



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:04 PM UTC

PDB ID : 3VVS / pdb_00003vvs
Title : Crystal structure of MATE in complex with MaD3S
Authors : Tanaka, Y.; Ishitani, R.; Nureki, O.
Deposited on : 2012-07-27
Resolution : 2.60 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

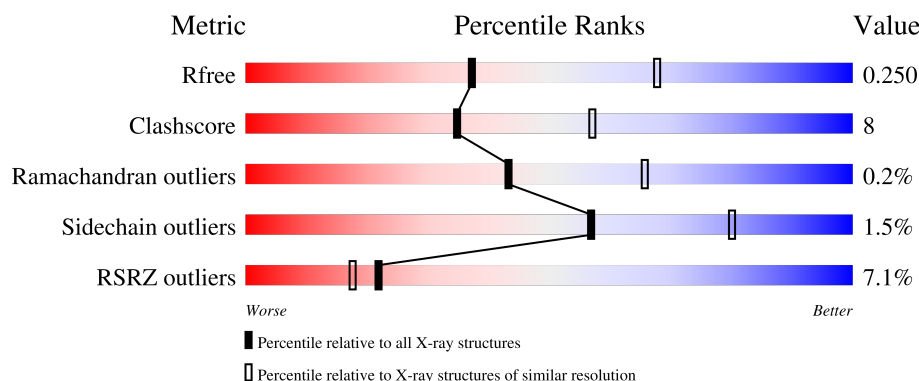
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	461	5% 85% 11% ..
2	B	11	18% 82% 82%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3583 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.

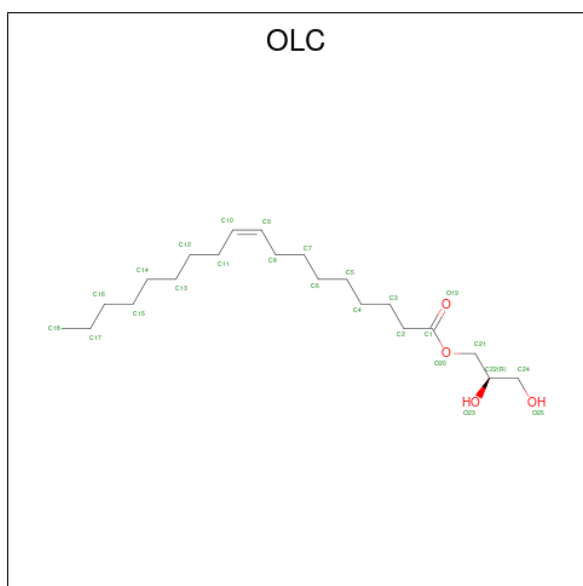
- Molecule 1 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	1	0
			3280	2161	528	569	22			

- Molecule 2 is a protein called macrocyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	S	0	0	0
			82	57	10	14	1			

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			13	13		
3	A	1	Total	C	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 18 1	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C O 19 18 1	0	0
3	A	1	Total C O 19 18 1	0	0
3	A	1	Total C O 19 18 1	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 11 11	0	0

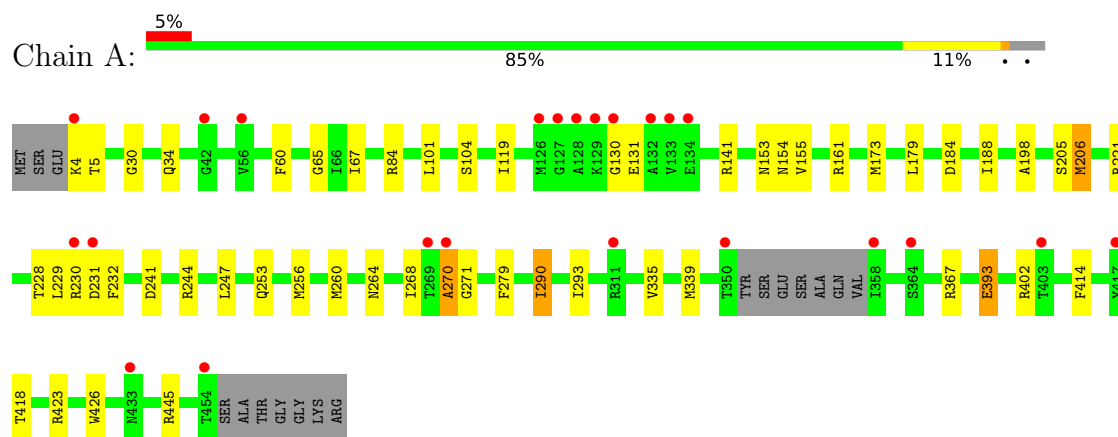
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0

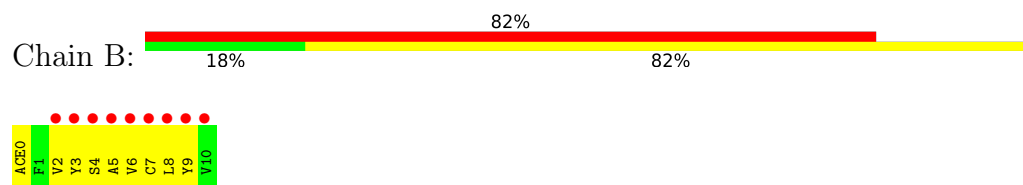
3 Residue-property plots [i](#)

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: Putative uncharacterized protein



- Molecule 2: macrocyclic peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.09Å 59.97Å 68.53Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	43.08 – 2.60 43.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.08-2.60) 95.5 (43.08-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.213 , 0.244 0.212 , 0.250	Depositor DCC
R_{free} test set	2009 reflections (9.22%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3583	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: ACE, DPN, OLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/3339	0.72	1/4537 (0.0%)
2	B	0.38	0/69	0.91	0/94
All	All	0.31	0/3408	0.73	1/4631 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ALA	N-CA-C	5.66	117.12	111.07

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	3280	0	3404	43	0
2	B	82	0	74	23	0
3	A	181	0	297	10	0
4	A	40	0	0	1	0
All	All	3583	0	3775	55	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 8.

All (55) 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:B:0:ACE:H1	2:B:4:SER:OG	1.51	1.08
1:A:256:MET:SD	2:B:6:VAL:HG21	2.02	0.99
2:B:7:CYS:H	2:B:8:LEU:HD23	1.27	0.96
1:A:253:GLN:OE1	2:B:6:VAL:HG23	1.71	0.90
1:A:34:GLN:HE22	2:B:3:TYR:HD1	1.25	0.83
1:A:256:MET:SD	2:B:6:VAL:CG2	2.67	0.82
2:B:7:CYS:N	2:B:8:LEU:HD23	2.01	0.75
2:B:0:ACE:CH3	2:B:4:SER:OG	2.33	0.74
1:A:34:GLN:NE2	2:B:3:TYR:HD1	1.85	0.73
1:A:153:ASN:HD22	1:A:206[A]:MET:HE3	1.54	0.71
2:B:5:ALA:O	2:B:8:LEU:CD2	2.42	0.67
1:A:290:ILE:HD13	1:A:293:ILE:HD12	1.76	0.66
2:B:6:VAL:HA	2:B:8:LEU:CD2	2.28	0.64
1:A:34:GLN:NE2	2:B:3:TYR:CD1	2.64	0.62
1:A:101:LEU:HB3	3:A:503:OLC:H8	1.83	0.60
1:A:229:LEU:HG	3:A:503:OLC:H5	1.85	0.58
1:A:84:ARG:NH1	1:A:241:ASP:OD2	2.33	0.58
2:B:6:VAL:HA	2:B:8:LEU:HD21	1.86	0.58
1:A:141:ARG:HD3	3:A:504:OLC:H3	1.84	0.57
1:A:228:THR:HA	3:A:503:OLC:H3	1.86	0.57
2:B:0:ACE:H1	2:B:4:SER:HG	1.65	0.57
1:A:154:ASN:HD21	2:B:2:VAL:HG12	1.72	0.55
1:A:65:GLY:HA2	3:A:506:OLC:H13A	1.87	0.54
1:A:279:PHE:HD1	1:A:426:TRP:HZ3	1.56	0.54
1:A:253:GLN:OE1	2:B:6:VAL:CG2	2.49	0.54
1:A:153:ASN:HD22	1:A:206[A]:MET:CE	2.22	0.53
1:A:161:ARG:NH1	4:A:612:HOH:O	2.42	0.53
2:B:5:ALA:O	2:B:8:LEU:HD22	2.08	0.52
1:A:393:GLU:HG2	3:A:512:OLC:H4A	1.93	0.51
1:A:256:MET:SD	2:B:6:VAL:HG22	2.51	0.50
2:B:5:ALA:O	2:B:8:LEU:HD23	2.10	0.50
1:A:414:PHE:O	1:A:418:THR:OG1	2.30	0.49
1:A:65:GLY:HA3	3:A:501:OLC:H8A	1.93	0.49
1:A:179:LEU:HD23	1:A:205:SER:HA	1.95	0.48
1:A:244:ARG:HG3	3:A:512:OLC:H6A	1.94	0.48
1:A:256:MET:HE2	1:A:402:ARG:HH12	1.78	0.48
2:B:6:VAL:HA	2:B:8:LEU:HD23	1.95	0.48
1:A:104:SER:HB3	1:A:155:VAL:HG21	1.96	0.47
1:A:270:ALA:N	1:A:271:GLY:HA3	2.31	0.46
2:B:7:CYS:H	2:B:8:LEU:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD11	1:A:198:ALA:HB2	1.97	0.46
1:A:339:MET:O	1:A:367:ARG:NE	2.49	0.45
1:A:60:PHE:CE1	2:B:9:TYR:HB3	2.52	0.45
1:A:230:ARG:HA	1:A:231:ASP:HA	1.56	0.45
1:A:130:GLY:HA2	1:A:131:GLU:C	2.41	0.45
1:A:221:ARG:HH22	3:A:503:OLC:H2	1.83	0.44
1:A:423:ARG:HA	1:A:426:TRP:CD1	2.53	0.43
1:A:4:LYS:HA	1:A:5:THR:HA	1.50	0.43
1:A:30:GLY:HA3	1:A:173:MET:HE3	2.00	0.43
1:A:260:MET:HE3	1:A:260:MET:HA	2.00	0.42
1:A:264:ASN:O	1:A:268:ILE:HG13	2.20	0.42
1:A:335:VAL:HG12	1:A:339:MET:HE2	2.03	0.40
1:A:119:ILE:HD12	1:A:119:ILE:HA	1.95	0.40
1:A:247:LEU:HD23	3:A:512:OLC:H9	2.03	0.40
1:A:67:ILE:HG23	2:B:2:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/461 (96%)	431 (98%)	9 (2%)	1 (0%)	43	66
2	B	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
All	All	449/472 (95%)	437 (97%)	11 (2%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	PHE

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	331/362 (91%)	325 (98%)	6 (2%)	51	76
2	B	7/8 (88%)	7 (100%)	0	100	100
All	All	338/370 (91%)	332 (98%)	6 (2%)	57	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	ASP
1	A	206[A]	MET
1	A	206[B]	MET
1	A	290	ILE
1	A	393	GLU
1	A	445	ARG

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

Mol	Chain	Res	Type
1	A	10	GLN
1	A	38	ASN
1	A	153	ASN
1	A	154	ASN
1	A	274	ASN
1	A	387	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	OLC	A	509	-	18,18,24	1.03	2 (11%)	17,17,25	0.68	0
3	OLC	A	507	-	18,18,24	1.03	2 (11%)	17,17,25	0.72	0
3	OLC	A	506	-	9,9,24	0.98	1 (11%)	8,8,25	0.57	0
3	OLC	A	505	-	11,11,24	0.90	1 (9%)	9,9,25	0.57	0
3	OLC	A	504	-	17,17,24	0.72	1 (5%)	16,16,25	0.55	0
3	OLC	A	508	-	18,18,24	1.03	2 (11%)	17,17,25	0.65	0
3	OLC	A	511	-	13,13,24	0.80	1 (7%)	10,10,25	0.52	0
3	OLC	A	503	-	18,18,24	1.02	2 (11%)	17,17,25	0.74	0
3	OLC	A	501	-	12,12,24	0.83	1 (8%)	11,11,25	0.59	0
3	OLC	A	510	-	14,14,24	0.79	1 (7%)	12,12,25	0.57	0
3	OLC	A	512	-	10,10,24	0.93	1 (10%)	9,9,25	0.60	0
3	OLC	A	502	-	7,7,24	1.11	1 (14%)	6,6,25	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	509	-	-	7/16/16/24	-
3	OLC	A	507	-	-	7/16/16/24	-
3	OLC	A	506	-	-	4/7/7/24	-
3	OLC	A	505	-	-	2/7/7/24	-
3	OLC	A	504	-	-	10/15/15/24	-
3	OLC	A	508	-	-	10/16/16/24	-
3	OLC	A	511	-	-	4/7/7/24	-
3	OLC	A	503	-	-	6/16/16/24	-
3	OLC	A	501	-	-	7/10/10/24	-
3	OLC	A	510	-	-	3/10/10/24	-
3	OLC	A	512	-	-	7/8/8/24	-
3	OLC	A	502	-	-	5/5/5/24	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	OLC	O20-C1	-3.27	1.25	1.42
3	A	503	OLC	O20-C1	-3.26	1.25	1.42
3	A	508	OLC	O20-C1	-3.26	1.25	1.42
3	A	509	OLC	O20-C1	-3.25	1.25	1.42
3	A	502	OLC	C10-C9	2.86	1.47	1.29
3	A	505	OLC	C10-C9	2.86	1.47	1.29
3	A	506	OLC	C9-C10	2.84	1.47	1.29
3	A	504	OLC	C9-C10	2.81	1.47	1.31
3	A	510	OLC	C9-C10	2.81	1.47	1.29
3	A	508	OLC	C9-C10	2.78	1.47	1.31
3	A	512	OLC	C9-C10	2.78	1.47	1.31
3	A	507	OLC	C9-C10	2.77	1.47	1.31
3	A	501	OLC	C9-C10	2.77	1.47	1.31
3	A	509	OLC	C9-C10	2.75	1.47	1.31
3	A	503	OLC	C9-C10	2.74	1.47	1.31
3	A	511	OLC	C9-C10	2.72	1.47	1.31

There are no bond angle outliers.

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	OLC	C1-C2-C3-C4
3	A	506	OLC	C11-C12-C13-C14
3	A	503	OLC	C1-C2-C3-C4
3	A	509	OLC	C3-C4-C5-C6
3	A	509	OLC	C1-C2-C3-C4
3	A	512	OLC	C3-C4-C5-C6
3	A	503	OLC	C4-C5-C6-C7
3	A	507	OLC	C5-C6-C7-C8
3	A	507	OLC	C1-C2-C3-C4
3	A	512	OLC	C4-C5-C6-C7
3	A	503	OLC	C3-C4-C5-C6
3	A	504	OLC	C12-C13-C14-C15
3	A	512	OLC	C5-C6-C7-C8
3	A	511	OLC	C11-C10-C9-C8
3	A	511	OLC	C6-C7-C8-C9
3	A	502	OLC	C3-C4-C5-C6
3	A	504	OLC	C11-C10-C9-C8
3	A	510	OLC	C3-C4-C5-C6
3	A	502	OLC	C4-C5-C6-C7
3	A	508	OLC	C10-C11-C12-C13
3	A	504	OLC	C3-C4-C5-C6
3	A	506	OLC	C14-C15-C16-C17
3	A	501	OLC	C11-C10-C9-C8
3	A	503	OLC	C11-C10-C9-C8
3	A	507	OLC	C11-C10-C9-C8
3	A	507	OLC	C10-C11-C12-C13
3	A	508	OLC	C11-C10-C9-C8
3	A	509	OLC	C11-C10-C9-C8
3	A	512	OLC	C11-C10-C9-C8
3	A	508	OLC	C3-C4-C5-C6
3	A	503	OLC	C11-C12-C13-C14
3	A	501	OLC	C2-C3-C4-C5
3	A	501	OLC	C1-C2-C3-C4
3	A	507	OLC	C3-C4-C5-C6
3	A	512	OLC	C2-C3-C4-C5
3	A	507	OLC	C4-C5-C6-C7
3	A	508	OLC	C11-C12-C13-C14
3	A	502	OLC	C5-C6-C7-C8
3	A	508	OLC	C4-C5-C6-C7
3	A	504	OLC	C11-C12-C13-C14
3	A	502	OLC	C6-C7-C8-C9
3	A	510	OLC	C1-C2-C3-C4
3	A	512	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	510	OLC	C14-C15-C16-C17
3	A	501	OLC	C9-C10-C11-C12
3	A	509	OLC	O20-C1-C2-C3
3	A	508	OLC	C13-C14-C15-C16
3	A	508	OLC	C7-C8-C9-C10
3	A	509	OLC	C9-C10-C11-C12
3	A	506	OLC	C9-C10-C11-C12
3	A	511	OLC	C9-C10-C11-C12
3	A	512	OLC	C7-C8-C9-C10
3	A	507	OLC	C12-C13-C14-C15
3	A	502	OLC	C7-C8-C9-C10
3	A	505	OLC	C7-C8-C9-C10
3	A	506	OLC	C12-C13-C14-C15
3	A	508	OLC	C5-C6-C7-C8
3	A	509	OLC	C4-C5-C6-C7
3	A	504	OLC	C5-C6-C7-C8
3	A	505	OLC	C14-C15-C16-C17
3	A	511	OLC	C7-C8-C9-C10
3	A	504	OLC	C4-C5-C6-C7
3	A	501	OLC	C7-C8-C9-C10
3	A	504	OLC	C1-C2-C3-C4
3	A	504	OLC	C9-C10-C11-C12
3	A	509	OLC	C7-C8-C9-C10
3	A	503	OLC	C5-C6-C7-C8
3	A	501	OLC	C6-C7-C8-C9
3	A	504	OLC	C7-C8-C9-C10
3	A	508	OLC	C12-C13-C14-C15
3	A	501	OLC	C4-C5-C6-C7
3	A	504	OLC	C14-C15-C16-C17

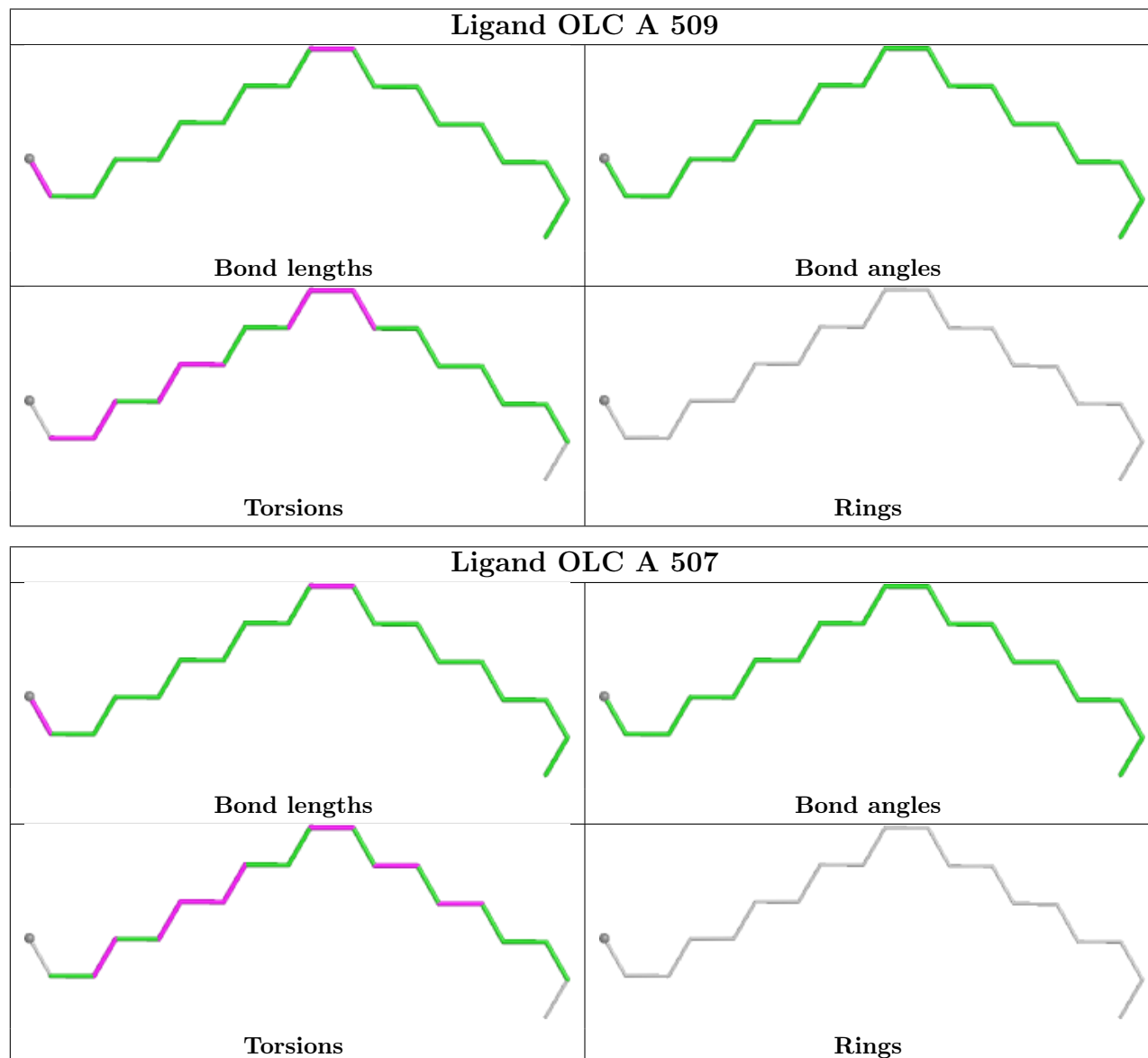
There are no ring outliers.

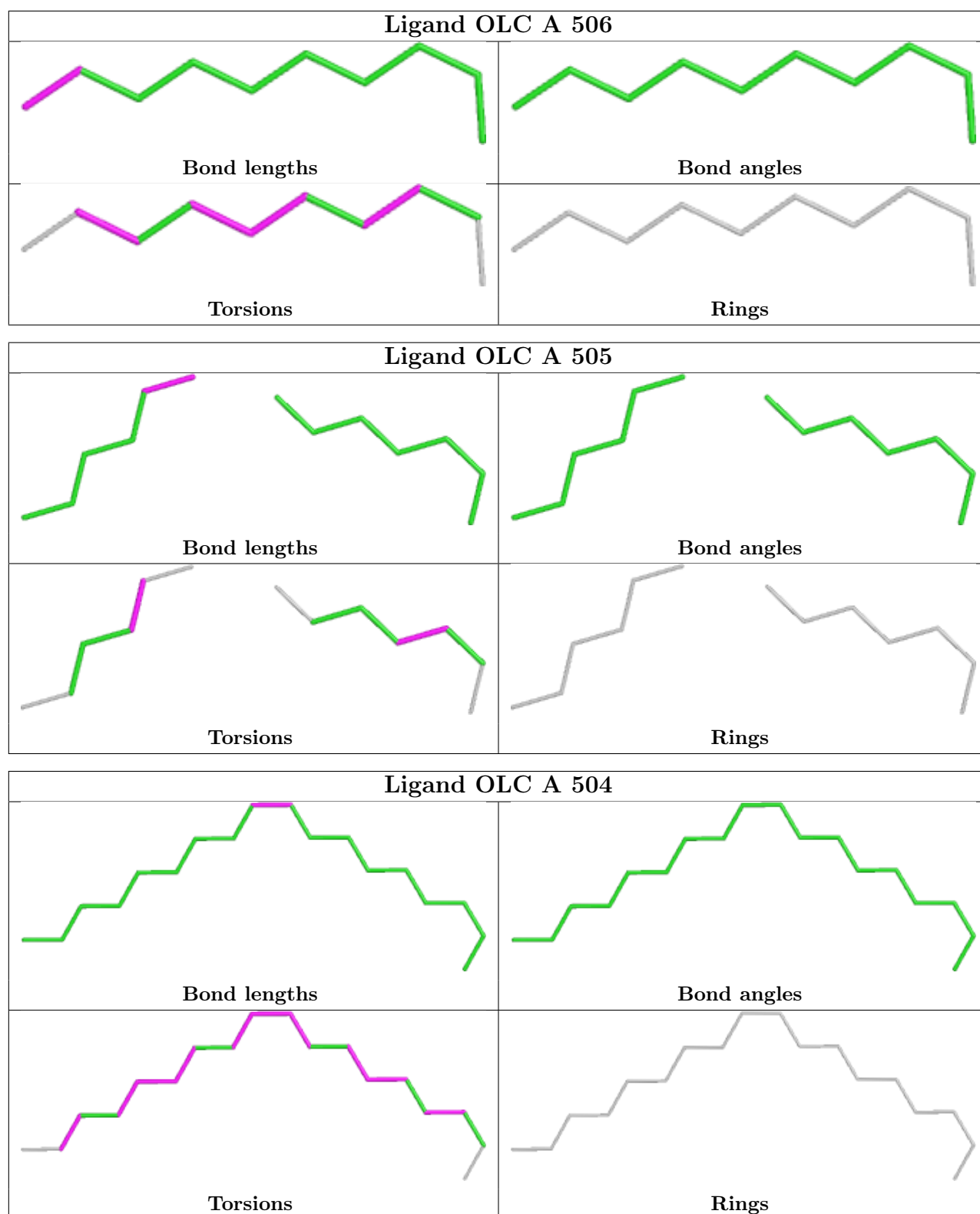
5 monomers are involved in 10 short contacts:

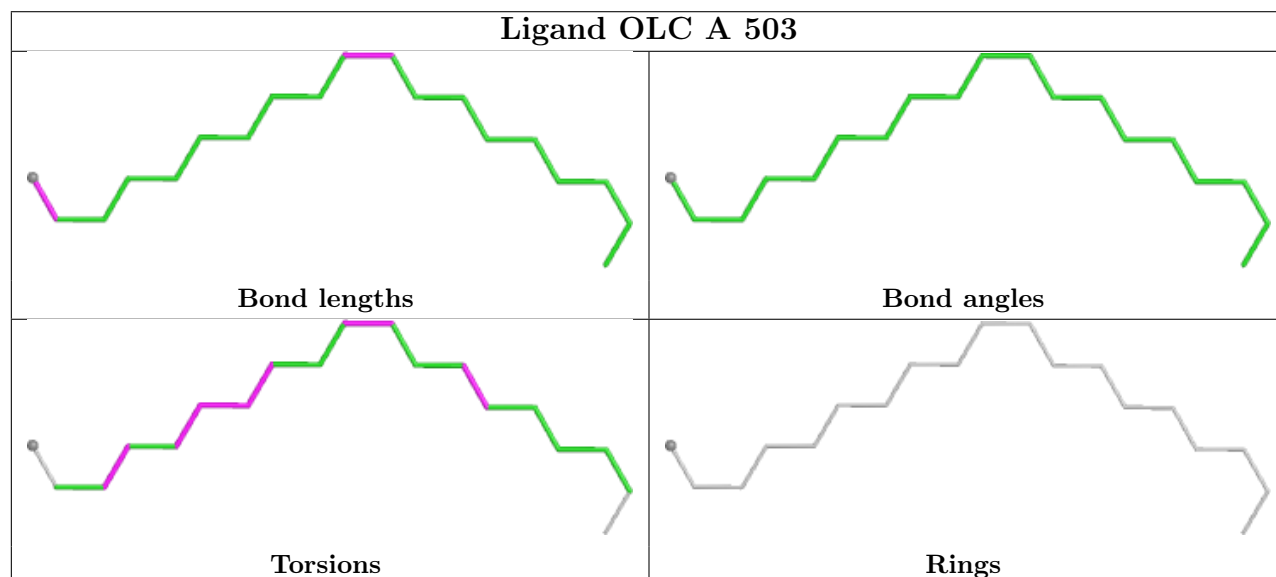
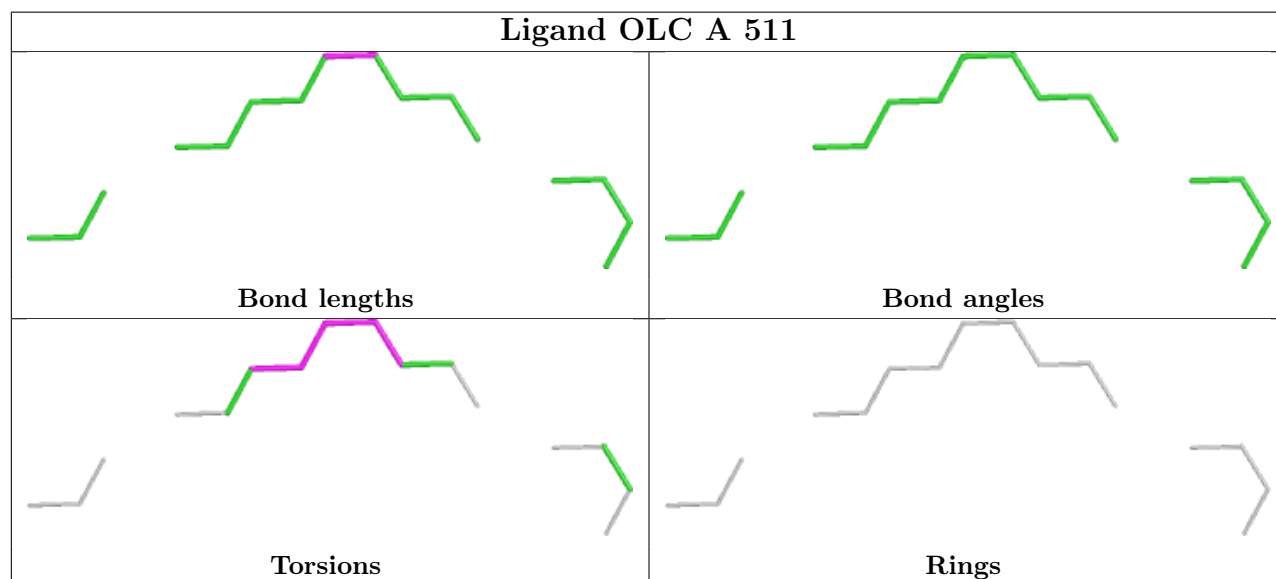
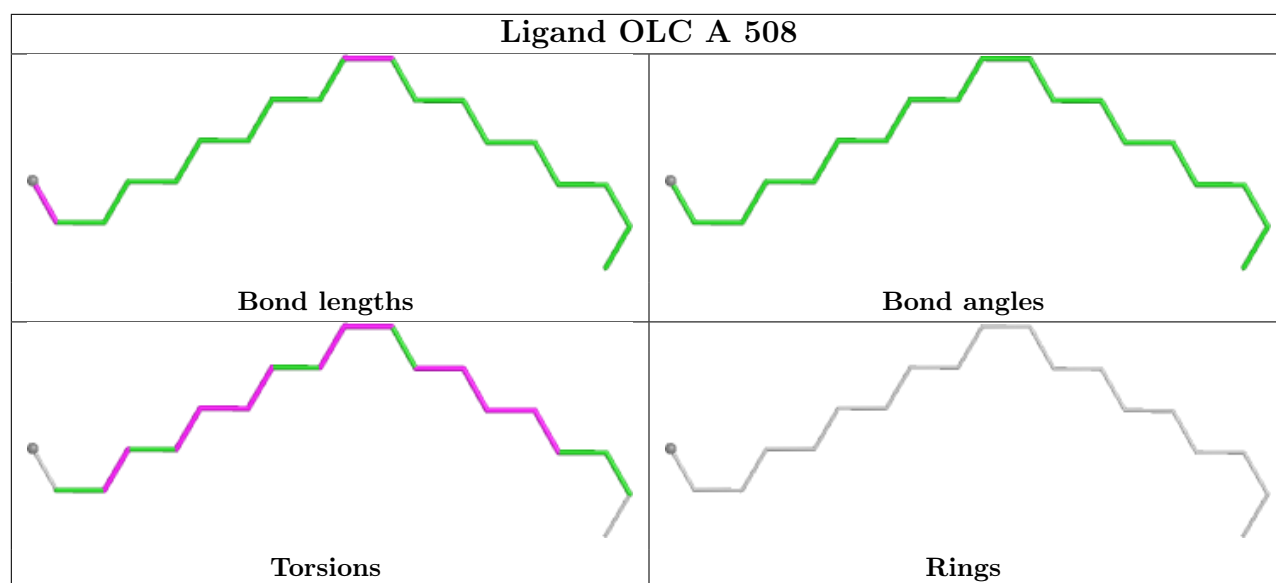
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	OLC	1	0
3	A	504	OLC	1	0
3	A	503	OLC	4	0
3	A	501	OLC	1	0
3	A	512	OLC	3	0

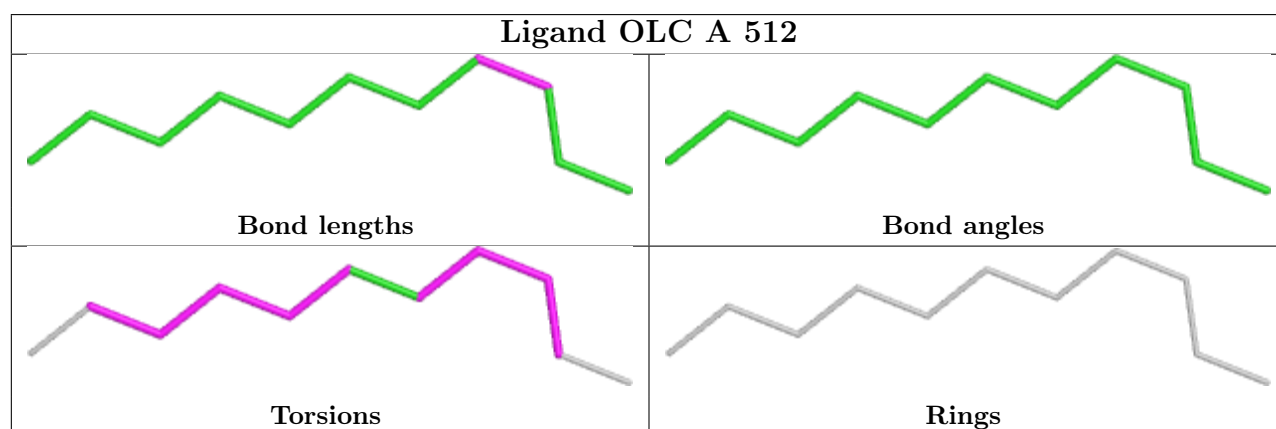
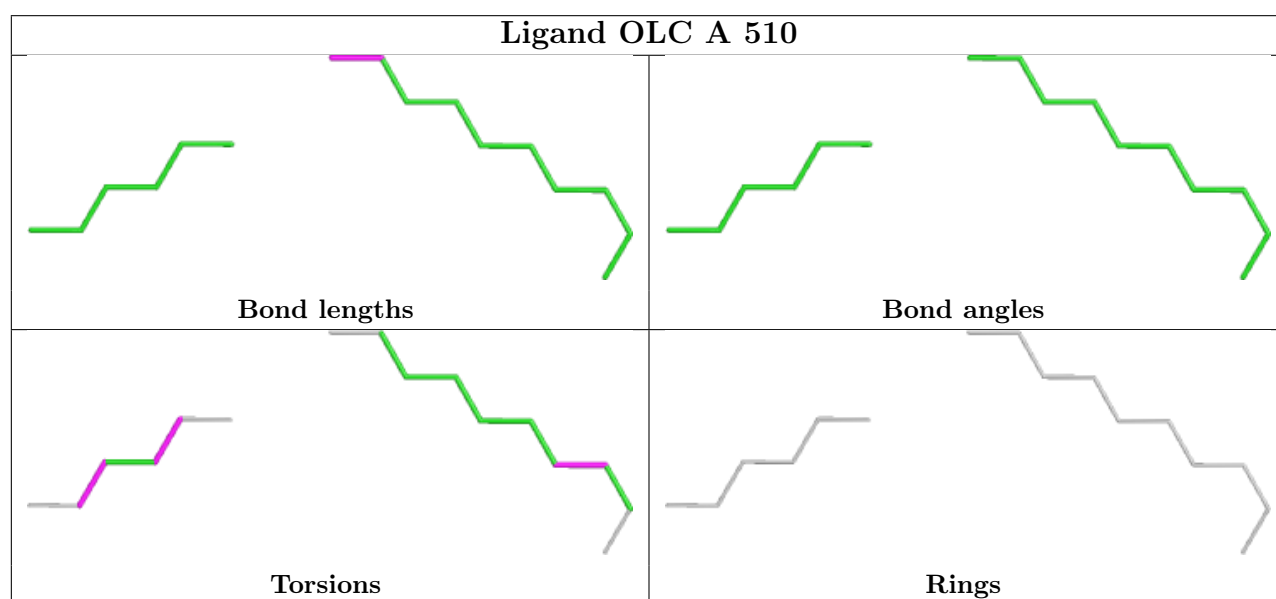
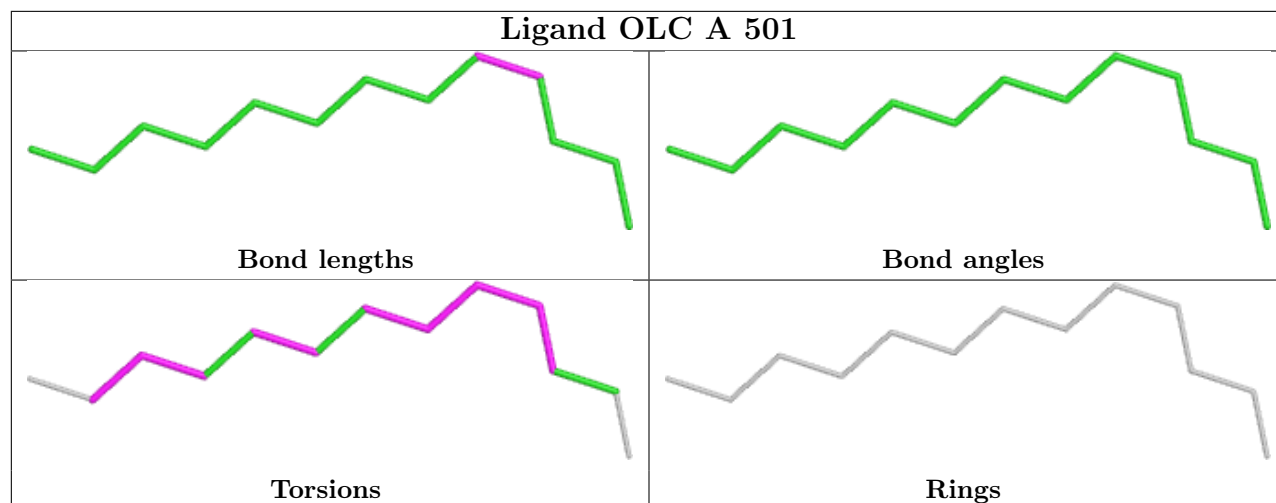
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

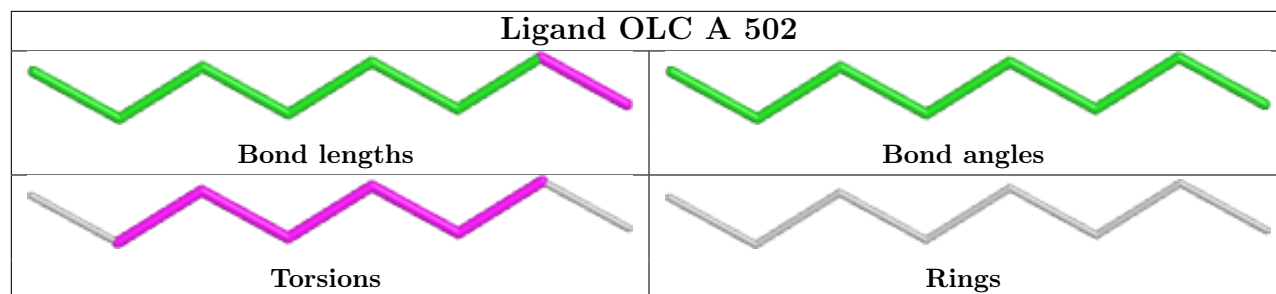
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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	444/461 (96%)	0.32	23 (5%) 33 27	14, 36, 68, 118	1 (0%)
2	B	9/11 (81%)	5.67	9 (100%) 0 0	74, 95, 143, 150	0
All	All	453/472 (95%)	0.42	32 (7%) 22 17	14, 36, 75, 150	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	SER	8.2
2	B	10	VAL	7.3
2	B	9	TYR	6.7
2	B	6	VAL	6.6
2	B	5	ALA	6.0
1	A	130	GLY	5.5
2	B	2	VAL	4.8
1	A	132	ALA	4.7
1	A	127	GLY	4.7
1	A	129	LYS	4.3
2	B	8	LEU	4.2
2	B	7	CYS	4.1
1	A	433	ASN	3.5
1	A	128	ALA	3.4
1	A	403	THR	3.3
2	B	3	TYR	3.2
1	A	350	THR	3.1
1	A	231	ASP	3.0
1	A	42	GLY	2.8
1	A	417	TYR	2.7
1	A	4	LYS	2.7
1	A	126	MET	2.5
1	A	311	ARG	2.5
1	A	134	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	454	THR	2.4
1	A	364	SER	2.4
1	A	358	ILE	2.3
1	A	269	THR	2.3
1	A	230	ARG	2.2
1	A	270	ALA	2.2
1	A	56	VAL	2.1
1	A	133	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DPN	B	1	11/12	0.80	0.27	78,86,94,96	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

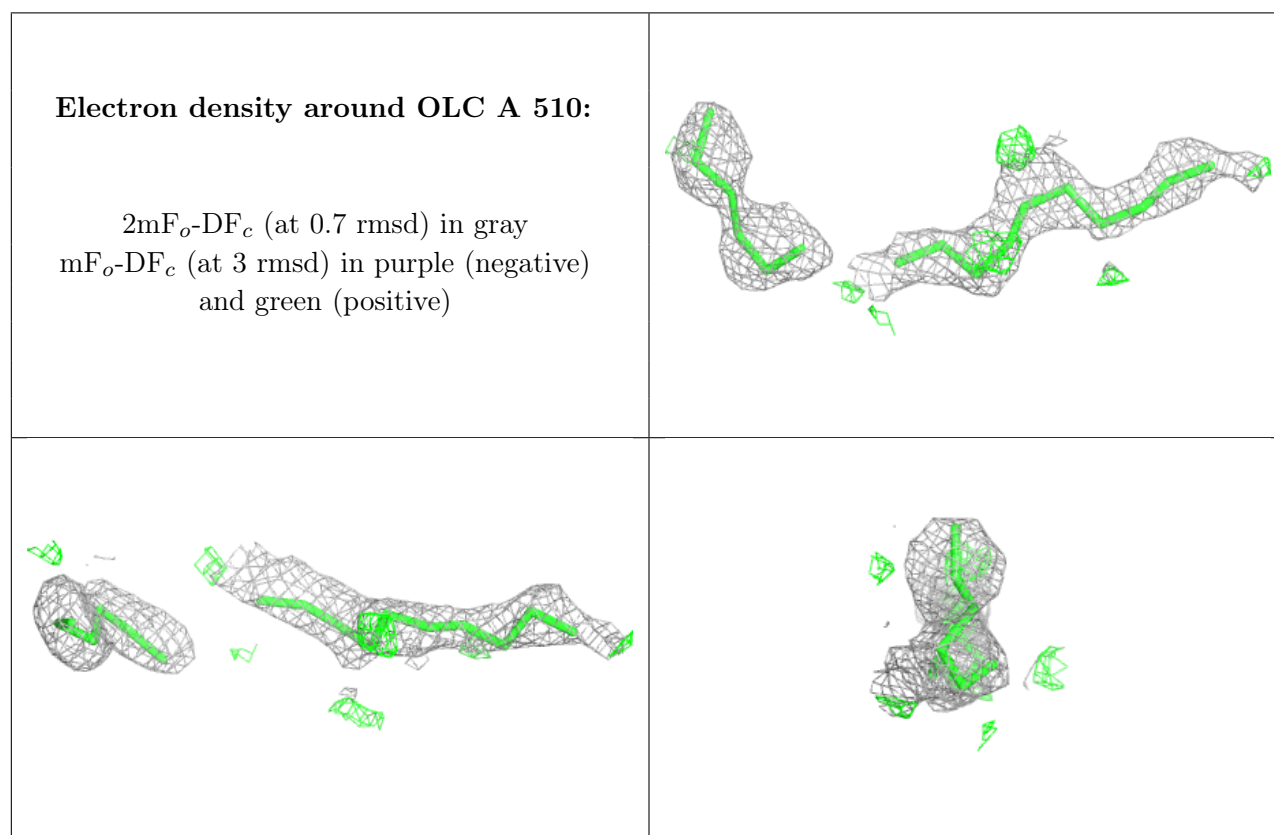
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLC	A	510	16/25	0.75	0.22	46,52,56,58	0
3	OLC	A	511	16/25	0.75	0.31	62,65,71,72	0
3	OLC	A	505	13/25	0.78	0.21	50,55,59,60	0
3	OLC	A	509	19/25	0.78	0.23	59,65,72,74	0
3	OLC	A	512	11/25	0.78	0.25	58,60,63,65	0
3	OLC	A	508	19/25	0.79	0.21	50,59,62,63	0
3	OLC	A	506	10/25	0.81	0.25	61,65,66,66	0
3	OLC	A	504	18/25	0.81	0.20	39,43,58,59	0
3	OLC	A	507	19/25	0.83	0.19	38,52,70,71	0

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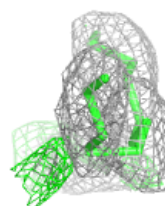
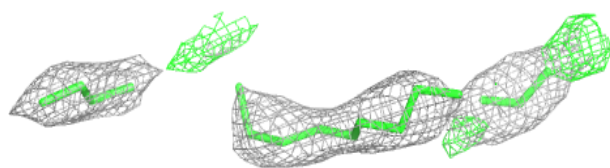
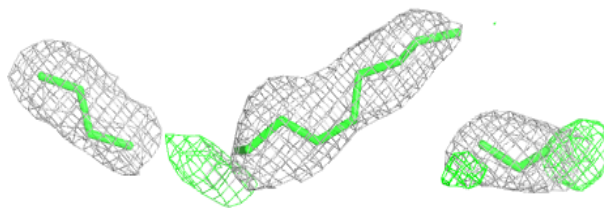
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLC	A	501	13/25	0.83	0.18	30,48,69,70	0
3	OLC	A	503	19/25	0.84	0.20	42,51,63,64	0
3	OLC	A	502	8/25	0.88	0.21	30,32,40,42	0

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

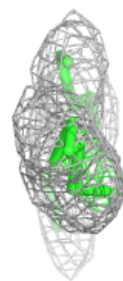
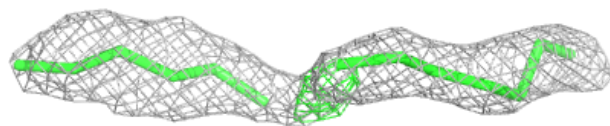
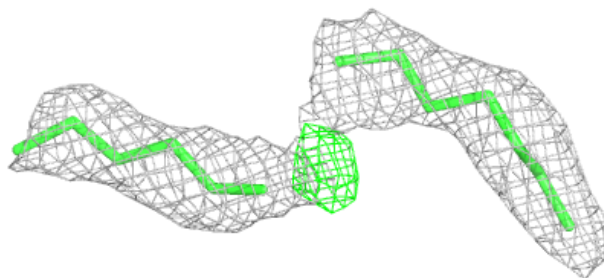


Electron density around OLC A 511:

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

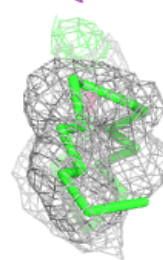
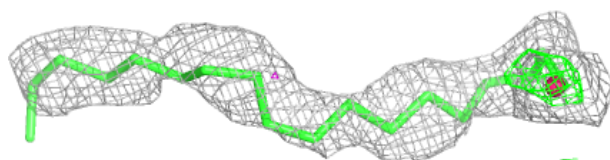
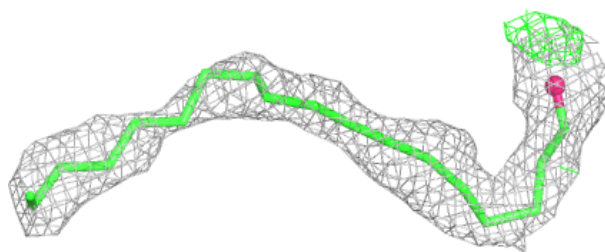
**Electron density around OLC A 505:**

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

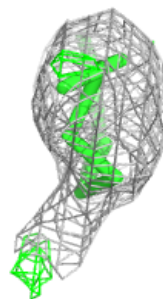
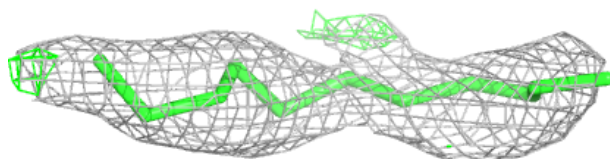
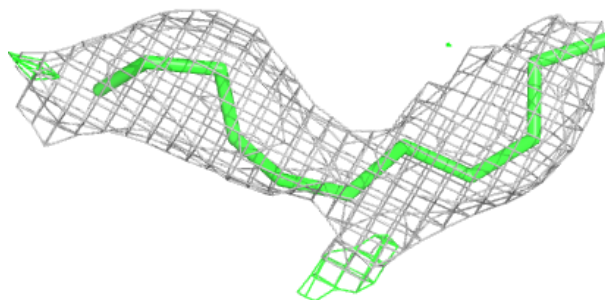


Electron density around OLC A 509:

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

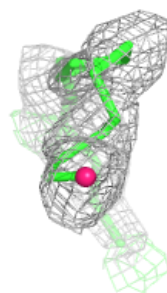
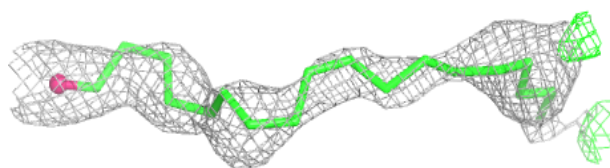
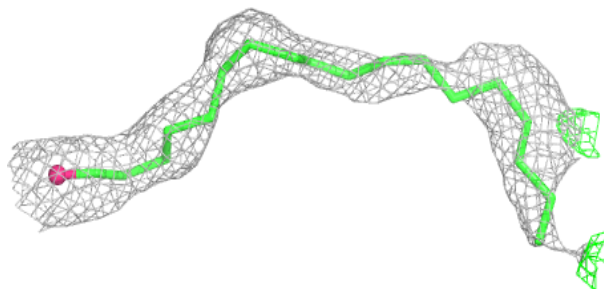
**Electron density around OLC A 512:**

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

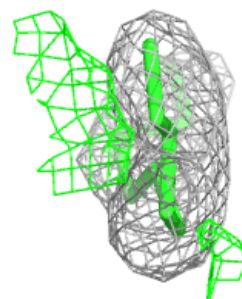
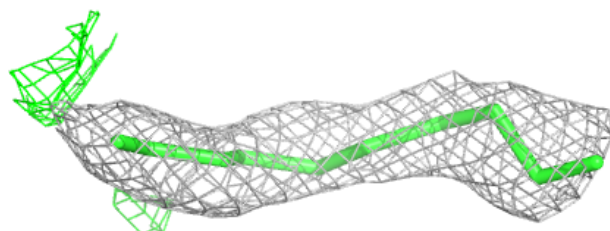
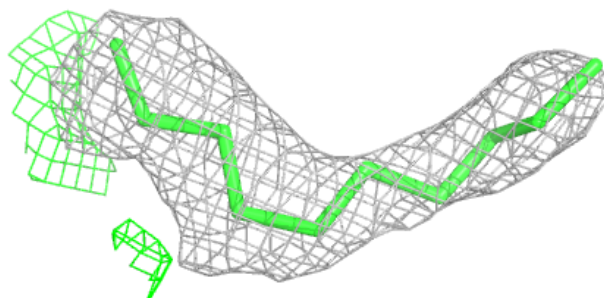


Electron density around OLC A 508:

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

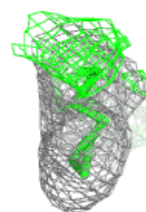
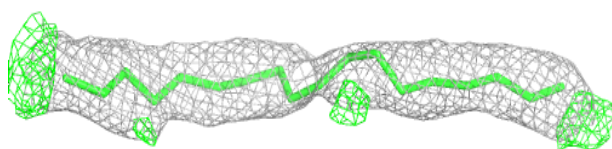
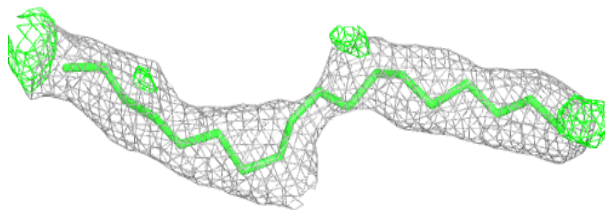
**Electron density around OLC A 506:**

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

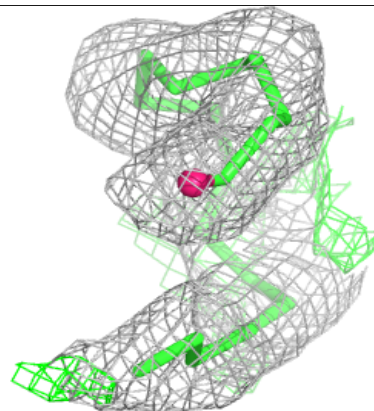
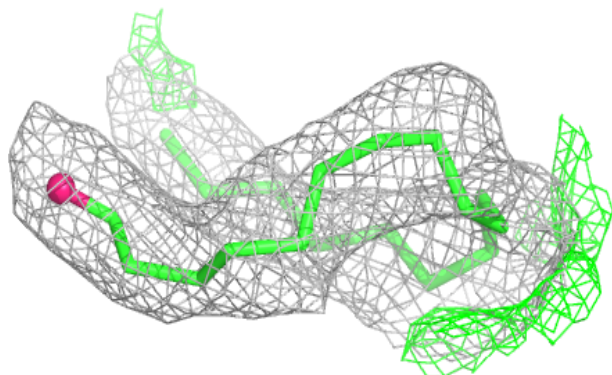
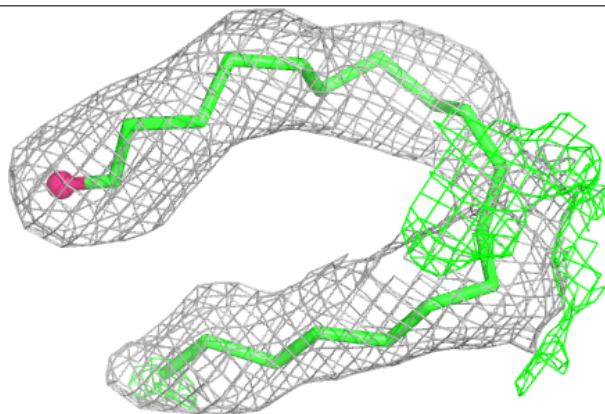


Electron density around OLC A 504:

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

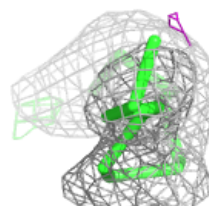
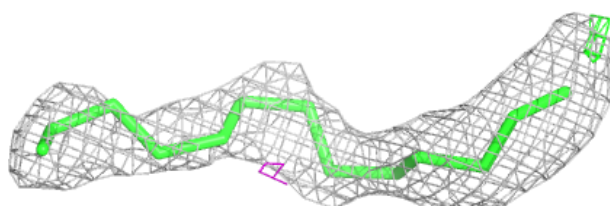
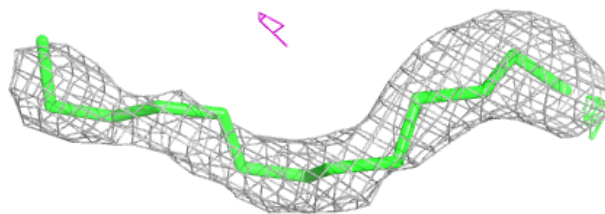
**Electron density around OLC A 507:**

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

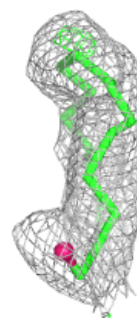
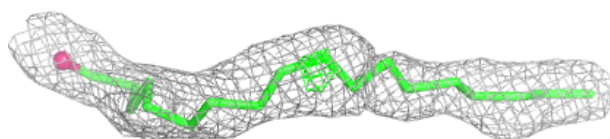
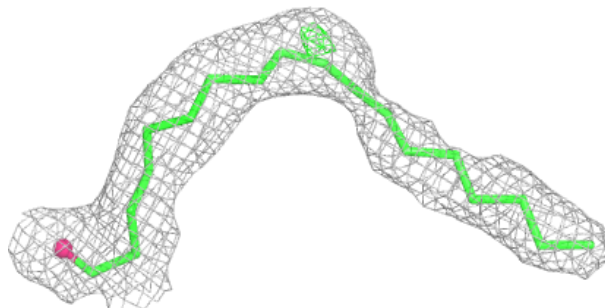


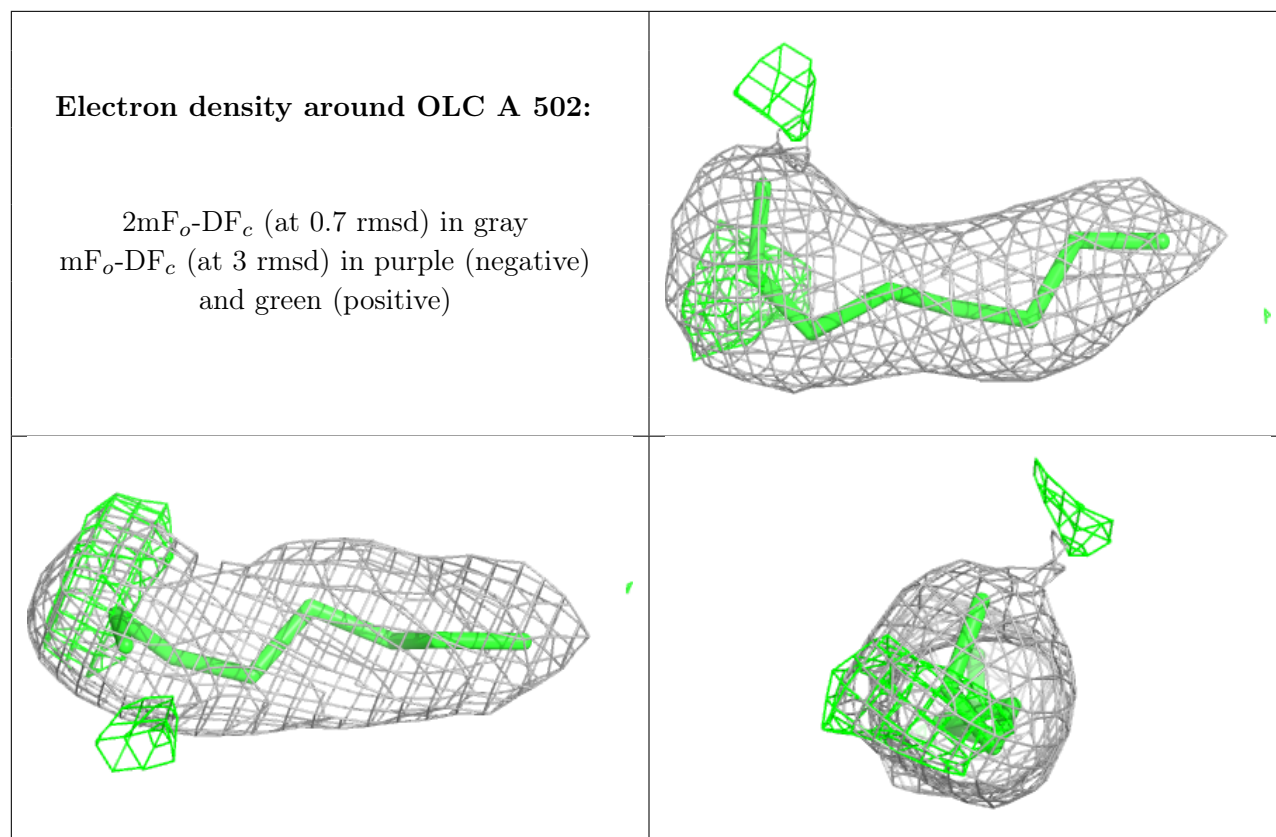
Electron density around OLC A 501:

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

**Electron density around OLC A 503:**

$2mF_o-DF_c$ (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.