C11-C12
4	A	310	OLA	C5-C6-C7-C8
4	A	307	OLA	C3-C4-C5-C6
4	E	303	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	E	308	OLA	C14-C15-C16-C17
4	C	304	OLA	C13-C14-C15-C16
4	E	303	OLA	C7-C8-C9-C10
4	E	303	OLA	C9-C10-C11-C12
4	F	309	OLA	C13-C14-C15-C16
4	A	303	OLA	C11-C12-C13-C14
4	A	311	OLA	C2-C3-C4-C5
4	C	308	OLA	C7-C8-C9-C10
4	D	308	OLA	C4-C5-C6-C7
4	A	303	OLA	C7-C8-C9-C10
4	A	307	OLA	C9-C10-C11-C12
4	D	308	OLA	C9-C10-C11-C12
4	E	309	OLA	C7-C8-C9-C10
4	F	307	OLA	C7-C8-C9-C10
4	B	305	OLA	C14-C15-C16-C17
4	B	303	OLA	C15-C16-C17-C18
4	D	307	OLA	C7-C8-C9-C10
4	C	307	OLA	C9-C10-C11-C12
2	D	302	LFA	C11-C10-C9-C8
4	E	307	OLA	C3-C4-C5-C6
4	E	304	OLA	C7-C8-C9-C10
4	A	310	OLA	C3-C4-C5-C6
4	E	308	OLA	C13-C14-C15-C16
4	A	305	OLA	O1-C1-C2-C3
4	C	306	OLA	C11-C12-C13-C14
4	B	305	OLA	C4-C5-C6-C7
4	B	306	OLA	C3-C4-C5-C6
4	D	308	OLA	C2-C3-C4-C5
4	A	306	OLA	C2-C3-C4-C5
4	F	309	OLA	C3-C4-C5-C6
4	B	305	OLA	O1-C1-C2-C3
4	B	306	OLA	O1-C1-C2-C3
4	A	306	OLA	C4-C5-C6-C7
5	C	309	RET	C1-C6-C7-C8
4	A	303	OLA	O1-C1-C2-C3
4	B	305	OLA	O2-C1-C2-C3
4	D	306	OLA	O1-C1-C2-C3
4	D	306	OLA	O2-C1-C2-C3
4	E	303	OLA	O1-C1-C2-C3
4	E	306	OLA	C6-C7-C8-C9
4	E	303	OLA	O2-C1-C2-C3
4	A	305	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	301	LFA	C1-C2-C3-C4
4	A	305	OLA	O2-C1-C2-C3
4	B	306	OLA	O2-C1-C2-C3
4	E	306	OLA	O2-C1-C2-C3
4	A	304	OLA	O2-C1-C2-C3
4	A	311	OLA	O1-C1-C2-C3
4	D	307	OLA	C6-C7-C8-C9
4	F	306	OLA	C12-C13-C14-C15
4	A	303	OLA	O2-C1-C2-C3
4	A	306	OLA	O2-C1-C2-C3
4	C	305	OLA	C5-C6-C7-C8
4	A	304	OLA	O1-C1-C2-C3
4	E	306	OLA	O1-C1-C2-C3
2	D	302	LFA	C4-C5-C6-C7
2	F	303	LFA	C3-C4-C5-C6
4	E	307	OLA	O2-C1-C2-C3
4	A	304	OLA	C9-C10-C11-C12
4	E	305	OLA	C7-C8-C9-C10
4	E	308	OLA	C7-C8-C9-C10
4	E	308	OLA	C9-C10-C11-C12
4	C	306	OLA	C9-C10-C11-C12
4	A	306	OLA	O1-C1-C2-C3
4	C	302	OLA	O2-C1-C2-C3
4	A	310	OLA	O1-C1-C2-C3
4	A	310	OLA	O2-C1-C2-C3
4	A	311	OLA	O2-C1-C2-C3
4	B	305	OLA	C7-C8-C9-C10
4	D	306	OLA	C7-C8-C9-C10
4	F	306	OLA	C7-C8-C9-C10
4	C	305	OLA	C7-C8-C9-C10
4	C	302	OLA	O1-C1-C2-C3
4	C	303	OLA	O1-C1-C2-C3
4	E	307	OLA	C6-C7-C8-C9
4	F	307	OLA	O2-C1-C2-C3
4	C	303	OLA	O2-C1-C2-C3
4	B	303	OLA	C7-C8-C9-C10
4	C	303	OLA	C7-C8-C9-C10
4	E	304	OLA	O2-C1-C2-C3
4	E	305	OLA	C12-C13-C14-C15
4	E	306	OLA	C14-C15-C16-C17
4	C	302	OLA	C11-C12-C13-C14
4	A	303	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	308	OLA	C9-C10-C11-C12
4	B	303	OLA	C9-C10-C11-C12
4	C	304	OLA	C9-C10-C11-C12
4	E	304	OLA	O1-C1-C2-C3
4	A	310	OLA	C9-C10-C11-C12
4	B	304	OLA	C9-C10-C11-C12
4	B	306	OLA	C7-C8-C9-C10
4	E	304	OLA	C9-C10-C11-C12
4	E	308	OLA	C12-C13-C14-C15
4	F	307	OLA	C14-C15-C16-C17
4	E	307	OLA	O1-C1-C2-C3
4	F	308	OLA	O2-C1-C2-C3
4	F	308	OLA	O1-C1-C2-C3
4	D	307	OLA	C9-C10-C11-C12
4	C	302	OLA	C7-C8-C9-C10
4	F	307	OLA	O1-C1-C2-C3
4	E	308	OLA	O2-C1-C2-C3
4	A	309	OLA	C7-C8-C9-C10
4	A	310	OLA	C7-C8-C9-C10
4	C	307	OLA	C12-C13-C14-C15
4	A	306	OLA	C7-C8-C9-C10
4	A	306	OLA	C9-C10-C11-C12
4	E	306	OLA	C9-C10-C11-C12
4	C	306	OLA	C7-C8-C9-C10
4	C	307	OLA	C7-C8-C9-C10
4	A	304	OLA	C6-C7-C8-C9
4	E	307	OLA	C14-C15-C16-C17
4	D	307	OLA	C13-C14-C15-C16
4	C	302	OLA	C13-C14-C15-C16
4	C	305	OLA	C10-C11-C12-C13
4	F	307	OLA	C2-C3-C4-C5
4	E	308	OLA	O1-C1-C2-C3
4	E	304	OLA	C12-C13-C14-C15
4	A	305	OLA	C5-C6-C7-C8
2	D	301	LFA	C1-C2-C3-C4
4	E	305	OLA	O2-C1-C2-C3
4	D	308	OLA	C6-C7-C8-C9
4	B	305	OLA	C12-C13-C14-C15
4	A	307	OLA	C13-C14-C15-C16
4	C	307	OLA	O2-C1-C2-C3
4	C	305	OLA	O2-C1-C2-C3
4	C	306	OLA	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	304	OLA	C5-C6-C7-C8
4	B	303	OLA	O2-C1-C2-C3
4	B	304	OLA	C5-C6-C7-C8
2	F	304	LFA	C7-C8-C9-C10
4	B	303	OLA	C6-C7-C8-C9
4	C	306	OLA	O1-C1-C2-C3

There are no ring outliers.

39 monomers are involved in 77 short contacts:

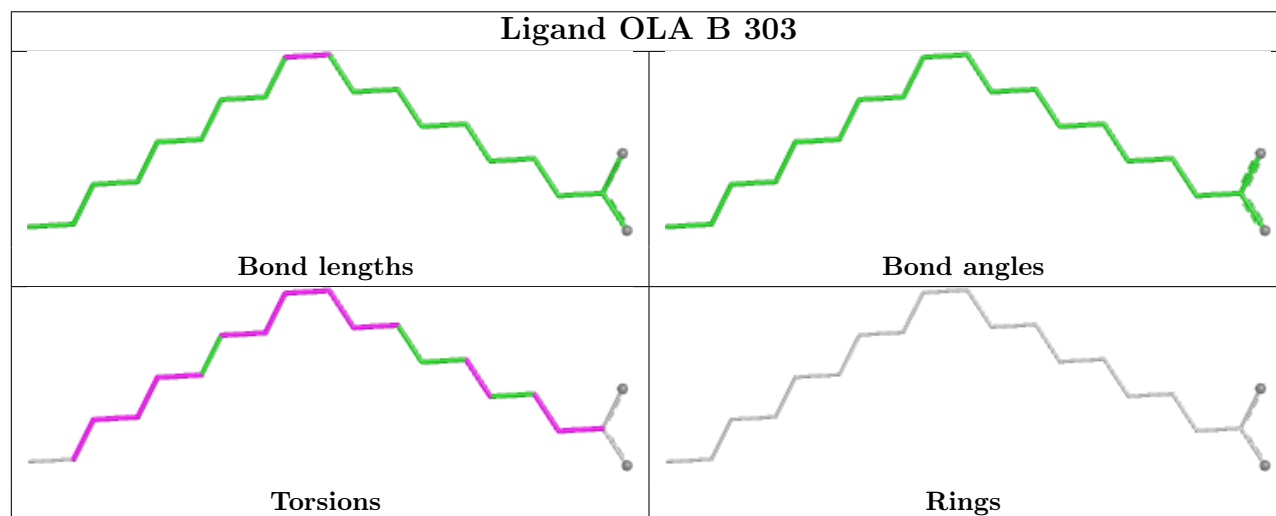
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	303	LFA	2	0
4	B	303	OLA	1	0
4	B	305	OLA	3	0
4	D	307	OLA	2	0
4	C	305	OLA	8	0
2	A	301	LFA	1	0
4	A	307	OLA	1	0
5	C	309	RET	1	0
5	E	310	RET	2	0
4	A	309	OLA	5	0
4	F	308	OLA	1	0
4	A	310	OLA	5	0
4	A	308	OLA	4	0
4	A	303	OLA	2	0
4	C	308	OLA	1	0
4	E	303	OLA	3	0
4	A	311	OLA	4	0
4	C	304	OLA	1	0
5	A	312	RET	1	0
4	D	308	OLA	5	0
2	F	304	LFA	1	0
2	D	301	LFA	1	0
4	F	309	OLA	1	0
4	E	304	OLA	1	0
4	A	304	OLA	1	0
2	B	301	LFA	1	0
2	F	302	LFA	1	0
2	F	303	LFA	1	0
4	F	307	OLA	4	0
4	E	309	OLA	2	0
5	D	309	RET	1	0

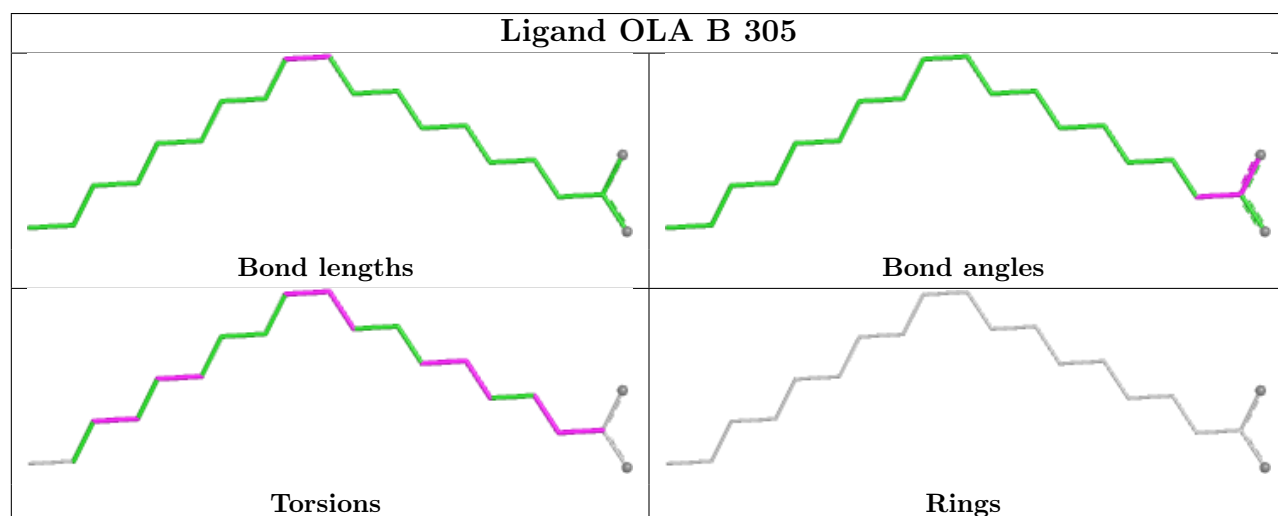
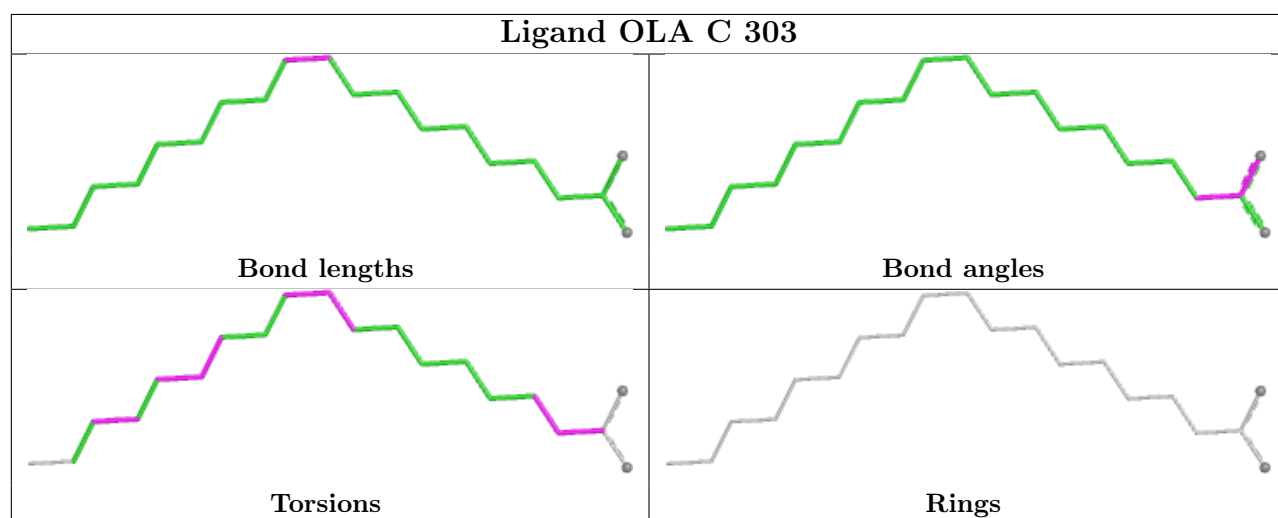
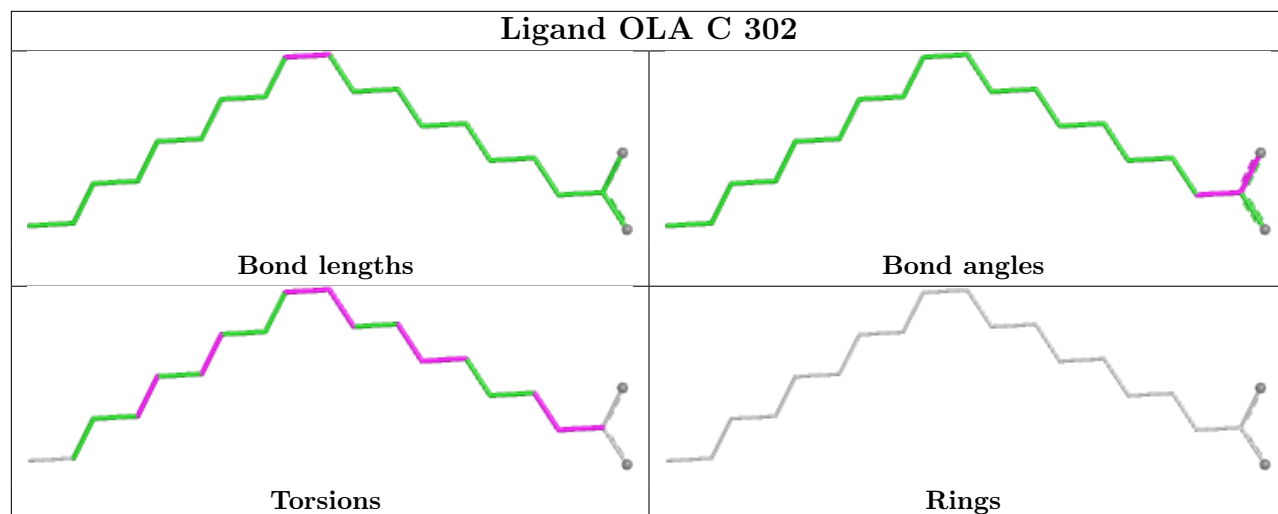
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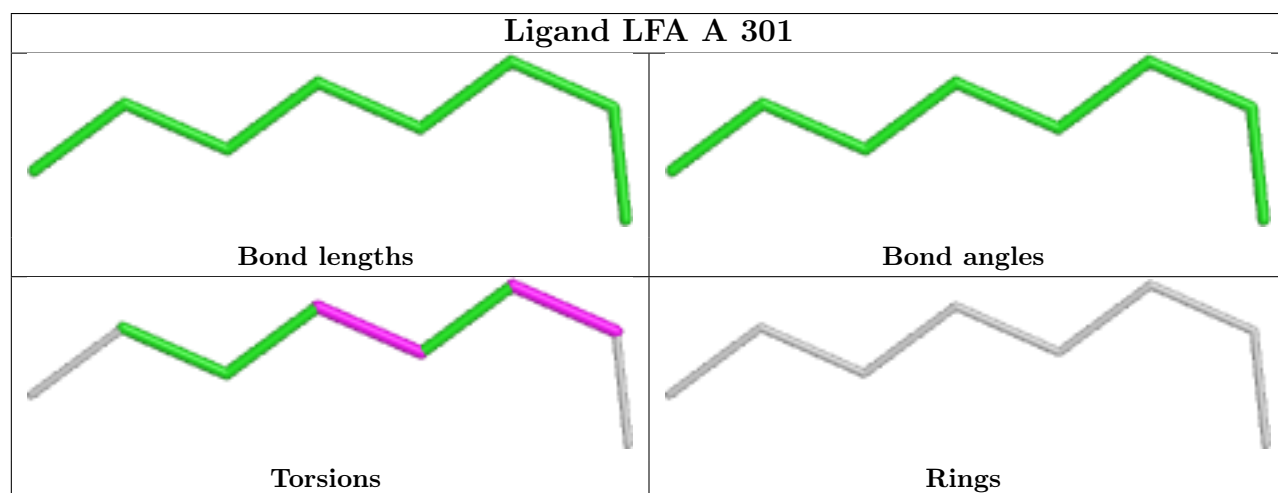
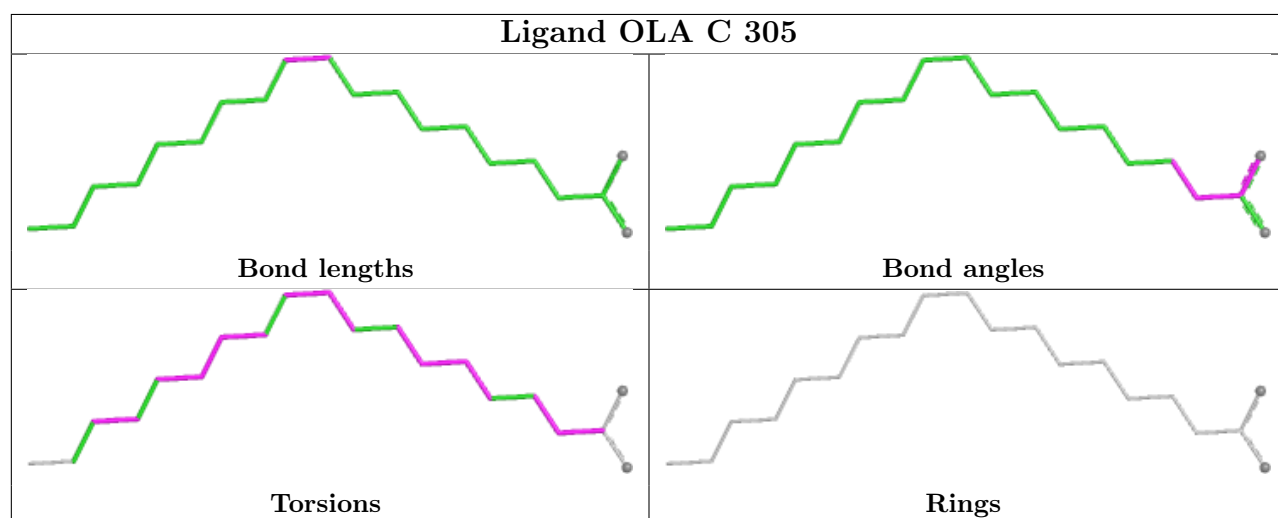
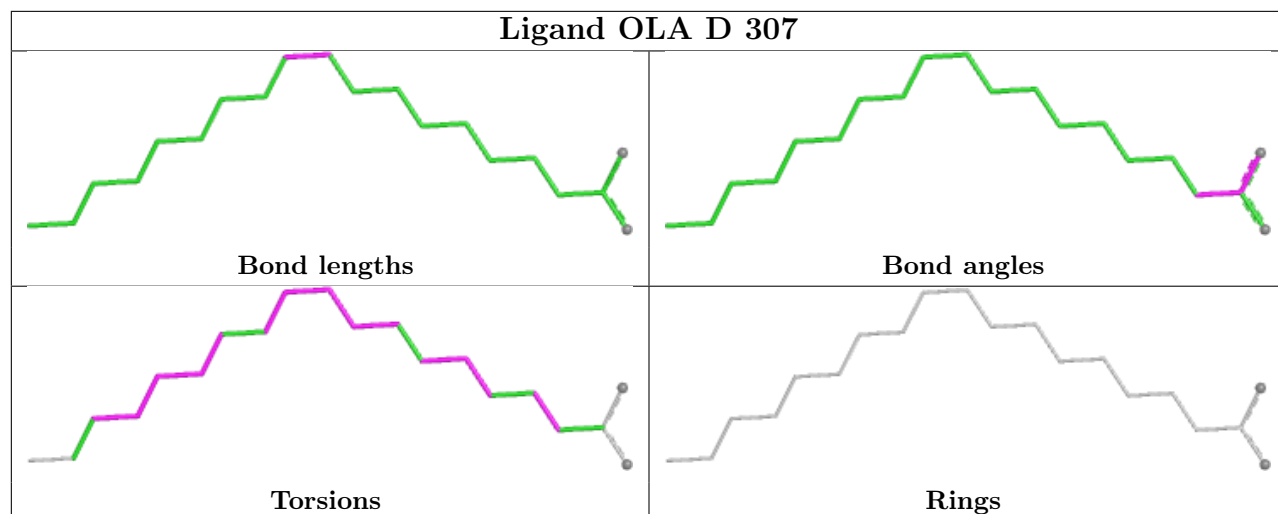
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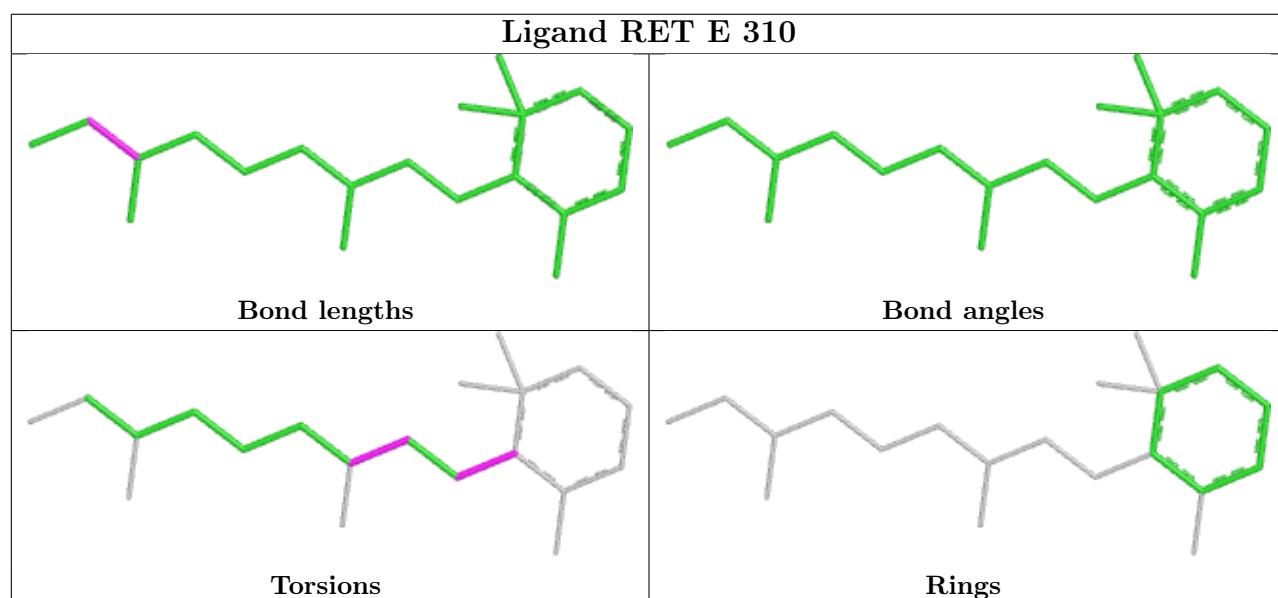
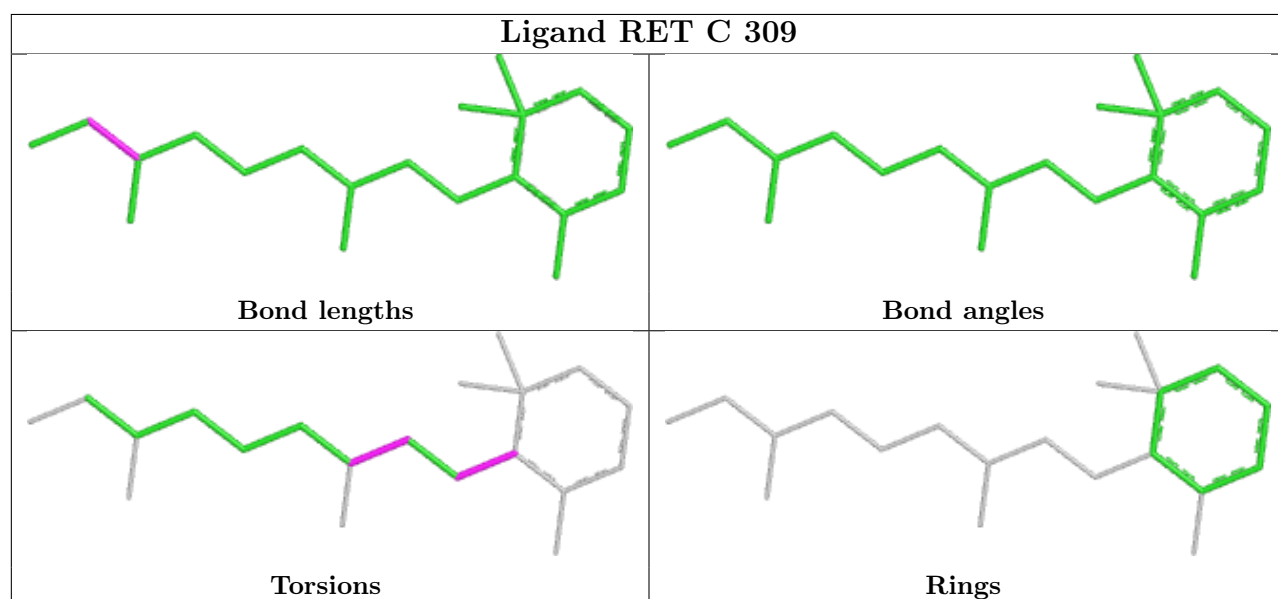
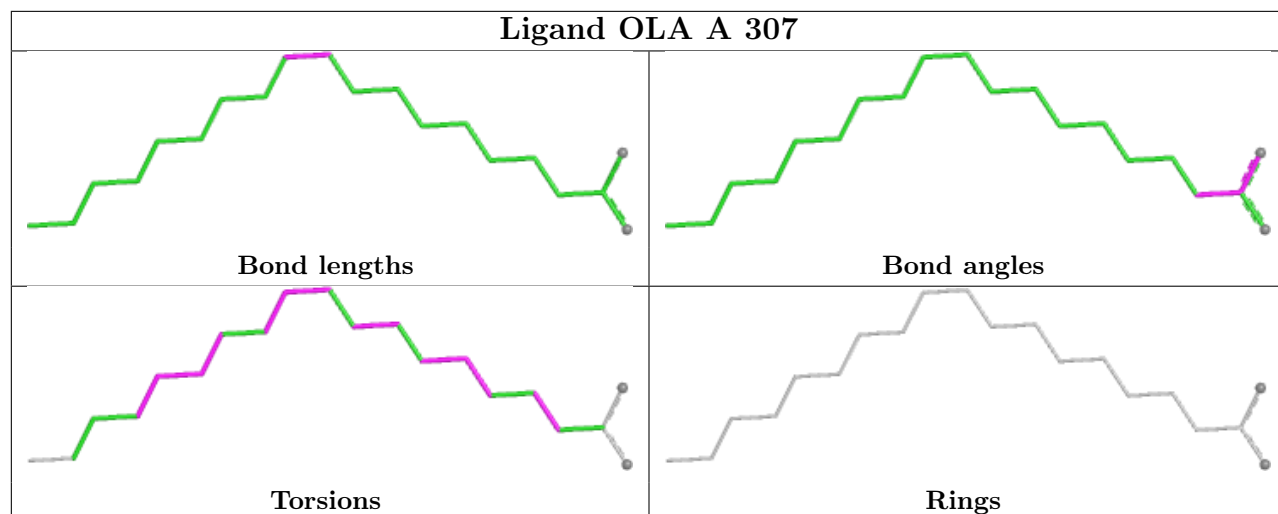
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	310	RET	1	0
4	E	308	OLA	2	0
4	C	306	OLA	1	0
2	E	301	LFA	4	0
5	B	307	RET	3	0
2	D	302	LFA	1	0
4	A	305	OLA	1	0
4	E	307	OLA	3	0

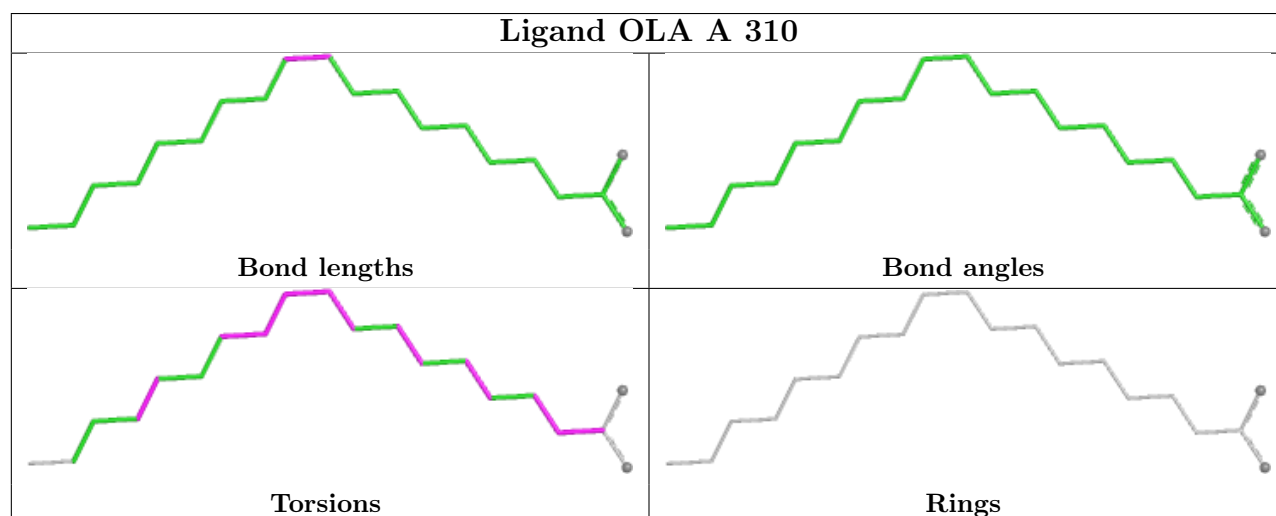
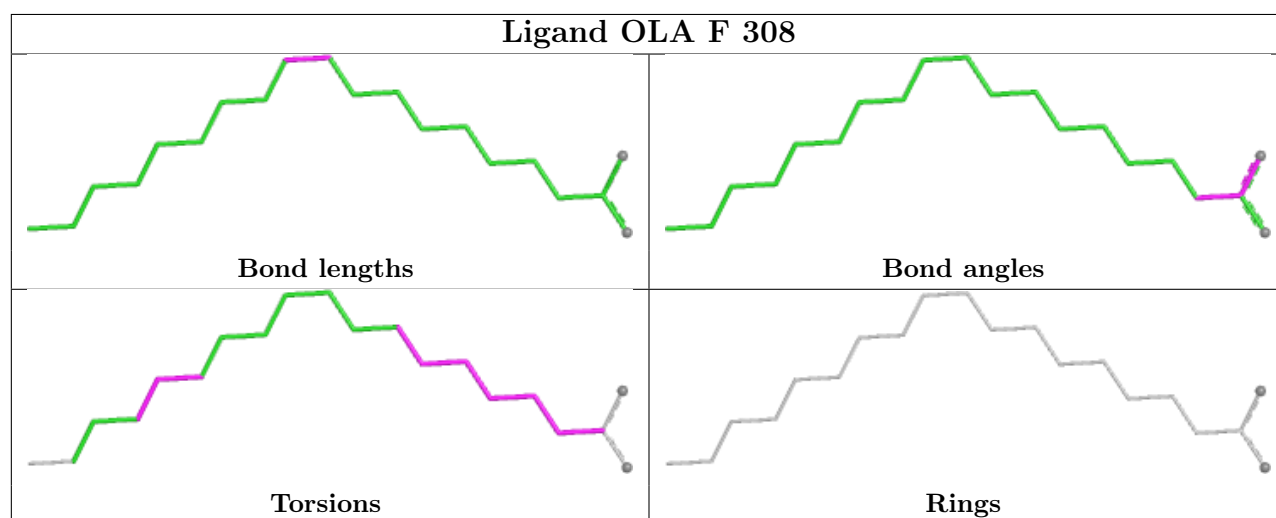
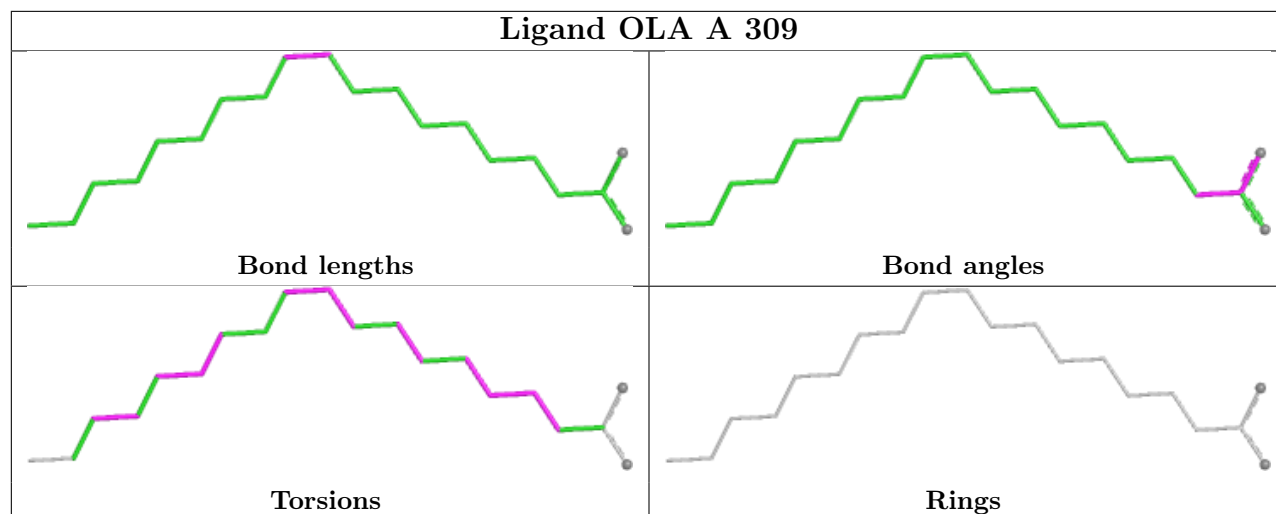
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

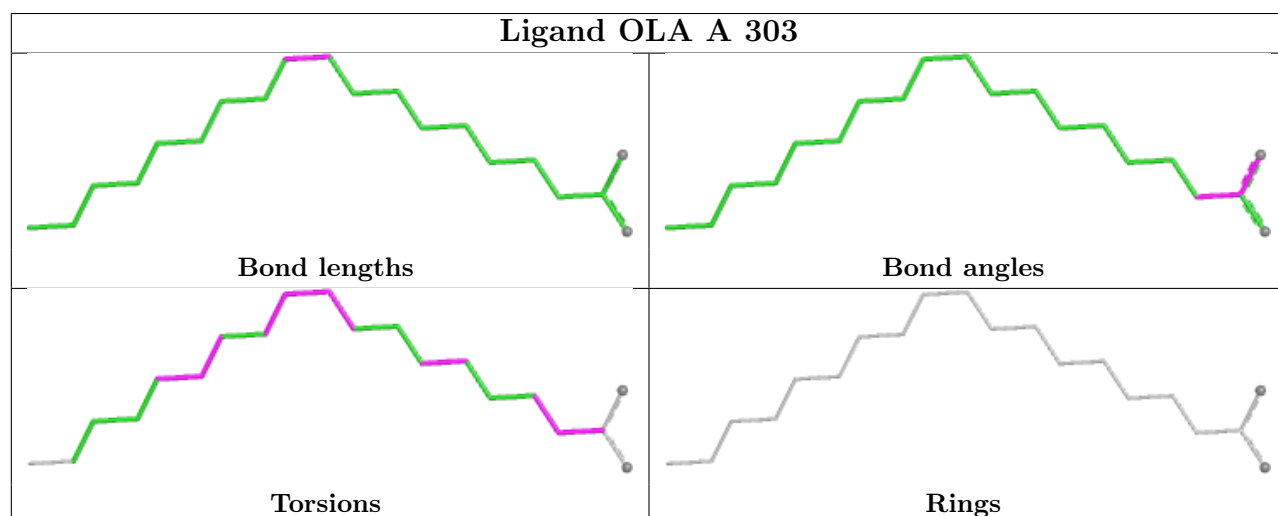
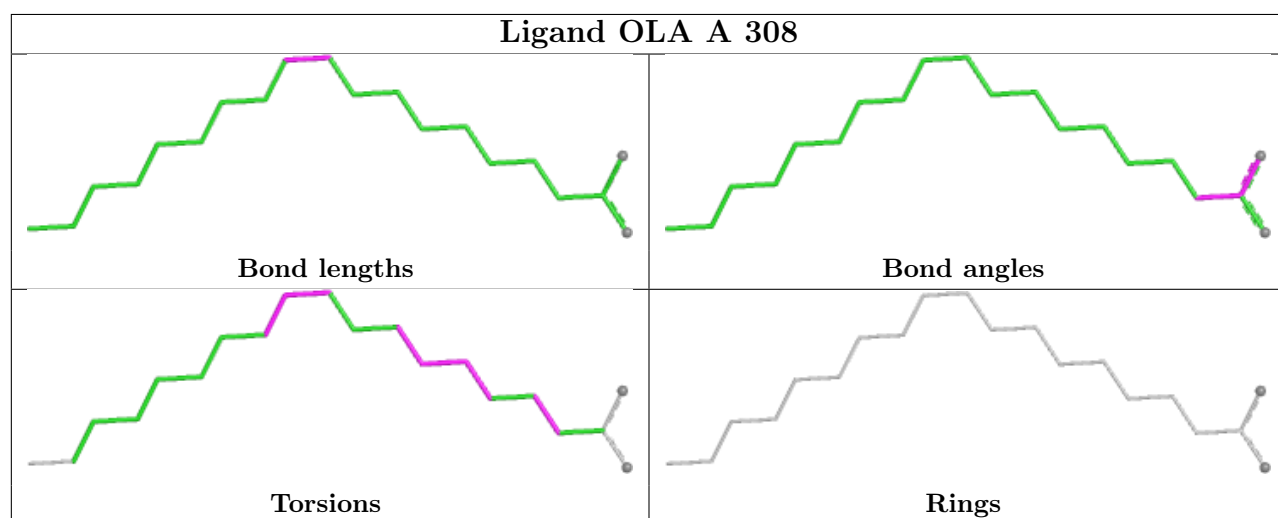
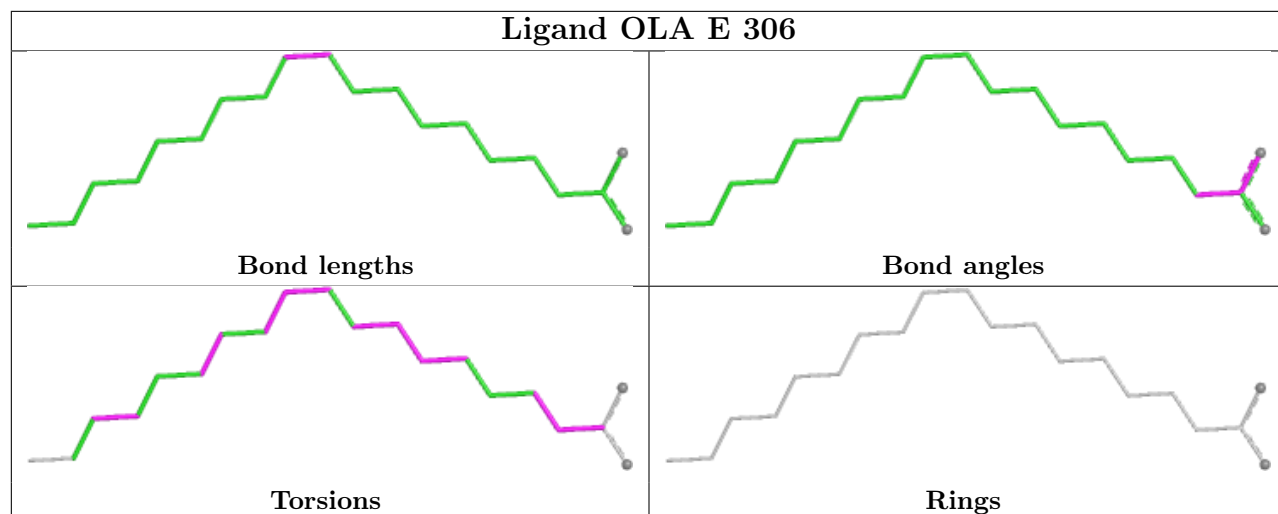


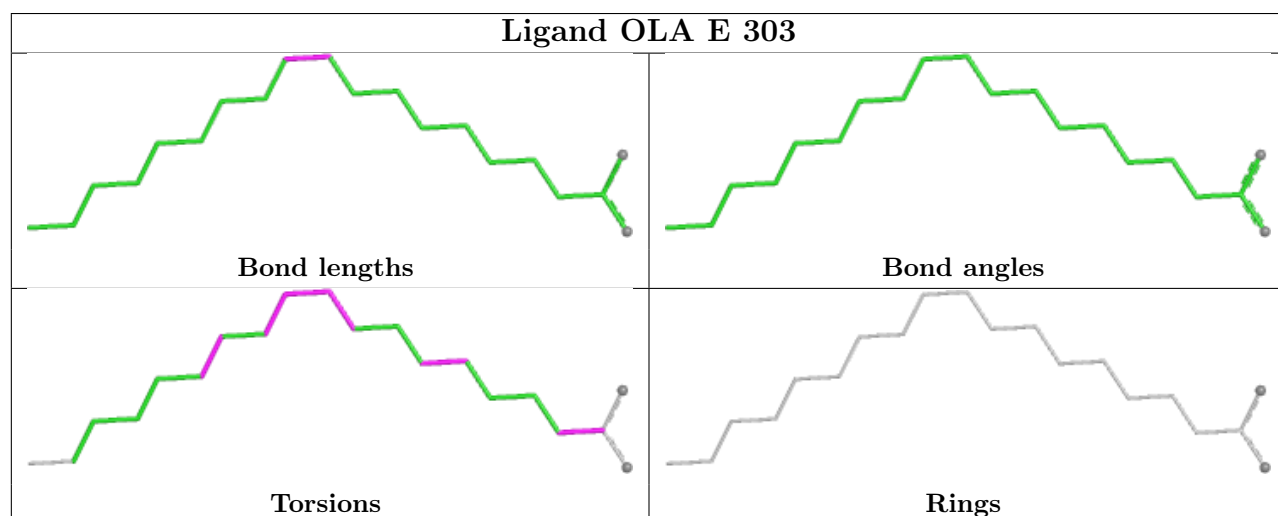
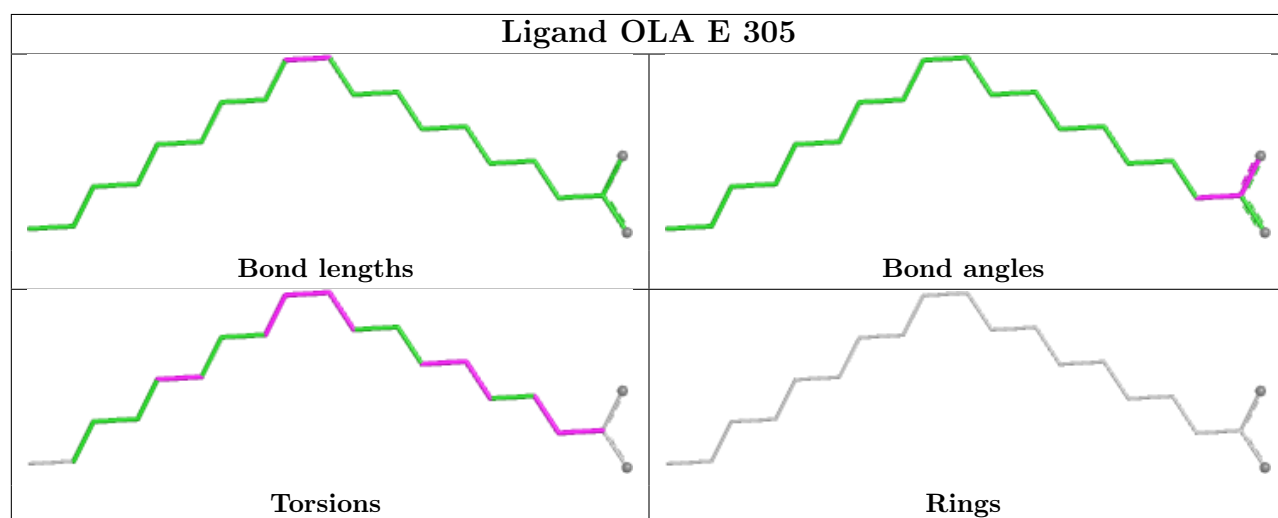
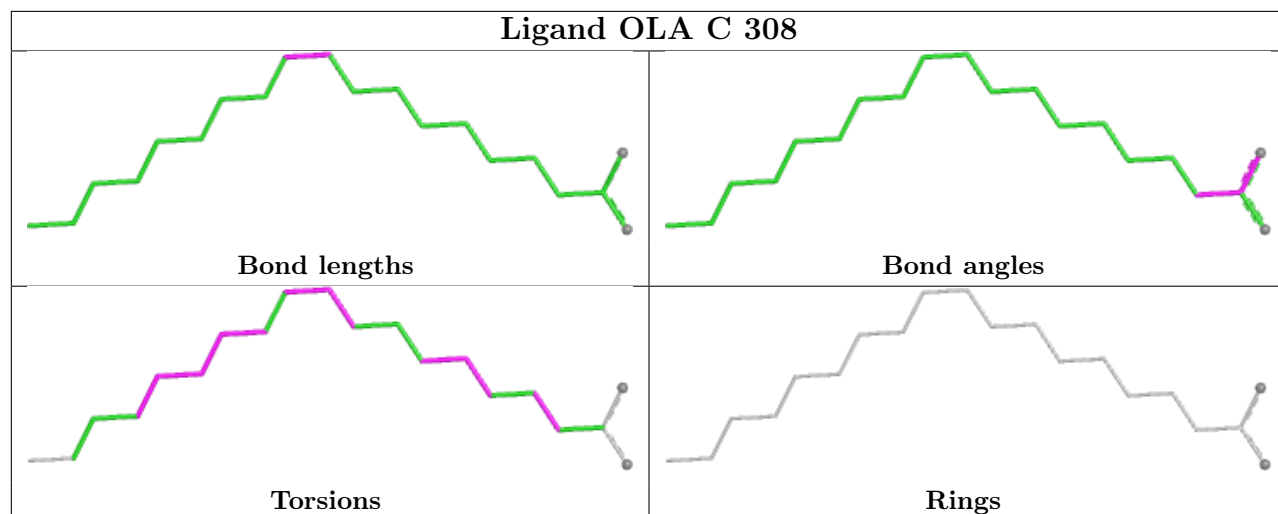


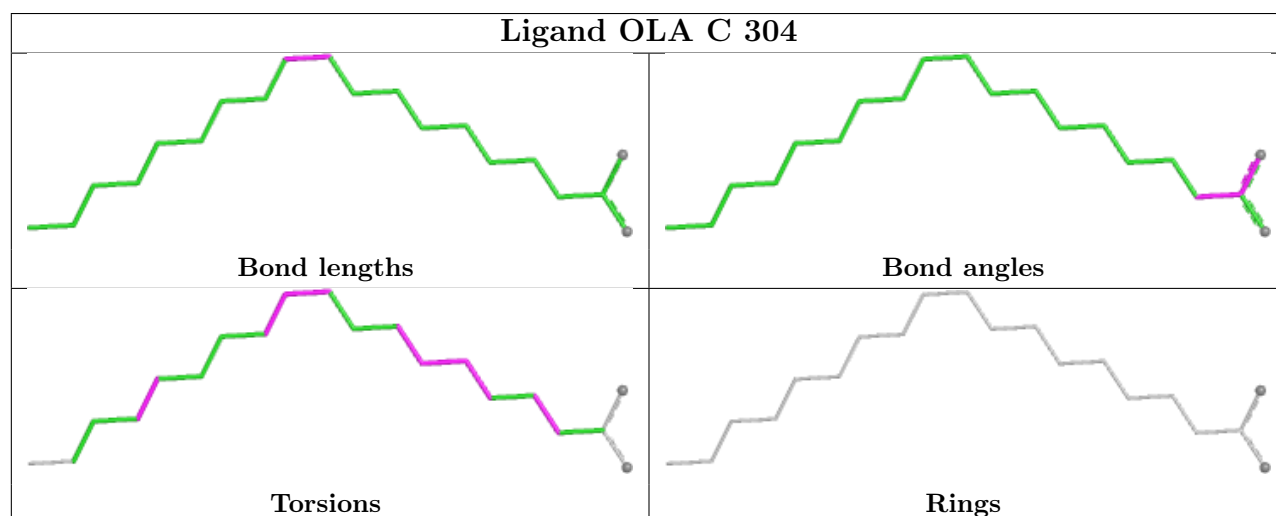
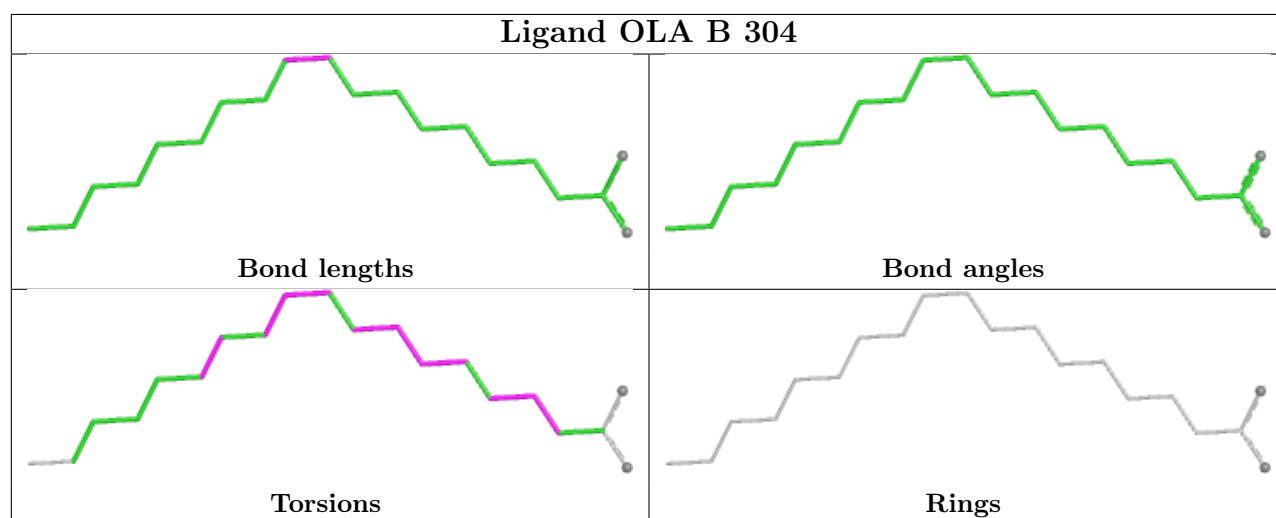
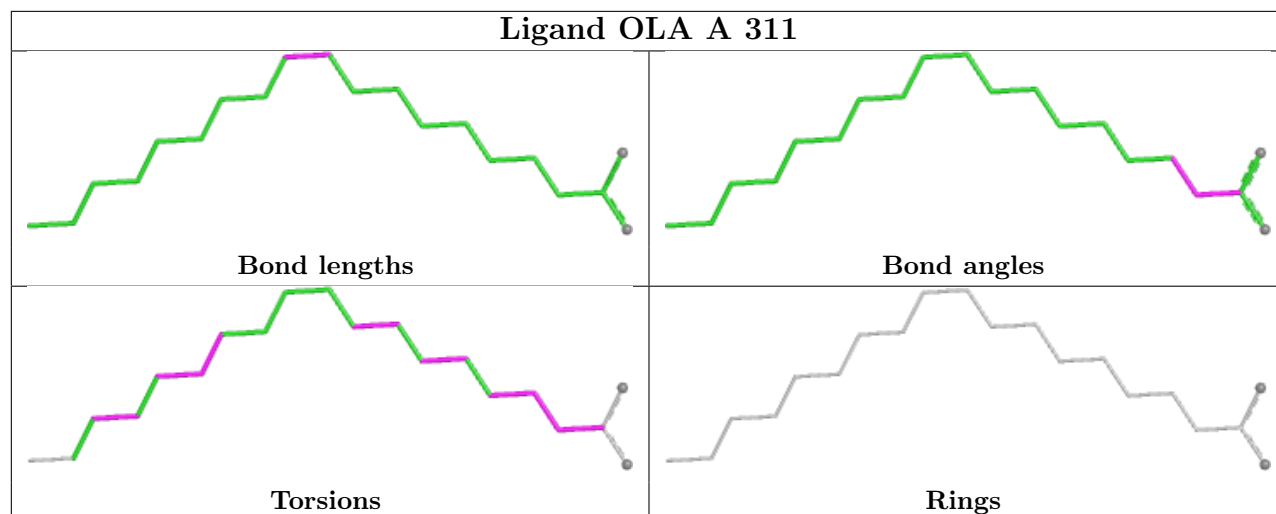


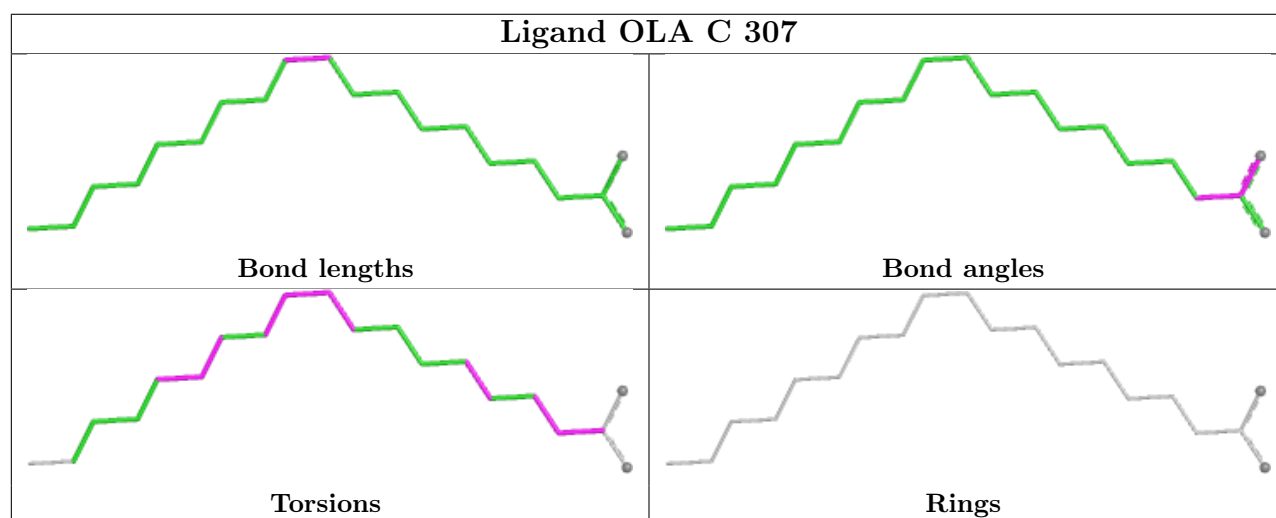
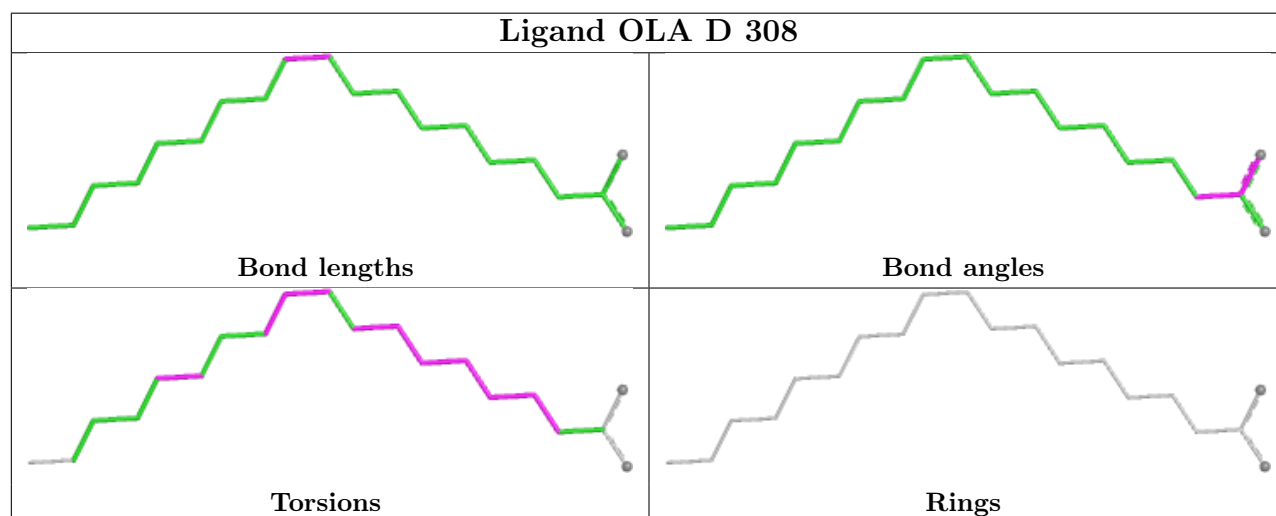
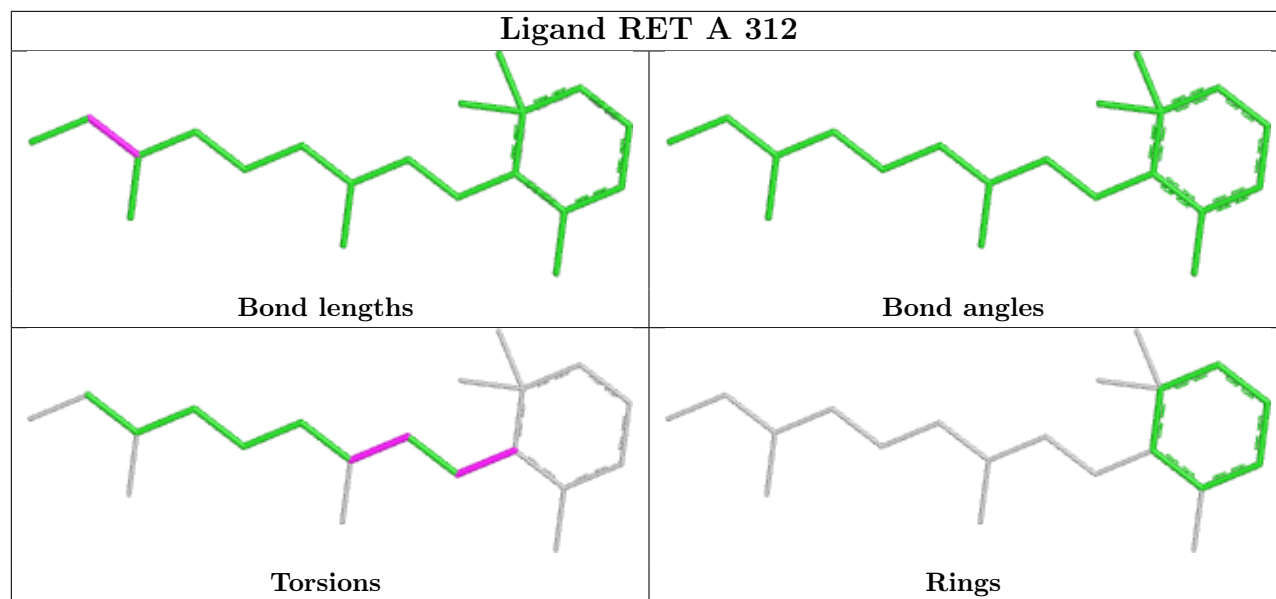


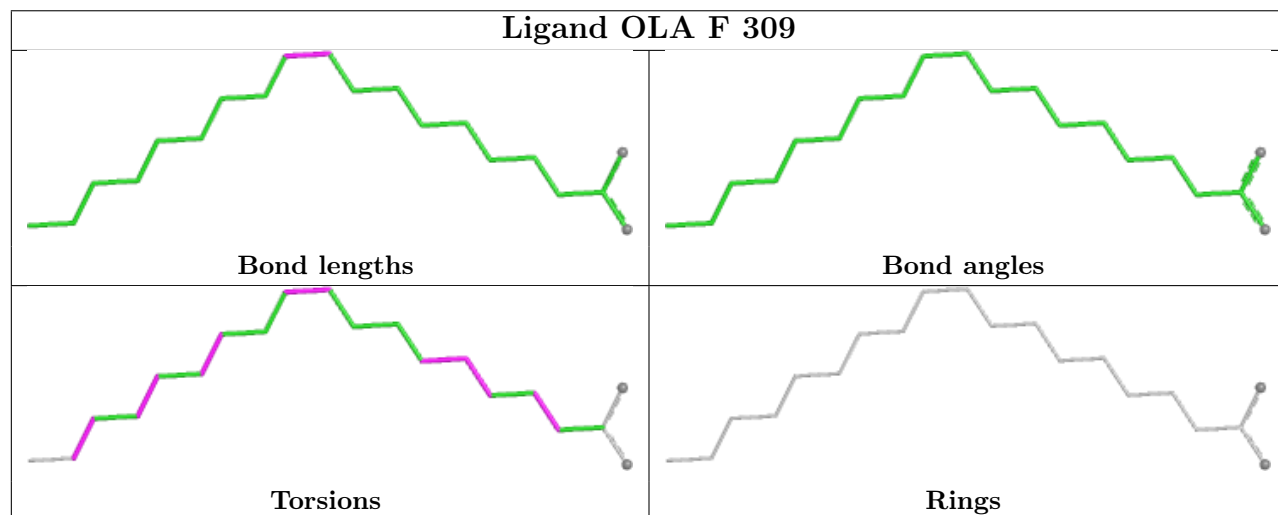
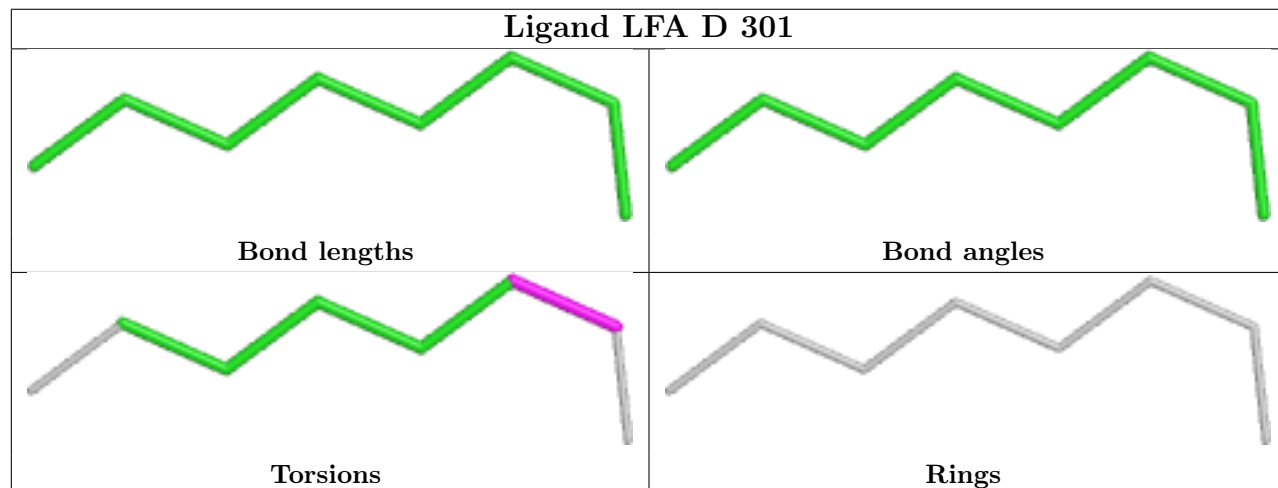
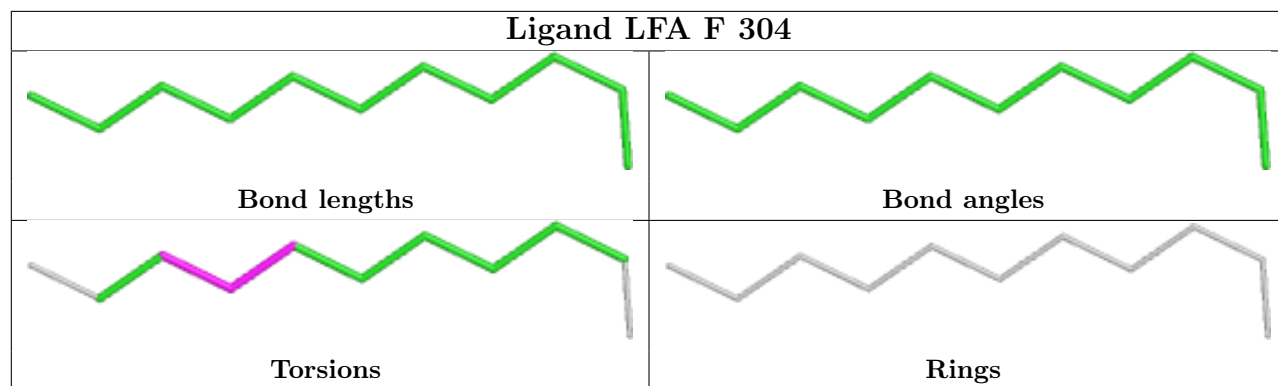


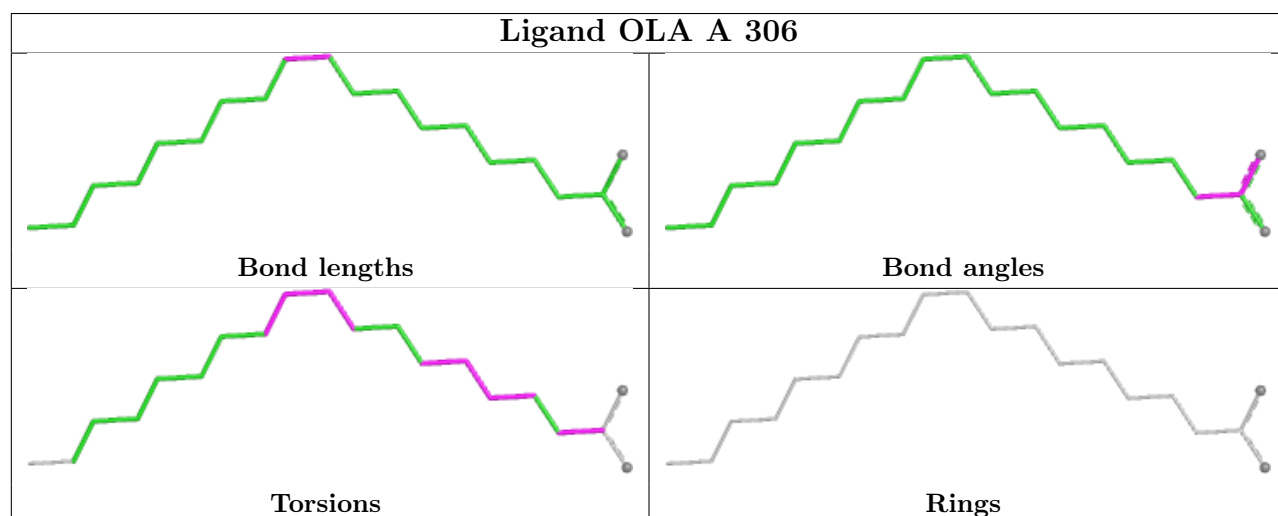
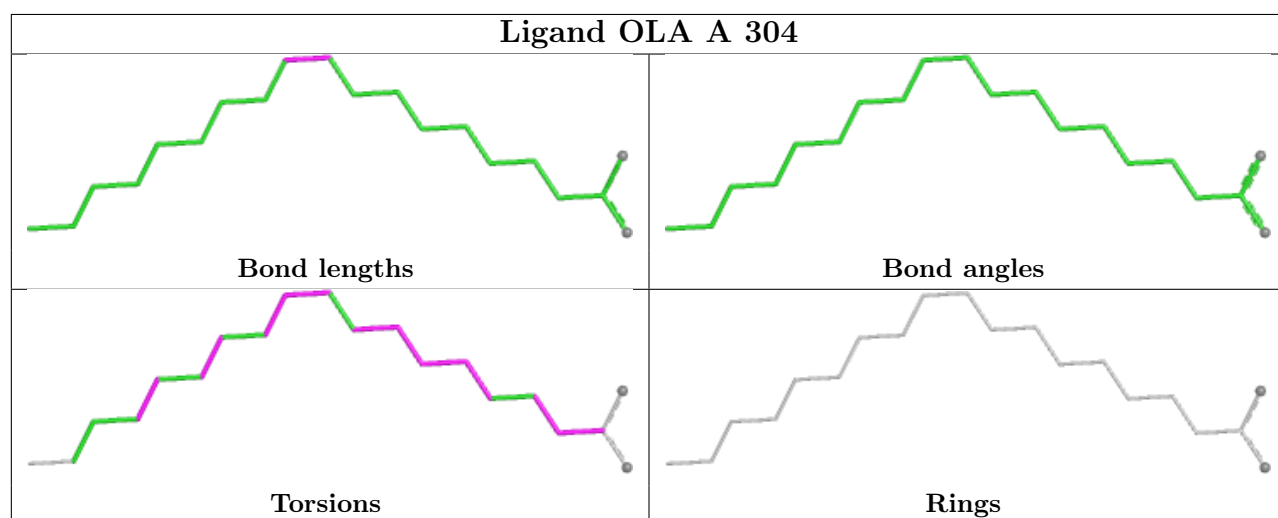
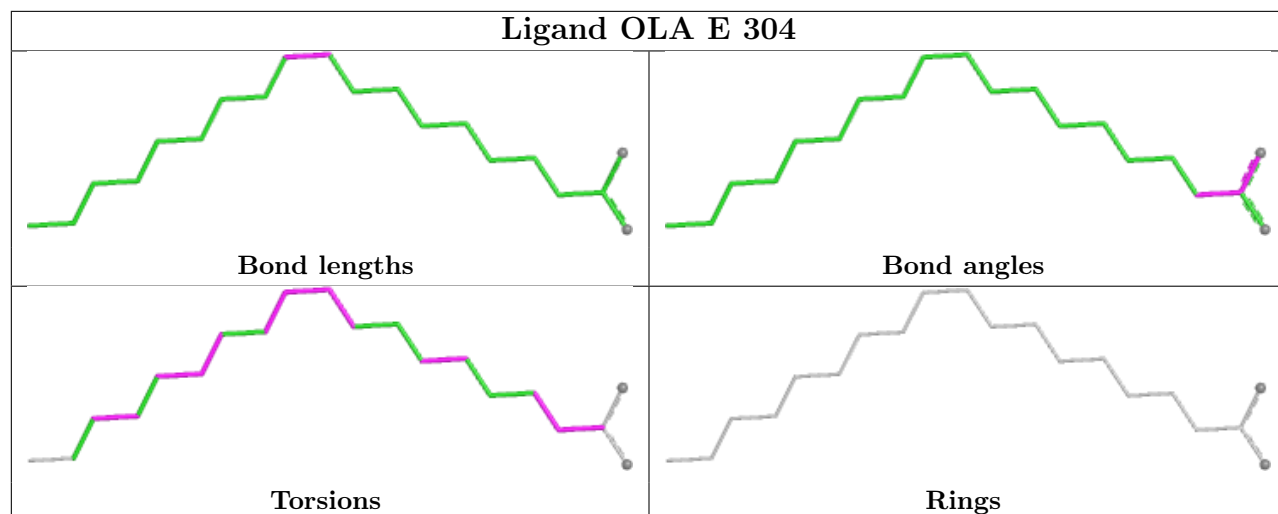


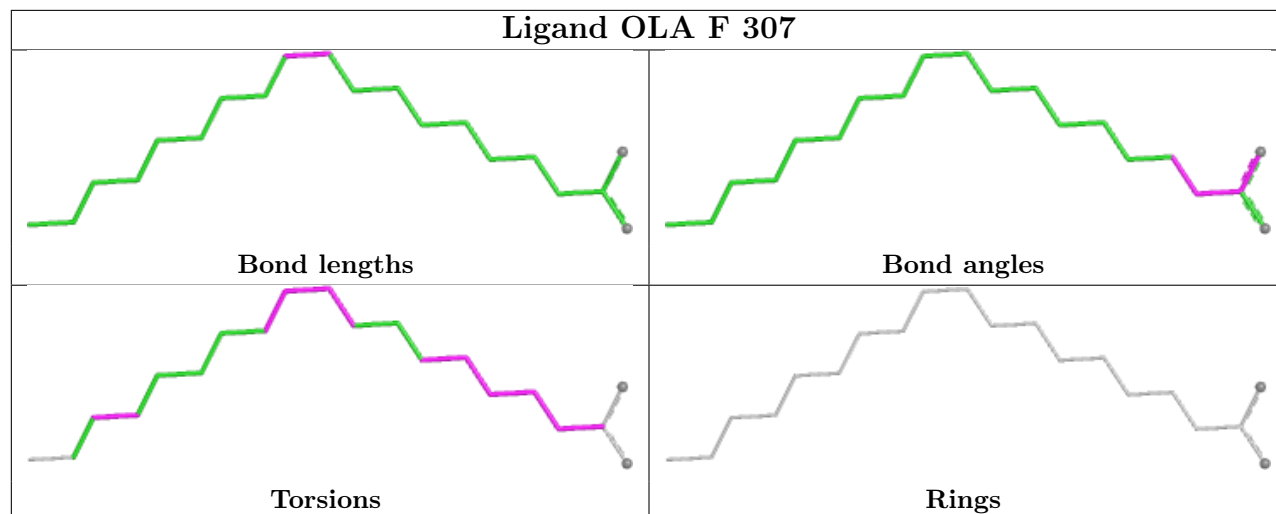
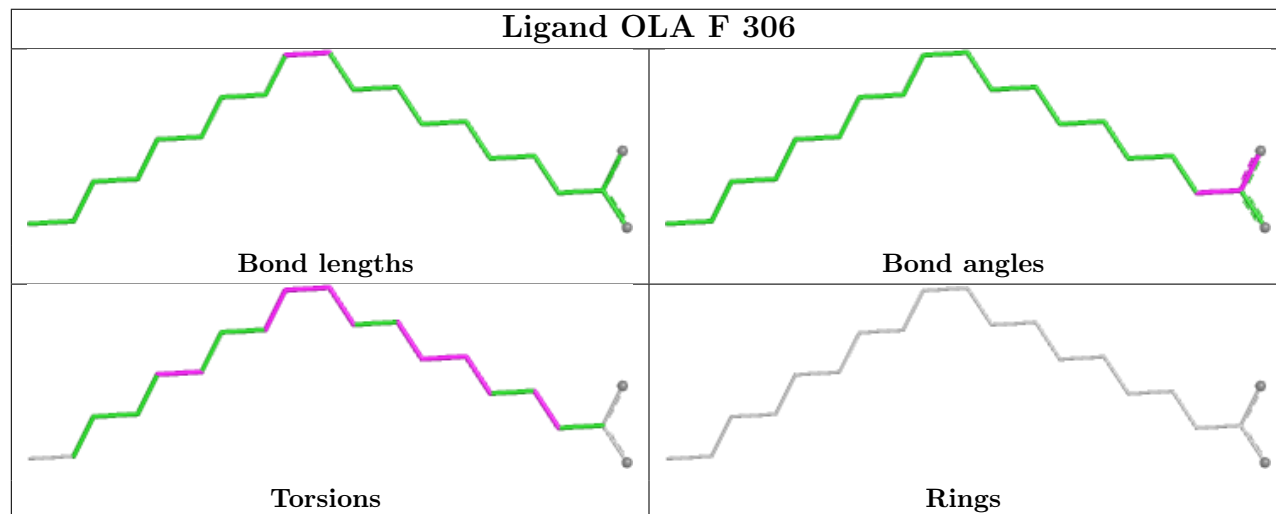
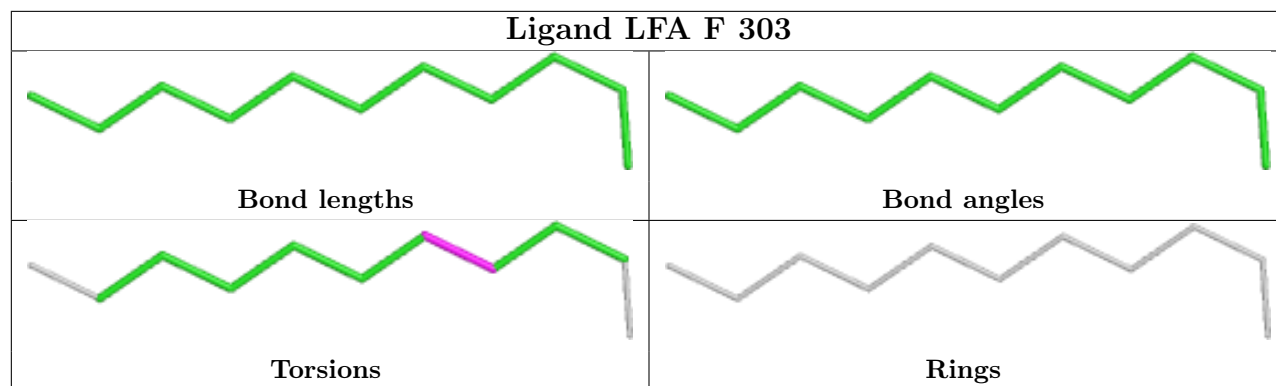


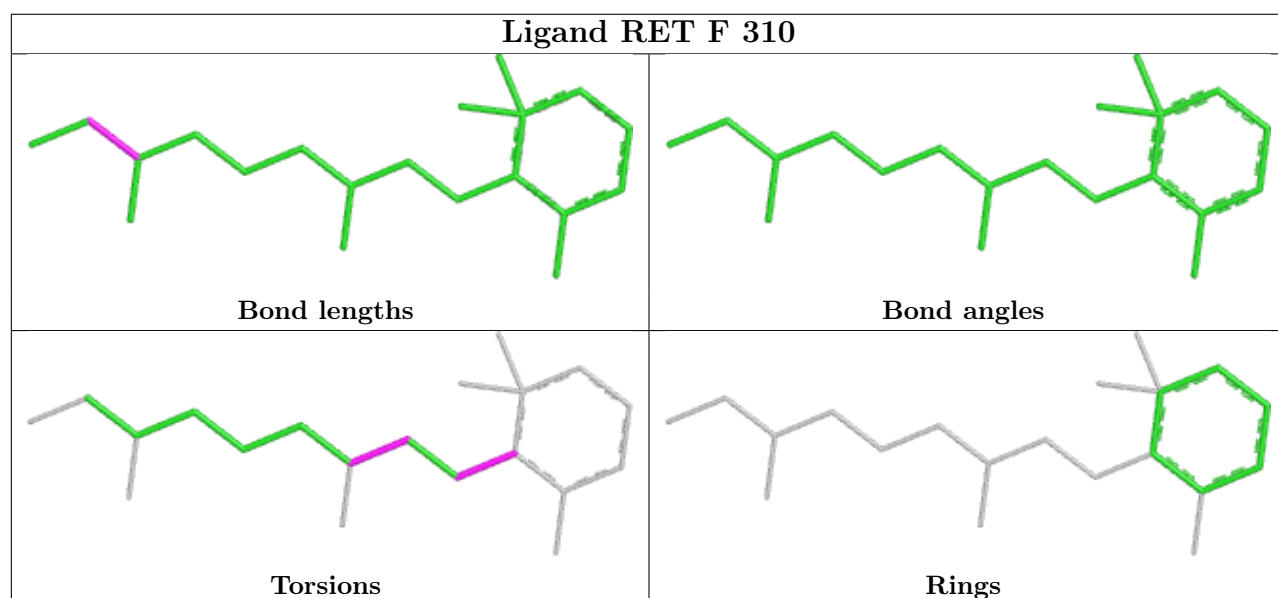
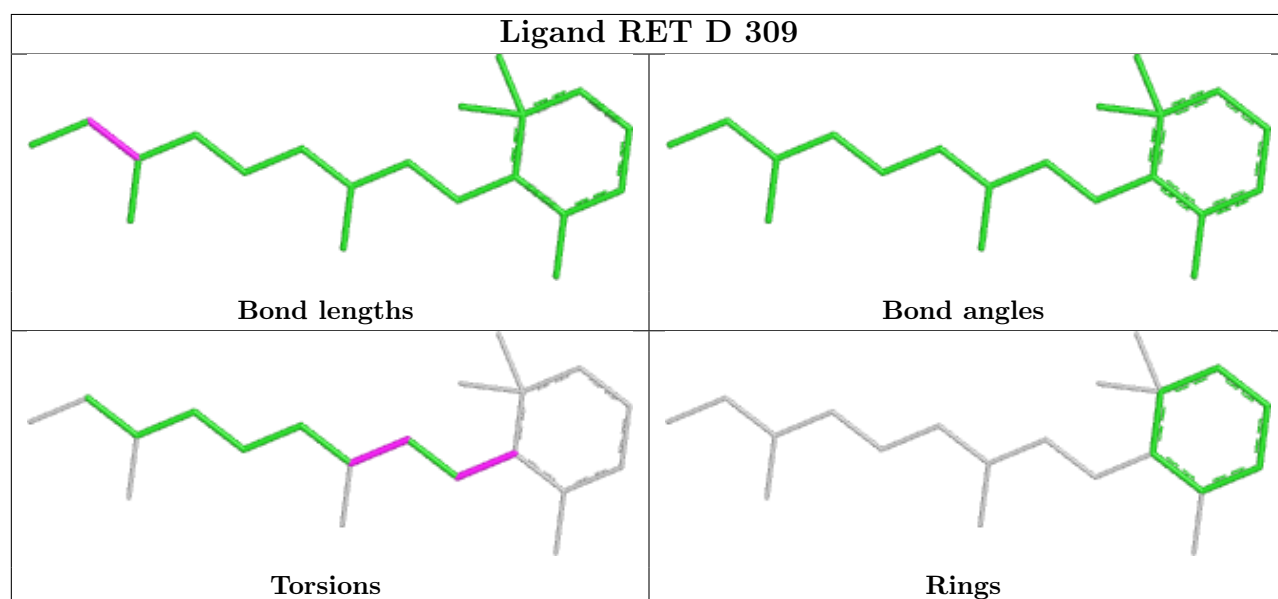
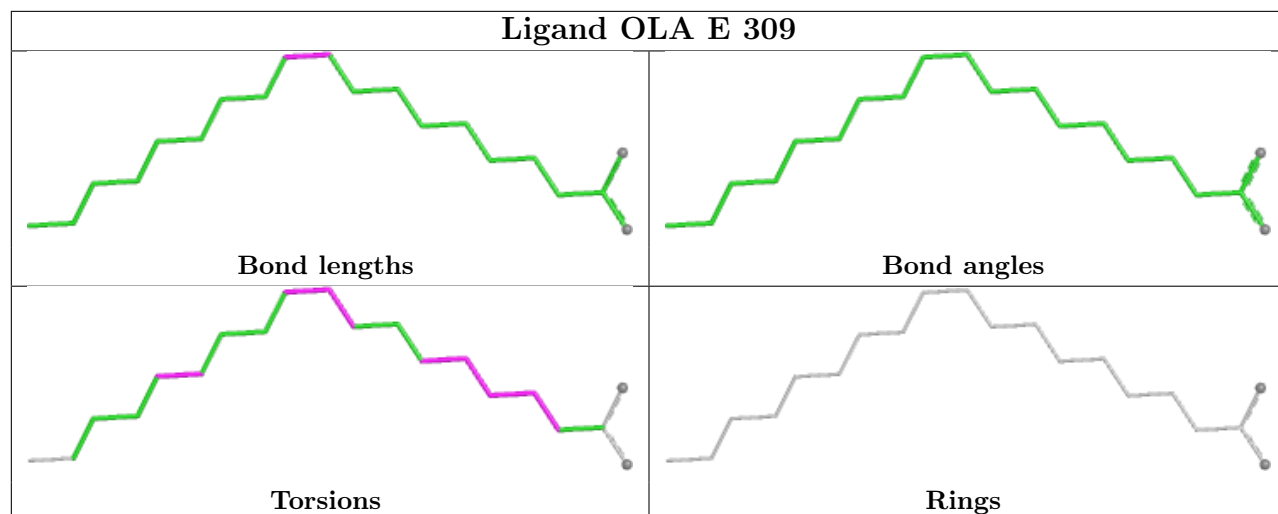


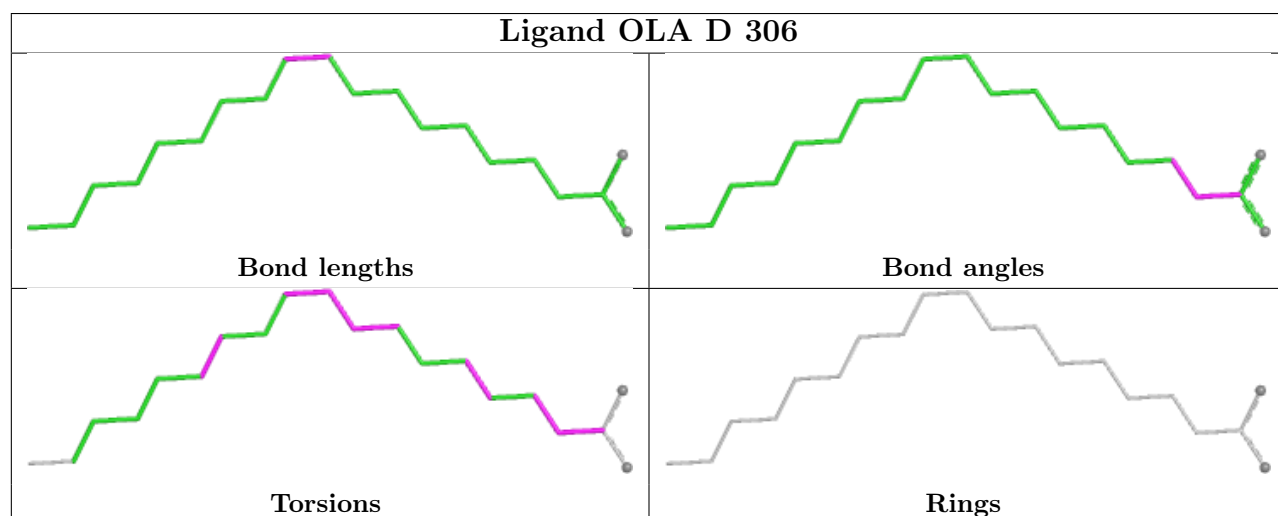
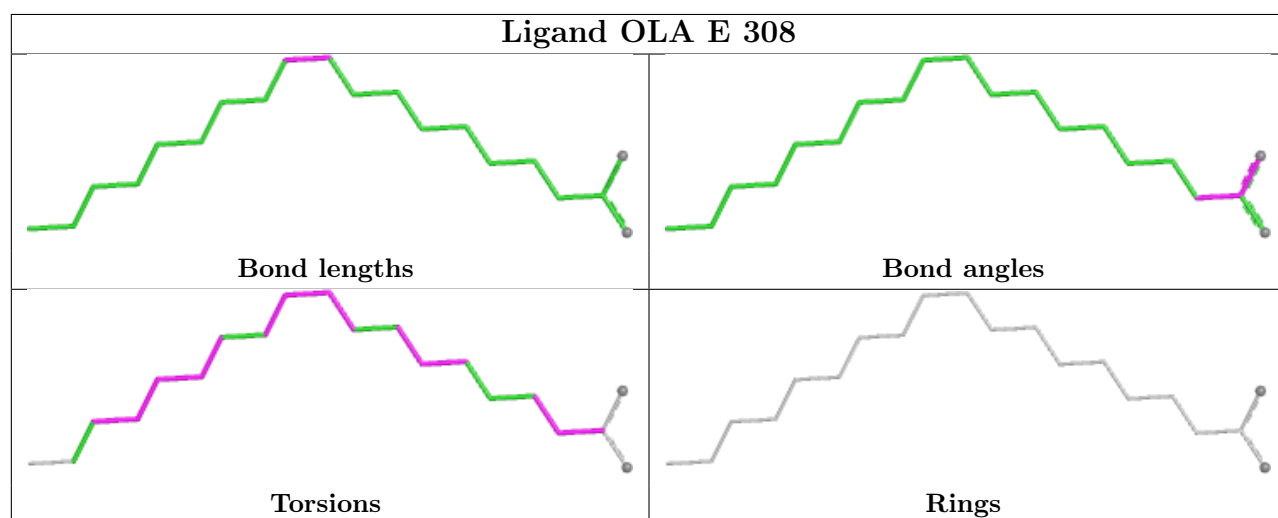
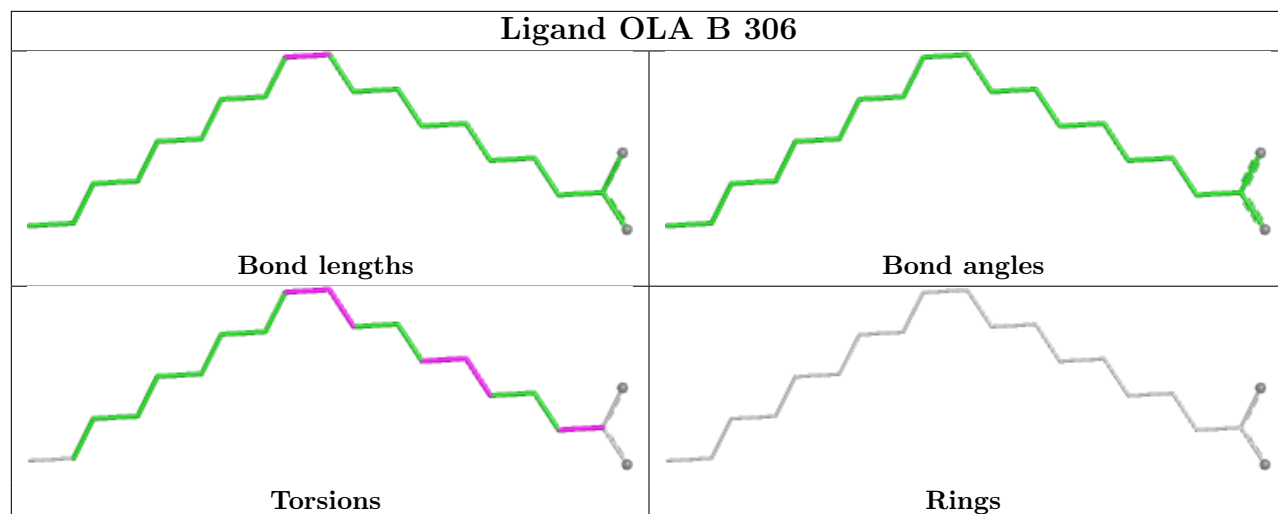


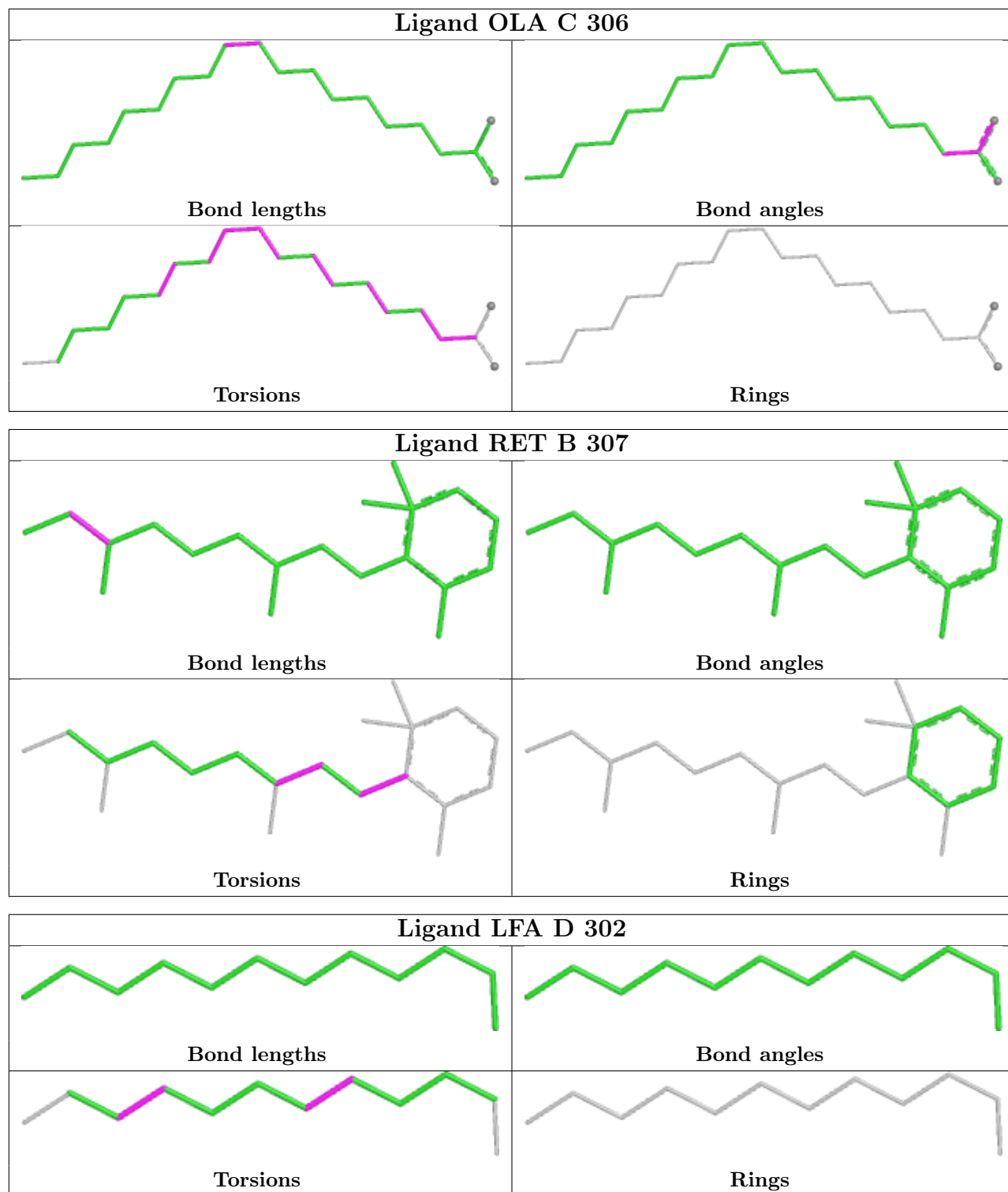


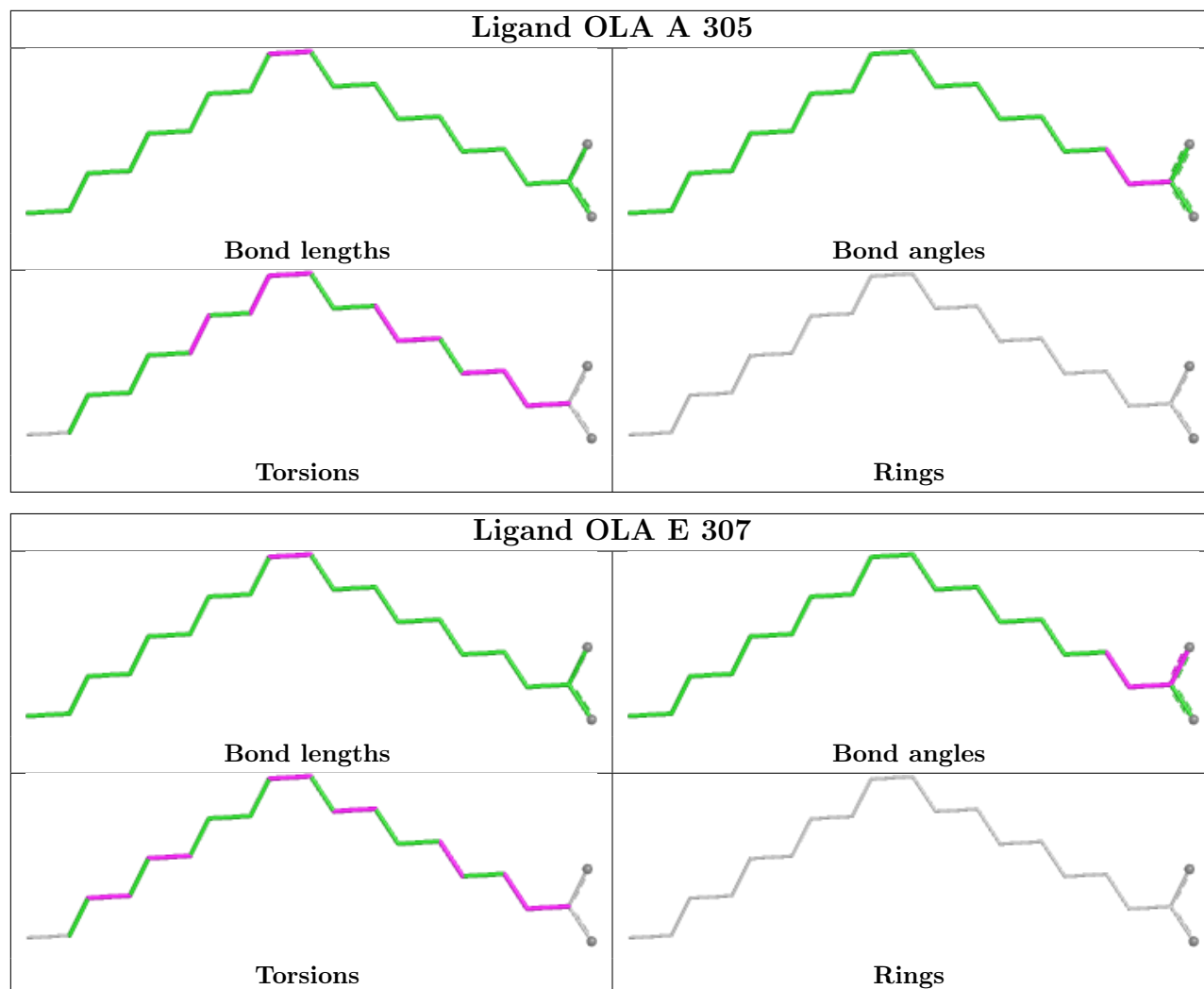












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	253/263 (96%)	0.24	7 (2%)	55 50	37, 46, 65, 78	0
1	B	252/263 (95%)	0.43	8 (3%)	50 44	22, 46, 68, 78	2 (0%)
1	C	255/263 (96%)	0.30	7 (2%)	56 51	37, 46, 67, 102	0
1	D	254/263 (96%)	0.22	6 (2%)	59 55	35, 46, 64, 83	0
1	E	253/263 (96%)	0.35	7 (2%)	55 50	38, 47, 69, 75	0
1	F	253/263 (96%)	0.35	8 (3%)	50 44	37, 47, 70, 84	0
All	All	1520/1578 (96%)	0.31	43 (2%)	55 50	22, 46, 68, 102	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256	THR	4.5
1	E	243	ALA	4.0
1	F	253	ALA	3.9
1	C	254	GLY	3.6
1	B	242	PRO	3.6
1	F	243	ALA	3.5
1	C	239	ALA	3.4
1	D	255	GLY	3.3
1	B	170[A]	ASP	3.1
1	B	105	THR	3.0
1	D	105	THR	2.9
1	E	242	PRO	2.8
1	F	242	PRO	2.8
1	D	240	GLY	2.8
1	B	243	ALA	2.7
1	A	168	GLY	2.6
1	F	68	LEU	2.6
1	E	105	THR	2.5
1	A	105	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	166	VAL	2.5
1	C	241	ALA	2.5
1	B	240	GLY	2.4
1	F	168	GLY	2.4
1	B	103	PRO	2.4
1	F	73	GLY	2.4
1	A	202	GLN	2.4
1	C	255	GLY	2.3
1	E	168	GLY	2.3
1	E	69	THR	2.2
1	A	166	VAL	2.2
1	F	134	GLY	2.2
1	D	16	VAL	2.2
1	D	238	ARG	2.2
1	F	240	GLY	2.2
1	B	241	ALA	2.2
1	E	4	ARG	2.2
1	C	251	ARG	2.1
1	E	167	THR	2.1
1	A	204	GLY	2.1
1	B	2	ASN	2.1
1	A	165	ARG	2.0
1	A	5	PRO	2.0
1	D	103	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LFA	A	301	8/20	0.69	0.27	52,57,57,61	0
4	OLA	A	310	20/20	0.74	0.27	61,75,77,80	0
2	LFA	E	301	7/20	0.75	0.29	55,56,58,59	0
2	LFA	F	301	15/20	0.76	0.25	44,53,58,58	0
2	LFA	D	303	7/20	0.76	0.29	48,51,55,57	0
2	LFA	B	301	7/20	0.77	0.25	49,55,58,59	0
4	OLA	E	309	20/20	0.77	0.24	58,65,76,76	0
4	OLA	A	311	20/20	0.78	0.21	50,64,70,73	0
4	OLA	E	308	20/20	0.78	0.20	53,59,71,74	0
4	OLA	A	309	20/20	0.78	0.24	46,56,63,67	0
2	LFA	F	304	11/20	0.79	0.26	54,64,74,74	0
2	LFA	D	302	12/20	0.79	0.23	55,59,72,74	0
4	OLA	F	309	20/20	0.79	0.18	55,62,67,75	0
4	OLA	B	303	20/20	0.80	0.21	44,55,67,69	0
2	LFA	F	302	7/20	0.80	0.23	45,46,49,49	0
2	LFA	D	304	6/20	0.80	0.22	43,44,47,49	0
4	OLA	A	308	20/20	0.80	0.19	51,61,70,72	0
4	OLA	C	304	20/20	0.80	0.22	44,55,78,80	0
4	OLA	A	306	20/20	0.81	0.21	57,67,76,80	0
4	OLA	D	308	20/20	0.81	0.21	46,55,63,63	0
4	OLA	C	307	20/20	0.81	0.19	40,51,58,61	0
4	OLA	E	303	20/20	0.82	0.22	43,57,69,71	0
2	LFA	D	301	8/20	0.83	0.23	48,53,55,61	0
4	OLA	E	307	20/20	0.83	0.18	51,58,65,67	0
4	OLA	F	308	20/20	0.83	0.20	58,65,74,74	0
4	OLA	C	308	20/20	0.83	0.20	51,59,74,75	0
4	OLA	E	306	20/20	0.84	0.18	48,57,74,77	0
4	OLA	A	307	20/20	0.85	0.15	50,54,75,76	0
4	OLA	B	305	20/20	0.85	0.19	39,52,87,87	0
4	OLA	C	303	20/20	0.85	0.20	46,57,64,69	0
4	OLA	C	306	20/20	0.86	0.18	41,55,70,71	0
4	OLA	A	303	20/20	0.86	0.17	43,50,71,76	0
4	OLA	D	306	20/20	0.86	0.17	38,50,65,66	0
4	OLA	C	305	20/20	0.87	0.17	41,51,63,65	0
4	OLA	F	307	20/20	0.87	0.18	46,56,68,69	0
4	OLA	B	306	20/20	0.88	0.15	47,51,59,67	0
4	OLA	E	304	20/20	0.89	0.15	40,48,65,72	0
4	OLA	E	305	20/20	0.89	0.16	41,54,81,81	0
4	OLA	B	304	20/20	0.89	0.17	40,46,66,69	0
2	LFA	F	303	11/20	0.90	0.16	54,60,66,68	0
4	OLA	A	305	20/20	0.91	0.13	41,53,66,71	0
4	OLA	A	304	20/20	0.91	0.14	37,47,64,65	0
4	OLA	F	306	20/20	0.91	0.13	36,42,66,67	0

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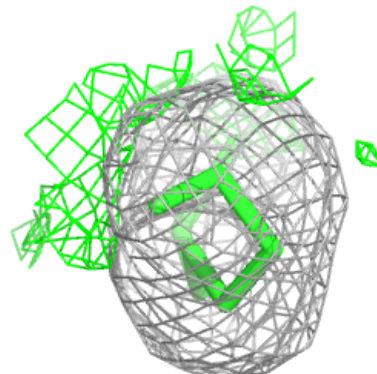
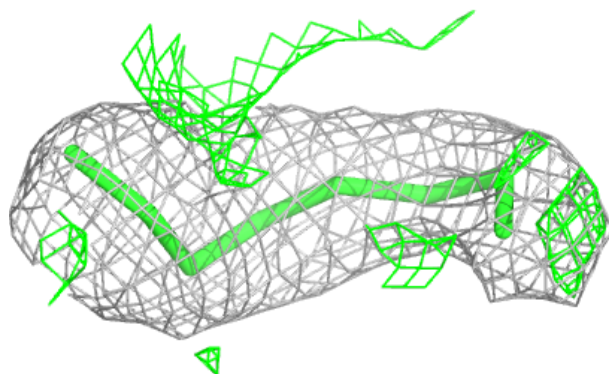
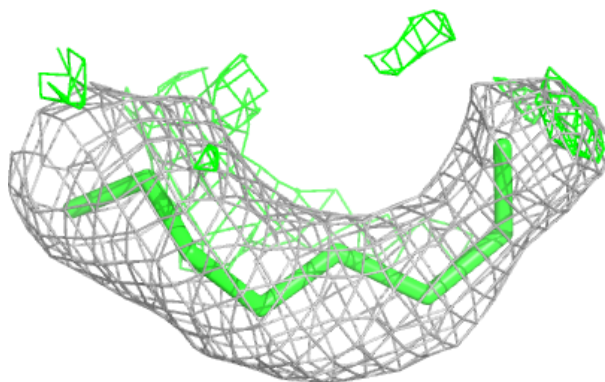
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OLA	D	307	20/20	0.91	0.13	34,56,72,77	0
5	RET	B	307	20/21	0.92	0.12	36,42,48,49	0
5	RET	E	310	20/21	0.92	0.12	37,41,44,44	0
4	OLA	C	302	20/20	0.93	0.13	37,43,68,69	0
5	RET	F	310	20/21	0.93	0.11	40,43,49,49	0
5	RET	A	312	20/21	0.94	0.11	31,38,42,44	0
5	RET	D	309	20/21	0.94	0.10	31,37,41,44	0
5	RET	C	309	20/21	0.94	0.10	34,42,46,47	0
3	CL	B	302	1/1	0.96	0.06	43,43,43,43	0
3	CL	C	301	1/1	0.96	0.06	43,43,43,43	0
3	CL	D	305	1/1	0.97	0.07	42,42,42,42	0
3	CL	F	305	1/1	0.98	0.04	44,44,44,44	0
3	CL	A	302	1/1	0.98	0.06	40,40,40,40	0
3	CL	E	302	1/1	0.98	0.05	43,43,43,43	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.

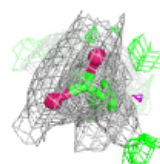
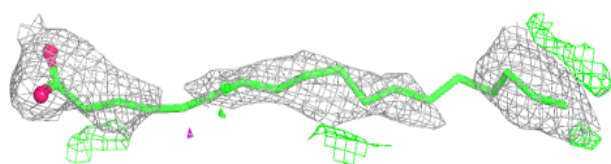
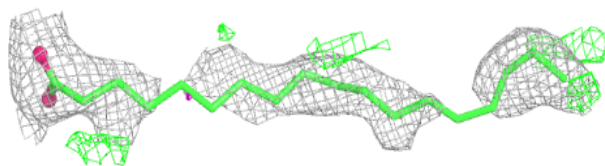
Electron density around LFA A 301:

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

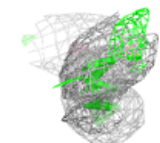
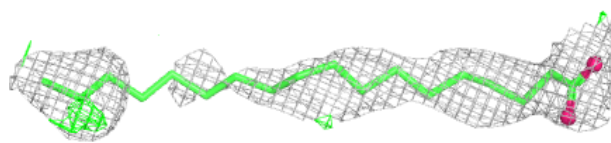
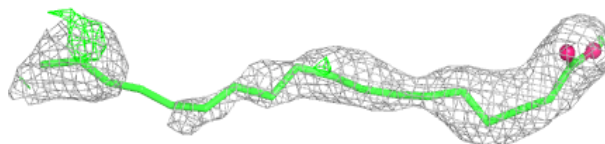


Electron density around OLA A 310:

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

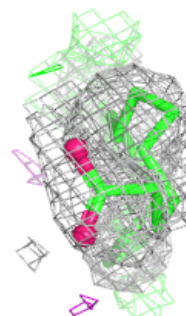
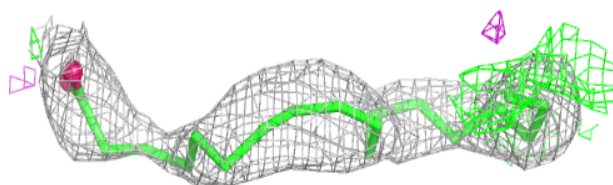
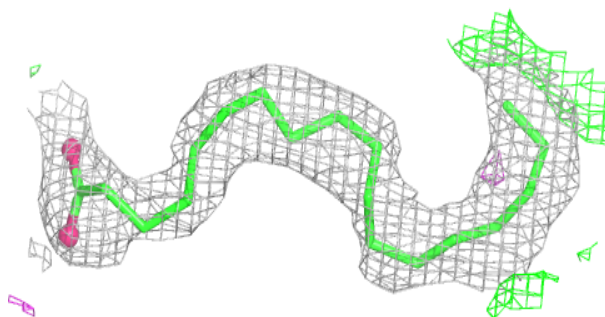
**Electron density around OLA E 309:**

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

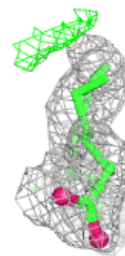
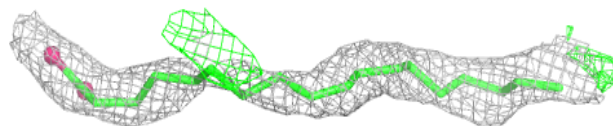
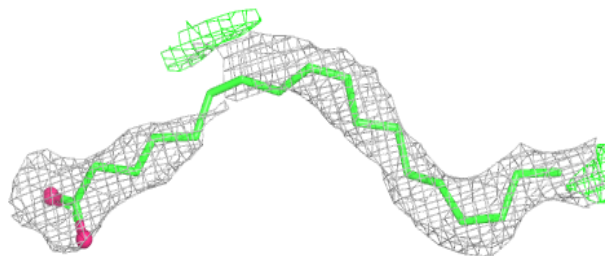


Electron density around OLA A 311:

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

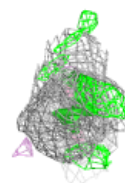
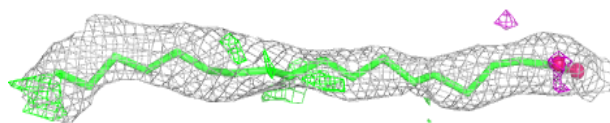
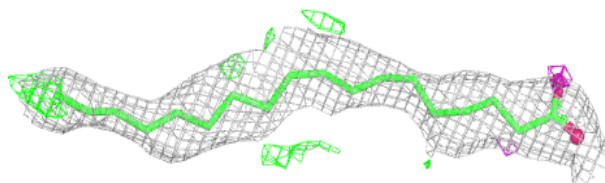
**Electron density around OLA E 308:**

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

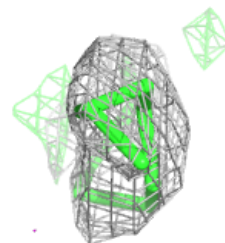
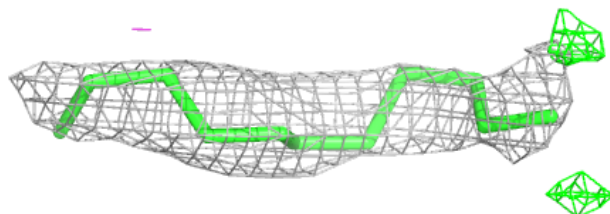
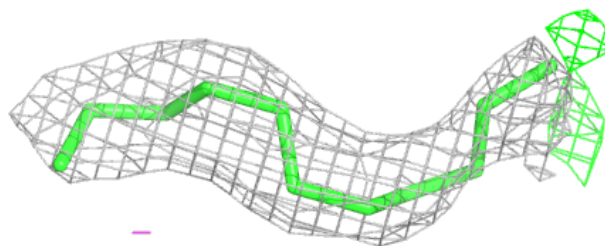


Electron density around OLA A 309:

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

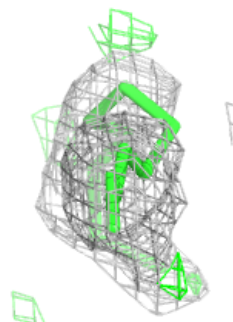
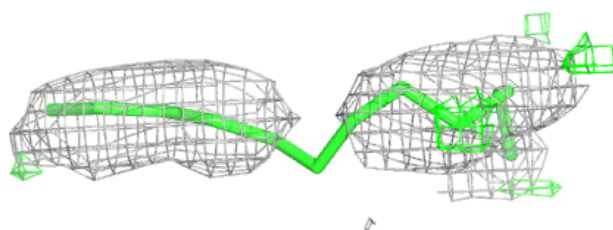
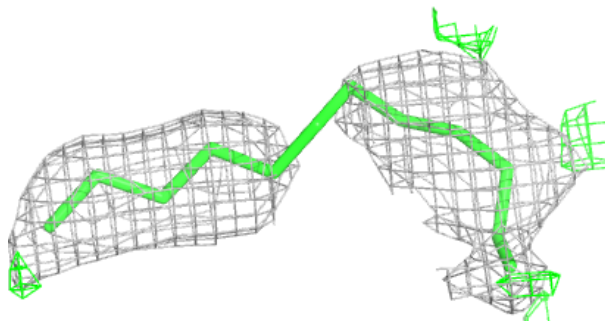
**Electron density around LFA F 304:**

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

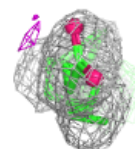
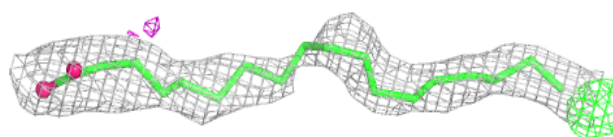
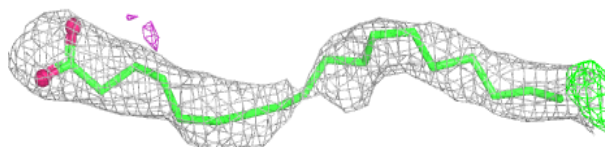


Electron density around LFA D 302:

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

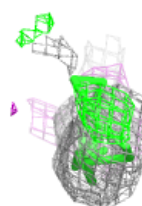
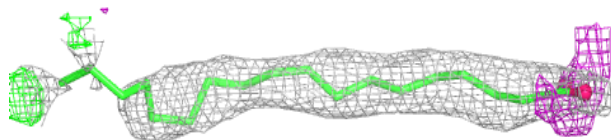
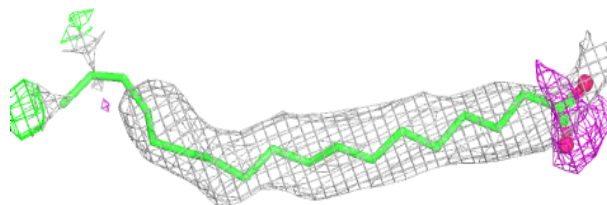
**Electron density around OLA F 309:**

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

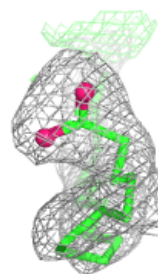
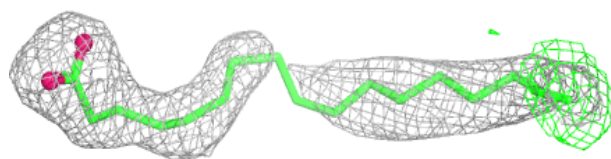
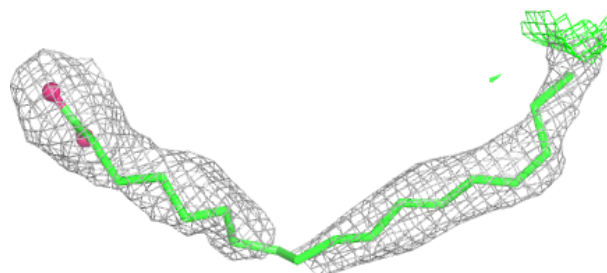


Electron density around OLA B 303:

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

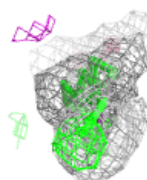
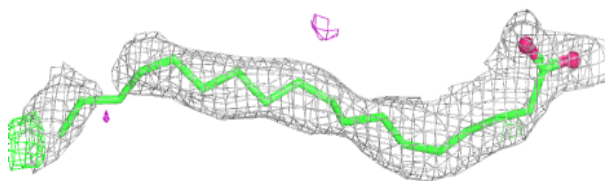
**Electron density around OLA A 308:**

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and green (positive)

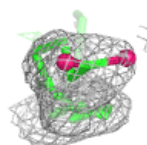
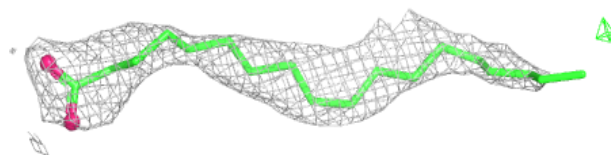
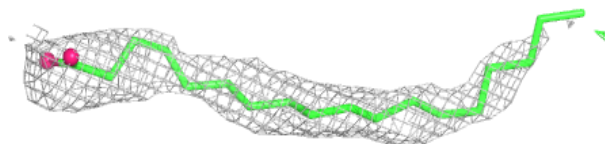


Electron density around OLA C 304:

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

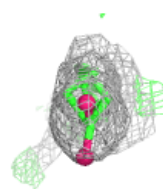
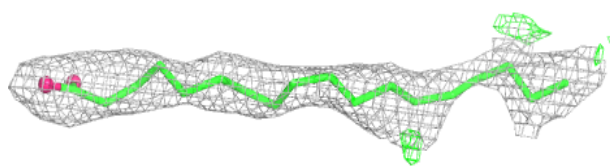
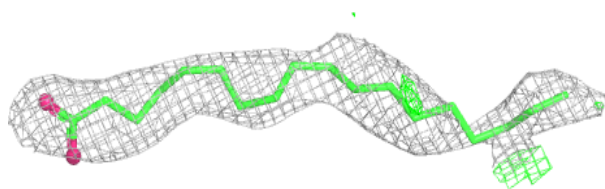
**Electron density around OLA A 306:**

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and green (positive)

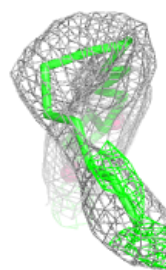
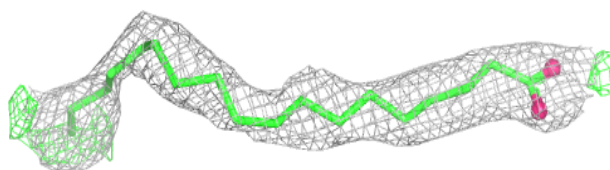
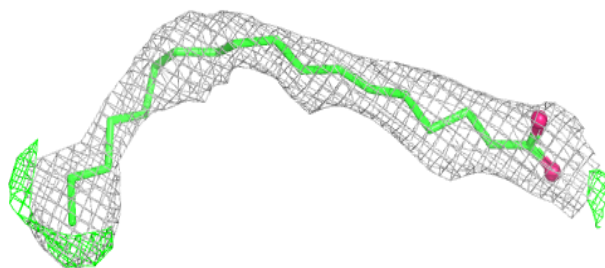


Electron density around OLA D 308:

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

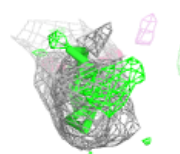
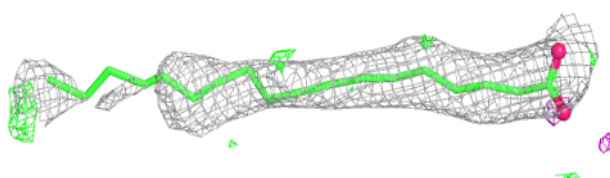
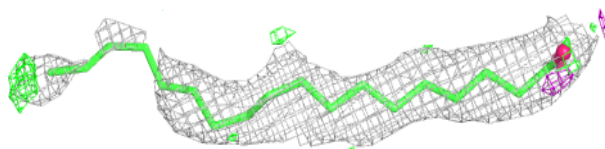
**Electron density around OLA C 307:**

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

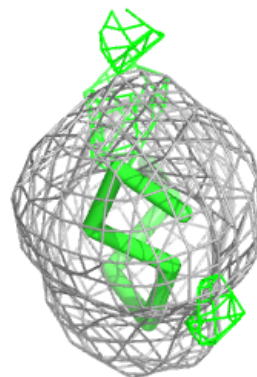
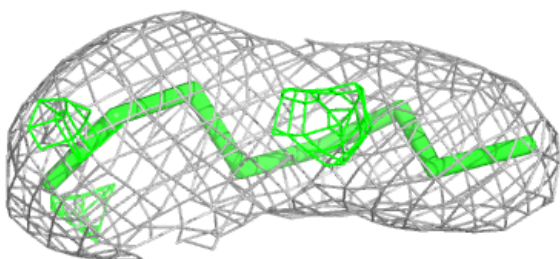
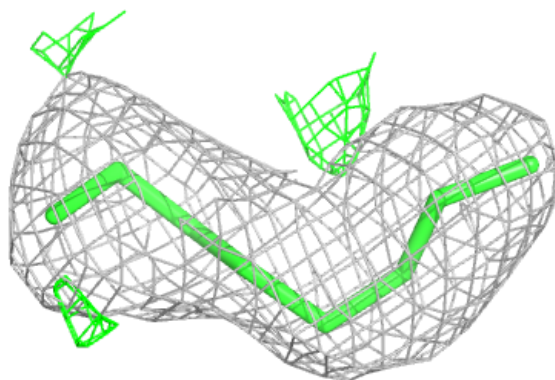


Electron density around OLA E 303:

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

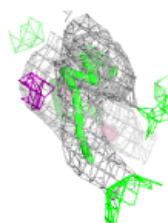
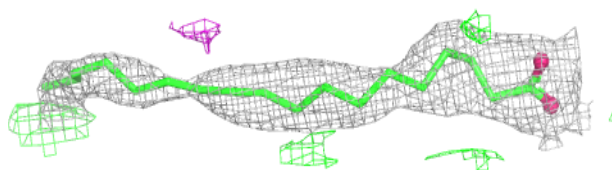
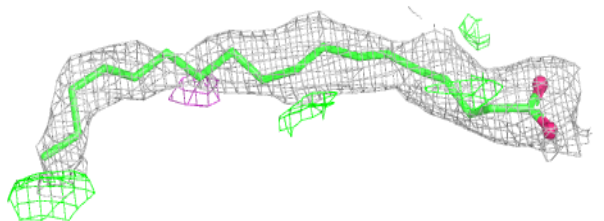
**Electron density around LFA D 301:**

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

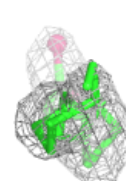
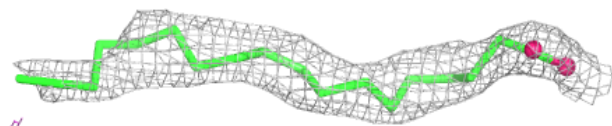
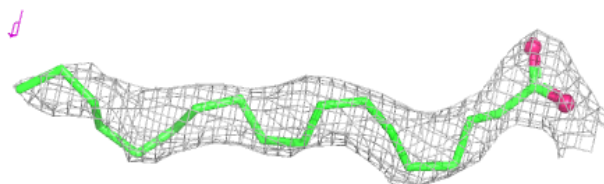


Electron density around OLA E 307:

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

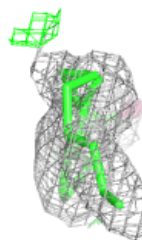
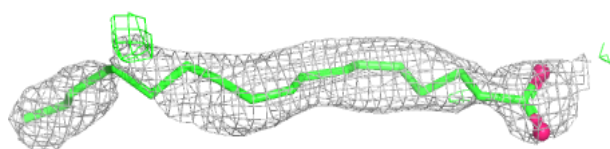
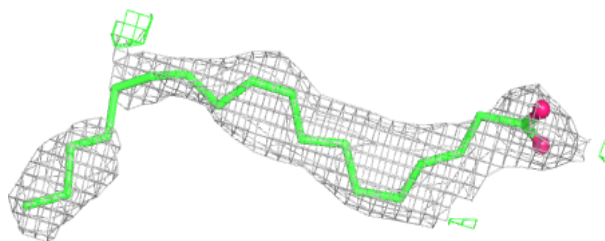
**Electron density around OLA F 308:**

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

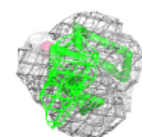
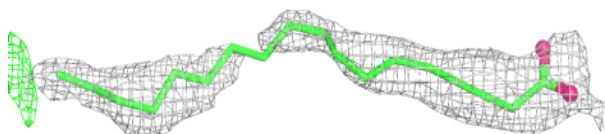


Electron density around OLA C 308:

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

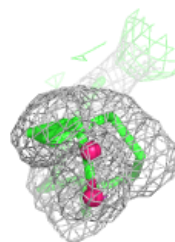
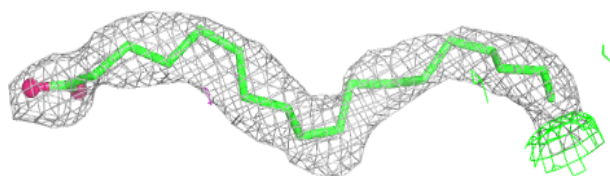
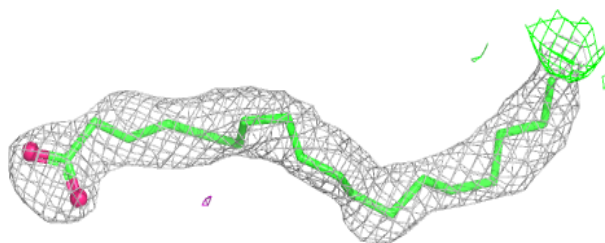
**Electron density around OLA E 306:**

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

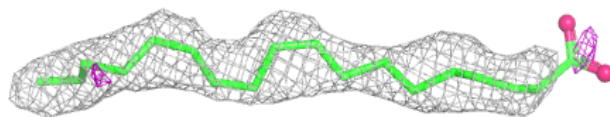
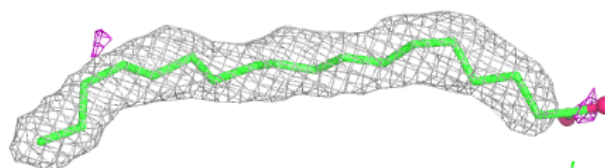


Electron density around OLA A 307:

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

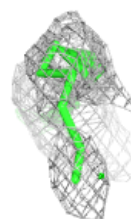
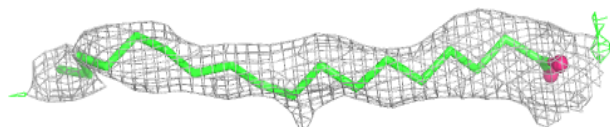
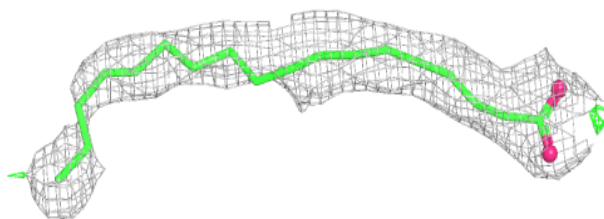
**Electron density around OLA B 305:**

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

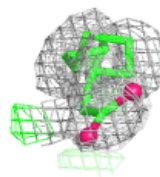
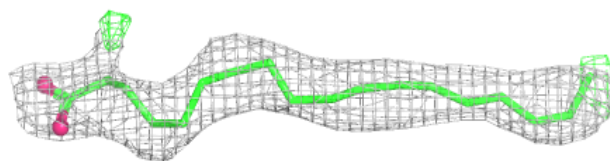
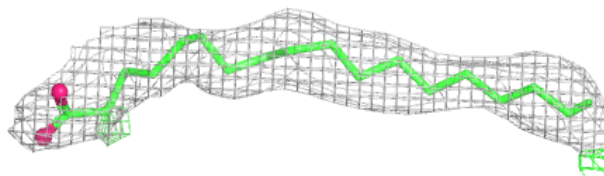


Electron density around OLA C 303:

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

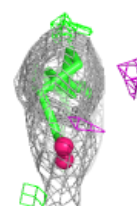
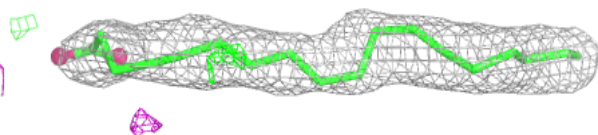
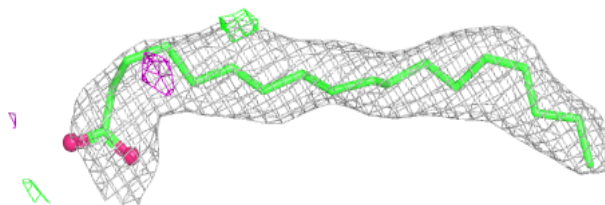
**Electron density around OLA C 306:**

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

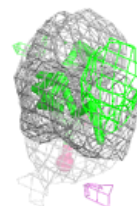
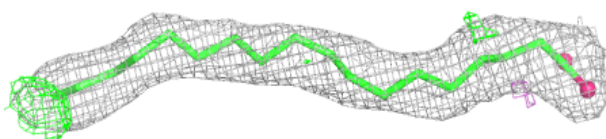
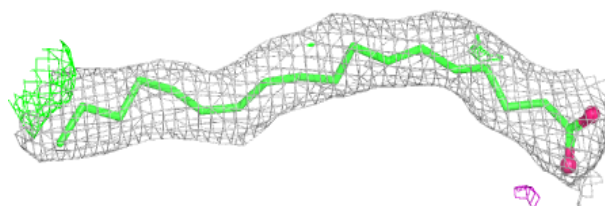


Electron density around OLA A 303:

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

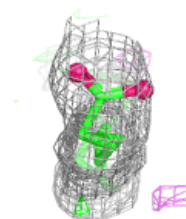
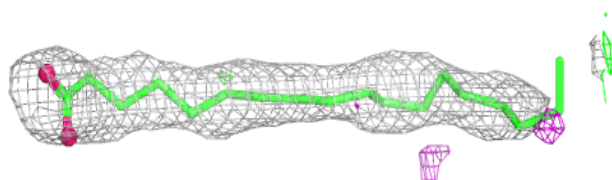
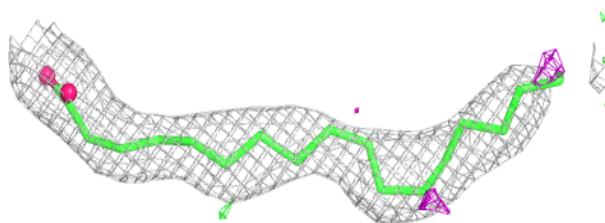
**Electron density around OLA D 306:**

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

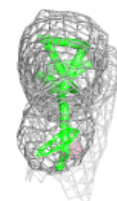
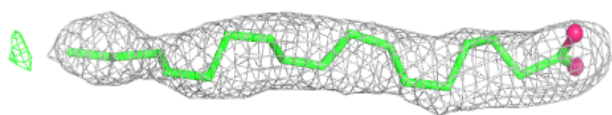
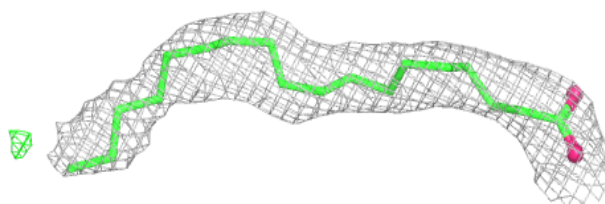


Electron density around OLA C 305:

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

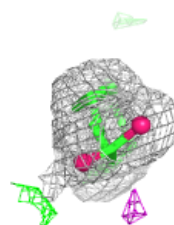
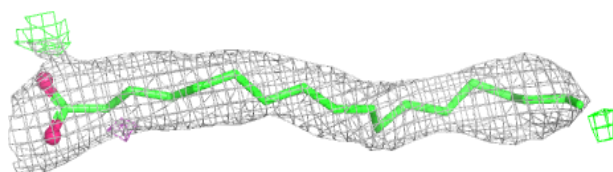
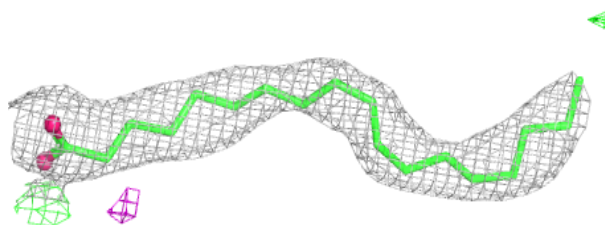
**Electron density around OLA F 307:**

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

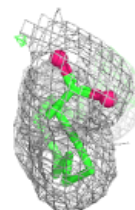
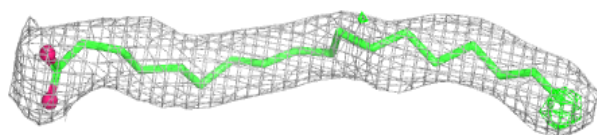
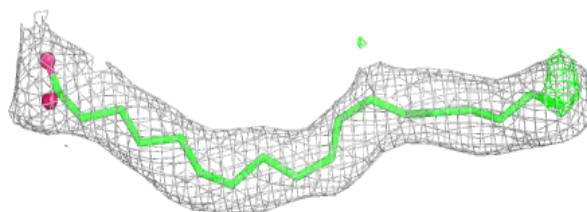


Electron density around OLA B 306:

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

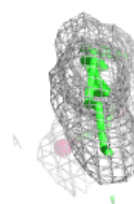
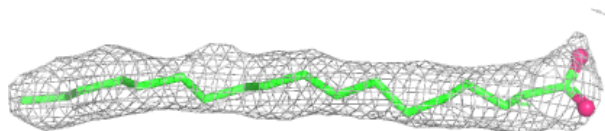
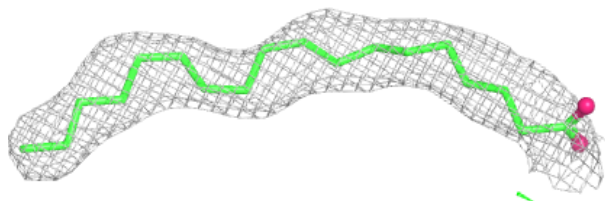
**Electron density around OLA E 304:**

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

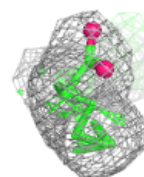
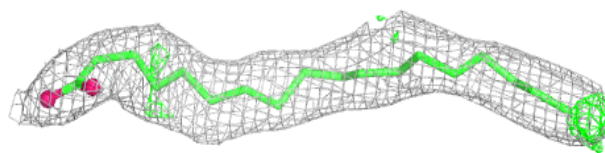
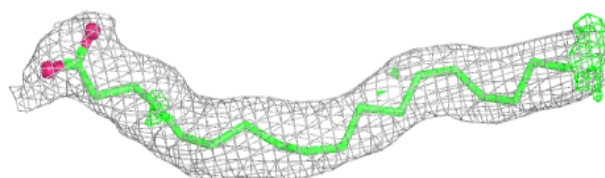


Electron density around OLA E 305:

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

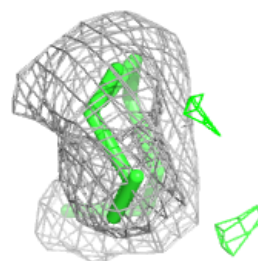
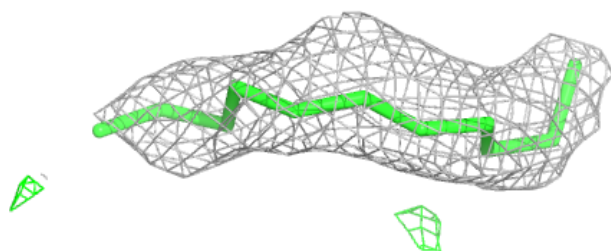
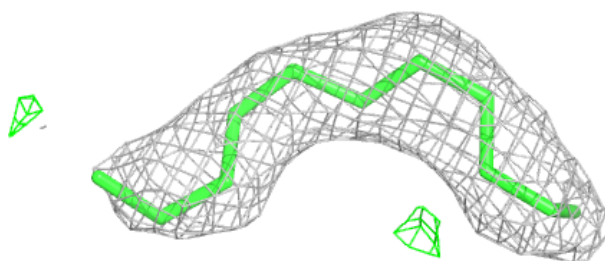
**Electron density around OLA B 304:**

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

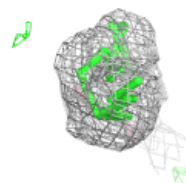
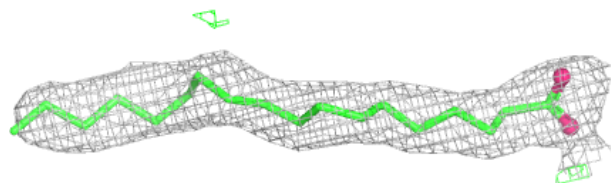
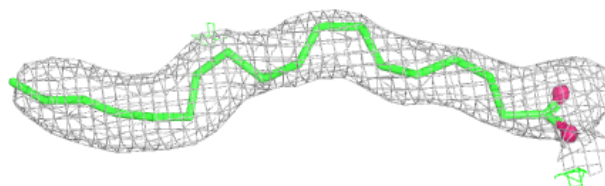


Electron density around LFA F 303:

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

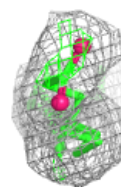
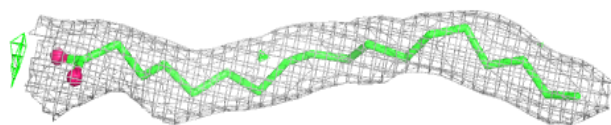
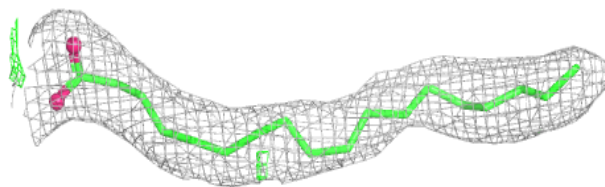
**Electron density around OLA A 305:**

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

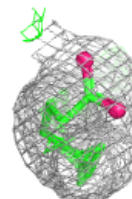
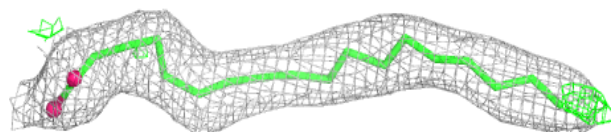
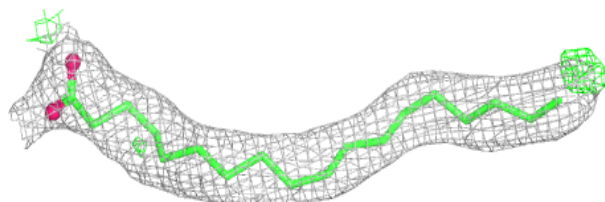


Electron density around OLA A 304:

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

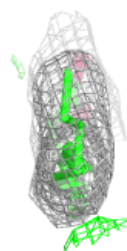
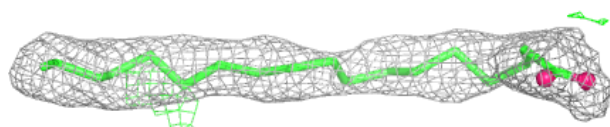
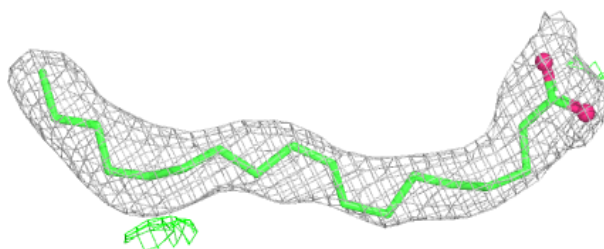
**Electron density around OLA F 306:**

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

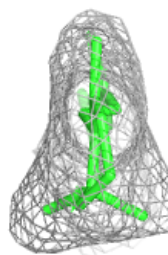
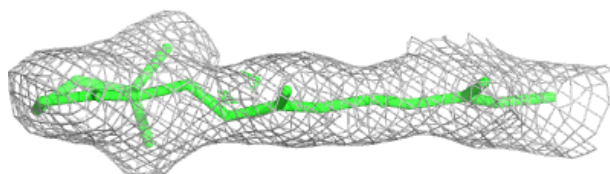
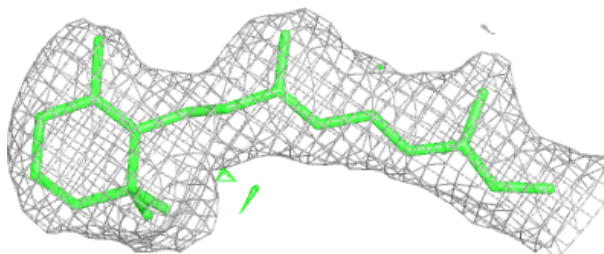


Electron density around OLA D 307:

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

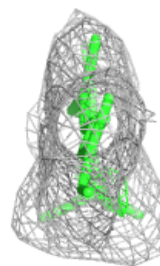
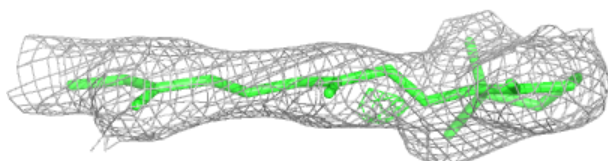
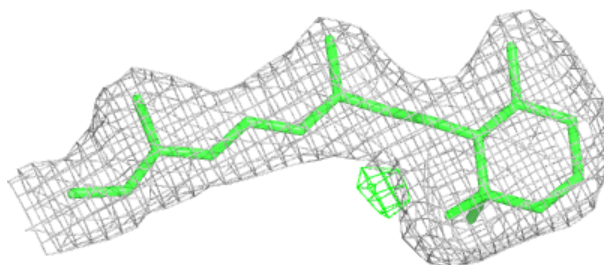
**Electron density around RET B 307:**

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

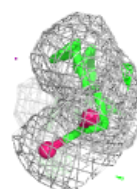
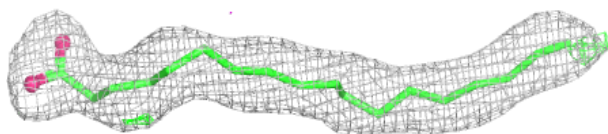
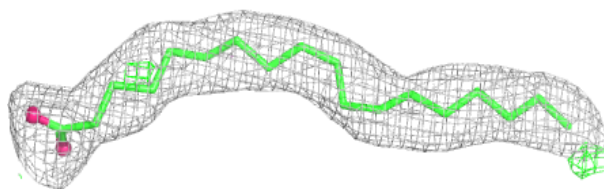


Electron density around RET E 310:

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

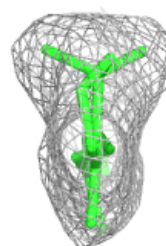
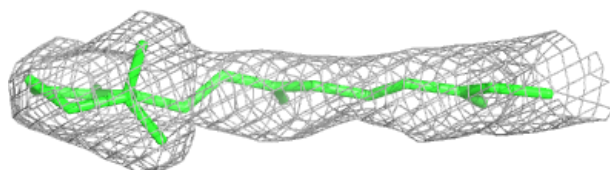
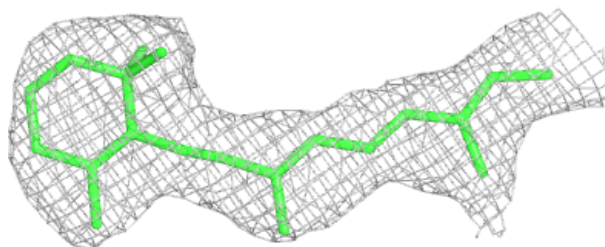
**Electron density around OLA C 302:**

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

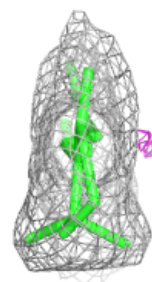
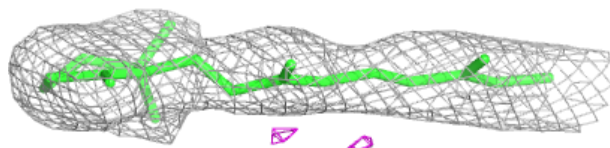
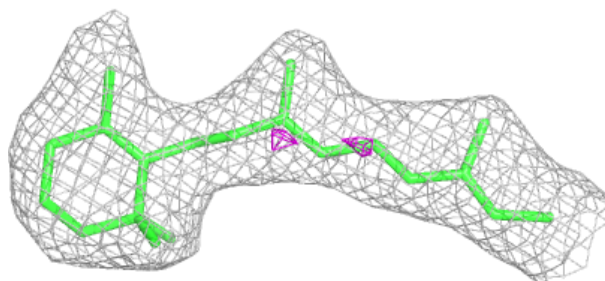


Electron density around RET F 310:

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

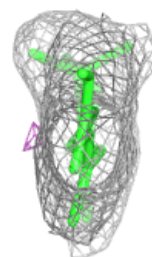
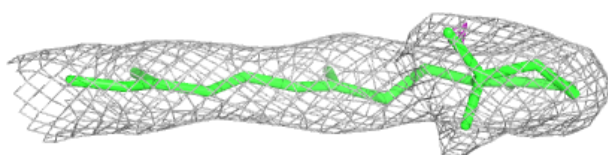
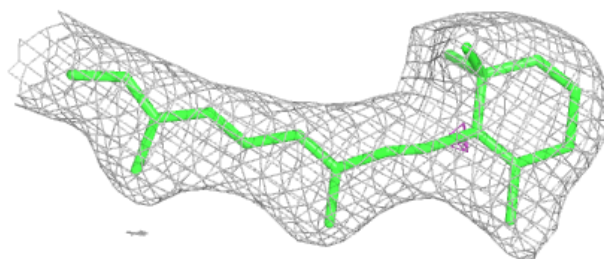
**Electron density around RET A 312:**

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

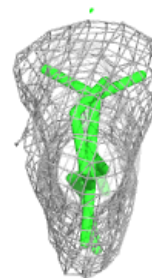
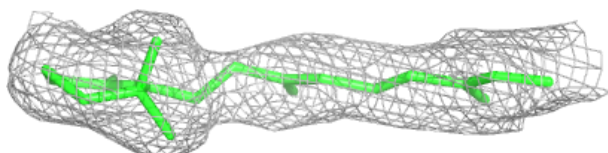
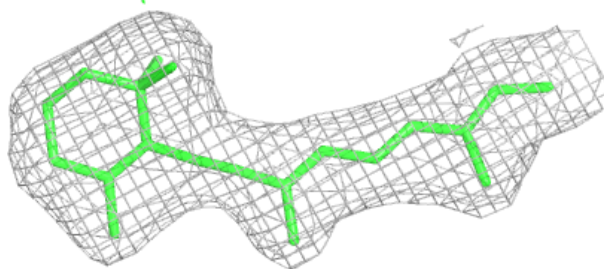


Electron density around RET D 309:

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

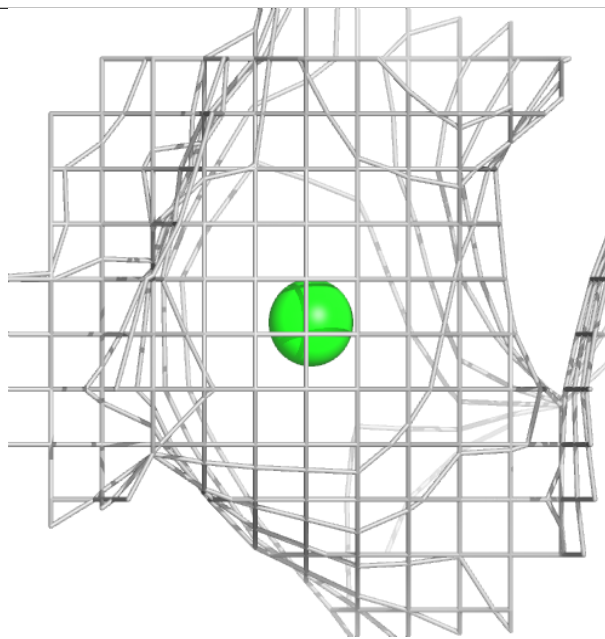
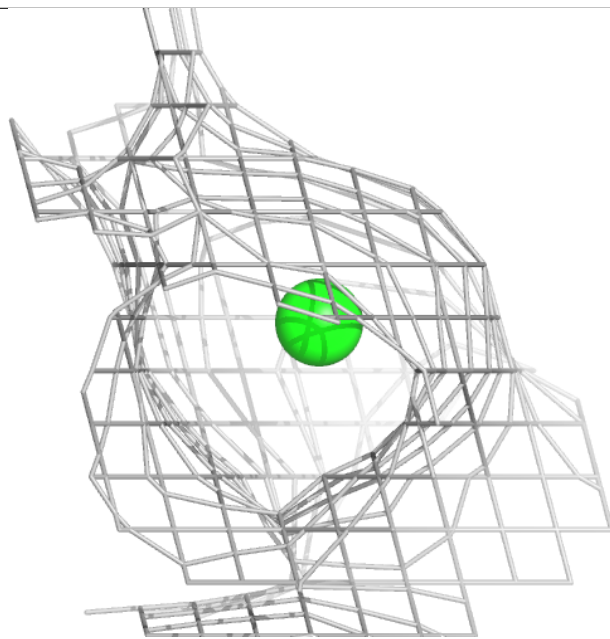
**Electron density around RET C 309:**

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



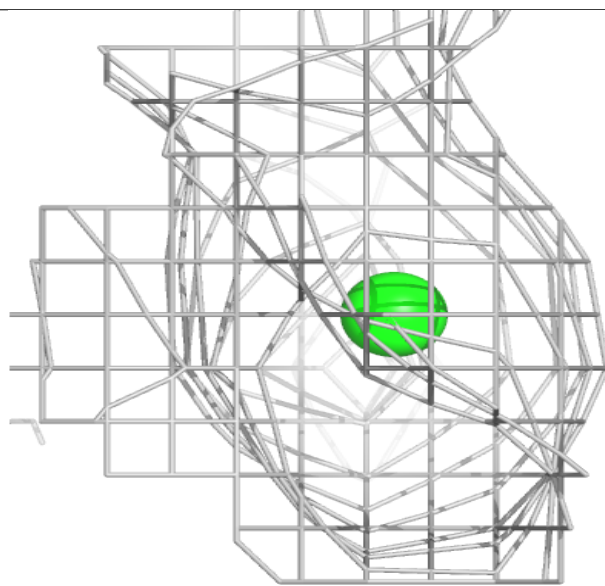
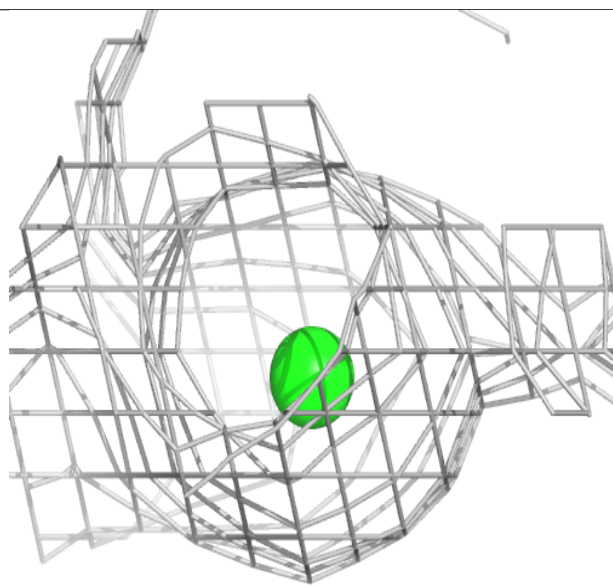
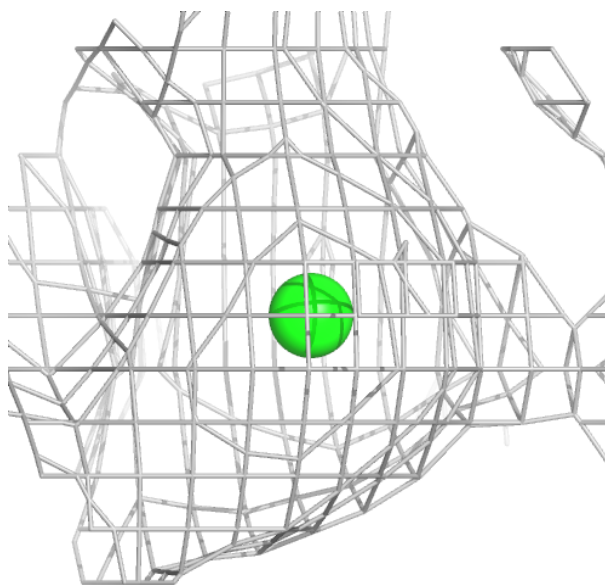
Electron density around CL B 302:

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



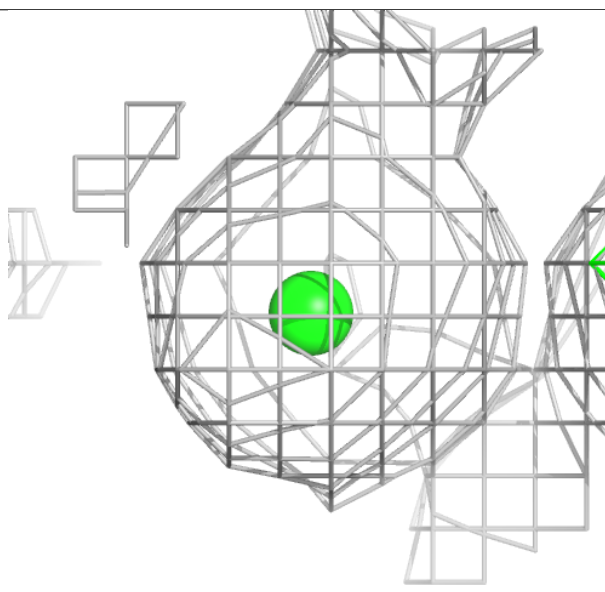
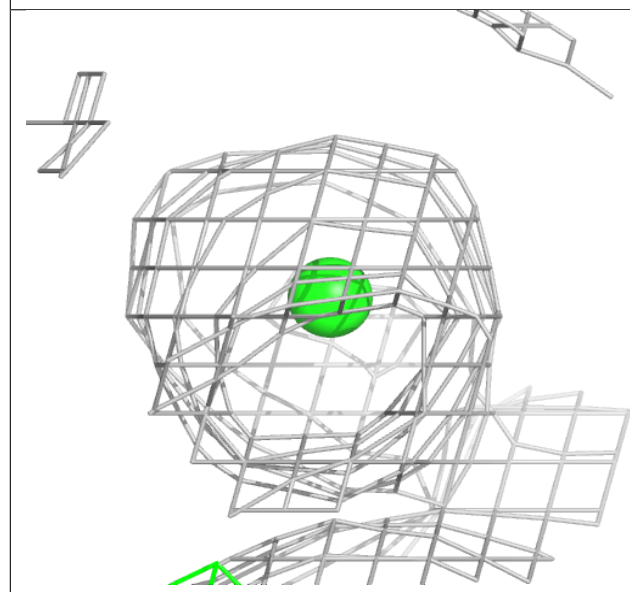
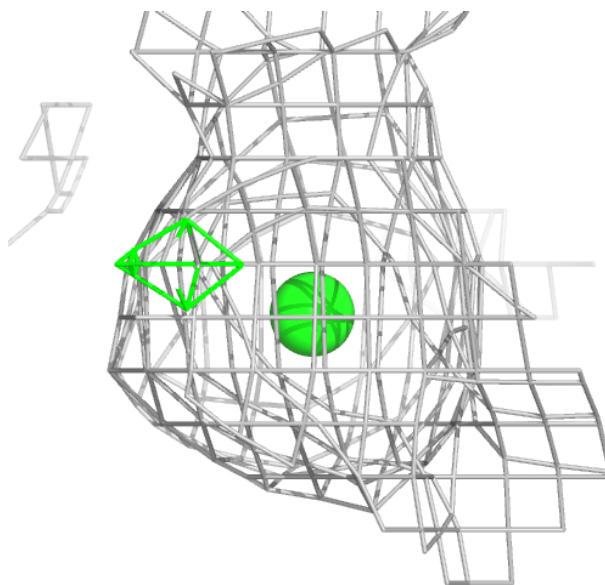
Electron density around CL C 301:

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



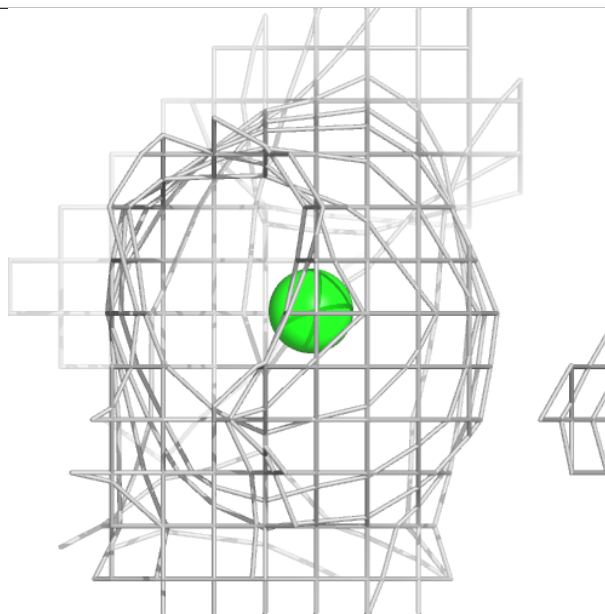
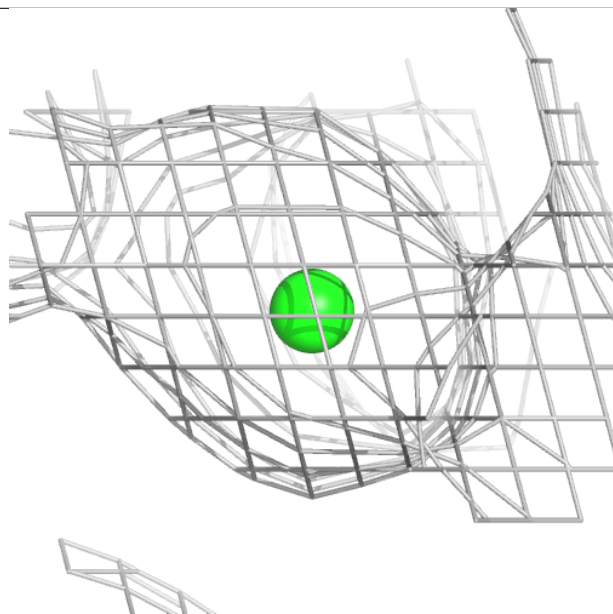
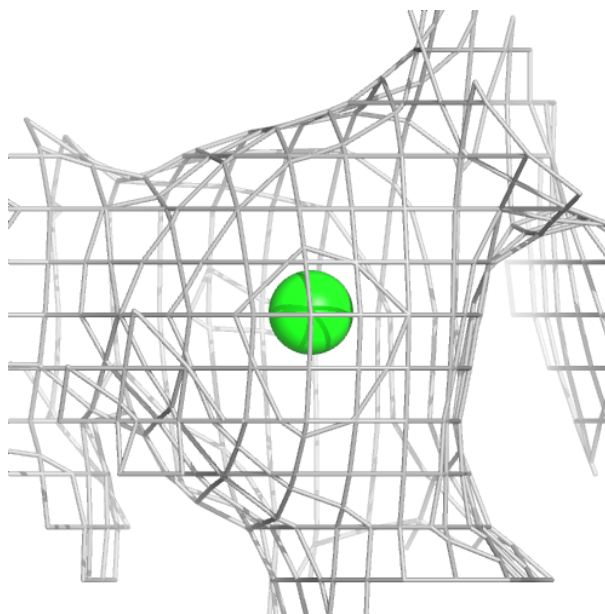
Electron density around CL D 305:

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



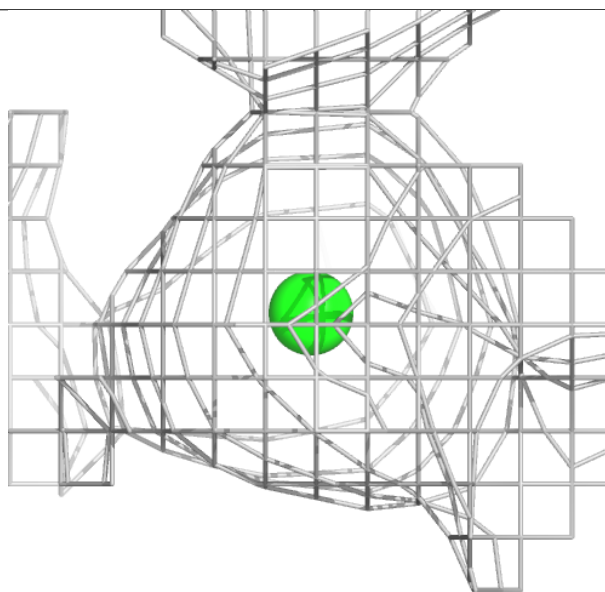
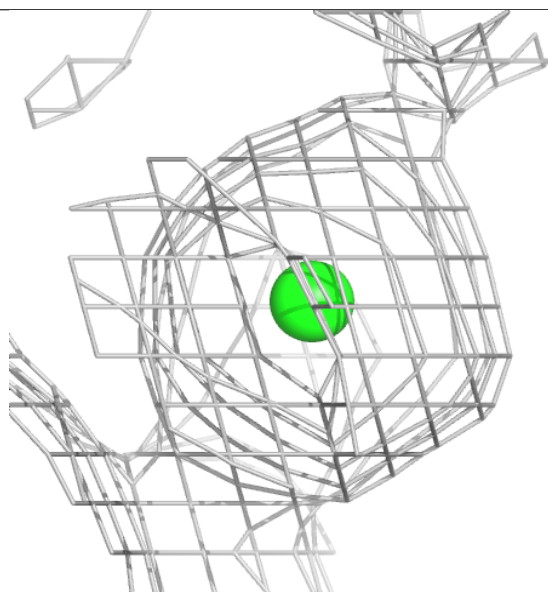
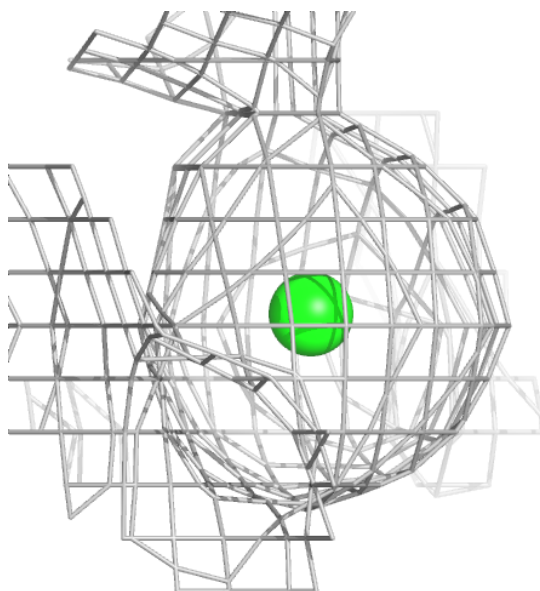
Electron density around CL F 305:

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



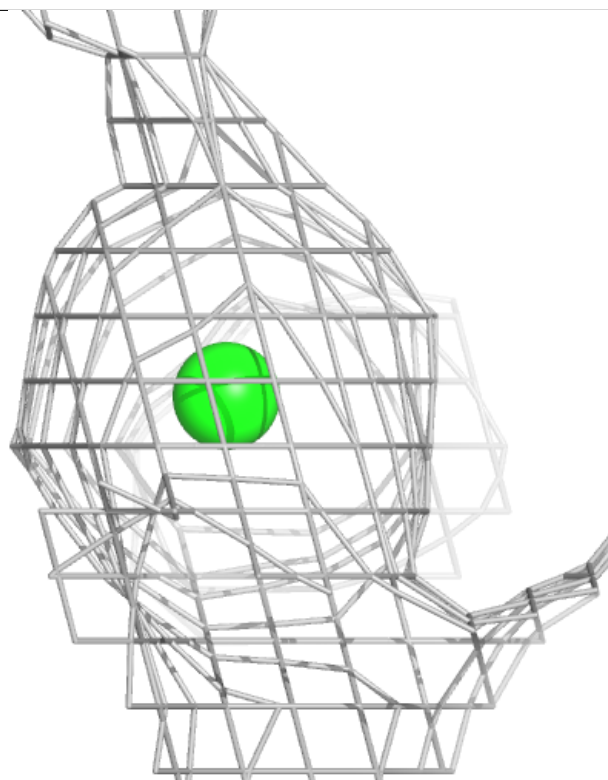
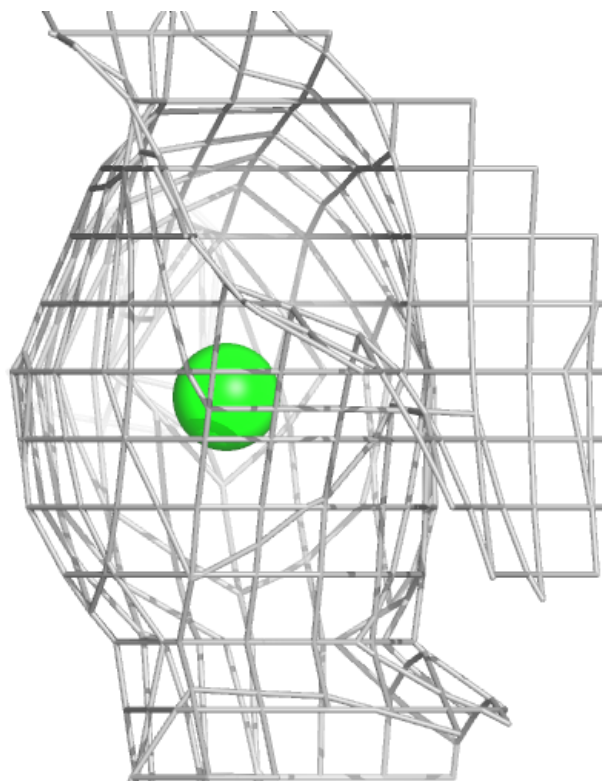
Electron density around CL A 302:

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



Electron density around CL E 302:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.