



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:52 AM UTC

PDB ID : 5N6L / pdb_00005n6l
Title : Structure of the membrane integral lipoprotein N-acyltransferase Lnt C387A mutant from E. coli
Authors : Huang, C.-Y.; Boland, C.; Howe, N.; Wiktor, M.; Vogeley, L.; Weichert, D.; Bailey, J.; Olieric, V.; Wang, M.; Caffrey, M.
Deposited on : 2017-02-15
Resolution : 2.90 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

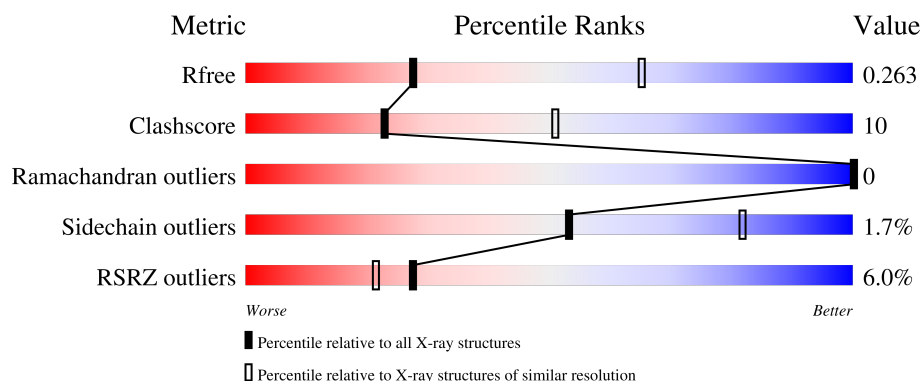
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	532	
1	B	532	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8371 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 Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3982	2621	659	688	14			
1	B	491	Total	C	N	O	S	0	0	0
			3863	2540	641	669	13			

There are 42 discrepancies between the modelled and reference sequences:

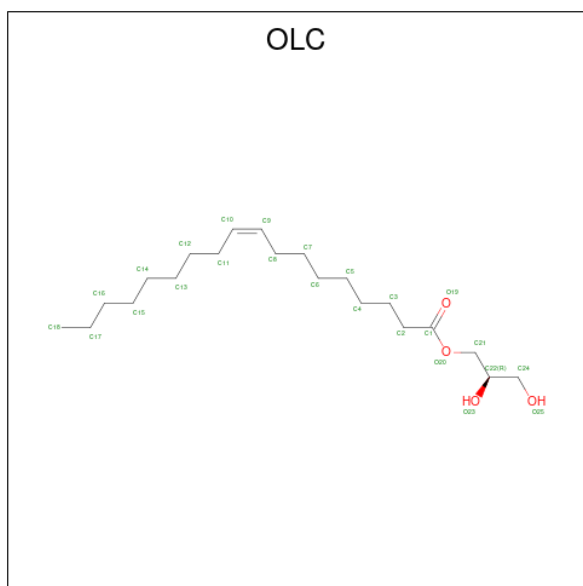
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23930
A	-18	GLY	-	expression tag	UNP P23930
A	-17	SER	-	expression tag	UNP P23930
A	-16	SER	-	expression tag	UNP P23930
A	-15	HIS	-	expression tag	UNP P23930
A	-14	HIS	-	expression tag	UNP P23930
A	-13	HIS	-	expression tag	UNP P23930
A	-12	HIS	-	expression tag	UNP P23930
A	-11	HIS	-	expression tag	UNP P23930
A	-10	HIS	-	expression tag	UNP P23930
A	-9	SER	-	expression tag	UNP P23930
A	-8	SER	-	expression tag	UNP P23930
A	-7	GLY	-	expression tag	UNP P23930
A	-6	LEU	-	expression tag	UNP P23930
A	-5	VAL	-	expression tag	UNP P23930
A	-4	PRO	-	expression tag	UNP P23930
A	-3	ARG	-	expression tag	UNP P23930
A	-2	GLY	-	expression tag	UNP P23930
A	-1	SER	-	expression tag	UNP P23930
A	0	HIS	-	expression tag	UNP P23930
A	387	ALA	CYS	engineered mutation	UNP P23930
B	-19	MET	-	initiating methionine	UNP P23930
B	-18	GLY	-	expression tag	UNP P23930
B	-17	SER	-	expression tag	UNP P23930
B	-16	SER	-	expression tag	UNP P23930

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P23930
B	-14	HIS	-	expression tag	UNP P23930
B	-13	HIS	-	expression tag	UNP P23930
B	-12	HIS	-	expression tag	UNP P23930
B	-11	HIS	-	expression tag	UNP P23930
B	-10	HIS	-	expression tag	UNP P23930
B	-9	SER	-	expression tag	UNP P23930
B	-8	SER	-	expression tag	UNP P23930
B	-7	GLY	-	expression tag	UNP P23930
B	-6	LEU	-	expression tag	UNP P23930
B	-5	VAL	-	expression tag	UNP P23930
B	-4	PRO	-	expression tag	UNP P23930
B	-3	ARG	-	expression tag	UNP P23930
B	-2	GLY	-	expression tag	UNP P23930
B	-1	SER	-	expression tag	UNP P23930
B	0	HIS	-	expression tag	UNP P23930
B	387	ALA	CYS	engineered mutation	UNP P23930

- 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	O	0	0
			15	11	4		
2	A	1	Total	C	O	0	0
			12	8	4		

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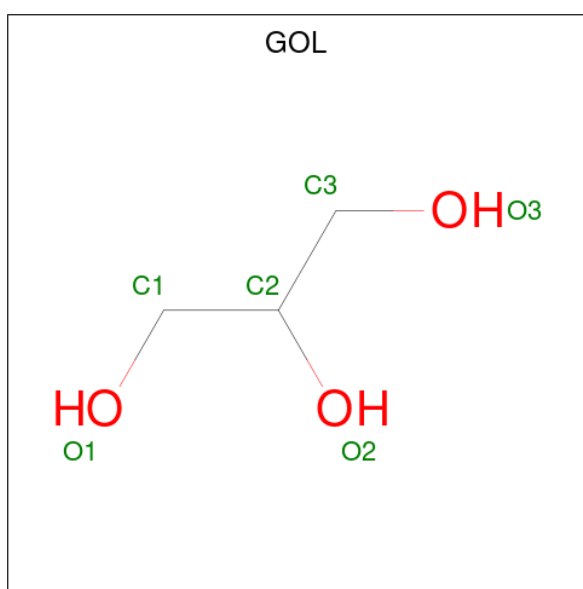
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			20	16	4		
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	B	1	Total	C	O	0	0
			14	10	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			11	7	4		
2	B	1	Total	C	O	0	0
			21	17	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			18	14	4		
2	B	1	Total	C	O	0	0
			13	9	4		
2	B	1	Total	C	O	0	0
			11	7	4		
2	B	1	Total	C	O	0	0
			16	12	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

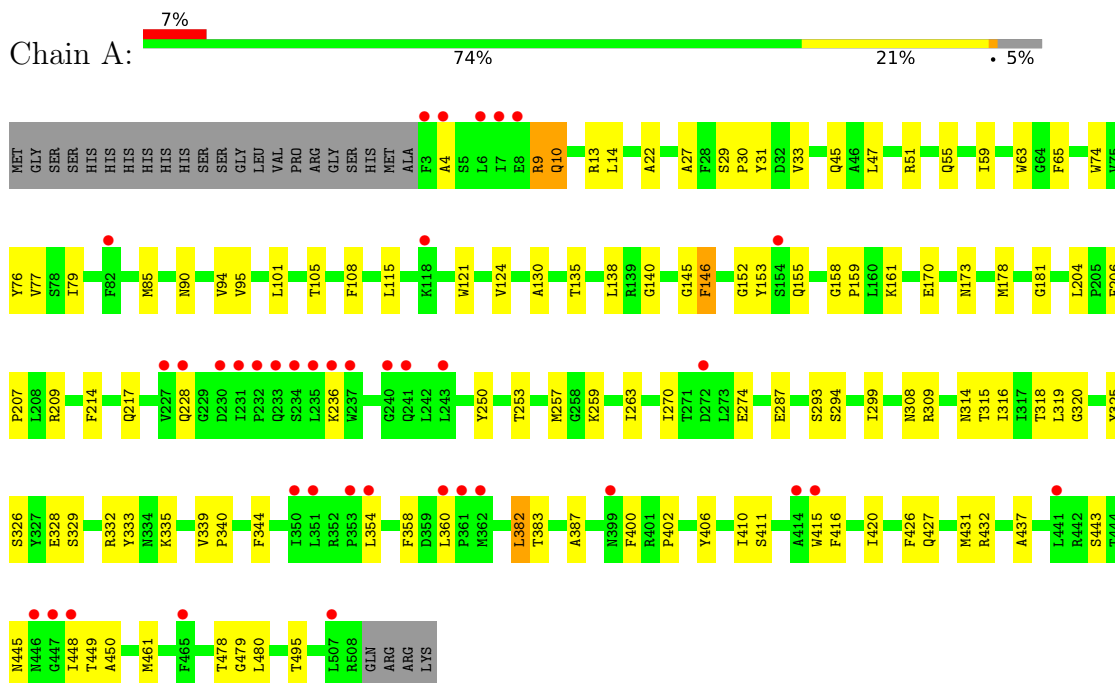
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	5	Total	O	0	0
			5	5		

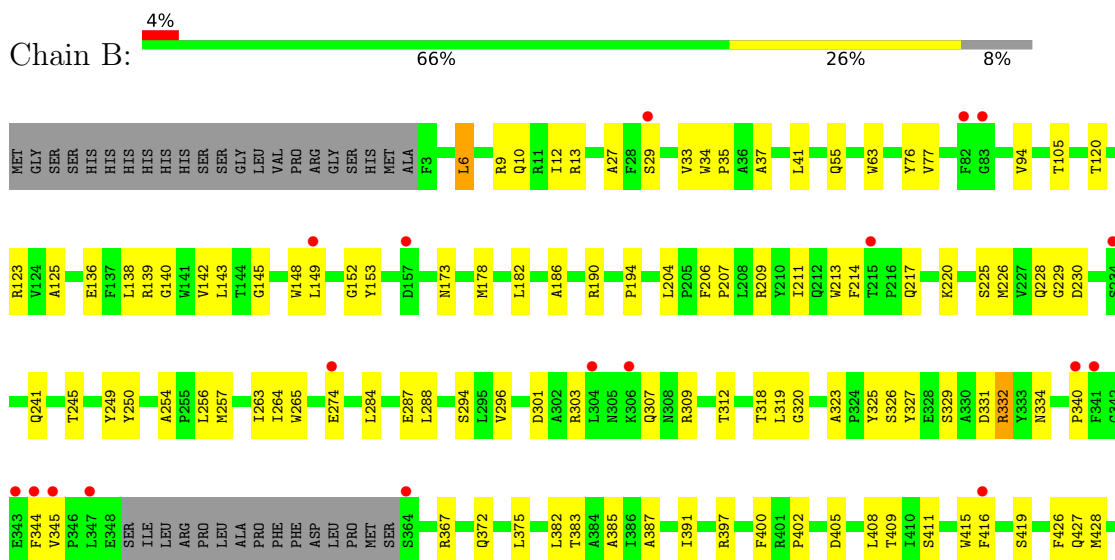
3 Residue-property plots [i](#)

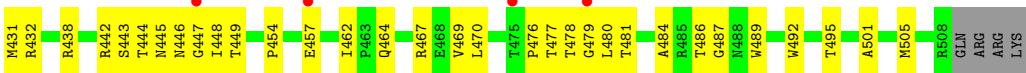
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Apolipoprotein N-acyltransferase



- Molecule 1: Apolipoprotein N-acyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.22Å 142.95Å 197.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.90 49.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.79-2.90) 97.7 (49.79-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.91Å)	Xtriage
Refinement program	BUSTER, PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.227 , 0.263 0.238 , 0.263	Depositor DCC
R_{free} test set	1699 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8371	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	1/4097 (0.0%)	0.46	0/5598
1	B	0.18	0/3972	0.44	0/5425
All	All	0.20	1/8069 (0.0%)	0.45	0/11023

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	PHE	C-N	6.93	1.50	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	0	4051	78	0
1	B	3863	0	3926	95	0
2	A	312	0	406	14	0
2	B	129	0	167	3	0
3	A	48	0	64	2	0
3	B	24	0	32	0	0
4	A	8	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8371	0	8646	176	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 10.

All (176) 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)
2:A:612:OLC:H2	2:A:613:OLC:H21A	1.66	0.76
1:B:214:PHE:HA	1:B:479:GLY:HA3	1.66	0.75
1:A:85:MET:HB2	1:A:90:ASN:HD21	1.51	0.75
1:A:214:PHE:HA	1:A:479:GLY:HA3	1.71	0.71
1:A:153:TYR:OH	1:A:432:ARG:NH2	2.25	0.69
1:A:140:GLY:O	1:A:145:GLY:HA2	1.92	0.69
1:B:153:TYR:OH	1:B:432:ARG:NH2	2.25	0.69
1:B:318:THR:OG1	1:B:331:ASP:OD2	2.04	0.68
1:A:443:SER:HA	1:A:449:THR:HG23	1.74	0.68
1:B:250:TYR:OH	1:B:287:GLU:OE2	2.11	0.68
1:A:354:LEU:HD11	1:A:360:LEU:H	1.58	0.68
1:B:228:GLN:NE2	1:B:446:ASN:O	2.27	0.67
1:B:405:ASP:OD2	1:B:476:PRO:HB3	1.95	0.66
1:A:77:VAL:HG21	1:A:416:PHE:HA	1.76	0.66
1:A:31:TYR:HD1	2:A:615:OLC:H21	1.62	0.65
1:B:397:ARG:NH1	1:B:484:ALA:O	2.30	0.65
1:A:14:LEU:HD23	1:A:59:ILE:HD13	1.78	0.65
1:B:178:MET:HE1	2:B:602:OLC:H13	1.81	0.63
1:A:29:SER:HB2	1:A:427:GLN:HB2	1.81	0.62
1:B:438:ARG:NH1	1:B:479:GLY:O	2.22	0.62
1:B:63:TRP:HE3	1:B:105:THR:HG21	1.65	0.61
1:A:257:MET:O	1:A:293:SER:OG	2.13	0.61
1:B:76:TYR:HB2	1:B:94:VAL:HG21	1.83	0.61
1:A:155:GLN:HG3	1:A:158:GLY:HA3	1.83	0.61
1:B:29:SER:HB2	1:B:427:GLN:HB2	1.83	0.61
1:B:257:MET:HE1	1:B:287:GLU:HB3	1.82	0.61
1:A:382:LEU:HD12	1:A:406:TYR:HB2	1.83	0.60
1:B:375:LEU:N	1:B:382:LEU:O	2.35	0.59
1:A:33:VAL:HG21	2:A:615:OLC:H4	1.85	0.59
1:A:63:TRP:HE3	1:A:105:THR:HG21	1.68	0.59
1:A:339:VAL:HG21	2:A:612:OLC:H24A	1.84	0.58
1:B:284:LEU:HD22	1:B:319:LEU:HD13	1.85	0.58
1:A:76:TYR:HB2	1:A:94:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:NH2	2:B:603:OLC:O23	2.37	0.58
1:A:340:PRO:HA	1:A:344:PHE:CE2	2.38	0.58
1:A:450:ALA:HB2	1:A:461:MET:HG3	1.86	0.58
1:B:344:PHE:HD1	1:B:345:VAL:N	2.02	0.57
1:A:178:MET:HE1	2:A:603:OLC:H8A	1.86	0.57
1:B:462:ILE:HD13	1:B:470:LEU:HB2	1.87	0.57
1:A:161:LYS:HD3	1:A:209:ARG:NH1	2.20	0.56
1:A:316:ILE:HG12	1:A:410:ILE:HD11	1.88	0.56
1:B:229:GLY:HA2	1:B:467:ARG:HG3	1.88	0.56
1:B:303:ARG:NH2	1:B:327:TYR:O	2.24	0.56
1:B:228:GLN:HE21	1:B:446:ASN:HA	1.71	0.56
1:A:214:PHE:HB3	1:A:437:ALA:HB1	1.88	0.55
1:A:294:SER:HA	1:A:320:GLY:HA3	1.88	0.55
1:B:63:TRP:CE3	1:B:105:THR:HG21	2.40	0.55
1:B:294:SER:HA	1:B:320:GLY:HA3	1.88	0.55
1:B:37:ALA:O	1:B:41:LEU:HD12	2.06	0.55
1:A:328:GLU:N	1:A:328:GLU:OE2	2.40	0.55
1:B:125:ALA:HB2	1:B:182:LEU:HD21	1.87	0.55
1:A:152:GLY:N	1:A:173:ASN:OD1	2.36	0.55
2:A:612:OLC:H5	2:A:618:OLC:H2	1.88	0.55
1:A:27:ALA:HA	1:A:33:VAL:O	2.06	0.55
1:A:383:THR:HG21	1:A:400:PHE:HA	1.88	0.54
1:B:10:GLN:NE2	1:B:55:GLN:HB2	2.22	0.54
1:A:250:TYR:OH	1:A:287:GLU:OE2	2.23	0.54
1:B:492:TRP:HA	1:B:495:THR:HG22	1.89	0.54
1:A:9:ARG:HG3	3:A:624:GOL:H31	1.89	0.53
1:B:138:LEU:O	1:B:142:VAL:HG12	2.07	0.53
1:B:344:PHE:HE2	1:B:367:ARG:HH12	1.56	0.53
1:B:402:PRO:O	1:B:438:ARG:NH2	2.42	0.53
1:A:13:ARG:NH2	2:A:602:OLC:O23	2.42	0.53
1:A:55:GLN:O	1:A:59:ILE:HG12	2.08	0.53
1:A:274:GLU:OE1	1:A:332:ARG:NH2	2.42	0.53
1:B:383:THR:HG21	1:B:400:PHE:HA	1.90	0.53
1:B:446:ASN:OD1	1:B:447:GLY:N	2.42	0.53
1:B:416:PHE:O	1:B:419:SER:OG	2.17	0.52
1:B:447:GLY:O	1:B:464:GLN:HB3	2.09	0.52
1:A:121:TRP:CE3	2:A:603:OLC:H3	2.45	0.52
1:B:27:ALA:HA	1:B:33:VAL:O	2.10	0.52
1:A:178:MET:HE1	2:A:603:OLC:H11	1.92	0.51
1:B:307:GLN:HG2	1:B:309:ARG:HG3	1.92	0.51
1:B:136:GLU:OE1	1:B:139:ARG:NH2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:SER:HB3	1:B:329:SER:HB2	1.92	0.51
1:B:501:ALA:O	1:B:505:MET:HG2	2.10	0.51
1:A:124:VAL:HB	1:A:181:GLY:HA3	1.93	0.51
1:A:204:LEU:O	1:A:207:PRO:HD2	2.11	0.51
1:A:431:MET:HA	1:A:431:MET:HE3	1.92	0.50
1:B:217:GLN:NE2	1:B:478:THR:HB	2.27	0.50
1:B:217:GLN:HB2	1:B:476:PRO:HG2	1.94	0.50
1:B:34:TRP:CG	1:B:35:PRO:HD3	2.47	0.50
1:A:74:TRP:O	1:A:77:VAL:HG22	2.11	0.50
1:B:152:GLY:N	1:B:173:ASN:OD1	2.43	0.50
1:B:397:ARG:CD	1:B:487:GLY:HA2	2.42	0.50
1:A:228:GLN:HG3	1:A:445:ASN:O	2.12	0.49
1:B:257:MET:HE3	1:B:288:LEU:HD23	1.94	0.49
1:A:326:SER:HB3	1:A:329:SER:HB2	1.94	0.49
1:B:274:GLU:OE1	1:B:332:ARG:NH2	2.46	0.49
1:B:9:ARG:HB2	1:B:12:ILE:HD13	1.95	0.48
1:B:229:GLY:O	1:B:445:ASN:ND2	2.46	0.48
1:B:120:THR:HG23	1:B:123:ARG:H	1.77	0.48
1:A:10:GLN:NE2	1:A:51:ARG:HH11	2.12	0.48
1:B:140:GLY:O	1:B:145:GLY:HA3	2.14	0.48
1:B:411:SER:O	1:B:444:THR:HA	2.13	0.48
1:B:301:ASP:O	1:B:312:THR:HA	2.14	0.47
1:A:135:THR:HA	1:A:138:LEU:HD12	1.97	0.47
1:B:143:LEU:C	1:B:145:GLY:H	2.22	0.47
1:A:4:ALA:HB3	1:A:9:ARG:HG2	1.97	0.47
1:A:217:GLN:NE2	1:A:478:THR:HB	2.30	0.47
1:B:405:ASP:CG	1:B:476:PRO:HB3	2.40	0.47
1:B:254:ALA:HA	1:B:257:MET:HG3	1.96	0.47
1:B:211:ILE:HG12	2:B:606:OLC:H3	1.97	0.46
1:B:340:PRO:O	1:B:344:PHE:HB3	2.14	0.46
1:A:85:MET:HB2	1:A:90:ASN:ND2	2.23	0.46
1:B:431:MET:HE3	1:B:431:MET:HA	1.96	0.46
1:B:387:ALA:HA	1:B:411:SER:HB2	1.97	0.46
1:B:220:LYS:HB2	1:B:476:PRO:HG3	1.97	0.46
1:B:426:PHE:CB	1:B:448:ILE:HD12	2.46	0.46
1:A:108:PHE:HB2	1:A:135:THR:HG21	1.97	0.46
1:A:270:ILE:HB	1:A:299:ILE:HG13	1.98	0.46
1:A:63:TRP:CE3	1:A:105:THR:HG21	2.48	0.46
1:A:47:LEU:HD23	2:A:602:OLC:H2A	1.98	0.45
1:A:65:PHE:HZ	1:A:95:VAL:HG13	1.81	0.45
1:A:319:LEU:HG	1:A:325:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PHE:HB2	1:B:477:THR:HB	1.98	0.45
1:B:402:PRO:HB3	1:B:480:LEU:HD11	1.98	0.45
1:B:204:LEU:O	1:B:207:PRO:HD2	2.16	0.45
1:A:22:ALA:HB1	2:A:601:OLC:H4A	1.98	0.45
1:B:241:GLN:O	1:B:245:THR:HG23	2.16	0.45
1:B:249:TYR:HB3	1:B:265:TRP:CZ2	2.52	0.45
1:A:318:THR:C	1:A:319:LEU:HD12	2.42	0.45
1:B:230:ASP:O	1:B:467:ARG:NH2	2.48	0.45
1:A:77:VAL:CG2	1:A:416:PHE:HA	2.45	0.45
1:B:10:GLN:HE21	1:B:55:GLN:HB2	1.82	0.45
1:B:213:TRP:HB2	1:B:481:THR:HG22	1.98	0.45
1:B:409:THR:O	1:B:442:ARG:HA	2.16	0.45
1:B:296:VAL:HG22	1:B:318:THR:HG22	1.99	0.45
1:B:186:ALA:HB2	1:B:194:PRO:HG2	1.99	0.44
1:B:226:MET:HE3	1:B:226:MET:HB2	1.87	0.44
1:A:426:PHE:CD2	1:A:448:ILE:HG21	2.52	0.44
1:B:319:LEU:HD23	1:B:325:TYR:HB2	2.00	0.44
1:B:334:ASN:H	1:B:372:GLN:HE22	1.65	0.44
1:B:385:ALA:O	1:B:409:THR:HA	2.18	0.44
1:B:318:THR:HB	1:B:323:ALA:HB1	2.00	0.43
1:A:79:ILE:HG22	1:A:90:ASN:ND2	2.32	0.43
1:A:402:PRO:HB3	1:A:480:LEU:HD21	2.00	0.43
1:A:155:GLN:OE1	1:A:159:PRO:HD2	2.18	0.43
1:B:206:PHE:O	1:B:209:ARG:HG2	2.18	0.43
1:B:382:LEU:HD23	1:B:408:LEU:HD13	2.00	0.43
1:A:206:PHE:O	1:A:209:ARG:HG2	2.18	0.43
1:A:101:LEU:HD11	1:A:146:PHE:CE2	2.53	0.43
1:B:426:PHE:HB2	1:B:448:ILE:HD12	2.00	0.43
1:A:274:GLU:CD	1:A:332:ARG:HH22	2.25	0.43
1:B:77:VAL:HG23	1:B:416:PHE:HA	2.00	0.42
1:A:253:THR:HG23	1:A:263:ILE:HG21	1.99	0.42
1:A:30:PRO:HG2	1:A:420:ILE:HB	2.01	0.42
1:A:101:LEU:HD11	1:A:146:PHE:HE2	1.84	0.42
1:B:148:TRP:HD1	1:B:149:LEU:HG	1.84	0.42
1:B:256:LEU:HD11	1:B:469:VAL:HG11	2.00	0.42
1:A:121:TRP:HA	1:A:124:VAL:HG22	2.01	0.42
1:A:315:THR:HA	1:A:333:TYR:O	2.20	0.42
1:B:77:VAL:CG2	1:B:416:PHE:HA	2.50	0.42
1:A:31:TYR:CD1	2:A:615:OLC:H21	2.47	0.42
1:A:314:ASN:HB3	1:A:335:LYS:HB2	2.02	0.42
1:B:153:TYR:CE2	1:B:428:MET:HE3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ILE:HB	1:B:428:MET:HE2	2.01	0.41
1:A:354:LEU:HD13	1:A:360:LEU:HB2	2.02	0.41
1:B:454:PRO:HD2	1:B:457:GLU:OE2	2.20	0.41
1:A:9:ARG:HG3	3:A:624:GOL:H11	2.01	0.41
1:A:130:ALA:HA	1:A:495:THR:HG23	2.03	0.41
1:B:226:MET:HG2	1:B:264:ILE:HB	2.02	0.41
1:B:6:LEU:HD13	1:B:12:ILE:HG12	2.01	0.41
1:B:34:TRP:CD2	1:B:35:PRO:HD3	2.55	0.41
1:A:206:PHE:HB3	1:A:207:PRO:HD3	2.03	0.41
1:A:236:LYS:HE2	1:A:236:LYS:HB2	1.85	0.41
1:A:76:TYR:HB3	2:A:611:OLC:H24A	2.03	0.41
1:B:432:ARG:HD3	1:B:432:ARG:HA	1.80	0.40
1:B:443:SER:HA	1:B:449:THR:HG23	2.03	0.40
1:B:486:THR:O	1:B:489:TRP:CD1	2.74	0.40
2:A:612:OLC:H8	2:A:612:OLC:H11	1.76	0.40
1:A:209:ARG:HH11	1:A:209:ARG:HD2	1.76	0.40
1:B:225:SER:O	1:B:263:ILE:HA	2.22	0.40
1:A:170:GLU:HA	1:A:173:ASN:ND2	2.36	0.40
1:A:387:ALA:HA	1:A:411:SER:HB2	2.04	0.40
1:B:33:VAL:HG12	1:B:35:PRO:HD2	2.04	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	504/532 (95%)	488 (97%)	16 (3%)	0	100	100
1	B	487/532 (92%)	479 (98%)	8 (2%)	0	100	100
All	All	991/1064 (93%)	967 (98%)	24 (2%)	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	421/443 (95%)	411 (98%)	10 (2%)	43	75
1	B	407/443 (92%)	403 (99%)	4 (1%)	68	89
All	All	828/886 (94%)	814 (98%)	14 (2%)	53	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	10	GLN
1	A	45	GLN
1	A	115	LEU
1	A	259	LYS
1	A	308	ASN
1	A	309	ARG
1	A	358	PHE
1	A	382	LEU
1	A	415	TRP
1	B	6	LEU
1	B	190	ARG
1	B	332	ARG
1	B	415	TRP

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

Mol	Chain	Res	Type
1	A	10	GLN
1	A	45	GLN
1	A	90	ASN
1	A	459	GLN
1	B	50	ASN
1	B	228	GLN
1	B	378	ASN
1	B	427	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 ⓘ

39 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	A	614	-	13,13,24	0.91	1 (7%)	14,14,25	1.15	1 (7%)
3	GOL	B	610	-	5,5,5	0.36	0	5,5,5	0.28	0
2	OLC	A	609	-	21,21,24	0.76	1 (4%)	22,22,25	0.94	1 (4%)
3	GOL	A	627	-	5,5,5	0.30	0	5,5,5	0.14	0
2	OLC	A	604	-	13,13,24	0.93	1 (7%)	14,14,25	1.13	1 (7%)
3	GOL	B	609	-	5,5,5	0.36	0	5,5,5	0.33	0
2	OLC	A	607	-	14,14,24	0.87	1 (7%)	15,15,25	1.05	1 (6%)
2	OLC	B	601	-	13,13,24	0.90	1 (7%)	14,14,25	0.98	1 (7%)
2	OLC	A	605	-	11,11,24	0.99	1 (9%)	12,12,25	1.19	1 (8%)
2	OLC	A	611	-	15,15,24	0.87	1 (6%)	16,16,25	0.96	1 (6%)
2	OLC	B	605	-	17,17,24	0.83	1 (5%)	18,18,25	1.10	1 (5%)
3	GOL	A	620	-	5,5,5	0.36	0	5,5,5	0.30	0
2	OLC	A	608	-	13,13,24	0.93	1 (7%)	14,14,25	1.07	1 (7%)
3	GOL	A	624	-	5,5,5	0.33	0	5,5,5	0.23	0
2	OLC	B	603	-	10,10,24	1.05	1 (10%)	11,11,25	1.16	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	A	613	-	13,13,24	0.91	1 (7%)	14,14,25	1.09	1 (7%)
2	OLC	A	616	-	12,12,24	0.89	1 (8%)	13,13,25	1.27	1 (7%)
2	OLC	A	618	-	13,13,24	0.85	1 (7%)	14,14,25	1.24	1 (7%)
2	OLC	A	610	-	11,11,24	1.00	1 (9%)	12,12,25	1.13	1 (8%)
2	OLC	B	607	-	10,10,24	0.97	1 (10%)	11,11,25	1.11	1 (9%)
2	OLC	A	617	-	13,13,24	0.88	1 (7%)	14,14,25	1.12	1 (7%)
3	GOL	A	622	-	5,5,5	0.37	0	5,5,5	0.38	0
3	GOL	A	625	-	5,5,5	0.31	0	5,5,5	0.26	0
2	OLC	B	604	-	20,20,24	0.77	1 (5%)	21,21,25	1.06	1 (4%)
3	GOL	A	626	-	5,5,5	0.32	0	5,5,5	0.21	0
2	OLC	A	612	-	21,21,24	0.74	1 (4%)	22,22,25	1.00	1 (4%)
2	OLC	A	602	-	11,11,24	0.98	1 (9%)	12,12,25	1.08	1 (8%)
3	GOL	B	611	-	5,5,5	0.42	0	5,5,5	0.07	0
2	OLC	B	602	-	24,24,24	0.69	1 (4%)	25,25,25	0.97	1 (4%)
2	OLC	A	603	-	21,21,24	0.75	1 (4%)	22,22,25	1.08	2 (9%)
2	OLC	A	601	-	14,14,24	0.87	1 (7%)	15,15,25	1.04	1 (6%)
2	OLC	B	608	-	15,15,24	0.81	1 (6%)	16,16,25	0.93	1 (6%)
3	GOL	A	621	-	5,5,5	0.35	0	5,5,5	0.29	0
2	OLC	A	606	-	24,24,24	0.70	1 (4%)	25,25,25	1.17	1 (4%)
3	GOL	A	623	-	5,5,5	0.36	0	5,5,5	0.38	0
2	OLC	B	606	-	12,12,24	0.94	1 (8%)	13,13,25	1.35	2 (15%)
3	GOL	B	612	-	5,5,5	0.27	0	5,5,5	0.67	0
2	OLC	A	619	-	21,21,24	0.73	1 (4%)	22,22,25	0.95	1 (4%)
2	OLC	A	615	-	19,19,24	0.81	1 (5%)	20,20,25	1.51	4 (20%)

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	OLC	A	614	-	-	8/13/13/24	-
3	GOL	B	610	-	-	0/4/4/4	-
2	OLC	A	609	-	-	5/21/21/24	-
3	GOL	A	627	-	-	0/4/4/4	-
2	OLC	A	604	-	-	4/13/13/24	-
3	GOL	B	609	-	-	0/4/4/4	-
2	OLC	A	607	-	-	10/14/14/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	601	-	-	5/13/13/24	-
2	OLC	A	605	-	-	2/11/11/24	-
2	OLC	A	611	-	-	7/15/15/24	-
2	OLC	B	605	-	-	8/17/17/24	-
3	GOL	A	620	-	-	0/4/4/4	-
2	OLC	A	608	-	-	5/13/13/24	-
3	GOL	A	624	-	-	2/4/4/4	-
2	OLC	B	603	-	-	7/10/10/24	-
2	OLC	A	613	-	-	4/13/13/24	-
2	OLC	A	616	-	-	0/12/12/24	-
2	OLC	A	618	-	-	4/13/13/24	-
2	OLC	A	610	-	-	1/11/11/24	-
2	OLC	B	607	-	-	6/10/10/24	-
2	OLC	A	617	-	-	4/13/13/24	-
3	GOL	A	622	-	-	2/4/4/4	-
3	GOL	A	625	-	-	2/4/4/4	-
2	OLC	B	604	-	-	8/20/20/24	-
3	GOL	A	626	-	-	1/4/4/4	-
2	OLC	A	612	-	-	10/21/21/24	-
2	OLC	A	602	-	-	4/11/11/24	-
3	GOL	B	611	-	-	1/4/4/4	-
2	OLC	B	602	-	-	9/24/24/24	-
2	OLC	A	603	-	-	7/21/21/24	-
2	OLC	A	601	-	-	5/14/14/24	-
2	OLC	B	608	-	-	11/15/15/24	-
3	GOL	A	621	-	-	0/4/4/4	-
2	OLC	A	606	-	-	8/24/24/24	-
3	GOL	A	623	-	-	1/4/4/4	-
2	OLC	B	606	-	-	2/12/12/24	-
3	GOL	B	612	-	-	4/4/4/4	-
2	OLC	A	619	-	-	9/21/21/24	-
2	OLC	A	615	-	-	7/19/19/24	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	615	OLC	O20-C1	3.00	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	OLC	O20-C1	2.78	1.41	1.33
2	B	606	OLC	O20-C1	2.76	1.41	1.33
2	B	604	OLC	O20-C1	2.74	1.41	1.33
2	A	603	OLC	O20-C1	2.74	1.41	1.33
2	A	611	OLC	O20-C1	2.73	1.41	1.33
2	A	614	OLC	O20-C1	2.70	1.41	1.33
2	A	609	OLC	O20-C1	2.69	1.41	1.33
2	B	603	OLC	O20-C1	2.69	1.41	1.33
2	A	604	OLC	O20-C1	2.68	1.41	1.33
2	A	608	OLC	O20-C1	2.68	1.41	1.33
2	A	610	OLC	O20-C1	2.67	1.41	1.33
2	A	613	OLC	O20-C1	2.67	1.41	1.33
2	A	612	OLC	O20-C1	2.66	1.41	1.33
2	B	602	OLC	O20-C1	2.66	1.41	1.33
2	A	605	OLC	O20-C1	2.64	1.41	1.33
2	B	605	OLC	O20-C1	2.64	1.41	1.33
2	A	601	OLC	O20-C1	2.64	1.41	1.33
2	A	607	OLC	O20-C1	2.63	1.41	1.33
2	A	602	OLC	O20-C1	2.62	1.41	1.33
2	B	601	OLC	O20-C1	2.62	1.41	1.33
2	A	616	OLC	O20-C1	2.61	1.41	1.33
2	A	619	OLC	O20-C1	2.60	1.40	1.33
2	B	608	OLC	O20-C1	2.60	1.40	1.33
2	A	617	OLC	O20-C1	2.58	1.40	1.33
2	B	607	OLC	O20-C1	2.49	1.40	1.33
2	A	618	OLC	O20-C1	2.49	1.40	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	615	OLC	O20-C1-C2	3.90	123.71	111.83
2	A	606	OLC	O20-C1-C2	3.62	122.86	111.83
2	A	603	OLC	O20-C1-C2	3.34	122.01	111.83
2	B	606	OLC	O20-C1-C2	3.28	121.82	111.83
2	B	604	OLC	O20-C1-C2	3.15	121.45	111.83
2	A	616	OLC	O20-C1-C2	3.14	121.40	111.83
2	A	618	OLC	O20-C1-C2	3.08	121.22	111.83
2	A	614	OLC	O20-C1-C2	2.94	120.81	111.83
2	A	605	OLC	O20-C1-C2	2.89	120.64	111.83
2	B	602	OLC	O20-C1-C2	2.85	120.52	111.83
2	A	604	OLC	O20-C1-C2	2.85	120.51	111.83
2	B	603	OLC	O20-C1-C2	2.78	120.32	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	610	OLC	O20-C1-C2	2.76	120.24	111.83
2	A	612	OLC	O20-C1-C2	2.75	120.23	111.83
2	A	617	OLC	O20-C1-C2	2.73	120.15	111.83
2	B	605	OLC	O20-C1-C2	2.71	120.09	111.83
2	A	607	OLC	O20-C1-C2	2.70	120.08	111.83
2	A	609	OLC	O20-C1-C2	2.69	120.03	111.83
2	A	613	OLC	O20-C1-C2	2.68	120.02	111.83
2	A	601	OLC	O20-C1-C2	2.65	119.90	111.83
2	B	607	OLC	O20-C1-C2	2.64	119.87	111.83
2	A	619	OLC	O20-C1-C2	2.63	119.87	111.83
2	A	608	OLC	O20-C1-C2	2.63	119.86	111.83
2	A	602	OLC	O20-C1-C2	2.55	119.61	111.83
2	B	601	OLC	O20-C1-C2	2.53	119.56	111.83
2	A	611	OLC	O20-C1-C2	2.51	119.48	111.83
2	A	615	OLC	C21-O20-C1	-2.45	108.16	117.12
2	A	615	OLC	O20-C21-C22	2.33	116.81	105.85
2	B	606	OLC	C3-C2-C1	-2.13	105.90	113.69
2	B	608	OLC	O20-C1-C2	2.12	118.28	111.83
2	A	603	OLC	O20-C1-O19	-2.04	118.52	123.63
2	A	615	OLC	C21-C22-C24	-2.02	104.96	111.77

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	OLC	C21-C22-C24-O25
2	A	603	OLC	O20-C21-C22-O23
2	A	607	OLC	O20-C21-C22-C24
2	A	608	OLC	C21-C22-C24-O25
2	A	608	OLC	O20-C21-C22-C24
2	A	612	OLC	O20-C21-C22-O23
2	A	615	OLC	O20-C21-C22-C24
2	A	615	OLC	O20-C21-C22-O23
2	A	619	OLC	O20-C21-C22-O23
2	B	602	OLC	O20-C21-C22-C24
2	B	604	OLC	O20-C21-C22-O23
2	B	607	OLC	C21-C22-C24-O25
2	B	607	OLC	O20-C21-C22-O23
3	A	622	GOL	C1-C2-C3-O3
3	A	622	GOL	O2-C2-C3-O3
3	A	625	GOL	C1-C2-C3-O3
3	B	612	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	612	GOL	O1-C1-C2-C3
2	B	607	OLC	O19-C1-O20-C21
2	B	607	OLC	C2-C1-O20-C21
2	B	608	OLC	C2-C1-O20-C21
2	B	608	OLC	O19-C1-O20-C21
2	B	603	OLC	C2-C1-O20-C21
2	A	607	OLC	O20-C21-C22-O23
2	A	608	OLC	O20-C21-C22-O23
2	B	602	OLC	O20-C21-C22-O23
2	B	603	OLC	O19-C1-O20-C21
2	A	604	OLC	C2-C1-O20-C21
2	A	605	OLC	C2-C1-O20-C21
2	A	606	OLC	C2-C1-O20-C21
2	A	611	OLC	C2-C1-O20-C21
2	A	614	OLC	C2-C1-O20-C21
2	B	604	OLC	C2-C1-O20-C21
2	B	606	OLC	C2-C1-O20-C21
2	B	604	OLC	O20-C21-C22-C24
2	B	608	OLC	O20-C21-C22-C24
2	B	603	OLC	O20-C21-C22-O23
2	A	605	OLC	O19-C1-O20-C21
2	A	606	OLC	O19-C1-O20-C21
2	B	604	OLC	O19-C1-O20-C21
2	B	606	OLC	O19-C1-O20-C21
2	A	618	OLC	C1-C2-C3-C4
2	B	608	OLC	O23-C22-C24-O25
2	A	614	OLC	O19-C1-O20-C21
2	A	613	OLC	C1-C2-C3-C4
2	A	608	OLC	C1-C2-C3-C4
2	A	609	OLC	C1-C2-C3-C4
2	B	605	OLC	C1-C2-C3-C4
2	A	604	OLC	O19-C1-O20-C21
2	A	611	OLC	O19-C1-O20-C21
2	A	612	OLC	C1-C2-C3-C4
2	A	614	OLC	C1-C2-C3-C4
2	A	613	OLC	O20-C21-C22-O23
2	A	618	OLC	O20-C21-C22-O23
2	B	608	OLC	O20-C21-C22-O23
2	A	603	OLC	O20-C21-C22-C24
2	A	612	OLC	O20-C21-C22-C24
2	A	619	OLC	O20-C21-C22-C24
2	A	611	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	604	OLC	C21-C22-C24-O25
2	A	607	OLC	C21-C22-C24-O25
2	A	612	OLC	C21-C22-C24-O25
2	A	614	OLC	C21-C22-C24-O25
2	B	603	OLC	C21-C22-C24-O25
2	B	608	OLC	C21-C22-C24-O25
3	B	612	GOL	C1-C2-C3-O3
2	A	612	OLC	C11-C12-C13-C14
2	A	606	OLC	C12-C13-C14-C15
2	B	601	OLC	C2-C3-C4-C5
2	B	608	OLC	C2-C3-C4-C5
2	A	602	OLC	O23-C22-C24-O25
2	A	608	OLC	O23-C22-C24-O25
2	A	614	OLC	O23-C22-C24-O25
2	A	603	OLC	C2-C3-C4-C5
2	A	602	OLC	C1-C2-C3-C4
2	A	614	OLC	C3-C4-C5-C6
2	B	605	OLC	C4-C5-C6-C7
2	A	611	OLC	C3-C4-C5-C6
2	B	608	OLC	C4-C5-C6-C7
2	B	601	OLC	C3-C4-C5-C6
2	A	601	OLC	C2-C1-O20-C21
2	B	602	OLC	C5-C6-C7-C8
2	B	608	OLC	C3-C4-C5-C6
2	A	612	OLC	C6-C7-C8-C9
2	A	619	OLC	C2-C1-O20-C21
2	A	612	OLC	C5-C6-C7-C8
2	A	609	OLC	C2-C3-C4-C5
2	A	614	OLC	C2-C3-C4-C5
2	A	619	OLC	C4-C5-C6-C7
2	A	613	OLC	C2-C3-C4-C5
2	A	612	OLC	C3-C4-C5-C6
2	A	607	OLC	C2-C3-C4-C5
2	B	602	OLC	C1-C2-C3-C4
2	A	609	OLC	C10-C11-C12-C13
2	A	607	OLC	C4-C5-C6-C7
2	A	603	OLC	C4-C5-C6-C7
2	A	601	OLC	O19-C1-O20-C21
2	A	611	OLC	C2-C3-C4-C5
2	B	605	OLC	C2-C3-C4-C5
2	B	608	OLC	C1-C2-C3-C4
2	B	604	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	B	604	OLC	C5-C6-C7-C8
2	A	617	OLC	C2-C1-O20-C21
2	A	604	OLC	O23-C22-C24-O25
2	A	617	OLC	C3-C4-C5-C6
2	A	609	OLC	C6-C7-C8-C9
2	A	619	OLC	O19-C1-O20-C21
2	A	603	OLC	C1-C2-C3-C4
2	A	607	OLC	C2-C1-O20-C21
2	A	619	OLC	C6-C7-C8-C9
2	B	601	OLC	C2-C1-O20-C21
2	A	601	OLC	C4-C5-C6-C7
2	B	605	OLC	C5-C6-C7-C8
2	B	602	OLC	C10-C11-C12-C13
2	A	617	OLC	O19-C1-O20-C21
2	A	615	OLC	C2-C1-O20-C21
2	A	603	OLC	C3-C4-C5-C6
2	A	611	OLC	C4-C5-C6-C7
2	A	607	OLC	O19-C1-O20-C21
2	B	605	OLC	C2-C1-O20-C21
2	A	602	OLC	C2-C3-C4-C5
2	A	607	OLC	C5-C6-C7-C8
2	A	601	OLC	C3-C4-C5-C6
2	A	606	OLC	O23-C22-C24-O25
2	B	607	OLC	O23-C22-C24-O25
3	B	611	GOL	O1-C1-C2-O2
2	A	618	OLC	C4-C5-C6-C7
2	B	601	OLC	O19-C1-O20-C21
2	A	614	OLC	C4-C5-C6-C7
2	A	612	OLC	C2-C3-C4-C5
2	B	601	OLC	C1-C2-C3-C4
2	B	607	OLC	O20-C21-C22-C24
2	A	607	OLC	C3-C4-C5-C6
2	B	602	OLC	C2-C3-C4-C5
2	A	607	OLC	O23-C22-C24-O25
2	B	603	OLC	O23-C22-C24-O25
3	A	624	GOL	O1-C1-C2-O2
3	A	625	GOL	O2-C2-C3-O3
2	B	608	OLC	C6-C7-C8-C9
2	A	615	OLC	O19-C1-O20-C21
2	B	605	OLC	O19-C1-O20-C21
2	A	619	OLC	C3-C4-C5-C6
2	A	609	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	606	OLC	C1-C2-C3-C4
2	B	605	OLC	C7-C8-C9-C10
2	A	619	OLC	C5-C6-C7-C8
2	A	612	OLC	O23-C22-C24-O25
2	B	602	OLC	C7-C8-C9-C10
2	A	603	OLC	C6-C7-C8-C9
2	A	615	OLC	C9-C10-C11-C12
2	A	606	OLC	C11-C12-C13-C14
2	A	618	OLC	O20-C21-C22-C24
2	A	615	OLC	C21-C22-C24-O25
2	A	601	OLC	C5-C6-C7-C8
3	A	623	GOL	O2-C2-C3-O3
3	B	612	GOL	O2-C2-C3-O3
2	A	617	OLC	C1-C2-C3-C4
2	B	603	OLC	C1-C2-C3-C4
2	A	610	OLC	C1-C2-C3-C4
2	A	606	OLC	C15-C16-C17-C18
2	B	604	OLC	C7-C8-C9-C10
2	B	603	OLC	O20-C21-C22-C24
2	A	611	OLC	O20-C21-C22-O23
2	B	605	OLC	O20-C21-C22-O23
3	A	624	GOL	O1-C1-C2-C3
2	A	606	OLC	C7-C8-C9-C10
2	A	619	OLC	C7-C8-C9-C10
2	A	615	OLC	C7-C8-C9-C10
2	B	602	OLC	O20-C1-C2-C3
3	A	626	GOL	O1-C1-C2-O2
2	B	604	OLC	C11-C12-C13-C14
2	B	602	OLC	O19-C1-C2-C3
2	A	613	OLC	O20-C21-C22-C24

There are no ring outliers.

12 monomers are involved in 19 short contacts:

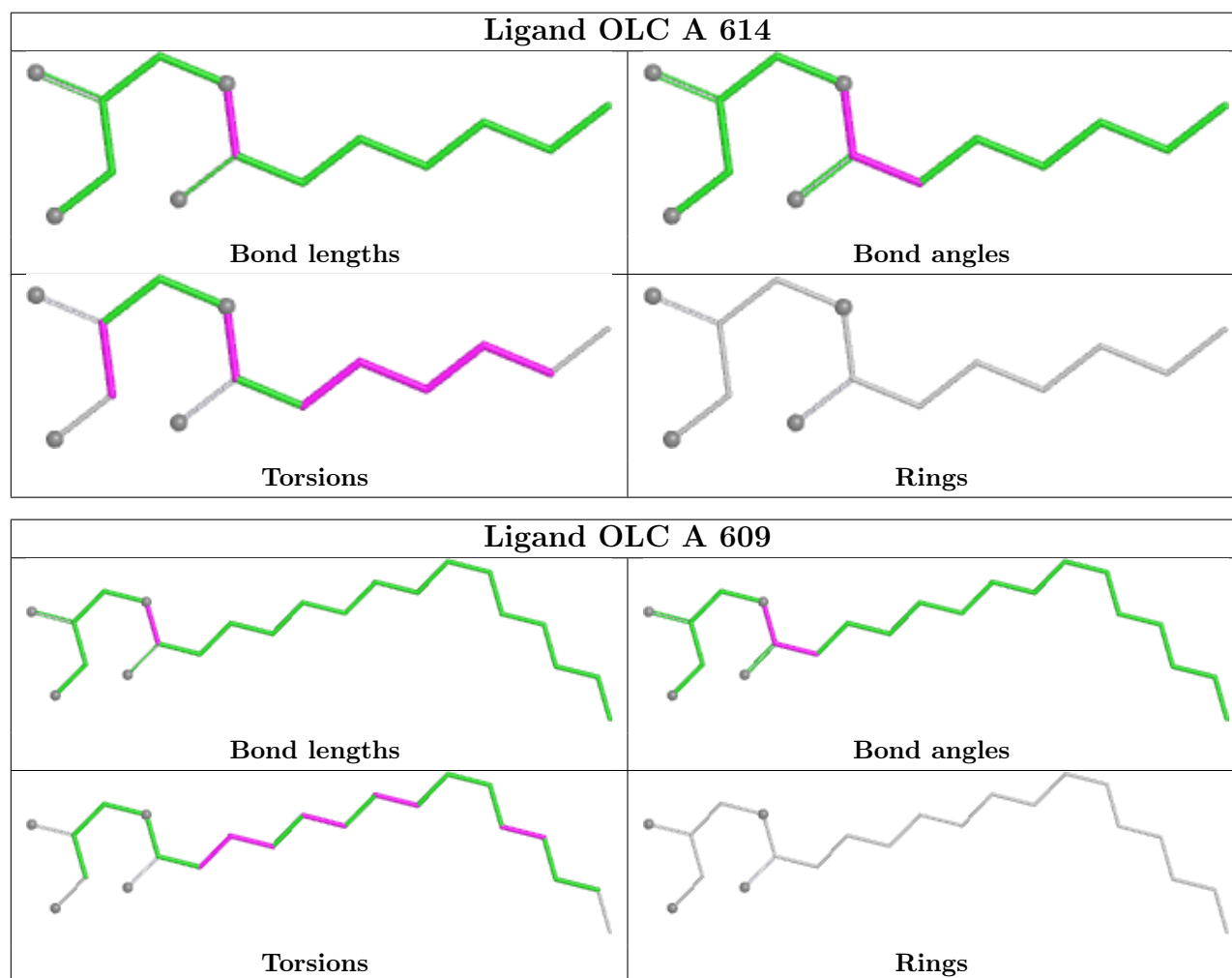
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	611	OLC	1	0
3	A	624	GOL	2	0
2	B	603	OLC	1	0
2	A	613	OLC	1	0
2	A	618	OLC	1	0
2	A	612	OLC	4	0
2	A	602	OLC	2	0

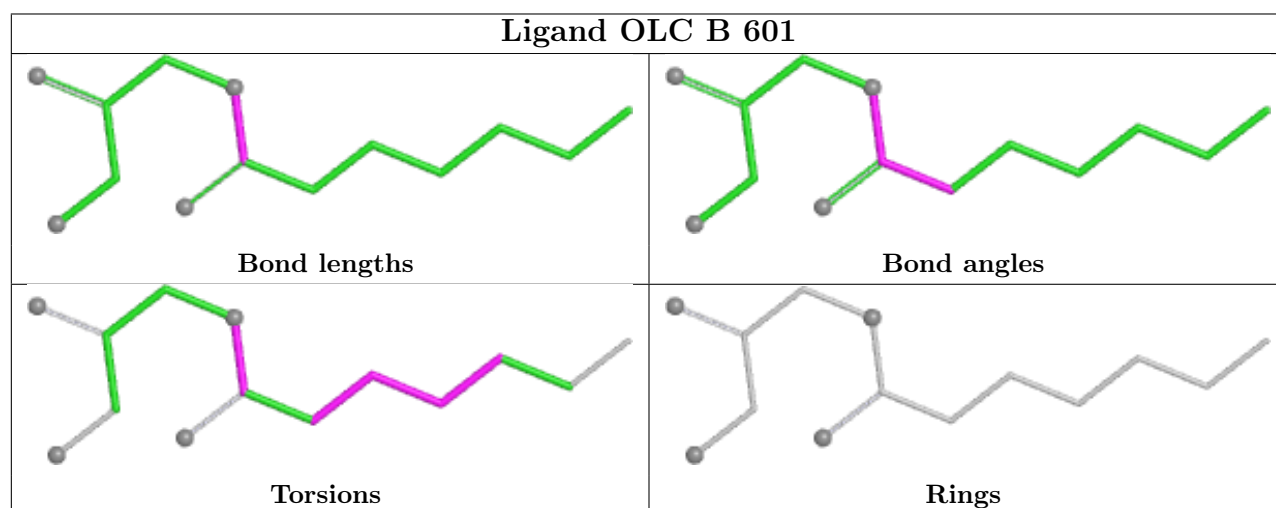
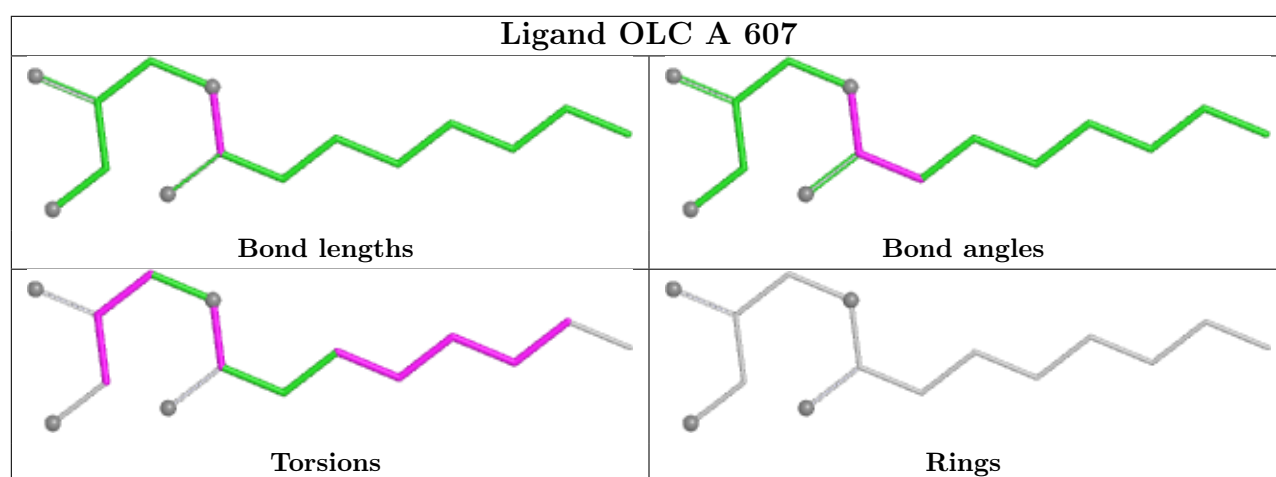
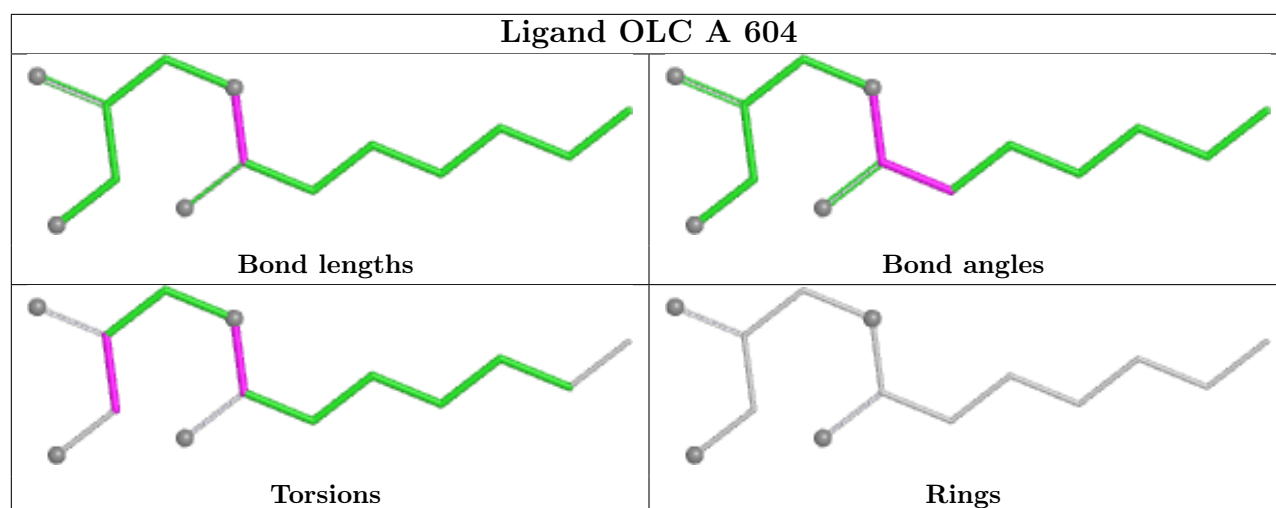
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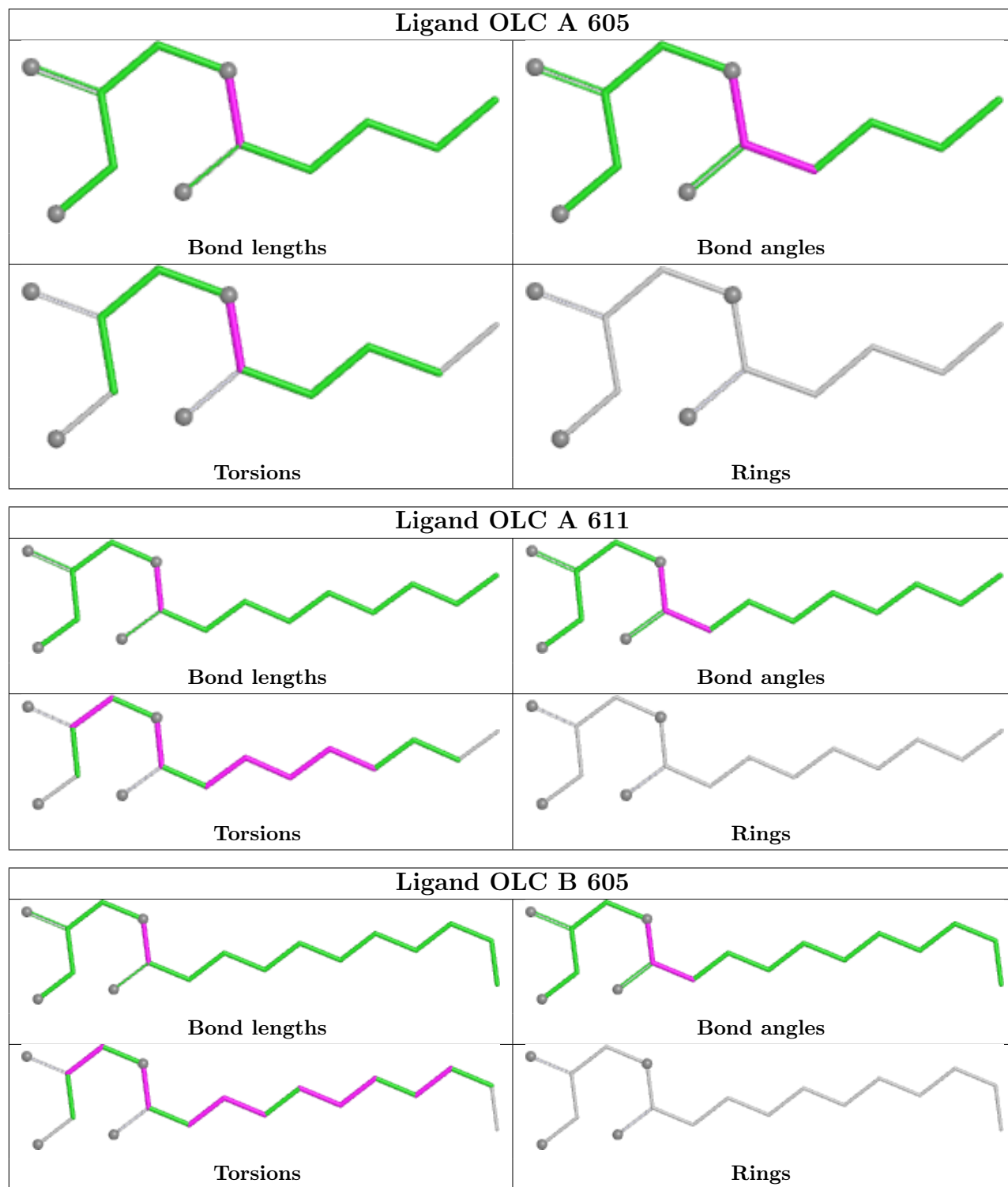
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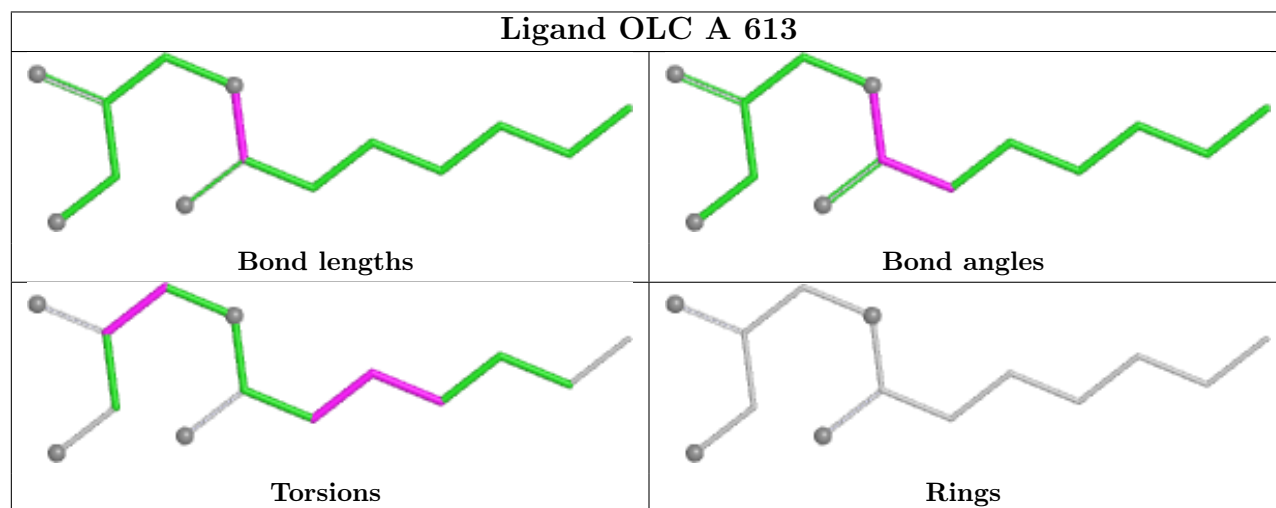
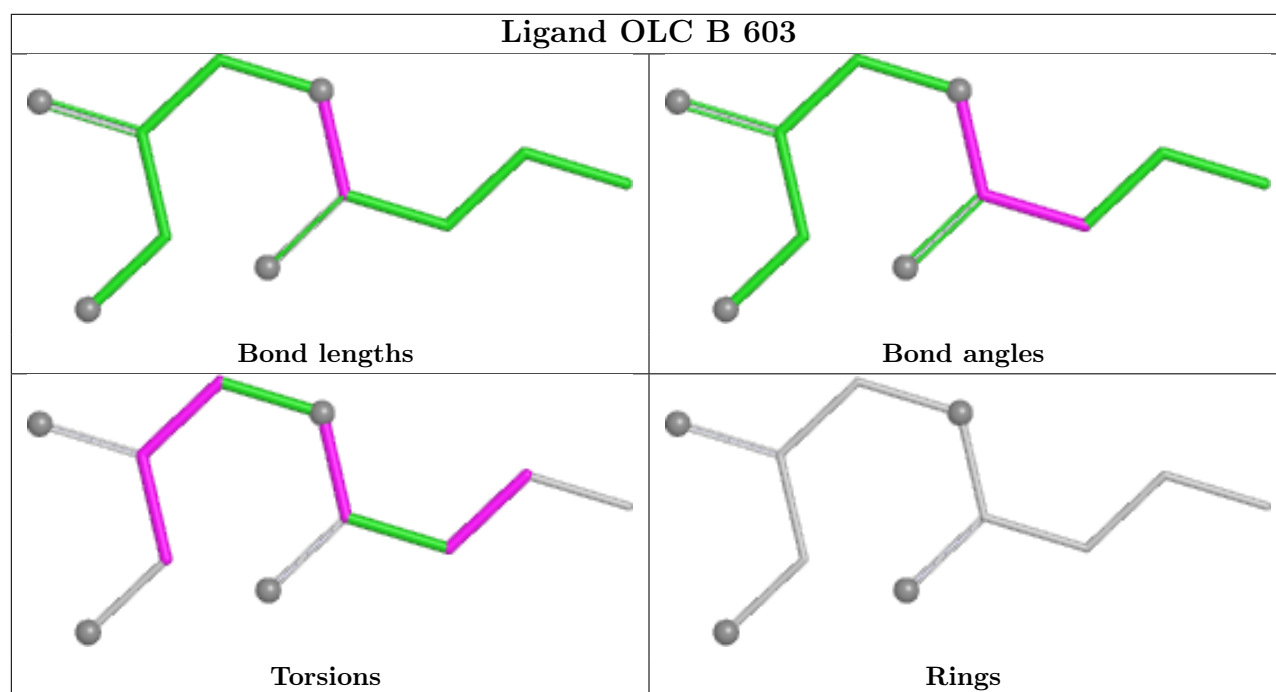
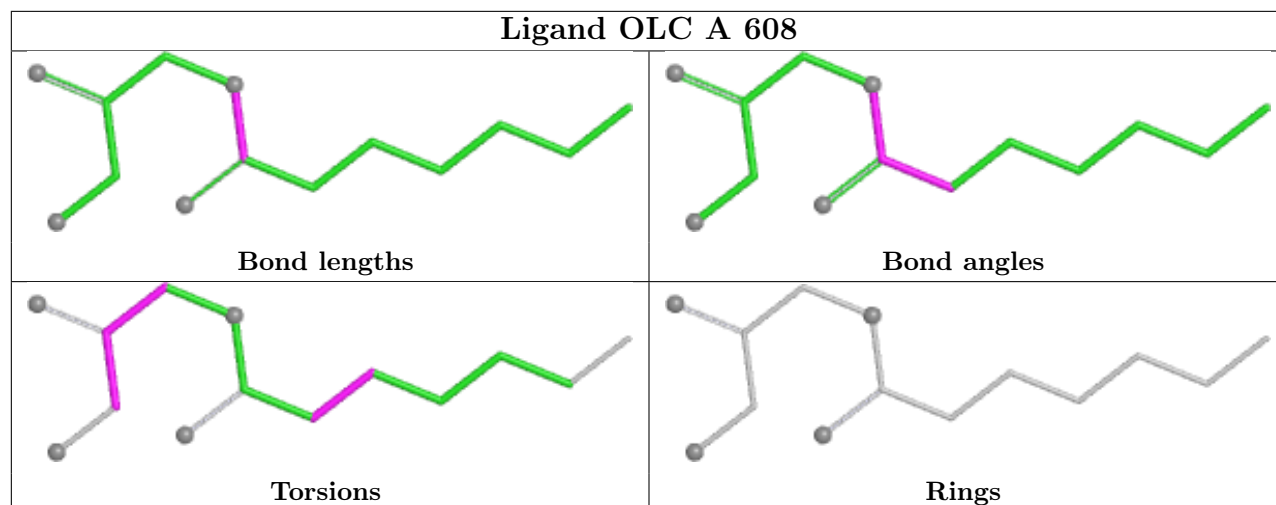
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	OLC	1	0
2	A	603	OLC	3	0
2	A	601	OLC	1	0
2	B	606	OLC	1	0
2	A	615	OLC	3	0

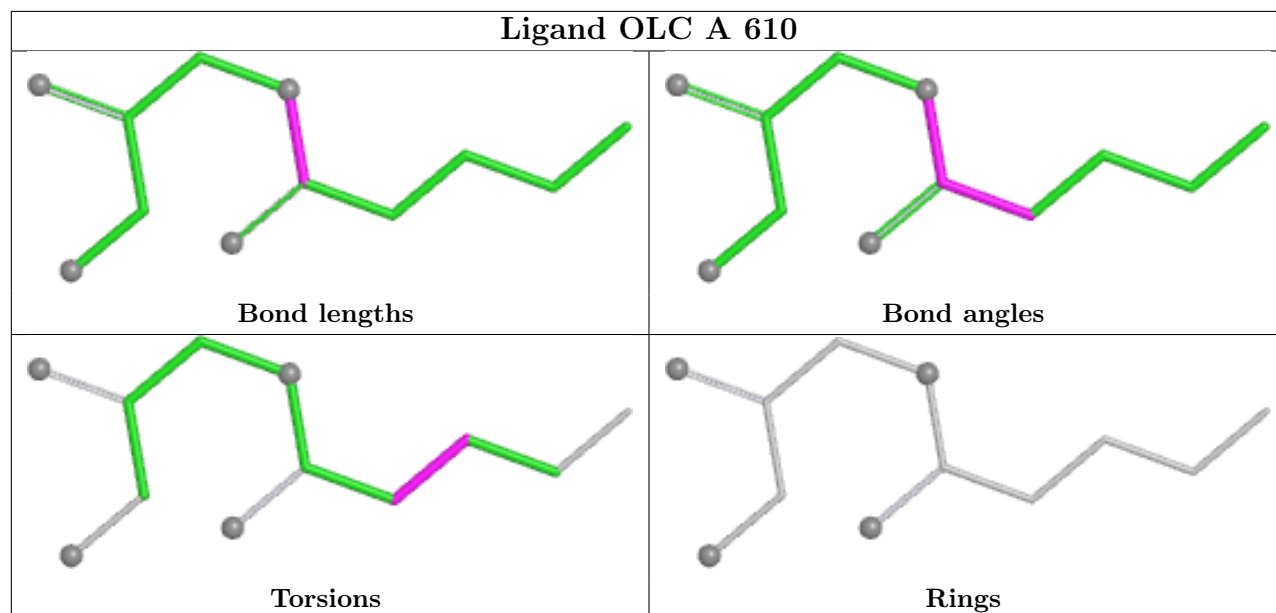
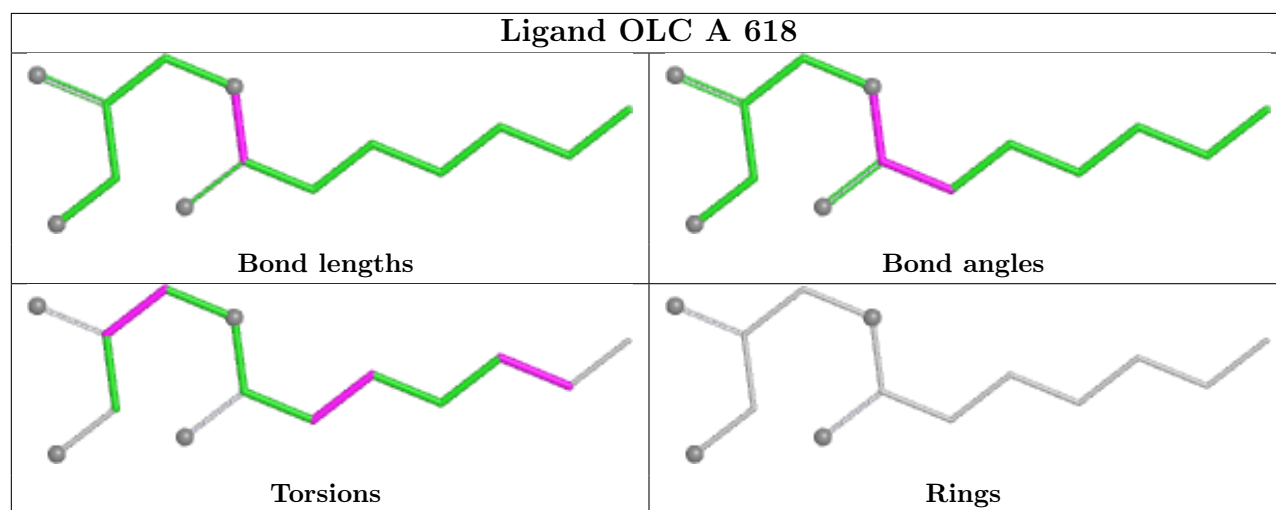
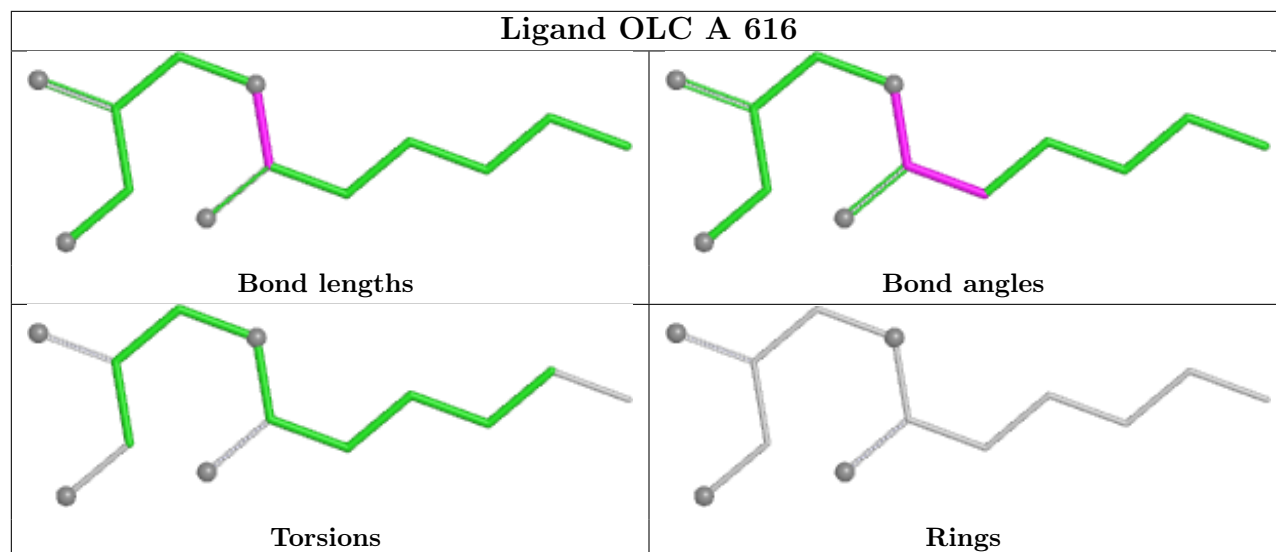
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

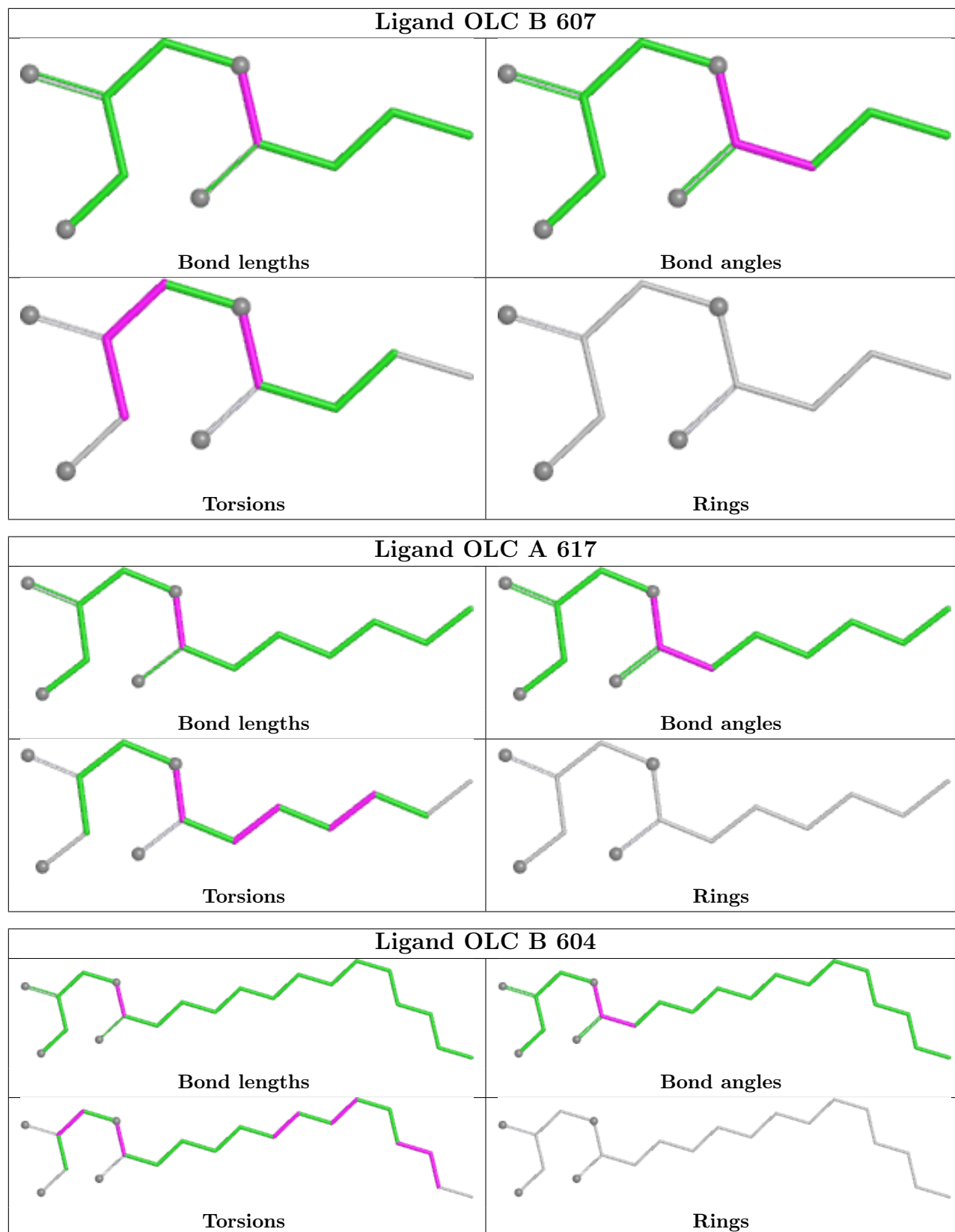


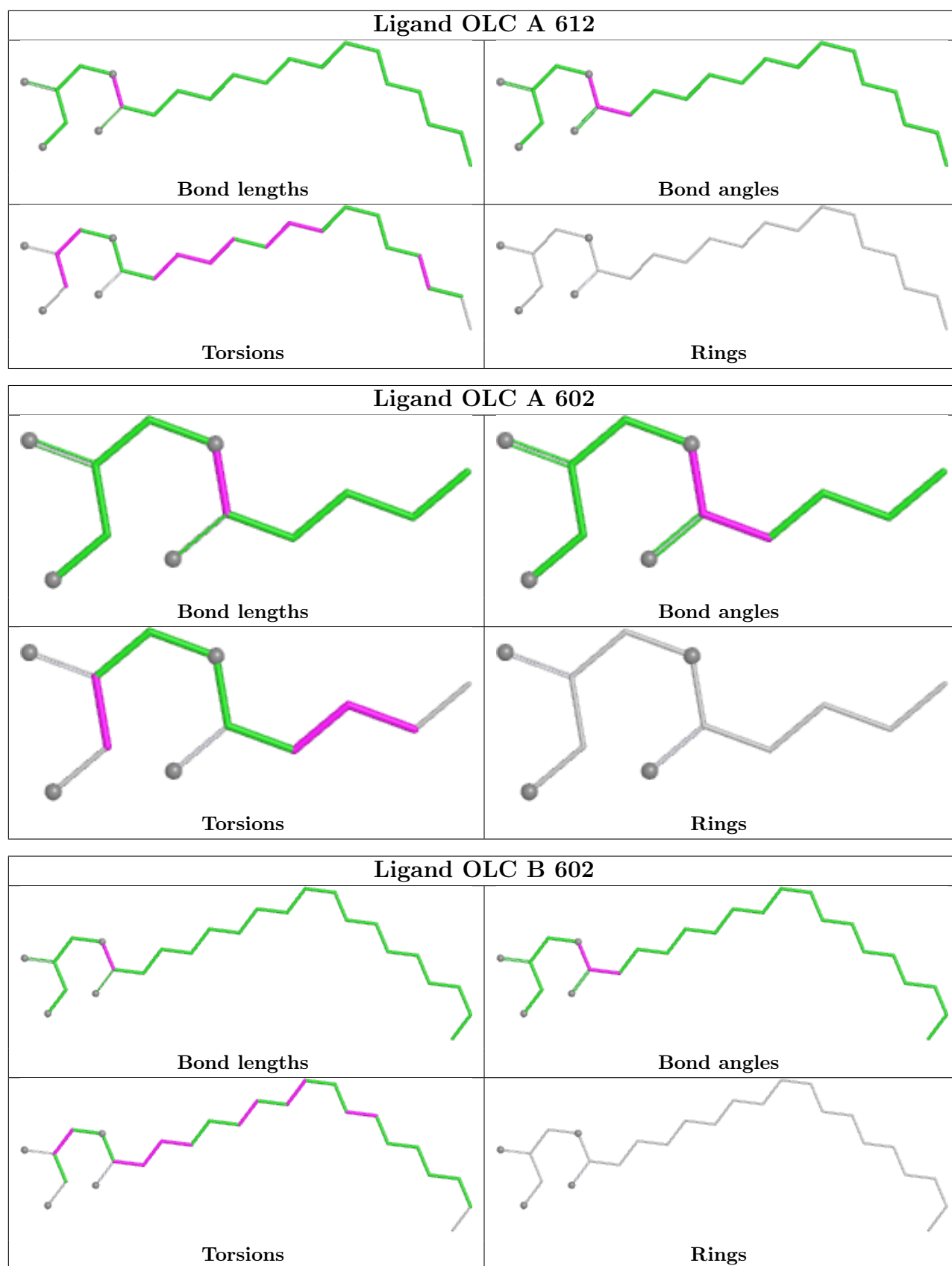


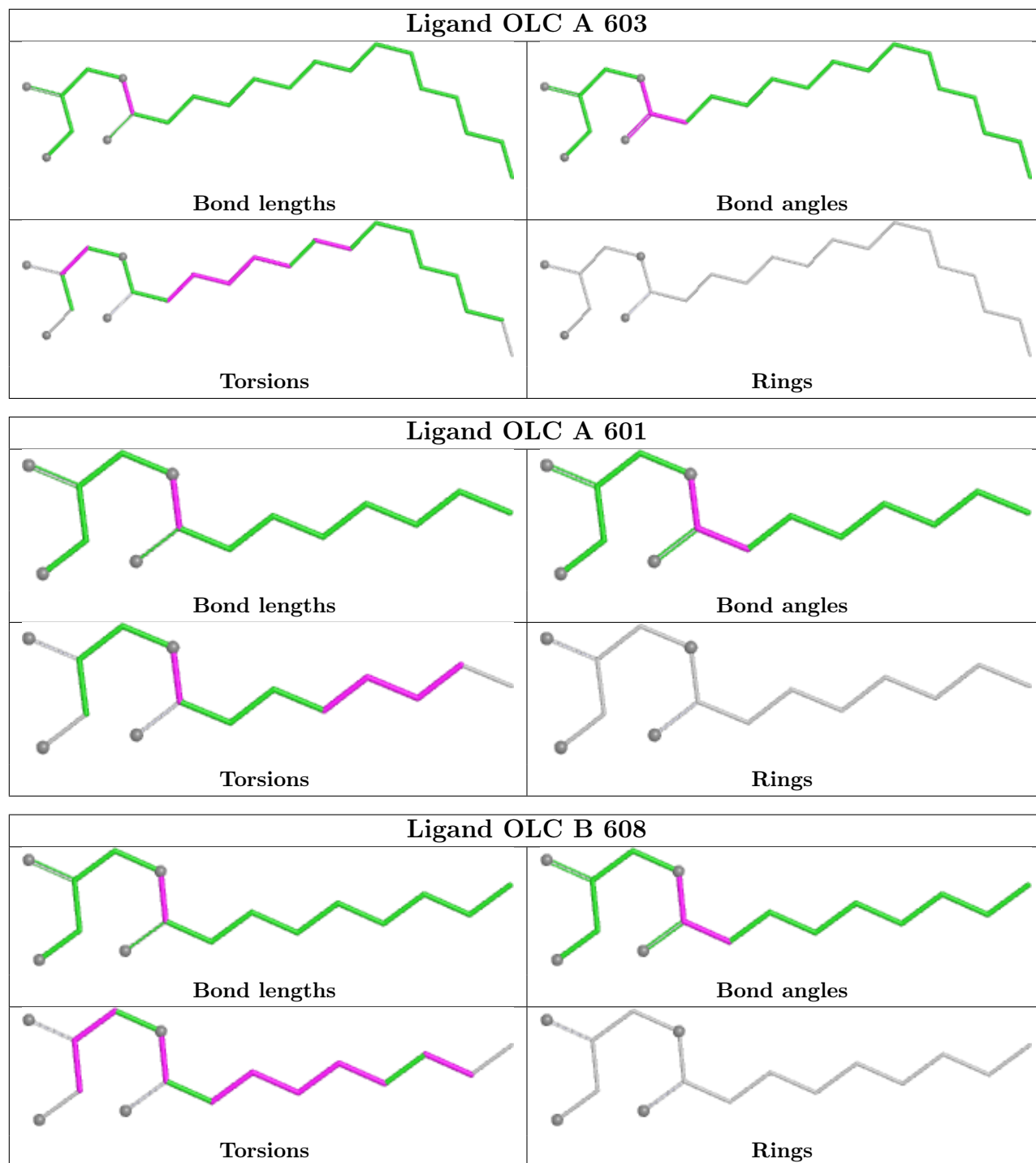


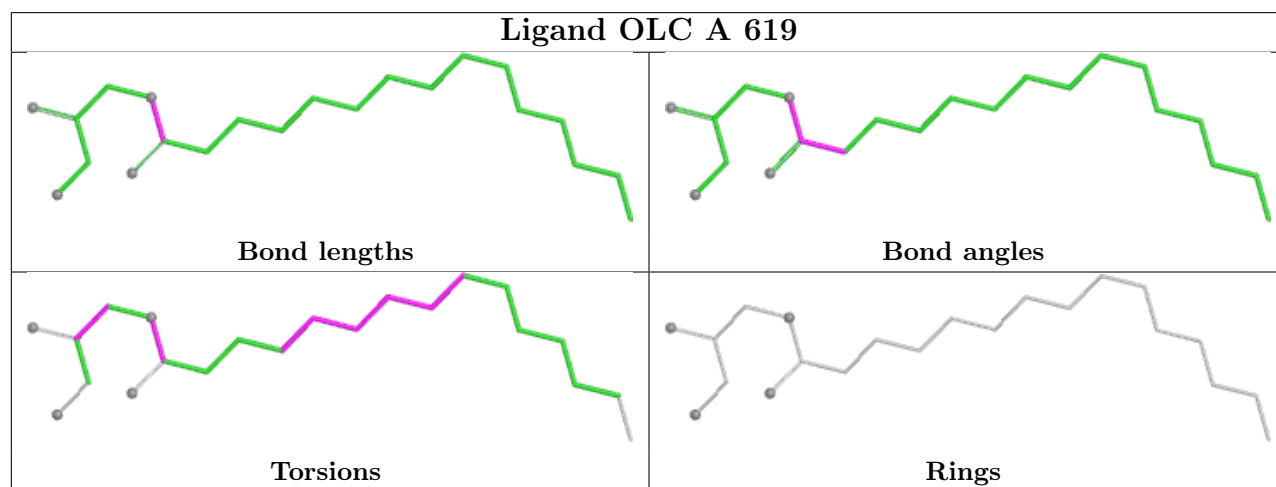
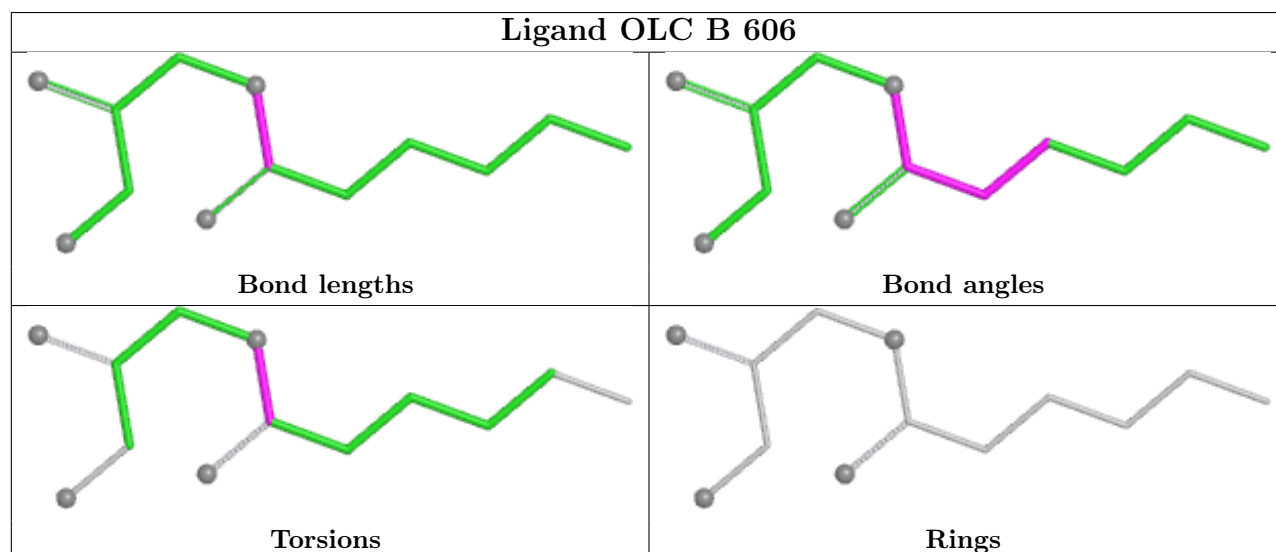
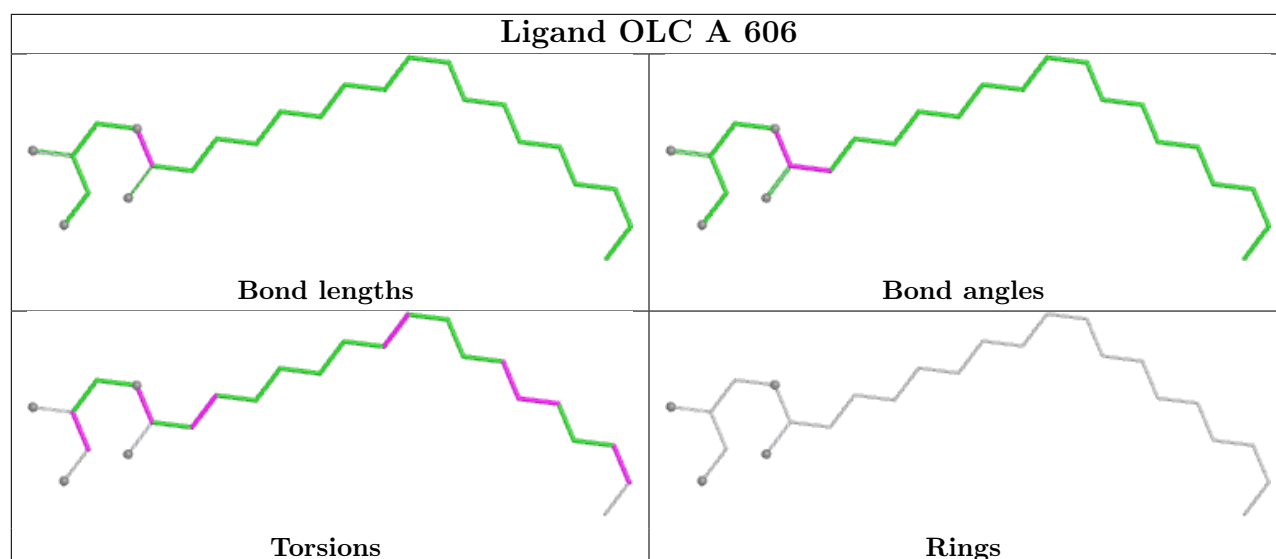


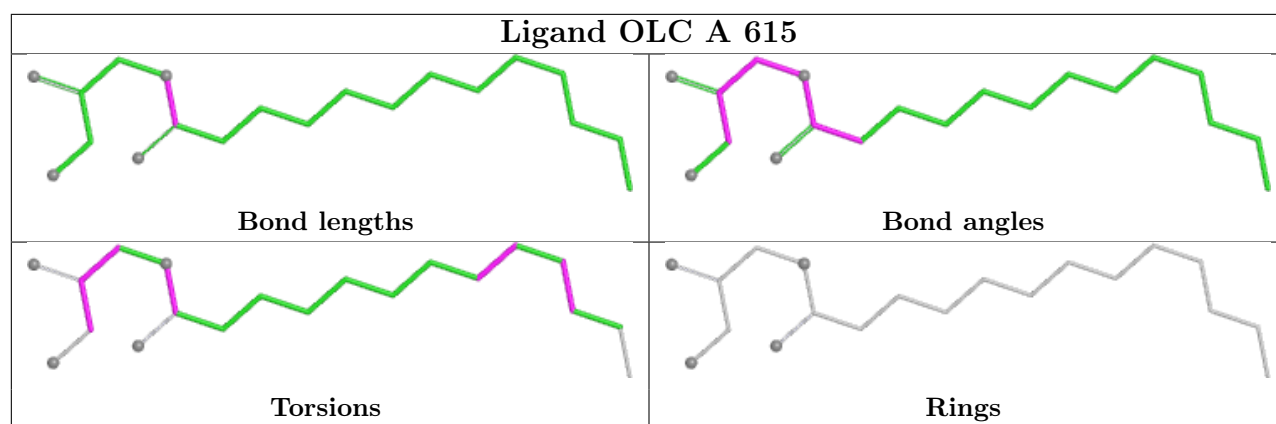












5.7 Other polymers [i](#)

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	506/532 (95%)	0.43	38 (7%)	20 16	52, 73, 121, 160	0
1	B	491/532 (92%)	0.40	22 (4%)	38 30	66, 87, 123, 156	0
All	All	997/1064 (93%)	0.41	60 (6%)	27 21	52, 81, 123, 160	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	ASN	5.1
1	A	447	GLY	5.1
1	B	345	VAL	5.1
1	B	29	SER	4.1
1	B	341	PHE	3.8
1	B	343	GLU	3.7
1	A	234	SER	3.7
1	A	236	LYS	3.6
1	A	3	PHE	3.6
1	B	82	PHE	3.5
1	A	237	TRP	3.4
1	A	448	ILE	3.2
1	B	447	GLY	3.2
1	A	232	PRO	3.2
1	A	360	LEU	3.1
1	A	6	LEU	3.0
1	A	235	LEU	3.0
1	A	118	LYS	3.0
1	B	344	PHE	2.9
1	B	83	GLY	2.9
1	A	414	ALA	2.9
1	A	351	LEU	2.8
1	B	416	PHE	2.8
1	A	272	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	233	GLN	2.8
1	B	457	GLU	2.8
1	B	340	PRO	2.7
1	A	231	ILE	2.6
1	A	240	GLY	2.6
1	A	399	ASN	2.6
1	A	353	PRO	2.6
1	A	8	GLU	2.6
1	A	7	ILE	2.5
1	A	4	ALA	2.5
1	B	215	THR	2.5
1	B	475	THR	2.4
1	A	361	PRO	2.4
1	B	234	SER	2.4
1	A	228	GLN	2.4
1	A	243	LEU	2.4
1	A	507	LEU	2.4
1	A	465	PHE	2.3
1	A	82	PHE	2.3
1	B	364	SER	2.3
1	B	306	LYS	2.2
1	A	350	ILE	2.2
1	A	154	SER	2.2
1	A	354	LEU	2.2
1	B	347	LEU	2.2
1	B	274	GLU	2.2
1	B	479	GLY	2.2
1	A	227	VAL	2.1
1	A	230	ASP	2.1
1	A	441	LEU	2.1
1	A	362	MET	2.1
1	B	149	LEU	2.1
1	A	241	GLN	2.1
1	B	157	ASP	2.1
1	B	304	LEU	2.0
1	A	415	TRP	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.

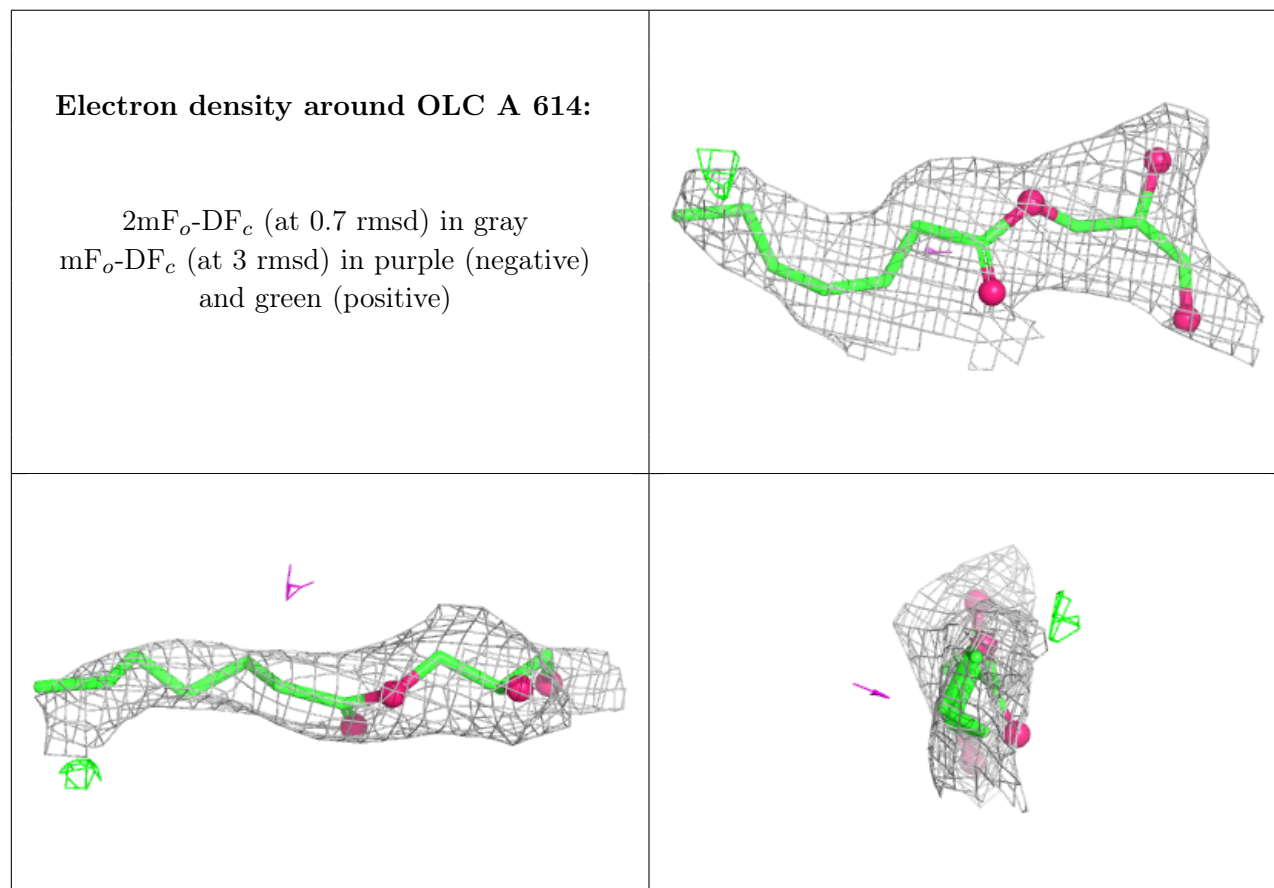
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	624	6/6	0.29	0.21	99,106,110,113	0
3	GOL	A	620	6/6	0.62	0.19	122,122,124,125	0
2	OLC	A	614	14/25	0.65	0.24	100,109,114,121	0
2	OLC	B	605	18/25	0.69	0.20	116,119,128,128	0
3	GOL	A	621	6/6	0.72	0.15	79,88,97,103	0
3	GOL	A	622	6/6	0.72	0.17	114,121,124,128	0
2	OLC	B	607	11/25	0.72	0.16	75,100,110,112	0
2	OLC	B	606	13/25	0.73	0.18	69,90,104,108	0
2	OLC	A	616	13/25	0.76	0.14	66,81,102,105	0
2	OLC	A	607	15/25	0.78	0.23	102,104,114,116	0
2	OLC	A	605	12/25	0.78	0.24	101,112,125,138	0
2	OLC	A	604	14/25	0.79	0.18	100,108,119,120	0
2	OLC	B	601	14/25	0.80	0.17	94,104,113,118	0
2	OLC	A	615	20/25	0.80	0.20	64,92,116,119	0
3	GOL	B	609	6/6	0.80	0.15	88,98,104,110	0
3	GOL	B	611	6/6	0.80	0.17	75,89,96,96	0
3	GOL	B	612	6/6	0.80	0.10	94,97,102,108	0
3	GOL	B	610	6/6	0.81	0.22	111,113,115,128	0
2	OLC	B	608	16/25	0.81	0.17	73,94,118,125	0
2	OLC	A	608	14/25	0.81	0.19	81,96,105,106	0
2	OLC	A	609	22/25	0.82	0.17	91,101,112,126	0
2	OLC	B	603	11/25	0.82	0.18	114,123,129,133	0
2	OLC	A	613	14/25	0.83	0.16	87,104,113,117	0
2	OLC	A	602	12/25	0.83	0.20	87,94,102,111	0
2	OLC	A	611	16/25	0.83	0.21	91,94,97,112	0
2	OLC	A	610	12/25	0.84	0.23	108,119,129,141	0
3	GOL	A	626	6/6	0.84	0.14	81,83,93,102	0
2	OLC	A	601	15/25	0.86	0.18	74,82,89,94	0
3	GOL	A	623	6/6	0.86	0.13	85,88,93,101	0
2	OLC	A	617	14/25	0.86	0.17	85,93,101,114	0
2	OLC	B	604	21/25	0.86	0.17	103,114,124,129	0
3	GOL	A	627	6/6	0.87	0.13	78,84,86,98	0

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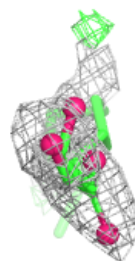
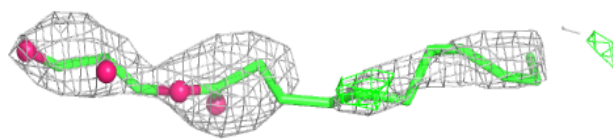
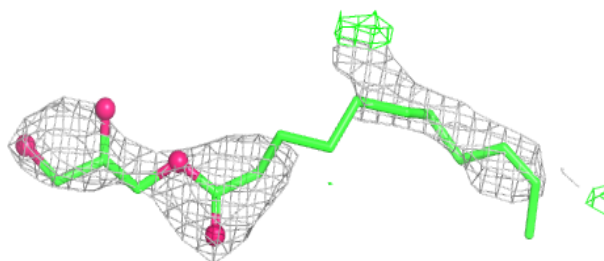
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	A	603	22/25	0.88	0.17	72,91,107,112	0
2	OLC	A	619	22/25	0.88	0.15	60,72,115,124	0
2	OLC	B	602	25/25	0.89	0.14	54,86,104,107	0
2	OLC	A	606	25/25	0.89	0.17	67,86,96,105	0
2	OLC	A	618	14/25	0.89	0.17	80,85,99,103	0
2	OLC	A	612	22/25	0.90	0.16	76,86,109,112	0
3	GOL	A	625	6/6	0.91	0.10	65,76,80,89	0

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

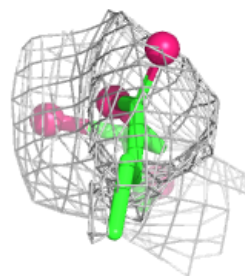
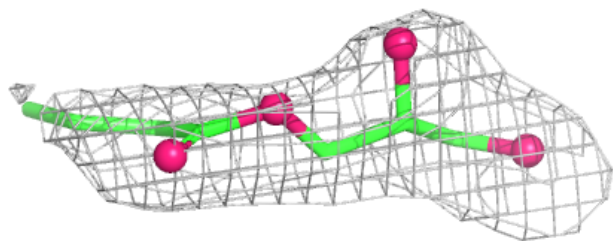
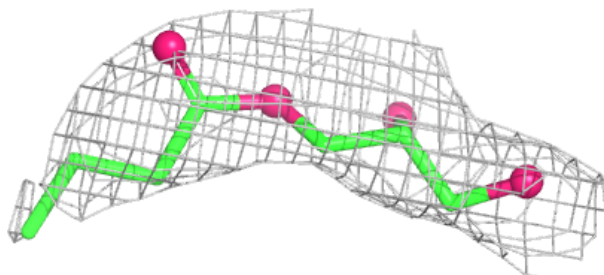


Electron density around OLC B 605:

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

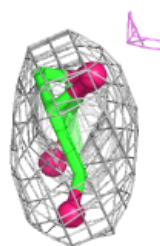
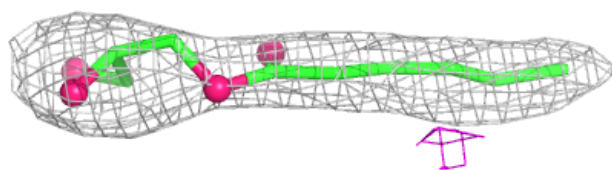
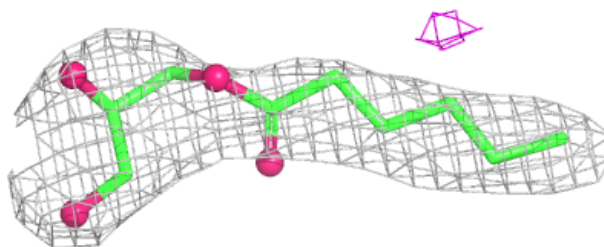
**Electron density around OLC B 607:**

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

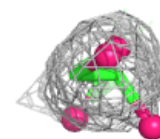
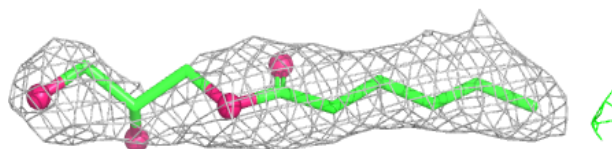
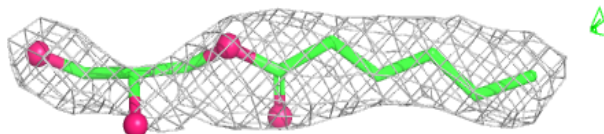


Electron density around OLC B 606:

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

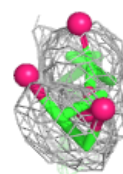
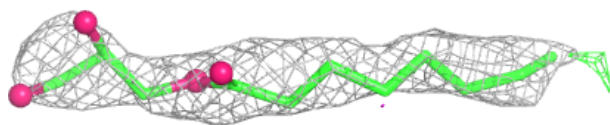
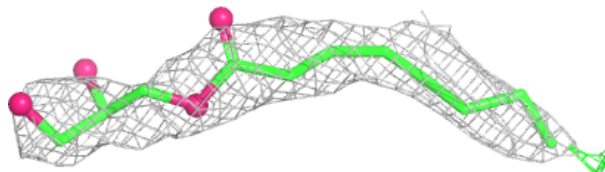
**Electron density around OLC A 616:**

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

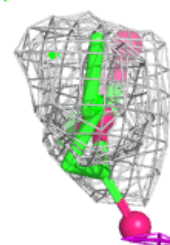
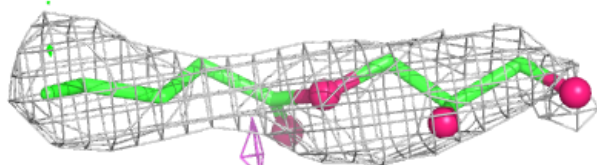
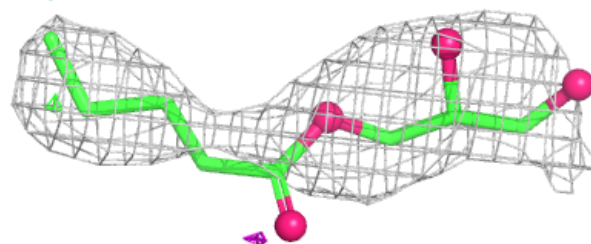


Electron density around OLC A 607:

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

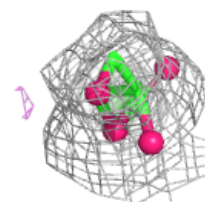
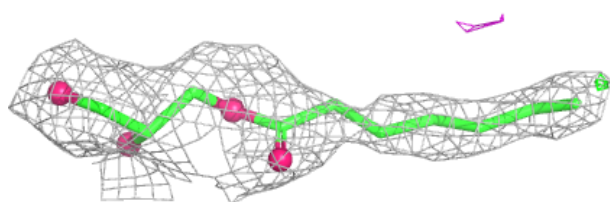
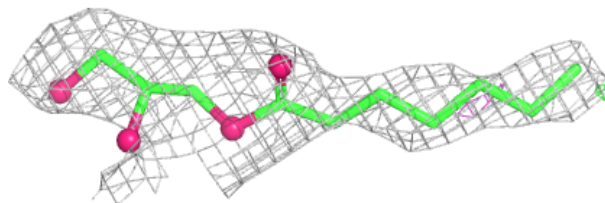
**Electron density around OLC A 605:**

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

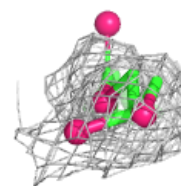
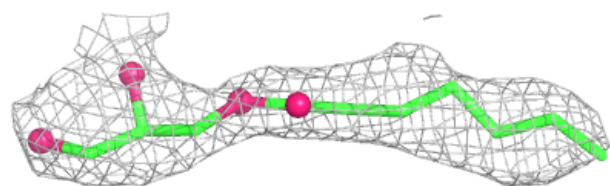
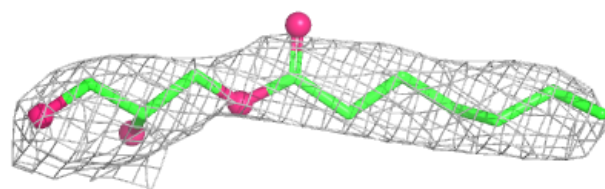


Electron density around OLC A 604:

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

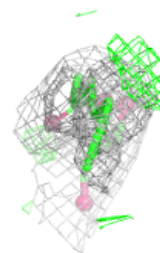
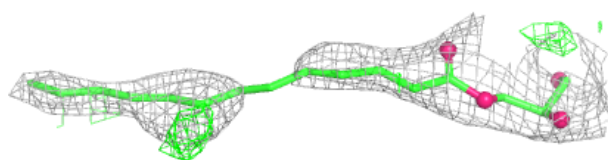
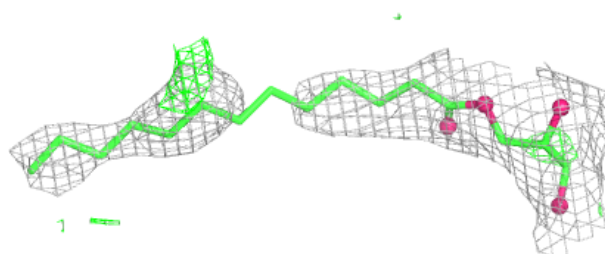
**Electron density around OLC B 601:**

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

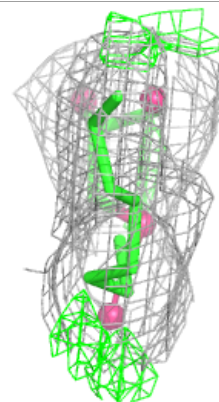
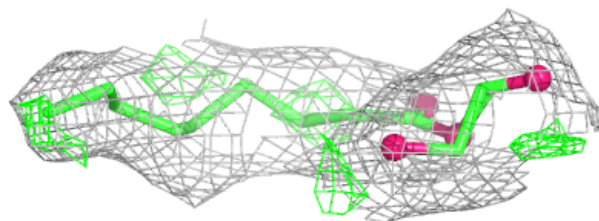
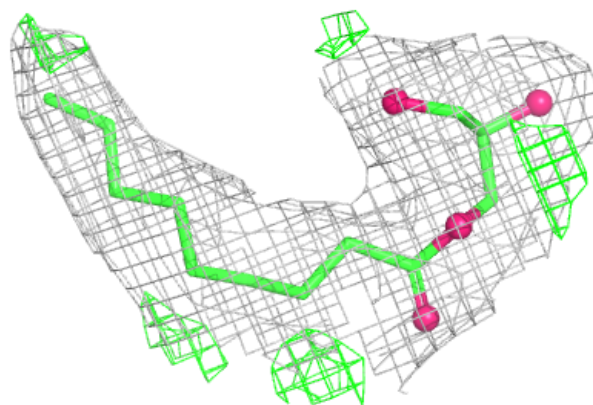


Electron density around OLC A 615:

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

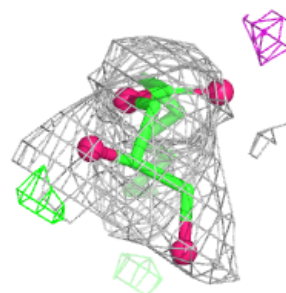
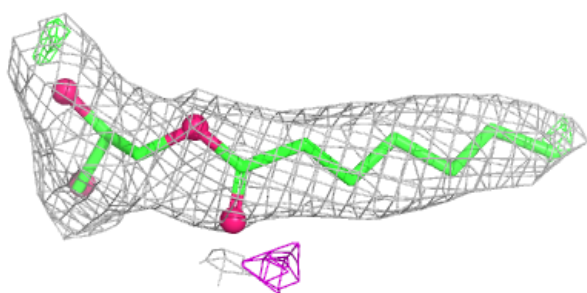
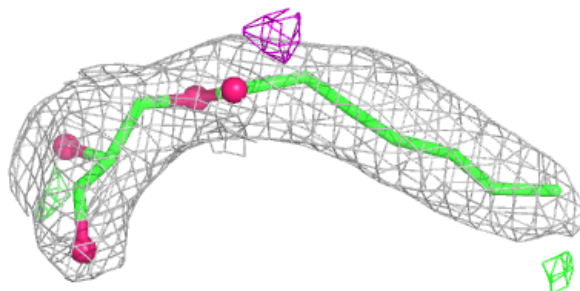
**Electron density around OLC B 608:**

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and green (positive)

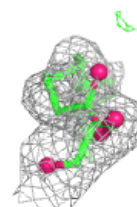
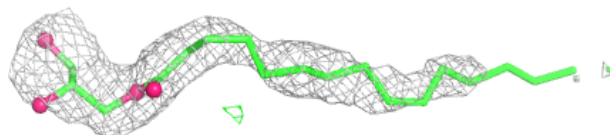
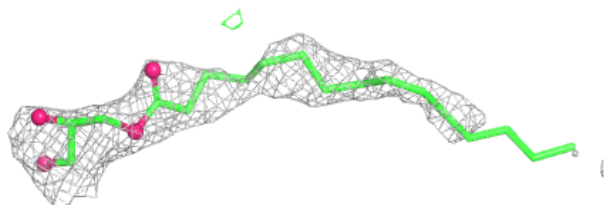


Electron density around OLC A 608:

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

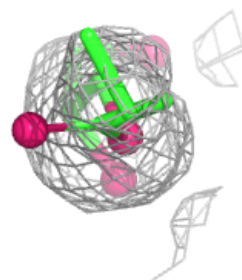
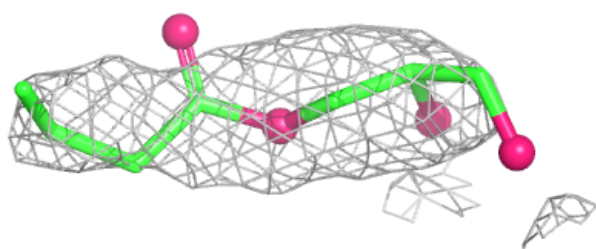
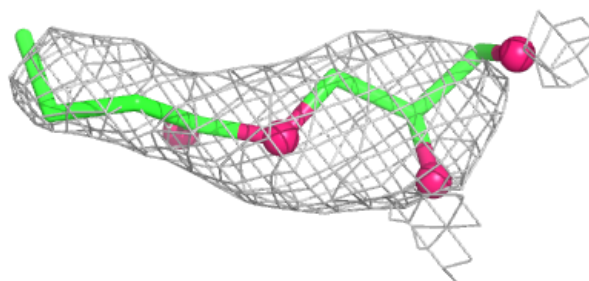
**Electron density around OLC A 609:**

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

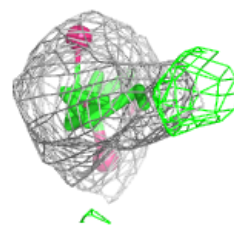
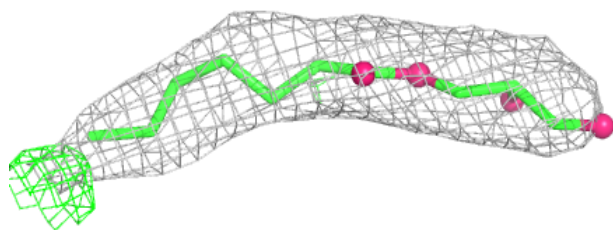
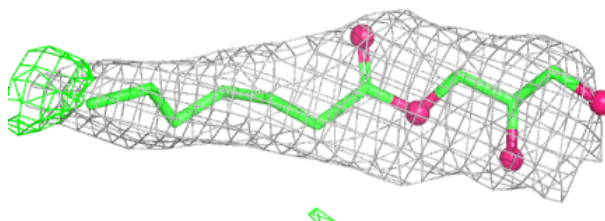


Electron density around OLC B 603:

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

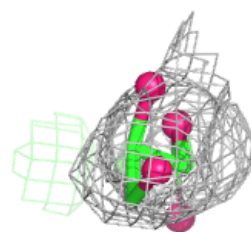
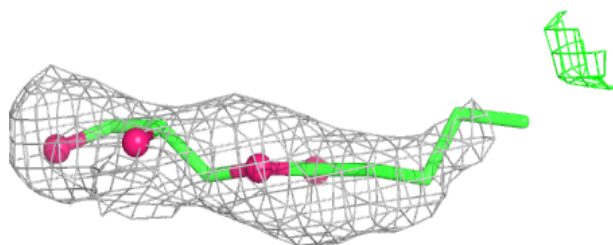
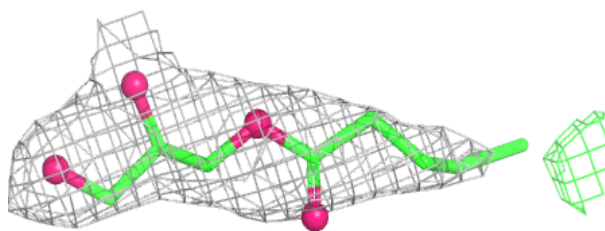
**Electron density around OLC A 613:**

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

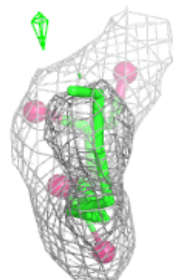
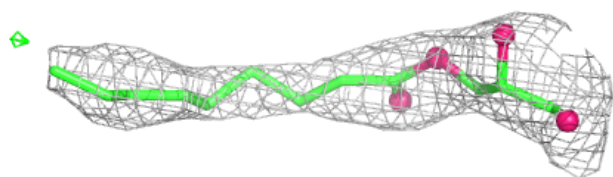
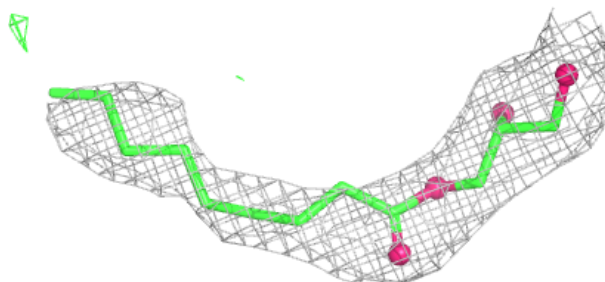


Electron density around OLC A 602:

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

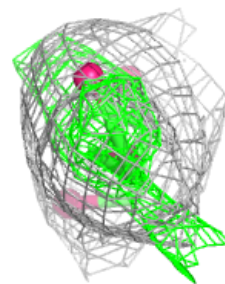
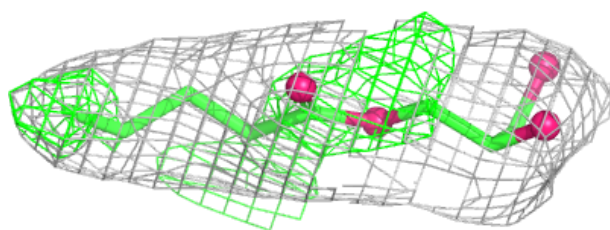
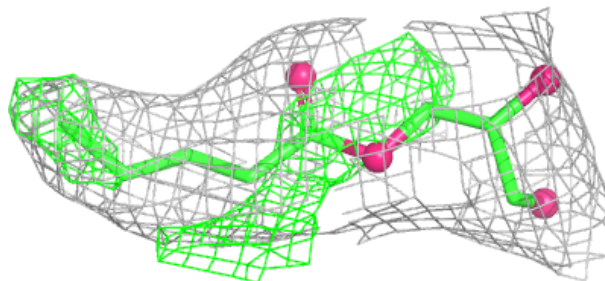
**Electron density around OLC A 611:**

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

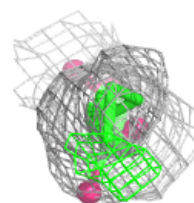
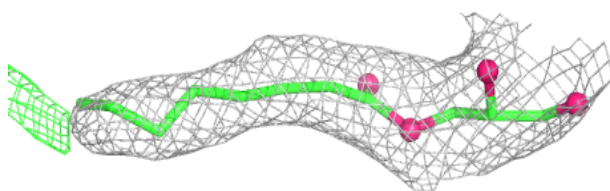
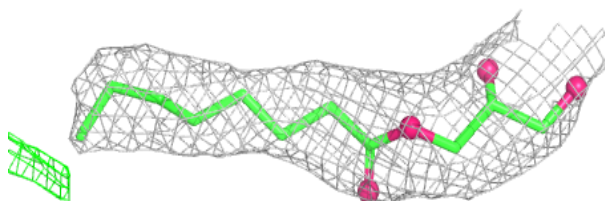


Electron density around OLC A 610:

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

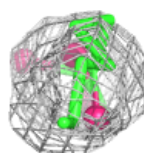
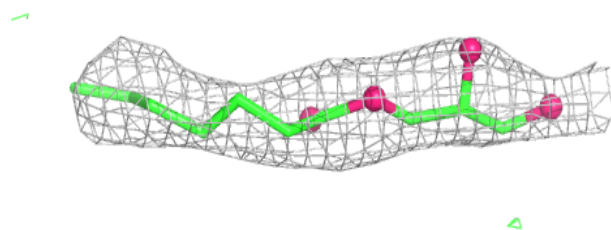
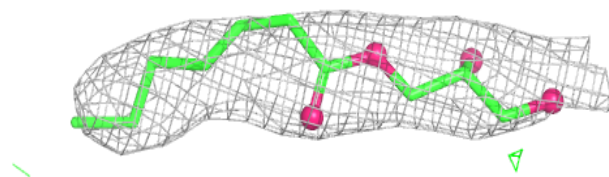
**Electron density around OLC A 601:**

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

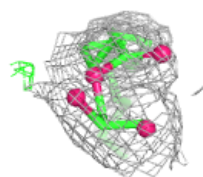
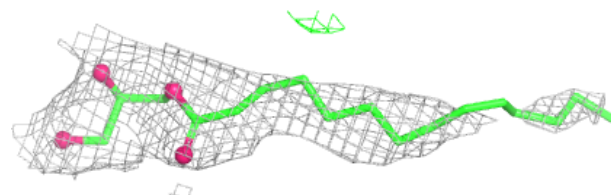
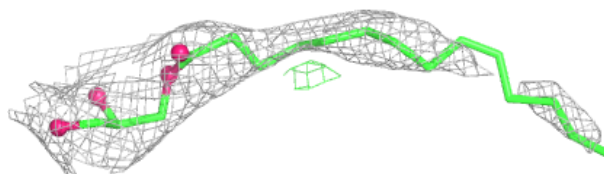


Electron density around OLC A 617:

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

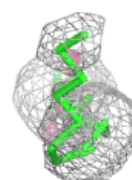
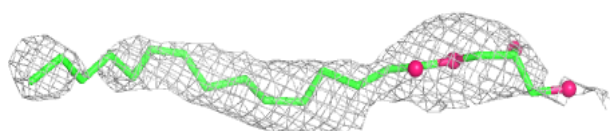
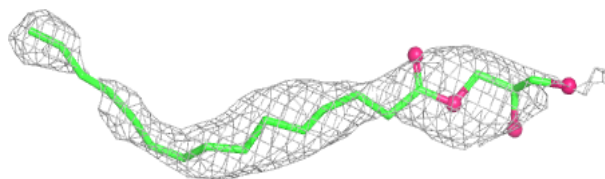
**Electron density around OLC B 604:**

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

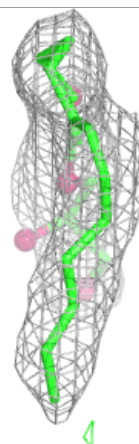
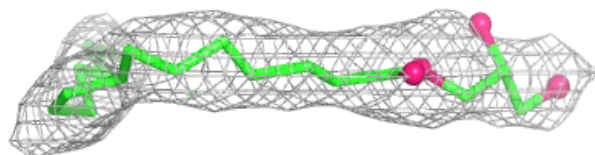


Electron density around OLC A 603:

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

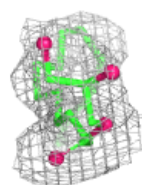
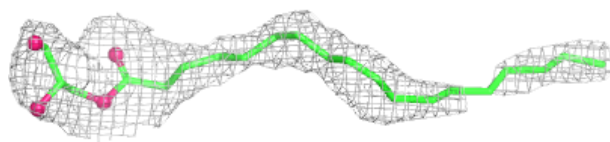
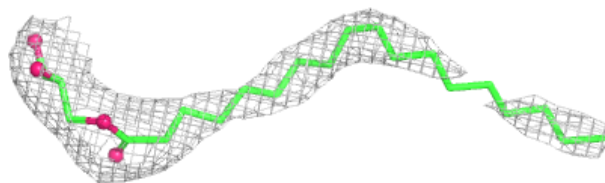
**Electron density around OLC A 619:**

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

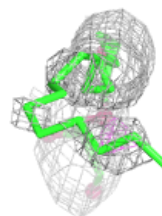
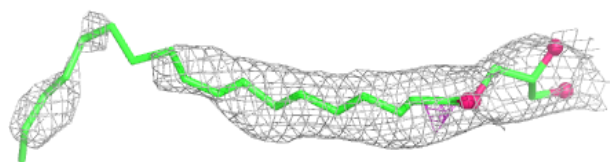
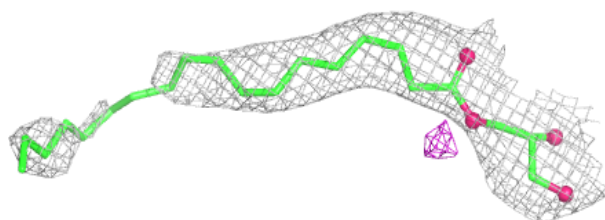


Electron density around OLC B 602:

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

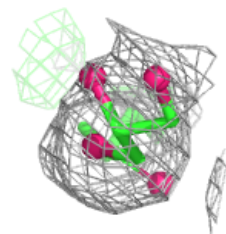
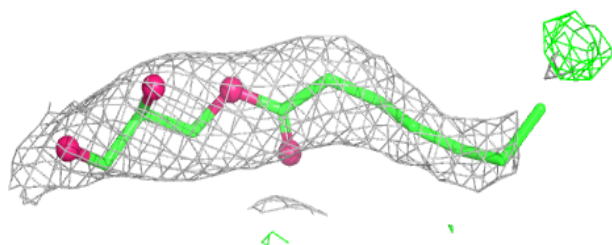
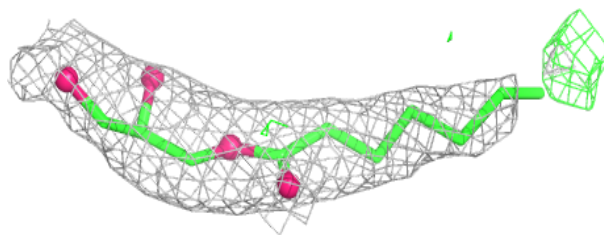
**Electron density around OLC A 606:**

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

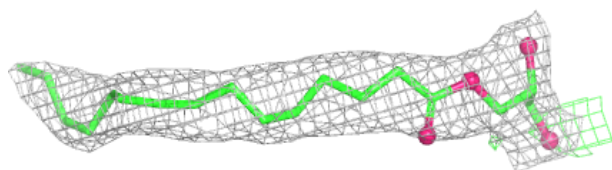
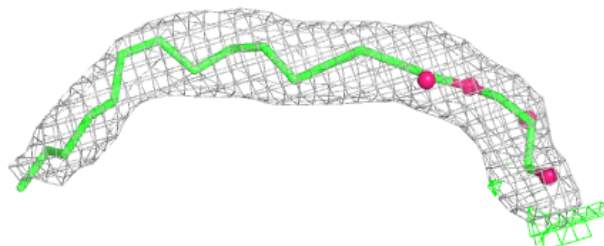


Electron density around OLC A 618:

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

**Electron density around OLC A 612:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.