



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:30 AM UTC

PDB ID : 6PS7 / pdb_00006ps7
Title : XFEL A2aR structure by ligand exchange from LUF5843 to ZM241385.
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Zatsepin, N.A.; Weierstall, U.; Liu, W.; Nango, E.; Nakane, T.; Tanaka, R.;
Tono, K.; Joti, Y.; Iwata, S.; Moraes, I.; Gati, C.; Cherezov, C.
Deposited on : 2019-07-12
Resolution : 1.85 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

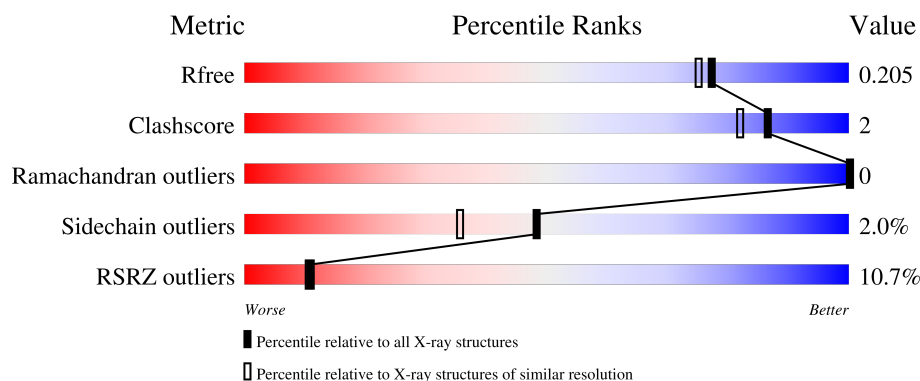
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	442	10% 83% 6% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3655 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 Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	20	0
			3131	2053	516	539	23			

There are 34 discrepancies between the modelled and reference sequences:

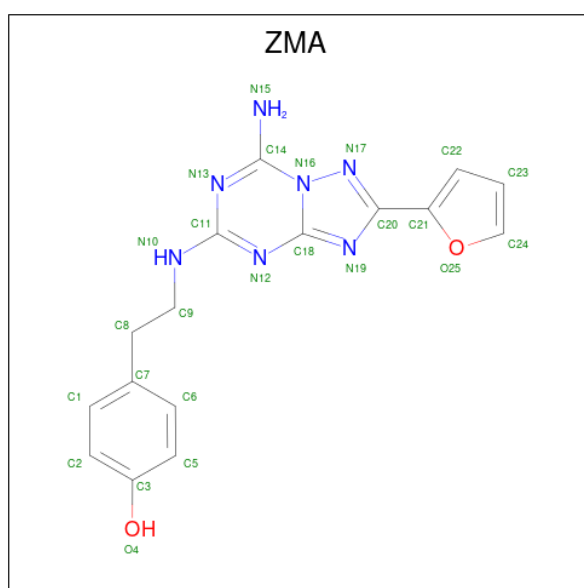
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl)[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl}phenol (CCD ID: ZMA) (formula: C₁₆H₁₅N₇O₂) (labeled as "Ligand of Interest" by depositor).



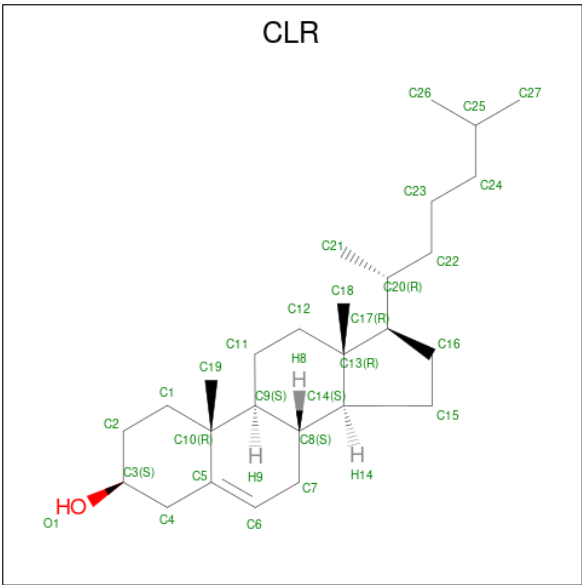
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



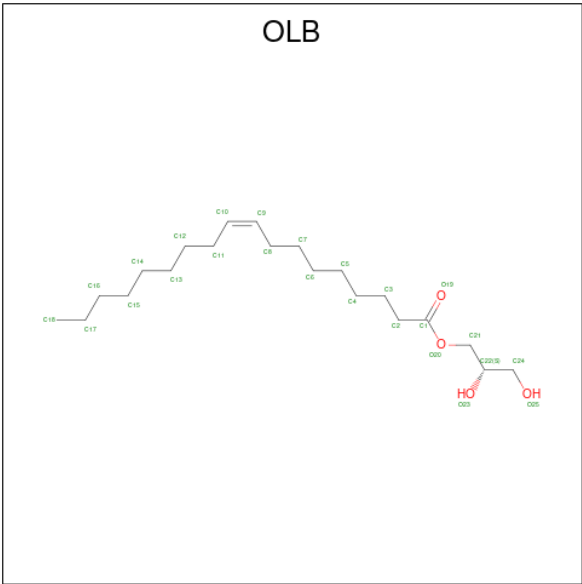
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	13	4		
3	A	1	Total	C	O	0	0
			16	12	4		
3	A	1	Total	C	O	0	0
			18	14	4		
3	A	1	Total	C	O	0	0
			17	13	4		
3	A	1	Total	C	O	0	0
			17	13	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			17	13	4		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



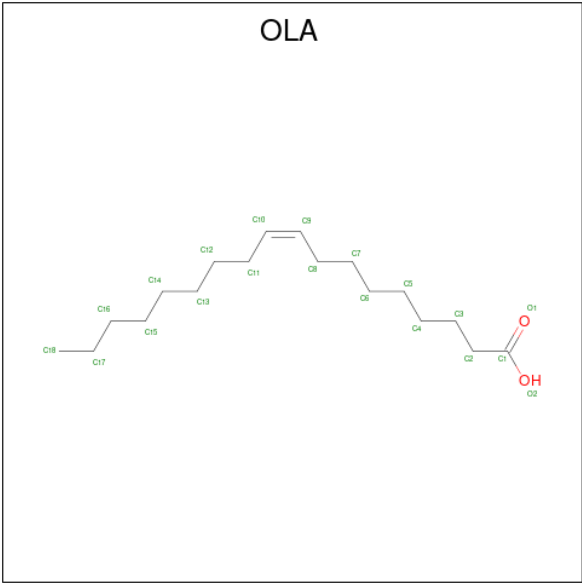
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	13	4		

- Molecule 6 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	14	2		
6	A	1	Total	C	O	0	0
			9	7	2		
6	A	1	Total	C	O	0	0
			9	7	2		
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C	O	0	0
			13	11	2		
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C		0	0
			9	9			
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

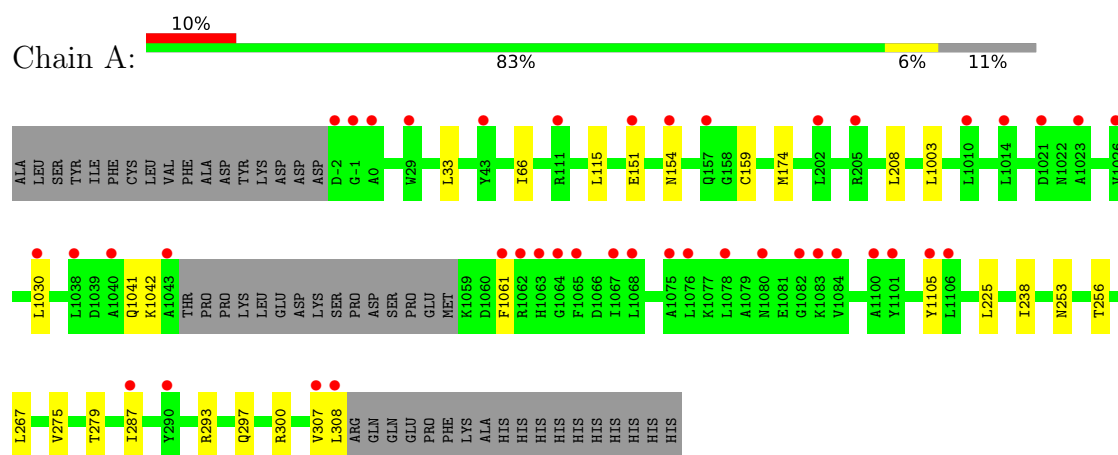
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	105	Total	O	0	0
			105	105		

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: Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.32Å 180.49Å 142.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.49 – 1.85 33.49 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.49-1.85) 99.9 (33.49-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.175 , 0.201 0.181 , 0.205	Depositor DCC
R_{free} test set	1236 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3655	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: CLR, ZMA, NA, OLC, OLB, OLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/3215	0.49	0/4381

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3131	0	3164	15	0
2	A	25	0	14	0	0
3	A	135	0	165	1	0
4	A	84	0	138	0	0
5	A	17	0	22	0	0
6	A	157	0	202	0	0
7	A	1	0	0	0	0
8	A	105	0	0	1	0
All	All	3655	0	3705	15	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 2.

All (15) 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:297:GLN:OE1	1:A:300[B]:ARG:NH1	2.31	0.63
1:A:275[B]:VAL:O	1:A:279:THR:HG23	2.03	0.58
1:A:66[B]:ILE:HD11	8:A:1348:HOH:O	2.04	0.56
1:A:174[B]:MET:HE2	1:A:256:THR:HB	1.92	0.52
1:A:154[B]:ASN:OD1	1:A:159:CYS:HB2	2.12	0.49
1:A:174[B]:MET:HE1	1:A:253:ASN:HA	1.95	0.48
1:A:1061:PHE:HA	1:A:1105[A]:TYR:CE2	2.51	0.46
1:A:275[A]:VAL:O	1:A:279:THR:HG23	2.16	0.46
1:A:293:ARG:O	1:A:297:GLN:HG2	2.17	0.45
1:A:238:ILE:HD13	1:A:287[B]:ILE:HD13	1.99	0.45
1:A:307:VAL:O	1:A:308:LEU:HD12	2.17	0.45
1:A:208:LEU:HG	1:A:225[B]:LEU:HD23	1.99	0.43
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.21	0.41
1:A:151:GLU:OE1	1:A:154[B]:ASN:ND2	2.54	0.41
1:A:267:LEU:HD21	3:A:1204:OLC:H22	2.03	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	408/442 (92%)	404 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	323/369 (88%)	317 (98%)	6 (2%)	50 38

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

Mol	Chain	Res	Type
1	A	33	LEU
1	A	115	LEU
1	A	1003	LEU
1	A	1030	LEU
1	A	1041	GLN
1	A	1042	LYS

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

Mol	Chain	Res	Type
1	A	1013	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	OLA	A	1219	-	10,10,19	0.67	0	10,10,19	0.89	0
6	OLA	A	1225	-	17,17,19	0.57	0	17,17,19	0.84	0
2	ZMA	A	1201	-	26,28,28	0.44	0	30,39,39	0.71	1 (3%)
6	OLA	A	1222	-	10,10,19	0.65	0	10,10,19	0.93	0
6	OLA	A	1215	-	15,15,19	0.56	0	15,15,19	0.75	0
6	OLA	A	1218	-	11,11,19	0.63	0	11,11,19	0.95	0
6	OLA	A	1227	-	16,16,19	0.51	0	16,16,19	0.98	1 (6%)
3	OLC	A	1205	-	16,16,24	0.59	0	17,17,25	1.17	1 (5%)
3	OLC	A	1209	-	10,10,24	0.66	0	11,11,25	1.16	1 (9%)
6	OLA	A	1217	-	8,8,19	0.68	0	8,8,19	0.96	0
4	CLR	A	1211	-	31,31,31	0.73	1 (3%)	48,48,48	0.93	1 (2%)
5	OLB	A	1214	-	16,16,24	0.31	0	17,17,25	0.33	0
6	OLA	A	1216	-	8,8,19	0.70	0	8,8,19	1.01	0
3	OLC	A	1204	-	17,17,24	0.57	0	18,18,25	1.08	1 (5%)
3	OLC	A	1208	-	10,10,24	0.65	0	11,11,25	1.14	1 (9%)
6	OLA	A	1224	-	7,7,19	0.74	0	7,7,19	0.81	0
6	OLA	A	1223	-	8,8,19	0.38	0	7,7,19	0.64	0
6	OLA	A	1220	-	12,12,19	0.63	0	12,12,19	0.97	0
3	OLC	A	1202	-	16,16,24	0.63	0	17,17,25	1.02	1 (5%)
6	OLA	A	1226	-	11,11,19	0.65	0	11,11,19	0.91	0
3	OLC	A	1206	-	16,16,24	0.56	0	17,17,25	1.24	2 (11%)
4	CLR	A	1213	-	31,31,31	0.60	0	48,48,48	0.79	2 (4%)
6	OLA	A	1221	-	11,11,19	0.64	0	11,11,19	0.97	0
3	OLC	A	1203	-	15,15,24	0.57	0	16,16,25	1.09	1 (6%)
3	OLC	A	1210	-	16,16,24	0.62	0	17,17,25	1.06	2 (11%)
4	CLR	A	1212	-	31,31,31	0.66	0	48,48,48	0.92	1 (2%)
3	OLC	A	1207	-	10,10,24	0.65	0	11,11,25	1.13	1 (9%)

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
6	OLA	A	1219	-	-	3/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLA	A	1225	-	-	7/15/15/17	-
2	ZMA	A	1201	-	-	0/10/10/10	0/4/4/4
6	OLA	A	1222	-	-	4/8/8/17	-
6	OLA	A	1215	-	-	4/13/13/17	-
6	OLA	A	1218	-	-	1/9/9/17	-
6	OLA	A	1227	-	-	7/14/14/17	-
3	OLC	A	1205	-	-	4/16/16/24	-
3	OLC	A	1209	-	-	3/10/10/24	-
6	OLA	A	1217	-	-	3/6/6/17	-
4	CLR	A	1211	-	-	1/10/68/68	0/4/4/4
5	OLB	A	1214	-	-	0/16/16/24	-
6	OLA	A	1216	-	-	1/6/6/17	-
3	OLC	A	1204	-	-	4/17/17/24	-
3	OLC	A	1208	-	-	5/10/10/24	-
6	OLA	A	1224	-	-	1/5/5/17	-
6	OLA	A	1223	-	-	1/6/6/17	-
6	OLA	A	1220	-	-	7/10/10/17	-
3	OLC	A	1202	-	-	5/16/16/24	-
6	OLA	A	1226	-	-	2/9/9/17	-
3	OLC	A	1206	-	-	4/16/16/24	-
4	CLR	A	1213	-	-	1/10/68/68	0/4/4/4
6	OLA	A	1221	-	-	4/9/9/17	-
3	OLC	A	1203	-	-	2/15/15/24	-
3	OLC	A	1210	-	-	11/16/16/24	-
4	CLR	A	1212	-	-	2/10/68/68	0/4/4/4
3	OLC	A	1207	-	-	1/10/10/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1211	CLR	C10-C9	-2.04	1.52	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1206	OLC	O20-C1-C2	3.30	121.89	111.83
3	A	1210	OLC	O20-C1-C2	3.16	121.46	111.83
3	A	1205	OLC	O20-C1-C2	3.10	121.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1203	OLC	O20-C1-C2	2.99	120.95	111.83
3	A	1209	OLC	O20-C1-C2	2.84	120.51	111.83
2	A	1201	ZMA	N15-C14-N16	2.76	121.78	118.32
3	A	1204	OLC	O20-C1-C2	2.73	120.15	111.83
3	A	1207	OLC	O20-C1-C2	2.70	120.06	111.83
3	A	1208	OLC	O20-C1-C2	2.69	120.03	111.83
3	A	1202	OLC	O20-C1-C2	2.68	120.01	111.83
6	A	1227	OLA	C3-C2-C1	-2.49	108.01	114.51
4	A	1213	CLR	C4-C5-C6	-2.46	117.23	120.57
4	A	1213	CLR	C4-C5-C10	2.44	119.54	116.42
4	A	1212	CLR	C4-C5-C10	2.16	119.19	116.42
3	A	1206	OLC	O20-C1-O19	-2.16	118.22	123.63
4	A	1211	CLR	C4-C5-C10	2.11	119.12	116.42
3	A	1210	OLC	O20-C1-O19	-2.05	118.50	123.63

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	OLC	C21-C22-C24-O25
3	A	1205	OLC	O20-C21-C22-O23
3	A	1204	OLC	C2-C1-O20-C21
3	A	1204	OLC	O19-C1-O20-C21
3	A	1206	OLC	O20-C21-C22-C24
3	A	1210	OLC	C1-C2-C3-C4
6	A	1222	OLA	C1-C2-C3-C4
6	A	1226	OLA	C1-C2-C3-C4
3	A	1209	OLC	C2-C1-O20-C21
3	A	1210	OLC	O20-C21-C22-O23
6	A	1217	OLA	C1-C2-C3-C4
3	A	1210	OLC	O20-C21-C22-C24
3	A	1206	OLC	O20-C21-C22-O23
3	A	1208	OLC	C21-C22-C24-O25
3	A	1209	OLC	O19-C1-O20-C21
3	A	1202	OLC	O23-C22-C24-O25
6	A	1220	OLA	C4-C5-C6-C7
6	A	1227	OLA	C11-C12-C13-C14
6	A	1220	OLA	C5-C6-C7-C8
6	A	1227	OLA	C6-C7-C8-C9
3	A	1203	OLC	C5-C6-C7-C8
3	A	1210	OLC	C2-C3-C4-C5
3	A	1210	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
6	A	1225	OLA	C12-C13-C14-C15
6	A	1225	OLA	C10-C11-C12-C13
3	A	1202	OLC	C2-C1-O20-C21
3	A	1206	OLC	C6-C7-C8-C9
6	A	1218	OLA	C4-C5-C6-C7
3	A	1202	OLC	O19-C1-O20-C21
3	A	1210	OLC	O19-C1-O20-C21
3	A	1207	OLC	O20-C21-C22-O23
3	A	1210	OLC	C6-C7-C8-C9
6	A	1220	OLA	C2-C3-C4-C5
6	A	1227	OLA	C2-C3-C4-C5
6	A	1224	OLA	C2-C3-C4-C5
6	A	1225	OLA	C5-C6-C7-C8
6	A	1217	OLA	C4-C5-C6-C7
3	A	1210	OLC	O23-C22-C24-O25
6	A	1217	OLA	C2-C3-C4-C5
6	A	1221	OLA	C1-C2-C3-C4
6	A	1216	OLA	C1-C2-C3-C4
6	A	1215	OLA	C6-C7-C8-C9
3	A	1203	OLC	C6-C7-C8-C9
6	A	1221	OLA	C4-C5-C6-C7
4	A	1213	CLR	C22-C23-C24-C25
6	A	1215	OLA	C4-C5-C6-C7
6	A	1225	OLA	C4-C5-C6-C7
6	A	1215	OLA	C1-C2-C3-C4
3	A	1209	OLC	O23-C22-C24-O25
6	A	1220	OLA	C6-C7-C8-C9
6	A	1223	OLA	C10-C11-C12-C13
6	A	1227	OLA	C5-C6-C7-C8
3	A	1205	OLC	O20-C21-C22-C24
3	A	1210	OLC	C5-C6-C7-C8
6	A	1225	OLA	C2-C3-C4-C5
6	A	1219	OLA	C3-C4-C5-C6
3	A	1205	OLC	C7-C8-C9-C10
3	A	1210	OLC	C3-C4-C5-C6
6	A	1222	OLA	C4-C5-C6-C7
6	A	1220	OLA	O1-C1-C2-C3
6	A	1219	OLA	O2-C1-C2-C3
6	A	1221	OLA	O1-C1-C2-C3
6	A	1219	OLA	O1-C1-C2-C3
6	A	1221	OLA	O2-C1-C2-C3
3	A	1204	OLC	C2-C3-C4-C5

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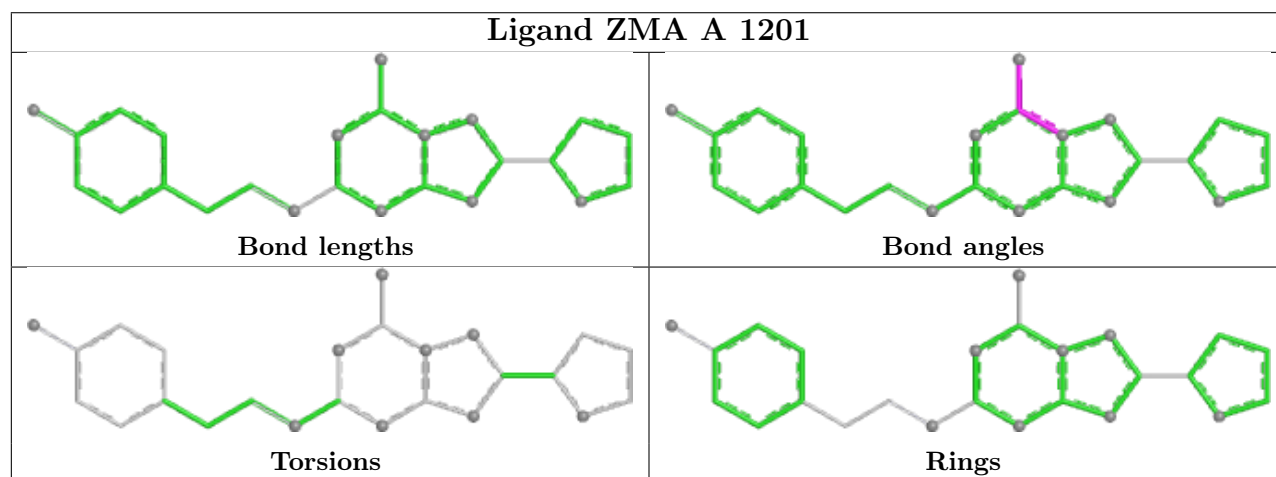
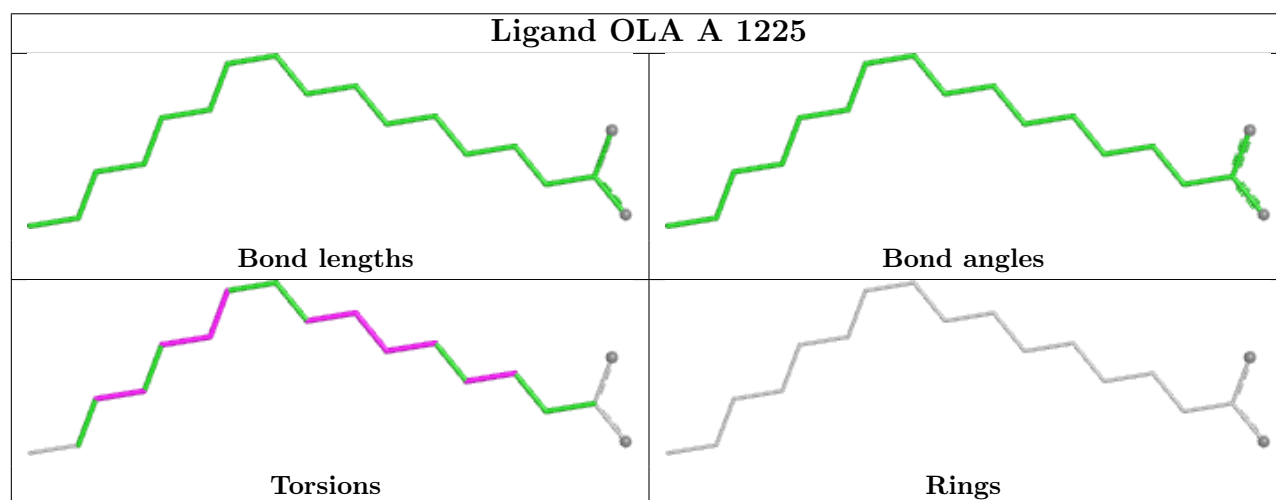
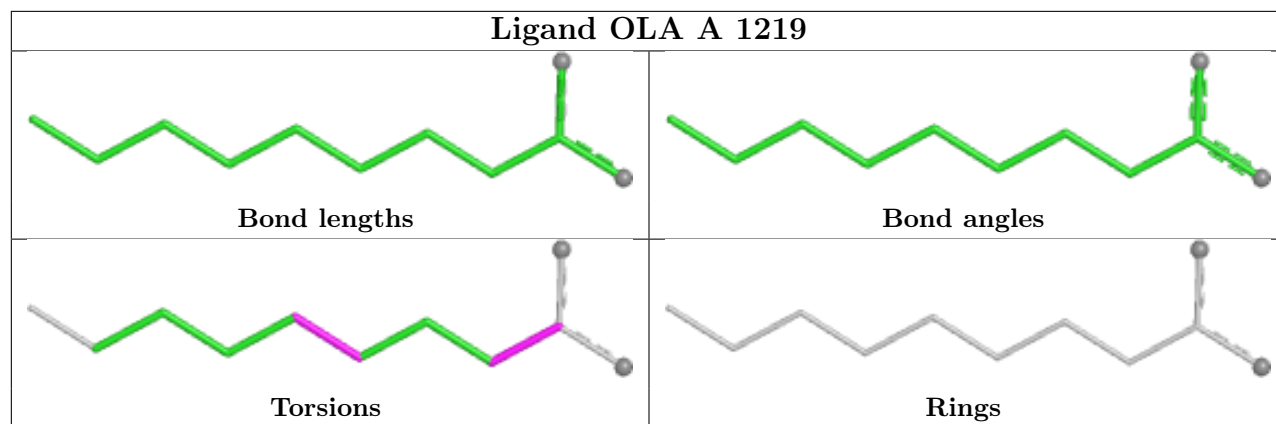
Mol	Chain	Res	Type	Atoms
3	A	1208	OLC	O23-C22-C24-O25
3	A	1205	OLC	C1-C2-C3-C4
4	A	1212	CLR	C23-C24-C25-C27
3	A	1206	OLC	C7-C8-C9-C10
3	A	1210	OLC	C7-C8-C9-C10
6	A	1220	OLA	O2-C1-C2-C3
6	A	1227	OLA	C1-C2-C3-C4
3	A	1204	OLC	C7-C8-C9-C10
6	A	1225	OLA	C9-C10-C11-C12
3	A	1208	OLC	O19-C1-O20-C21
6	A	1222	OLA	O1-C1-C2-C3
4	A	1211	CLR	C22-C23-C24-C25
6	A	1222	OLA	O2-C1-C2-C3
6	A	1215	OLA	C9-C10-C11-C12
6	A	1227	OLA	C9-C10-C11-C12
3	A	1208	OLC	C2-C1-O20-C21
6	A	1220	OLA	C7-C8-C9-C10
6	A	1227	OLA	C4-C5-C6-C7
4	A	1212	CLR	C23-C24-C25-C26
6	A	1226	OLA	C5-C6-C7-C8
3	A	1208	OLC	O20-C21-C22-O23
3	A	1202	OLC	C7-C8-C9-C10
6	A	1225	OLA	C6-C7-C8-C9

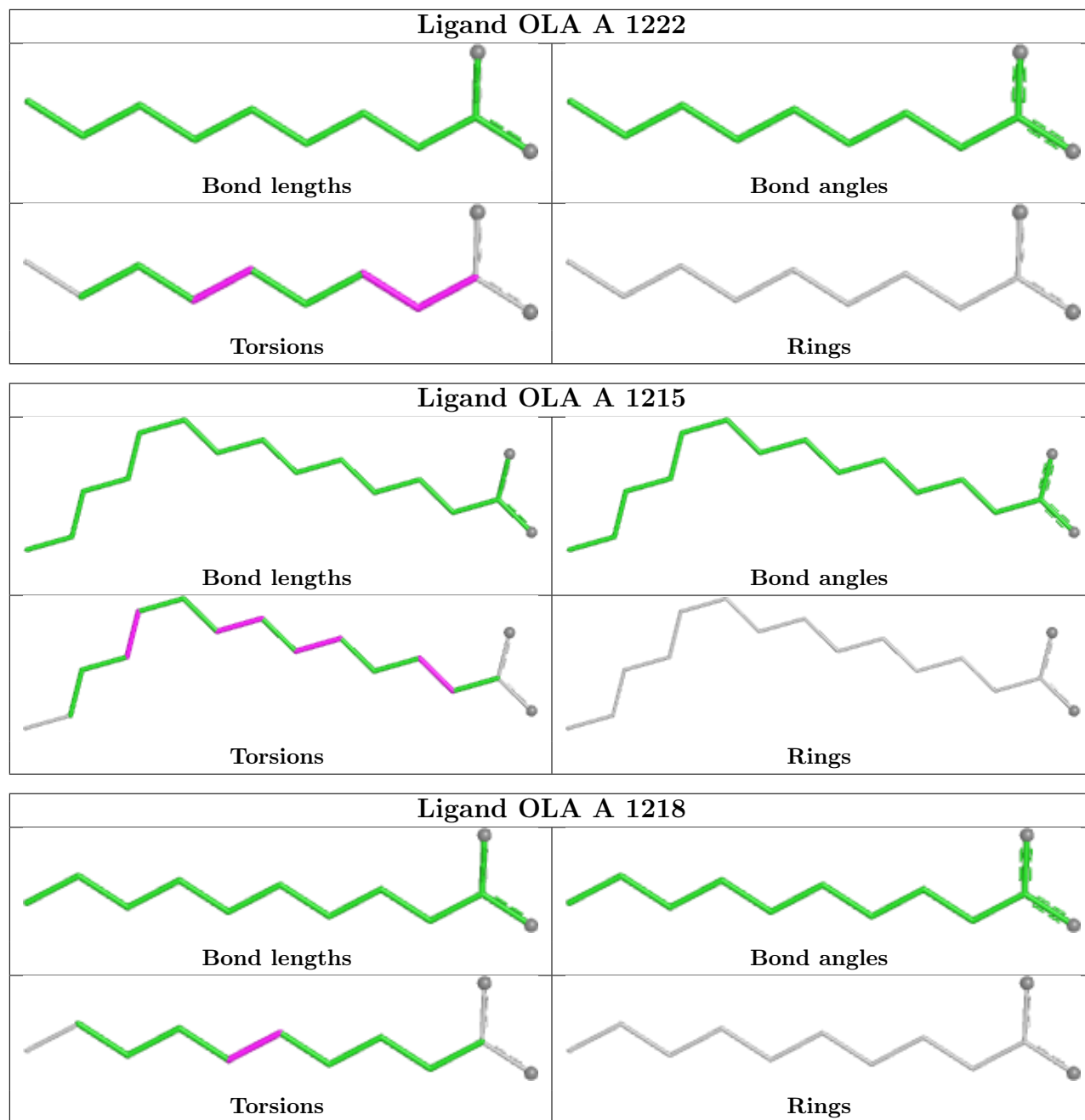
There are no ring outliers.

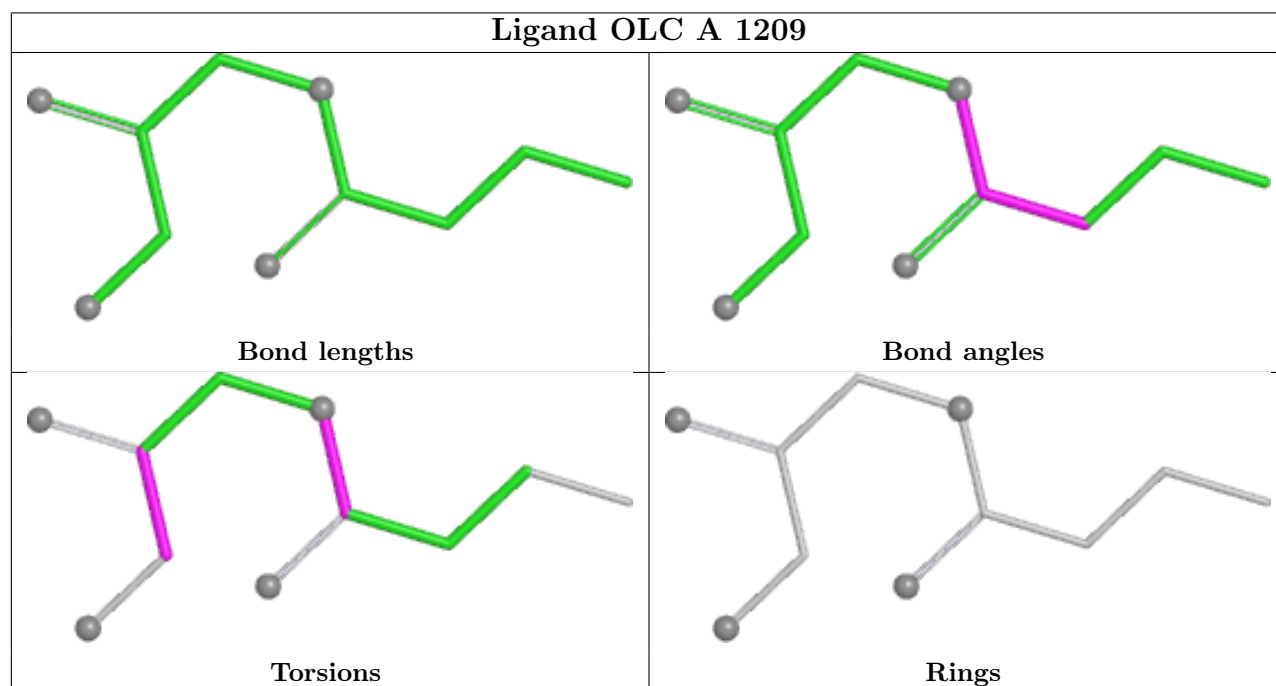
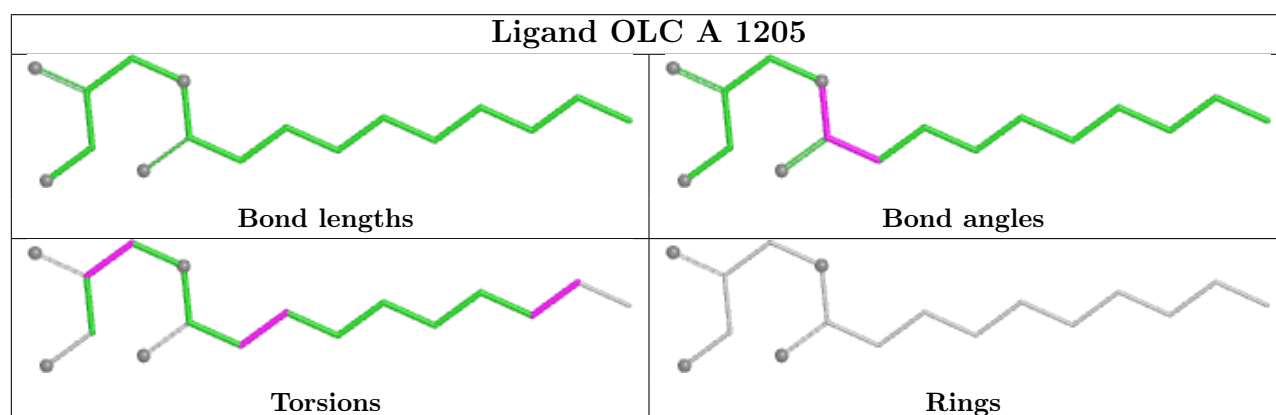
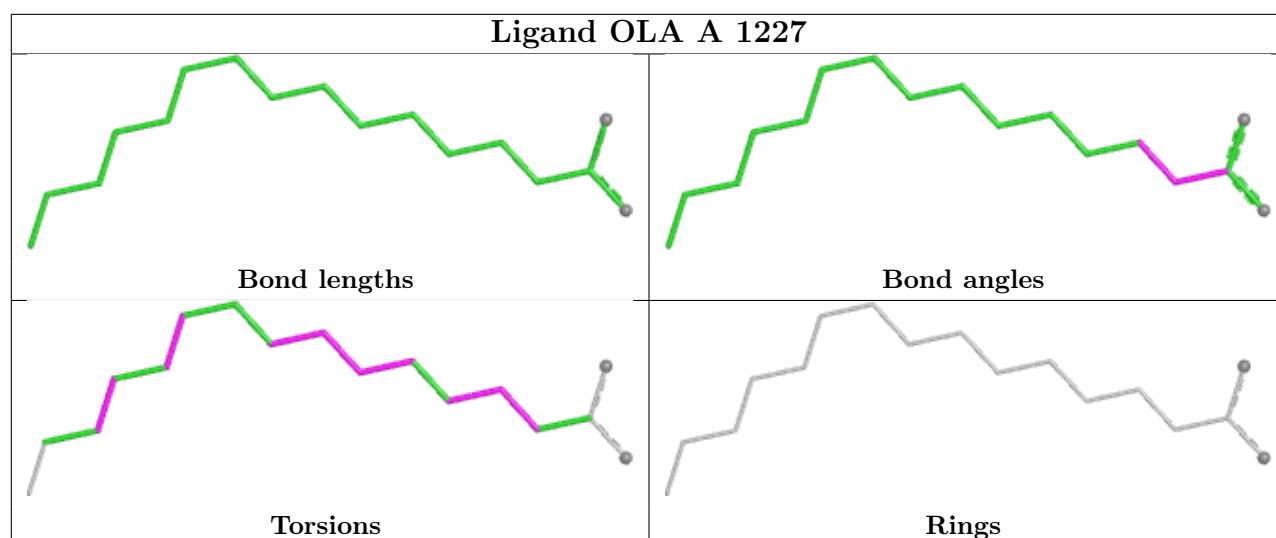
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	OLC	1	0

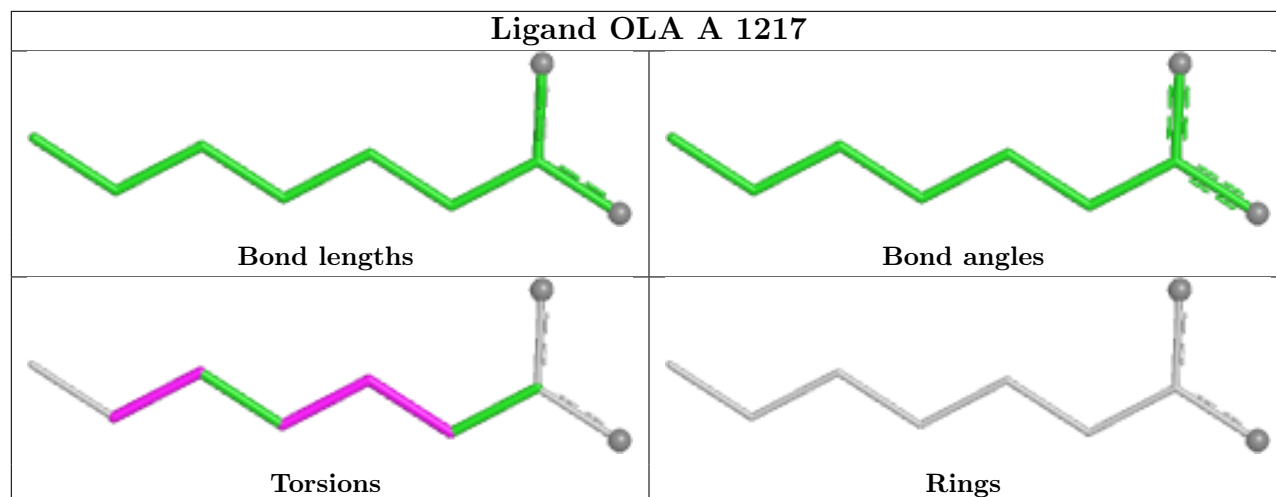
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



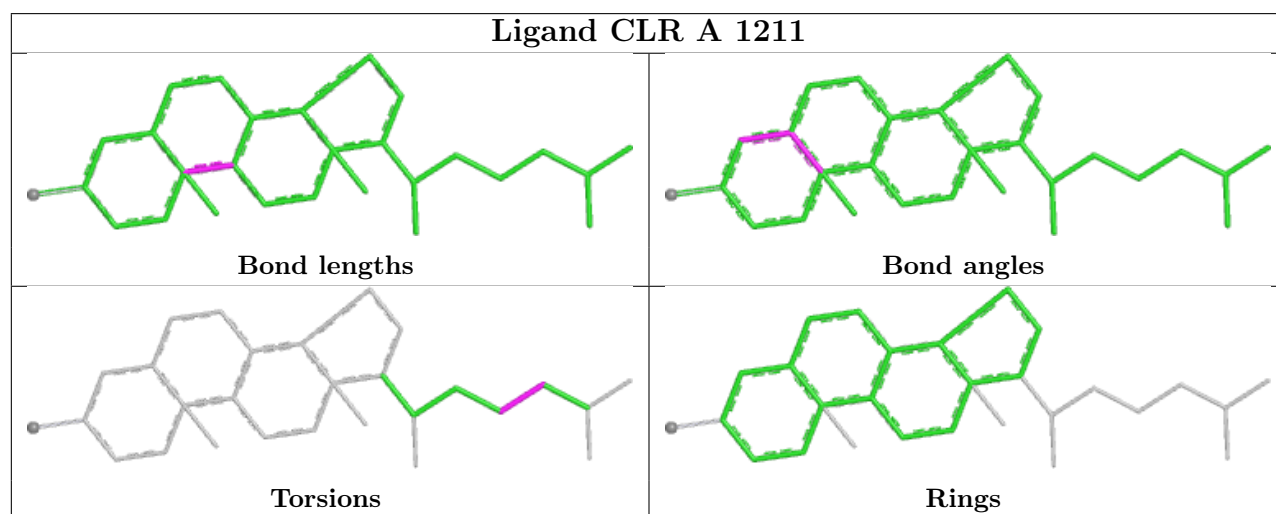




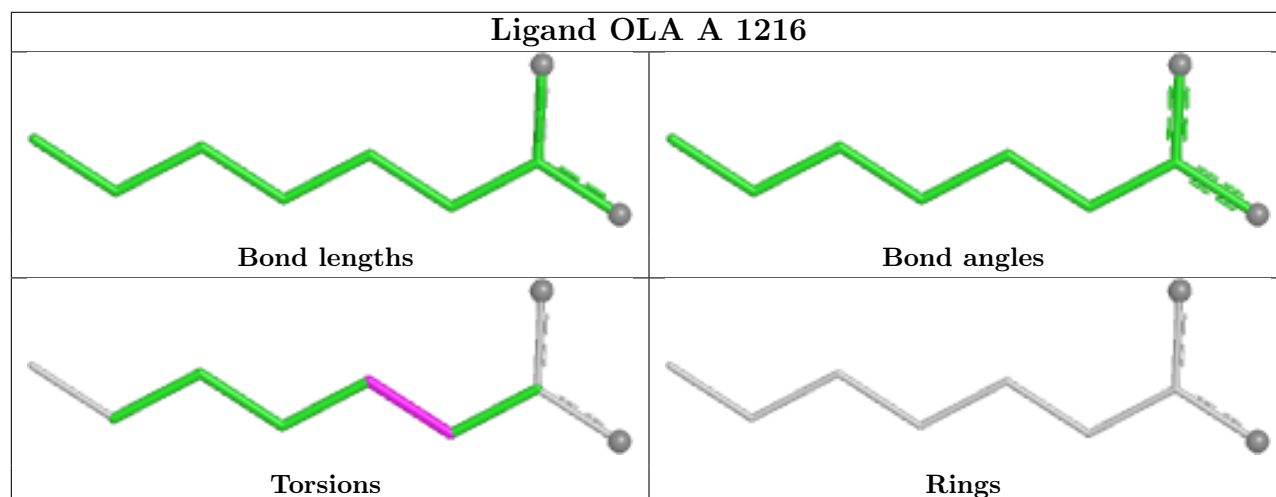
Ligand OLA A 1217

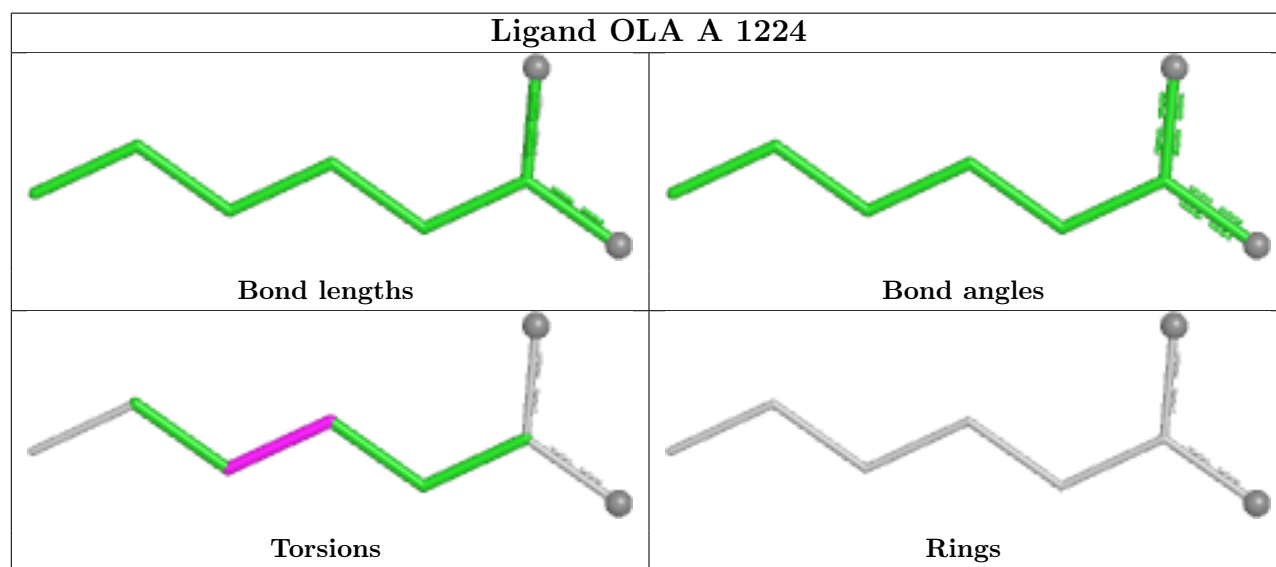
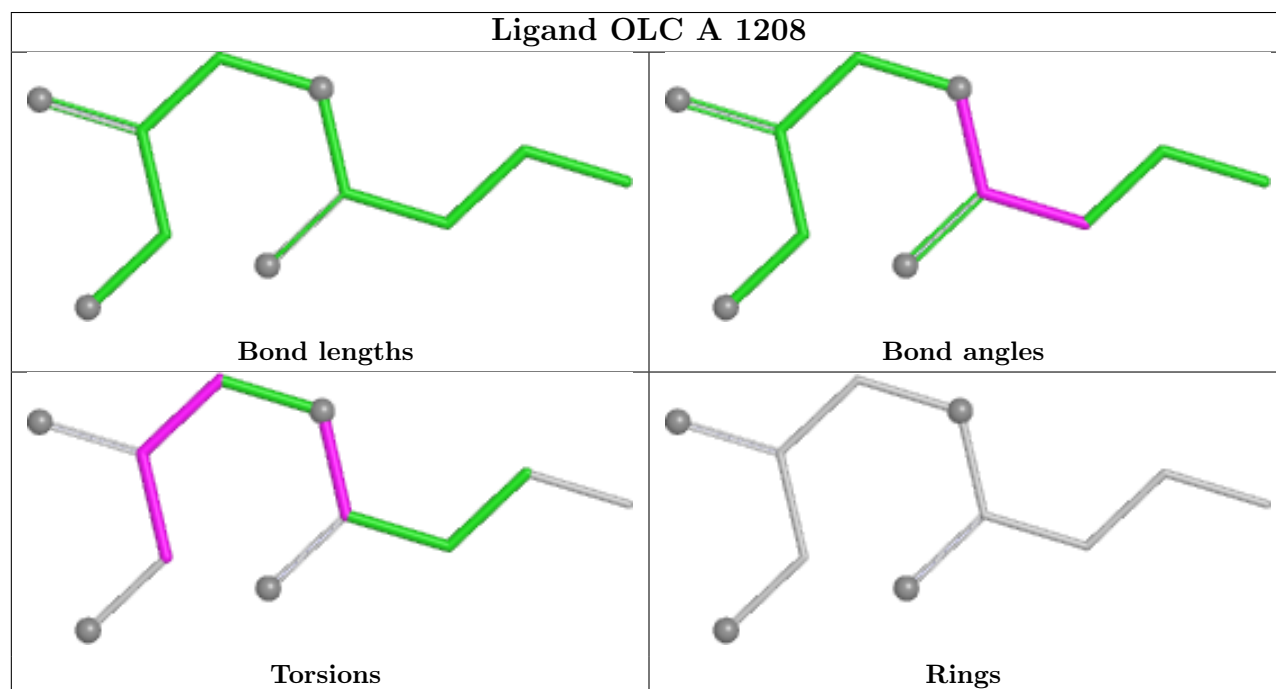
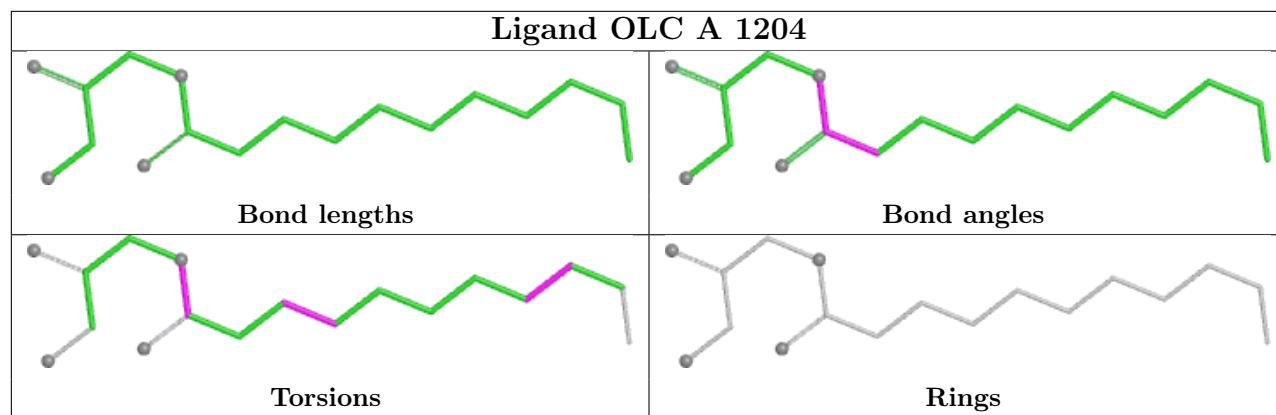


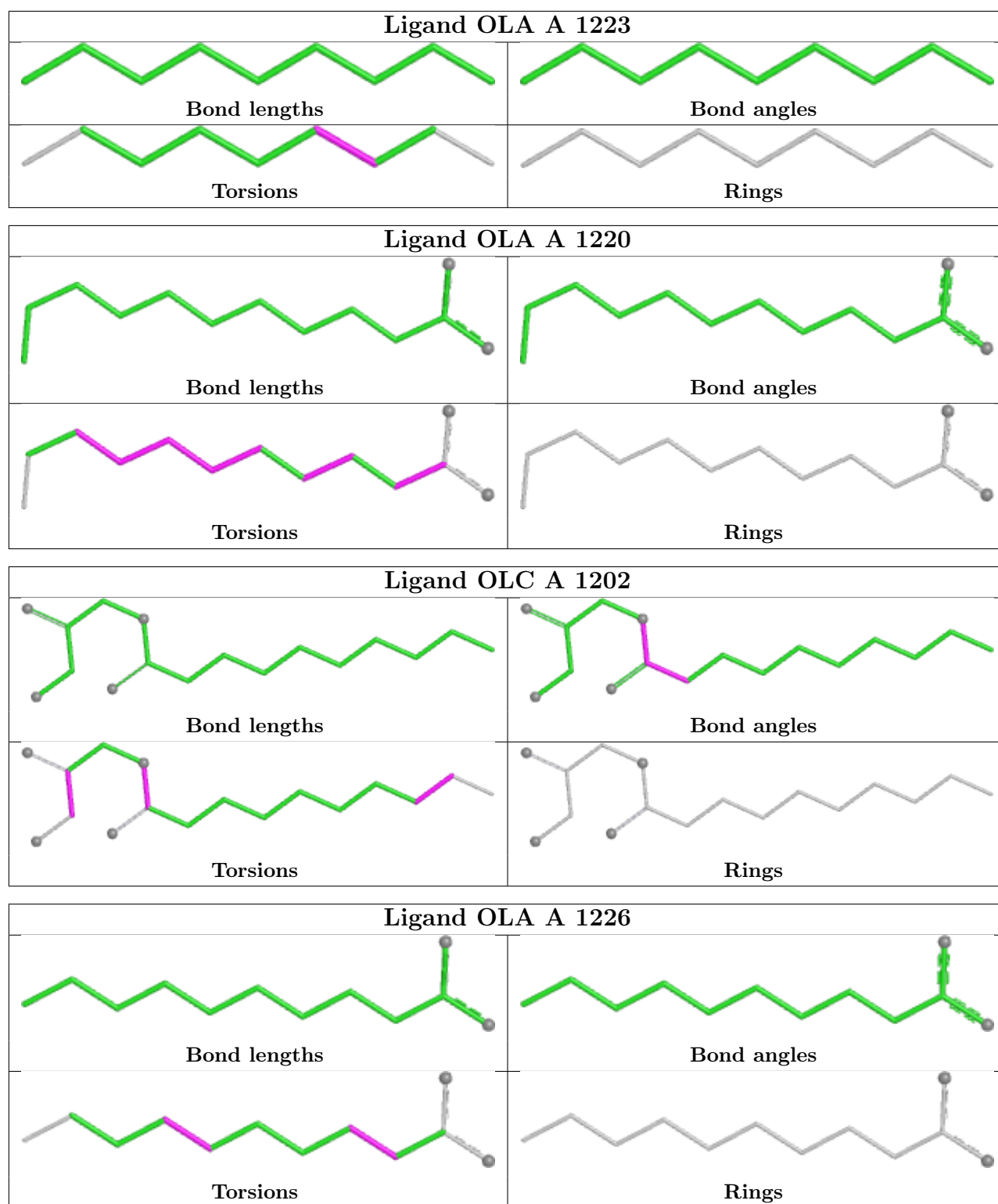
Ligand CLR A 1211

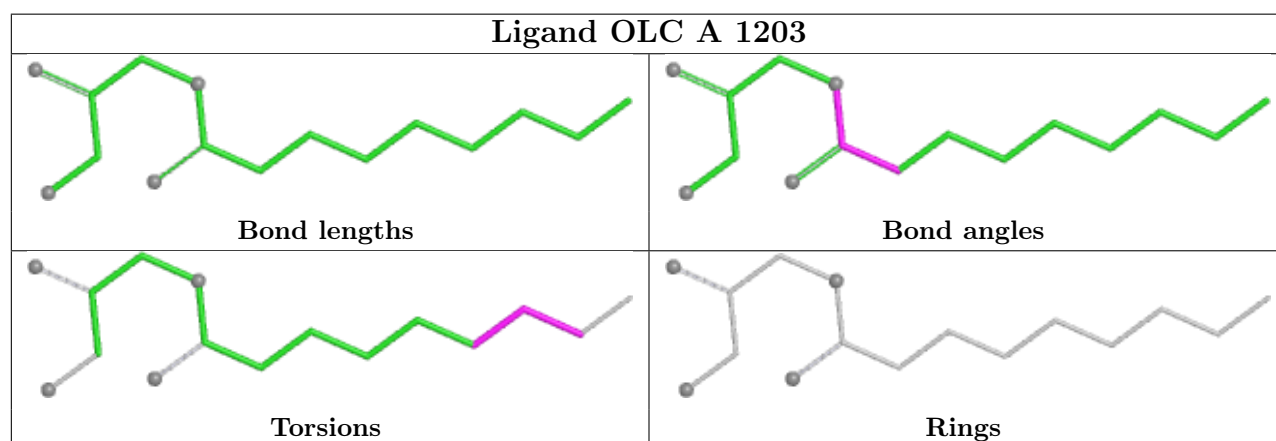
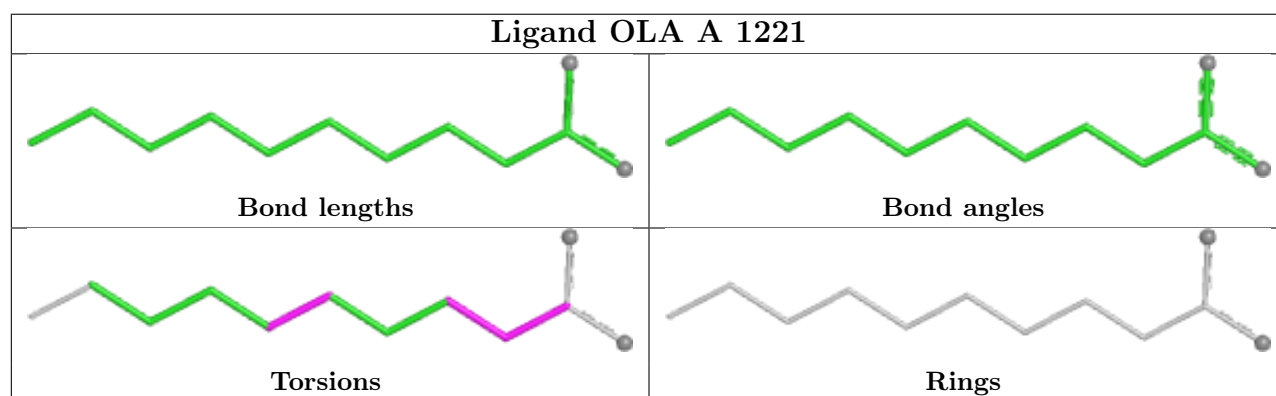
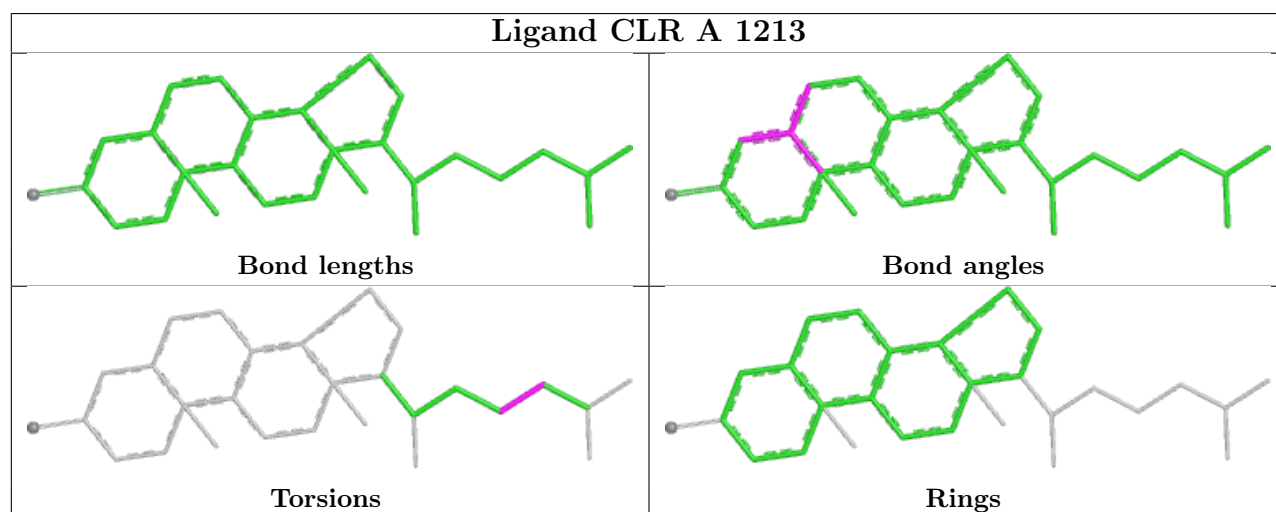
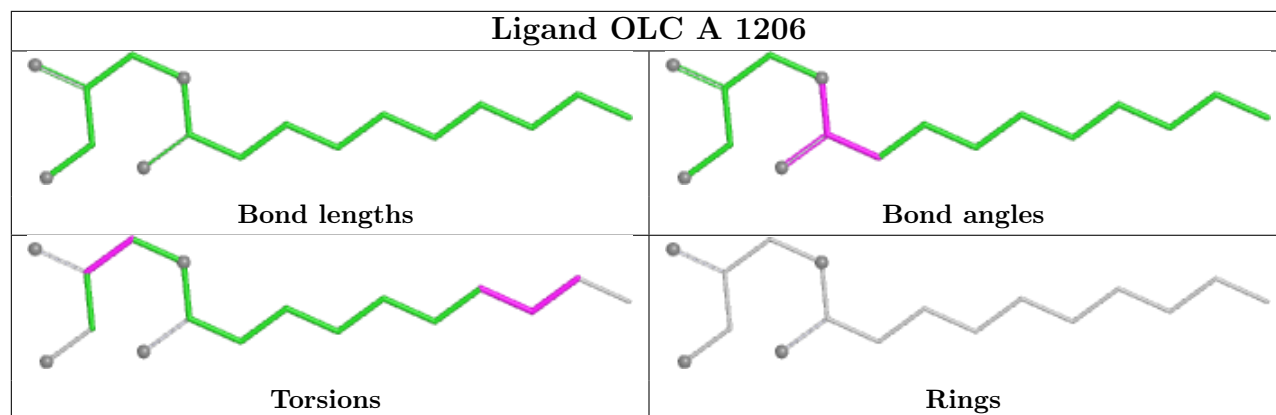


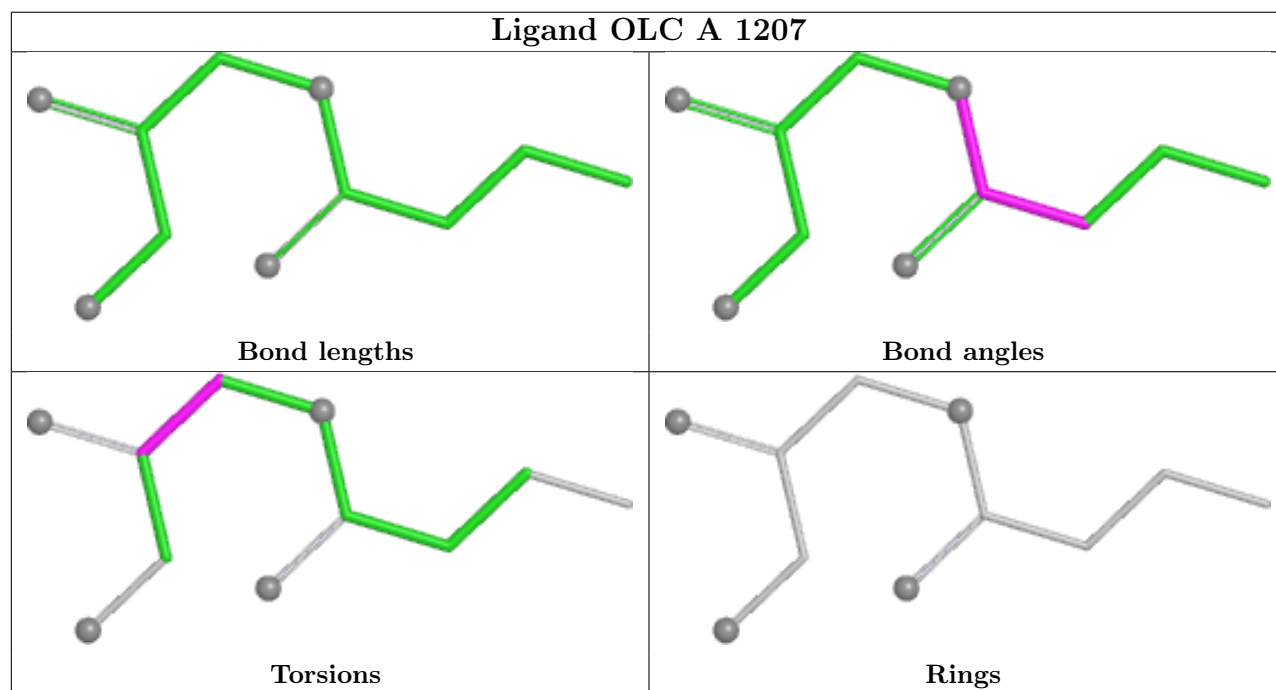
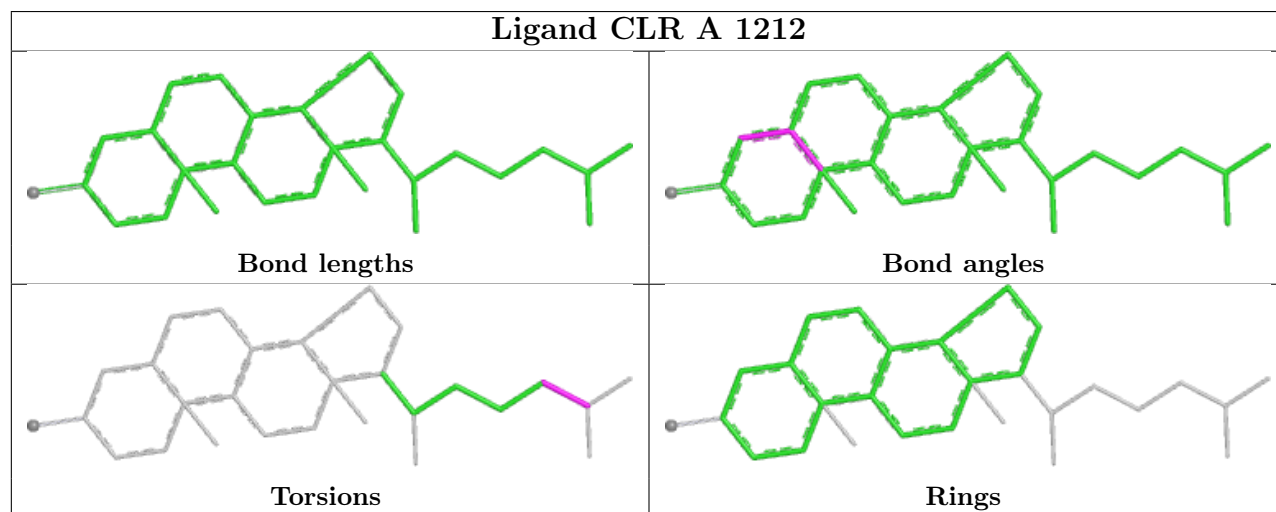
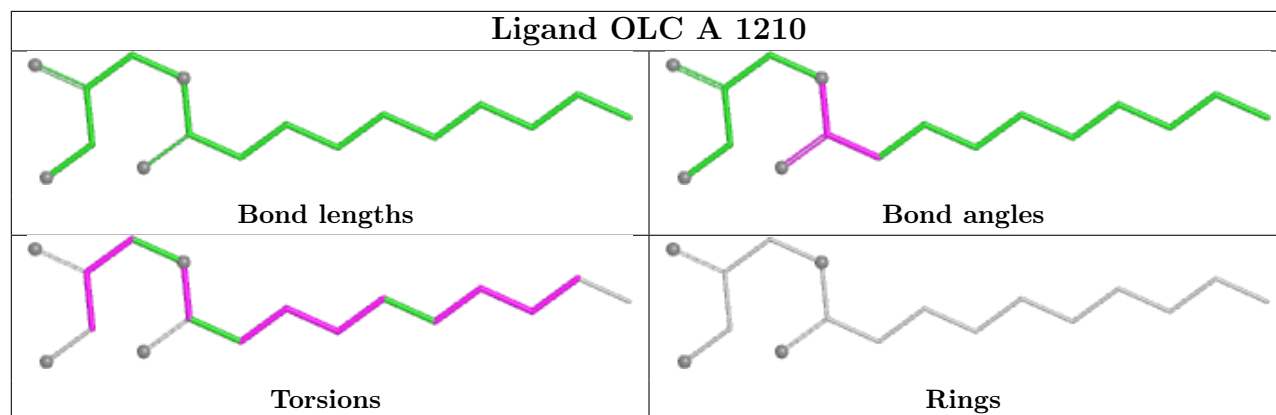
Ligand OLA A 1216











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	392/442 (88%)	0.59	42 (10%)	11 10	13, 36, 99, 128	20 (5%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1106[A]	LEU	5.4
1	A	1105[A]	TYR	4.6
1	A	1078	LEU	4.2
1	A	-2	ASP	3.9
1	A	1067	ILE	3.8
1	A	29	TRP	3.6
1	A	-1	GLY	3.3
1	A	0	ALA	3.3
1	A	308	LEU	3.3
1	A	307	VAL	3.1
1	A	1065	PHE	3.0
1	A	1023	ALA	2.9
1	A	1061	PHE	2.8
1	A	157	GLN	2.7
1	A	1026	VAL	2.7
1	A	1084	VAL	2.7
1	A	1064	GLY	2.7
1	A	1063	HIS	2.7
1	A	43	TYR	2.7
1	A	1040	ALA	2.6
1	A	151	GLU	2.5
1	A	1068	LEU	2.5
1	A	1076	LEU	2.3
1	A	290	TYR	2.3
1	A	111	ARG	2.3
1	A	202	LEU	2.2
1	A	1101	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1021	ASP	2.2
1	A	1043	ALA	2.2
1	A	1100	ALA	2.2
1	A	205[A]	ARG	2.2
1	A	1075	ALA	2.1
1	A	1080	ASN	2.1
1	A	287[A]	ILE	2.1
1	A	1062	ARG	2.1
1	A	1082	GLY	2.1
1	A	1030	LEU	2.1
1	A	1038	LEU	2.1
1	A	154[A]	ASN	2.0
1	A	1010	LEU	2.0
1	A	1014	LEU	2.0
1	A	1083	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLC	A	1210	17/25	0.71	0.25	77,117,146,149	0
6	OLA	A	1220	13/20	0.73	0.17	72,77,103,104	0
6	OLA	A	1222	11/20	0.73	0.19	85,88,95,99	0
5	OLB	A	1214	17/25	0.74	0.24	69,81,99,100	0
6	OLA	A	1217	9/20	0.76	0.20	67,70,92,93	0
6	OLA	A	1223	9/20	0.77	0.19	73,76,80,81	0
3	OLC	A	1207	11/25	0.78	0.17	81,87,93,93	0
6	OLA	A	1225	18/20	0.78	0.17	74,77,83,83	0

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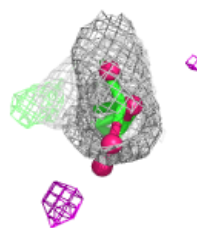
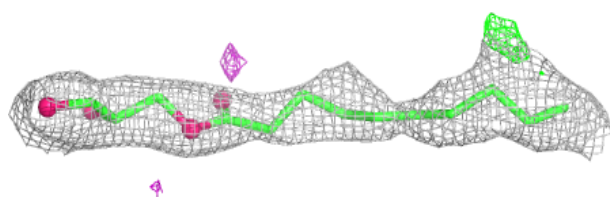
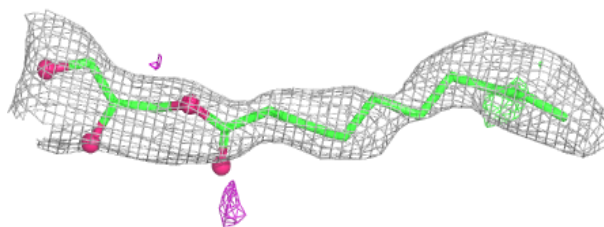
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLC	A	1209	11/25	0.80	0.19	69,84,95,105	0
3	OLC	A	1208	11/25	0.80	0.13	78,80,85,85	0
6	OLA	A	1218	12/20	0.81	0.16	70,77,84,84	0
6	OLA	A	1221	12/20	0.82	0.16	64,74,102,110	0
6	OLA	A	1224	8/20	0.83	0.17	72,74,77,81	0
3	OLC	A	1203	16/25	0.83	0.20	58,70,85,88	0
6	OLA	A	1226	12/20	0.85	0.16	56,63,74,78	0
3	OLC	A	1204	18/25	0.86	0.17	64,75,88,93	0
3	OLC	A	1206	17/25	0.86	0.15	50,60,82,86	0
3	OLC	A	1202	17/25	0.87	0.15	58,75,88,92	0
6	OLA	A	1219	11/20	0.88	0.18	46,62,92,94	0
6	OLA	A	1215	16/20	0.88	0.17	57,75,108,111	0
6	OLA	A	1227	17/20	0.88	0.23	55,63,151,152	0
6	OLA	A	1216	9/20	0.89	0.16	56,64,71,76	0
3	OLC	A	1205	17/25	0.89	0.15	61,71,78,84	0
4	CLR	A	1212	28/28	0.92	0.11	41,46,64,69	0
4	CLR	A	1213	28/28	0.94	0.10	38,47,78,82	0
4	CLR	A	1211	28/28	0.95	0.08	37,40,74,77	0
7	NA	A	1228	1/1	0.96	0.07	33,33,33,33	0
2	ZMA	A	1201	25/25	0.97	0.06	22,25,44,54	0

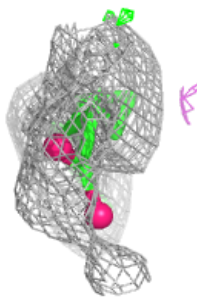
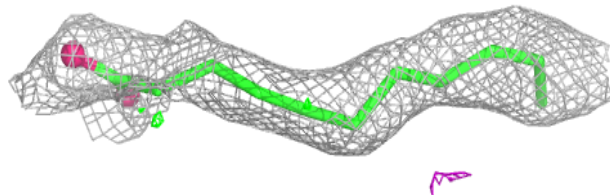
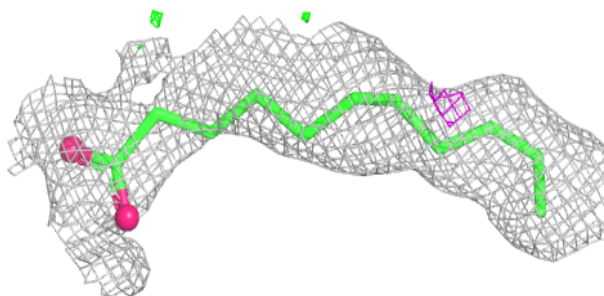
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 1210:

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

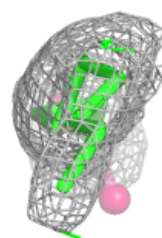
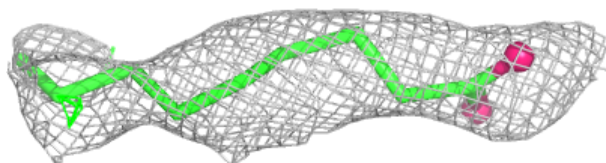
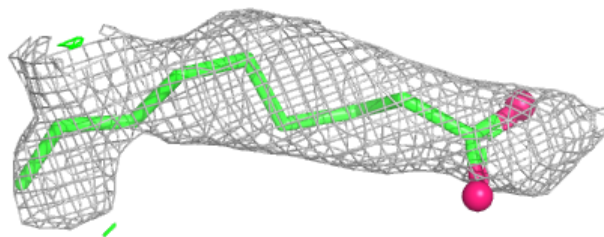
**Electron density around OLA A 1220:**

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

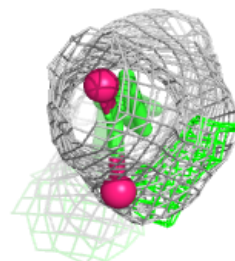
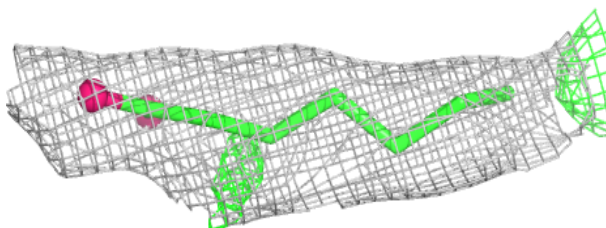
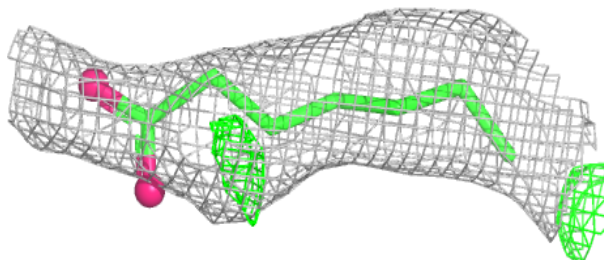


Electron density around OLA A 1222:

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

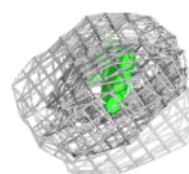
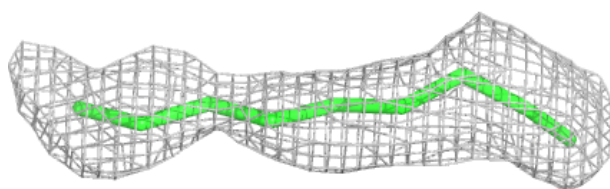
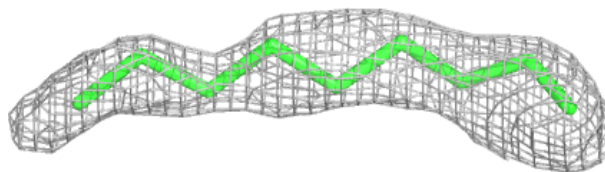
**Electron density around OLA A 1217:**

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

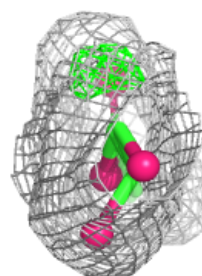
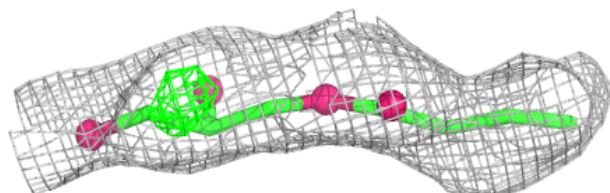
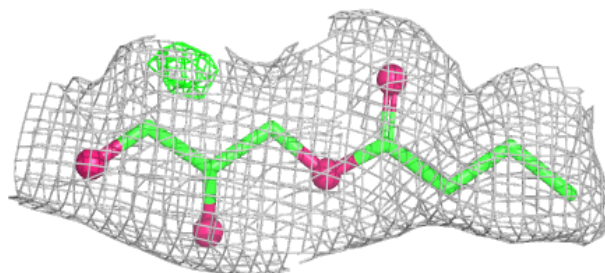


Electron density around OLA A 1223:

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

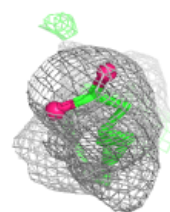
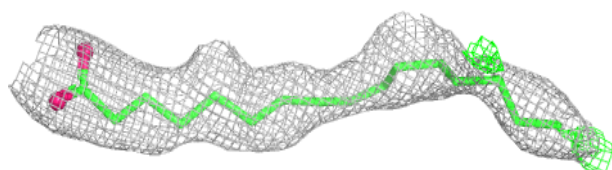
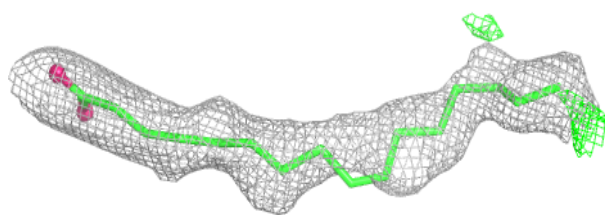
**Electron density around OLC A 1207:**

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

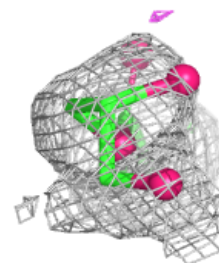
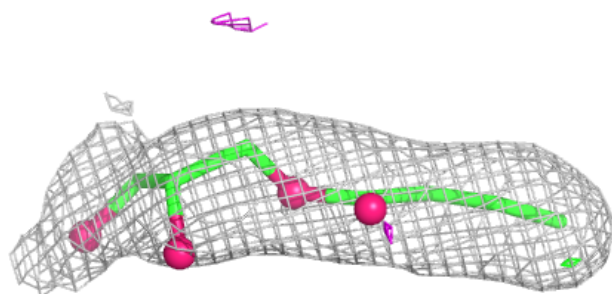
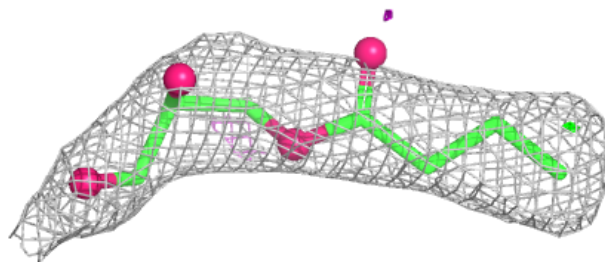


Electron density around OLA A 1225:

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

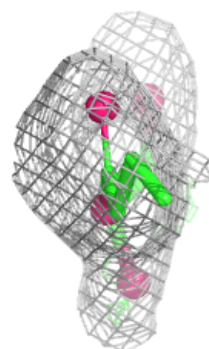
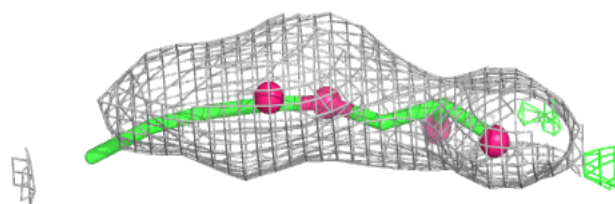
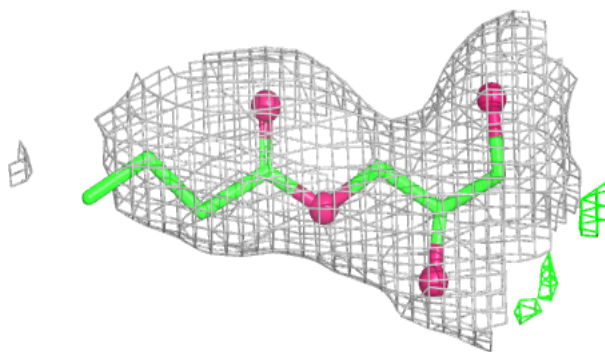
**Electron density around OLC A 1209:**

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

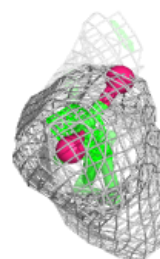
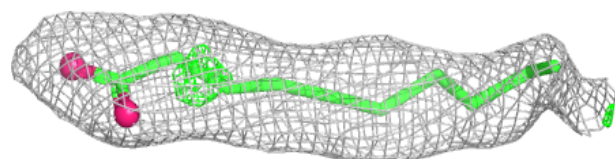
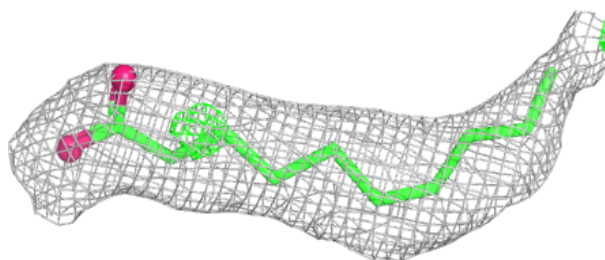


Electron density around OLC A 1208:

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

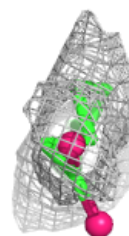
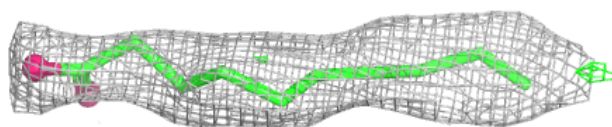
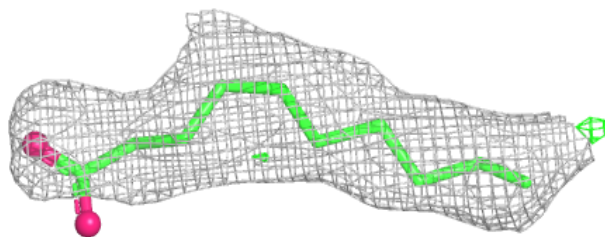
**Electron density around OLA A 1218:**

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

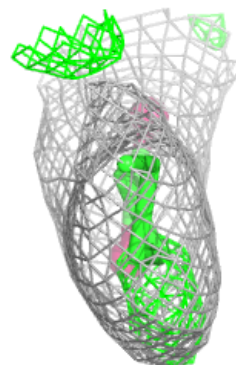
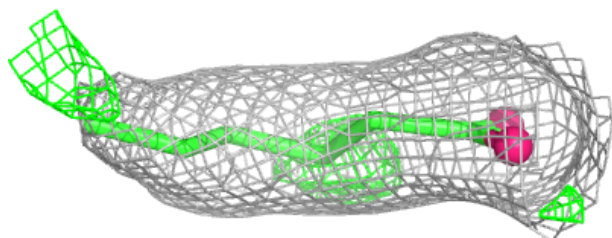
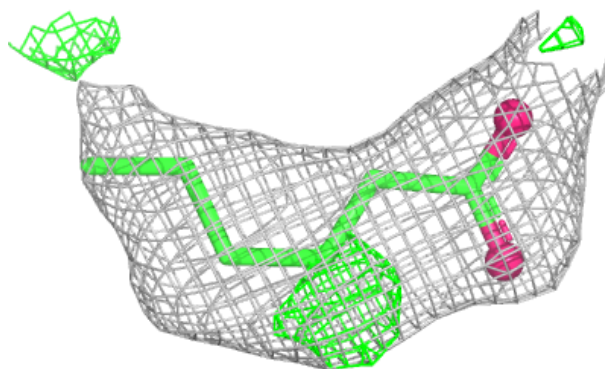


Electron density around OLA A 1221:

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

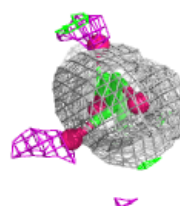
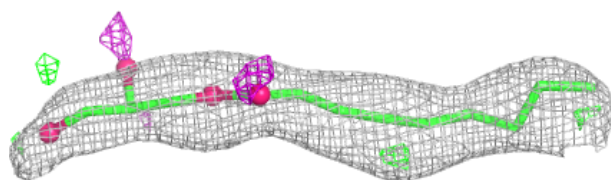
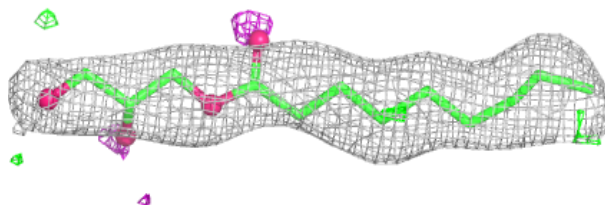
**Electron density around OLA A 1224:**

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

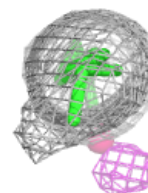
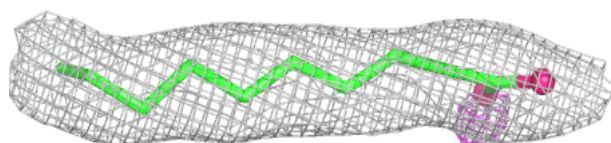
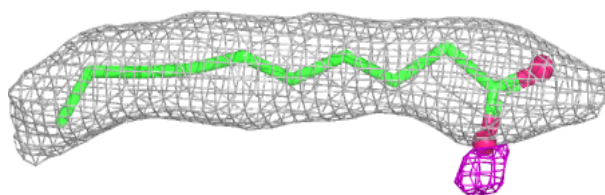


Electron density around OLC A 1203:

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

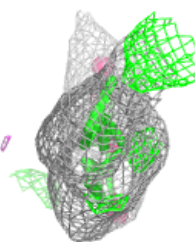
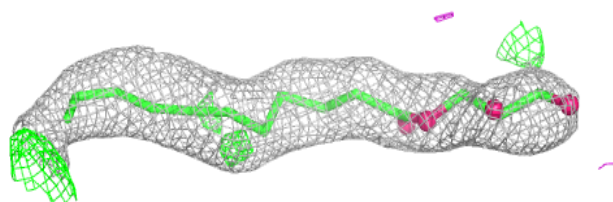
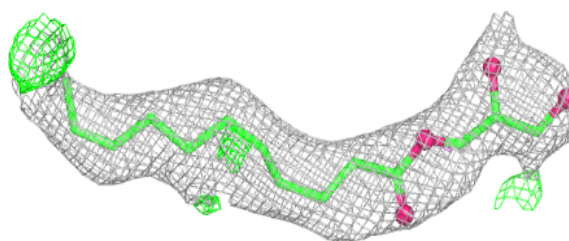
**Electron density around OLA A 1226:**

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

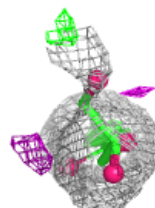
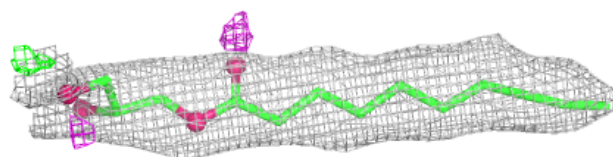
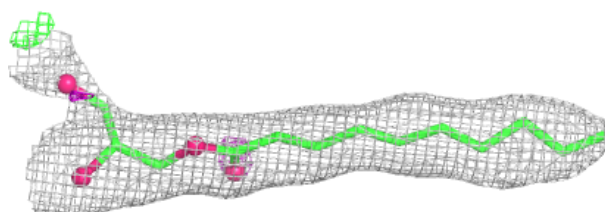


Electron density around OLC A 1204:

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

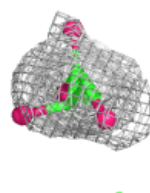
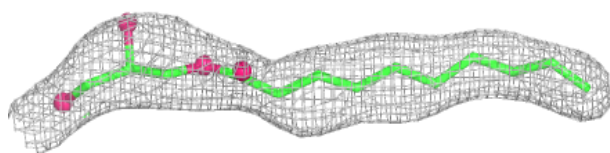
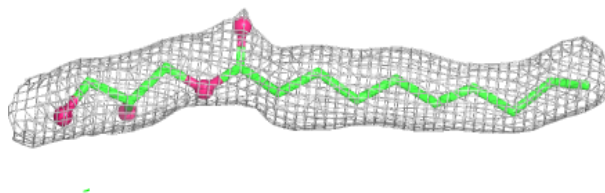
**Electron density around OLC A 1206:**

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

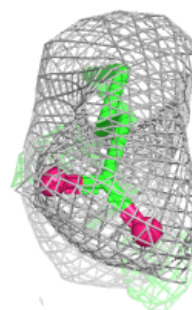
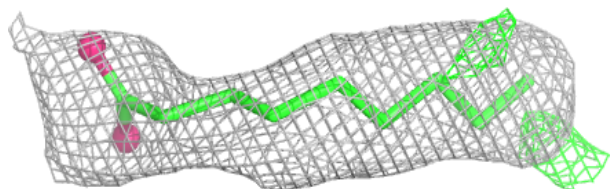
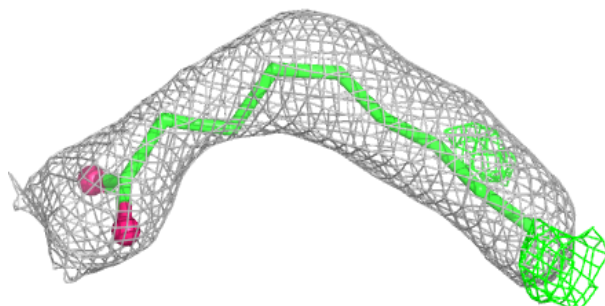


Electron density around OLC A 1202:

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

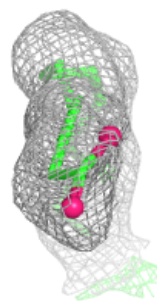
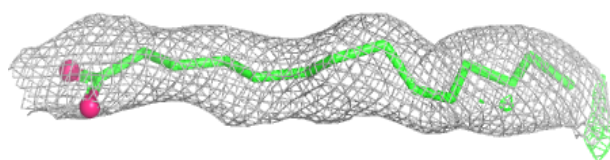
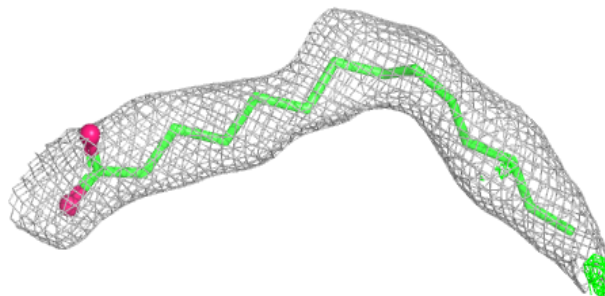
**Electron density around OLA A 1219:**

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

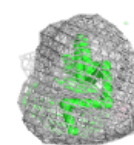
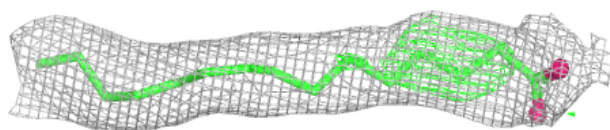
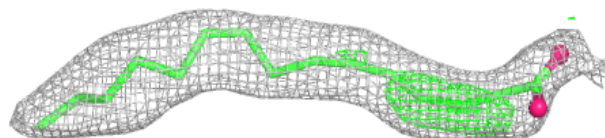


Electron density around OLA A 1215:

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

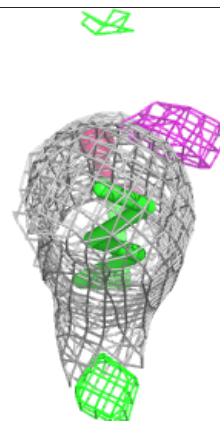
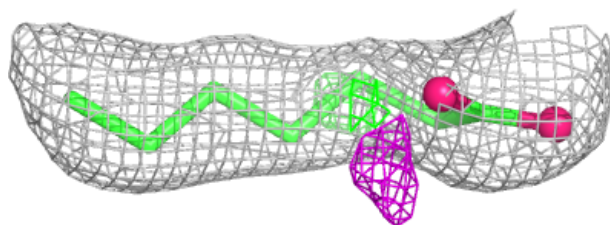
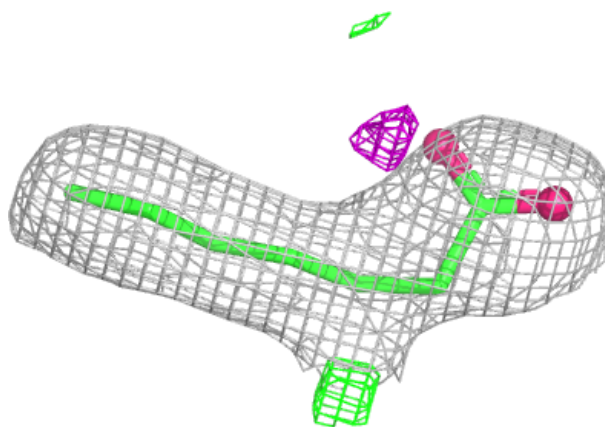
**Electron density around OLA A 1227:**

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

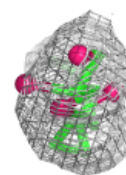
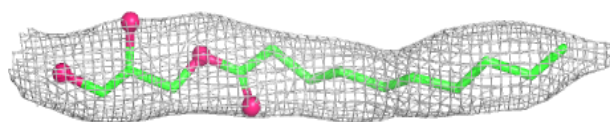
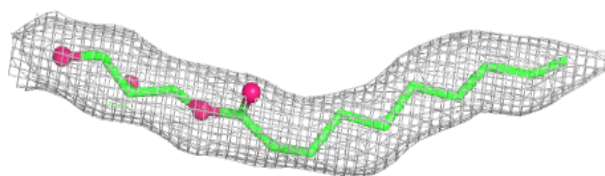


Electron density around OLA A 1216:

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

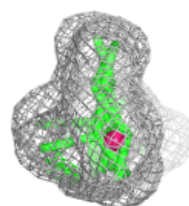
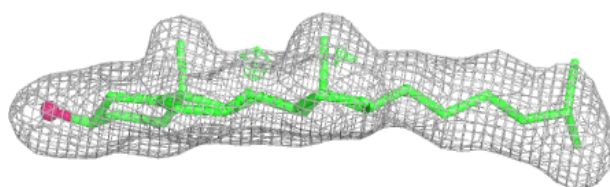
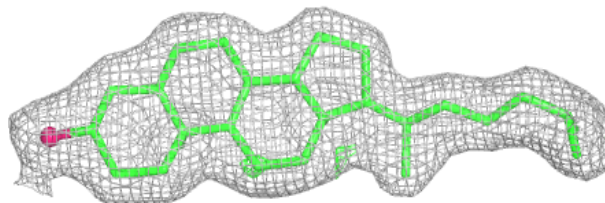
**Electron density around OLC A 1205:**

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

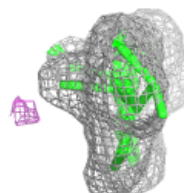
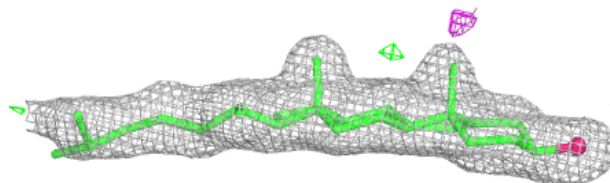
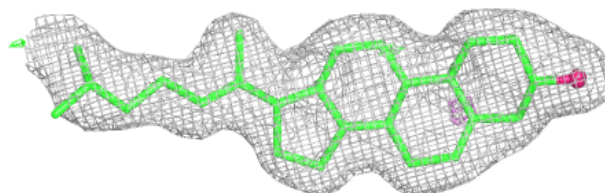


Electron density around CLR A 1212:

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

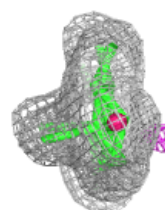
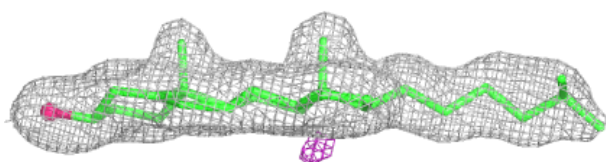
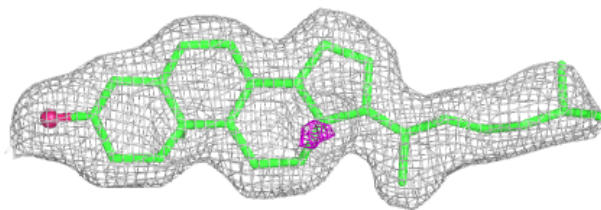
**Electron density around CLR A 1213:**

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

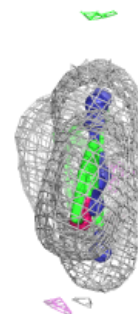
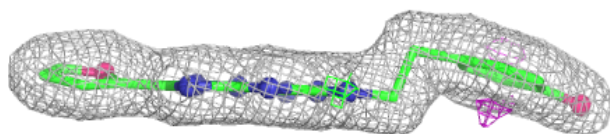
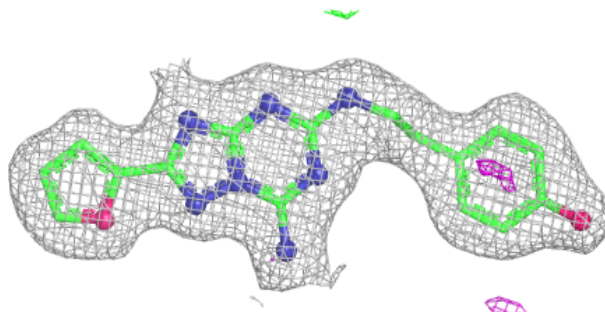


Electron density around CLR A 1211:

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

**Electron density around ZMA A 1201:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.