



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 12:34 PM EDT

PDB ID : 7INU / pdb\_00007inu  
Title : Crystal structure of A2A in complex with F336  
Authors : Huang, C.-Y.; Cheng, R.Y.K.; Metz, A.  
Deposited on : 2025-08-21  
Resolution : 2.46 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](mailto: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

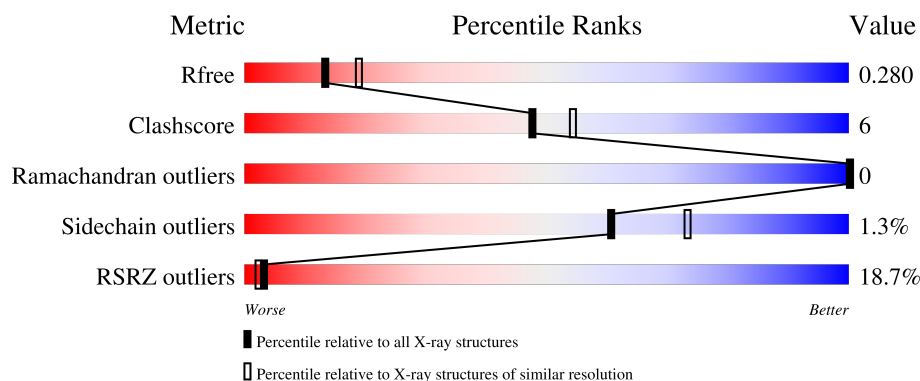
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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  $\geq 3$ , 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	433	

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
7	TEP	A	1235	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3704 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 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	13	0
			3126	2035	532	536	23			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P0ABE7
A	1102	ILE	-	linker	UNP P0ABE7
A	1103	GLN	-	linker	UNP P0ABE7
A	1104	LYS	-	linker	UNP P0ABE7
A	1105	TYR	-	linker	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	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274

*Continued on next page...*

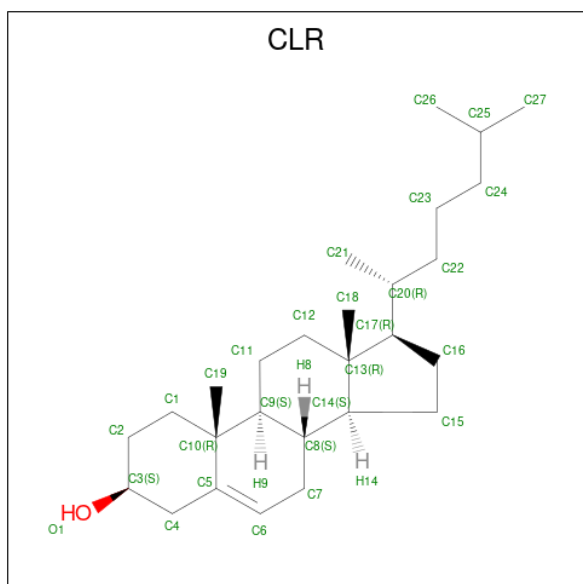
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



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
			10	8	2		
4	A	1	Total	C	O	0	0
			9	7	2		
4	A	1	Total	C	O	0	0
			18	16	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
			12	10	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			15	13	2		
4	A	1	Total	C	O	0	0
			11	9	2		
4	A	1	Total	C	O	0	0
			19	17	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C		0	0
			12	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 10 10	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C O 15 13 2	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C O 13 11 2	0	0
4	A	1	Total C O 20 18 2	0	0

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula:  $C_{21}H_{40}O_4$ ).



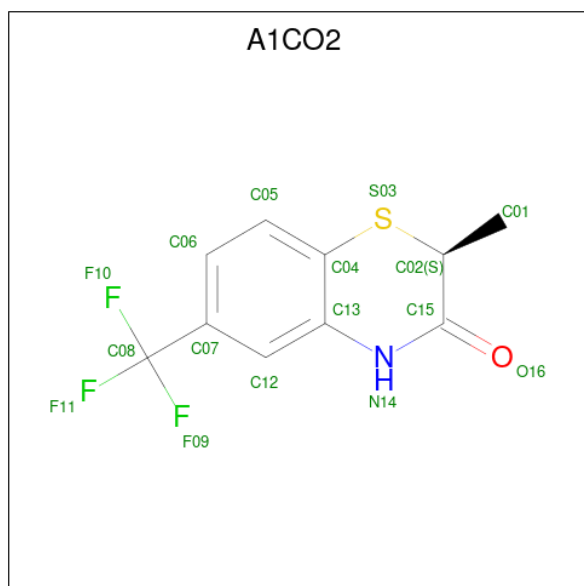
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 12 4	0	0
5	A	1	Total C O 17 13 4	0	0

Continued on next page...

Continued from previous page...

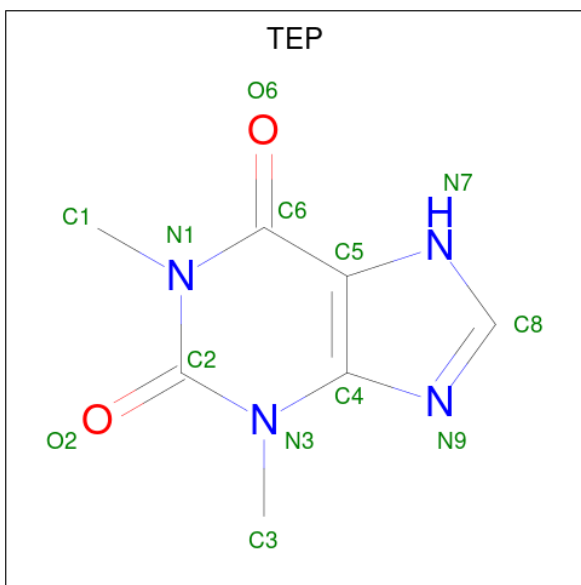
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	19	4		
5	A	1	Total	C	O	0	0
			23	19	4		
5	A	1	Total	C	O	0	0
			23	19	4		
5	A	1	Total	C	O	0	0
			18	14	4		
5	A	1	Total	C	O	0	0
			16	12	4		

- Molecule 6 is (2S)-2-methyl-6-(trifluoromethyl)-2H-1,4-benzothiazin-3(4H)-one (CCD ID: A1CO2) (formula: C<sub>10</sub>H<sub>8</sub>F<sub>3</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	S	
			16	10	3	1	1	1	

- Molecule 7 is THEOPHYLLINE (CCD ID: TEP) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			13	7	4	2		

- Molecule 8 is water.

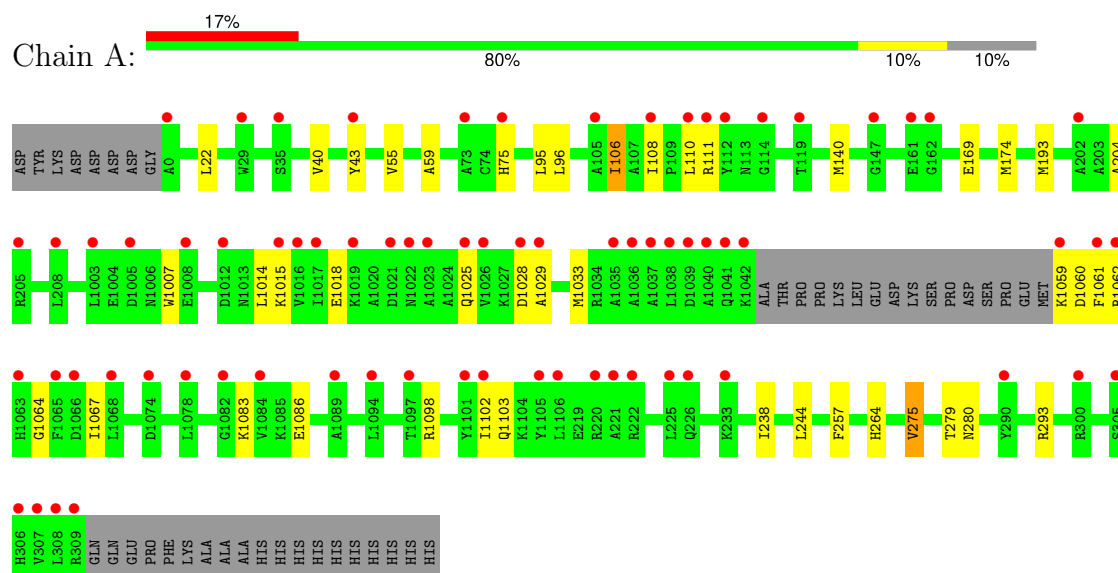
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	21	Total	O	0	0
			21	21		



### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Adenosine receptor A2a/Soluble cytochrome b562/Adenosine receptor A2a chimera



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.40Å 179.24Å 139.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.13 – 2.46 55.13 – 2.46	Depositor EDS
% Data completeness (in resolution range)	73.2 (55.13-2.46) 73.2 (55.13-2.46)	Depositor EDS
$R_{merge}$	0.74	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, $R_{free}$	0.254 , 0.279 0.255 , 0.280	Depositor DCC
$R_{free}$ test set	649 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, TEP, OLA, NA, A1CO2, OLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.15	0/3191	0.28	0/4338

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3126	0	3206	31	0
2	A	1	0	0	0	0
3	A	84	0	138	0	0
4	A	307	0	459	12	0
5	A	136	0	186	5	0
6	A	16	0	0	0	0
7	A	13	0	8	0	0
8	A	21	0	0	1	0
All	All	3704	0	3997	43	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 6.

All (43) 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:108:ILE:HD12	1:A:111:ARG:HB3	1.56	0.87
5:A:1229:OLC:H4A	5:A:1230:OLC:H2	1.71	0.71
1:A:1007:TRP:CH2	1:A:1103:GLN:HG3	2.28	0.68
1:A:1083:LYS:HB3	1:A:1086:GLU:HB2	1.78	0.65
4:A:1222:OLA:H51	4:A:1226:OLA:H131	1.83	0.61
1:A:106:ILE:HD11	1:A:204:ALA:HB2	1.84	0.58
1:A:1098:ARG:HA	1:A:1102:ILE:HB	1.84	0.58
1:A:280:ASN:ND2	8:A:1305:HOH:O	2.35	0.57
1:A:1029:ALA:O	1:A:1033:MET:HG3	2.04	0.57
1:A:1064:GLY:HA2	1:A:1067:ILE:HD12	1.85	0.56
1:A:40:VAL:HA	1:A:43:TYR:HD1	1.72	0.55
1:A:1007:TRP:HZ3	1:A:1102:ILE:HG22	1.70	0.55
1:A:1015:LYS:HA	1:A:1018:GLU:HG3	1.91	0.53
4:A:1210:OLA:H183	4:A:1221:OLA:H121	1.92	0.52
4:A:1225:OLA:H62	5:A:1233:OLC:H3A	1.93	0.51
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.76	0.50
1:A:1059:LYS:NZ	1:A:1060:ASP:OD1	2.43	0.50
1:A:75:HIS:CD2	4:A:1225:OLA:H22	2.47	0.49
1:A:1007:TRP:HH2	1:A:1103:GLN:HG3	1.76	0.48
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.95	0.48
1:A:110:LEU:HD23	1:A:110:LEU:H	1.79	0.48
1:A:169:GLU:OE1	1:A:264:HIS:HE1	1.97	0.48
5:A:1231:OLC:H10	5:A:1231:OLC:H13A	1.60	0.48
4:A:1209:OLA:H21	4:A:1216:OLA:H32	1.96	0.47
4:A:1209:OLA:H122	4:A:1216:OLA:H151	1.97	0.47
1:A:40:VAL:HA	1:A:43:TYR:CD1	2.50	0.46
1:A:22:LEU:HB3	4:A:1211:OLA:H71	1.95	0.46
1:A:1059:LYS:HA	1:A:1062:ARG:HD3	1.98	0.46
1:A:140[B]:MET:HE3	4:A:1225:OLA:H71	1.96	0.46
1:A:1007:TRP:CZ3	1:A:1102:ILE:HG22	2.51	0.45
4:A:1216:OLA:H10	4:A:1216:OLA:H132	1.83	0.45
1:A:275[B]:VAL:O	1:A:279[B]:THR:HG23	2.17	0.44
1:A:174[A]:MET:HG3	1:A:257:PHE:HB2	1.99	0.44
1:A:244[B]:LEU:HD23	1:A:244[B]:LEU:HA	1.86	0.43
1:A:43:TYR:HE2	5:A:1232:OLC:H24	1.83	0.43
5:A:1229:OLC:H15	5:A:1230:OLC:H14	2.00	0.43
1:A:1014:LEU:O	1:A:1018:GLU:HG3	2.19	0.43
4:A:1210:OLA:H82	4:A:1210:OLA:H112	1.90	0.42
4:A:1215:OLA:H82	4:A:1215:OLA:H111	1.84	0.42
4:A:1224:OLA:H112	4:A:1224:OLA:H81	1.67	0.42
1:A:95:LEU:HD21	1:A:238:ILE:HG22	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HB2	1:A:193:MET:HE2	2.02	0.41
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.55	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	399/433 (92%)	396 (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	329/354 (93%)	324 (98%)	5 (2%)	57	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ILE
1	A	1025	GLN
1	A	1061	PHE
1	A	275[A]	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	275[B]	VAL

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	157	GLN
1	A	264	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 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 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	$\# Z  > 2$
4	OLA	A	1205	-	19,19,19	0.60	0	19,19,19	0.99	0
3	CLR	A	1202	-	31,31,31	0.31	0	48,48,48	0.47	0
4	OLA	A	1208	-	17,17,19	0.62	0	17,17,19	1.03	0
4	OLA	A	1218	-	9,9,19	0.41	0	8,8,19	0.77	0
5	OLC	A	1229	-	22,22,24	1.06	1 (4%)	23,23,25	1.19	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	A1CO2	A	1234	-	17,17,17	7.24	5 (29%)	23,26,26	1.66	4 (17%)
4	OLA	A	1209	-	19,19,19	0.63	0	19,19,19	0.96	1 (5%)
4	OLA	A	1222	-	7,7,19	0.31	0	6,6,19	0.80	0
5	OLC	A	1233	-	15,15,24	1.27	1 (6%)	16,16,25	0.99	1 (6%)
4	OLA	A	1211	-	11,11,19	0.75	0	11,11,19	1.18	0
5	OLC	A	1227	-	15,15,24	1.25	1 (6%)	16,16,25	1.26	1 (6%)
4	OLA	A	1207	-	8,8,19	0.81	0	8,8,19	1.30	1 (12%)
4	OLA	A	1214	-	10,10,19	0.73	0	10,10,19	1.23	1 (10%)
4	OLA	A	1213	-	14,14,19	0.67	0	14,14,19	1.08	0
4	OLA	A	1226	-	19,19,19	0.59	0	19,19,19	1.05	0
3	CLR	A	1204	-	31,31,31	0.29	0	48,48,48	0.39	0
5	OLC	A	1230	-	22,22,24	1.06	1 (4%)	23,23,25	1.21	3 (13%)
4	OLA	A	1223	-	14,14,19	0.66	0	14,14,19	1.08	2 (14%)
5	OLC	A	1228	-	16,16,24	1.31	1 (6%)	17,17,25	1.33	2 (11%)
4	OLA	A	1206	-	9,9,19	0.79	0	9,9,19	1.19	0
4	OLA	A	1224	-	14,14,19	0.35	0	13,13,19	0.73	0
3	CLR	A	1203	-	31,31,31	0.29	0	48,48,48	0.45	0
4	OLA	A	1215	-	18,18,19	0.60	0	18,18,19	1.07	1 (5%)
4	OLA	A	1217	-	11,11,19	0.36	0	10,10,19	0.72	0
4	OLA	A	1216	-	19,19,19	0.64	0	19,19,19	0.88	0
4	OLA	A	1210	-	19,19,19	0.58	0	19,19,19	1.04	1 (5%)
4	OLA	A	1212	-	7,7,19	0.89	0	7,7,19	1.27	0
5	OLC	A	1231	-	22,22,24	1.05	1 (4%)	23,23,25	1.25	3 (13%)
4	OLA	A	1221	-	8,8,19	0.31	0	7,7,19	0.79	0
4	OLA	A	1225	-	12,12,19	0.74	0	12,12,19	1.18	0
7	TEP	A	1235	-	14,14,14	1.87	5 (35%)	21,21,21	3.35	11 (52%)
4	OLA	A	1220	-	11,11,19	0.39	0	10,10,19	0.75	0
4	OLA	A	1219	-	10,10,19	0.42	0	9,9,19	0.83	0
5	OLC	A	1232	-	17,17,24	1.21	1 (5%)	18,18,25	1.25	2 (11%)

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
4	OLA	A	1205	-	-	10/17/17/17	-
3	CLR	A	1202	-	-	0/10/68/68	0/4/4/4
4	OLA	A	1208	-	-	9/15/15/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1218	-	-	1/7/7/17	-
5	OLC	A	1229	-	-	13/22/22/24	-
6	A1CO2	A	1234	-	-	0/6/18/18	0/2/2/2
4	OLA	A	1209	-	-	11/17/17/17	-
4	OLA	A	1222	-	-	0/5/5/17	-
5	OLC	A	1233	-	-	7/15/15/24	-
4	OLA	A	1211	-	-	4/9/9/17	-
5	OLC	A	1227	-	-	7/15/15/24	-
4	OLA	A	1207	-	-	3/6/6/17	-
4	OLA	A	1214	-	-	3/8/8/17	-
4	OLA	A	1213	-	-	4/12/12/17	-
4	OLA	A	1226	-	-	9/17/17/17	-
3	CLR	A	1204	-	-	3/10/68/68	0/4/4/4
5	OLC	A	1230	-	-	11/22/22/24	-
4	OLA	A	1223	-	-	5/12/12/17	-
5	OLC	A	1228	-	-	9/16/16/24	-
4	OLA	A	1206	-	-	3/7/7/17	-
4	OLA	A	1224	-	-	1/12/12/17	-
3	CLR	A	1203	-	-	1/10/68/68	0/4/4/4
4	OLA	A	1215	-	-	3/16/16/17	-
4	OLA	A	1217	-	-	4/9/9/17	-
4	OLA	A	1216	-	-	8/17/17/17	-
4	OLA	A	1210	-	-	7/17/17/17	-
4	OLA	A	1212	-	-	2/5/5/17	-
5	OLC	A	1231	-	-	11/22/22/24	-
4	OLA	A	1221	-	-	2/6/6/17	-
4	OLA	A	1225	-	-	8/10/10/17	-
7	TEP	A	1235	-	-	-	0/2/2/2
4	OLA	A	1220	-	-	3/9/9/17	-
4	OLA	A	1219	-	-	6/8/8/17	-
5	OLC	A	1232	-	-	8/17/17/24	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1234	A1CO2	C15-N14	24.26	1.61	1.34

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1234	A1CO2	C02-S03	-12.28	1.70	1.82
6	A	1234	A1CO2	C13-N14	11.37	1.59	1.39
7	A	1235	TEP	C6-N1	-3.71	1.32	1.40
5	A	1233	OLC	O20-C1	3.05	1.42	1.33
5	A	1228	OLC	O20-C1	3.00	1.42	1.33
5	A	1227	OLC	O20-C1	2.93	1.41	1.33
5	A	1232	OLC	O20-C1	2.78	1.41	1.33
5	A	1229	OLC	O20-C1	2.78	1.41	1.33
5	A	1230	OLC	O20-C1	2.75	1.41	1.33
5	A	1231	OLC	O20-C1	2.63	1.41	1.33
6	A	1234	A1CO2	C04-S03	-2.55	1.73	1.76
7	A	1235	TEP	C5-N7	-2.54	1.34	1.38
6	A	1234	A1CO2	O16-C15	-2.41	1.18	1.23
7	A	1235	TEP	C5-C6	-2.36	1.38	1.42
7	A	1235	TEP	C5-C4	-2.31	1.34	1.37
7	A	1235	TEP	O6-C6	-2.11	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1235	TEP	C8-N9-C4	6.55	107.83	103.45
7	A	1235	TEP	C5-C6-N1	5.97	120.08	112.07
7	A	1235	TEP	C4-C5-N7	5.91	108.20	105.29
7	A	1235	TEP	C5-C4-N9	-5.25	107.95	111.63
7	A	1235	TEP	C6-C5-C4	-4.08	119.91	123.13
7	A	1235	TEP	N7-C8-N9	-3.98	108.36	112.98
6	A	1234	A1CO2	C01-C02-C15	-3.95	108.04	112.03
7	A	1235	TEP	N3-C4-N9	3.62	131.96	126.27
5	A	1228	OLC	C8-C9-C10	3.52	152.31	126.65
7	A	1235	TEP	C6-N1-C2	-3.47	120.01	125.66
7	A	1235	TEP	O6-C6-C5	-3.34	119.83	126.64
5	A	1231	OLC	C8-C9-C10	3.30	149.55	124.83
5	A	1230	OLC	C8-C9-C10	3.21	148.92	124.83
5	A	1227	OLC	O20-C1-C2	3.21	121.63	111.83
5	A	1229	OLC	C8-C9-C10	3.21	148.89	124.83
6	A	1234	A1CO2	C04-S03-C02	3.16	108.28	101.19
6	A	1234	A1CO2	O16-C15-N14	3.13	125.68	122.16
7	A	1235	TEP	C5-C4-N3	-2.90	120.09	121.73
5	A	1232	OLC	C8-C9-C10	2.85	152.08	130.48
5	A	1228	OLC	O20-C1-C2	2.55	119.61	111.83
5	A	1233	OLC	O20-C1-C2	2.47	119.38	111.83
5	A	1231	OLC	O20-C1-C2	2.36	119.03	111.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1215	OLA	C3-C2-C1	-2.33	108.44	114.51
7	A	1235	TEP	N3-C2-N1	2.29	119.99	117.14
6	A	1234	A1CO2	F10-C08-C07	-2.21	108.16	112.90
4	A	1210	OLA	C3-C2-C1	-2.18	108.81	114.51
5	A	1232	OLC	O20-C1-C2	2.17	118.44	111.83
4	A	1223	OLA	C3-C2-C1	-2.13	108.95	114.51
5	A	1230	OLC	C11-C10-C9	-2.12	108.96	124.83
5	A	1229	OLC	C11-C10-C9	-2.10	109.06	124.83
4	A	1209	OLA	O2-C1-C2	2.09	120.61	114.00
4	A	1207	OLA	C3-C2-C1	-2.06	109.13	114.51
4	A	1214	OLA	C3-C2-C1	-2.05	109.15	114.51
5	A	1230	OLC	O20-C1-C2	2.05	118.10	111.83
5	A	1229	OLC	O20-C1-C2	2.04	118.07	111.83
4	A	1223	OLA	O2-C1-C2	2.02	120.38	114.00
5	A	1231	OLC	C11-C10-C9	-2.01	109.74	124.83

There are no chirality outliers.

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1213	OLA	C10-C11-C12-C13
4	A	1217	OLA	C6-C7-C8-C9
5	A	1229	OLC	C21-C22-C24-O25
5	A	1230	OLC	O20-C21-C22-O23
5	A	1231	OLC	O20-C21-C22-C24
5	A	1232	OLC	O19-C1-O20-C21
5	A	1232	OLC	C2-C1-O20-C21
5	A	1231	OLC	O19-C1-O20-C21
5	A	1231	OLC	C2-C1-O20-C21
5	A	1228	OLC	O20-C21-C22-O23
5	A	1231	OLC	O20-C21-C22-O23
5	A	1232	OLC	O20-C21-C22-O23
5	A	1230	OLC	O20-C21-C22-C24
5	A	1229	OLC	O23-C22-C24-O25
4	A	1225	OLA	C1-C2-C3-C4
4	A	1223	OLA	C1-C2-C3-C4
5	A	1230	OLC	C1-C2-C3-C4
5	A	1230	OLC	C2-C1-O20-C21
5	A	1231	OLC	C1-C2-C3-C4
5	A	1233	OLC	C1-C2-C3-C4
3	A	1204	CLR	C20-C22-C23-C24
4	A	1210	OLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1227	OLC	O20-C21-C22-O23
5	A	1231	OLC	C10-C11-C12-C13
3	A	1203	CLR	C21-C20-C22-C23
5	A	1227	OLC	O20-C21-C22-C24
4	A	1226	OLA	C15-C16-C17-C18
5	A	1230	OLC	O19-C1-O20-C21
4	A	1215	OLA	C5-C6-C7-C8
4	A	1223	OLA	C5-C6-C7-C8
5	A	1228	OLC	C1-C2-C3-C4
4	A	1217	OLA	C12-C13-C14-C15
4	A	1226	OLA	C11-C12-C13-C14
5	A	1230	OLC	C3-C4-C5-C6
4	A	1216	OLA	C5-C6-C7-C8
4	A	1219	OLA	C11-C12-C13-C14
4	A	1205	OLA	C14-C15-C16-C17
5	A	1232	OLC	C6-C7-C8-C9
5	A	1230	OLC	C12-C13-C14-C15
4	A	1207	OLA	C3-C4-C5-C6
5	A	1232	OLC	C3-C4-C5-C6
5	A	1232	OLC	C5-C6-C7-C8
4	A	1206	OLA	C3-C4-C5-C6
4	A	1205	OLA	C4-C5-C6-C7
4	A	1223	OLA	C3-C4-C5-C6
4	A	1224	OLA	C6-C7-C8-C9
4	A	1210	OLA	C15-C16-C17-C18
5	A	1228	OLC	C3-C4-C5-C6
4	A	1214	OLA	C4-C5-C6-C7
5	A	1233	OLC	C2-C3-C4-C5
4	A	1208	OLA	C6-C7-C8-C9
4	A	1219	OLA	C10-C11-C12-C13
4	A	1226	OLA	C6-C7-C8-C9
5	A	1231	OLC	C6-C7-C8-C9
4	A	1210	OLA	C5-C6-C7-C8
4	A	1211	OLA	C4-C5-C6-C7
4	A	1226	OLA	C4-C5-C6-C7
4	A	1216	OLA	C3-C4-C5-C6
4	A	1221	OLA	C12-C13-C14-C15
4	A	1205	OLA	C2-C3-C4-C5
5	A	1232	OLC	C4-C5-C6-C7
4	A	1226	OLA	C12-C13-C14-C15
4	A	1205	OLA	C12-C13-C14-C15
4	A	1205	OLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1229	OLC	C10-C11-C12-C13
5	A	1229	OLC	C3-C4-C5-C6
4	A	1226	OLA	C1-C2-C3-C4
4	A	1216	OLA	C11-C12-C13-C14
4	A	1210	OLA	C10-C11-C12-C13
5	A	1230	OLC	C10-C11-C12-C13
4	A	1208	OLA	C4-C5-C6-C7
4	A	1220	OLA	C4-C5-C6-C7
4	A	1225	OLA	C5-C6-C7-C8
4	A	1209	OLA	C4-C5-C6-C7
4	A	1226	OLA	C14-C15-C16-C17
5	A	1229	OLC	C2-C3-C4-C5
4	A	1209	OLA	C13-C14-C15-C16
5	A	1233	OLC	C6-C7-C8-C9
4	A	1210	OLA	C1-C2-C3-C4
4	A	1209	OLA	C14-C15-C16-C17
5	A	1228	OLC	C4-C5-C6-C7
4	A	1205	OLA	C11-C12-C13-C14
5	A	1231	OLC	C3-C4-C5-C6
4	A	1225	OLA	C4-C5-C6-C7
4	A	1225	OLA	C6-C7-C8-C9
4	A	1223	OLA	C4-C5-C6-C7
5	A	1228	OLC	C2-C1-O20-C21
5	A	1229	OLC	C2-C1-O20-C21
5	A	1229	OLC	C12-C13-C14-C15
4	A	1205	OLA	C15-C16-C17-C18
5	A	1230	OLC	C4-C5-C6-C7
5	A	1227	OLC	C2-C1-O20-C21
4	A	1208	OLA	C1-C2-C3-C4
5	A	1228	OLC	C7-C8-C9-C10
4	A	1208	OLA	C12-C13-C14-C15
4	A	1217	OLA	C11-C12-C13-C14
4	A	1223	OLA	C2-C3-C4-C5
5	A	1231	OLC	C4-C5-C6-C7
4	A	1221	OLA	C15-C16-C17-C18
4	A	1218	OLA	C9-C10-C11-C12
5	A	1228	OLC	C2-C3-C4-C5
4	A	1209	OLA	C3-C4-C5-C6
4	A	1216	OLA	C6-C7-C8-C9
4	A	1211	OLA	C1-C2-C3-C4
5	A	1227	OLC	C6-C7-C8-C9
4	A	1219	OLA	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1231	OLC	C5-C6-C7-C8
4	A	1219	OLA	C15-C16-C17-C18
5	A	1227	OLC	O19-C1-O20-C21
5	A	1229	OLC	O19-C1-O20-C21
5	A	1228	OLC	O19-C1-O20-C21
4	A	1205	OLA	C10-C11-C12-C13
5	A	1232	OLC	O20-C21-C22-C24
4	A	1205	OLA	C3-C4-C5-C6
4	A	1208	OLA	C10-C11-C12-C13
4	A	1220	OLA	C7-C8-C9-C10
4	A	1226	OLA	C3-C4-C5-C6
4	A	1209	OLA	C11-C12-C13-C14
5	A	1230	OLC	C6-C7-C8-C9
4	A	1212	OLA	C1-C2-C3-C4
5	A	1229	OLC	C5-C6-C7-C8
4	A	1214	OLA	C1-C2-C3-C4
5	A	1233	OLC	C2-C1-O20-C21
5	A	1229	OLC	C9-C10-C11-C12
5	A	1233	OLC	O19-C1-O20-C21
4	A	1220	OLA	C9-C10-C11-C12
4	A	1213	OLA	C4-C5-C6-C7
4	A	1209	OLA	C10-C11-C12-C13
5	A	1228	OLC	O20-C21-C22-C24
5	A	1229	OLC	C4-C5-C6-C7
4	A	1213	OLA	C7-C8-C9-C10
4	A	1209	OLA	C12-C13-C14-C15
5	A	1233	OLC	C3-C4-C5-C6
4	A	1216	OLA	C4-C5-C6-C7
4	A	1213	OLA	C2-C3-C4-C5
5	A	1230	OLC	O23-C22-C24-O25
4	A	1208	OLA	C3-C4-C5-C6
4	A	1214	OLA	C5-C6-C7-C8
5	A	1233	OLC	C4-C5-C6-C7
4	A	1217	OLA	C10-C11-C12-C13
5	A	1229	OLC	C6-C7-C8-C9
4	A	1219	OLA	C13-C14-C15-C16
4	A	1211	OLA	C2-C3-C4-C5
4	A	1210	OLA	C12-C13-C14-C15
4	A	1207	OLA	O2-C1-C2-C3
4	A	1208	OLA	O2-C1-C2-C3
4	A	1219	OLA	C9-C10-C11-C12
4	A	1211	OLA	C3-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	1216	OLA	C7-C8-C9-C10
4	A	1225	OLA	C7-C8-C9-C10
4	A	1226	OLA	C7-C8-C9-C10
4	A	1225	OLA	O2-C1-C2-C3
4	A	1208	OLA	O1-C1-C2-C3
4	A	1208	OLA	C7-C8-C9-C10
4	A	1207	OLA	O1-C1-C2-C3
5	A	1229	OLC	C11-C12-C13-C14
4	A	1210	OLA	C7-C8-C9-C10
4	A	1209	OLA	O1-C1-C2-C3
4	A	1215	OLA	C11-C12-C13-C14
4	A	1225	OLA	O1-C1-C2-C3
4	A	1209	OLA	C9-C10-C11-C12
4	A	1215	OLA	C7-C8-C9-C10
3	A	1204	CLR	C16-C17-C20-C22
4	A	1212	OLA	C2-C3-C4-C5
4	A	1209	OLA	C7-C8-C9-C10
4	A	1216	OLA	C15-C16-C17-C18
4	A	1209	OLA	O2-C1-C2-C3
5	A	1227	OLC	C3-C4-C5-C6
5	A	1231	OLC	C9-C10-C11-C12
3	A	1204	CLR	C22-C23-C24-C25
4	A	1205	OLA	O2-C1-C2-C3
4	A	1206	OLA	O2-C1-C2-C3
4	A	1216	OLA	C13-C14-C15-C16
4	A	1225	OLA	C2-C3-C4-C5
4	A	1206	OLA	O1-C1-C2-C3
5	A	1227	OLC	C1-C2-C3-C4

There are no ring outliers.

15 monomers are involved in 16 short contacts:

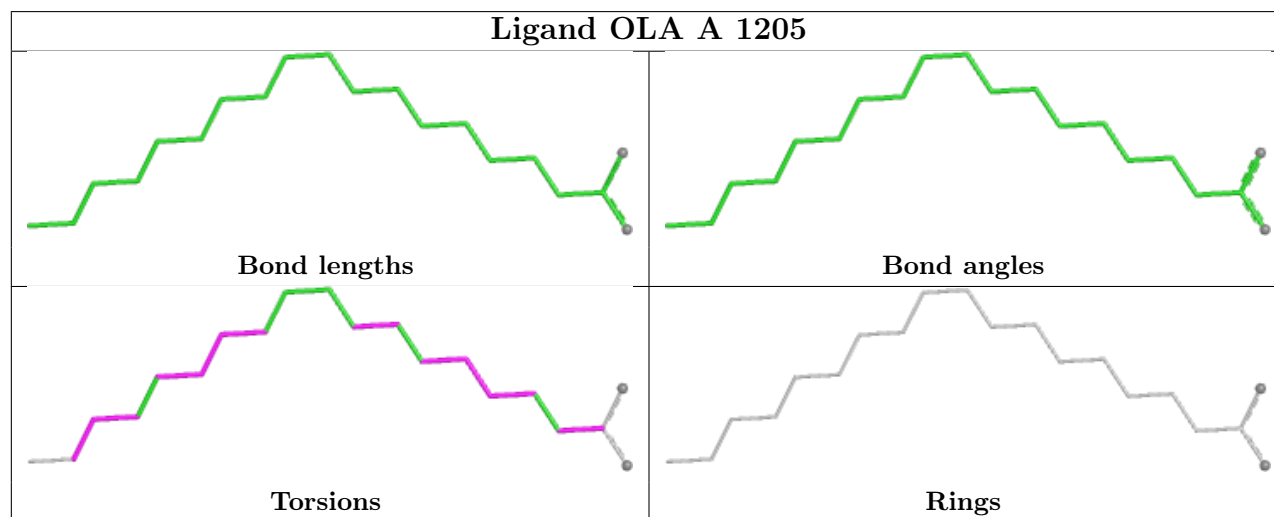
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1229	OLC	2	0
4	A	1209	OLA	2	0
4	A	1222	OLA	1	0
5	A	1233	OLC	1	0
4	A	1211	OLA	1	0
4	A	1226	OLA	1	0
5	A	1230	OLC	2	0
4	A	1224	OLA	1	0
4	A	1215	OLA	1	0

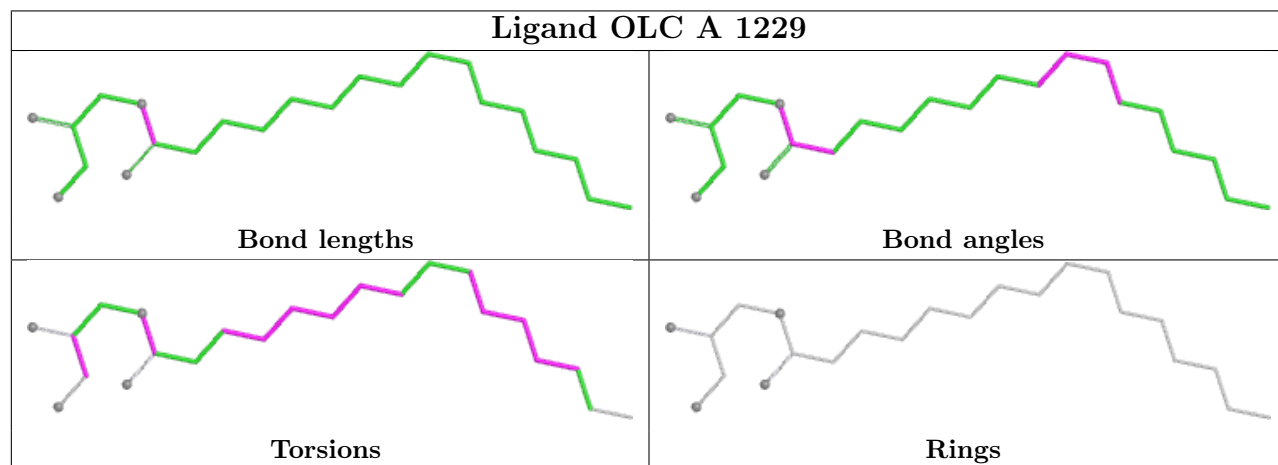
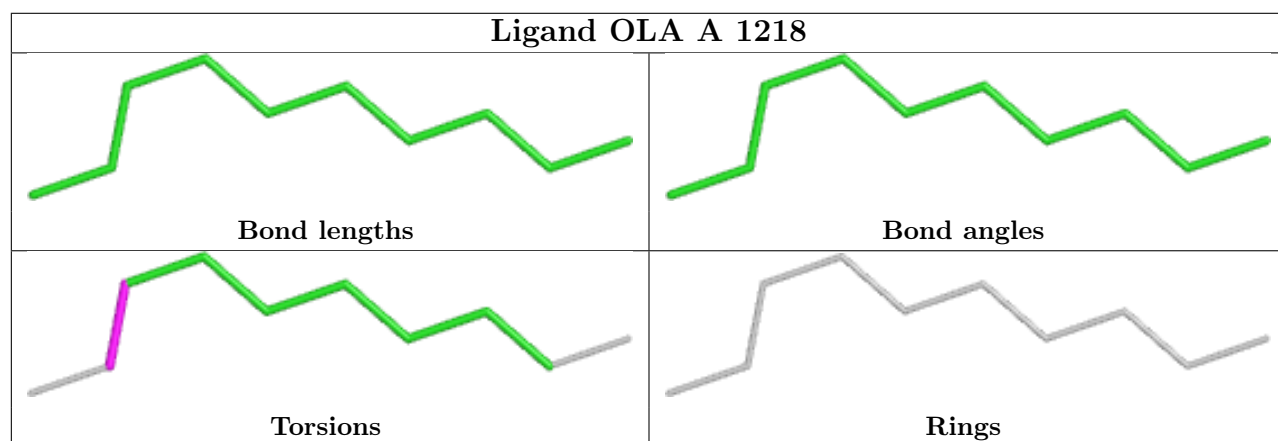
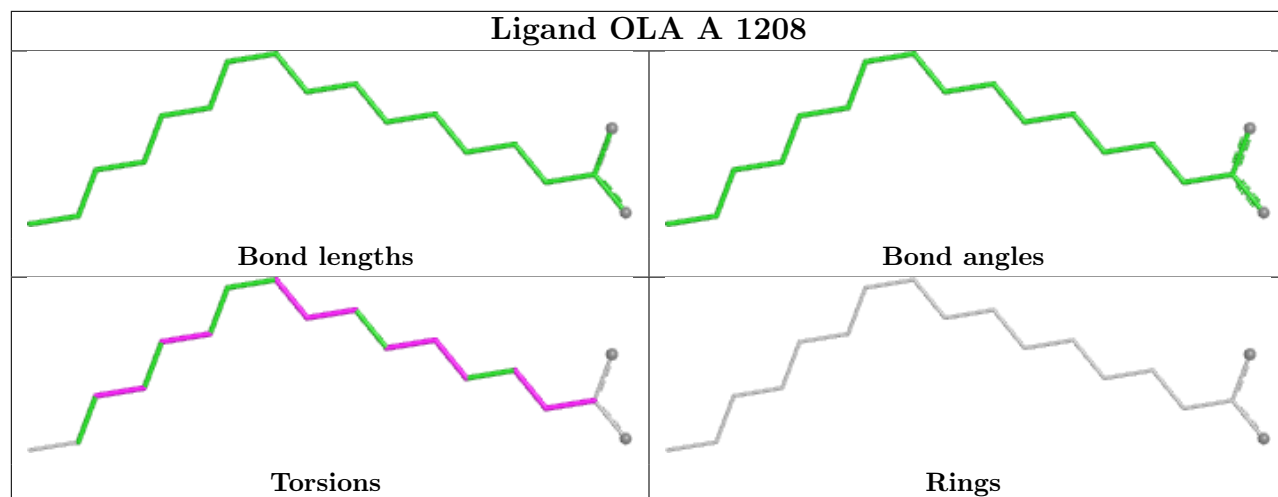
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1216	OLA	3	0
4	A	1210	OLA	2	0
5	A	1231	OLC	1	0
4	A	1221	OLA	1	0
4	A	1225	OLA	3	0
5	A	1232	OLC	1	0

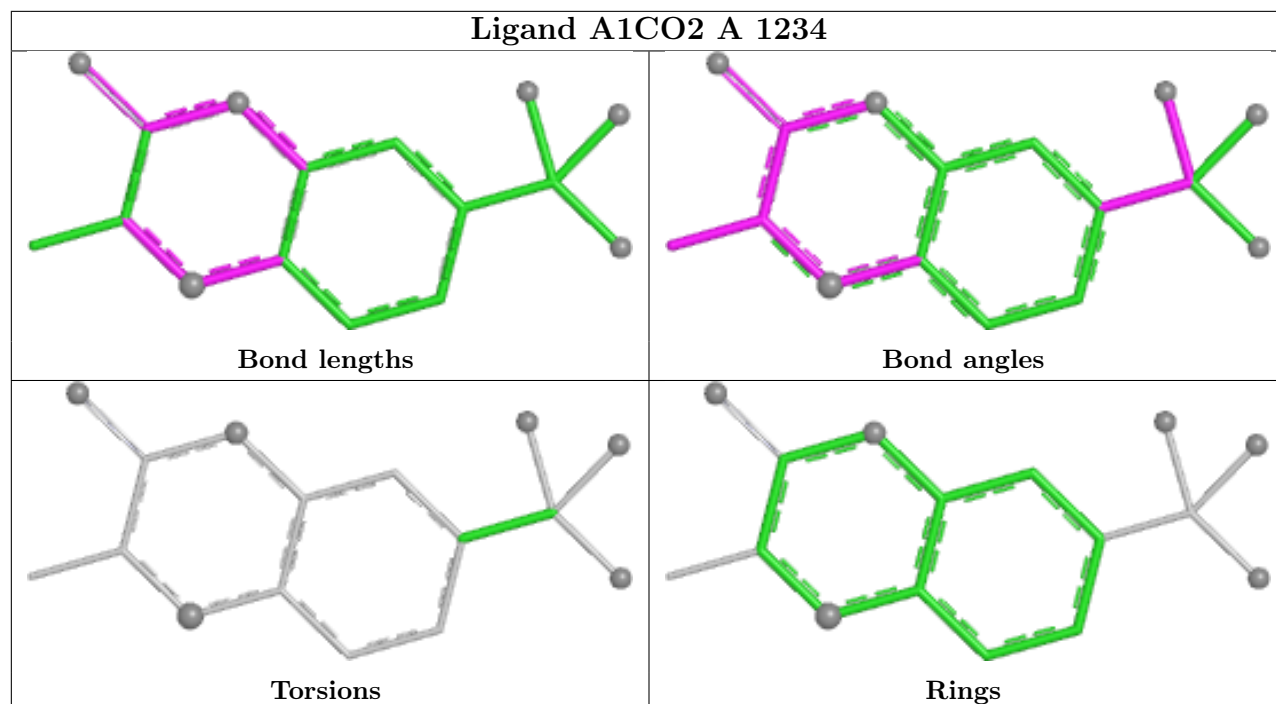
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



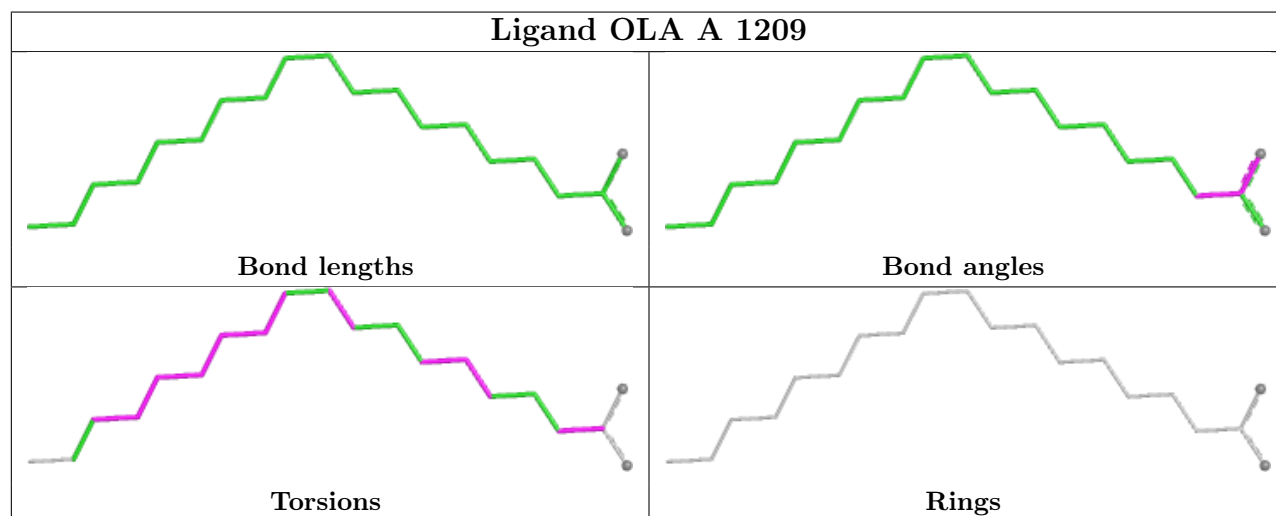




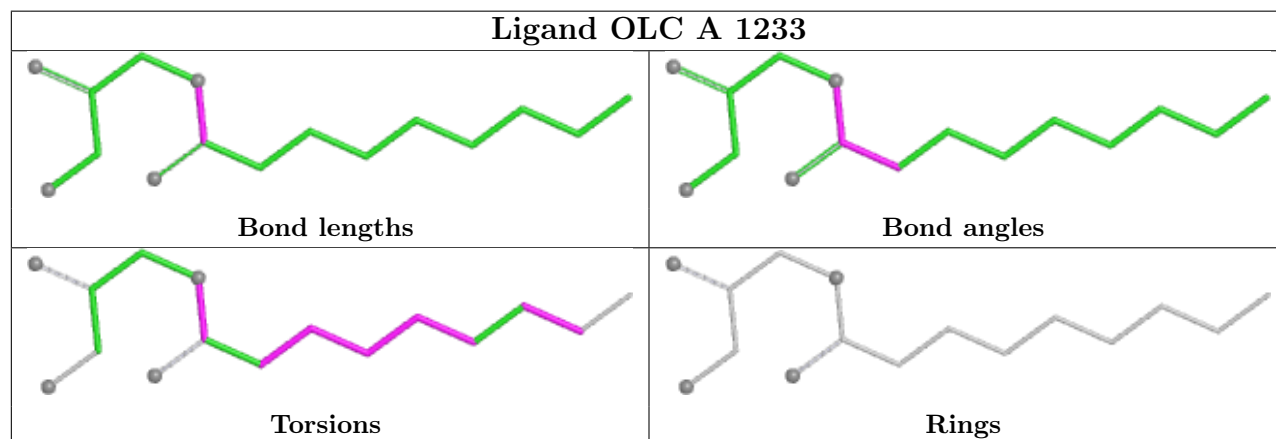
## Ligand A1CO2 A 1234

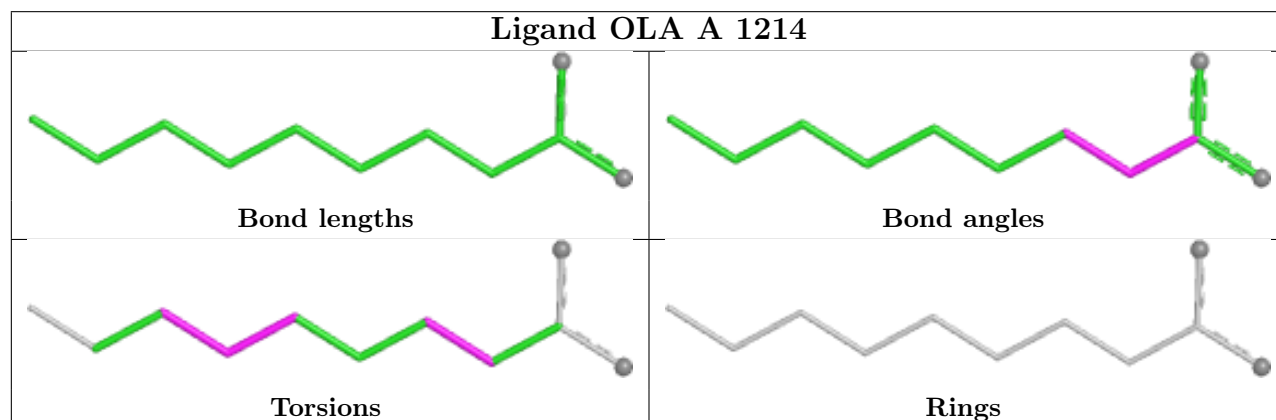
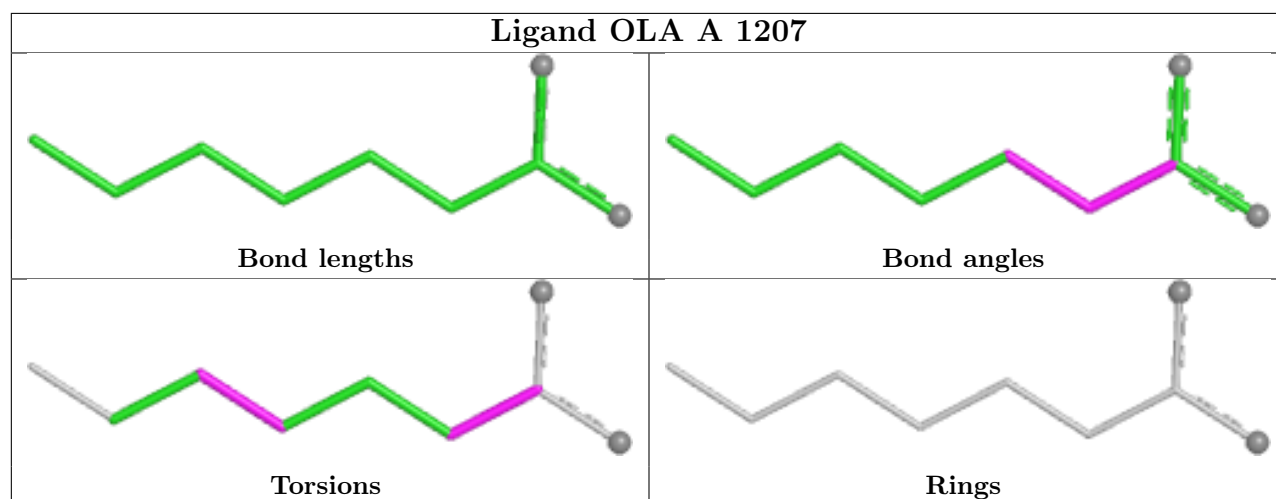
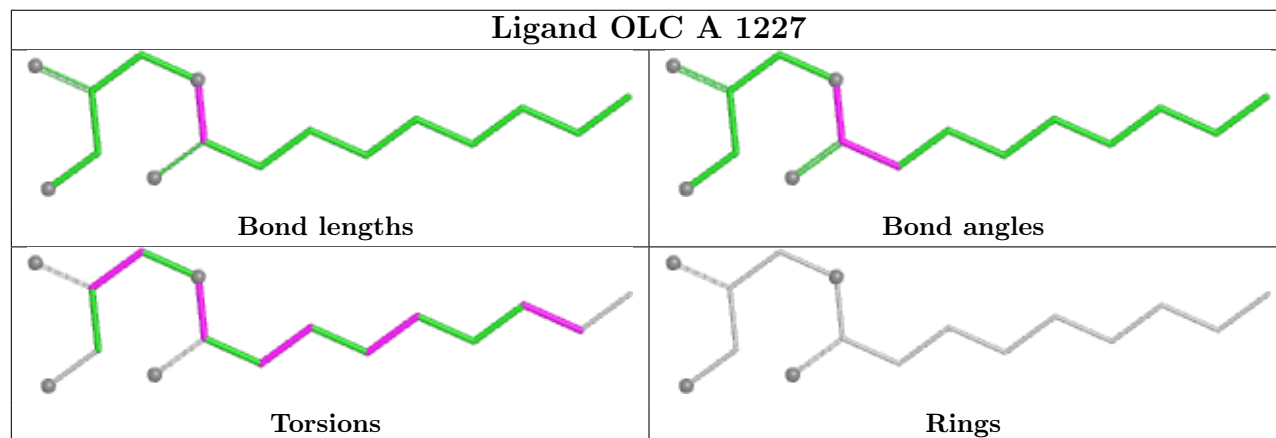
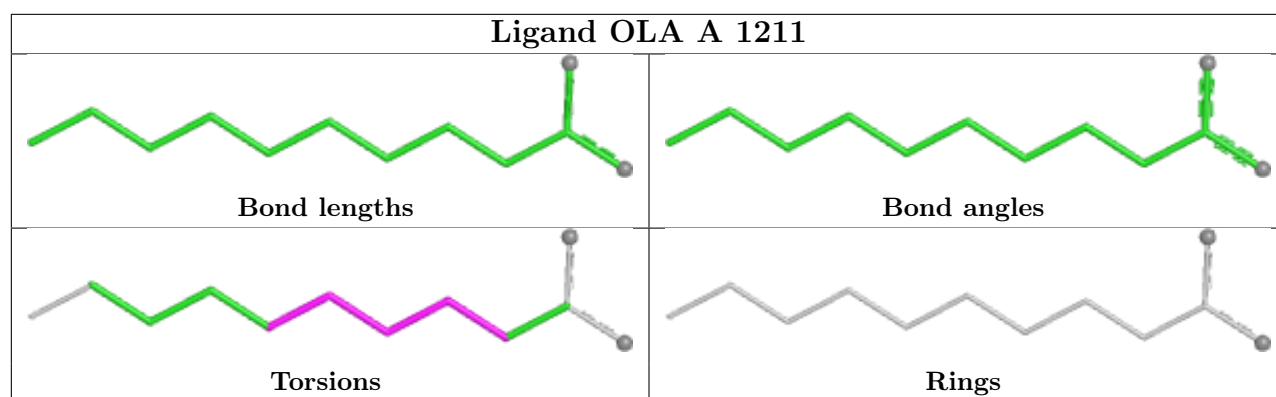


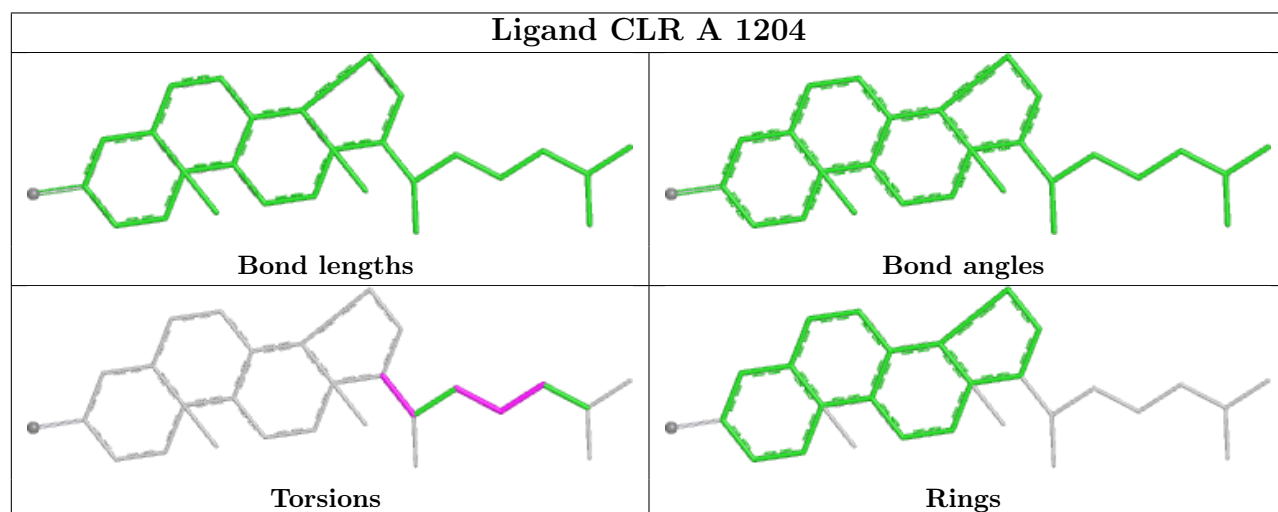
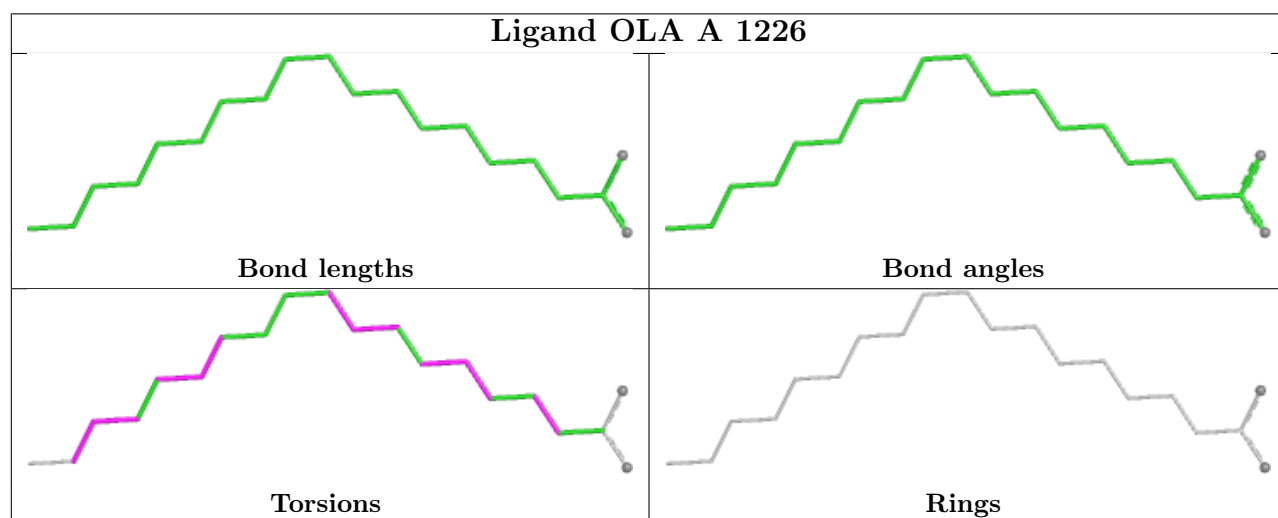
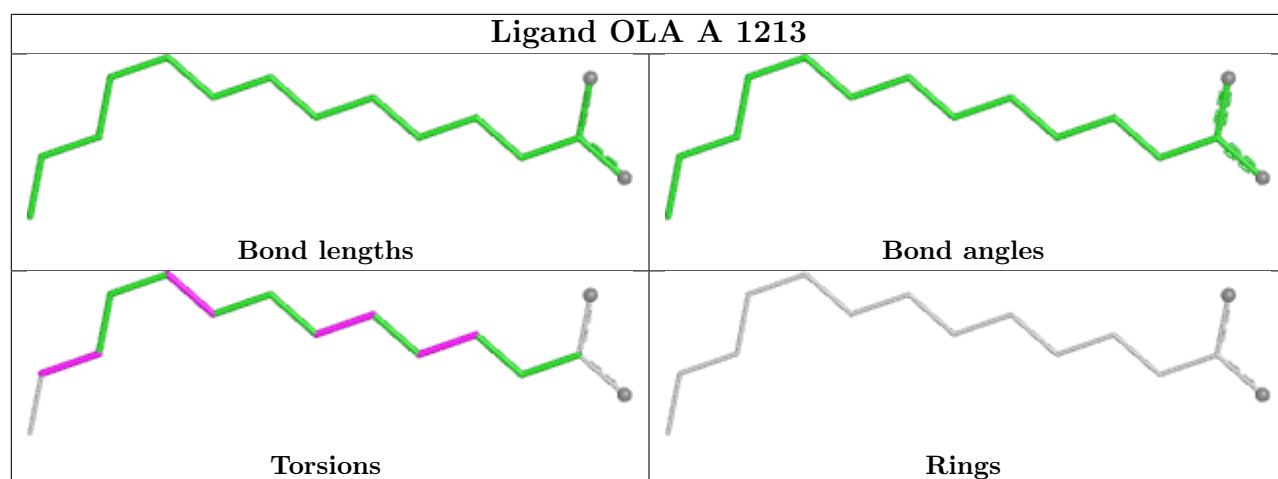
## Ligand OLA A 1209

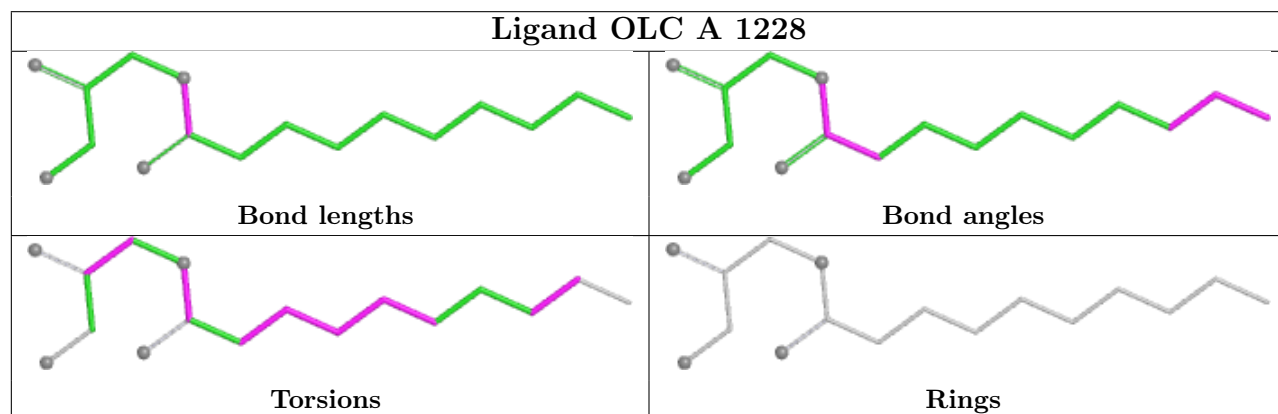
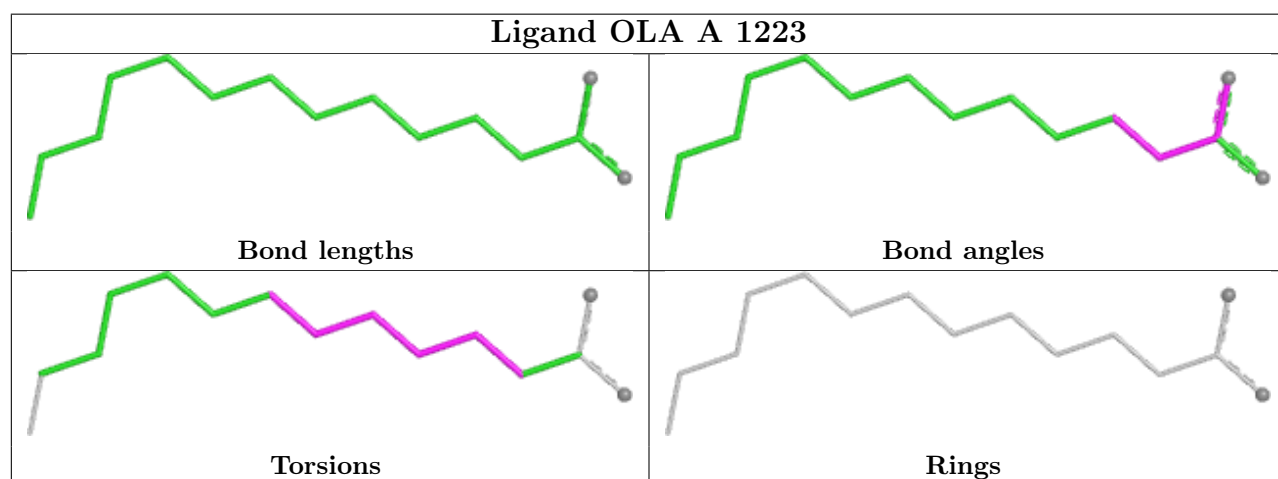
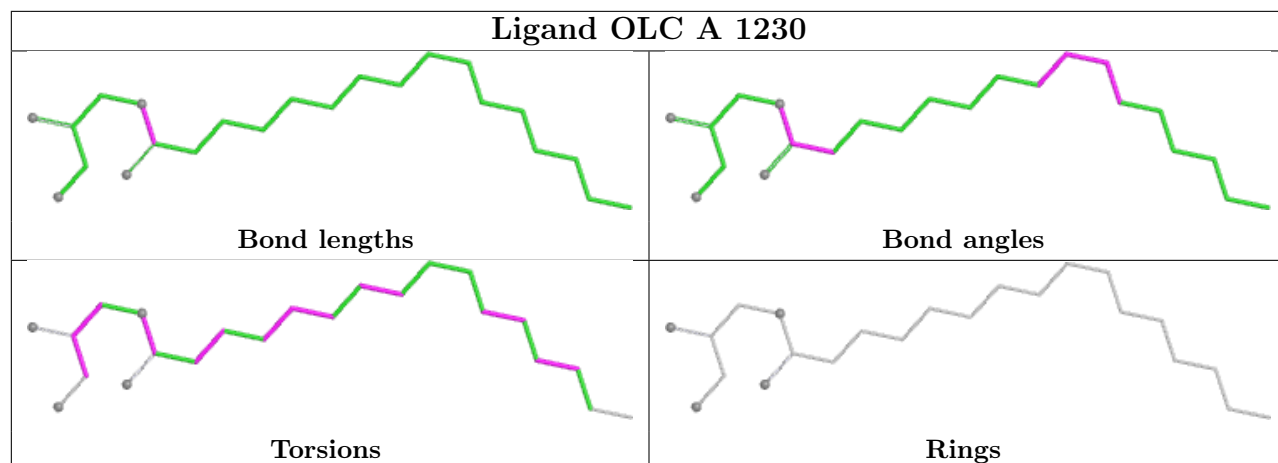


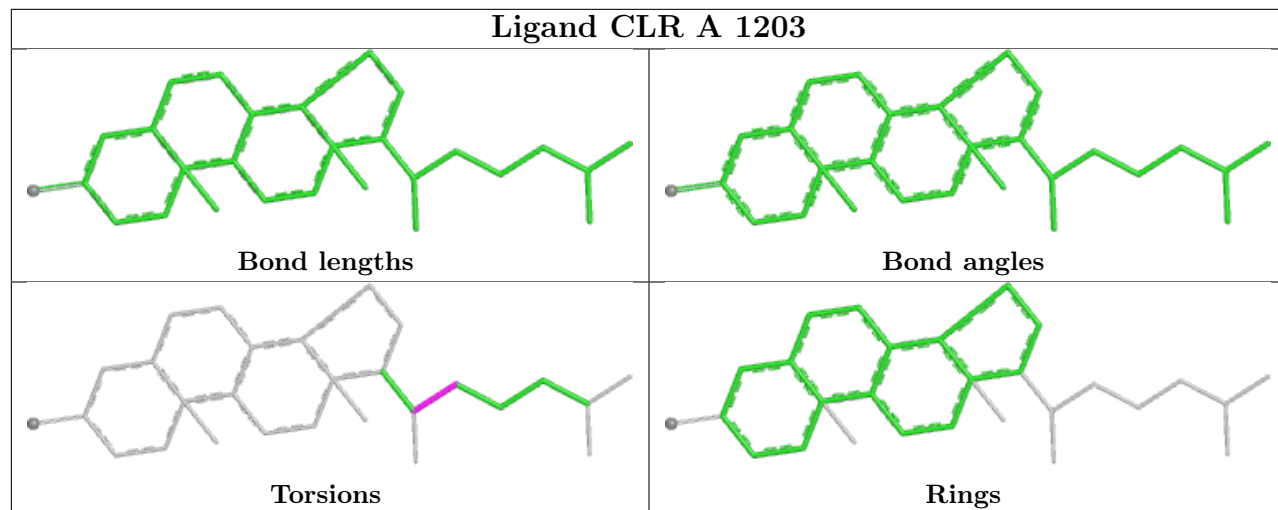
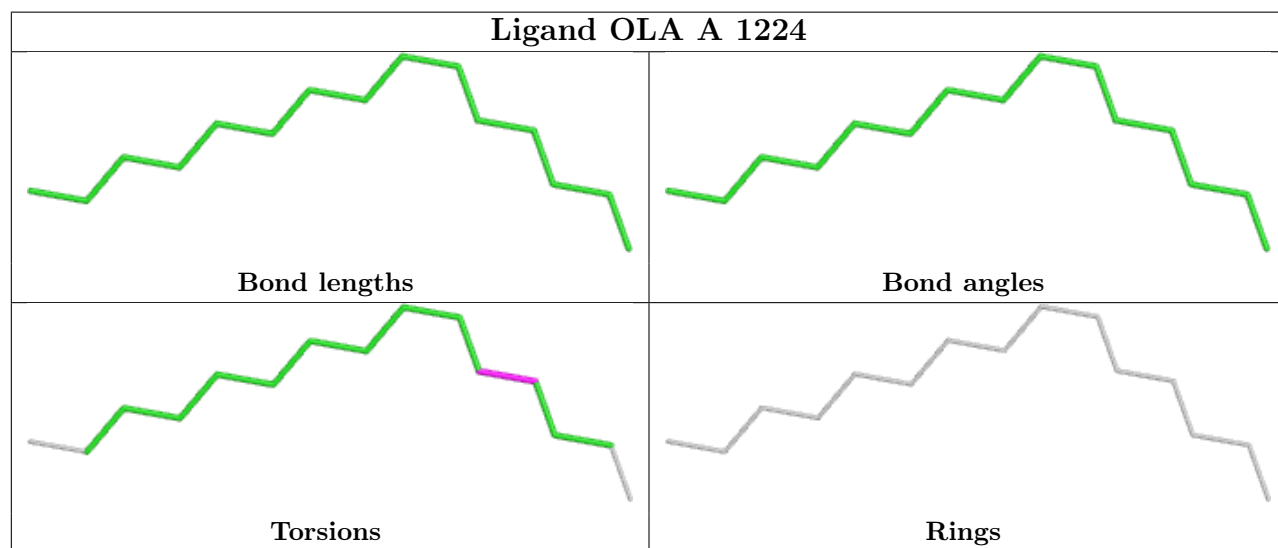
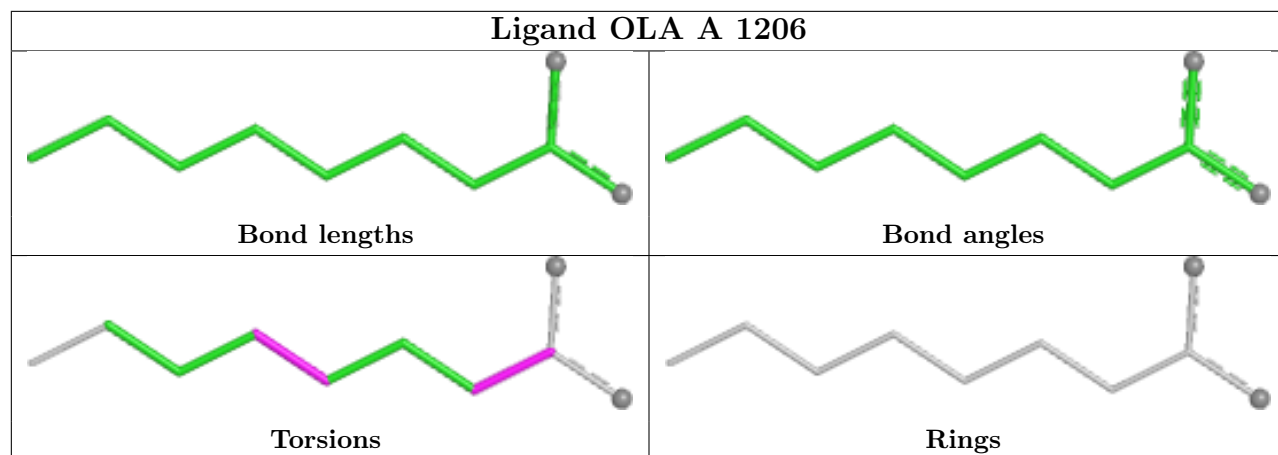
## Ligand OLC A 1233

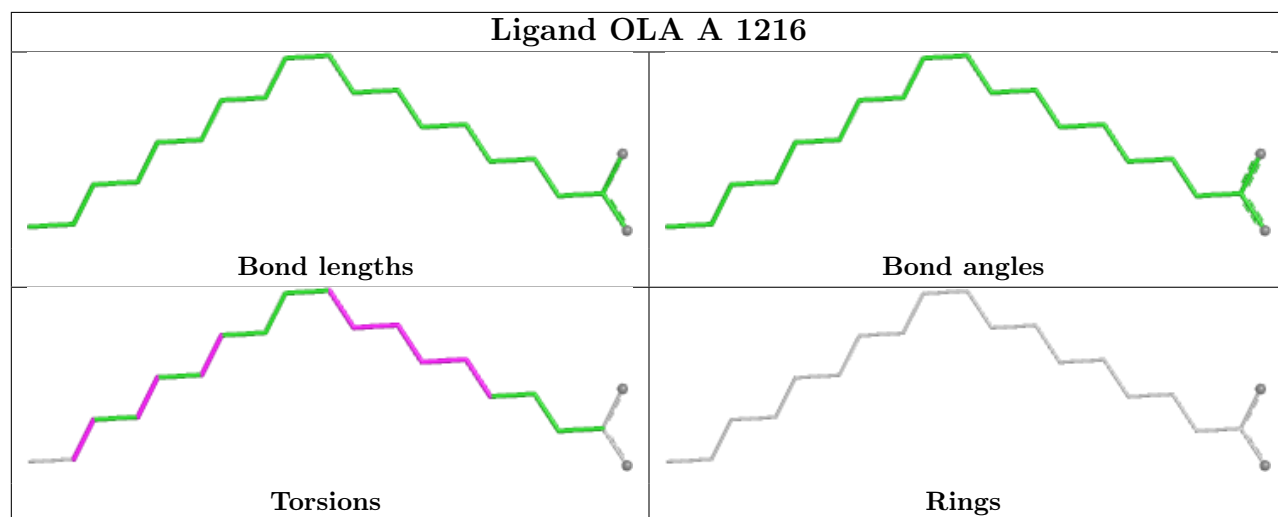
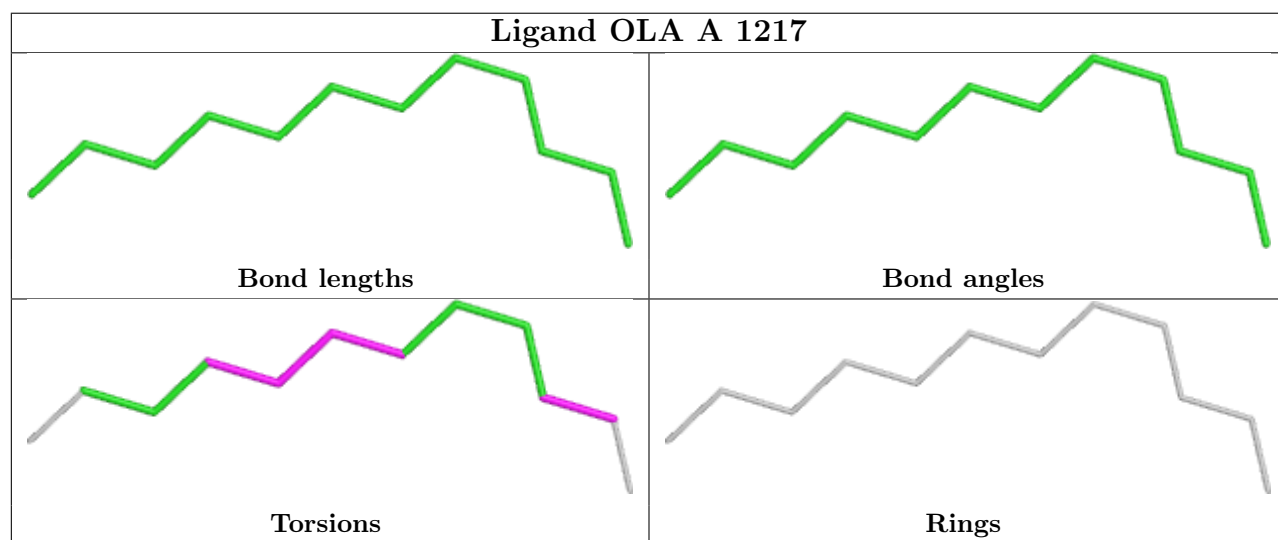
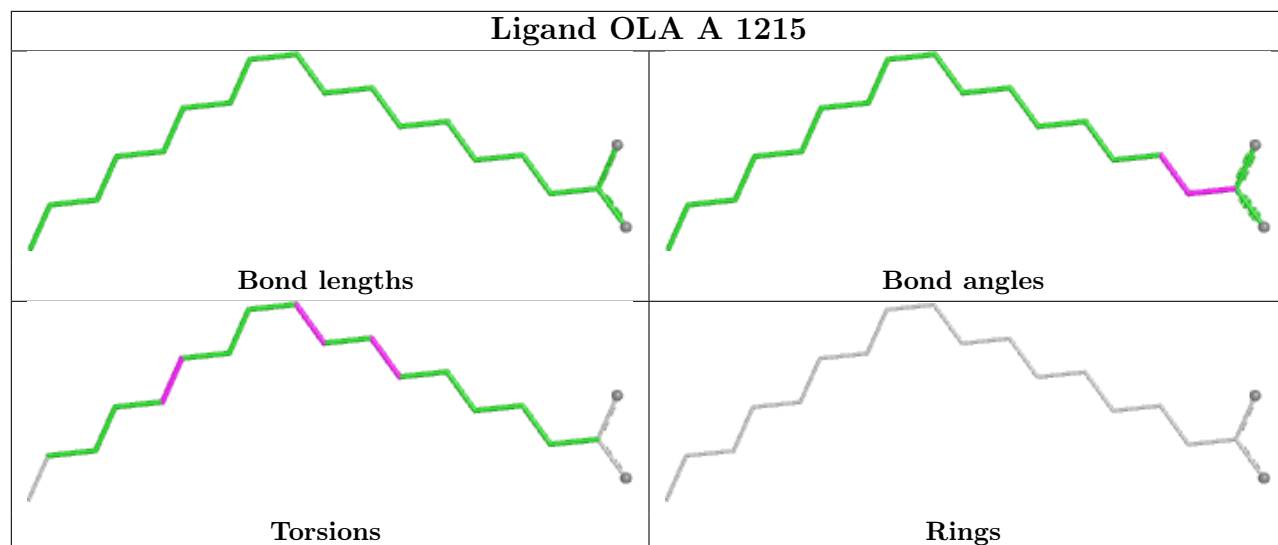


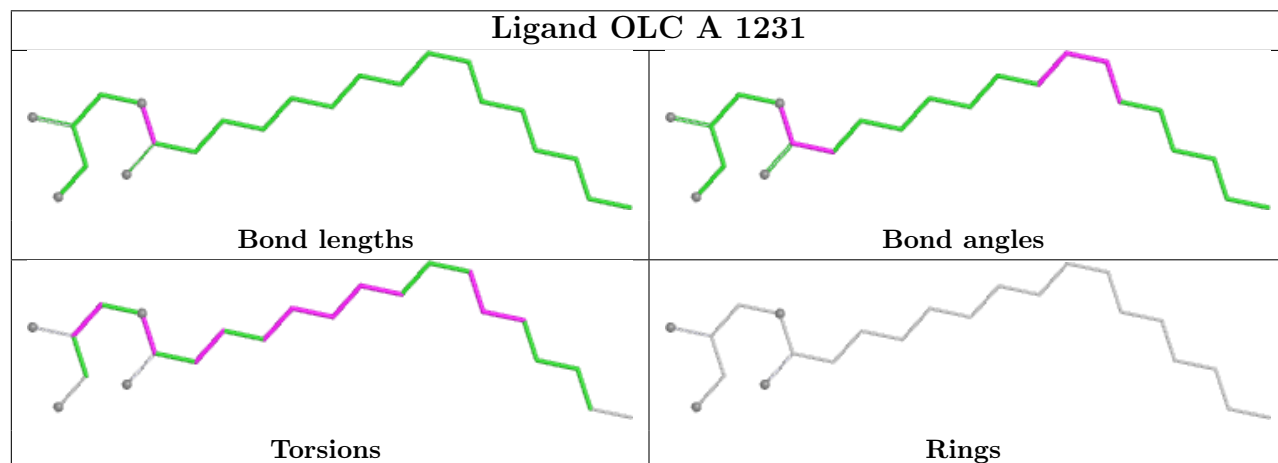
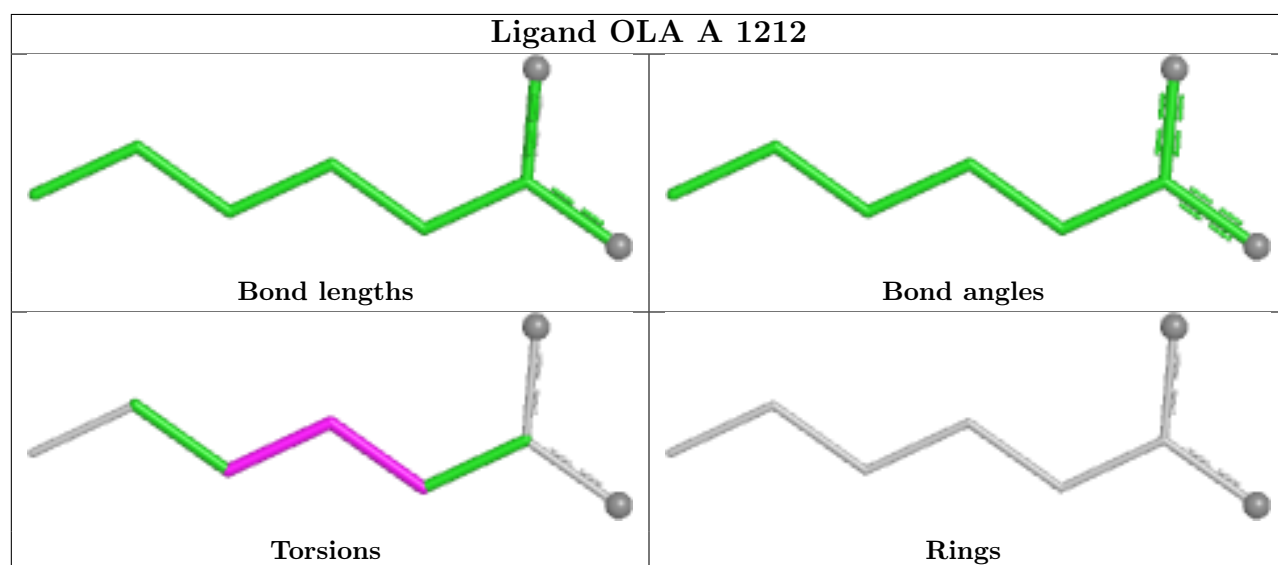
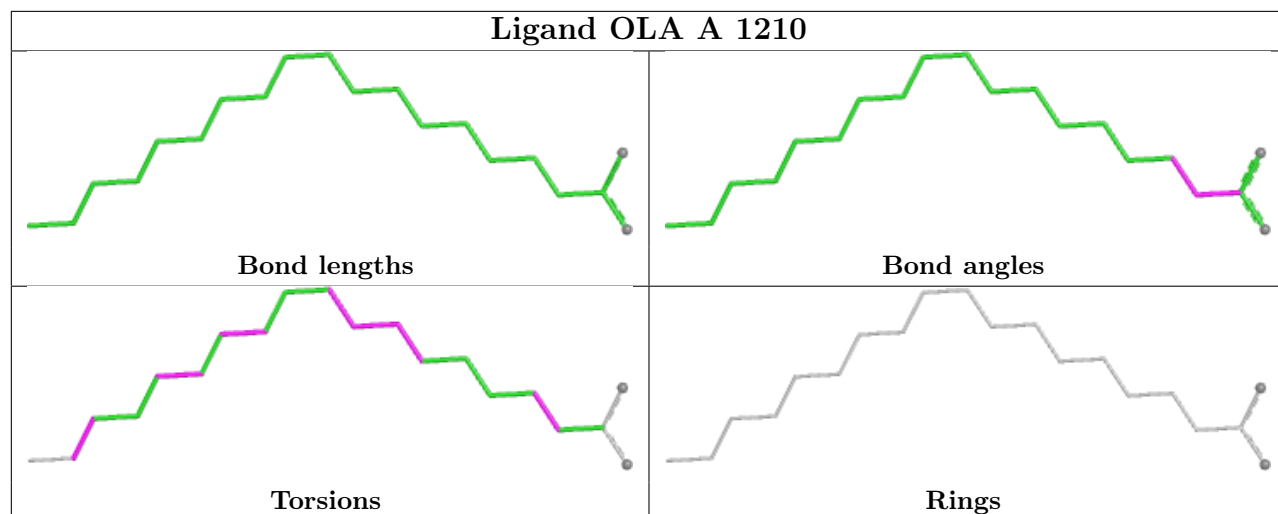


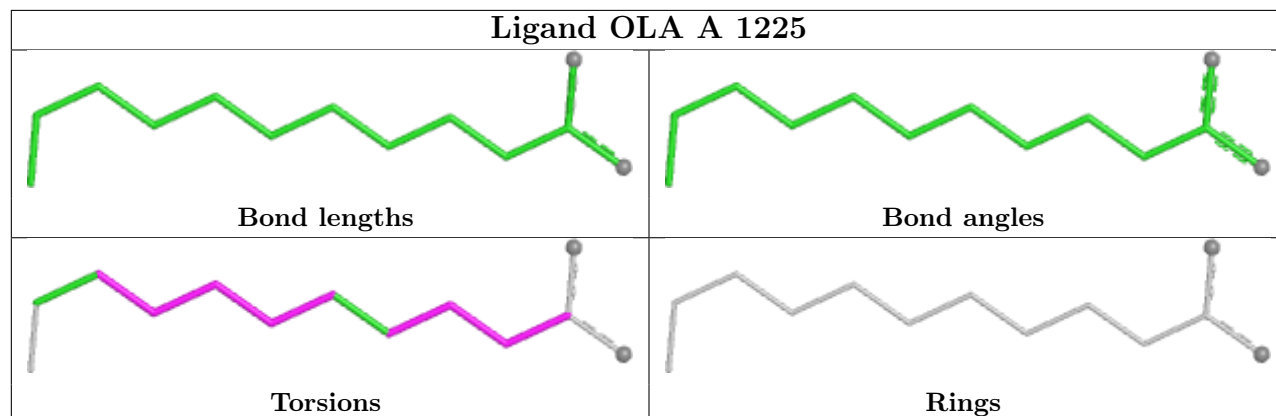
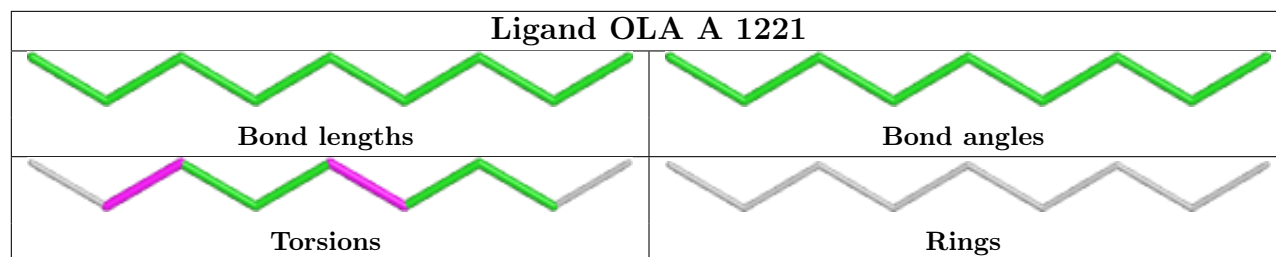




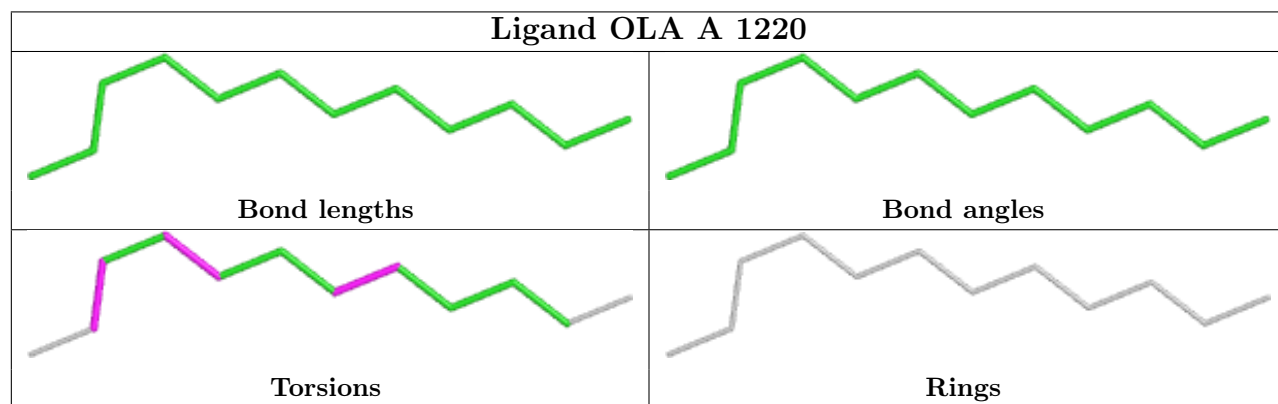
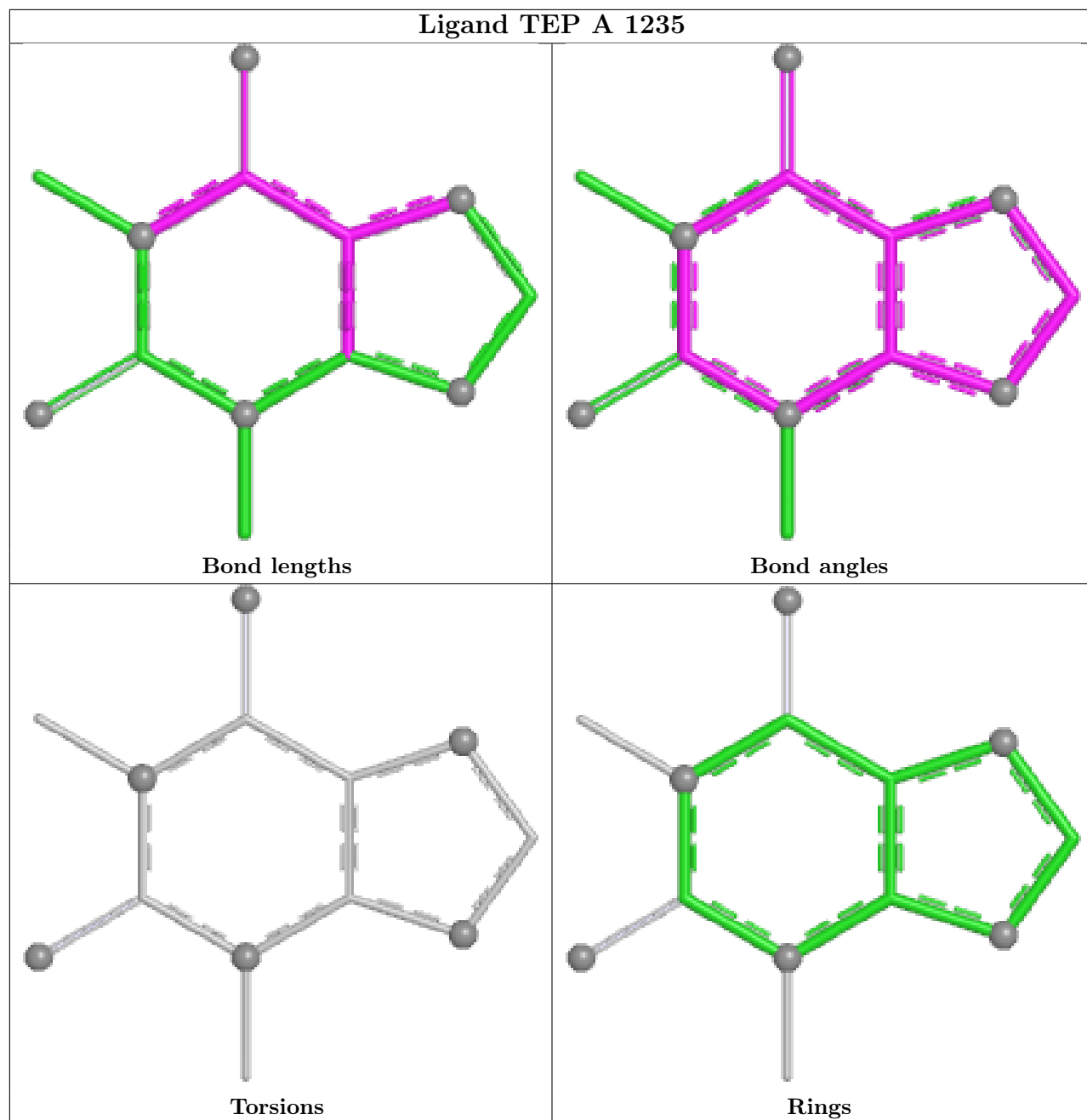


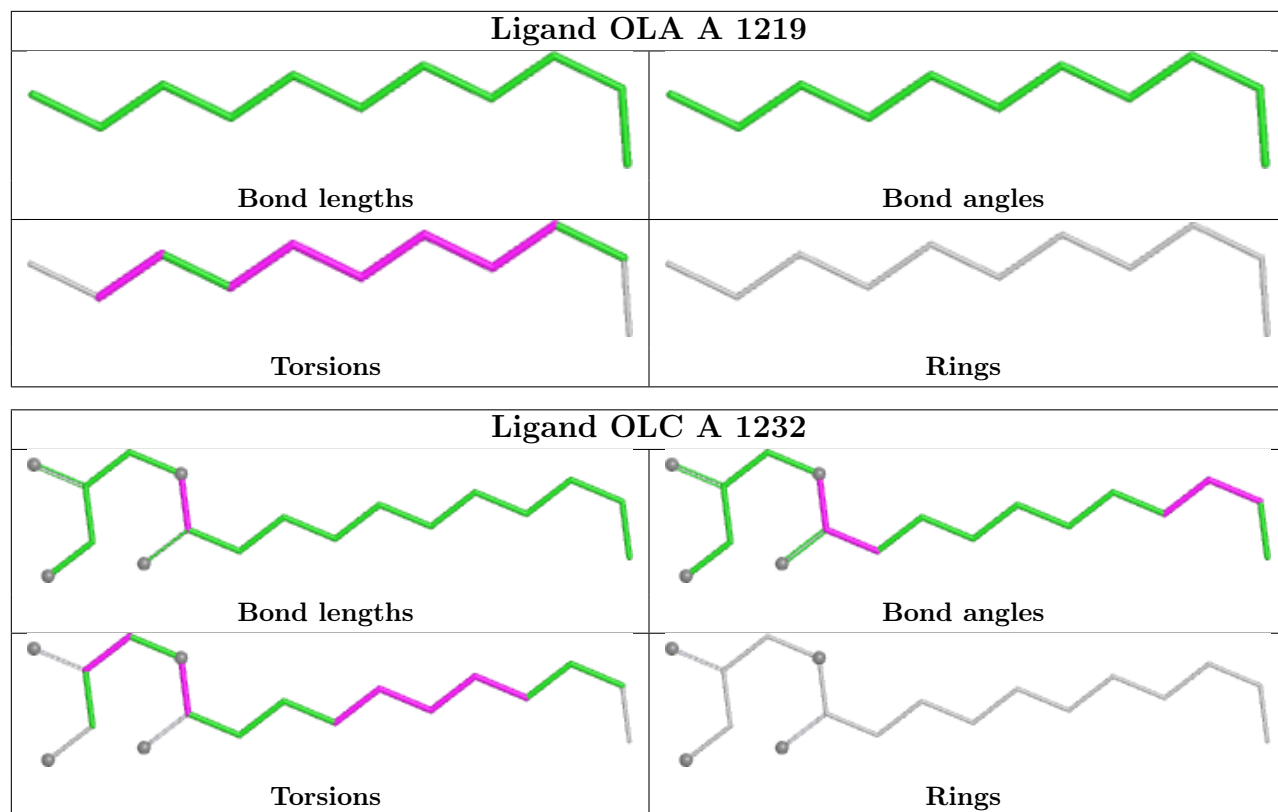












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	390/433 (90%)	1.11	73 (18%) 3 2	14, 42, 86, 119	13 (3%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	6.2
1	A	306	HIS	5.0
1	A	307	VAL	4.9
1	A	1021	ASP	4.2
1	A	1040	ALA	3.8
1	A	1106	LEU	3.7
1	A	1084	VAL	3.7
1	A	1042	LYS	3.7
1	A	1023	ALA	3.5
1	A	308	LEU	3.5
1	A	1036	ALA	3.5
1	A	1037	ALA	3.4
1	A	309	ARG	3.3
1	A	1041	GLN	3.3
1	A	1012	ASP	3.3
1	A	1026	VAL	3.2
1	A	29	TRP	3.1
1	A	1065	PHE	3.1
1	A	1094	LEU	2.9
1	A	1105	TYR	2.9
1	A	305	SER	2.9
1	A	1003	LEU	2.8
1	A	1015	LYS	2.8
1	A	222	ARG	2.8
1	A	111	ARG	2.8
1	A	1059	LYS	2.8
1	A	43	TYR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1097	THR	2.8
1	A	221	ALA	2.8
1	A	1016	VAL	2.7
1	A	1005	ASP	2.7
1	A	1063	HIS	2.7
1	A	1062	ARG	2.7
1	A	1017	ILE	2.7
1	A	300[A]	ARG	2.7
1	A	1082	GLY	2.6
1	A	1025	GLN	2.6
1	A	220	ARG	2.6
1	A	1078	LEU	2.6
1	A	208	LEU	2.6
1	A	75	HIS	2.6
1	A	1039	ASP	2.6
1	A	105	ALA	2.6
1	A	1038	LEU	2.5
1	A	0	ALA	2.5
1	A	1035	ALA	2.5
1	A	1022	ASN	2.5
1	A	202	ALA	2.5
1	A	205[A]	ARG	2.4
1	A	114	GLY	2.4
1	A	1068	LEU	2.4
1	A	290	TYR	2.3
1	A	108	ILE	2.3
1	A	35	SER	2.3
1	A	225	LEU	2.3
1	A	1074	ASP	2.2
1	A	73	ALA	2.2
1	A	119	THR	2.2
1	A	1028	ASP	2.2
1	A	112	TYR	2.2
1	A	233	LYS	2.2
1	A	110	LEU	2.2
1	A	1101	TYR	2.2
1	A	162	GLY	2.1
1	A	1008	GLU	2.1
1	A	1089	ALA	2.1
1	A	1066	ASP	2.1
1	A	147	GLY	2.1
1	A	161	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1102	ILE	2.1
1	A	226	GLN	2.0
1	A	1029	ALA	2.0
1	A	1019	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

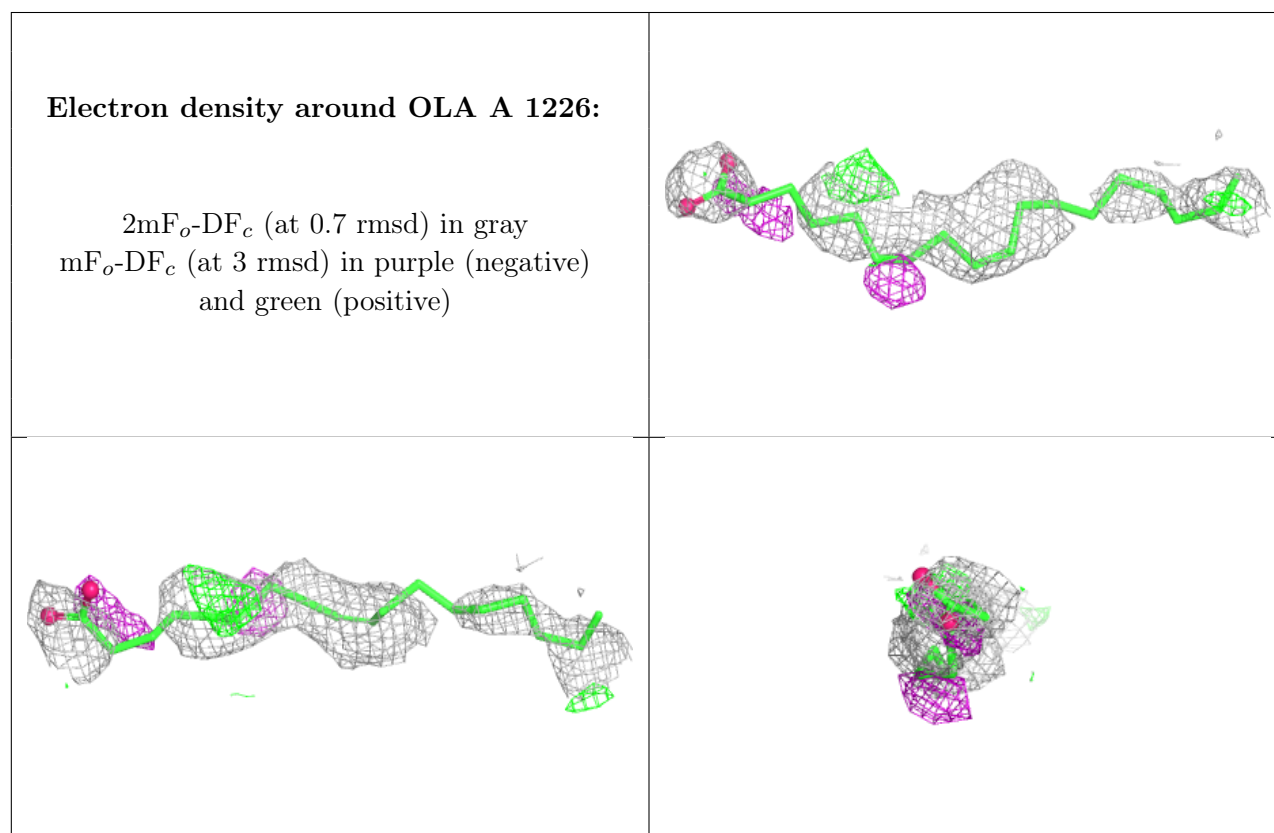
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OLA	A	1226	20/20	0.47	0.26	42,47,55,60	0
4	OLA	A	1225	13/20	0.59	0.20	35,41,60,63	0
4	OLA	A	1216	20/20	0.61	0.21	29,45,50,51	0
4	OLA	A	1223	15/20	0.63	0.18	36,38,47,50	0
5	OLC	A	1228	17/25	0.65	0.18	41,48,60,63	0
4	OLA	A	1213	15/20	0.66	0.18	41,45,55,56	0
4	OLA	A	1212	8/20	0.67	0.17	33,41,44,45	0
4	OLA	A	1222	8/20	0.67	0.22	37,41,42,42	0
4	OLA	A	1218	10/20	0.69	0.19	39,46,48,48	0
4	OLA	A	1220	12/20	0.70	0.16	29,36,37,39	0
4	OLA	A	1206	10/20	0.71	0.16	32,48,59,65	0
5	OLC	A	1233	16/25	0.71	0.20	31,40,48,49	0
4	OLA	A	1210	20/20	0.72	0.19	38,44,58,60	0
4	OLA	A	1208	18/20	0.72	0.16	31,39,48,53	0
5	OLC	A	1229	23/25	0.74	0.17	38,43,57,60	0
5	OLC	A	1232	18/25	0.74	0.18	32,48,57,63	0
4	OLA	A	1209	20/20	0.74	0.17	28,42,49,50	0
4	OLA	A	1214	11/20	0.75	0.15	29,36,46,51	0
5	OLC	A	1231	23/25	0.75	0.16	31,36,60,65	0

*Continued on next page...*

Continued from previous page...

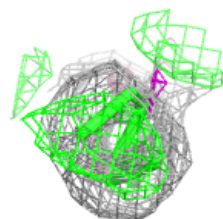
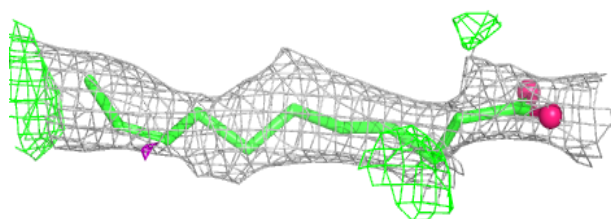
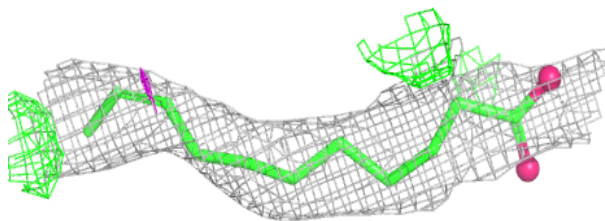
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OLA	A	1207	9/20	0.76	0.19	32,37,47,50	0
4	OLA	A	1219	11/20	0.76	0.17	31,33,43,45	0
4	OLA	A	1215	19/20	0.76	0.17	30,49,60,61	0
4	OLA	A	1211	12/20	0.76	0.15	35,41,46,49	0
4	OLA	A	1217	12/20	0.77	0.15	32,36,44,45	0
4	OLA	A	1224	15/20	0.77	0.16	30,33,39,40	0
5	OLC	A	1230	23/25	0.77	0.17	33,42,50,54	0
6	A1CO2	A	1234	16/16	0.77	0.21	39,49,69,77	16
4	OLA	A	1221	9/20	0.78	0.28	36,43,52,54	0
4	OLA	A	1205	20/20	0.80	0.16	32,38,50,52	0
5	OLC	A	1227	16/25	0.84	0.14	31,35,43,47	0
3	CLR	A	1202	28/28	0.86	0.15	30,35,46,59	0
3	CLR	A	1203	28/28	0.87	0.15	36,40,46,48	0
7	TEP	A	1235	13/13	0.88	0.11	25,26,29,31	0
2	NA	A	1201	1/1	0.90	0.13	33,33,33,33	0
3	CLR	A	1204	28/28	0.92	0.11	31,33,37,37	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.

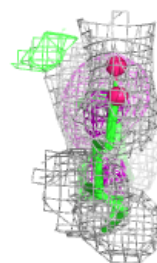
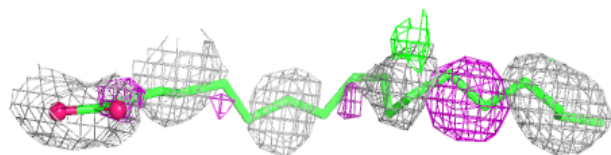
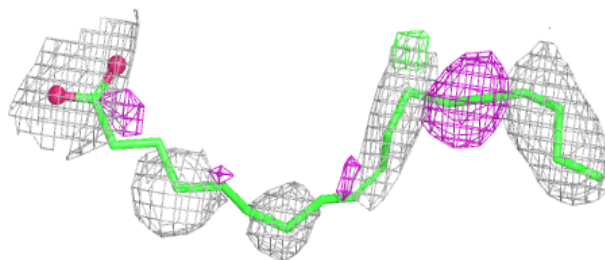


**Electron density around OLA A 1225:**

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

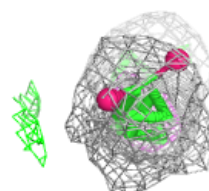
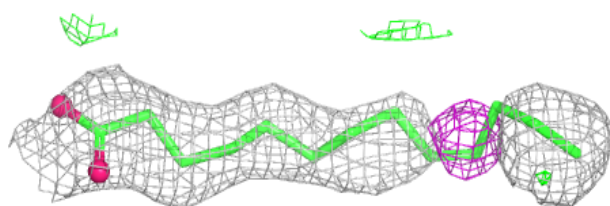
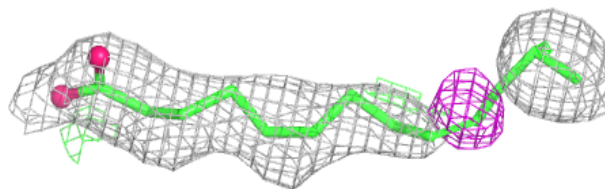
**Electron density around OLA A 1216:**

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

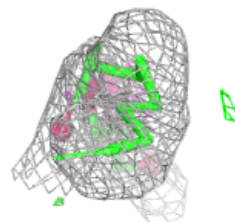
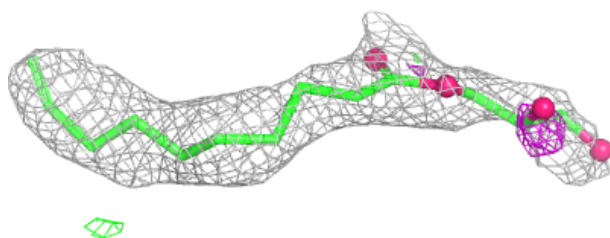
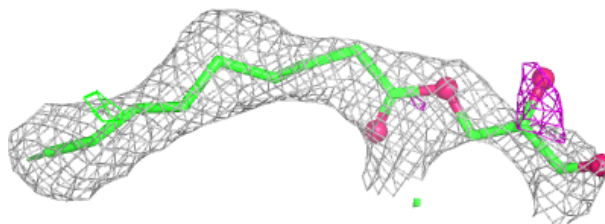


**Electron density around OLA A 1223:**

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

**Electron density around OLC A 1228:**

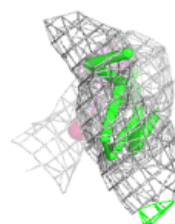
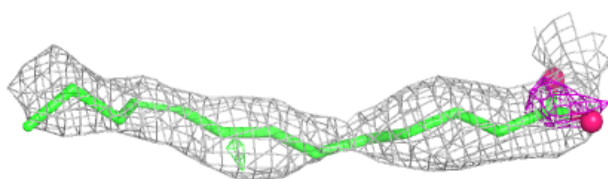
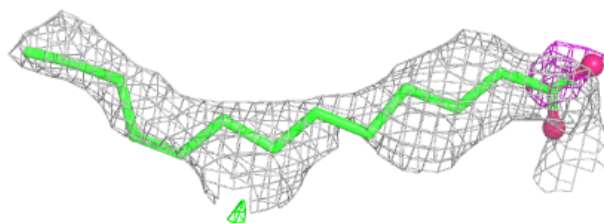
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



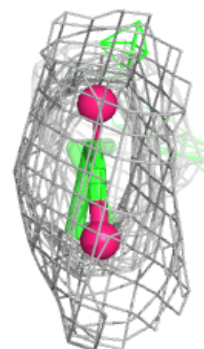
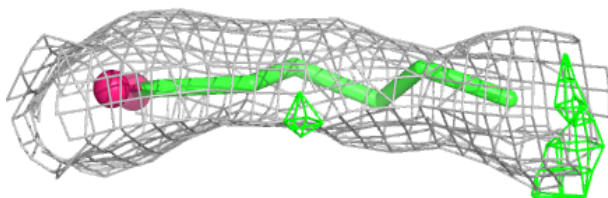


**Electron density around OLA A 1213:**

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

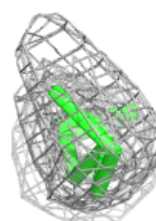
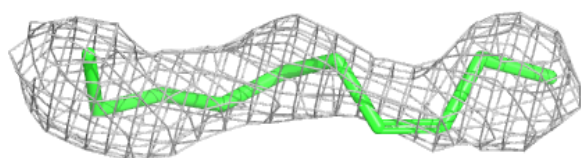
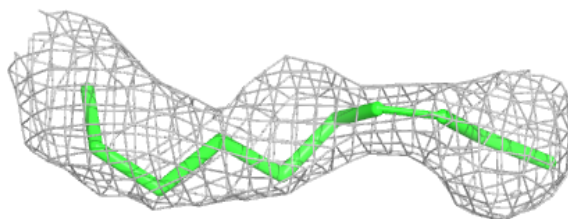
**Electron density around OLA A 1212:**

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

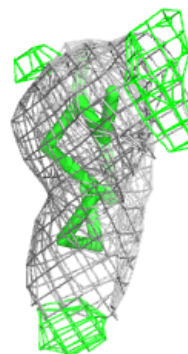
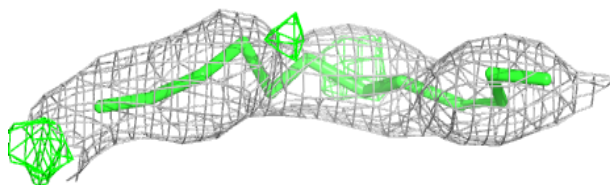
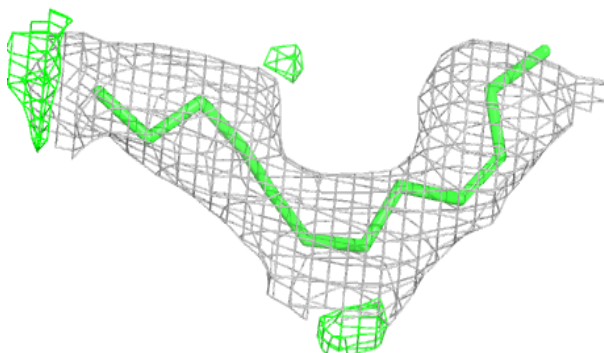


**Electron density around OLA A 1218:**

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

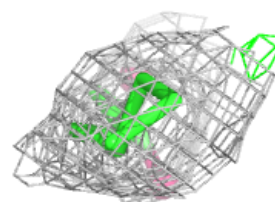
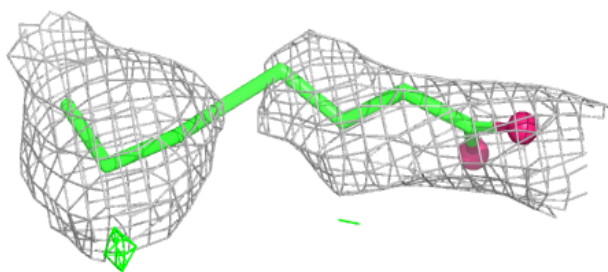
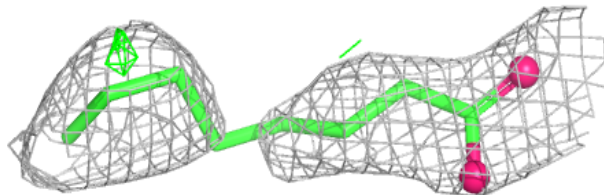
**Electron density around OLA A 1220:**

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

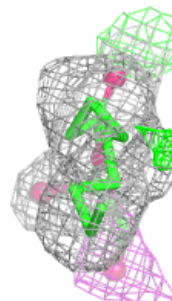
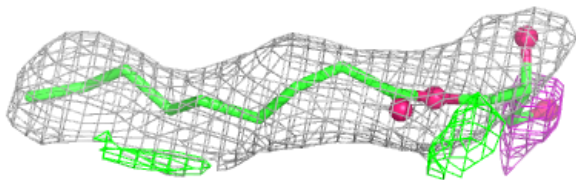
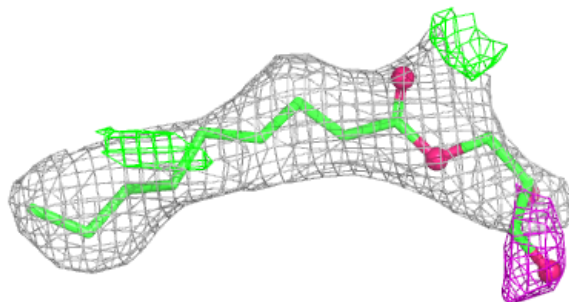


**Electron density around OLA A 1206:**

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

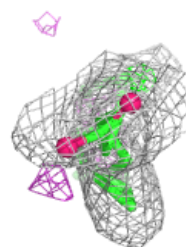
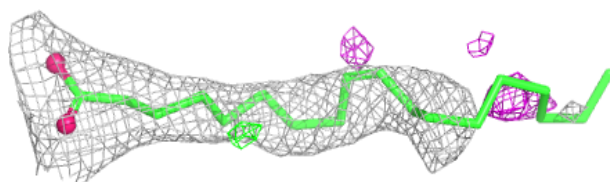
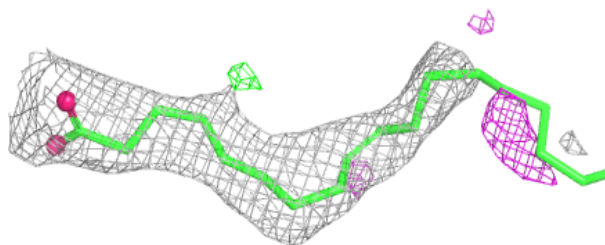
**Electron density around OLC A 1233:**

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

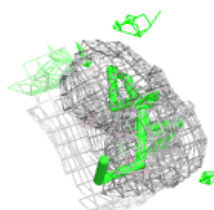
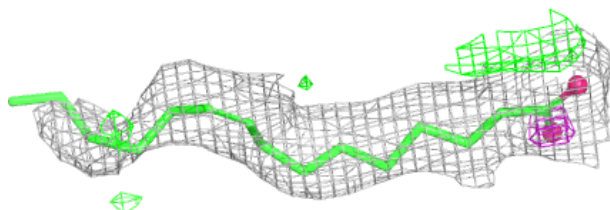
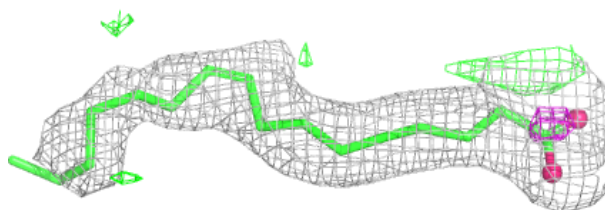


**Electron density around OLA A 1210:**

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

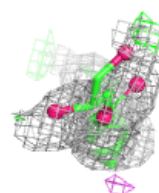
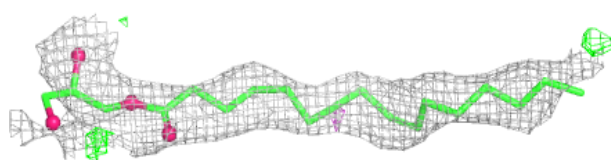
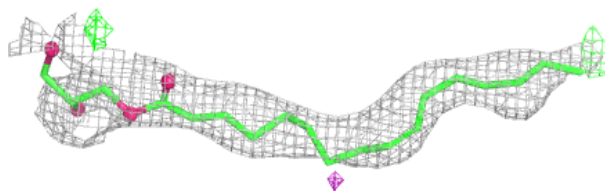
**Electron density around OLA A 1208:**

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

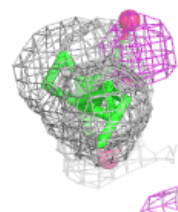
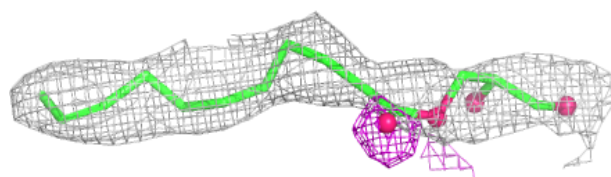
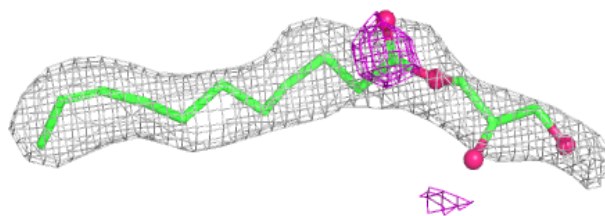


**Electron density around OLC A 1229:**

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

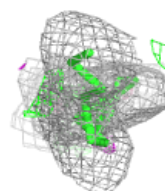
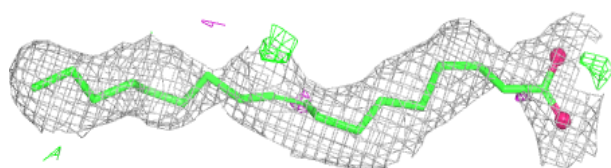
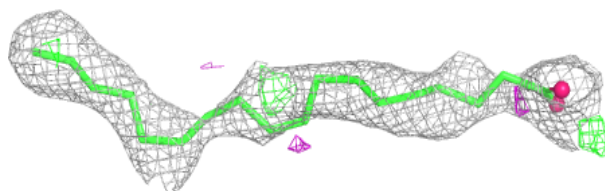
**Electron density around OLC A 1232:**

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

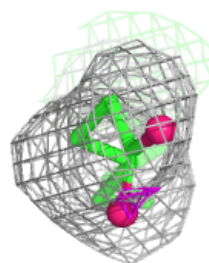
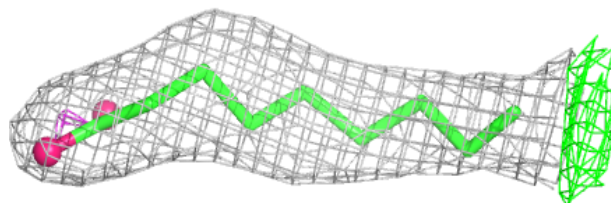
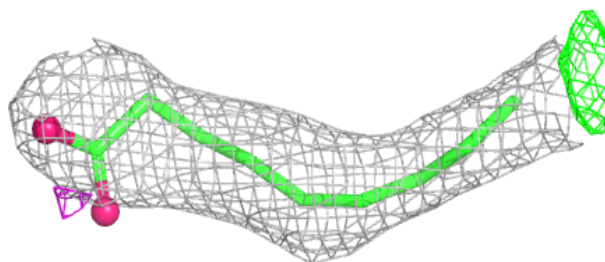


**Electron density around OLA A 1209:**

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

**Electron density around OLA A 1214:**

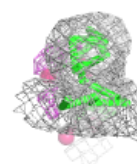
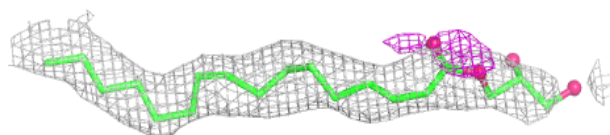
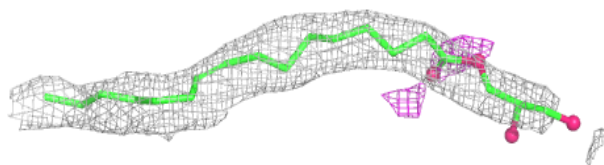
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



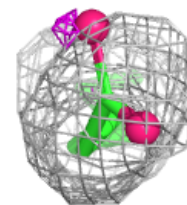
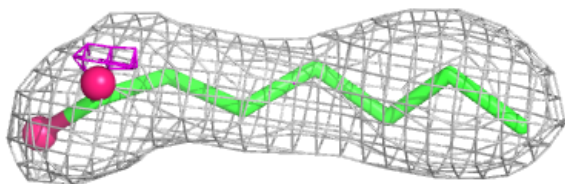
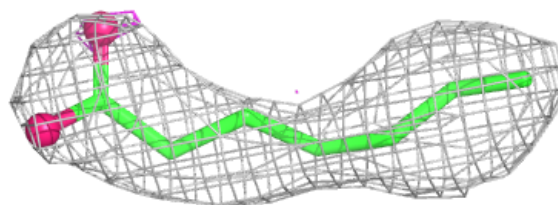


**Electron density around OLC A 1231:**

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

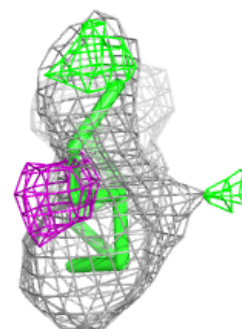
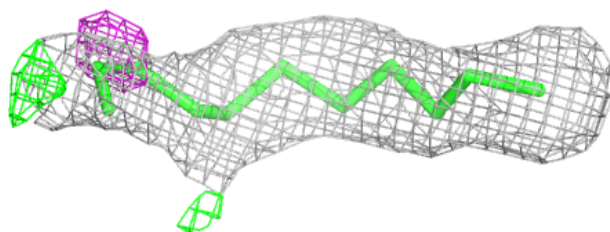
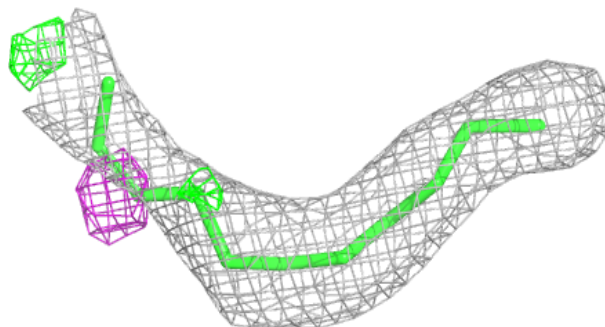
**Electron density around OLA A 1207:**

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

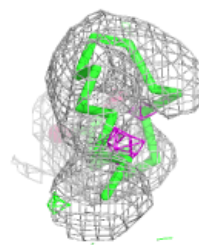
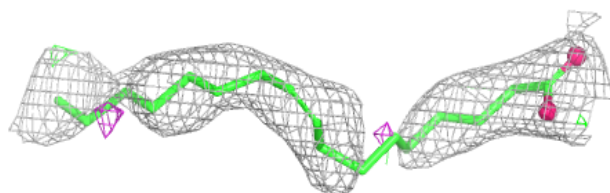
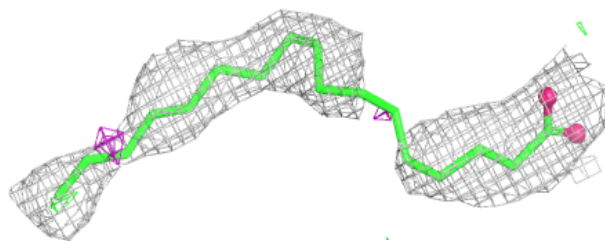


**Electron density around OLA A 1219:**

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

**Electron density around OLA A 1215:**

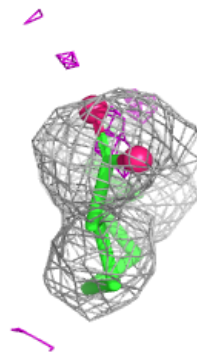
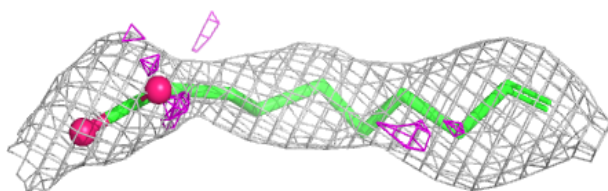
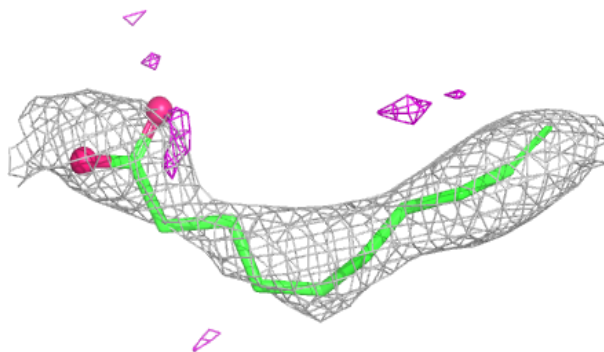
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



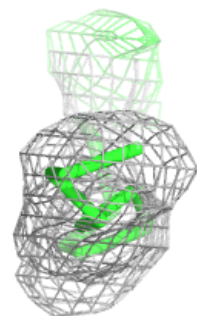
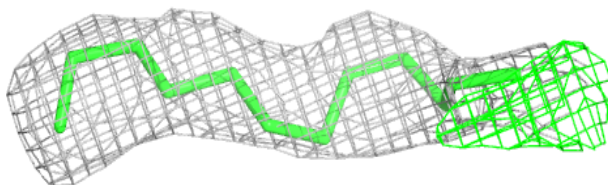
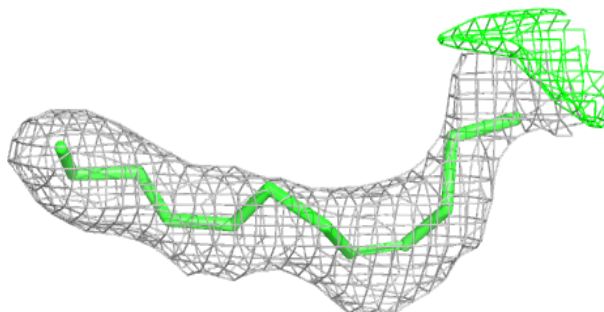


**Electron density around OLA A 1211:**

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

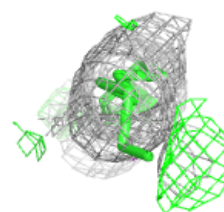
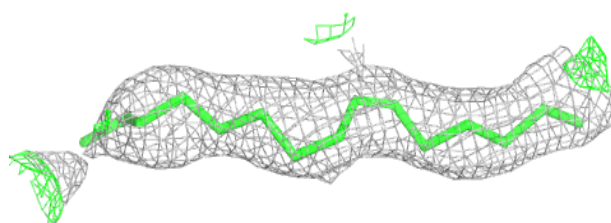
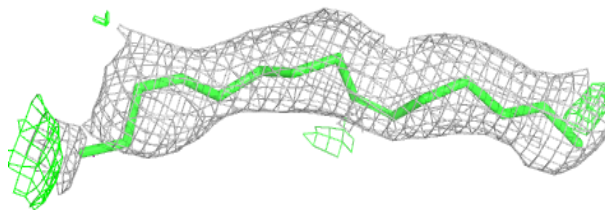
**Electron density around OLA A 1217:**

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

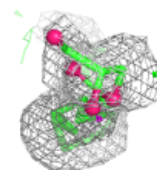
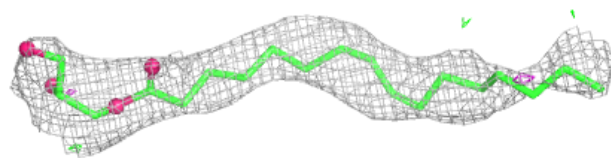
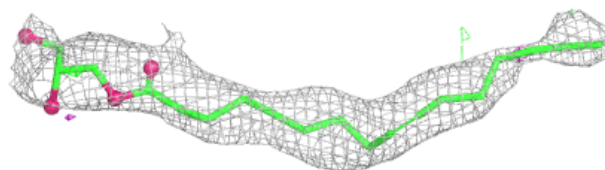


**Electron density around OLA A 1224:**

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

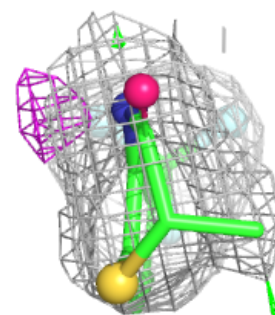
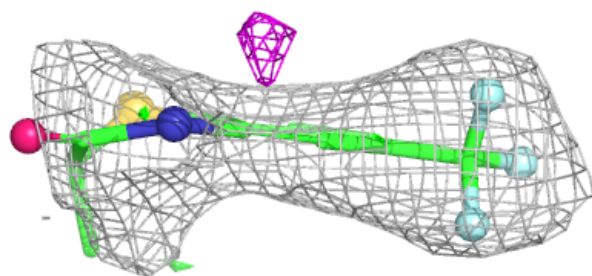
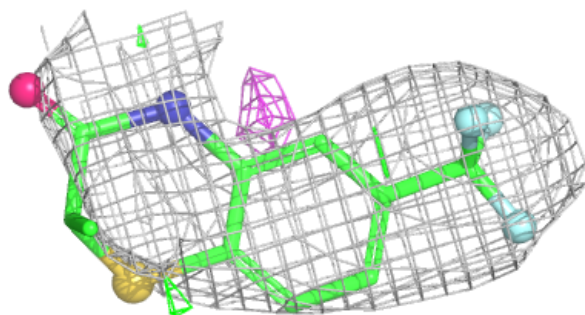
**Electron density around OLC A 1230:**

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

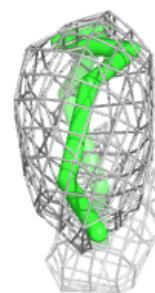
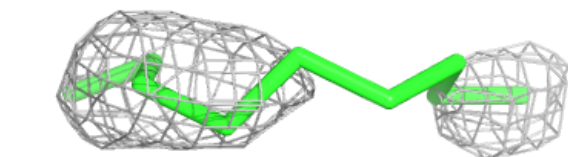
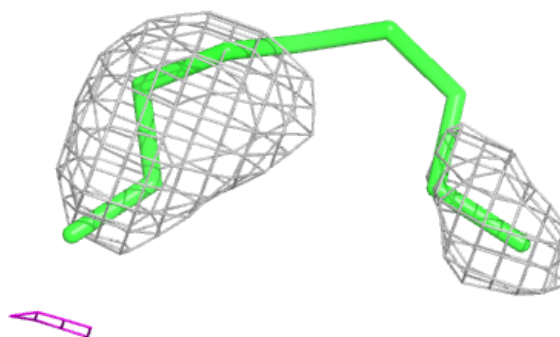


**Electron density around A1CO2 A 1234:**

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

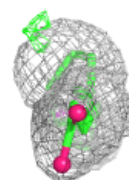
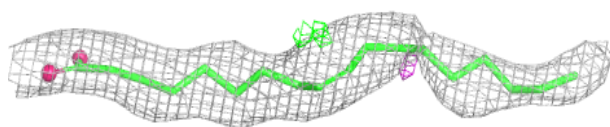
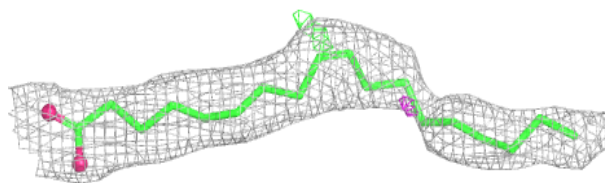
**Electron density around OLA A 1221:**

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

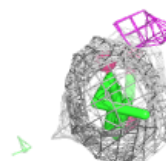
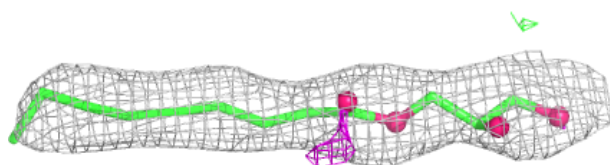
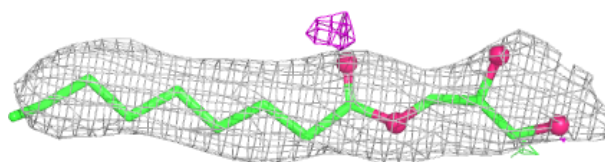


**Electron density around OLA A 1205:**

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

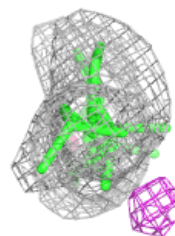
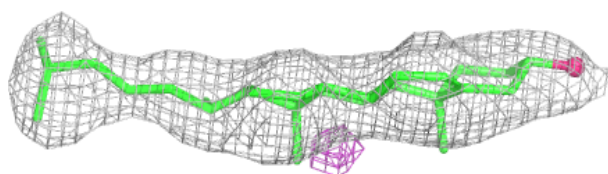
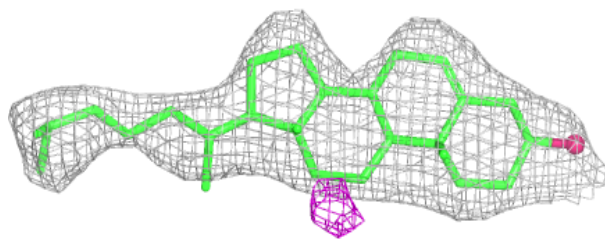
**Electron density around OLC A 1227:**

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



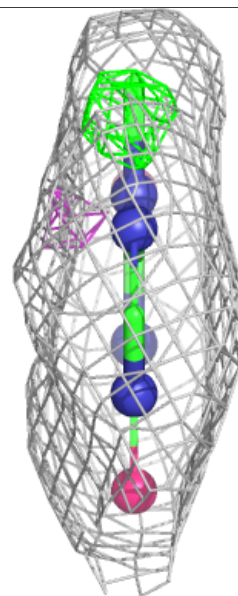
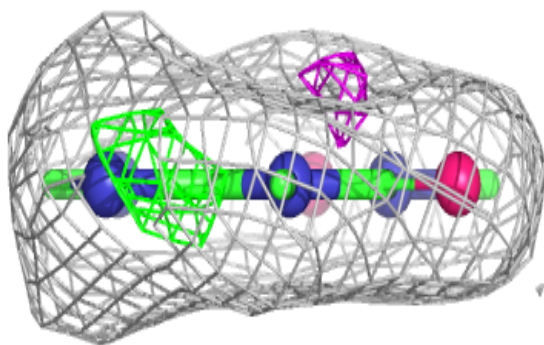
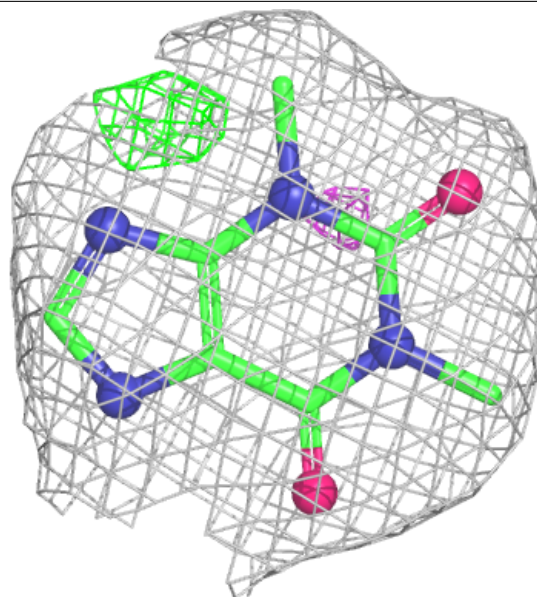
**Electron density around CLR A 1203:**

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

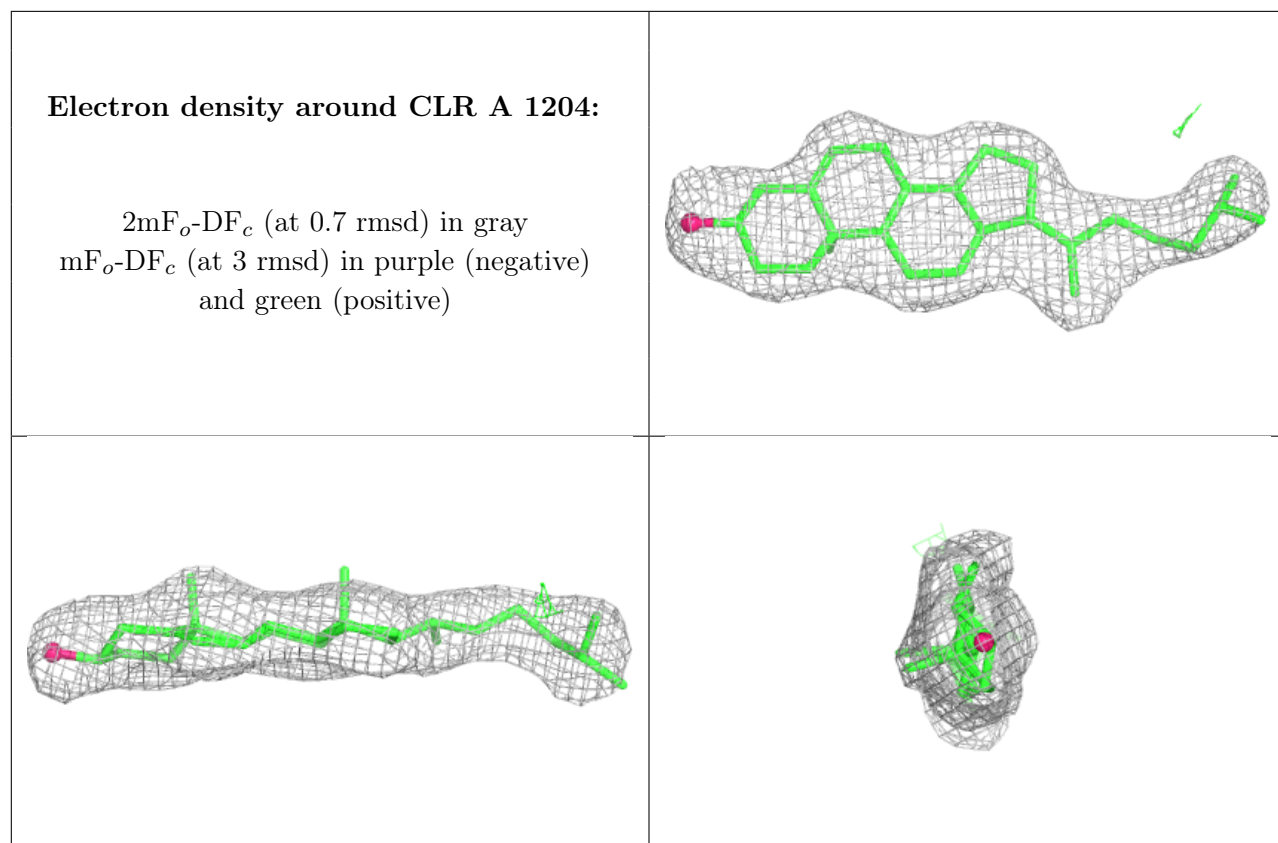


**Electron density around TEP A 1235:**

$2mF_o-DF_c$  (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.