



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:08 PM UTC

PDB ID : 6RZ8 / pdb_00006rz8
Title : Crystal structure of the human cysteinyl leukotriene receptor 2 in complex with ONO-2080365
Authors : Gusach, A.; Luginina, A.; Marin, E.; Brouillette, R.L.; Besserer-Offroy, E.; Longpre, J.M.; Ishchenko, A.; Popov, P.; Fujimoto, T.; Maruyama, T.; Stauch, B.; Ergasheva, M.; Romanovskaya, D.; Stepko, A.; Kovalev, K.; Shevtsov, M.; Gordeliy, V.; Han, G.W.; Sarret, P.; Katritch, V.; Borshchevskiy, V.; Mishin, A.; Cherezov, V.
Deposited on : 2019-06-12
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

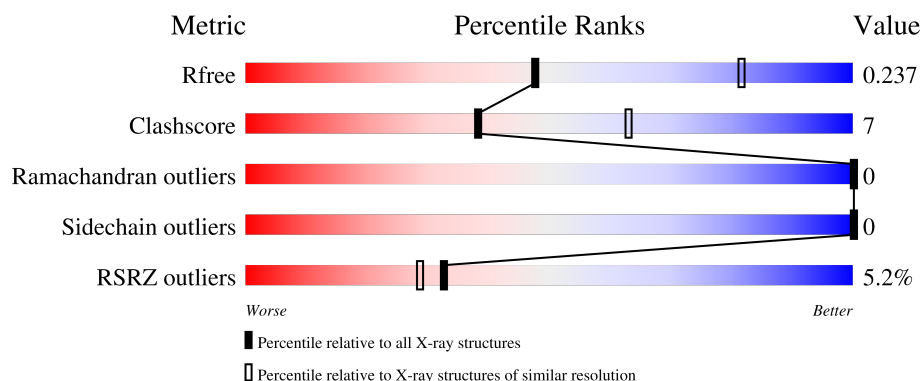
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	405	5% 76% 15% 10%

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3003 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.

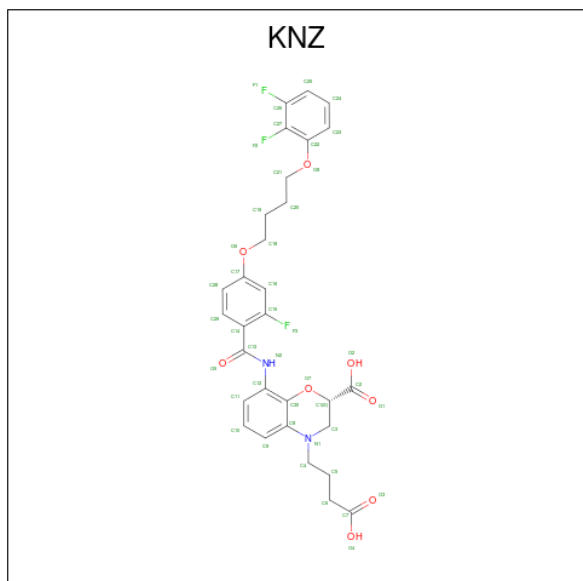
- Molecule 1 is a protein called Cysteinyl leukotriene receptor 2, Soluble cytochrome b562, Cysteinyl leukotriene receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2764	1812	445	490	17			

There are 6 discrepancies between the modelled and reference sequences:

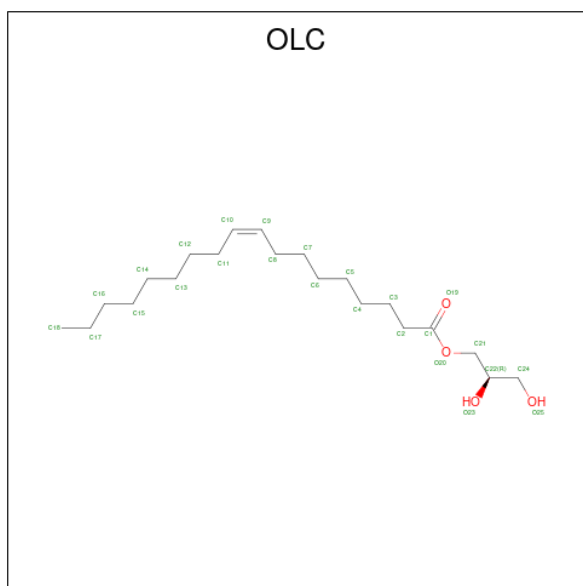
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	VAL	TRP	engineered mutation	UNP Q9NS75
A	84	ASN	ASP	engineered mutation	UNP Q9NS75
A	137	TYR	PHE	engineered mutation	UNP Q9NS75
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7

- Molecule 2 is (2 {S})-8-[[4-[4-[2,3-bis(fluoranyl)phenoxy]butoxy]-2-fluoranyl-phenyl]carbonyl amino]-4-(4-oxidanyl-4-oxidanylidene-but yl)-2,3-dihydro-1,4-benzoxazine-2-carboxylic acid (CCD ID: KNZ) (formula: C₃₀H₂₉F₃N₂O₈) (labeled as "Ligand of Interest" by depositor).



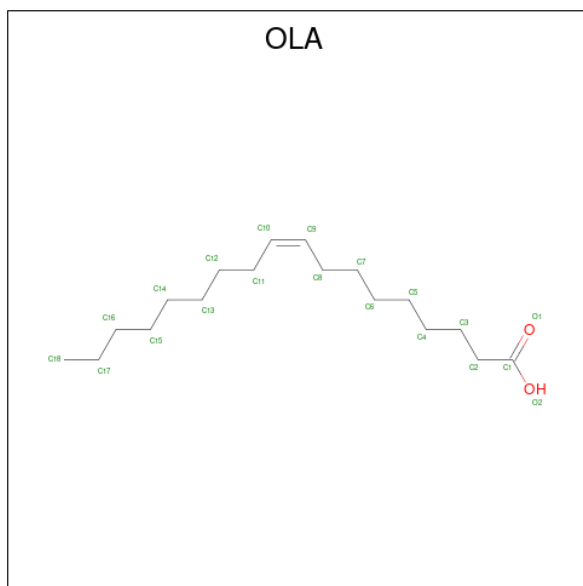
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			43	30	3	2	8		

- 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	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			21	17	4		
3	A	1	Total	C	O	0	0
			14	10	4		
3	A	1	Total	C		0	0
			13	13			
3	A	1	Total	C		0	0
			9	9			
3	A	1	Total	C		0	0
			5	5			
3	A	1	Total	C		0	0
			15	15			
3	A	1	Total	C		0	0
			4	4			
3	A	1	Total	C	O	0	0
			21	17	4		

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 14 14	0	0
4	A	1	Total C O 9 7 2	0	0
4	A	1	Total C O 7 5 2	0	0

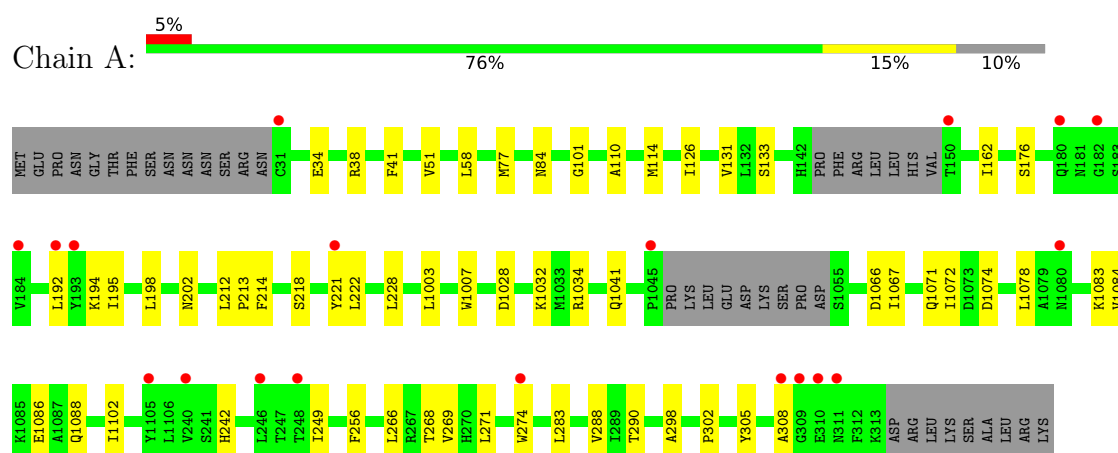
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0

3 Residue-property plots

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: Cysteinyl leukotriene receptor 2, Soluble cytochrome b562, Cysteinyl leukotriene receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	78.44Å 78.44Å 172.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.70 29.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.92-2.70) 92.5 (29.92-2.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.12-2829, BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.246 0.196 , 0.237	Depositor DCC
R_{free} test set	711 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 91.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3003	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: OLA, OLC, KNZ

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	0.22	0/2818	0.43	0/3846

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

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	2764	0	2718	39	0
2	A	43	0	0	1	0
3	A	149	0	218	5	0
4	A	30	0	38	0	0
5	A	17	0	0	0	0
All	All	3003	0	2974	41	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 (41) 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:A:1084:VAL:HG12	1:A:1088:GLN:HE21	1.52	0.74
1:A:38:ARG:HD3	1:A:101:GLY:HA2	1.74	0.69
1:A:269:VAL:HG12	1:A:283:LEU:HD11	1.77	0.67
1:A:1028:ASP:OD2	1:A:1032:LYS:NZ	2.34	0.61
1:A:126:ILE:HG23	1:A:256:PHE:HE1	1.66	0.61
1:A:198:LEU:O	1:A:202:ASN:N	2.31	0.59
1:A:283:LEU:HD12	3:A:2004:OLC:H3	1.86	0.58
1:A:1003:LEU:HD21	1:A:1102:ILE:HD12	1.89	0.55
1:A:266:LEU:HD12	1:A:290:THR:HG21	1.87	0.54
1:A:1084:VAL:O	1:A:1088:GLN:HG3	2.07	0.54
1:A:221:TYR:CG	1:A:249:ILE:HG23	2.44	0.53
1:A:176:SER:HB3	1:A:194:LYS:HE2	1.91	0.52
1:A:41:PHE:CZ	1:A:288:VAL:HG13	2.44	0.52
1:A:195:ILE:HD12	1:A:274:TRP:CE3	2.45	0.51
1:A:212:LEU:HB3	1:A:213:PRO:HD3	1.93	0.50
1:A:1041:GLN:NE2	1:A:1066:ASP:OD1	2.44	0.50
1:A:271:LEU:HD11	2:A:2001:KNZ:O5	2.12	0.49
1:A:126:ILE:HG23	1:A:256:PHE:CE1	2.46	0.49
1:A:51:VAL:HG11	3:A:2009:OLC:H9	1.94	0.49
1:A:1067:ILE:O	1:A:1071:GLN:HG3	2.12	0.49
1:A:110:ALA:O	1:A:114:MET:HG2	2.13	0.48
1:A:131:VAL:HG21	1:A:162:ILE:HD11	1.96	0.48
1:A:214:PHE:HB2	1:A:256:PHE:HE2	1.79	0.47
1:A:34:GLU:O	1:A:38:ARG:HG3	2.15	0.47
1:A:192:LEU:O	1:A:195:ILE:HG22	2.14	0.47
1:A:1007:TRP:CZ3	1:A:1102:ILE:HG13	2.51	0.45
1:A:133:SER:HG	1:A:221:TYR:HH	1.63	0.45
1:A:202:ASN:ND2	1:A:268:THR:HA	2.32	0.45
1:A:77:MET:HE1	1:A:308:ALA:HB3	1.98	0.45
1:A:218:SER:O	1:A:222:LEU:HG	2.16	0.45
1:A:58:LEU:HD12	3:A:2011:OLC:H3	1.99	0.45
1:A:84:ASN:HB3	1:A:298:ALA:HB1	1.99	0.44
1:A:1074:ASP:O	1:A:1078:LEU:HD13	2.18	0.44
1:A:1034:ARG:HB2	1:A:1072:ILE:HG21	2.01	0.43
3:A:2009:OLC:H9	3:A:2009:OLC:H6A	1.70	0.42
1:A:228:LEU:HB3	1:A:242:HIS:HE1	1.85	0.42
1:A:1083:LYS:HB3	1:A:1086:GLU:OE1	2.20	0.42
1:A:302:PRO:HA	1:A:305:TYR:CD2	2.54	0.42
1:A:1078:LEU:CD2	1:A:1086:GLU:HB3	2.50	0.42
1:A:1078:LEU:HD23	1:A:1086:GLU:HB3	2.02	0.40
3:A:2002:OLC:H14A	3:A:2002:OLC:H17	1.82	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	360/405 (89%)	351 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	280/356 (79%)	280 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1063	HIS
1	A	1088	GLN
1	A	242	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	2003	-	21,21,24	0.63	0	22,22,25	1.01	1 (4%)
4	OLA	A	2012	-	13,13,19	0.26	0	12,12,19	0.51	0
3	OLC	A	2009	-	14,14,24	0.40	0	13,13,25	0.68	0
3	OLC	A	2006	-	12,12,24	0.35	0	11,11,25	0.78	0
3	OLC	A	2005	-	13,13,24	0.73	0	14,14,25	1.04	1 (7%)
4	OLA	A	2013	-	8,8,19	0.73	0	8,8,19	0.96	0
2	KNZ	A	2001	-	46,46,46	0.70	1 (2%)	56,63,63	1.19	3 (5%)
3	OLC	A	2002	-	24,24,24	0.57	0	25,25,25	1.04	1 (4%)
3	OLC	A	2004	-	20,20,24	0.67	0	21,21,25	1.03	1 (4%)
3	OLC	A	2010	-	3,3,24	0.42	0	2,2,25	0.74	0
3	OLC	A	2011	-	20,20,24	0.64	0	21,21,25	0.97	1 (4%)
4	OLA	A	2014	-	6,6,19	0.82	0	6,6,19	1.01	0
3	OLC	A	2008	-	4,4,24	0.33	0	3,3,25	0.57	0
3	OLC	A	2007	-	8,8,24	0.35	0	7,7,25	0.66	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	2003	-	-	8/21/21/24	-
4	OLA	A	2012	-	-	3/11/11/17	-
3	OLC	A	2009	-	-	5/12/12/24	-
3	OLC	A	2006	-	-	5/10/10/24	-
3	OLC	A	2005	-	-	4/13/13/24	-
4	OLA	A	2013	-	-	5/6/6/17	-
2	KNZ	A	2001	-	-	4/27/39/39	0/4/4/4
3	OLC	A	2002	-	-	12/24/24/24	-
3	OLC	A	2004	-	-	10/20/20/24	-
3	OLC	A	2010	-	-	0/1/1/24	-
3	OLC	A	2011	-	-	11/20/20/24	-
4	OLA	A	2014	-	-	2/4/4/17	-
3	OLC	A	2008	-	-	0/2/2/24	-
3	OLC	A	2007	-	-	3/6/6/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	KNZ	O2-C2	-3.00	1.21	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	KNZ	O8-C22-C27	5.96	124.92	115.92
2	A	2001	KNZ	O8-C22-C23	-3.12	117.13	123.95
3	A	2004	OLC	O20-C1-C2	3.03	121.07	111.83
3	A	2011	OLC	O20-C1-C2	2.86	120.57	111.83
2	A	2001	KNZ	O2-C2-C1	2.81	120.03	112.71
3	A	2002	OLC	O20-C1-C2	2.70	120.06	111.83
3	A	2003	OLC	O20-C1-C2	2.67	119.98	111.83
3	A	2005	OLC	O20-C1-C2	2.59	119.72	111.83

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	KNZ	C27-C22-O8-C21
3	A	2003	OLC	C21-C22-C24-O25
3	A	2003	OLC	O23-C22-C24-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2002	OLC	O19-C1-O20-C21
3	A	2002	OLC	C2-C1-O20-C21
3	A	2002	OLC	O20-C21-C22-O23
3	A	2004	OLC	O20-C21-C22-O23
3	A	2004	OLC	C2-C1-O20-C21
2	A	2001	KNZ	C23-C22-O8-C21
3	A	2004	OLC	O19-C1-O20-C21
3	A	2011	OLC	C1-C2-C3-C4
3	A	2003	OLC	O20-C21-C22-O23
3	A	2011	OLC	O20-C21-C22-O23
3	A	2002	OLC	C21-C22-C24-O25
3	A	2005	OLC	C21-C22-C24-O25
3	A	2002	OLC	C2-C3-C4-C5
4	A	2013	OLA	C3-C4-C5-C6
3	A	2005	OLC	O23-C22-C24-O25
3	A	2011	OLC	C2-C1-O20-C21
3	A	2011	OLC	C4-C5-C6-C7
3	A	2009	OLC	C11-C12-C13-C14
3	A	2011	OLC	O19-C1-O20-C21
3	A	2003	OLC	C10-C11-C12-C13
3	A	2003	OLC	C6-C7-C8-C9
3	A	2011	OLC	C2-C3-C4-C5
3	A	2007	OLC	C6-C7-C8-C9
3	A	2004	OLC	C10-C11-C12-C13
3	A	2004	OLC	C6-C7-C8-C9
3	A	2011	OLC	C10-C11-C12-C13
3	A	2006	OLC	C6-C7-C8-C9
3	A	2009	OLC	C13-C14-C15-C16
3	A	2006	OLC	C12-C13-C14-C15
3	A	2009	OLC	C15-C16-C17-C18
3	A	2006	OLC	C11-C12-C13-C14
3	A	2002	OLC	C4-C5-C6-C7
3	A	2009	OLC	C10-C11-C12-C13
3	A	2002	OLC	O20-C21-C22-C24
3	A	2002	OLC	O23-C22-C24-O25
3	A	2011	OLC	C11-C12-C13-C14
3	A	2004	OLC	C11-C12-C13-C14
3	A	2011	OLC	C7-C8-C9-C10
4	A	2013	OLA	C4-C5-C6-C7
3	A	2004	OLC	O20-C21-C22-C24
3	A	2003	OLC	C2-C1-O20-C21
3	A	2004	OLC	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2007	OLC	C7-C8-C9-C10
3	A	2003	OLC	O19-C1-O20-C21
3	A	2005	OLC	C3-C4-C5-C6
3	A	2011	OLC	C3-C4-C5-C6
2	A	2001	KNZ	C5-C6-C7-O4
4	A	2012	OLA	C5-C6-C7-C8
2	A	2001	KNZ	C5-C6-C7-O3
3	A	2006	OLC	C5-C6-C7-C8
4	A	2013	OLA	O2-C1-C2-C3
3	A	2006	OLC	C9-C10-C11-C12
3	A	2011	OLC	C9-C10-C11-C12
3	A	2002	OLC	C14-C15-C16-C17
4	A	2013	OLA	O1-C1-C2-C3
4	A	2012	OLA	C7-C8-C9-C10
4	A	2014	OLA	C2-C3-C4-C5
4	A	2013	OLA	C2-C3-C4-C5
3	A	2002	OLC	C6-C7-C8-C9
4	A	2012	OLA	C3-C4-C5-C6
3	A	2002	OLC	C7-C8-C9-C10
3	A	2007	OLC	C9-C10-C11-C12
3	A	2002	OLC	C9-C10-C11-C12
4	A	2014	OLA	C1-C2-C3-C4
3	A	2004	OLC	C4-C5-C6-C7
3	A	2009	OLC	C5-C6-C7-C8
3	A	2005	OLC	C1-C2-C3-C4
3	A	2003	OLC	C9-C10-C11-C12
3	A	2004	OLC	O23-C22-C24-O25

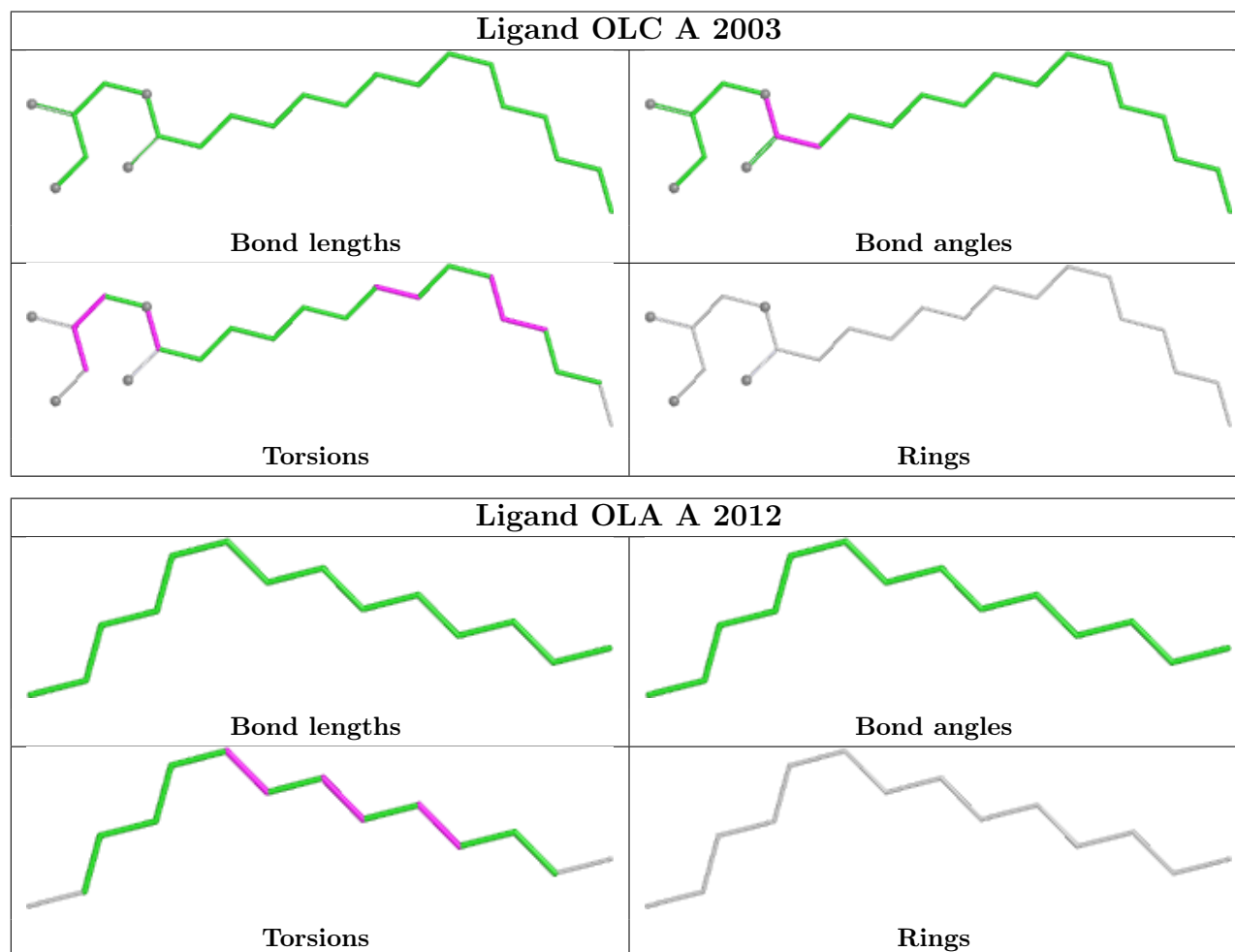
There are no ring outliers.

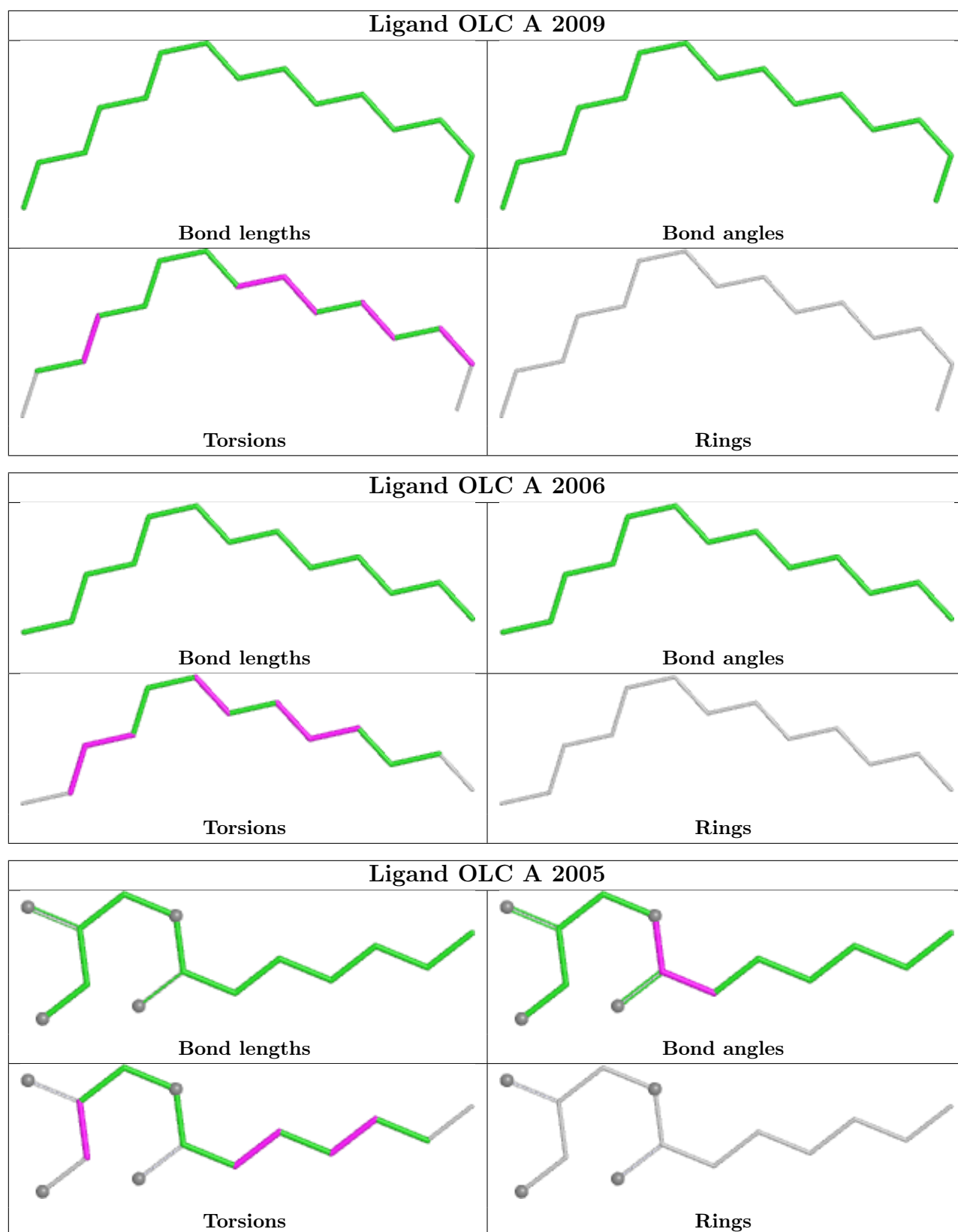
5 monomers are involved in 6 short contacts:

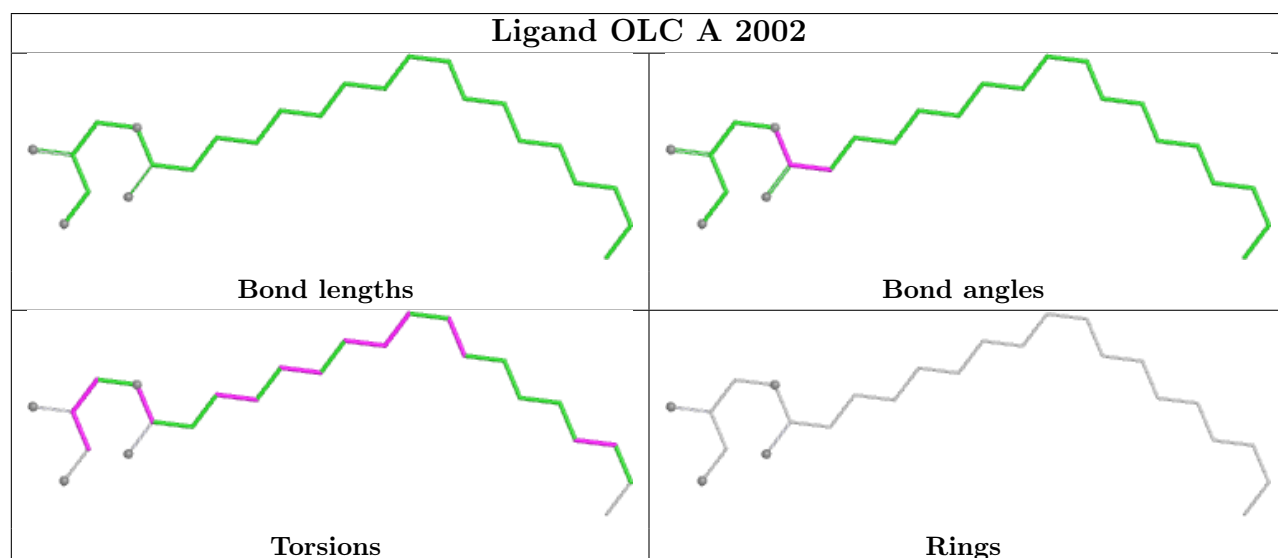
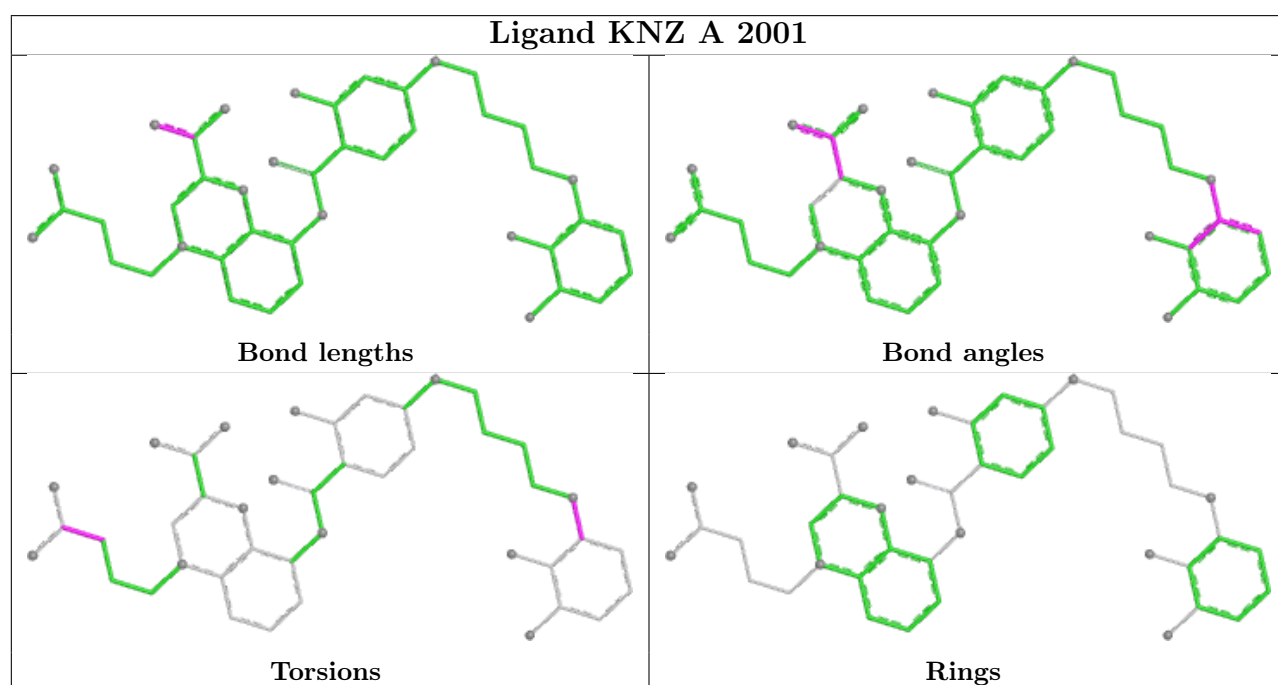
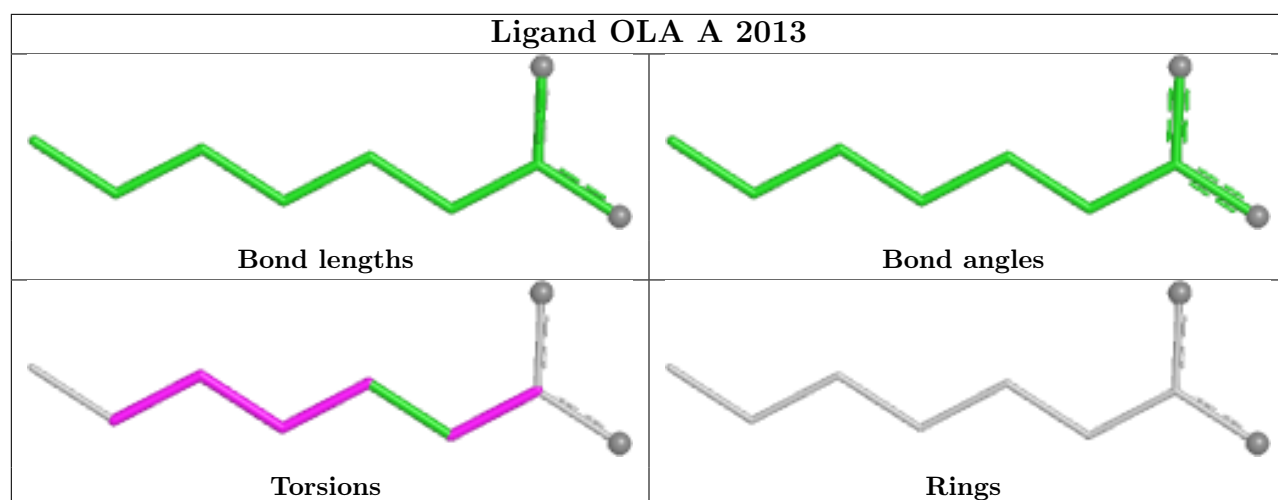
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2009	OLC	2	0
2	A	2001	KNZ	1	0
3	A	2002	OLC	1	0
3	A	2004	OLC	1	0
3	A	2011	OLC	1	0

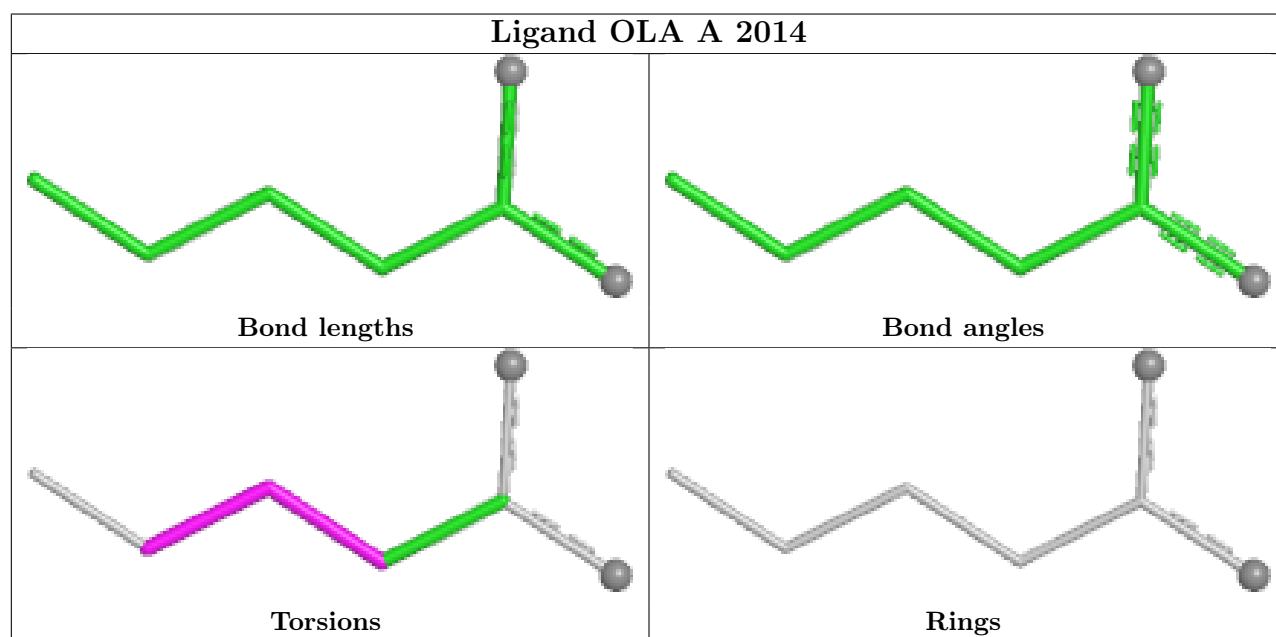
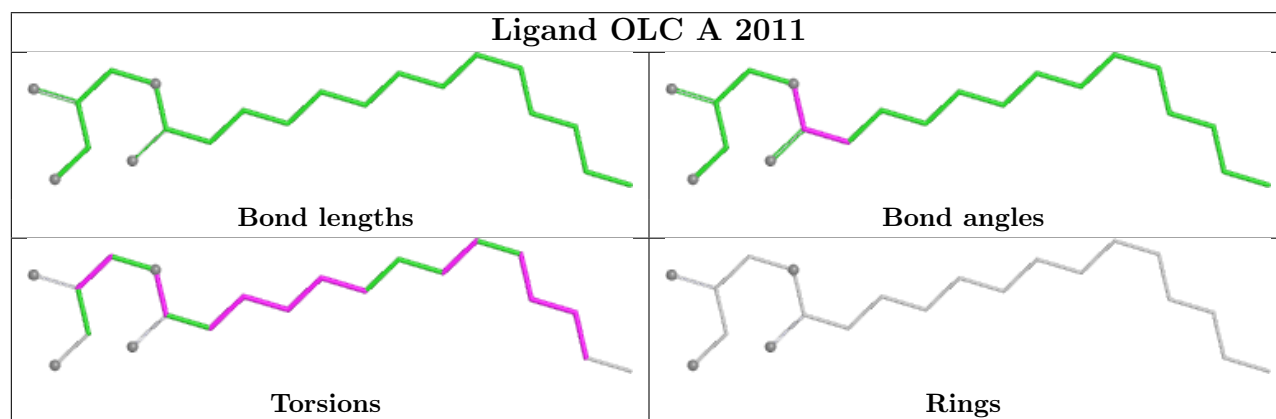
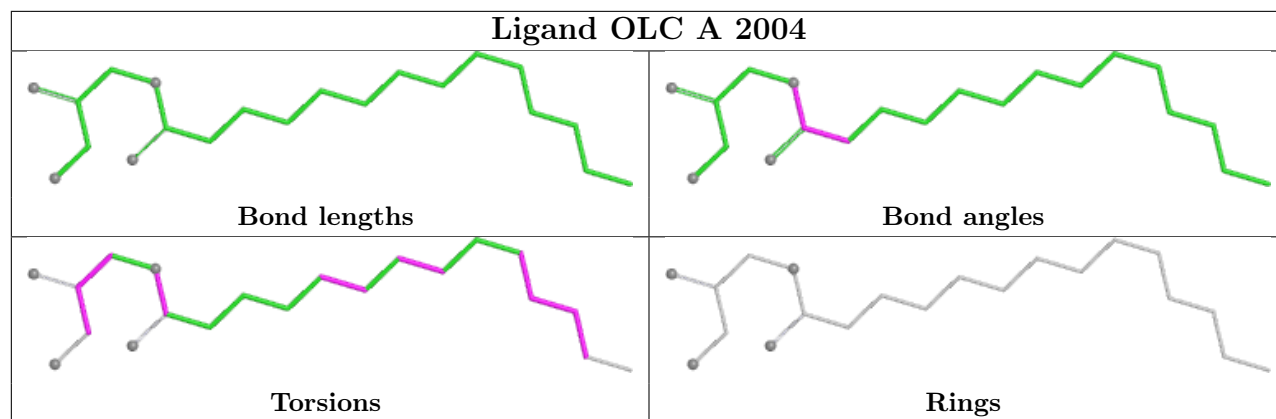
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

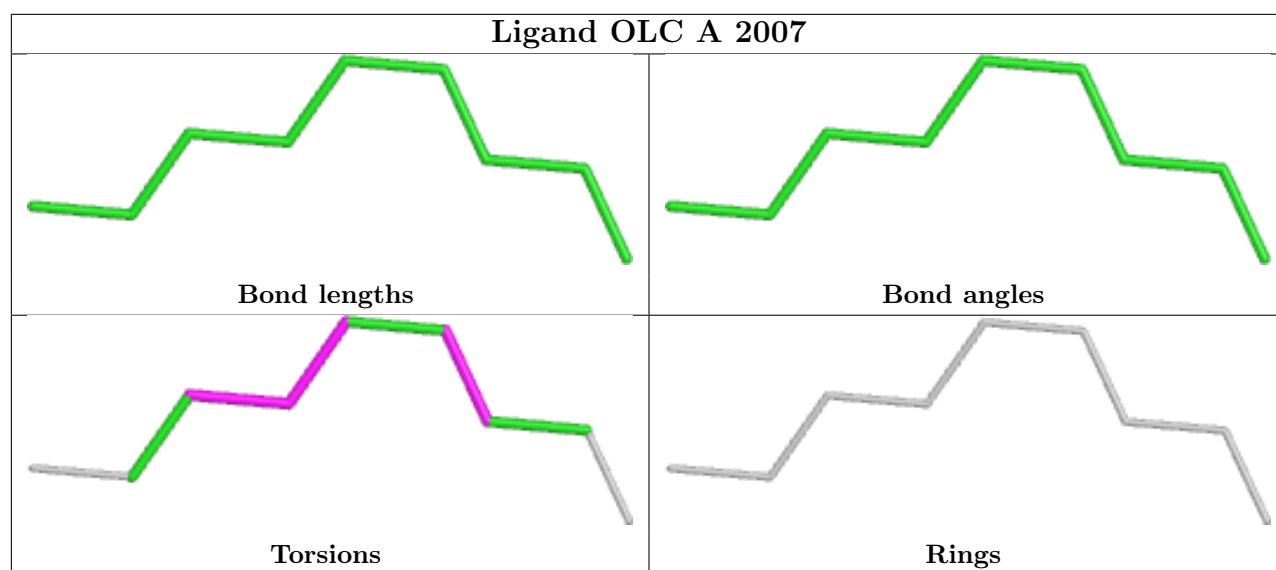
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	366/405 (90%)	0.31	19 (5%) 33 29	37, 72, 155, 203	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	VAL	4.0
1	A	193	TYR	3.8
1	A	246	LEU	3.4
1	A	274	TRP	3.3
1	A	182	GLY	2.8
1	A	1045	PRO	2.8
1	A	1105	TYR	2.7
1	A	192	LEU	2.7
1	A	184	VAL	2.5
1	A	310	GLU	2.4
1	A	1080	ASN	2.4
1	A	180	GLN	2.4
1	A	150	THR	2.3
1	A	309	GLY	2.3
1	A	311	ASN	2.2
1	A	31	CYS	2.1
1	A	221	TYR	2.1
1	A	248	THR	2.1
1	A	308	ALA	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

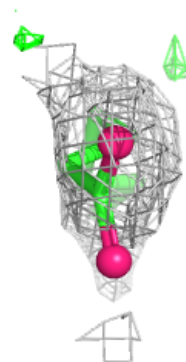
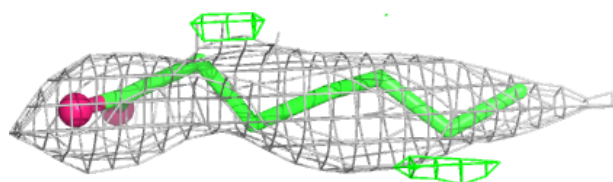
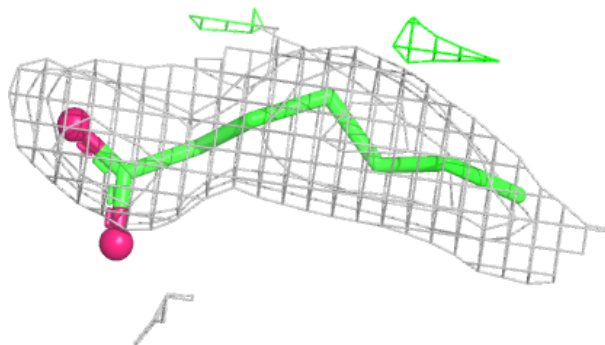
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OLA	A	2013	9/20	0.73	0.20	91,96,122,125	0
3	OLC	A	2008	5/25	0.83	0.25	76,80,85,92	0
3	OLC	A	2009	15/25	0.86	0.15	48,66,101,102	0
3	OLC	A	2002	25/25	0.86	0.17	52,78,111,126	0
3	OLC	A	2010	4/25	0.87	0.20	66,67,70,72	0
3	OLC	A	2011	21/25	0.88	0.17	81,101,125,131	0
3	OLC	A	2005	14/25	0.88	0.14	74,101,117,133	0
4	OLA	A	2012	14/20	0.89	0.18	85,93,104,105	0
3	OLC	A	2004	21/25	0.90	0.14	53,65,110,118	0
3	OLC	A	2007	9/25	0.90	0.15	68,78,89,98	0
4	OLA	A	2014	7/20	0.90	0.13	67,71,85,97	0
3	OLC	A	2006	13/25	0.91	0.15	68,86,99,106	0
3	OLC	A	2003	22/25	0.92	0.12	34,66,94,100	0
2	KNZ	A	2001	43/43	0.95	0.09	37,57,88,106	0

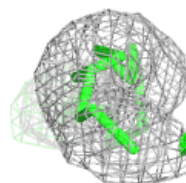
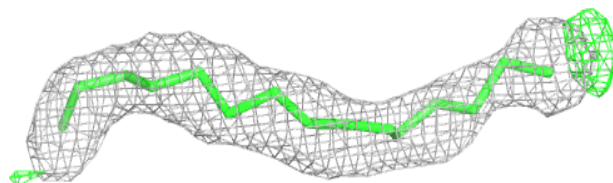
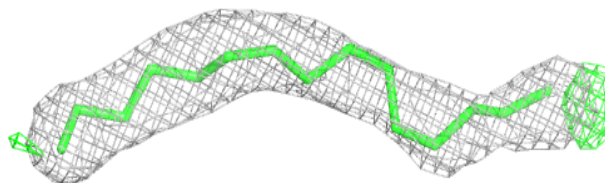
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 2013:

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

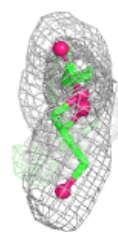
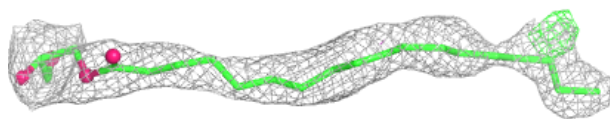
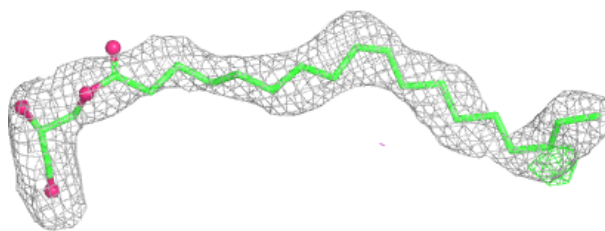
**Electron density around OLC A 2009:**

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

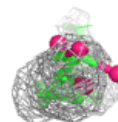
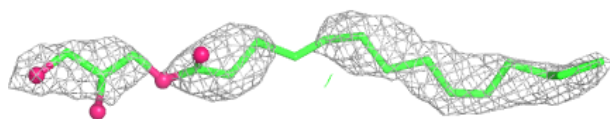
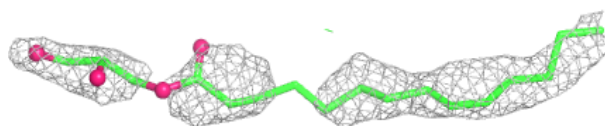


Electron density around OLC A 2002:

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

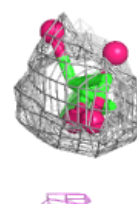
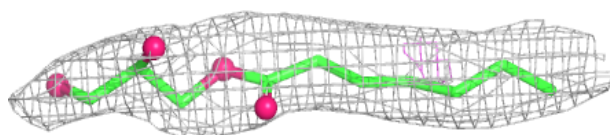
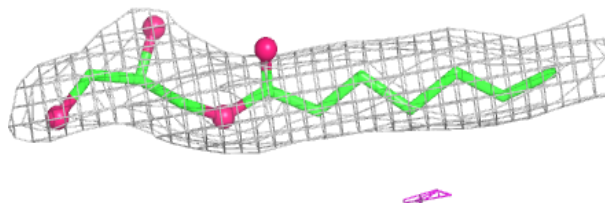
**Electron density around OLC A 2011:**

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

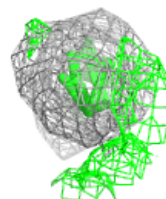
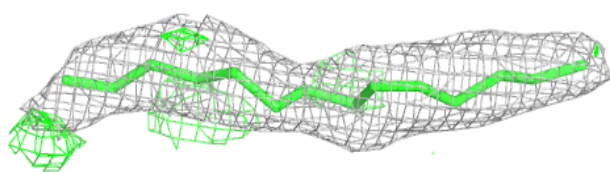
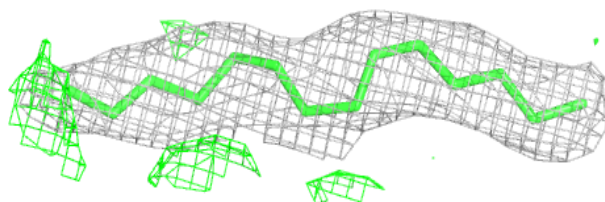


Electron density around OLC A 2005:

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

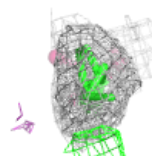
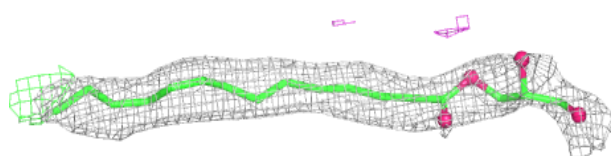
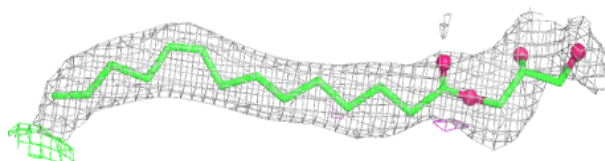
**Electron density around OLA A 2012:**

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

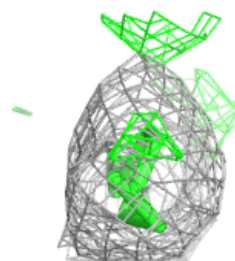
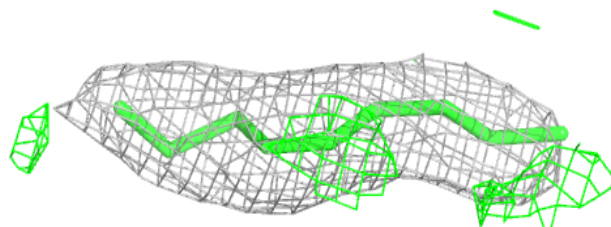
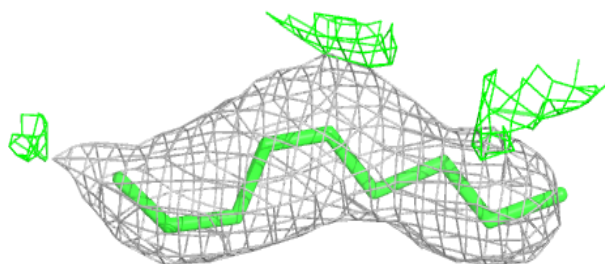


Electron density around OLC A 2004:

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

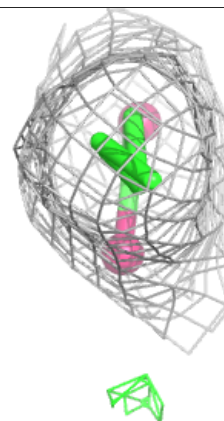
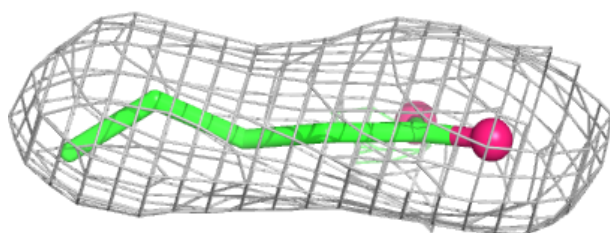
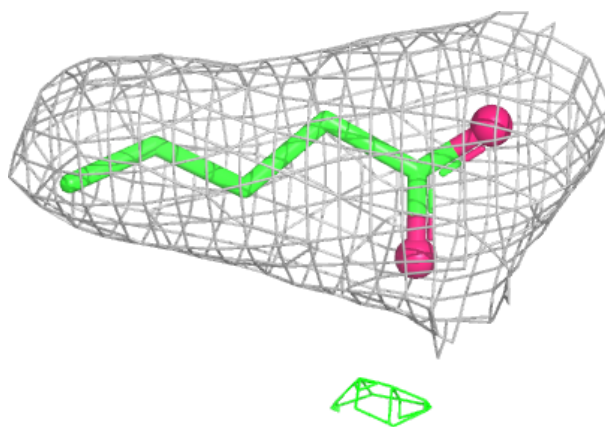
**Electron density around OLC A 2007:**

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

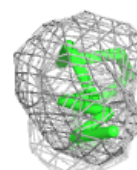
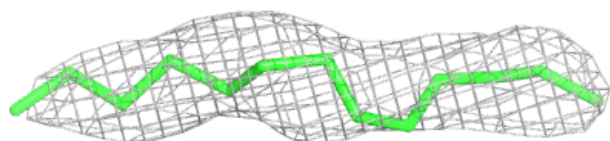
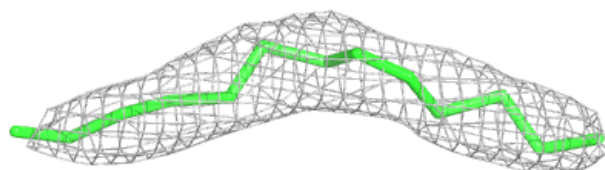


Electron density around OLA A 2014:

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

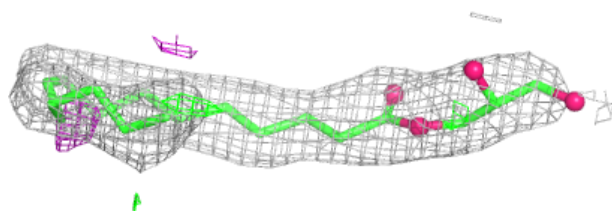
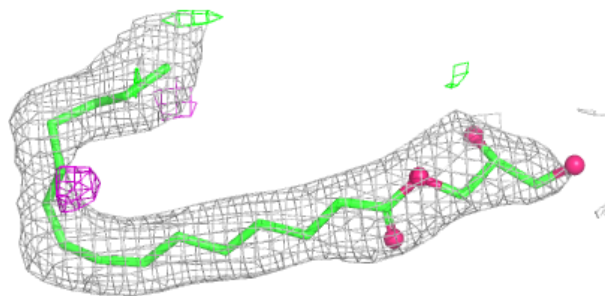
**Electron density around OLC A 2006:**

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

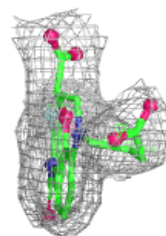
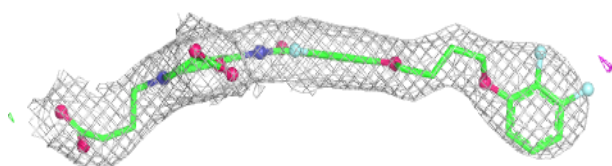
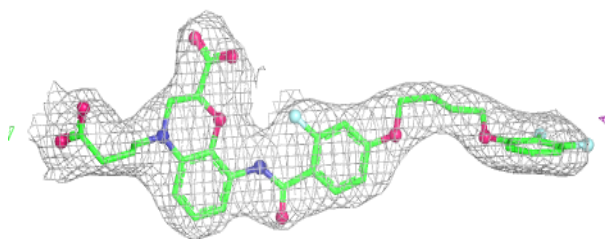


Electron density around OLC A 2003:

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

**Electron density around KNZ A 2001:**

$2mF_o-DF_c$ (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.