



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:42 PM UTC

PDB ID : 5OLG / pdb_00005olg
Title : Structure of the A2A-StaR2-bRIL562-ZM241385 complex at 1.86Å 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 : 1.87 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	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

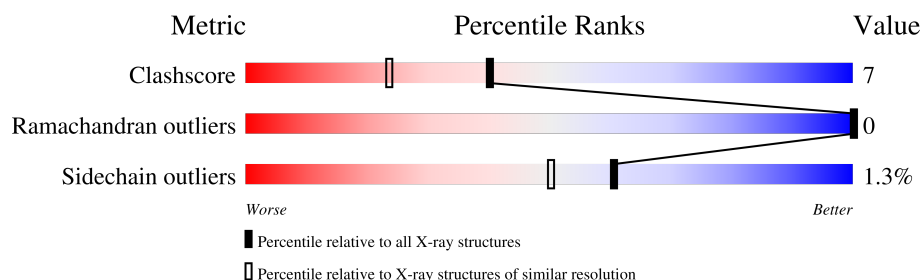
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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))
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	434	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLA	A	1221	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3719 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	11	0
			3097	2024	520	531	22			

There are 34 discrepancies between the modelled and reference sequences:

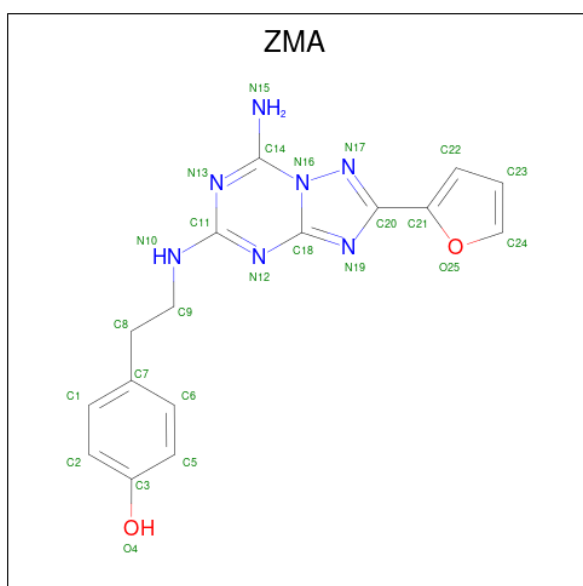
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
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	conflict	UNP P0ABE7
A	1106	LEU	-	linker	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 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).



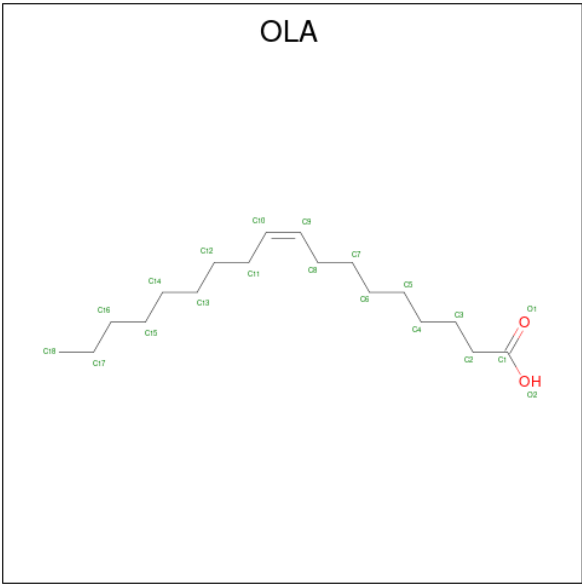
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



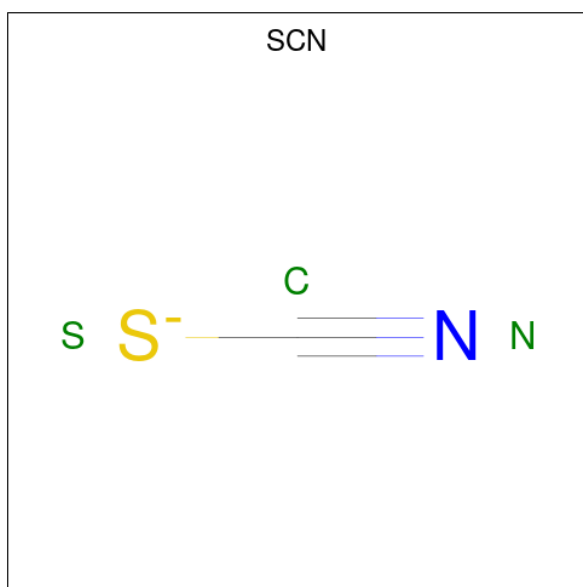
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



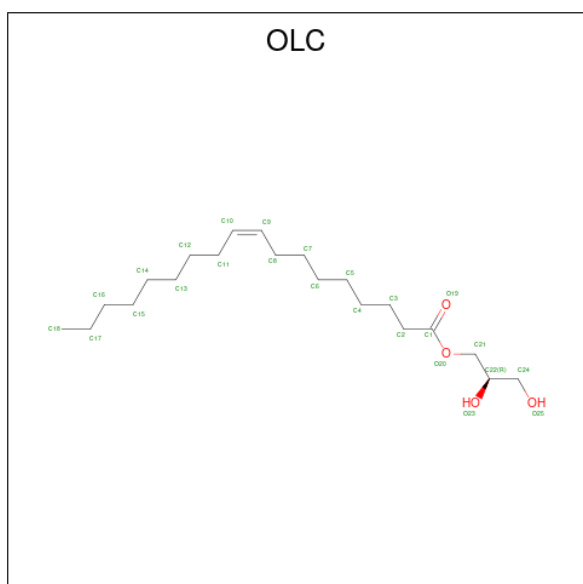
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			11	9	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			15	13	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



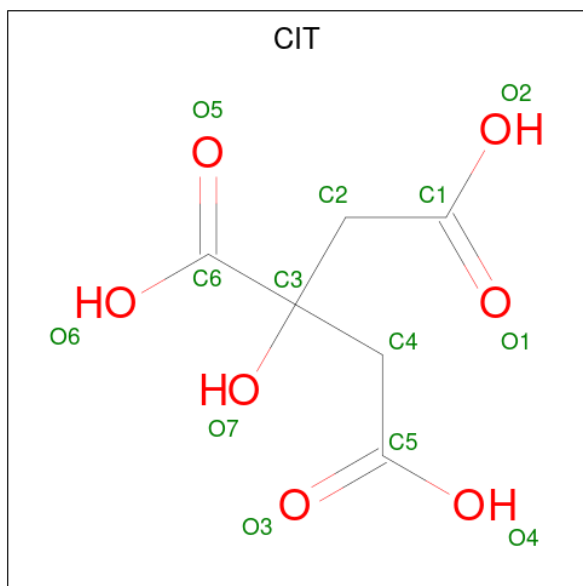
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			25	21	4		
6	A	1	Total	C	O	0	0
			9	5	4		
6	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

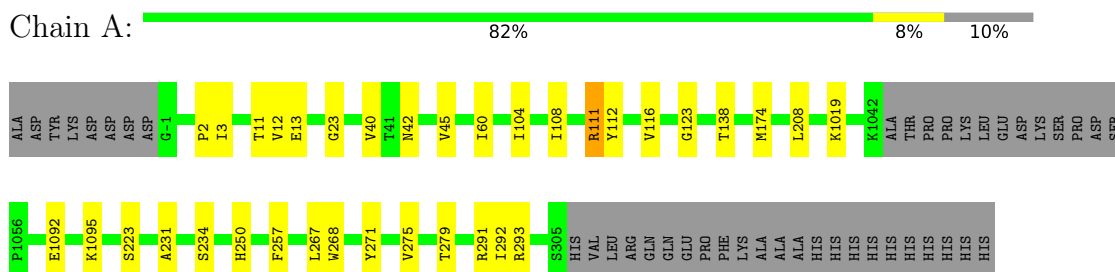
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	88	Total	O	0	0
			88	88		

i

Note EDS failed to run properly.

- Molecule 1: Adenosine receptor A2a, Soluble cytochrome b562, Adenosine receptor A2a



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.45Å 179.39Å 139.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.31 – 1.87	Depositor
% Data completeness (in resolution range)	97.7 (41.31-1.87)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.87Å)	Xtriage
Refinement program	PHENIX (1.12RC2_2821)	Depositor
R, R_{free}	0.189 , 0.224	Depositor
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.087	Xtriage
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
Total number of atoms	3719	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: OLC, OLA, ZMA, NA, CLR, SCN, CIT

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	0.51	0/3173	0.59	0/4317

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	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	3097	0	3181	36	0
2	A	25	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	112	0	184	8	0
4	A	312	0	500	29	0
5	A	12	0	0	1	0
6	A	59	0	87	1	0
7	A	13	0	5	1	0
8	A	1	0	0	0	0
9	A	88	0	0	3	0
All	All	3719	0	3972	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (50) 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:293:ARG:HG3	4:A:1221:OLA:C14	1.22	1.58
1:A:293:ARG:CG	4:A:1221:OLA:C14	1.84	1.49
1:A:293:ARG:CG	4:A:1221:OLA:H142	1.39	1.44
1:A:293:ARG:CG	4:A:1221:OLA:H141	1.58	1.17
1:A:293:ARG:HG2	4:A:1221:OLA:H141	1.06	1.01
1:A:123:GLY:HA3	7:A:1230:CIT:H22	1.58	0.85
4:A:1221:OLA:O2	9:A:1301:HOH:O	2.06	0.72
1:A:1092:GLU:OE2	1:A:1095:LYS:NZ	2.25	0.69
1:A:231:ALA:HA	4:A:1221:OLA:H71	1.79	0.65
1:A:293:ARG:CD	4:A:1221:OLA:H142	2.21	0.65
4:A:1219:OLA:H9	4:A:1220:OLA:H10	1.79	0.64
1:A:293:ARG:HG3	4:A:1221:OLA:C13	2.21	0.63
1:A:292:ILE:HG23	4:A:1221:OLA:H111	1.81	0.60
1:A:11:THR:HG23	4:A:1217:OLA:H81	1.83	0.59
1:A:268:TRP:CD1	3:A:1205:CLR:H3	2.38	0.58
1:A:293:ARG:HG3	4:A:1221:OLA:H142	0.58	0.58
4:A:1206:OLA:H162	4:A:1220:OLA:H152	1.85	0.58
1:A:250:HIS:CE1	2:A:1201:ZMA:H24	2.40	0.57
1:A:108:ILE:HB	1:A:111:ARG:HG3	1.88	0.55
1:A:292:ILE:HG12	4:A:1221:OLA:H72	1.88	0.55
4:A:1208:OLA:H31	9:A:1377:HOH:O	2.06	0.54
1:A:2:PRO:HD2	5:A:1225:SCN:S	2.47	0.54
3:A:1203:CLR:H161	4:A:1208:OLA:H141	1.90	0.54
1:A:12:VAL:HG22	6:A:1229:OLC:H7	1.89	0.53
1:A:234:SER:OG	1:A:291:ARG:NE	2.33	0.53
4:A:1212:OLA:H9	4:A:1216:OLA:H141	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1216:OLA:H152	4:A:1216:OLA:H111	1.92	0.51
1:A:293:ARG:HG2	4:A:1221:OLA:C14	1.78	0.50
1:A:42:ASN:HA	1:A:45:VAL:HB	1.94	0.50
1:A:293:ARG:H	4:A:1221:OLA:C13	2.25	0.49
1:A:1019:LYS:HE2	1:A:1019:LYS:HB3	1.66	0.47
1:A:267:LEU:HD11	1:A:271:TYR:HE2	1.79	0.46
3:A:1205:CLR:H213	4:A:1215:OLA:H132	1.97	0.46
1:A:293:ARG:H	4:A:1221:OLA:H132	1.80	0.46
1:A:275[B]:VAL:O	1:A:279[B]:THR:HG23	2.18	0.44
3:A:1204:CLR:H263	4:A:1209:OLA:H161	2.00	0.44
3:A:1205:CLR:H161	4:A:1218:OLA:H122	1.99	0.43
1:A:174:MET:HG3	1:A:257:PHE:HB2	2.01	0.43
1:A:104:ILE:HG22	1:A:112:TYR:HD1	1.84	0.43
3:A:1205:CLR:H193	3:A:1205:CLR:H111	1.87	0.42
1:A:293:ARG:HG3	4:A:1221:OLA:C12	2.49	0.42
4:A:1208:OLA:H52	4:A:1208:OLA:H21	1.84	0.42
1:A:292:ILE:HA	4:A:1221:OLA:H132	2.01	0.42
3:A:1204:CLR:H272	3:A:1204:CLR:H231	1.73	0.42
1:A:23:GLY:HA3	9:A:1362:HOH:O	2.20	0.41
1:A:268:TRP:CB	3:A:1205:CLR:H12	2.50	0.41
1:A:13:GLU:HB3	1:A:60:ILE:HG23	2.03	0.41
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.51	0.41
4:A:1216:OLA:H183	4:A:1216:OLA:H151	1.77	0.41
1:A:40:VAL:HG11	1:A:116:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/434 (92%)	394 (99%)	3 (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	325/353 (92%)	321 (99%)	4 (1%)	63 53

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	111	ARG
1	A	138	THR
1	A	223	SER

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	230	HIS

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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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
2	ZMA	A	1201	-	26,28,28	1.31	4 (15%)	30,39,39	1.99	9 (30%)
4	OLA	A	1215	-	19,19,19	0.49	0	19,19,19	0.85	0
3	CLR	A	1202	-	31,31,31	0.71	0	48,48,48	1.28	6 (12%)
3	CLR	A	1204	-	31,31,31	0.64	0	48,48,48	0.91	2 (4%)
3	CLR	A	1203	-	31,31,31	0.59	0	48,48,48	1.12	4 (8%)
7	CIT	A	1230	-	12,12,12	1.09	0	17,17,17	1.84	4 (23%)
4	OLA	A	1208	-	19,19,19	0.43	0	19,19,19	1.09	1 (5%)
5	SCN	A	1223	-	1,2,2	0.29	0	0,1,1	-	-
6	OLC	A	1229	-	24,24,24	0.95	1 (4%)	25,25,25	1.11	2 (8%)
3	CLR	A	1205	-	31,31,31	0.71	1 (3%)	48,48,48	1.15	3 (6%)
4	OLA	A	1214	-	10,10,19	0.56	0	10,10,19	1.48	2 (20%)
4	OLA	A	1213	-	19,19,19	0.62	0	19,19,19	0.53	0
4	OLA	A	1222	-	5,5,19	1.02	0	5,5,19	0.77	0
4	OLA	A	1216	-	19,19,19	0.42	0	19,19,19	0.98	0
4	OLA	A	1212	-	19,19,19	0.50	0	19,19,19	0.80	0
4	OLA	A	1217	-	19,19,19	0.55	0	19,19,19	0.94	1 (5%)
4	OLA	A	1218	-	14,14,19	0.64	0	14,14,19	0.94	0
5	SCN	A	1225	-	1,2,2	0.27	0	0,1,1	-	-
4	OLA	A	1221	-	19,19,19	0.59	0	19,19,19	0.88	0
4	OLA	A	1211	-	19,19,19	0.49	0	19,19,19	1.03	1 (5%)
6	OLC	A	1228	-	8,8,24	1.07	1 (12%)	9,9,25	0.99	0
4	OLA	A	1209	-	19,19,19	0.46	0	19,19,19	1.16	3 (15%)
4	OLA	A	1210	-	19,19,19	0.58	0	19,19,19	1.16	1 (5%)
4	OLA	A	1219	-	19,19,19	0.52	0	19,19,19	0.79	0
5	SCN	A	1226	-	1,2,2	0.08	0	0,1,1	-	-
5	SCN	A	1224	-	1,2,2	0.17	0	0,1,1	-	-
6	OLC	A	1227	-	24,24,24	1.03	1 (4%)	25,25,25	1.06	2 (8%)
4	OLA	A	1207	-	19,19,19	0.53	0	19,19,19	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLA	A	1206	-	19,19,19	0.58	0	19,19,19	0.82	0
4	OLA	A	1220	-	19,19,19	0.50	0	19,19,19	0.71	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
2	ZMA	A	1201	-	-	0/10/10/10	0/4/4/4
4	OLA	A	1215	-	-	9/17/17/17	-
3	CLR	A	1202	-	-	2/10/68/68	0/4/4/4
3	CLR	A	1204	-	-	2/10/68/68	0/4/4/4
3	CLR	A	1203	-	-	0/10/68/68	0/4/4/4
7	CIT	A	1230	-	-	7/16/16/16	-
4	OLA	A	1208	-	-	6/17/17/17	-
6	OLC	A	1229	-	-	6/24/24/24	-
3	CLR	A	1205	-	-	1/10/68/68	0/4/4/4
4	OLA	A	1214	-	-	6/8/8/17	-
4	OLA	A	1213	-	-	7/17/17/17	-
4	OLA	A	1222	-	-	0/3/3/17	-
4	OLA	A	1216	-	-	8/17/17/17	-
4	OLA	A	1212	-	-	4/17/17/17	-
4	OLA	A	1217	-	-	6/17/17/17	-
4	OLA	A	1218	-	-	6/12/12/17	-
4	OLA	A	1221	-	-	8/17/17/17	-
4	OLA	A	1211	-	-	7/17/17/17	-
6	OLC	A	1228	-	-	2/7/7/24	-
4	OLA	A	1209	-	-	4/17/17/17	-
4	OLA	A	1210	-	-	3/17/17/17	-
4	OLA	A	1219	-	-	2/17/17/17	-
6	OLC	A	1227	-	-	5/24/24/24	-
4	OLA	A	1207	-	-	4/17/17/17	-
4	OLA	A	1206	-	-	5/17/17/17	-
4	OLA	A	1220	-	-	6/17/17/17	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1227	OLC	O20-C1	4.63	1.46	1.33
6	A	1229	OLC	O20-C1	4.34	1.46	1.33
2	A	1201	ZMA	C18-N16	-2.69	1.34	1.38
6	A	1228	OLC	O20-C1	2.69	1.46	1.33
2	A	1201	ZMA	C20-N17	2.64	1.37	1.33
3	A	1205	CLR	C10-C9	-2.25	1.52	1.56
2	A	1201	ZMA	C14-N16	-2.17	1.34	1.37
2	A	1201	ZMA	C23-C24	2.06	1.40	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1230	CIT	O6-C6-C3	4.95	122.64	113.14
2	A	1201	ZMA	C9-C8-C7	-4.59	102.49	112.83
4	A	1210	OLA	C3-C2-C1	-4.43	102.94	114.51
2	A	1201	ZMA	C18-N16-N17	4.02	113.41	110.41
2	A	1201	ZMA	N13-C11-N12	-4.01	119.84	126.79
6	A	1229	OLC	O20-C1-C2	3.84	123.54	111.83
3	A	1202	CLR	C7-C8-C9	3.62	113.90	109.72
6	A	1227	OLC	O20-C1-C2	3.54	122.62	111.83
2	A	1201	ZMA	O25-C21-C22	3.35	114.90	109.96
6	A	1229	OLC	O20-C1-O19	-3.21	115.59	123.63
3	A	1202	CLR	C3-C4-C5	-3.17	107.00	112.05
3	A	1202	CLR	C18-C13-C17	-2.95	106.33	111.68
2	A	1201	ZMA	C23-C22-C21	-2.92	101.94	106.52
2	A	1201	ZMA	N10-C11-N13	2.78	120.84	116.54
4	A	1217	OLA	C3-C2-C1	-2.72	107.40	114.51
3	A	1202	CLR	C11-C12-C13	-2.66	108.25	112.74
4	A	1214	OLA	C3-C2-C1	-2.65	107.59	114.51
3	A	1205	CLR	C4-C5-C10	2.64	119.80	116.42
2	A	1201	ZMA	N15-C14-N16	2.64	121.62	118.32
2	A	1201	ZMA	C20-N17-N16	-2.62	98.68	101.39
3	A	1204	CLR	C12-C13-C17	2.53	120.33	116.60
4	A	1208	OLA	C3-C2-C1	-2.45	108.12	114.51
6	A	1227	OLC	O20-C1-O19	-2.45	117.50	123.63
3	A	1203	CLR	C19-C10-C9	-2.45	108.92	111.66
7	A	1230	CIT	O2-C1-C2	2.44	122.08	114.35
3	A	1203	CLR	C21-C20-C22	-2.43	106.57	110.34
3	A	1204	CLR	C11-C9-C10	-2.35	110.19	113.08
4	A	1209	OLA	O1-C1-C2	-2.35	115.64	123.09
3	A	1203	CLR	C4-C5-C10	2.33	119.40	116.42
2	A	1201	ZMA	N10-C11-N12	2.32	119.31	116.95
3	A	1202	CLR	C15-C14-C8	-2.27	115.48	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	CLR	C19-C10-C9	-2.26	109.12	111.66
4	A	1207	OLA	C6-C5-C4	-2.25	102.98	114.37
4	A	1209	OLA	C3-C2-C1	-2.25	108.64	114.51
3	A	1205	CLR	C19-C10-C9	-2.17	109.22	111.66
4	A	1211	OLA	C3-C2-C1	-2.17	108.84	114.51
3	A	1203	CLR	C15-C14-C13	2.17	106.39	103.84
7	A	1230	CIT	O2-C1-O1	-2.15	117.81	123.33
4	A	1214	OLA	O1-C1-C2	-2.14	116.30	123.09
7	A	1230	CIT	O6-C6-O5	-2.09	117.16	123.86
4	A	1209	OLA	O2-C1-C2	2.09	120.61	114.00
3	A	1205	CLR	C11-C9-C10	-2.01	110.61	113.08

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1228	OLC	O20-C21-C22-O23
7	A	1230	CIT	O7-C3-C4-C5
7	A	1230	CIT	C6-C3-C4-C5
6	A	1227	OLC	O20-C21-C22-O23
7	A	1230	CIT	C2-C3-C4-C5
4	A	1211	OLA	C1-C2-C3-C4
4	A	1206	OLA	C1-C2-C3-C4
4	A	1214	OLA	C1-C2-C3-C4
4	A	1215	OLA	C1-C2-C3-C4
4	A	1220	OLA	C1-C2-C3-C4
4	A	1216	OLA	C15-C16-C17-C18
4	A	1215	OLA	C11-C12-C13-C14
4	A	1206	OLA	C11-C12-C13-C14
4	A	1211	OLA	C2-C3-C4-C5
4	A	1220	OLA	C14-C15-C16-C17
6	A	1227	OLC	C10-C11-C12-C13
4	A	1220	OLA	C5-C6-C7-C8
4	A	1216	OLA	C2-C3-C4-C5
4	A	1216	OLA	C11-C12-C13-C14
4	A	1221	OLA	C3-C4-C5-C6
4	A	1214	OLA	C2-C3-C4-C5
4	A	1216	OLA	C14-C15-C16-C17
4	A	1221	OLA	C12-C13-C14-C15
4	A	1213	OLA	C4-C5-C6-C7
4	A	1216	OLA	C13-C14-C15-C16
6	A	1227	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
4	A	1213	OLA	C10-C11-C12-C13
4	A	1215	OLA	C5-C6-C7-C8
4	A	1218	OLA	C2-C3-C4-C5
6	A	1229	OLC	C14-C15-C16-C17
6	A	1227	OLC	C4-C5-C6-C7
4	A	1208	OLA	C4-C5-C6-C7
4	A	1221	OLA	C1-C2-C3-C4
4	A	1216	OLA	C4-C5-C6-C7
4	A	1211	OLA	C6-C7-C8-C9
4	A	1212	OLA	C6-C7-C8-C9
4	A	1213	OLA	C6-C7-C8-C9
4	A	1208	OLA	C11-C12-C13-C14
4	A	1207	OLA	C10-C11-C12-C13
4	A	1215	OLA	C6-C7-C8-C9
4	A	1221	OLA	C14-C15-C16-C17
4	A	1212	OLA	C2-C3-C4-C5
4	A	1211	OLA	C15-C16-C17-C18
4	A	1218	OLA	C3-C4-C5-C6
3	A	1202	CLR	C23-C24-C25-C26
4	A	1210	OLA	C3-C4-C5-C6
4	A	1216	OLA	C1-C2-C3-C4
4	A	1213	OLA	C15-C16-C17-C18
4	A	1218	OLA	C1-C2-C3-C4
4	A	1210	OLA	C5-C6-C7-C8
4	A	1211	OLA	C12-C13-C14-C15
6	A	1228	OLC	O20-C21-C22-C24
4	A	1209	OLA	C13-C14-C15-C16
4	A	1209	OLA	C14-C15-C16-C17
3	A	1204	CLR	C22-C23-C24-C25
3	A	1202	CLR	C23-C24-C25-C27
4	A	1217	OLA	C1-C2-C3-C4
6	A	1229	OLC	C11-C12-C13-C14
4	A	1211	OLA	C11-C12-C13-C14
4	A	1212	OLA	C10-C11-C12-C13
7	A	1230	CIT	C1-C2-C3-O7
4	A	1215	OLA	C4-C5-C6-C7
4	A	1211	OLA	C9-C10-C11-C12
4	A	1217	OLA	C4-C5-C6-C7
4	A	1208	OLA	C7-C8-C9-C10
4	A	1213	OLA	C9-C10-C11-C12
4	A	1206	OLA	C12-C13-C14-C15
6	A	1229	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	A	1217	OLA	C9-C10-C11-C12
4	A	1207	OLA	C7-C8-C9-C10
4	A	1220	OLA	C9-C10-C11-C12
4	A	1215	OLA	C12-C13-C14-C15
4	A	1220	OLA	C2-C3-C4-C5
4	A	1213	OLA	C13-C14-C15-C16
4	A	1214	OLA	O1-C1-C2-C3
4	A	1207	OLA	O2-C1-C2-C3
4	A	1207	OLA	O1-C1-C2-C3
6	A	1229	OLC	C2-C3-C4-C5
4	A	1221	OLA	O1-C1-C2-C3
4	A	1221	OLA	O2-C1-C2-C3
3	A	1205	CLR	C21-C20-C22-C23
6	A	1229	OLC	O20-C21-C22-O23
4	A	1214	OLA	C6-C7-C8-C9
4	A	1214	OLA	O2-C1-C2-C3
3	A	1204	CLR	C20-C22-C23-C24
4	A	1206	OLA	C9-C10-C11-C12
4	A	1212	OLA	C14-C15-C16-C17
4	A	1206	OLA	C7-C8-C9-C10
4	A	1209	OLA	C7-C8-C9-C10
4	A	1209	OLA	C9-C10-C11-C12
4	A	1218	OLA	C7-C8-C9-C10
4	A	1215	OLA	C7-C8-C9-C10
4	A	1213	OLA	C11-C12-C13-C14
6	A	1229	OLC	C1-C2-C3-C4
4	A	1215	OLA	O2-C1-C2-C3
4	A	1208	OLA	O1-C1-C2-C3
4	A	1217	OLA	C2-C3-C4-C5
4	A	1216	OLA	C7-C8-C9-C10
4	A	1218	OLA	O1-C1-C2-C3
4	A	1217	OLA	C3-C4-C5-C6
4	A	1215	OLA	O1-C1-C2-C3
4	A	1217	OLA	C14-C15-C16-C17
4	A	1221	OLA	C9-C10-C11-C12
4	A	1220	OLA	C7-C8-C9-C10
7	A	1230	CIT	C1-C2-C3-C4
4	A	1214	OLA	C3-C4-C5-C6
7	A	1230	CIT	O1-C1-C2-C3
4	A	1219	OLA	O1-C1-C2-C3
4	A	1208	OLA	O2-C1-C2-C3
4	A	1219	OLA	O2-C1-C2-C3

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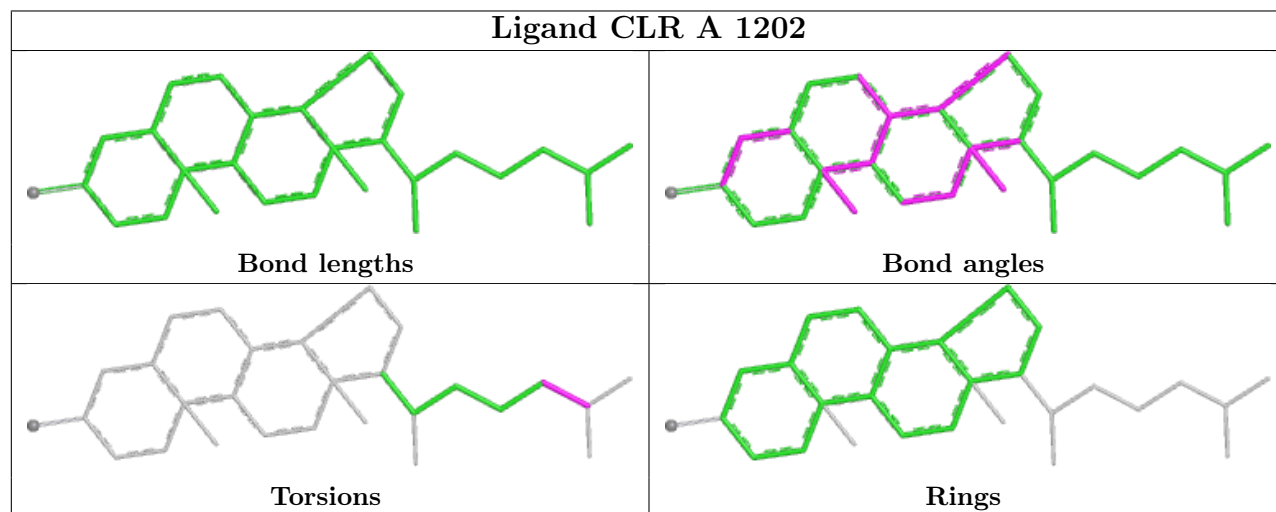
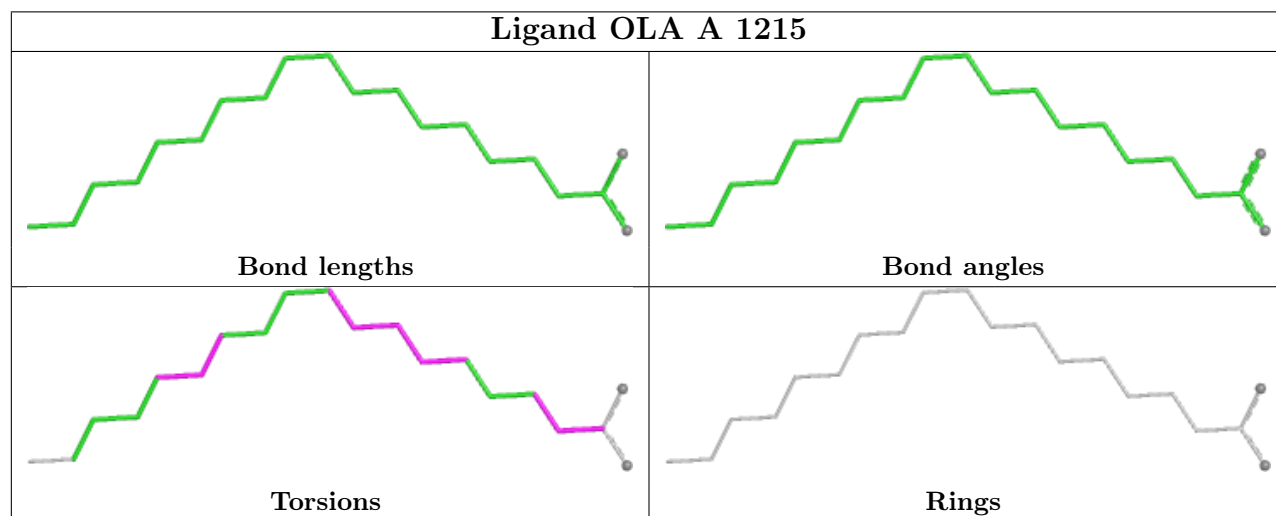
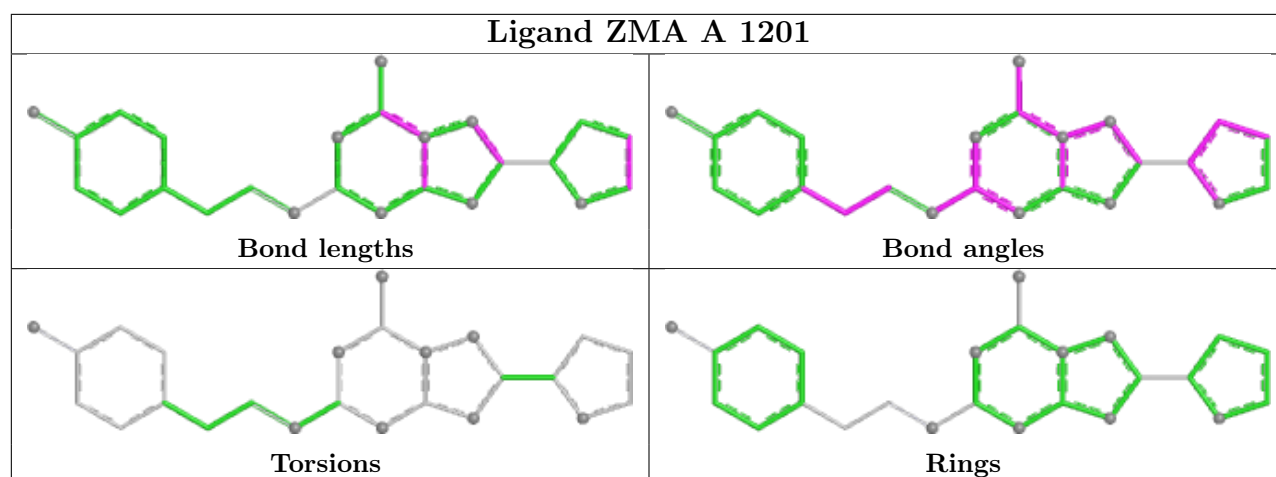
Mol	Chain	Res	Type	Atoms
4	A	1218	OLA	O2-C1-C2-C3
4	A	1208	OLA	C15-C16-C17-C18
7	A	1230	CIT	O2-C1-C2-C3
4	A	1210	OLA	O2-C1-C2-C3
4	A	1221	OLA	C15-C16-C17-C18
6	A	1227	OLC	C7-C8-C9-C10

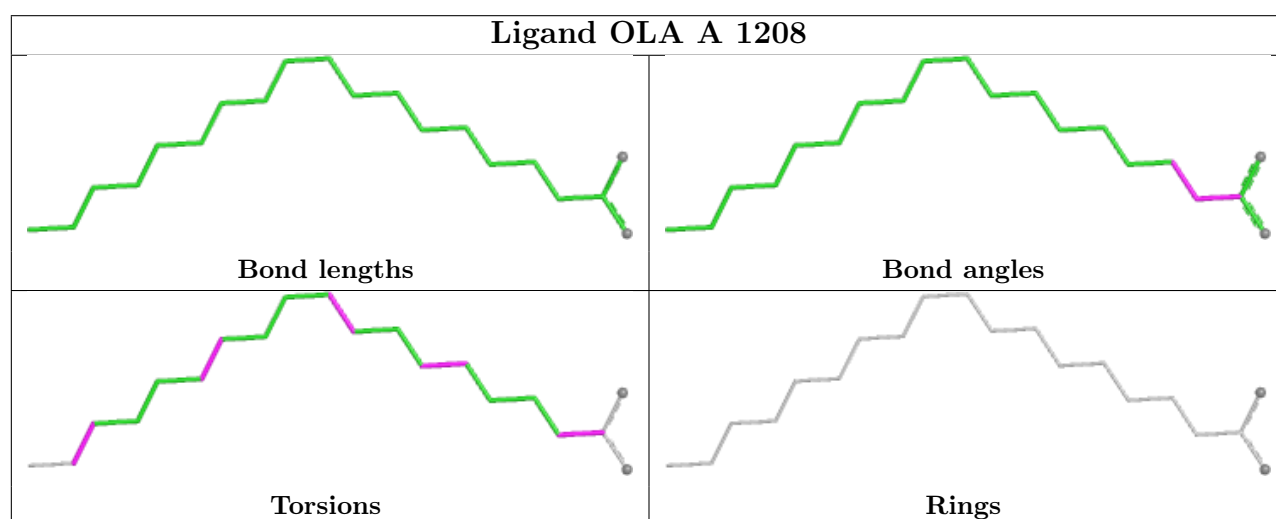
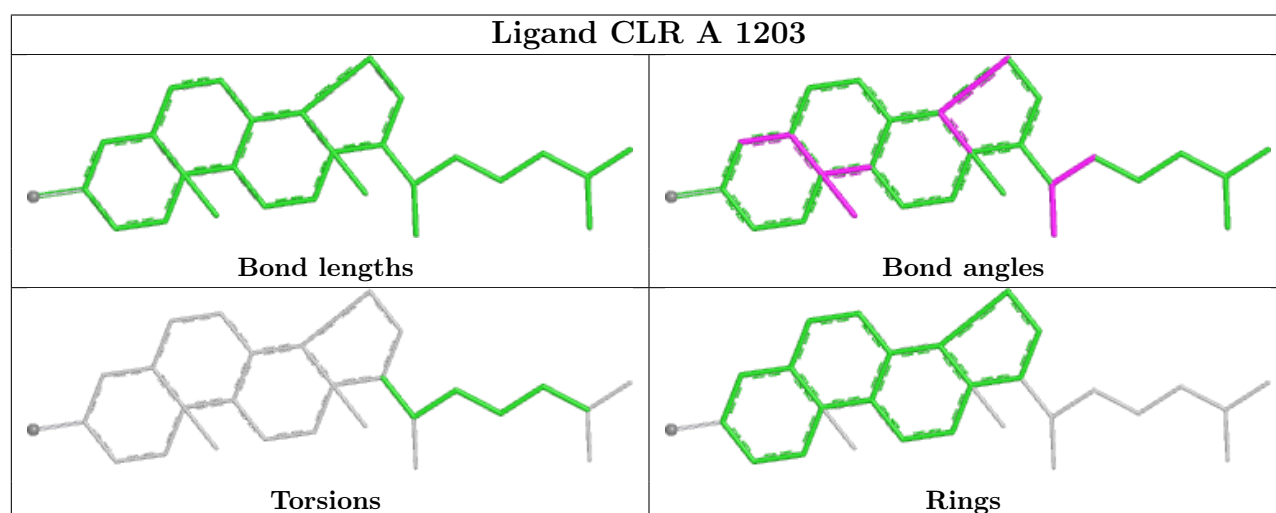
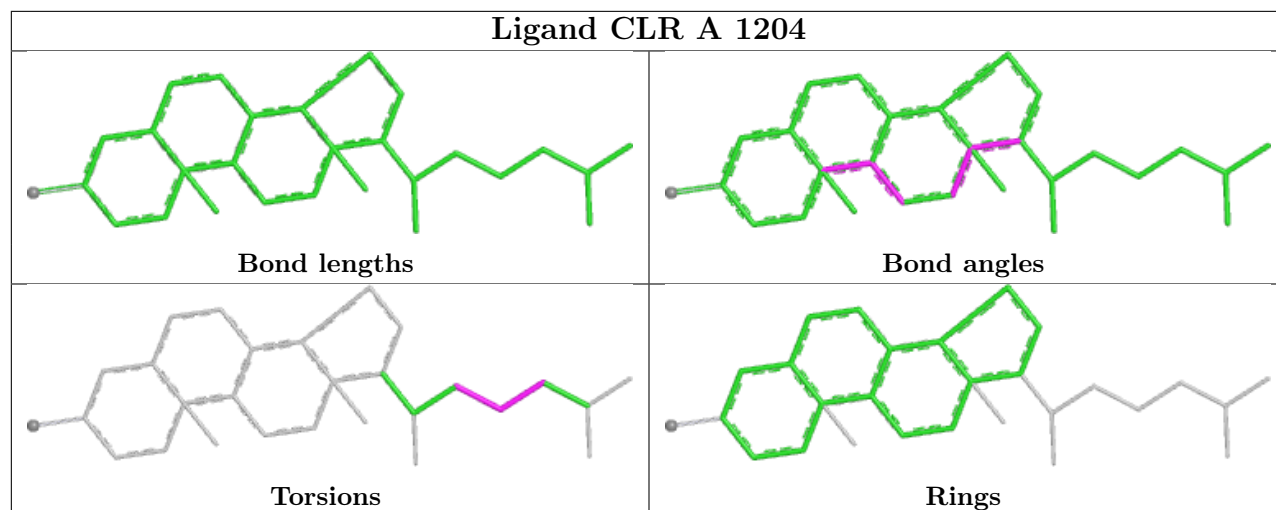
There are no ring outliers.

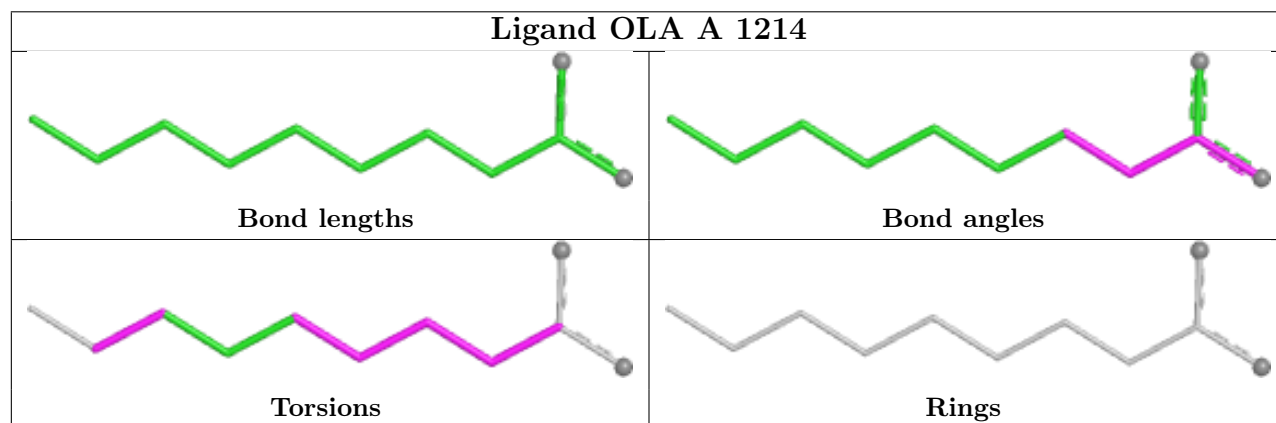
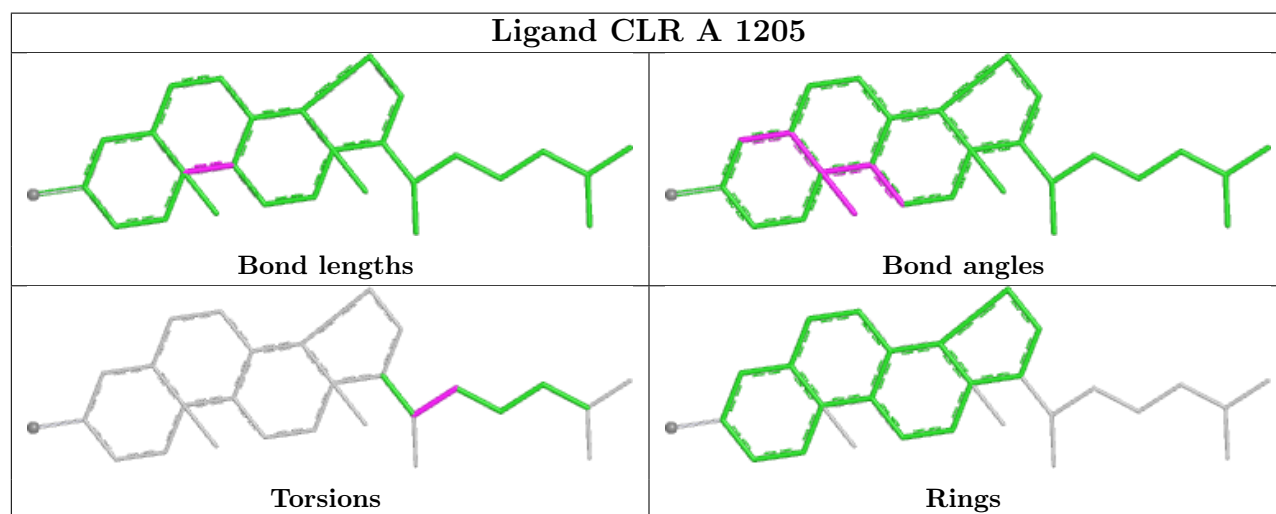
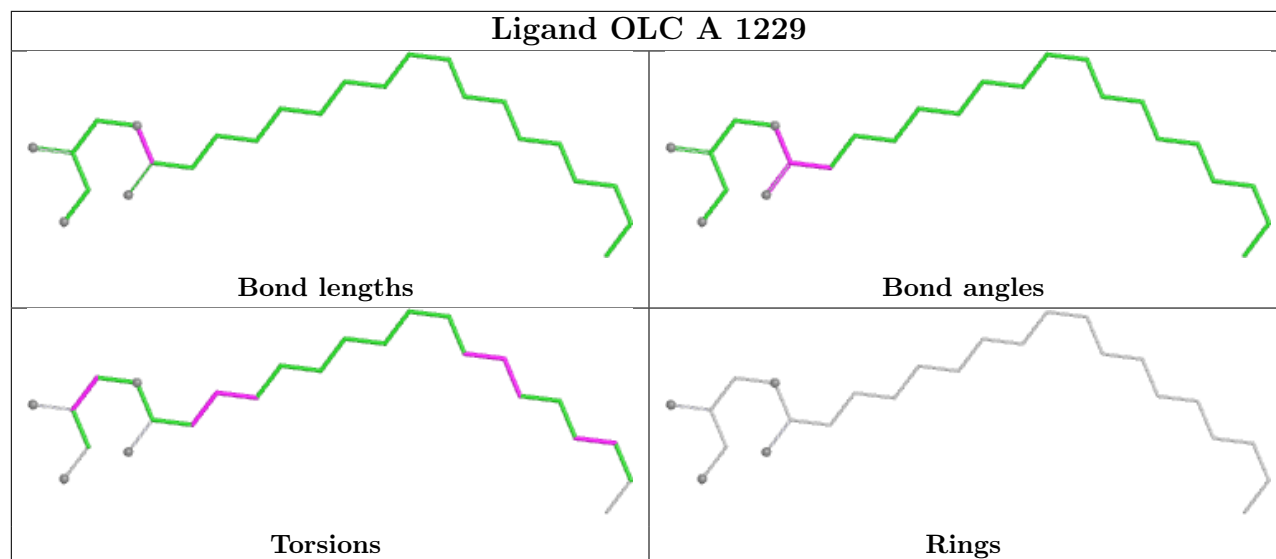
18 monomers are involved in 37 short contacts:

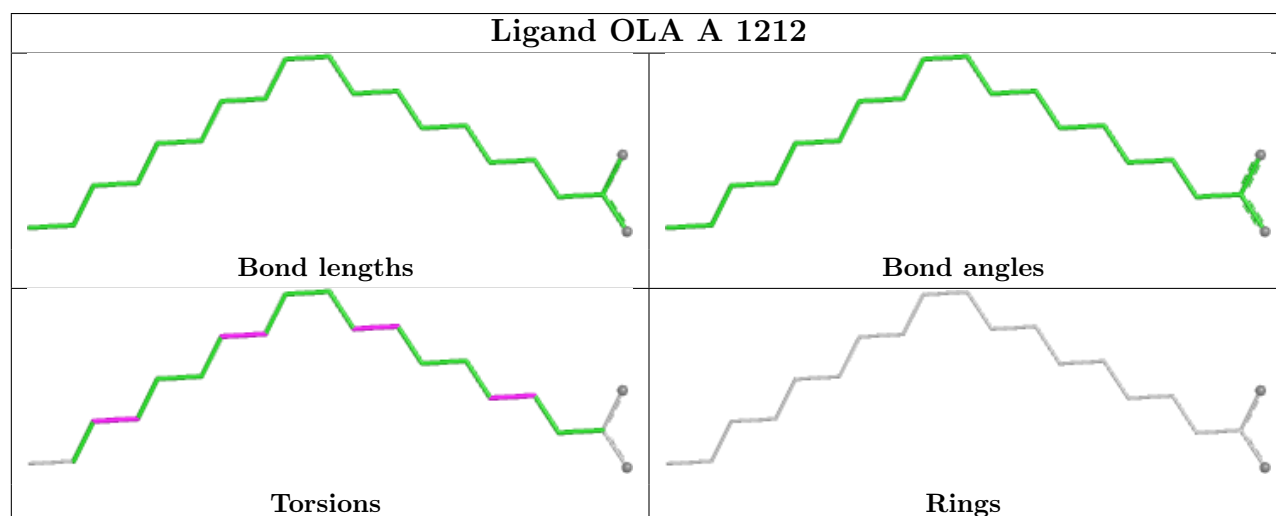
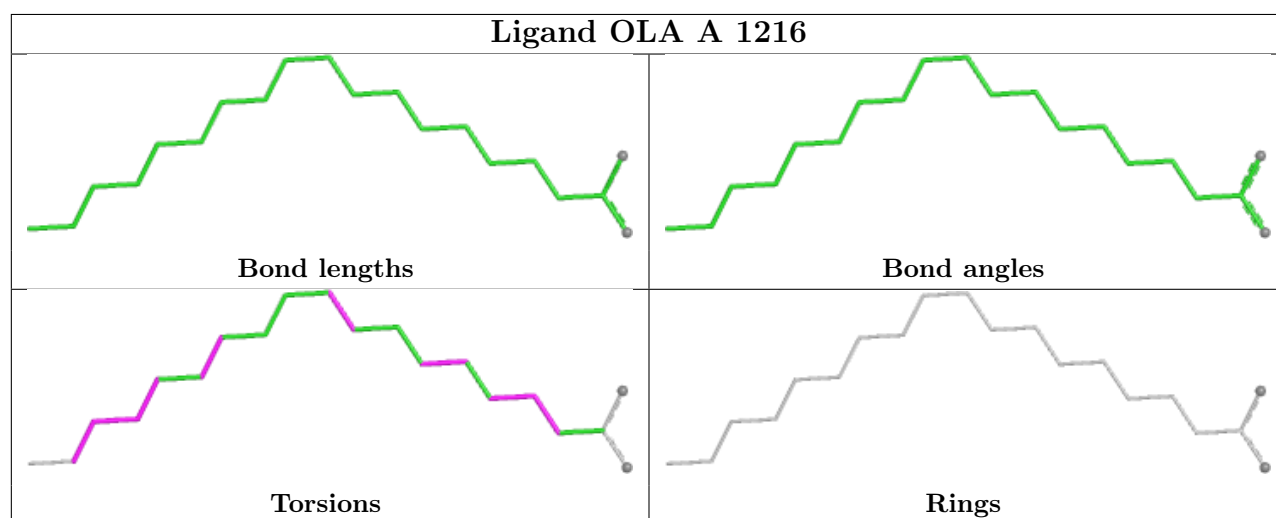
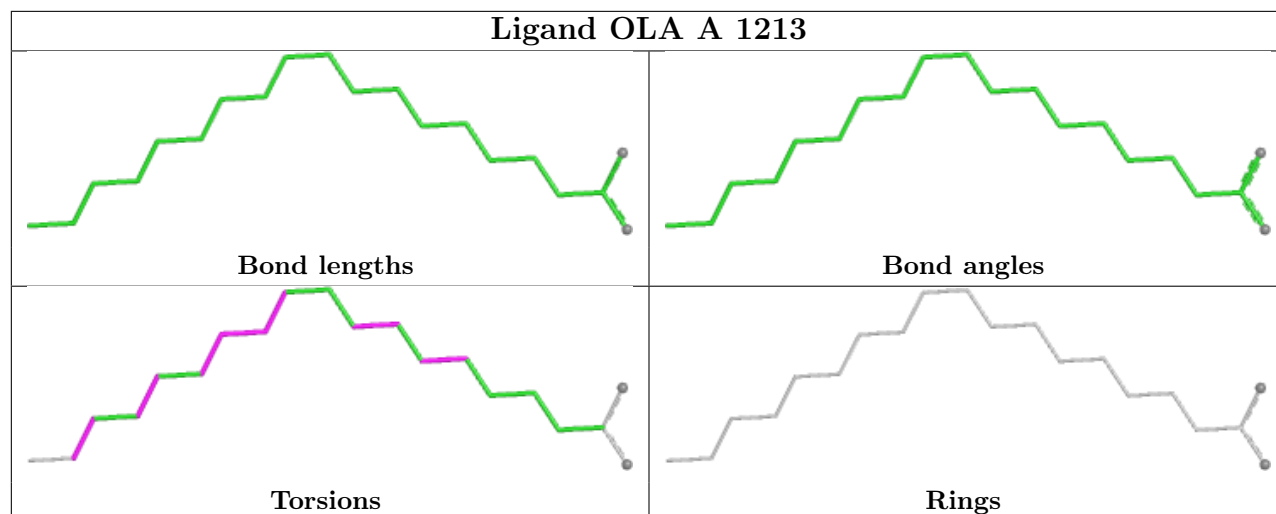
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ZMA	1	0
4	A	1215	OLA	1	0
3	A	1204	CLR	2	0
3	A	1203	CLR	1	0
7	A	1230	CIT	1	0
4	A	1208	OLA	3	0
6	A	1229	OLC	1	0
3	A	1205	CLR	5	0
4	A	1216	OLA	3	0
4	A	1212	OLA	1	0
4	A	1217	OLA	1	0
4	A	1218	OLA	1	0
5	A	1225	SCN	1	0
4	A	1221	OLA	17	0
4	A	1209	OLA	1	0
4	A	1219	OLA	1	0
4	A	1206	OLA	1	0
4	A	1220	OLA	2	0

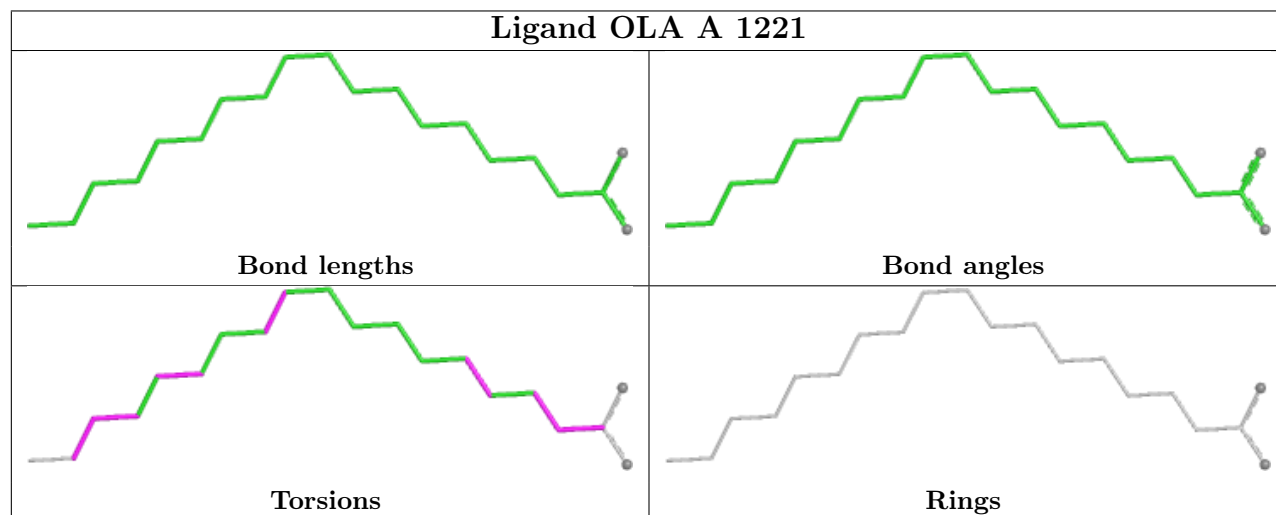
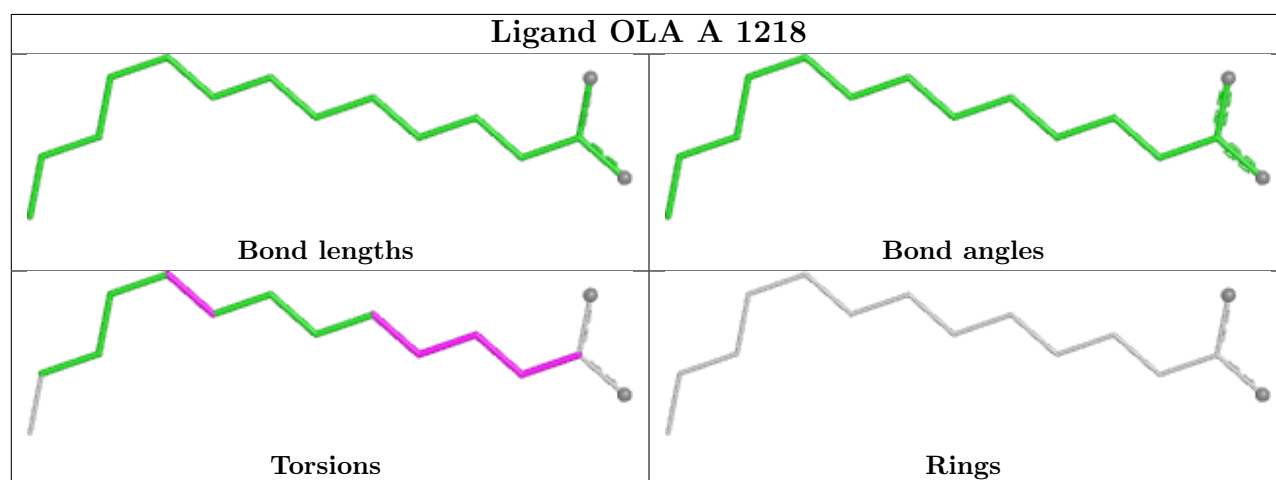
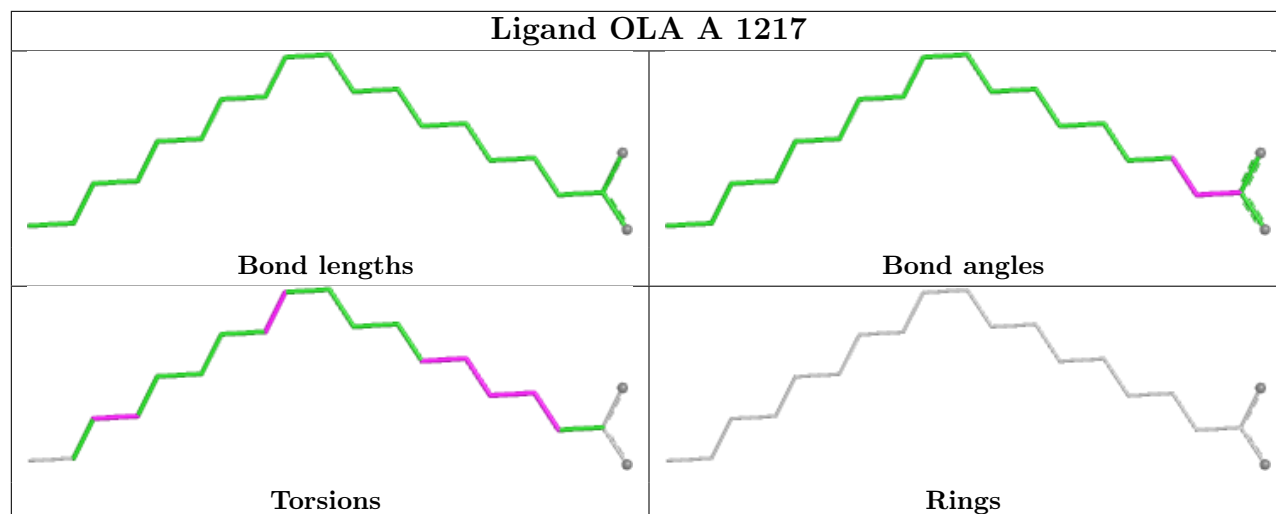
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

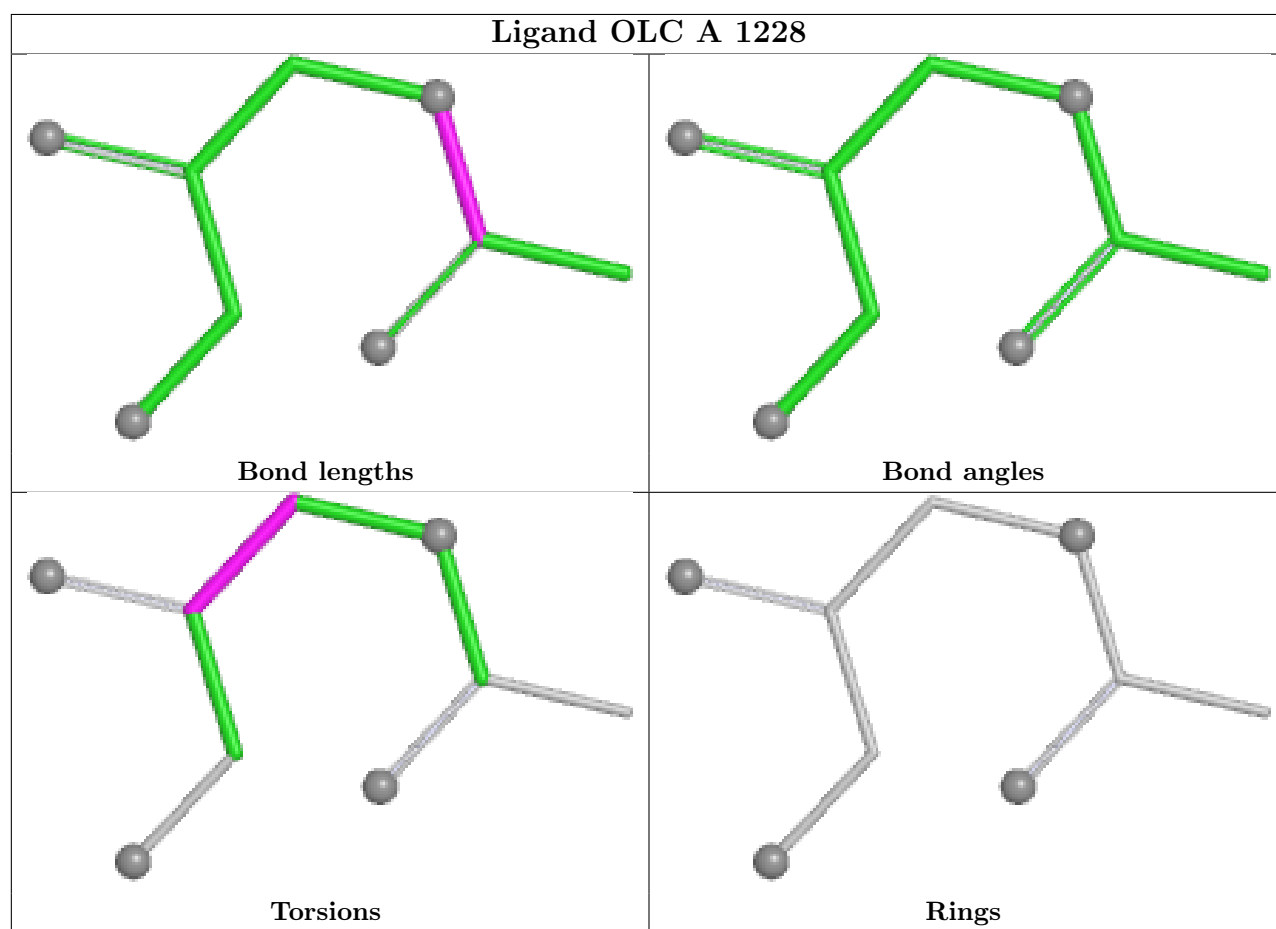
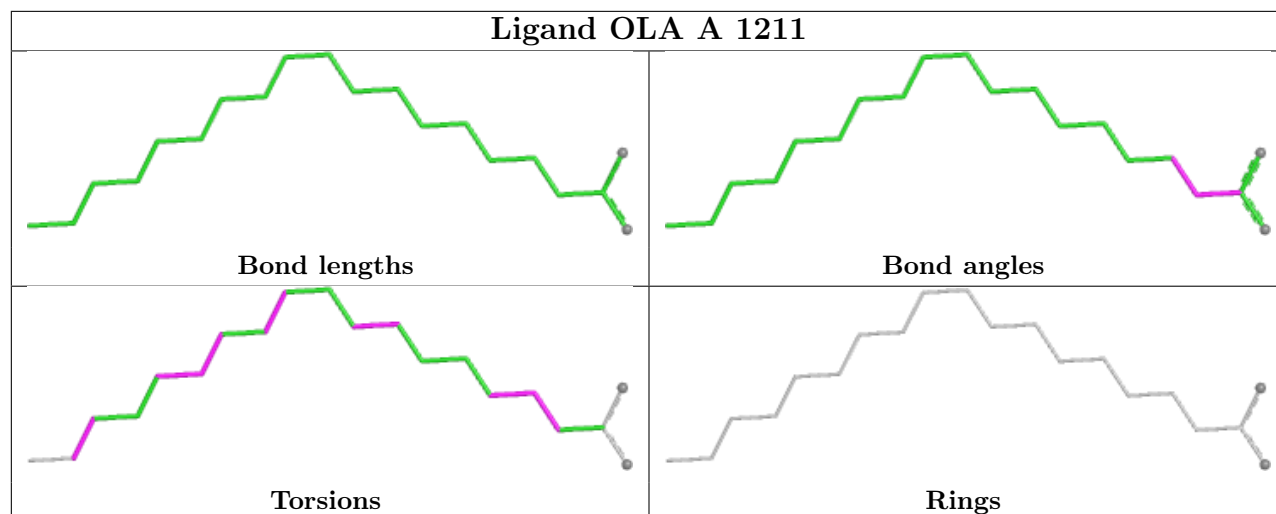


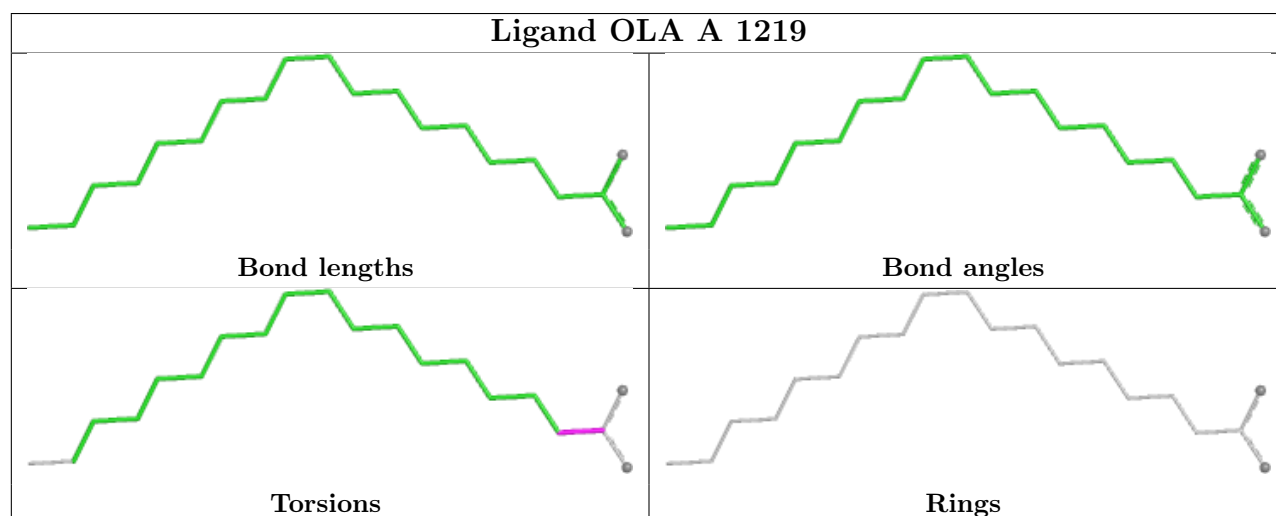
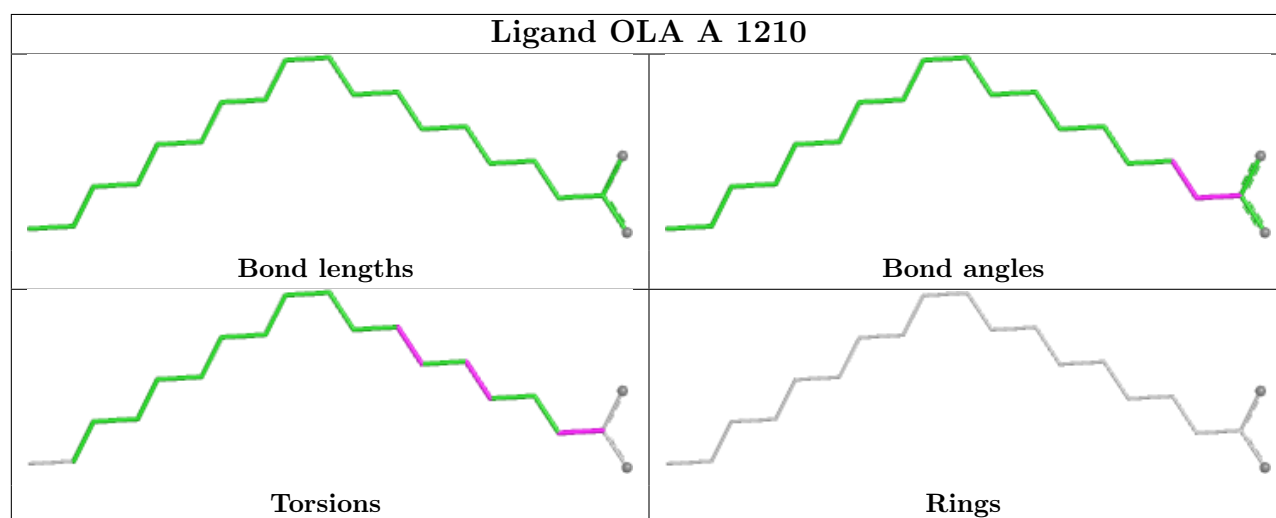
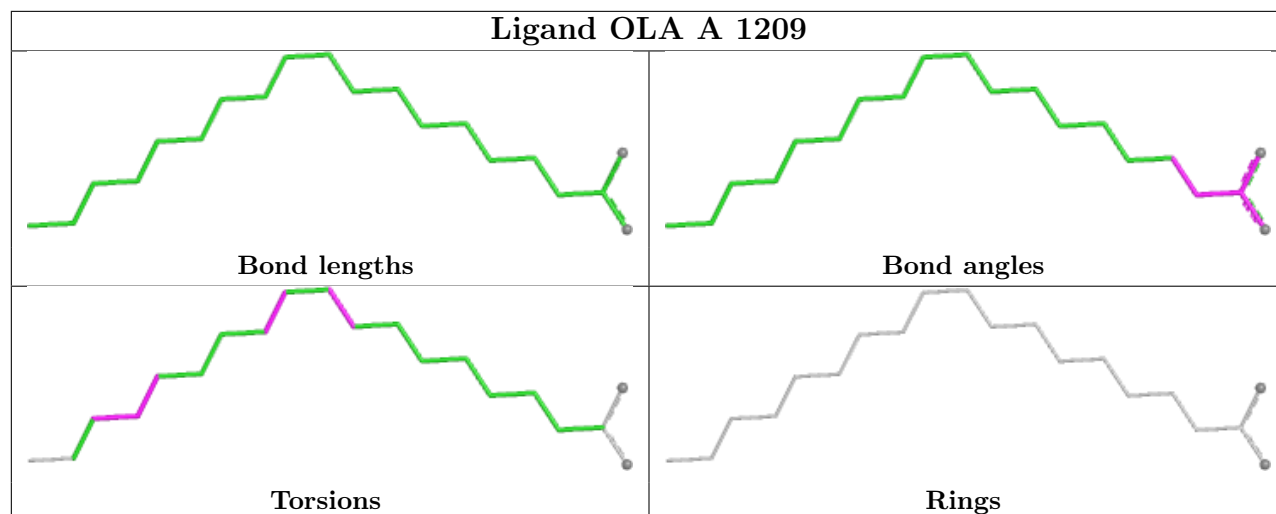


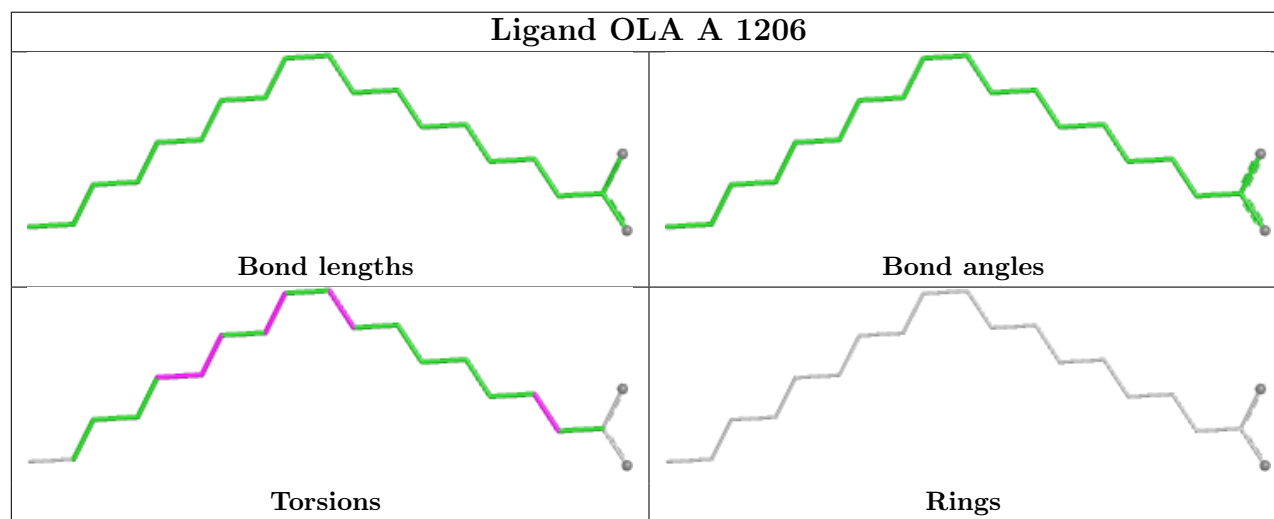
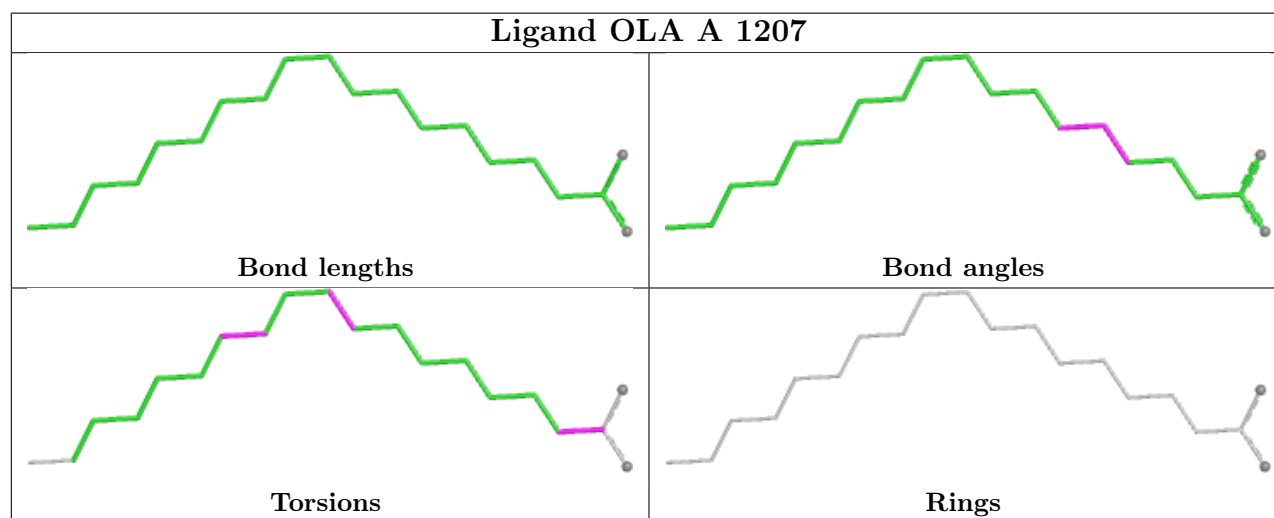
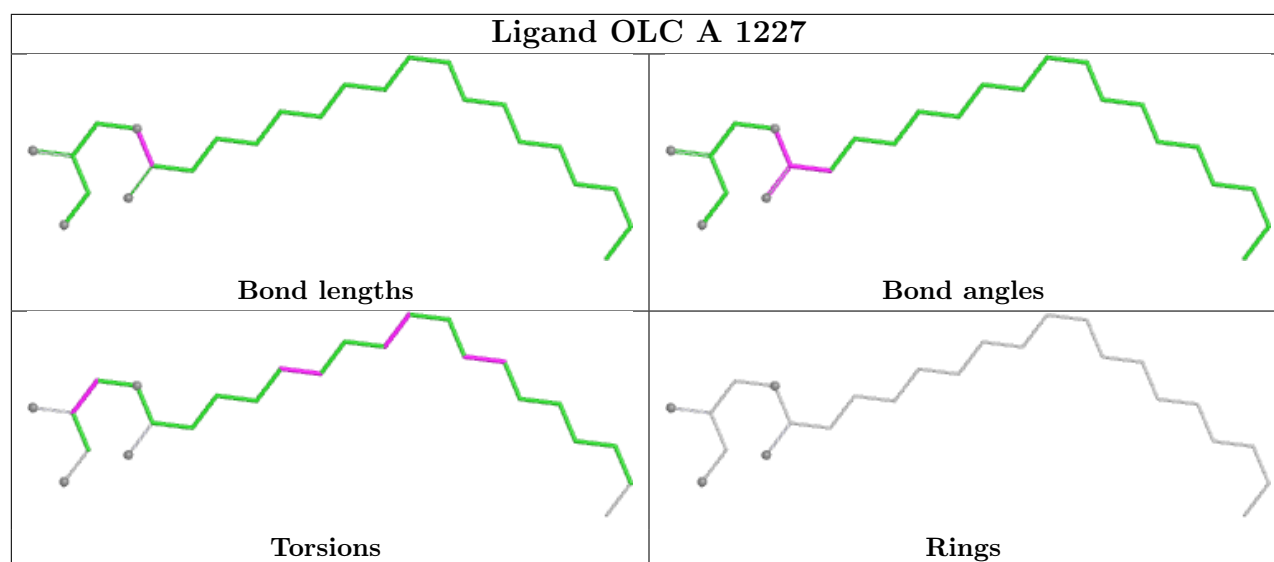


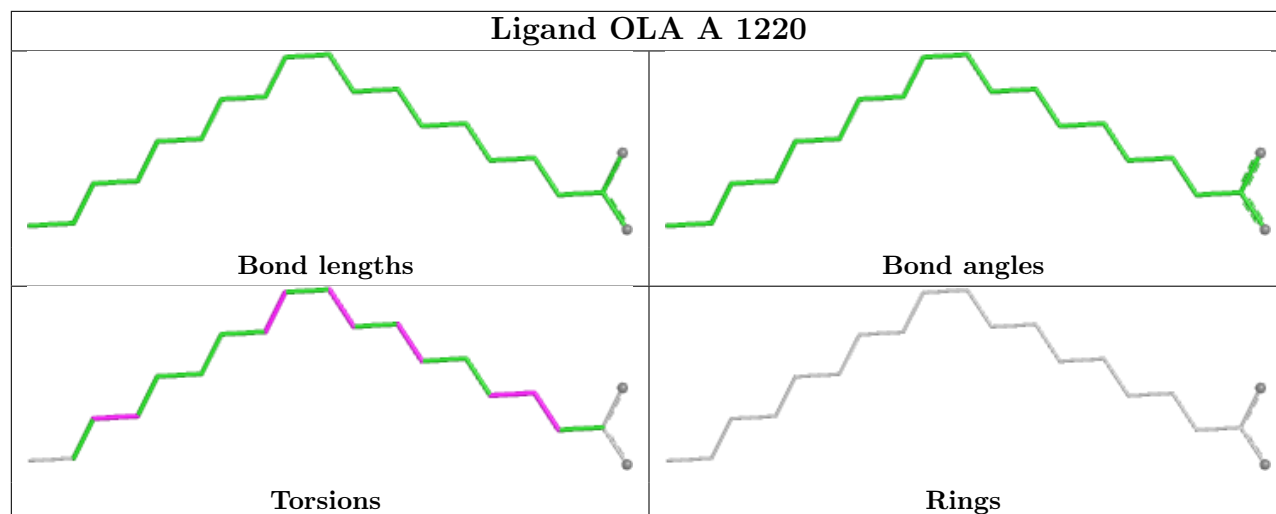












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

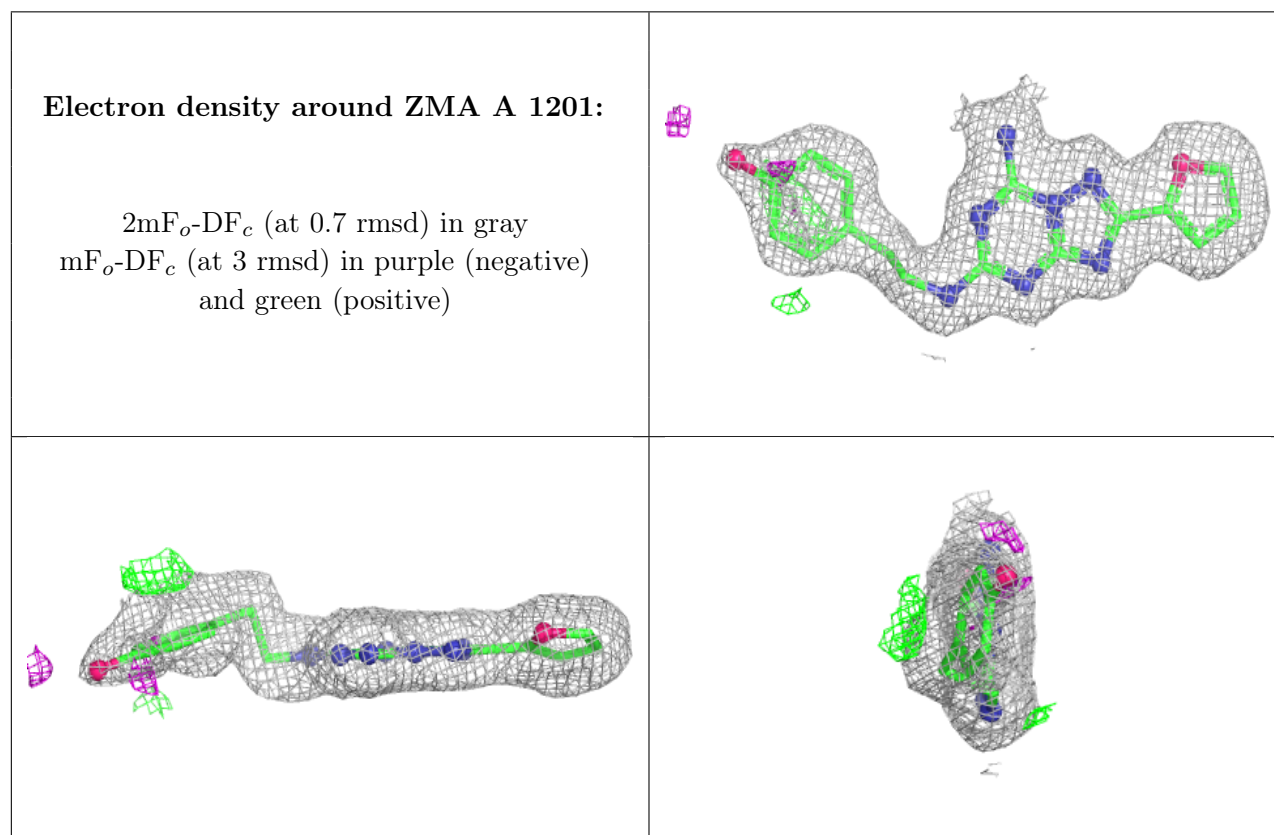
6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

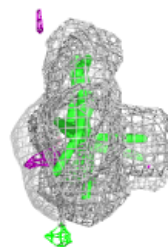
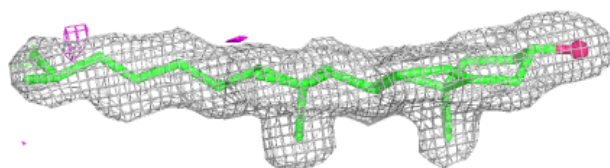
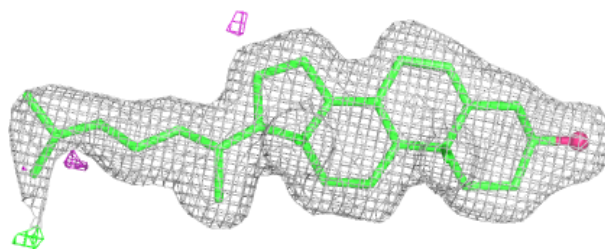
EDS failed to run properly - this section is therefore empty.

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.

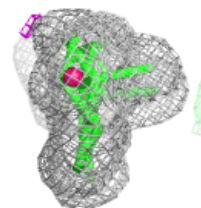
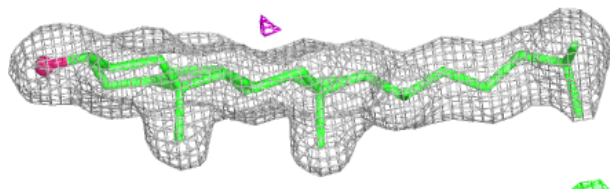
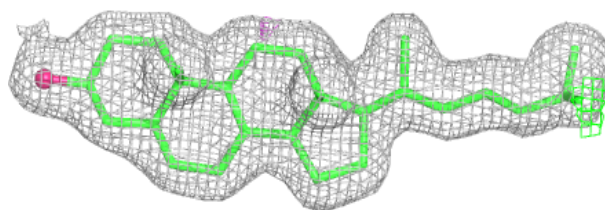


Electron density around CLR A 1202:

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

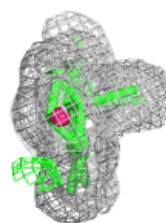
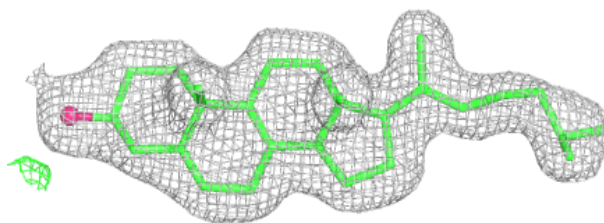
**Electron density around CLR A 1203:**

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

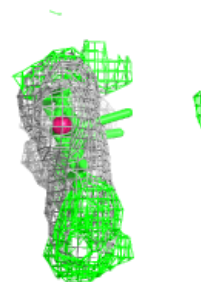
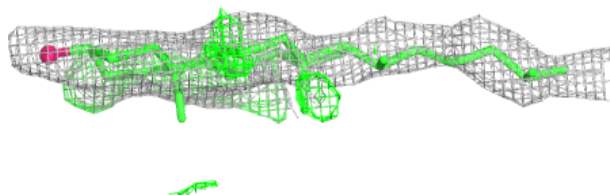
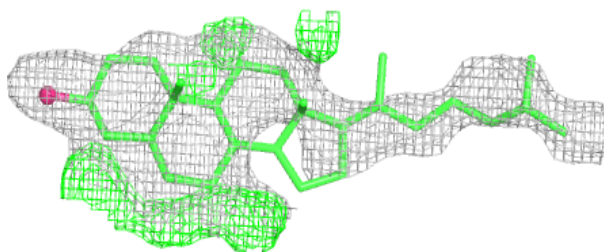


Electron density around CLR A 1204:

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

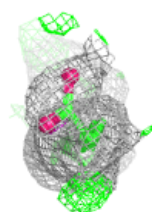
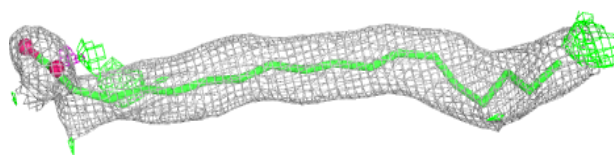
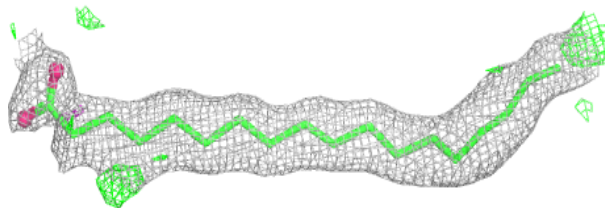
**Electron density around CLR A 1205:**

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

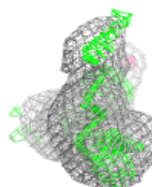
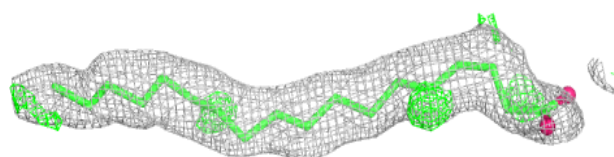
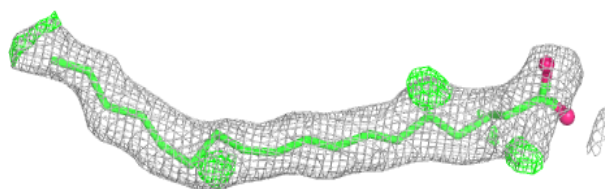


Electron density around OLA A 1206:

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

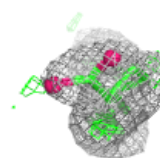
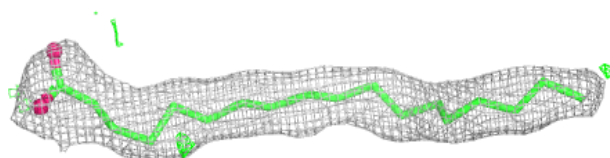
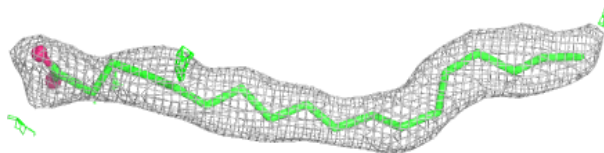
**Electron density around OLA A 1207:**

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

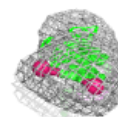
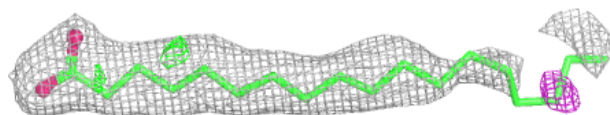
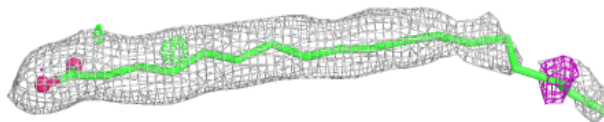


Electron density around OLA A 1208:

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

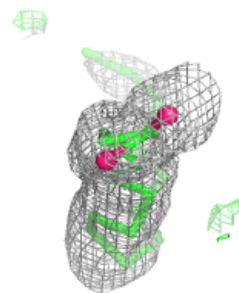
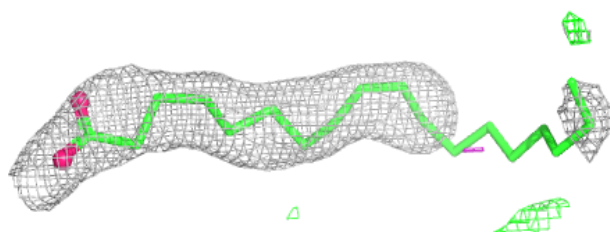
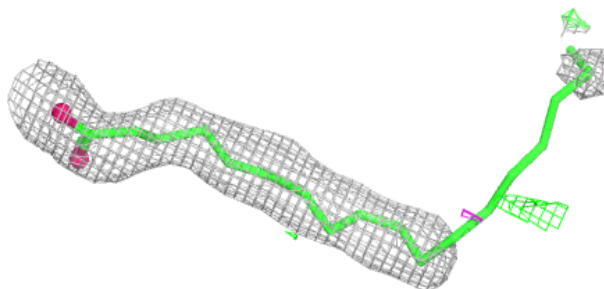
**Electron density around OLA A 1209:**

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

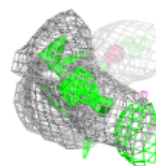
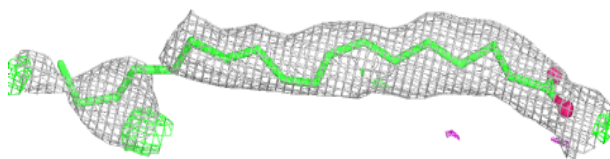
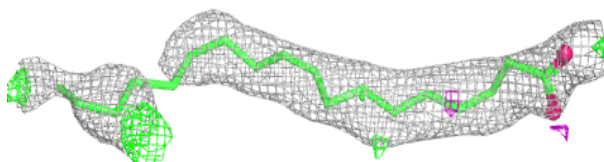


Electron density around OLA A 1210:

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

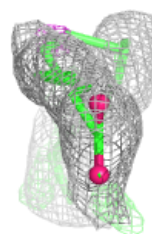
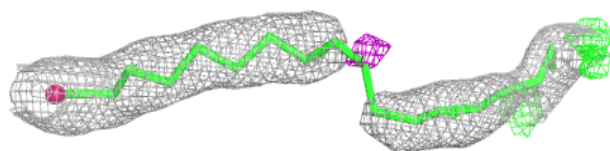
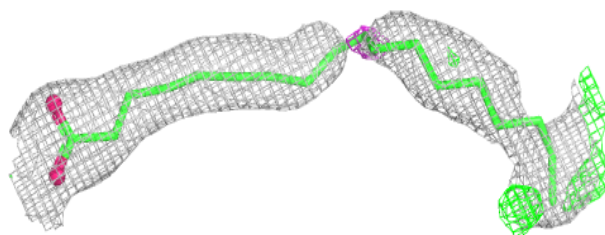
**Electron density around OLA A 1211:**

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

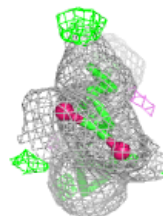
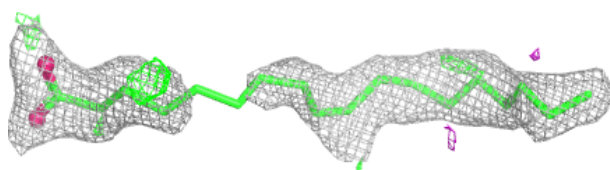
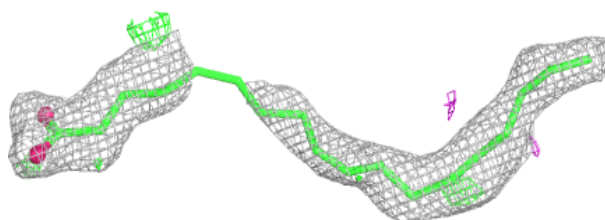


Electron density around OLA A 1212:

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

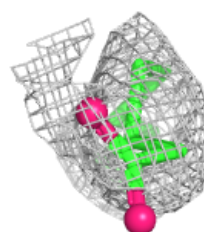
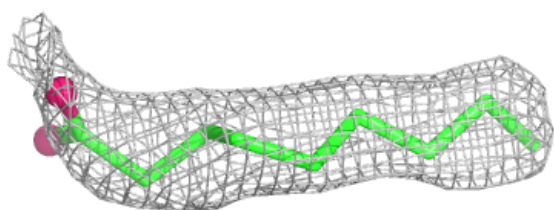
**Electron density around OLA A 1213:**

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

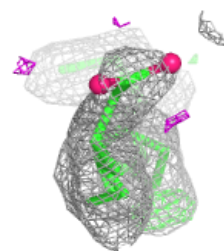
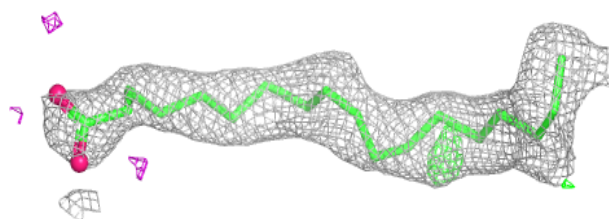
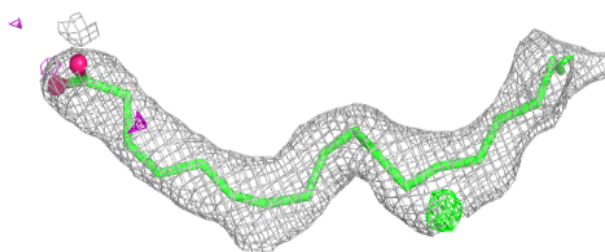


Electron density around OLA A 1214:

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

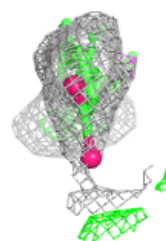
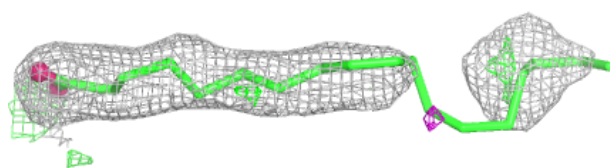
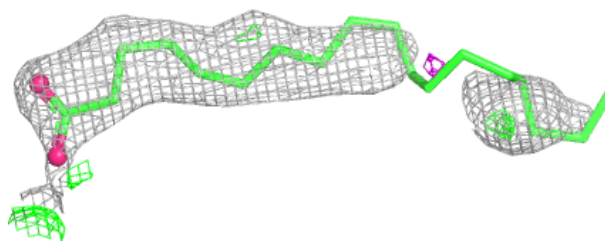
**Electron density around OLA A 1215:**

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

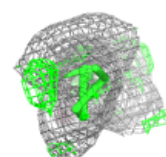
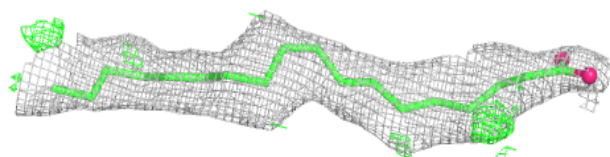
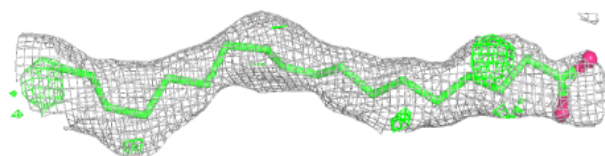


Electron density around OLA A 1216:

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

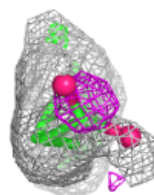
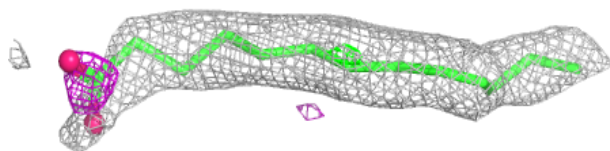
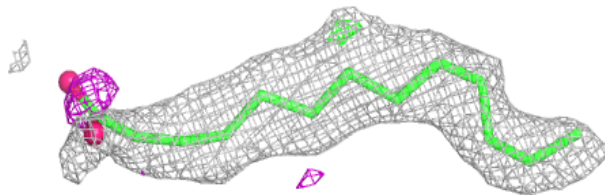
**Electron density around OLA A 1217:**

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

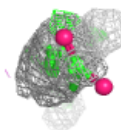
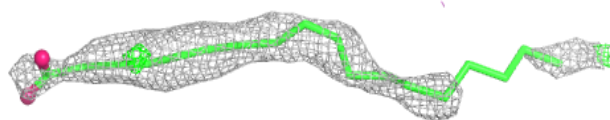
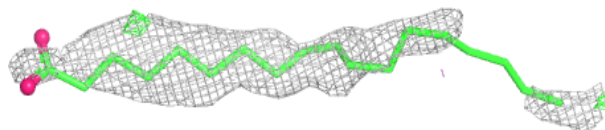


Electron density around OLA A 1218:

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

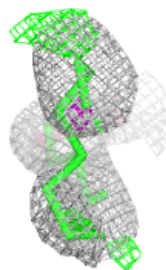
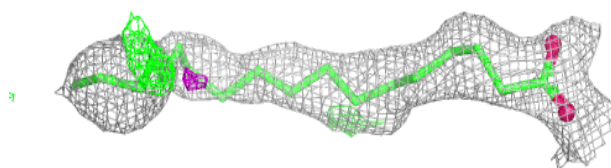
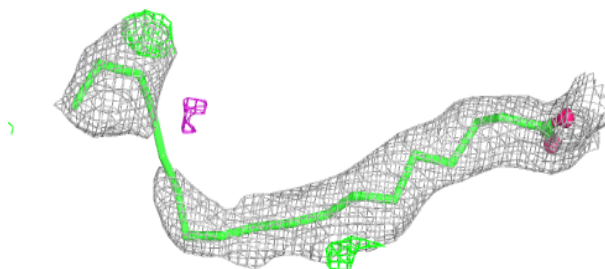
**Electron density around OLA A 1219:**

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

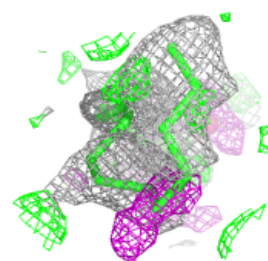
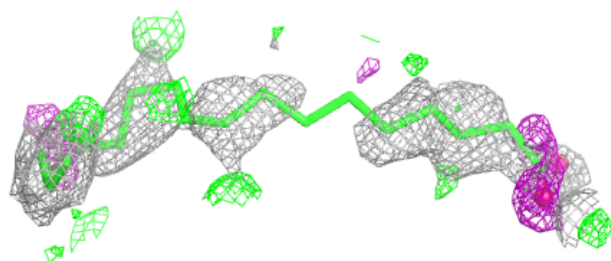
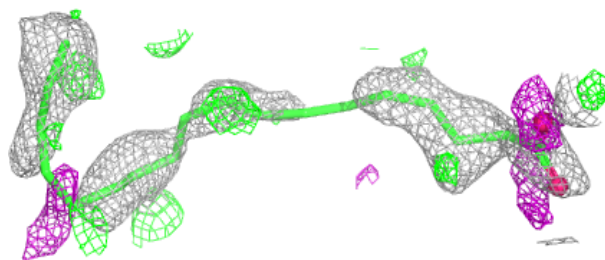


Electron density around OLA A 1220:

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

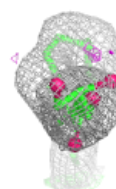
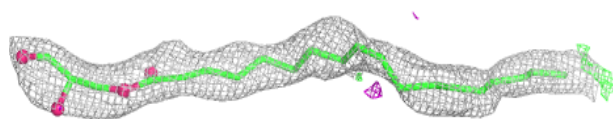
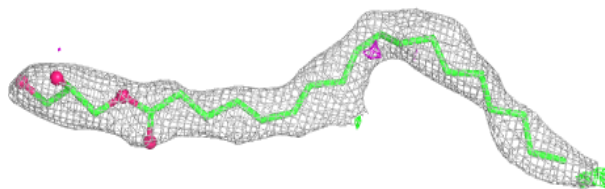
**Electron density around OLA A 1221:**

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

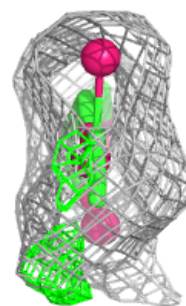
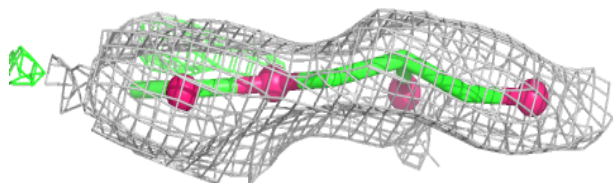
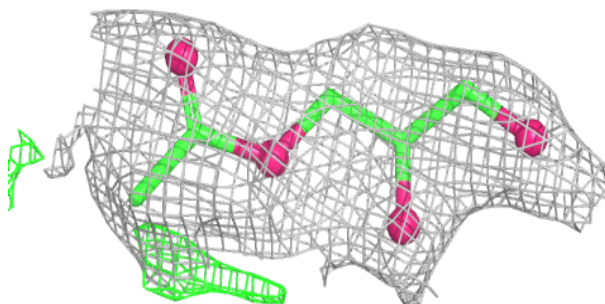


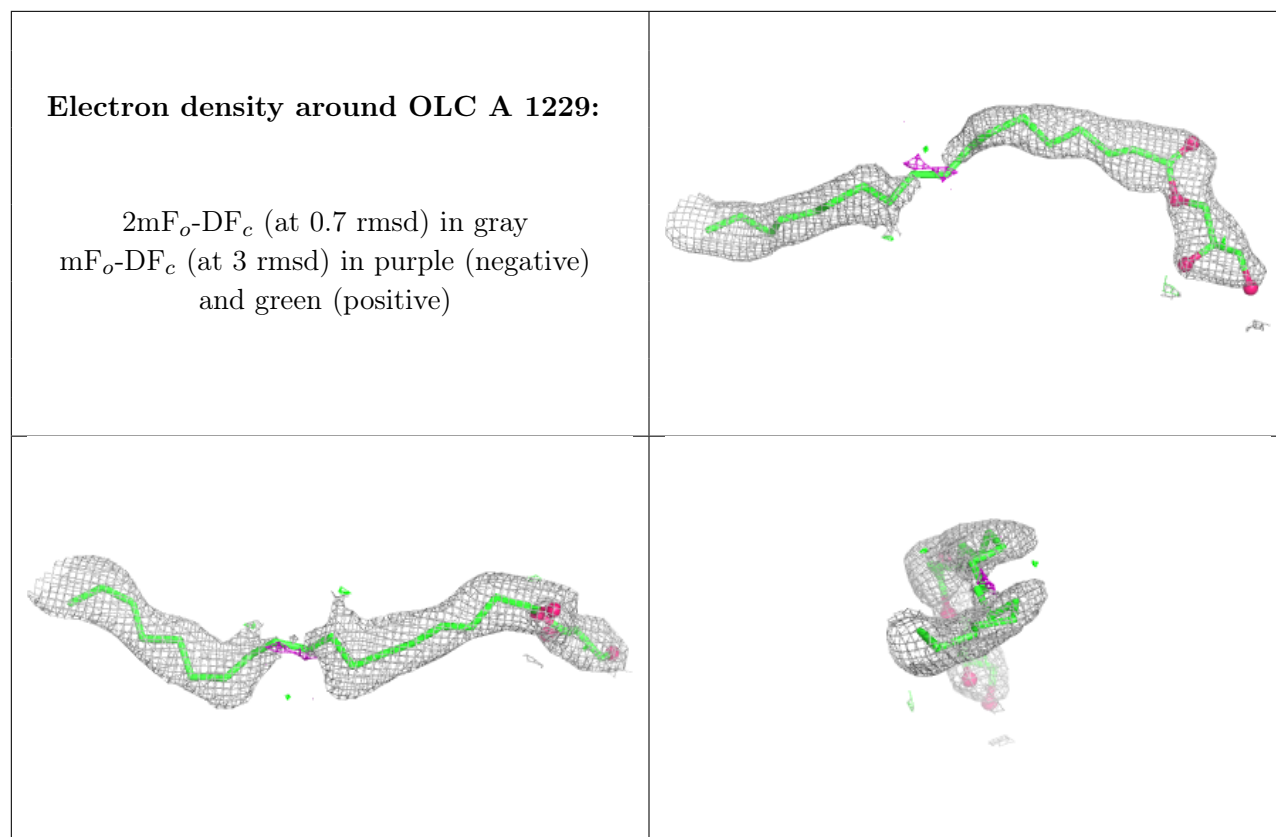
Electron density around OLC A 1227:

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

**Electron density around OLC A 1228:**

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





6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.