



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:07 PM UTC

PDB ID : 5OLH / pdb_00005olh
Title : Structure of the A2A-StaR2-bRIL562-Vipadenant complex at 2.6Å obtained from in meso soaking experiments.
Authors : Rucktooa, P.; Cheng, R.K.Y.; Segala, E.; Geng, T.; Errey, J.C.; Brown, G.A.; Cooke, R.; Marshall, F.H.; Dore, A.S.
Deposited on : 2017-07-27
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

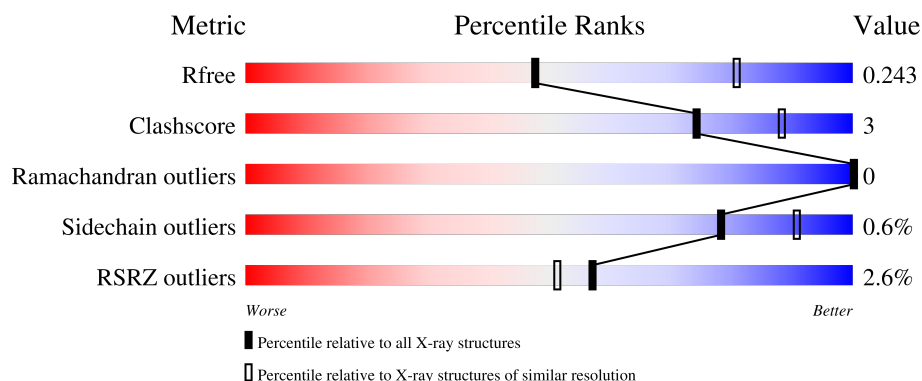
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

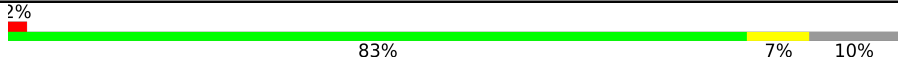
The reported resolution of this entry is 2.60 Å.

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	434	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3559 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	390	Total	C	N	O	S	0	3	0
			3047	1986	515	524	22			

There are 34 discrepancies between the modelled and reference sequences:

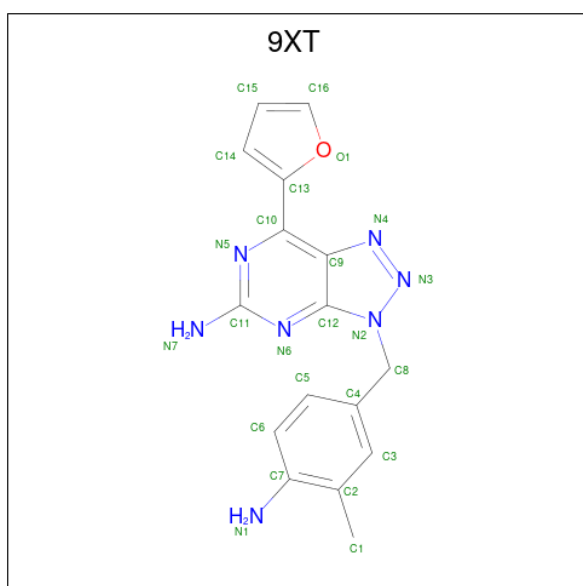
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
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	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	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	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274

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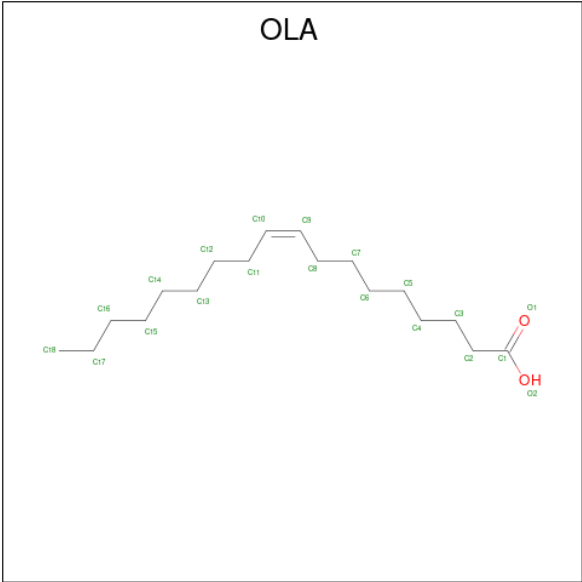
Chain	Residue	Modelled	Actual	Comment	Reference
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is 3-[(4-azanyl-3-methyl-phenyl)methyl]-7-(furan-2-yl)-[1,2,3]triazolo[4,5-d]pyrimidin-5-amine (CCD ID: 9XT) (formula: C₁₆H₁₅N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	16	7	1		

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 9 7 2	0	0
3	A	1	Total C O 18 16 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 12 10 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C O 19 17 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 13 13	0	0

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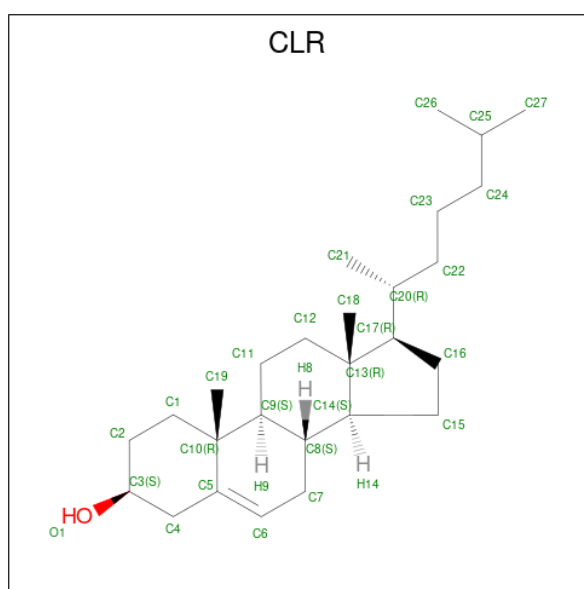
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

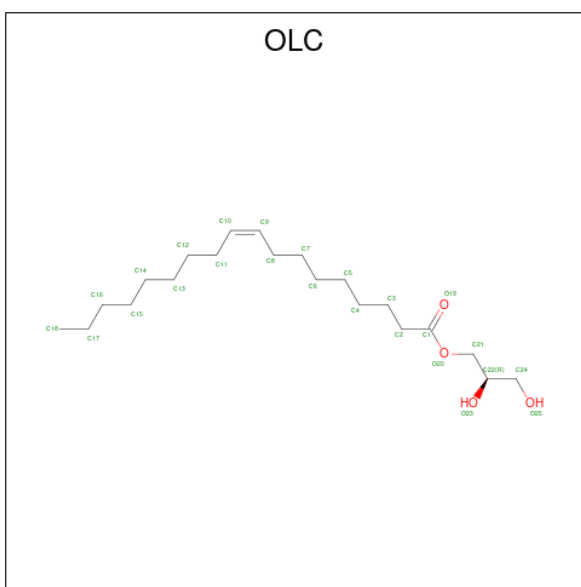
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Na		0	0
			1	1			

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	12	4		
6	A	1	Total	C	O	0	0
			17	13	4		
6	A	1	Total	C	O	0	0
			17	15	2		
6	A	1	Total	C	O	0	0
			20	18	2		
6	A	1	Total	C	O	0	0
			24	20	4		
6	A	1	Total	C	O	0	0
			22	18	4		
6	A	1	Total	C	O	0	0
			20	18	2		
6	A	1	Total	C	O	0	0
			20	18	2		

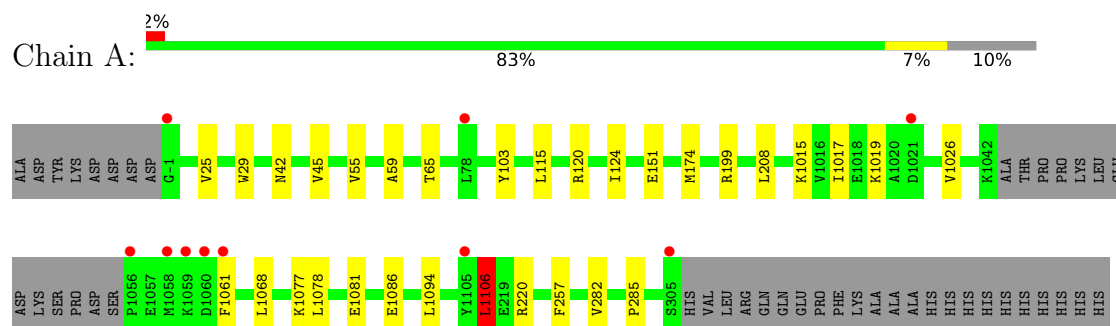
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	29	Total	O	0	1
			30	30		

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	39.40Å 179.33Å 141.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.60 29.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.82-2.60) 99.2 (29.82-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.12RC2_2821)	Depositor
R, R_{free}	0.200 , 0.249 0.194 , 0.243	Depositor DCC
R_{free} test set	815 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3559	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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, 9XT, OLC, OLA, NA

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	0.14	0/3114	0.32	3/4235 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LEU	CA-C-N	5.09	127.11	120.28
1	A	208	LEU	C-N-CA	5.09	127.11	120.28
1	A	1106	LEU	O-C-N	-5.02	116.34	122.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1106	LEU	Mainchain

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	3047	0	3112	18	0
2	A	24	0	0	0	0
3	A	217	0	329	6	0
4	A	1	0	0	0	0
5	A	84	0	138	1	0
6	A	156	0	232	4	0
7	A	30	0	0	0	0
All	All	3559	0	3811	23	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 3.

All (23) 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:25:VAL:HG22	3:A:1214:OLA:H132	1.75	0.68
6:A:1223:OLC:H17A	6:A:1227:OLC:H17	1.81	0.62
1:A:65:THR:HG23	6:A:1227:OLC:H4A	1.83	0.61
1:A:174:MET:HG3	1:A:257:PHE:HB2	1.85	0.58
1:A:29[A]:TRP:HZ3	3:A:1214:OLA:H62	1.74	0.52
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.93	0.51
6:A:1220:OLC:H7A	6:A:1221:OLC:H6	1.93	0.51
3:A:1202:OLA:H141	6:A:1224:OLC:H9	1.94	0.50
3:A:1208:OLA:H122	3:A:1217:OLA:H181	1.92	0.50
1:A:103:TYR:OH	1:A:199[B]:ARG:NH2	2.46	0.48
1:A:29[A]:TRP:HH2	3:A:1214:OLA:H22	1.79	0.47
1:A:1061:PHE:HZ	1:A:220:ARG:HE	1.62	0.46
1:A:42:ASN:HA	1:A:45:VAL:HB	1.99	0.44
1:A:282:VAL:O	1:A:285:PRO:HD2	2.18	0.43
1:A:1019:LYS:HB3	1:A:1019:LYS:HE2	1.79	0.43
1:A:1068:LEU:HD12	1:A:1094:LEU:HD22	2.00	0.43
1:A:115:LEU:O	1:A:120:ARG:NH2	2.50	0.43
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.00	0.42
1:A:124:ILE:HD13	3:A:1207:OLA:H31	2.01	0.42
1:A:1015:LYS:O	1:A:1019:LYS:HG2	2.20	0.41
1:A:1077:LYS:NZ	1:A:1081:GLU:OE2	2.47	0.41
5:A:1206:CLR:H232	5:A:1206:CLR:H211	1.68	0.41
1:A:1017:ILE:HG23	1:A:1026:VAL:HG13	2.01	0.41

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	389/434 (90%)	386 (99%)	3 (1%)	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	317/353 (90%)	315 (99%)	2 (1%)	78	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	1106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	75	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](#)

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	$\# Z > 2$
3	OLA	A	1215	-	13,13,19	1.00	1 (7%)	13,13,19	0.97	1 (7%)
3	OLA	A	1209	-	19,19,19	0.81	1 (5%)	19,19,19	0.90	1 (5%)
6	OLC	A	1221	-	16,16,24	1.14	1 (6%)	17,17,25	1.20	2 (11%)
6	OLC	A	1224	-	23,23,24	0.96	1 (4%)	24,24,25	0.97	1 (4%)
6	OLC	A	1223	-	19,19,24	1.04	1 (5%)	19,19,25	0.98	2 (10%)
3	OLA	A	1217	-	12,12,19	0.85	1 (8%)	11,11,19	0.53	0
3	OLA	A	1210	-	19,19,19	0.81	1 (5%)	19,19,19	0.96	2 (10%)
6	OLC	A	1226	-	19,19,24	1.08	1 (5%)	19,19,25	0.91	0
3	OLA	A	1207	-	8,8,19	0.71	0	8,8,19	1.25	1 (12%)
5	CLR	A	1205	-	31,31,31	0.71	1 (3%)	48,48,48	0.91	0
3	OLA	A	1214	-	18,18,19	0.81	1 (5%)	18,18,19	0.99	2 (11%)
6	OLC	A	1220	-	15,15,24	1.15	1 (6%)	16,16,25	1.13	2 (12%)
3	OLA	A	1202	-	19,19,19	0.81	1 (5%)	19,19,19	0.94	0
3	OLA	A	1216	-	9,9,19	0.98	1 (11%)	8,8,19	0.63	0
3	OLA	A	1208	-	17,17,19	0.84	1 (5%)	17,17,19	0.94	0
6	OLC	A	1225	-	21,21,24	0.99	1 (4%)	22,22,25	0.92	2 (9%)
5	CLR	A	1206	-	31,31,31	0.65	0	48,48,48	0.90	1 (2%)
3	OLA	A	1211	-	11,11,19	1.05	1 (9%)	11,11,19	1.16	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9XT	A	1201	-	27,27,27	1.37	3 (11%)	38,39,39	3.21	13 (34%)
5	CLR	A	1204	-	31,31,31	0.69	0	48,48,48	0.94	2 (4%)
3	OLA	A	1219	-	12,12,19	0.84	1 (8%)	11,11,19	0.59	0
3	OLA	A	1212	-	7,7,19	0.77	0	7,7,19	1.32	1 (14%)
6	OLC	A	1227	-	19,19,24	1.07	1 (5%)	19,19,25	0.97	1 (5%)
6	OLC	A	1222	-	16,16,24	1.19	1 (6%)	16,16,25	0.95	1 (6%)
3	OLA	A	1213	-	8,8,19	0.38	0	7,7,19	0.77	0
3	OLA	A	1228	-	19,19,19	0.81	1 (5%)	19,19,19	0.91	1 (5%)
3	OLA	A	1218	-	11,11,19	0.88	1 (9%)	10,10,19	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	OLA	A	1215	-	-	9/11/11/17	-
3	OLA	A	1209	-	-	7/17/17/17	-
6	OLC	A	1221	-	-	2/16/16/24	-
6	OLC	A	1224	-	-	3/23/23/24	-
6	OLC	A	1223	-	-	2/17/17/24	-
3	OLA	A	1217	-	-	2/10/10/17	-
3	OLA	A	1210	-	-	10/17/17/17	-
6	OLC	A	1226	-	-	3/17/17/24	-
3	OLA	A	1207	-	-	3/6/6/17	-
5	CLR	A	1205	-	-	1/10/68/68	0/4/4/4
3	OLA	A	1214	-	-	8/16/16/17	-
6	OLC	A	1220	-	-	0/15/15/24	-
3	OLA	A	1202	-	-	9/17/17/17	-
3	OLA	A	1216	-	-	7/7/7/17	-
3	OLA	A	1208	-	-	6/15/15/17	-
6	OLC	A	1225	-	-	2/21/21/24	-
5	CLR	A	1206	-	-	2/10/68/68	0/4/4/4
3	OLA	A	1211	-	-	4/9/9/17	-
2	9XT	A	1201	-	-	0/8/8/8	0/4/4/4
5	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
3	OLA	A	1219	-	-	5/10/10/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	A	1212	-	-	2/5/5/17	-
6	OLC	A	1227	-	-	8/17/17/24	-
6	OLC	A	1222	-	-	3/14/14/24	-
3	OLA	A	1213	-	-	1/6/6/17	-
3	OLA	A	1228	-	-	10/17/17/17	-
3	OLA	A	1218	-	-	6/9/9/17	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1222	OLC	O20-C1	4.66	1.46	1.30
6	A	1227	OLC	O20-C1	4.60	1.46	1.30
6	A	1226	OLC	O20-C1	4.59	1.46	1.30
6	A	1223	OLC	O20-C1	4.42	1.45	1.30
6	A	1224	OLC	O20-C1	4.35	1.46	1.33
6	A	1221	OLC	O20-C1	4.30	1.45	1.33
6	A	1225	OLC	O20-C1	4.28	1.45	1.33
2	A	1201	9XT	N2-N3	4.28	1.40	1.36
6	A	1220	OLC	O20-C1	4.25	1.45	1.33
3	A	1215	OLA	C10-C9	2.87	1.48	1.31
3	A	1211	OLA	C10-C9	2.83	1.47	1.29
3	A	1219	OLA	C10-C9	2.81	1.47	1.31
3	A	1217	OLA	C10-C9	2.81	1.47	1.31
3	A	1210	OLA	C10-C9	2.80	1.47	1.31
3	A	1216	OLA	C10-C9	2.79	1.47	1.31
3	A	1228	OLA	C10-C9	2.77	1.47	1.31
3	A	1209	OLA	C10-C9	2.77	1.47	1.31
3	A	1202	OLA	C10-C9	2.76	1.47	1.31
3	A	1214	OLA	C10-C9	2.76	1.47	1.31
3	A	1218	OLA	C10-C9	2.76	1.47	1.31
3	A	1208	OLA	C10-C9	2.75	1.47	1.31
2	A	1201	9XT	C12-N2	2.60	1.38	1.35
2	A	1201	9XT	C11-N7	2.53	1.39	1.33
5	A	1205	CLR	C10-C9	-2.08	1.52	1.56

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	9XT	N6-C12-N2	13.89	135.16	126.31
2	A	1201	9XT	C9-C12-N6	-8.15	118.60	127.18
2	A	1201	9XT	C12-N2-N3	-5.15	106.18	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	9XT	C8-N2-N3	3.52	126.69	120.27
2	A	1201	9XT	O1-C13-C10	3.44	125.46	117.16
2	A	1201	9XT	C10-N5-C11	3.35	120.98	116.80
6	A	1221	OLC	O20-C1-C2	3.28	121.84	111.83
6	A	1224	OLC	O20-C1-C2	3.15	121.45	111.83
6	A	1220	OLC	O20-C1-C2	3.15	121.42	111.83
2	A	1201	9XT	C11-N6-C12	2.90	121.29	113.51
6	A	1225	OLC	O20-C1-C2	2.83	120.48	111.83
2	A	1201	9XT	C10-C13-C14	-2.78	126.02	133.05
2	A	1201	9XT	C10-C9-C12	2.53	117.83	116.55
2	A	1201	9XT	C9-C12-N2	2.52	106.25	104.25
5	A	1204	CLR	C4-C5-C10	2.30	119.37	116.42
6	A	1223	OLC	O20-C1-C2	2.19	120.91	114.00
5	A	1206	CLR	C4-C5-C10	2.18	119.21	116.42
6	A	1220	OLC	O20-C1-O19	-2.17	118.20	123.63
3	A	1214	OLA	C3-C2-C1	-2.17	108.86	114.51
6	A	1221	OLC	O20-C1-O19	-2.14	118.27	123.63
3	A	1210	OLA	O2-C1-C2	2.13	120.73	114.00
3	A	1210	OLA	C3-C2-C1	-2.11	109.01	114.51
3	A	1211	OLA	O2-C1-C2	2.10	120.62	114.00
3	A	1207	OLA	O2-C1-C2	2.10	120.62	114.00
3	A	1215	OLA	O2-C1-C2	2.09	120.60	114.00
2	A	1201	9XT	C12-C9-N4	-2.08	107.70	109.31
6	A	1222	OLC	O20-C1-C2	2.06	120.51	114.00
3	A	1214	OLA	O2-C1-C2	2.05	120.47	114.00
3	A	1212	OLA	C3-C2-C1	-2.05	109.17	114.51
2	A	1201	9XT	N6-C11-N5	-2.04	122.36	125.48
5	A	1204	CLR	C4-C5-C6	-2.03	117.82	120.57
6	A	1227	OLC	C3-C2-C1	-2.02	109.23	114.51
3	A	1209	OLA	O2-C1-C2	2.02	120.39	114.00
3	A	1228	OLA	O2-C1-C2	2.02	120.38	114.00
2	A	1201	9XT	C2-C3-C4	-2.02	119.94	122.22
6	A	1223	OLC	C3-C2-C1	-2.01	109.26	114.51
6	A	1225	OLC	O20-C1-O19	-2.01	118.61	123.63

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1221	OLC	O20-C21-C22-C24
3	A	1210	OLA	C11-C10-C9-C8
5	A	1205	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	1209	OLA	C1-C2-C3-C4
6	A	1221	OLC	O20-C21-C22-O23
3	A	1213	OLA	C3-C4-C5-C6
3	A	1207	OLA	C1-C2-C3-C4
3	A	1210	OLA	C1-C2-C3-C4
3	A	1211	OLA	C1-C2-C3-C4
3	A	1212	OLA	C1-C2-C3-C4
3	A	1228	OLA	C1-C2-C3-C4
5	A	1206	CLR	C20-C22-C23-C24
3	A	1215	OLA	C5-C6-C7-C8
3	A	1218	OLA	C5-C6-C7-C8
3	A	1215	OLA	C1-C2-C3-C4
3	A	1202	OLA	C2-C3-C4-C5
3	A	1214	OLA	C11-C12-C13-C14
3	A	1214	OLA	C11-C10-C9-C8
3	A	1202	OLA	C4-C5-C6-C7
3	A	1215	OLA	C2-C3-C4-C5
3	A	1219	OLA	C11-C12-C13-C14
3	A	1228	OLA	C4-C5-C6-C7
3	A	1211	OLA	C4-C5-C6-C7
3	A	1209	OLA	C11-C12-C13-C14
3	A	1211	OLA	C3-C4-C5-C6
3	A	1215	OLA	C3-C4-C5-C6
3	A	1216	OLA	C5-C6-C7-C8
6	A	1222	OLC	C5-C6-C7-C8
3	A	1210	OLA	C4-C5-C6-C7
3	A	1216	OLA	C9-C10-C11-C12
3	A	1216	OLA	C4-C5-C6-C7
3	A	1218	OLA	C3-C4-C5-C6
6	A	1226	OLC	C10-C11-C12-C13
3	A	1218	OLA	C11-C10-C9-C8
6	A	1225	OLC	C2-C3-C4-C5
3	A	1202	OLA	C11-C12-C13-C14
3	A	1209	OLA	C10-C11-C12-C13
3	A	1202	OLA	C11-C10-C9-C8
3	A	1209	OLA	C11-C10-C9-C8
6	A	1226	OLC	C12-C13-C14-C15
6	A	1223	OLC	C11-C12-C13-C14
3	A	1228	OLA	C12-C13-C14-C15
3	A	1208	OLA	C11-C10-C9-C8
3	A	1216	OLA	C11-C10-C9-C8
3	A	1219	OLA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
6	A	1222	OLC	C2-C3-C4-C5
3	A	1210	OLA	C3-C4-C5-C6
3	A	1215	OLA	C11-C10-C9-C8
3	A	1217	OLA	C11-C10-C9-C8
3	A	1228	OLA	C11-C10-C9-C8
3	A	1228	OLA	C3-C4-C5-C6
3	A	1214	OLA	C4-C5-C6-C7
3	A	1208	OLA	C3-C4-C5-C6
3	A	1216	OLA	C3-C4-C5-C6
6	A	1227	OLC	C1-C2-C3-C4
3	A	1218	OLA	C1-C2-C3-C4
3	A	1214	OLA	C3-C4-C5-C6
3	A	1215	OLA	C9-C10-C11-C12
3	A	1218	OLA	C9-C10-C11-C12
3	A	1212	OLA	C3-C4-C5-C6
3	A	1228	OLA	C14-C15-C16-C17
3	A	1202	OLA	C13-C14-C15-C16
6	A	1224	OLC	C11-C12-C13-C14
3	A	1215	OLA	C4-C5-C6-C7
6	A	1224	OLC	C12-C13-C14-C15
3	A	1207	OLA	C4-C5-C6-C7
3	A	1208	OLA	C11-C12-C13-C14
6	A	1223	OLC	C5-C6-C7-C8
6	A	1225	OLC	C7-C8-C9-C10
6	A	1227	OLC	C7-C8-C9-C10
3	A	1202	OLA	C9-C10-C11-C12
3	A	1219	OLA	C9-C10-C11-C12
3	A	1208	OLA	O1-C1-C2-C3
3	A	1219	OLA	C6-C7-C8-C9
3	A	1202	OLA	C12-C13-C14-C15
6	A	1227	OLC	O19-C1-C2-C3
3	A	1207	OLA	C3-C4-C5-C6
3	A	1215	OLA	O2-C1-C2-C3
3	A	1208	OLA	O2-C1-C2-C3
3	A	1215	OLA	O1-C1-C2-C3
3	A	1228	OLA	C11-C12-C13-C14
6	A	1227	OLC	O20-C1-C2-C3
3	A	1209	OLA	C9-C10-C11-C12
3	A	1219	OLA	C7-C8-C9-C10
3	A	1211	OLA	C7-C8-C9-C10
3	A	1202	OLA	C6-C7-C8-C9
3	A	1210	OLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	1214	OLA	C5-C6-C7-C8
6	A	1227	OLC	C9-C10-C11-C12
3	A	1210	OLA	O2-C1-C2-C3
3	A	1228	OLA	C7-C8-C9-C10
3	A	1210	OLA	O1-C1-C2-C3
3	A	1210	OLA	C9-C10-C11-C12
3	A	1202	OLA	C7-C8-C9-C10
3	A	1216	OLA	C7-C8-C9-C10
3	A	1218	OLA	C7-C8-C9-C10
6	A	1227	OLC	C12-C13-C14-C15
6	A	1227	OLC	C10-C11-C12-C13
3	A	1209	OLA	C7-C8-C9-C10
3	A	1210	OLA	C7-C8-C9-C10
6	A	1226	OLC	C3-C4-C5-C6
5	A	1206	CLR	C13-C17-C20-C21
3	A	1214	OLA	C7-C8-C9-C10
3	A	1228	OLA	C9-C10-C11-C12
6	A	1222	OLC	C7-C8-C9-C10
6	A	1224	OLC	C9-C10-C11-C12
3	A	1208	OLA	C9-C10-C11-C12
3	A	1214	OLA	C9-C10-C11-C12
3	A	1216	OLA	C6-C7-C8-C9
3	A	1210	OLA	C15-C16-C17-C18
3	A	1209	OLA	C3-C4-C5-C6
3	A	1214	OLA	C1-C2-C3-C4
3	A	1228	OLA	C5-C6-C7-C8
3	A	1217	OLA	C12-C13-C14-C15
6	A	1227	OLC	C5-C6-C7-C8

There are no ring outliers.

11 monomers are involved in 10 short contacts:

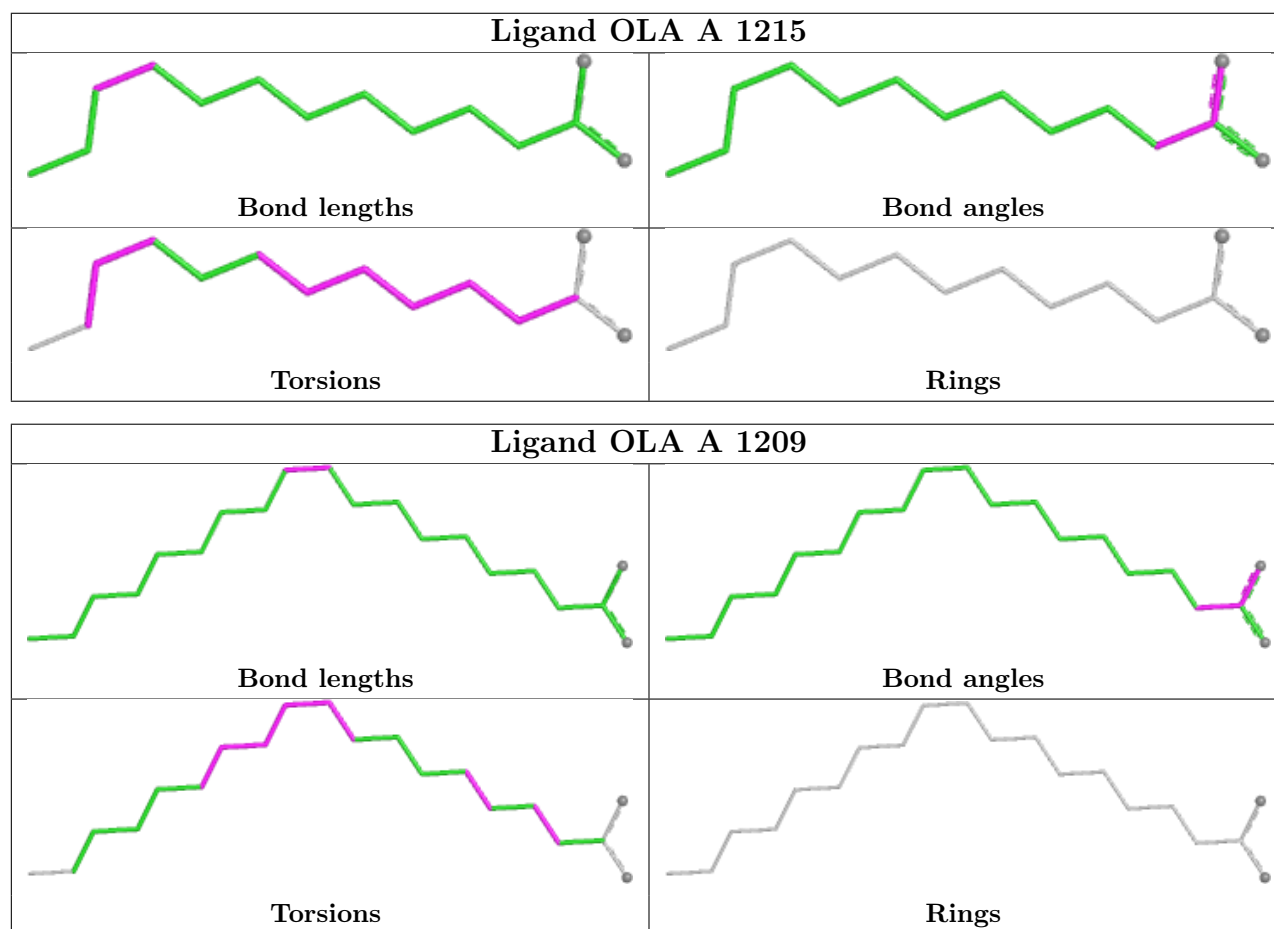
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1221	OLC	1	0
6	A	1224	OLC	1	0
6	A	1223	OLC	1	0
3	A	1217	OLA	1	0
3	A	1207	OLA	1	0
3	A	1214	OLA	3	0
6	A	1220	OLC	1	0
3	A	1202	OLA	1	0
3	A	1208	OLA	1	0

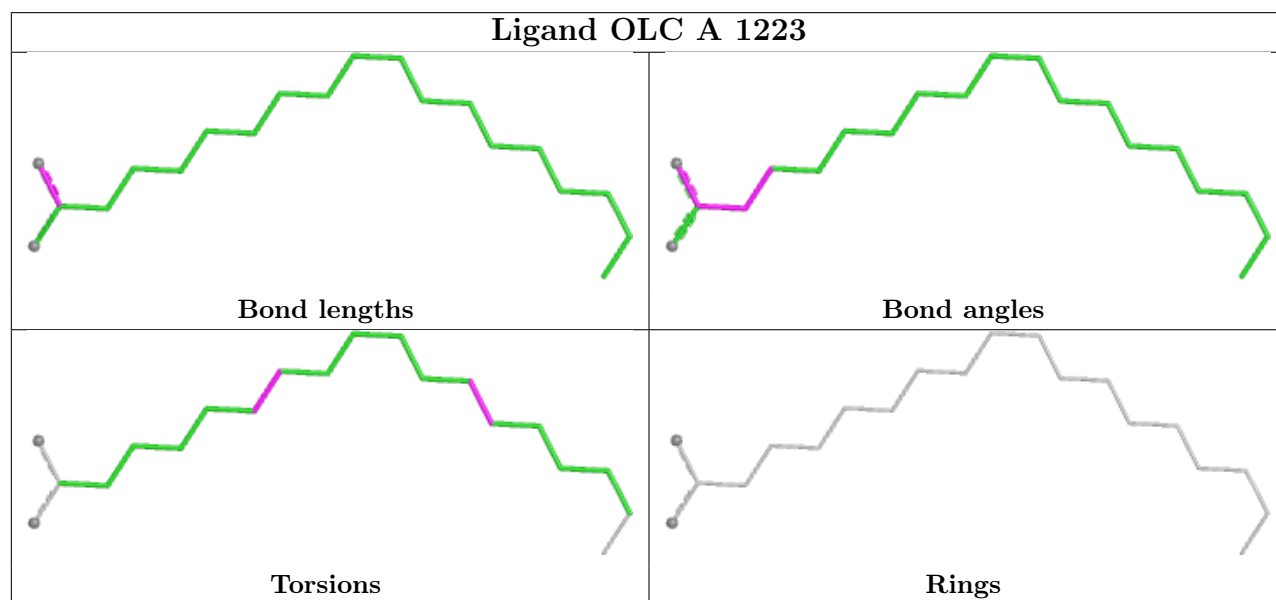
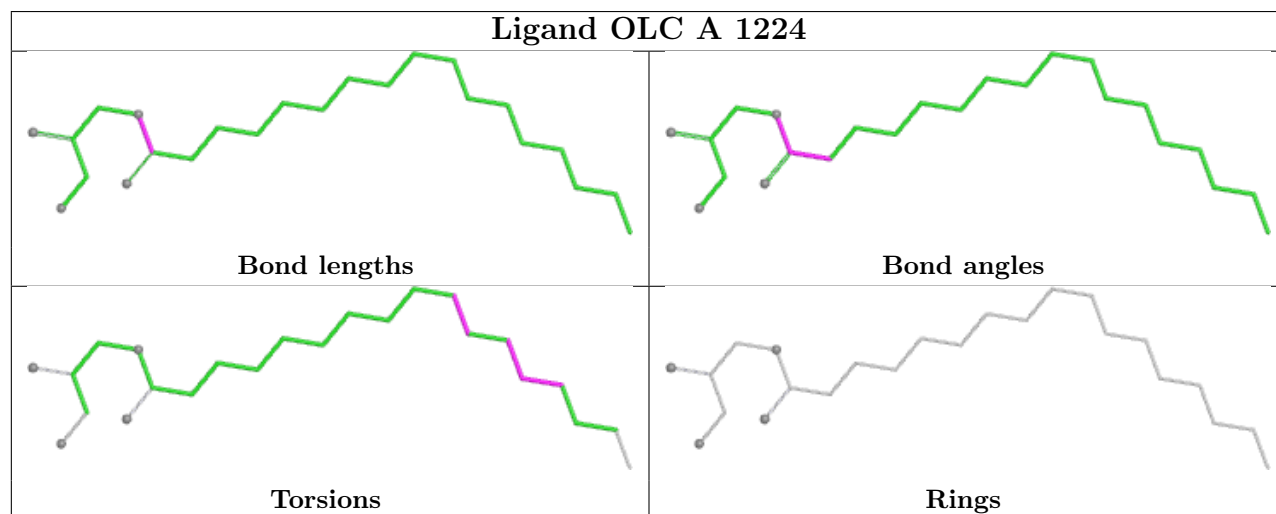
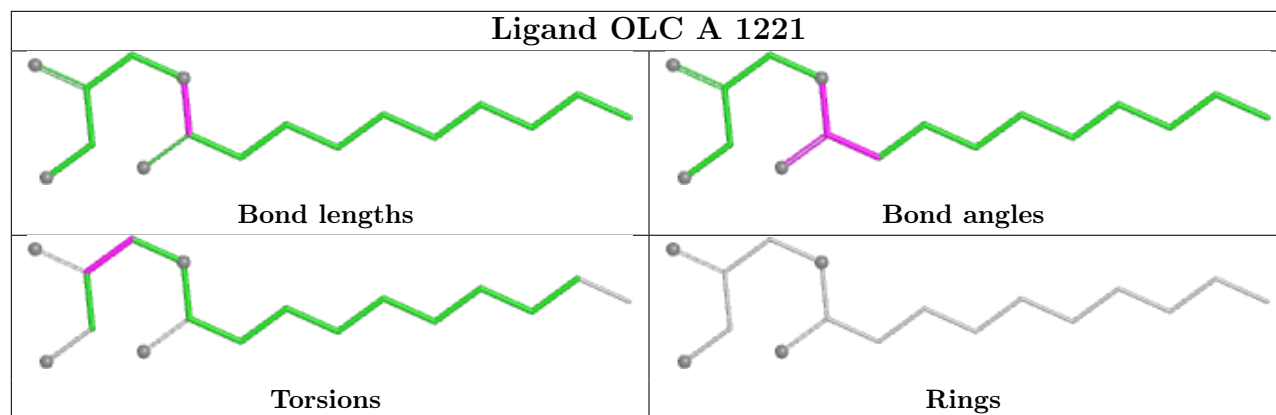
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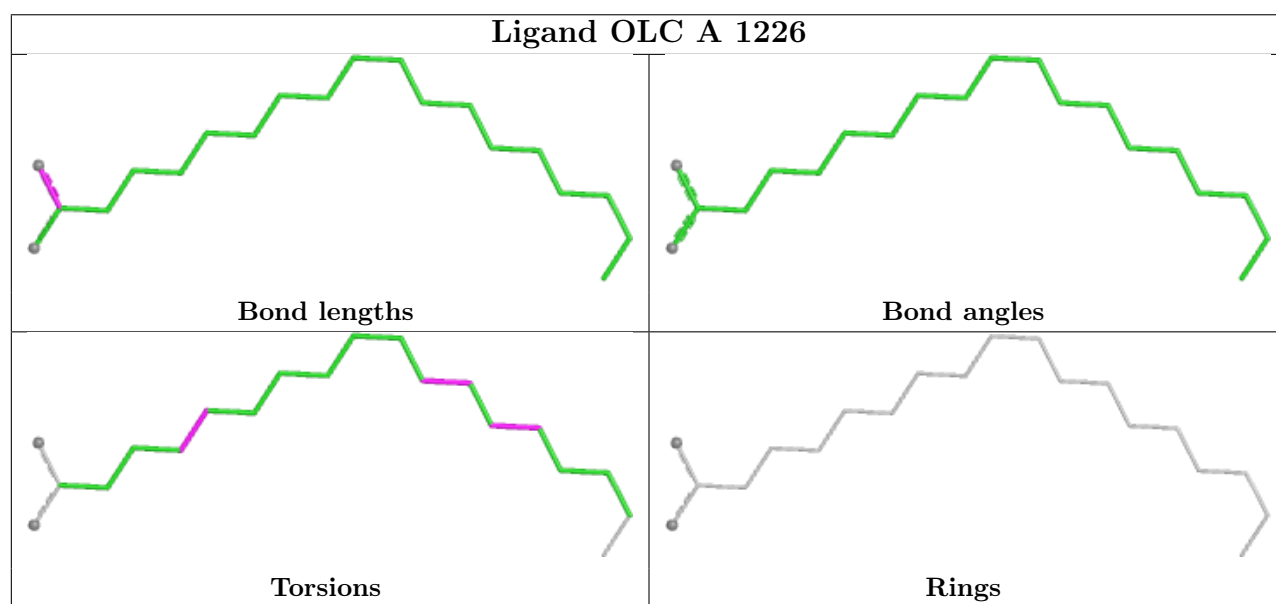
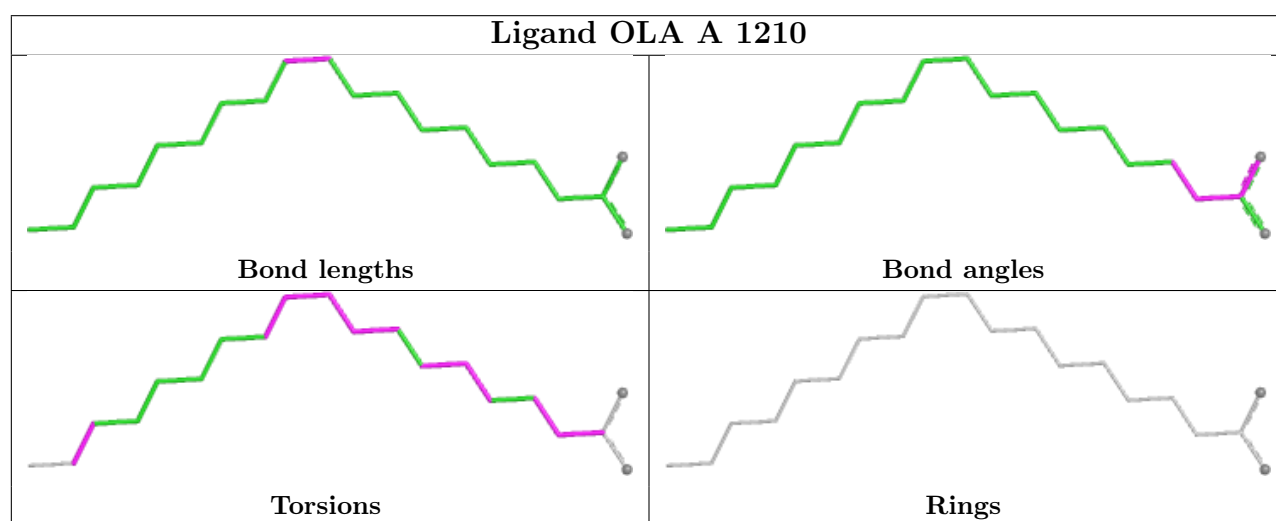
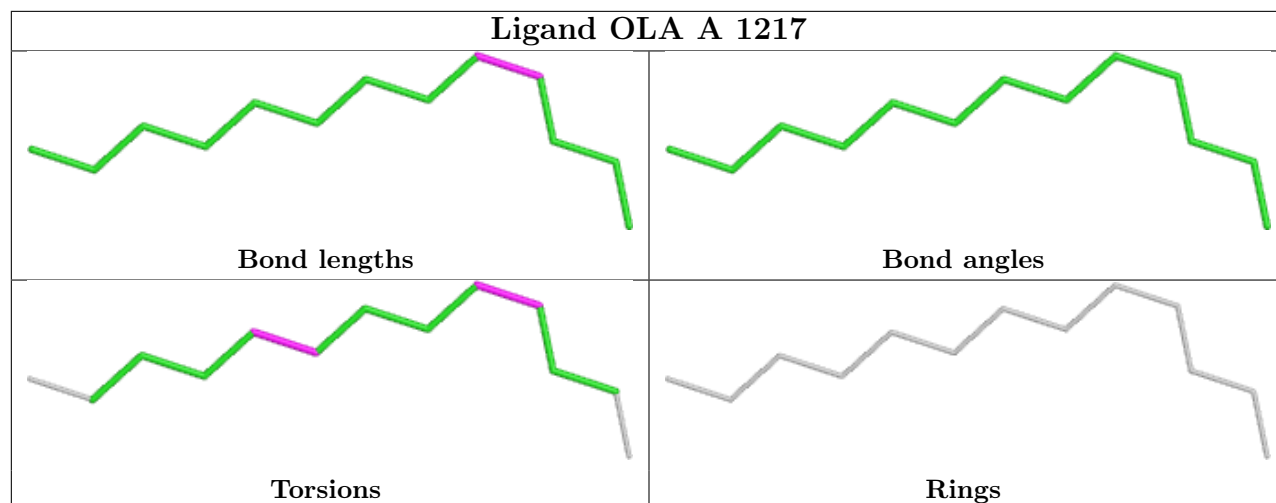
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1206	CLR	1	0
6	A	1227	OLC	2	0

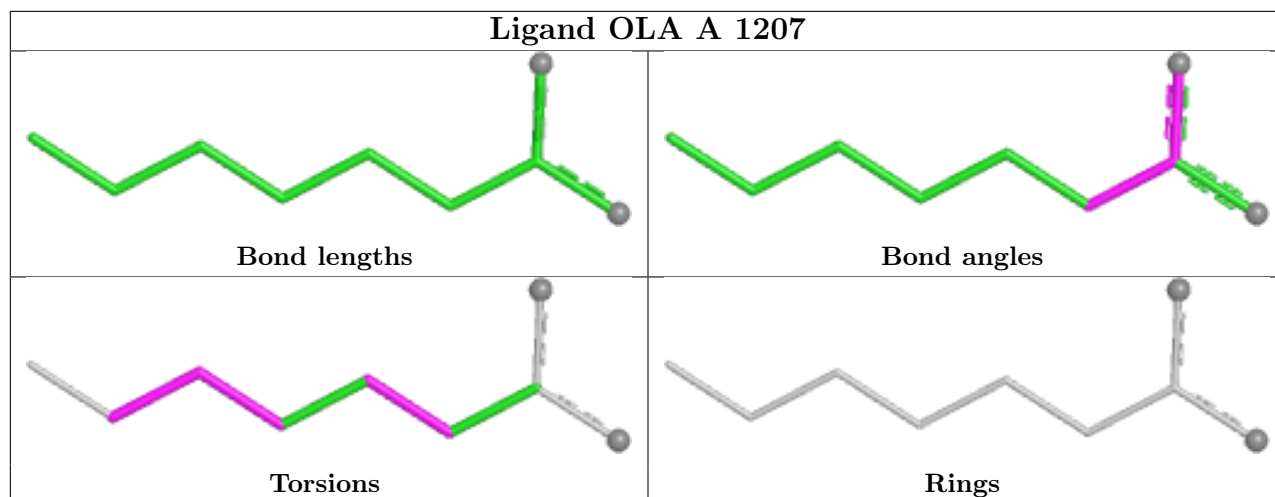
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



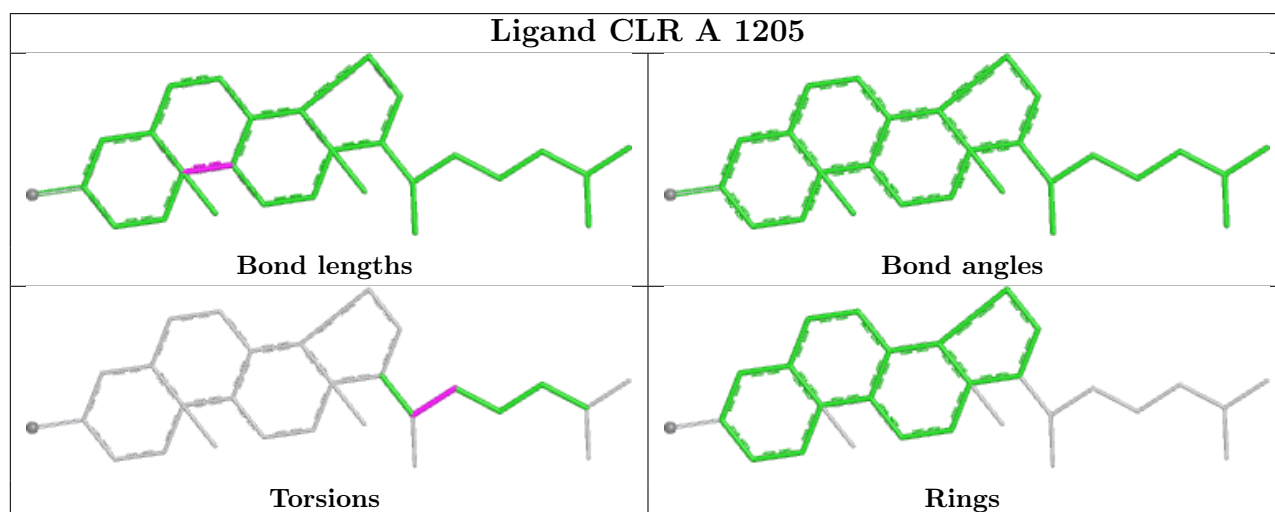




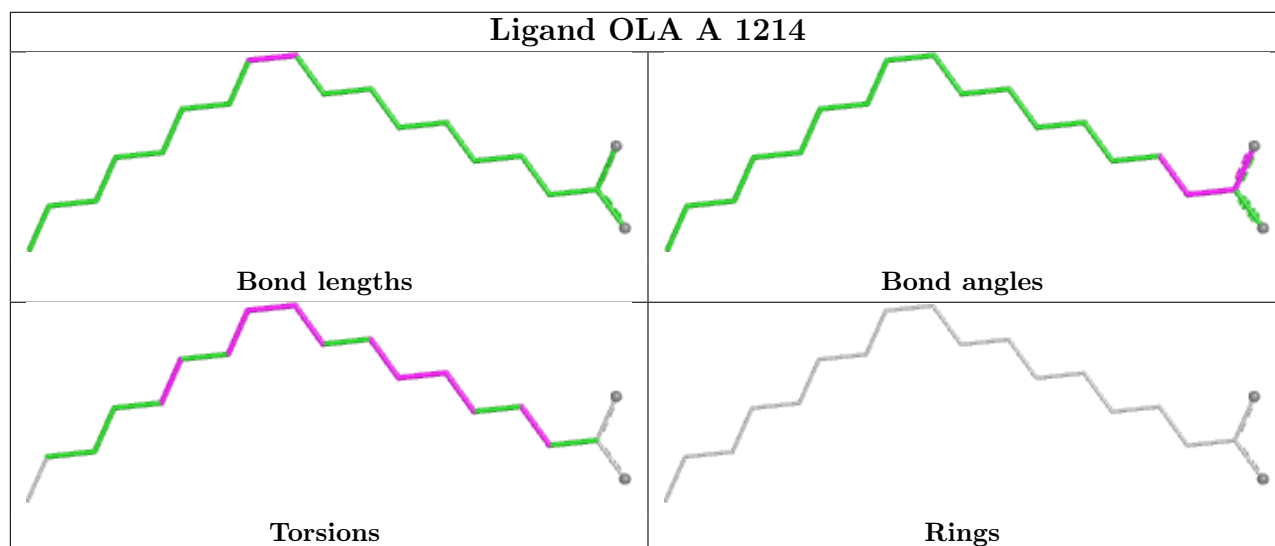
Ligand OLA A 1207

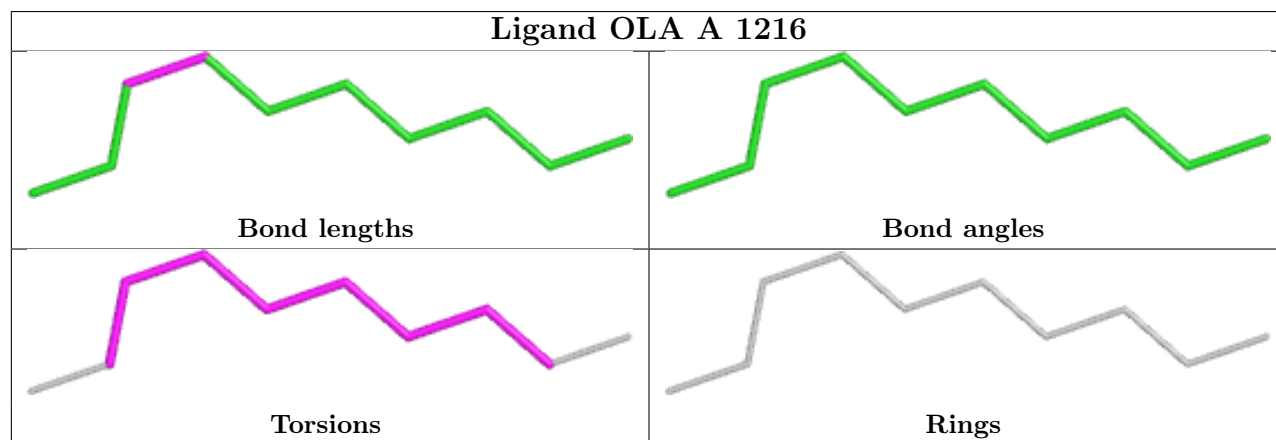
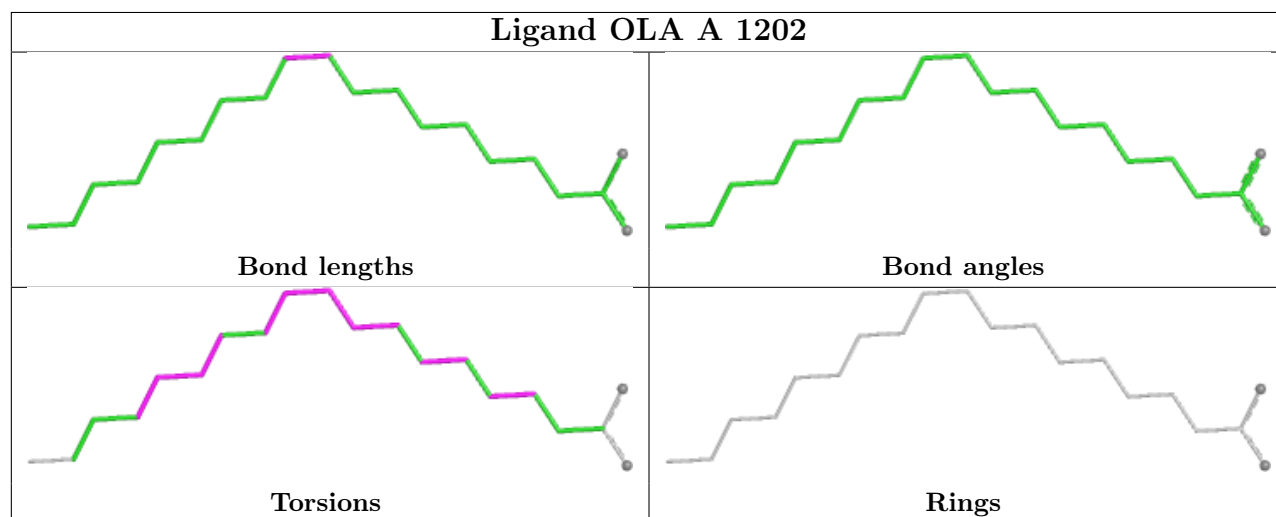
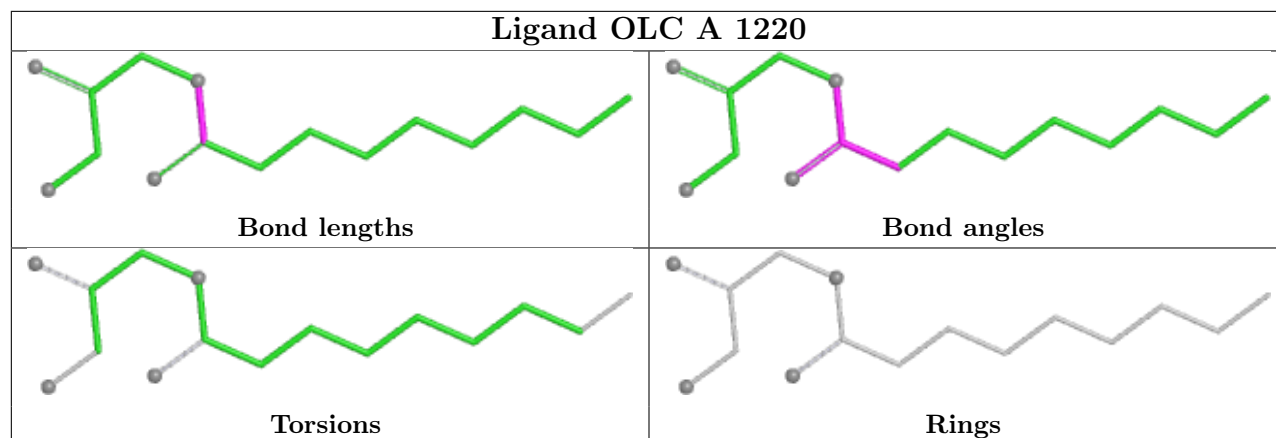


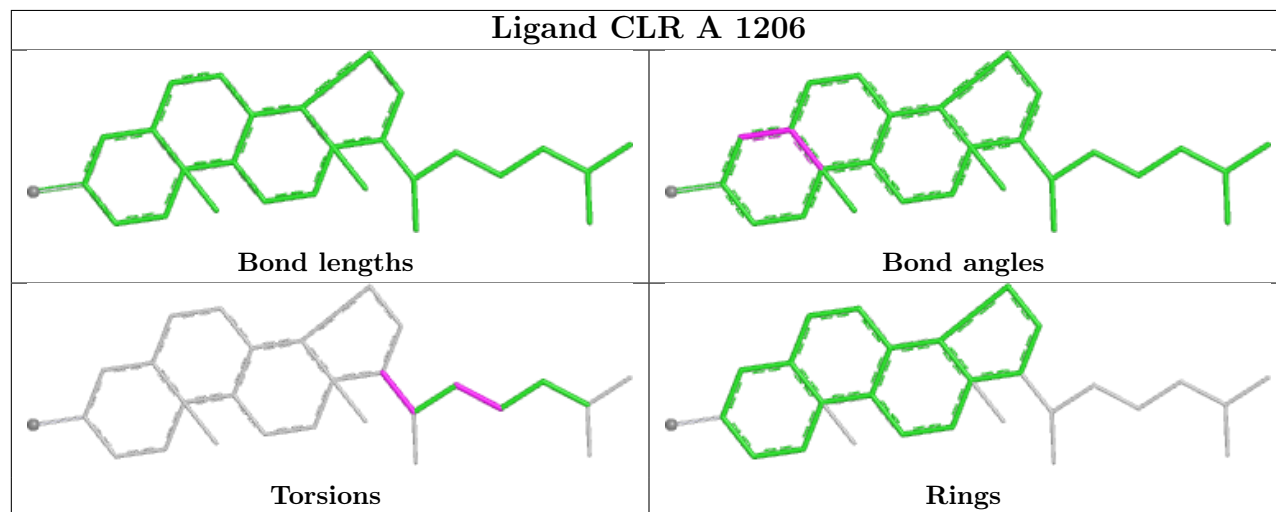
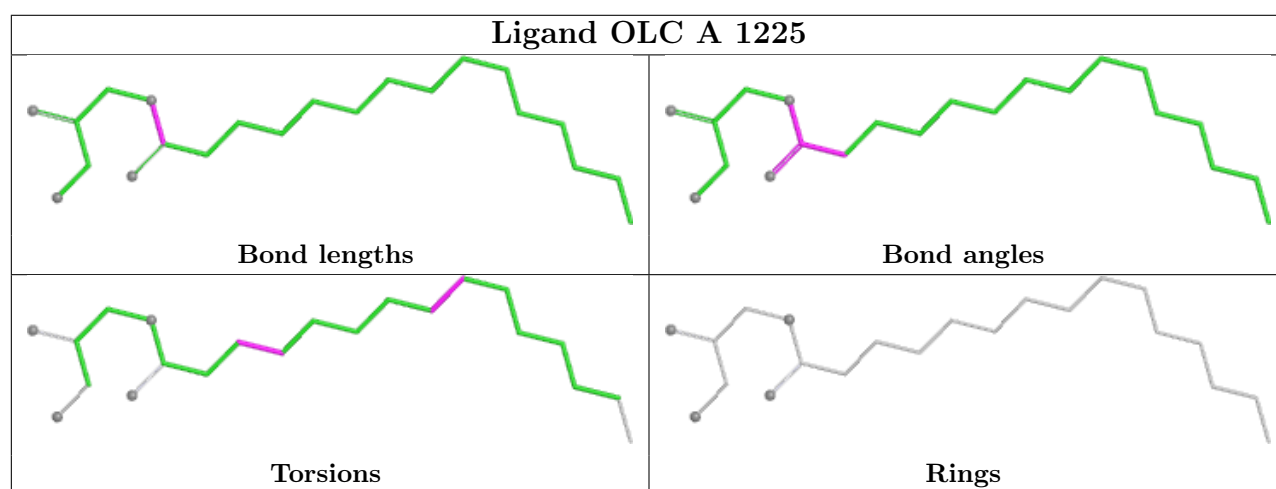
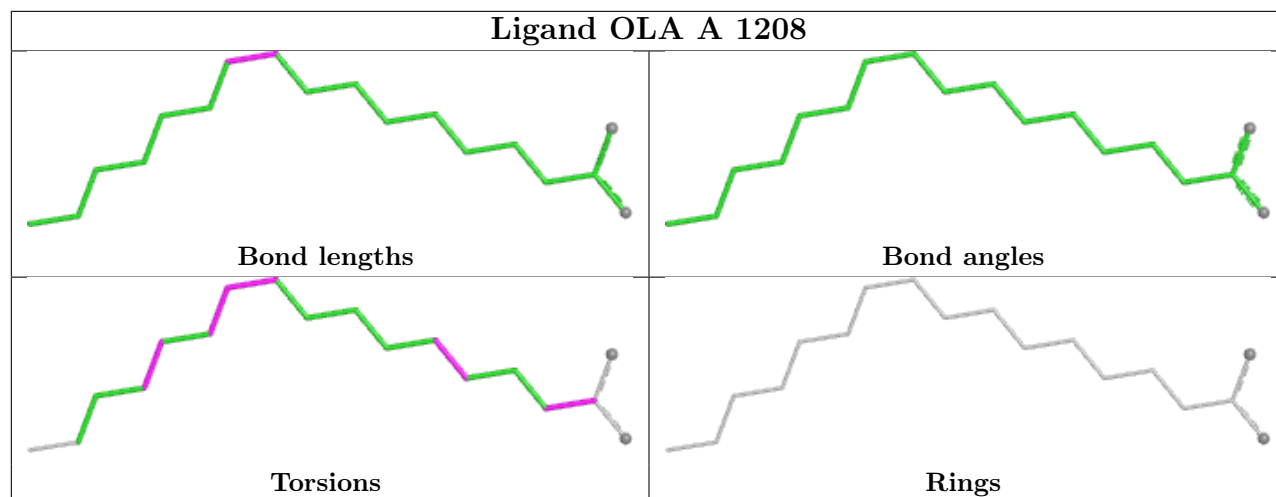
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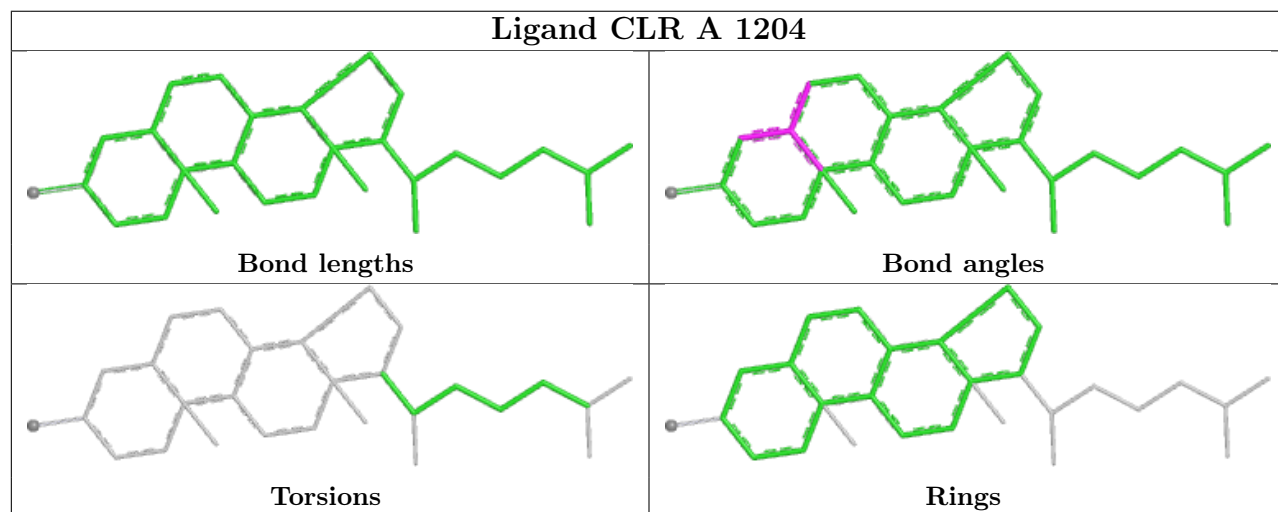
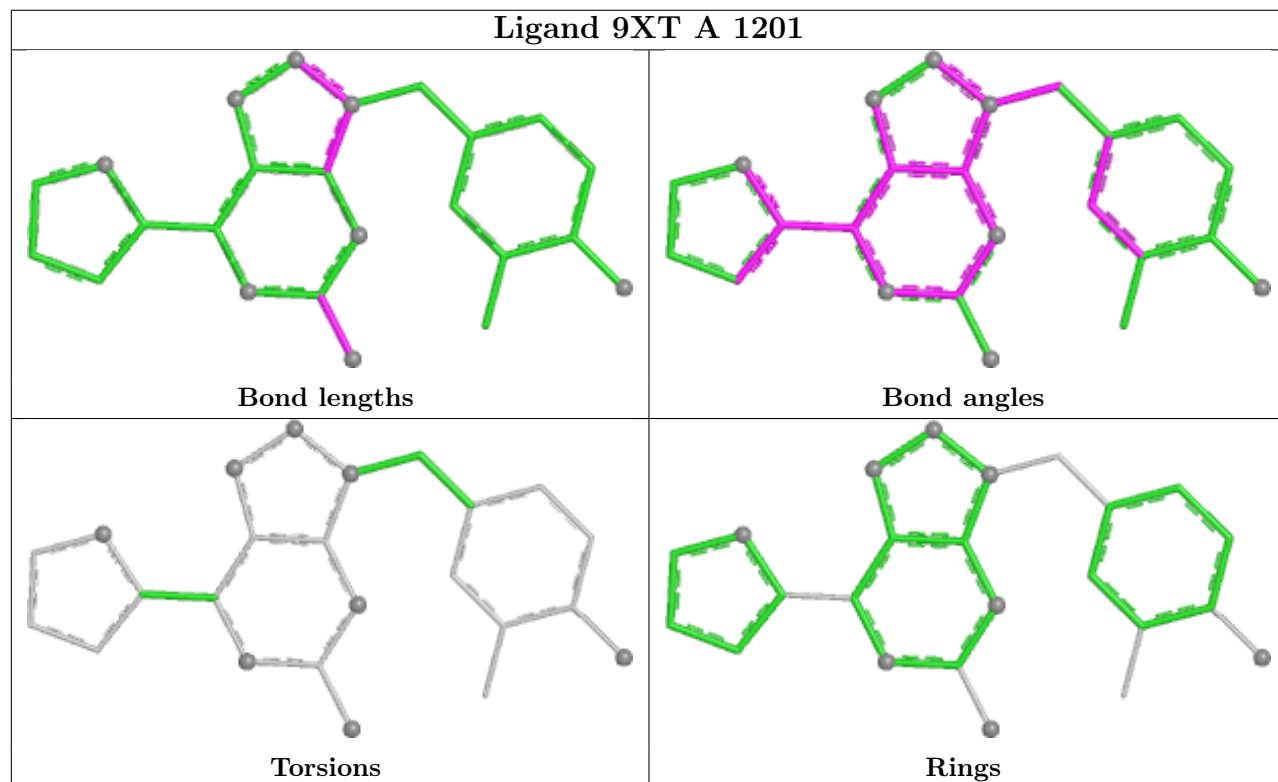
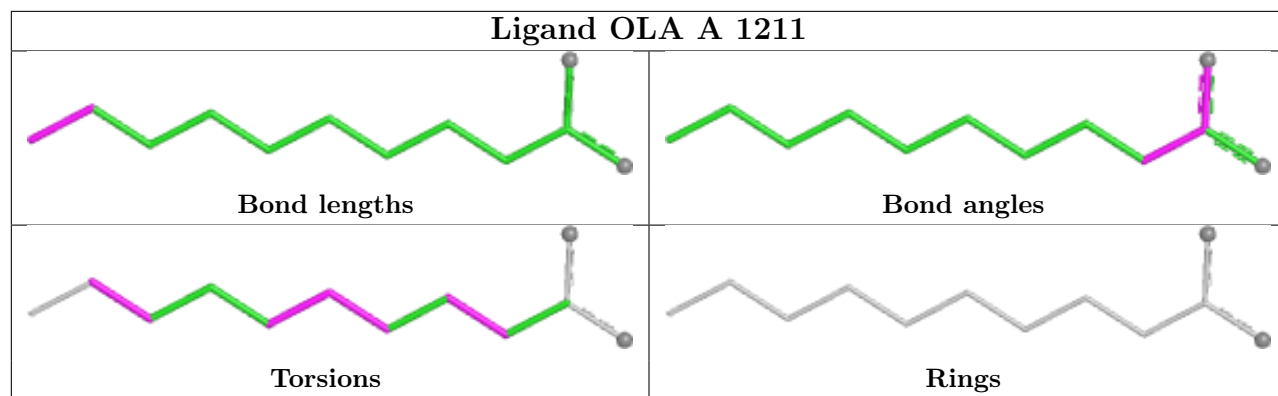


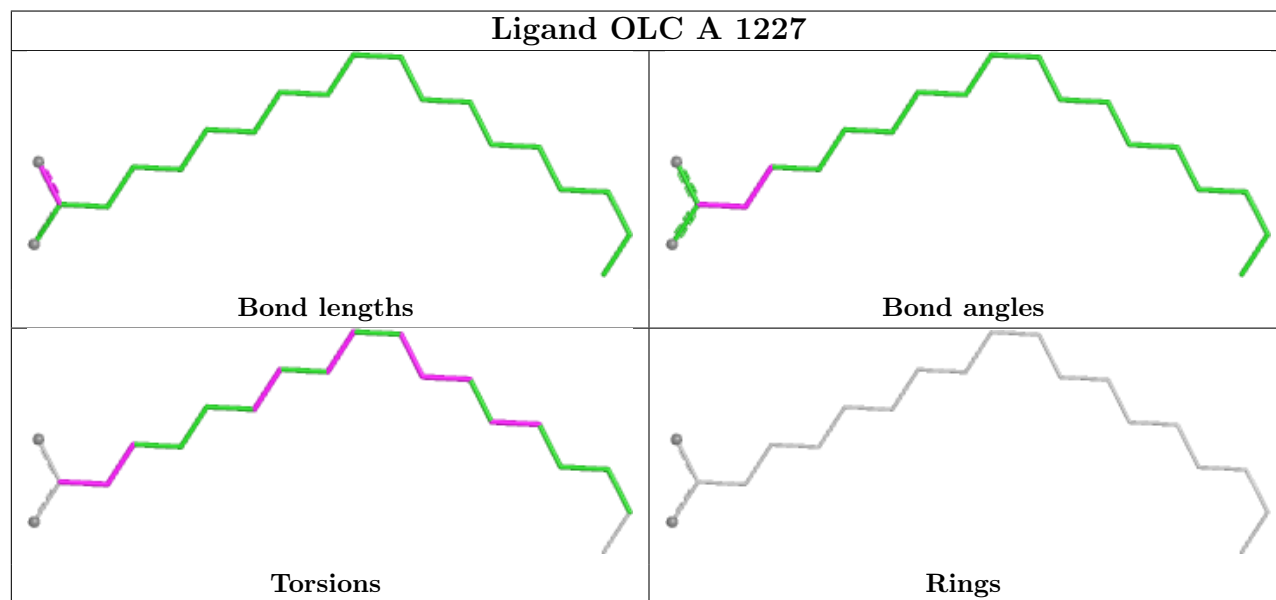
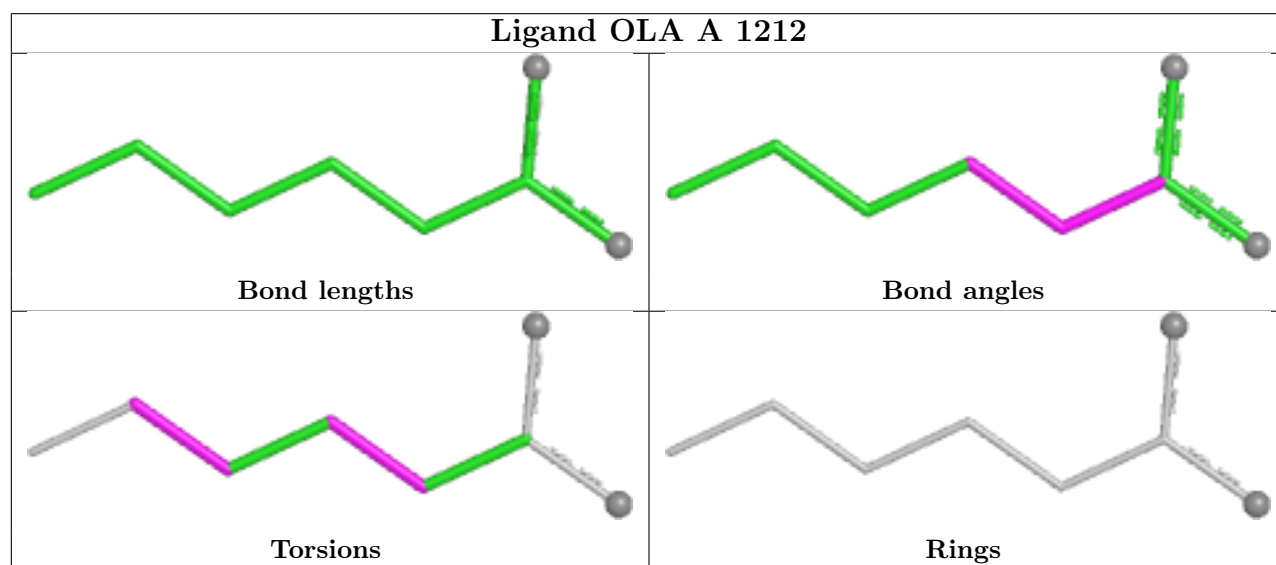
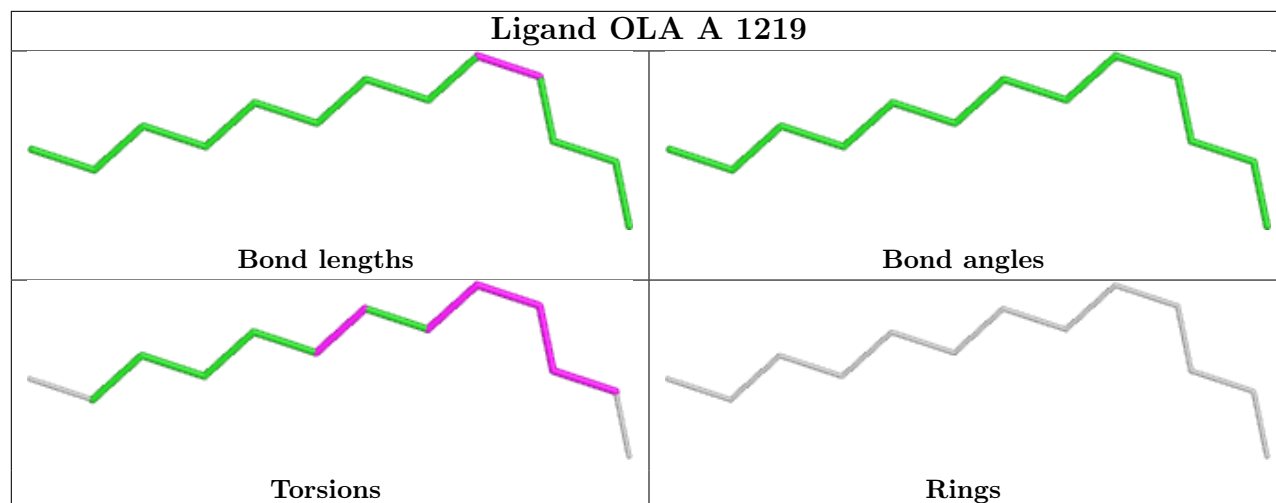
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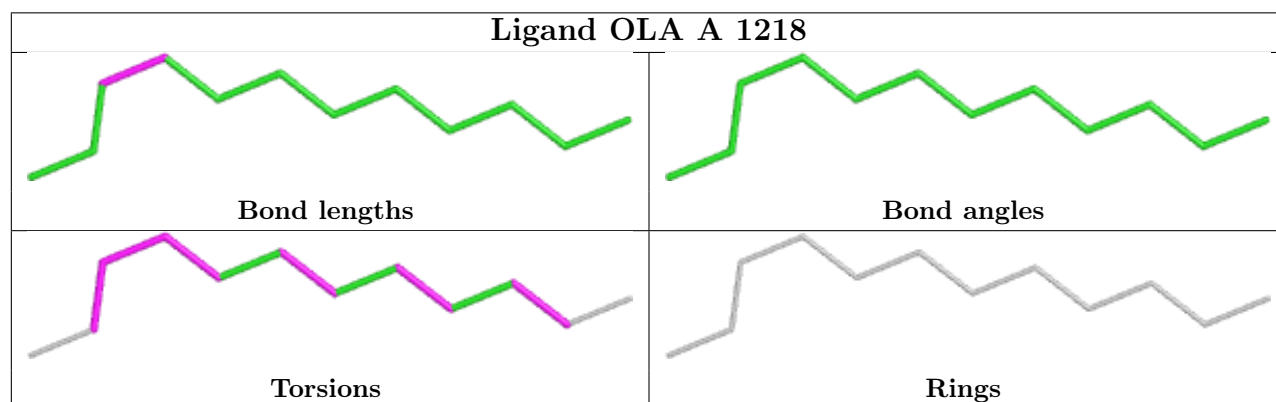
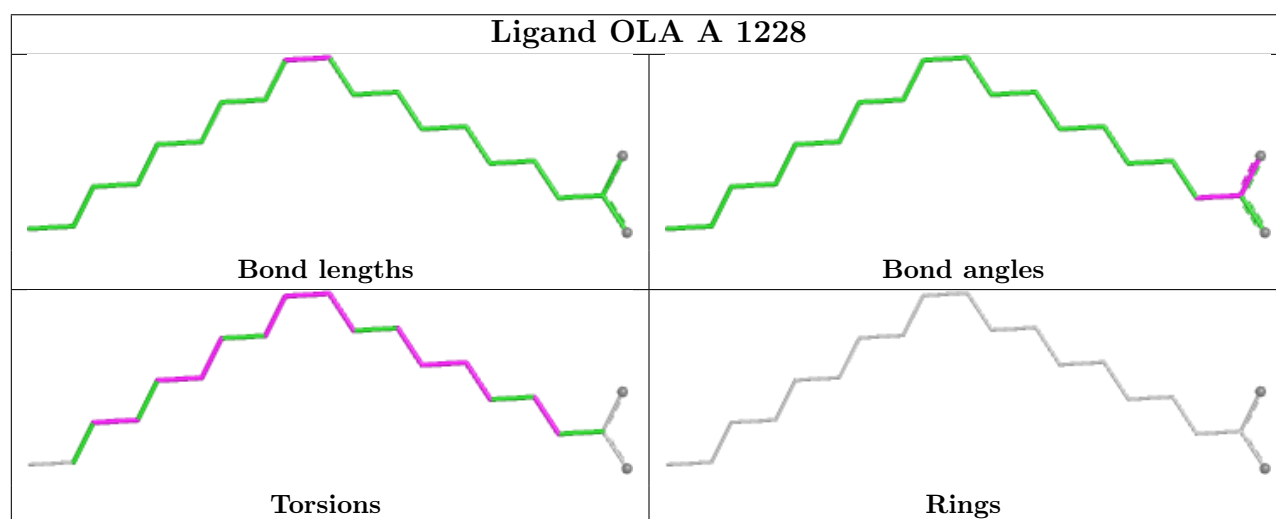
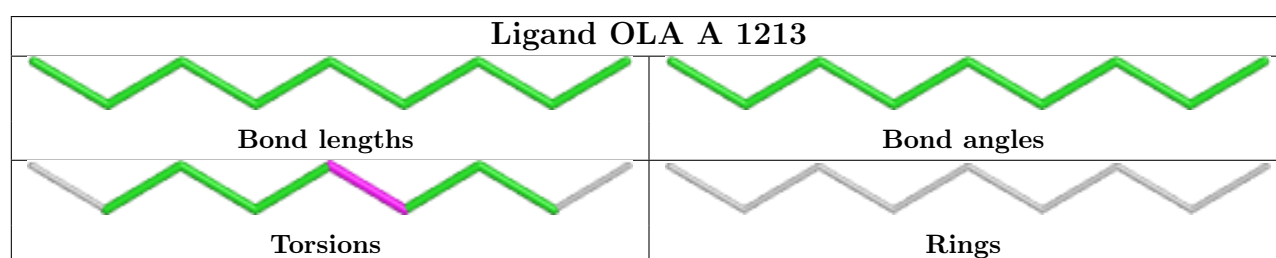
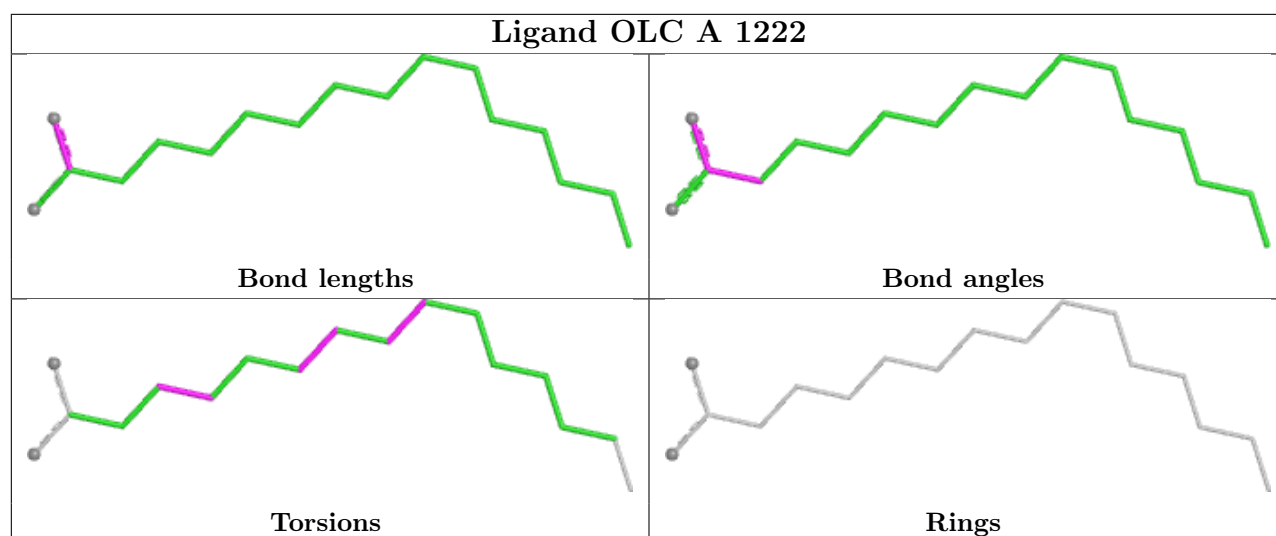












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	390/434 (89%)	-0.08	10 (2%) 57 51	10, 36, 80, 139	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	GLY	4.1
1	A	1061	PHE	3.5
1	A	1021	ASP	3.4
1	A	1056	PRO	3.0
1	A	1060	ASP	2.5
1	A	1105	TYR	2.5
1	A	1058	MET	2.2
1	A	305	SER	2.2
1	A	1059	LYS	2.1
1	A	78[A]	LEU	2.1

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](#)

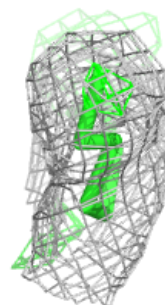
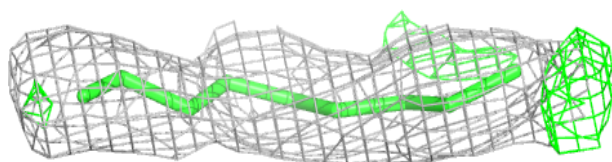
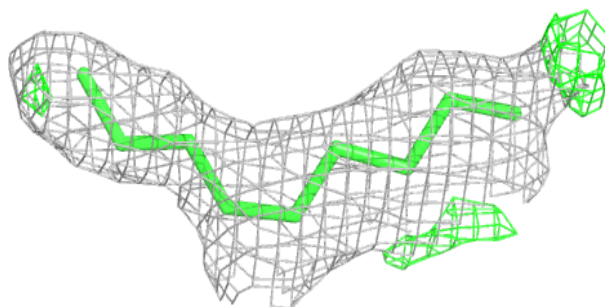
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	OLA	A	1213	9/20	0.62	0.18	55,56,58,60	0
3	OLA	A	1218	12/20	0.72	0.22	51,57,62,62	0
3	OLA	A	1217	13/20	0.75	0.24	54,59,68,69	0
3	OLA	A	1215	14/20	0.75	0.21	49,69,73,74	0
3	OLA	A	1210	20/20	0.76	0.15	46,61,68,69	0
3	OLA	A	1209	20/20	0.78	0.20	36,62,76,77	0
3	OLA	A	1216	10/20	0.79	0.19	54,59,61,61	0
3	OLA	A	1202	20/20	0.80	0.14	36,48,50,53	0
3	OLA	A	1214	19/20	0.80	0.18	58,62,67,68	0
3	OLA	A	1219	13/20	0.80	0.18	43,47,60,61	0
6	OLC	A	1221	17/25	0.81	0.17	55,63,70,78	0
6	OLC	A	1225	22/25	0.81	0.20	52,64,73,80	0
6	OLC	A	1224	24/25	0.82	0.17	34,56,67,72	0
3	OLA	A	1212	8/20	0.83	0.17	56,69,75,76	0
6	OLC	A	1227	20/25	0.83	0.17	38,58,74,78	0
3	OLA	A	1208	18/20	0.84	0.17	40,59,71,74	0
3	OLA	A	1228	20/20	0.85	0.13	62,63,64,65	20
6	OLC	A	1220	16/25	0.85	0.16	38,48,57,71	0
6	OLC	A	1226	20/25	0.85	0.18	25,54,78,85	0
3	OLA	A	1211	12/20	0.85	0.15	37,55,69,70	0
6	OLC	A	1223	20/25	0.89	0.14	30,41,68,69	0
6	OLC	A	1222	17/25	0.90	0.12	34,45,62,62	0
3	OLA	A	1207	9/20	0.90	0.12	36,44,61,62	0
4	NA	A	1203	1/1	0.91	0.11	54,54,54,54	0
5	CLR	A	1205	28/28	0.91	0.10	27,33,36,41	0
5	CLR	A	1204	28/28	0.93	0.10	28,32,62,67	0
5	CLR	A	1206	28/28	0.93	0.08	20,32,49,52	0
2	9XT	A	1201	24/24	0.98	0.06	12,22,26,32	0

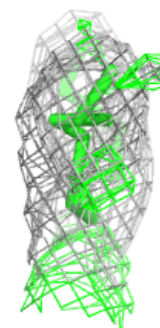
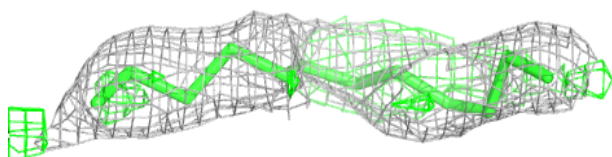
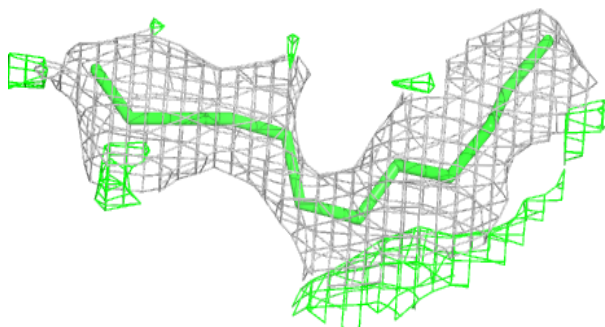
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1213:

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

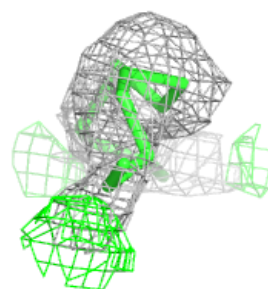
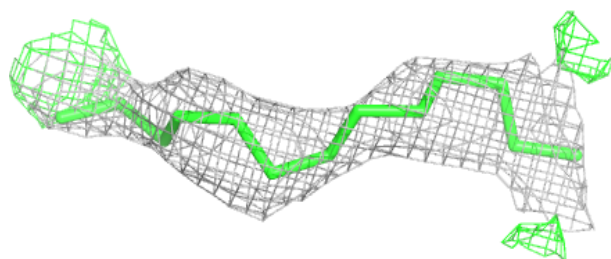
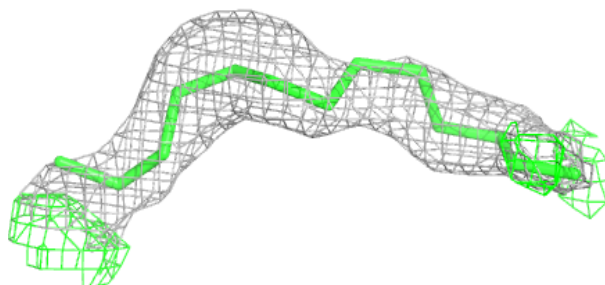
**Electron density around OLA A 1218:**

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

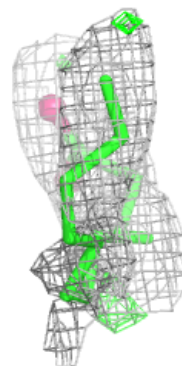
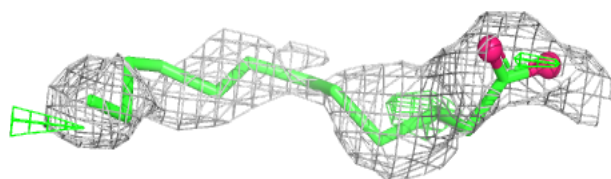
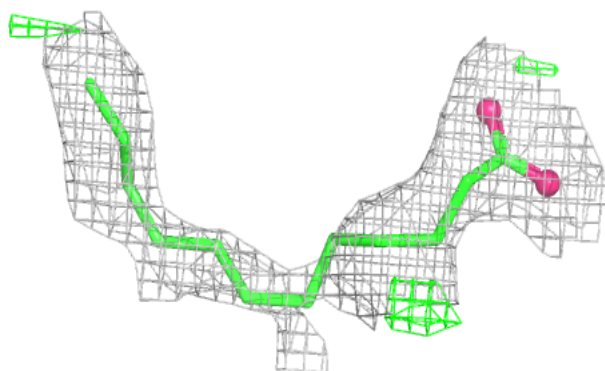


Electron density around OLA A 1217:

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

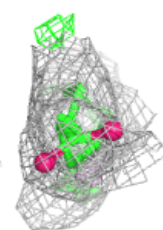
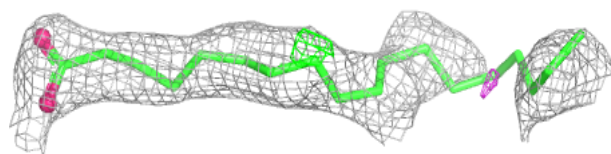
**Electron density around OLA A 1215:**

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

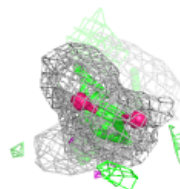
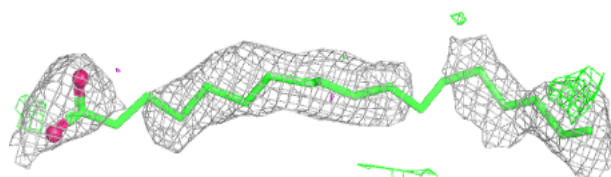
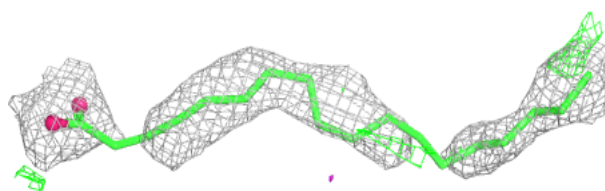


Electron density around OLA A 1210:

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

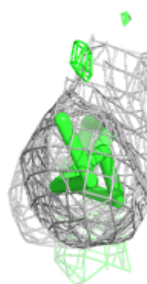
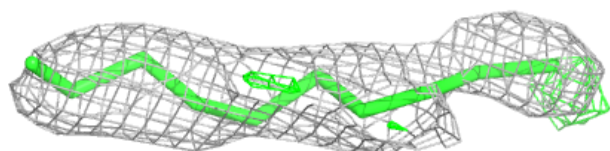
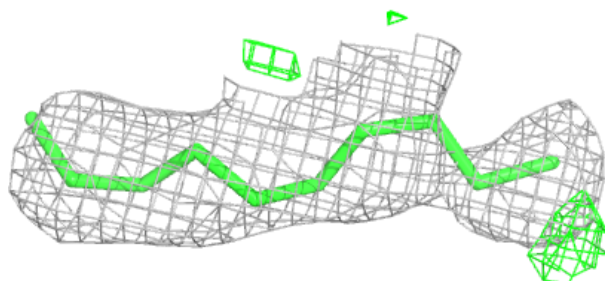
**Electron density around OLA A 1209:**

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

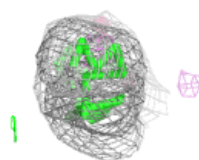
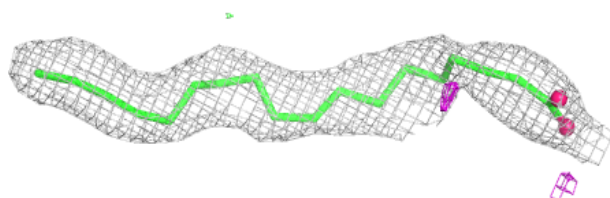
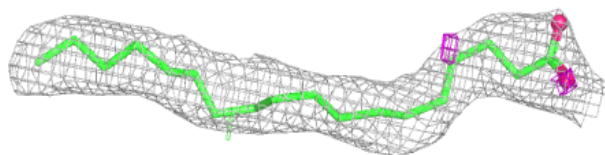


Electron density around OLA A 1216:

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

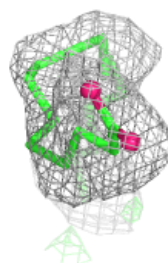
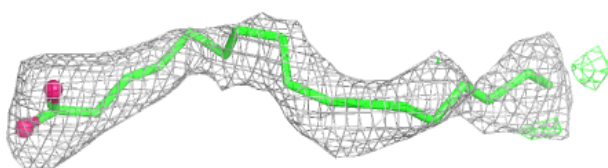
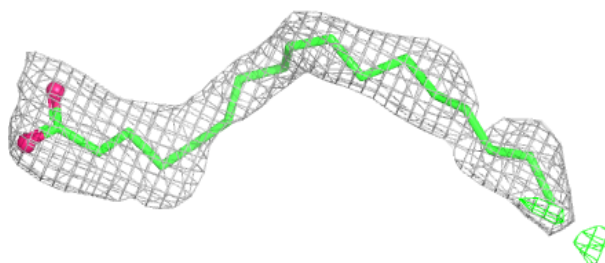
**Electron density around OLA A 1202:**

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

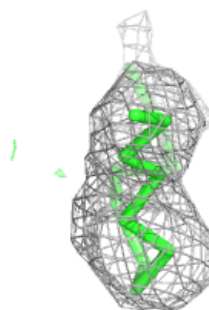
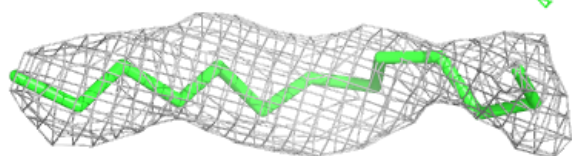
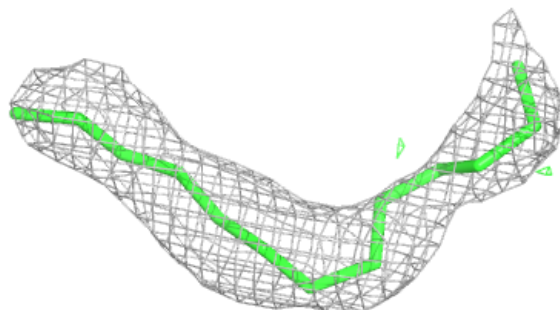


Electron density around OLA A 1214:

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and green (positive)

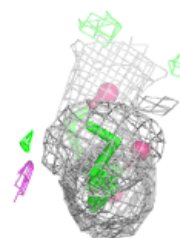
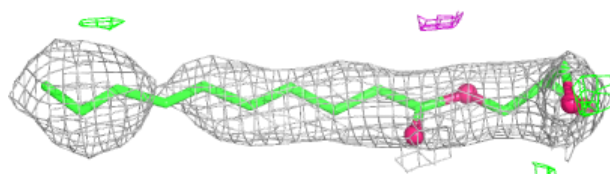
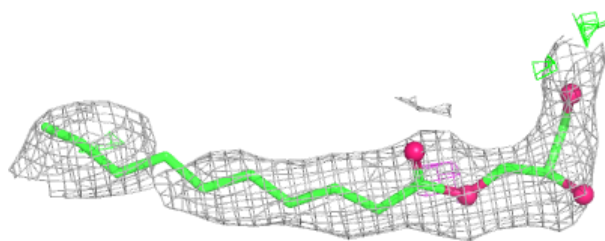
**Electron density around OLA A 1219:**

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

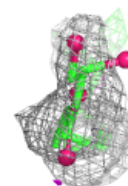
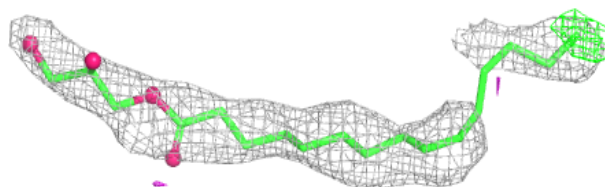


Electron density around OLC A 1221:

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

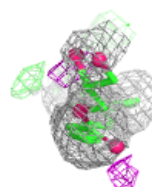
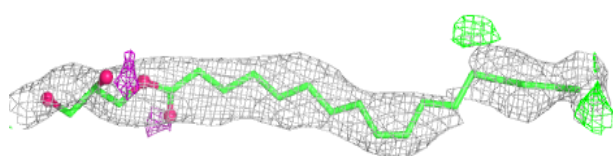
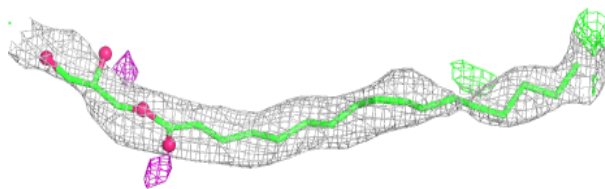
**Electron density around OLC A 1225:**

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

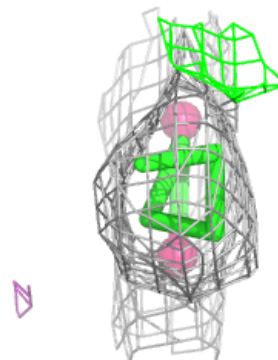
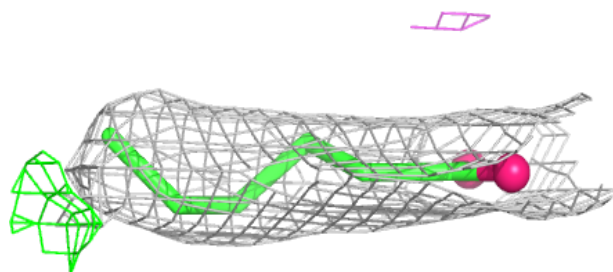
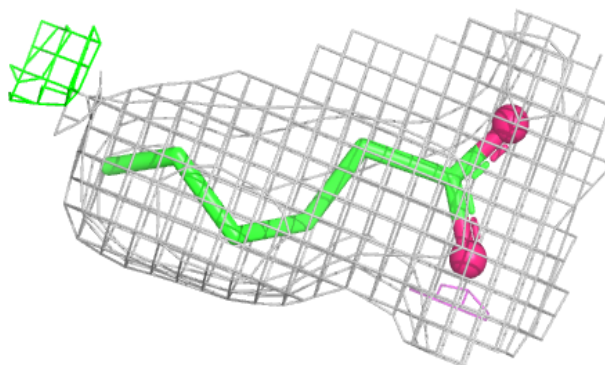


Electron density around OLC A 1224:

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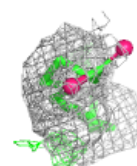
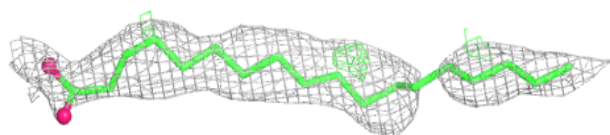
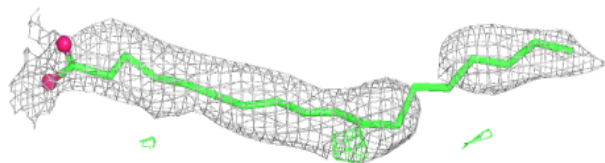
**Electron density around OLA A 1212:**

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and green (positive)

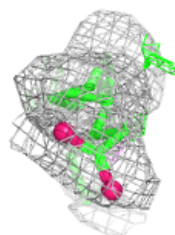
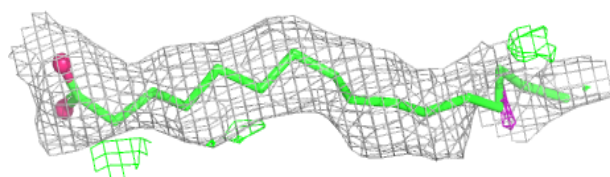
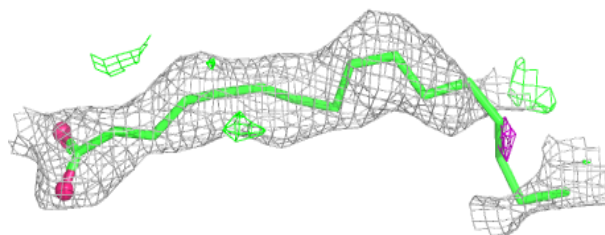


Electron density around OLC A 1227:

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and green (positive)

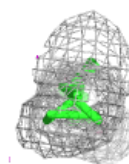
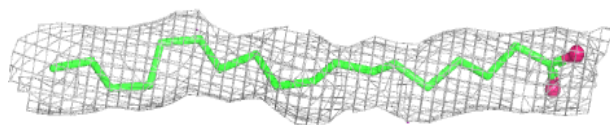
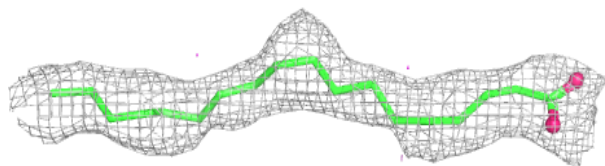
**Electron density around OLA A 1208:**

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and green (positive)

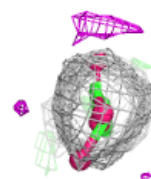
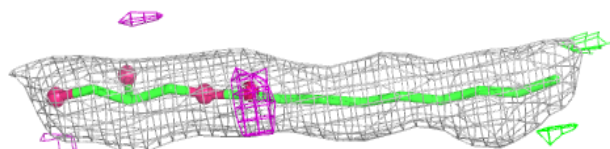
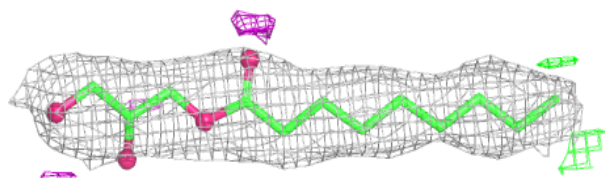


Electron density around OLA A 1228:

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and green (positive)

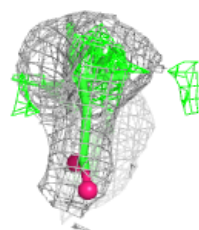
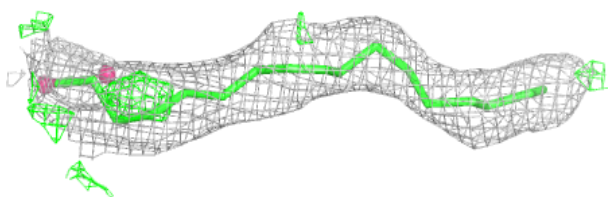
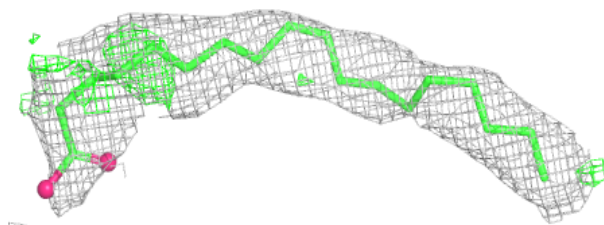
**Electron density around OLC A 1220:**

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and green (positive)

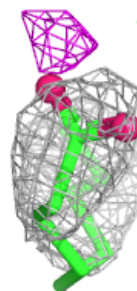
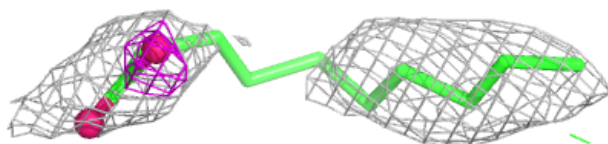
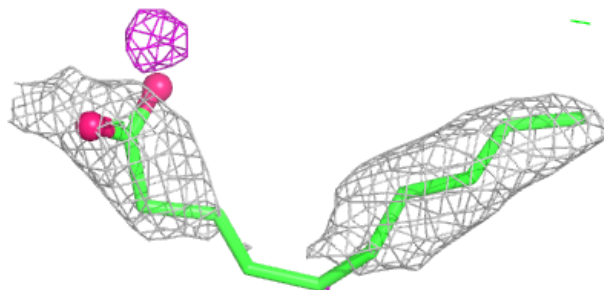


Electron density around OLC A 1226:

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and green (positive)

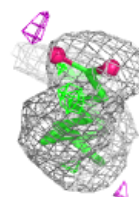
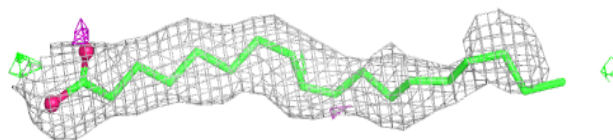
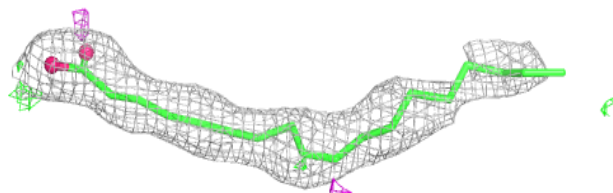
**Electron density around OLA A 1211:**

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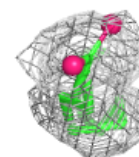
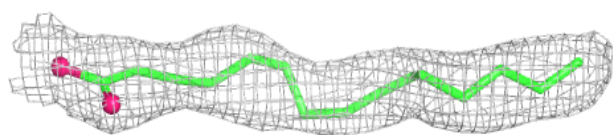
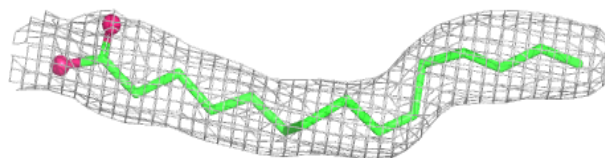


Electron density around OLC A 1223:

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

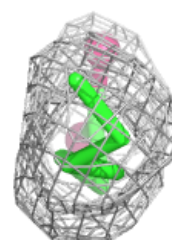
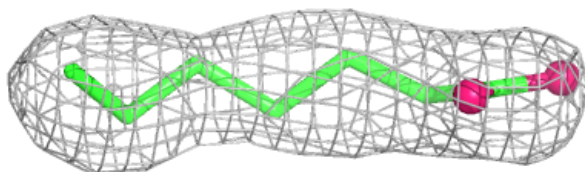
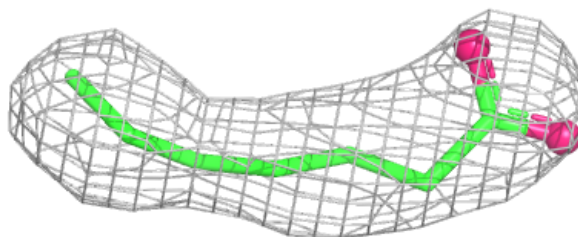
**Electron density around OLC A 1222:**

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

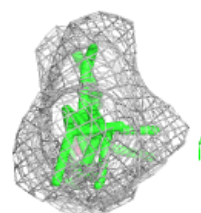
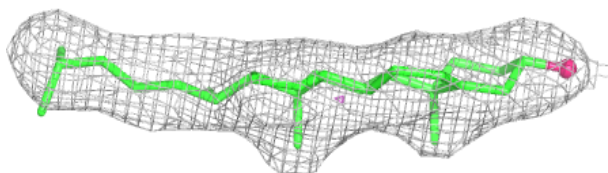
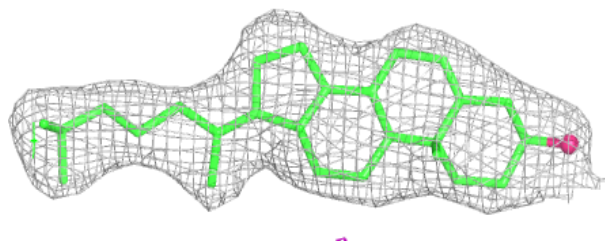


Electron density around OLA A 1207:

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

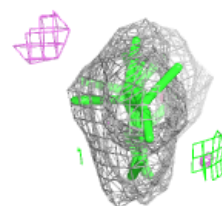
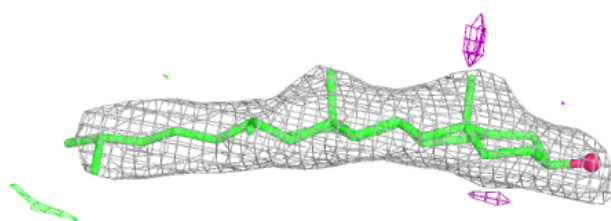
**Electron density around CLR A 1205:**

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

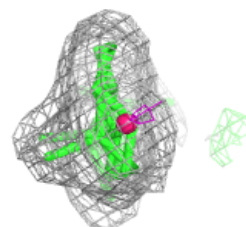
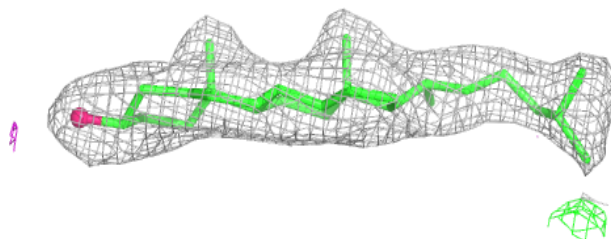
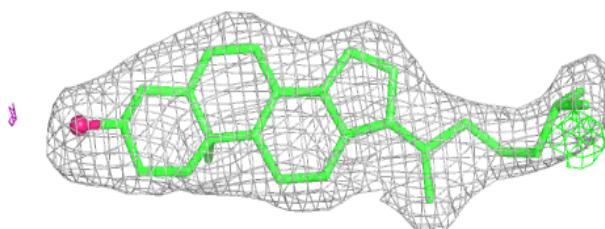


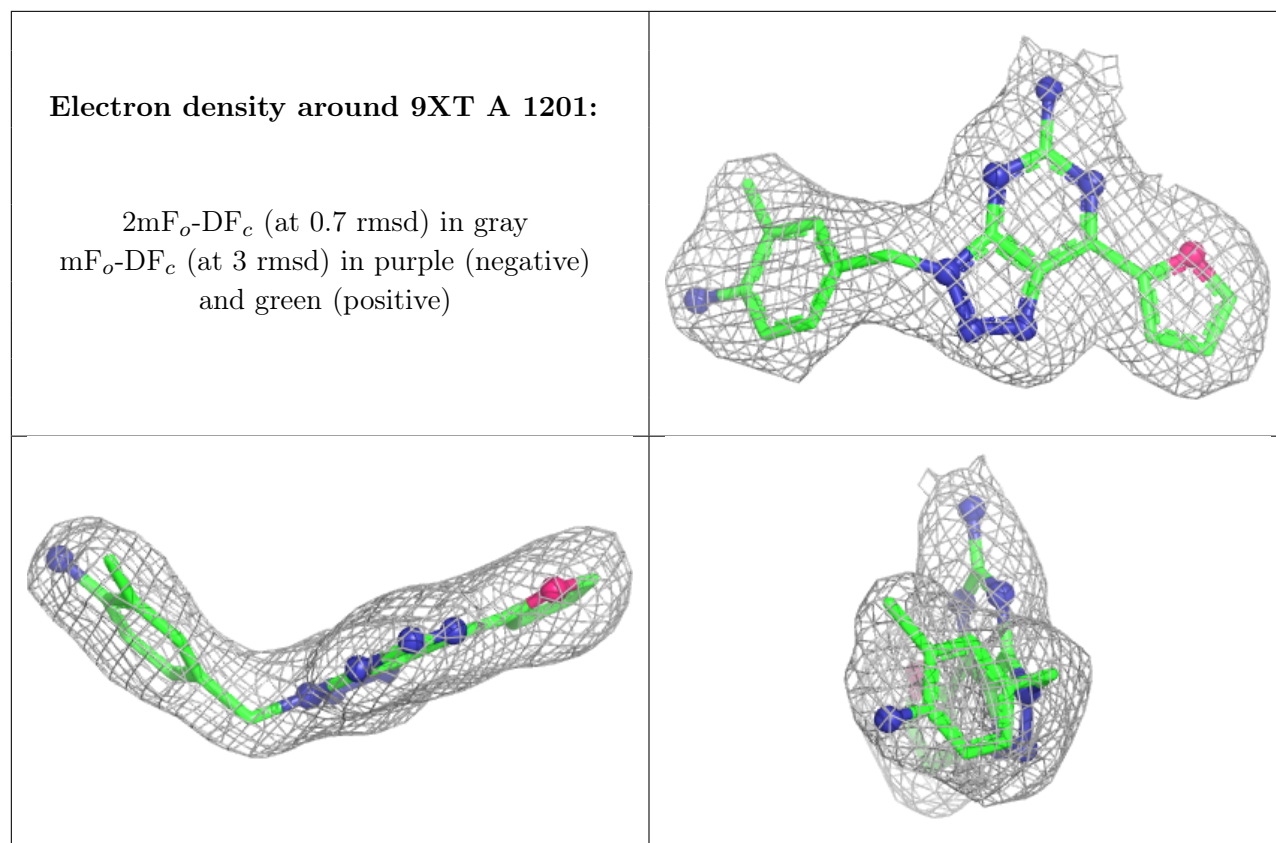
Electron density around CLR A 1204:

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

**Electron density around CLR 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.