



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 05:35 PM EDT

PDB ID : 7IOM / pdb\_00007iom  
Title : Crystal structure of A2A in complex with FU18-82  
Authors : Huang, C.-Y.; Cheng, R.Y.K.; Metz, A.  
Deposited on : 2025-08-21  
Resolution : 2.10 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>.

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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

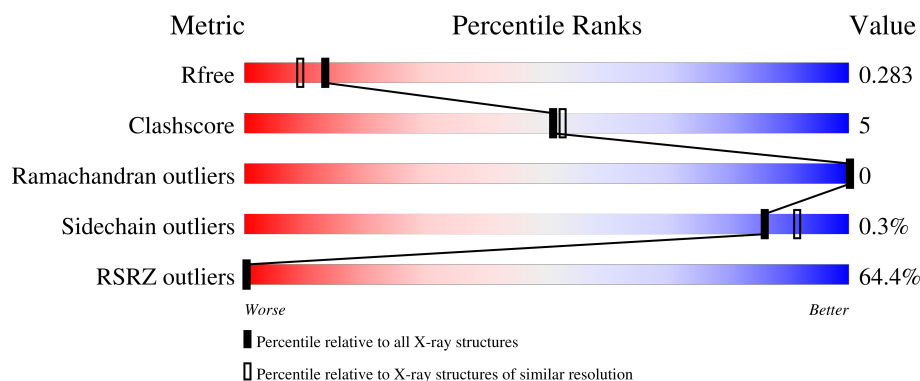
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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
3	TEP	A	2401	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3752 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	12	0
			3119	2030	531	535	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

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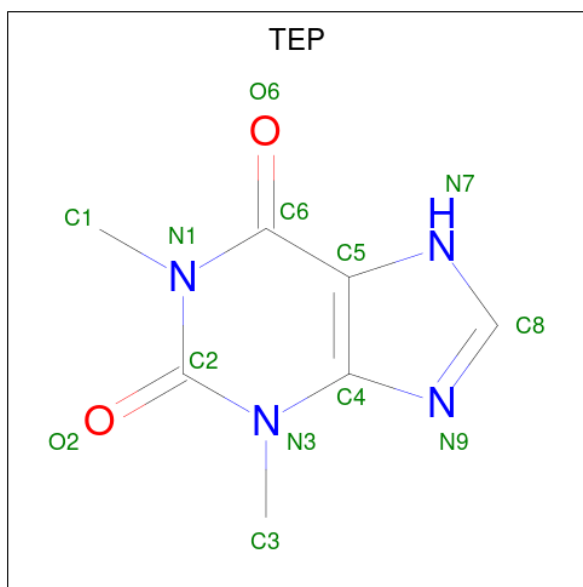
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Chain	Residue	Modelled	Actual	Comment	Reference
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS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

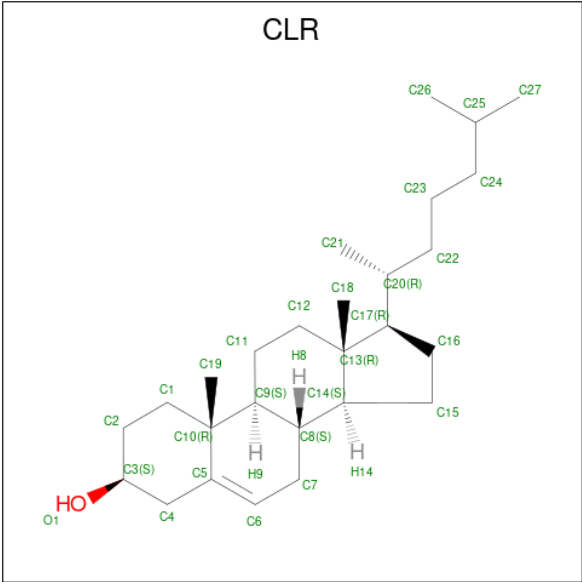
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 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).



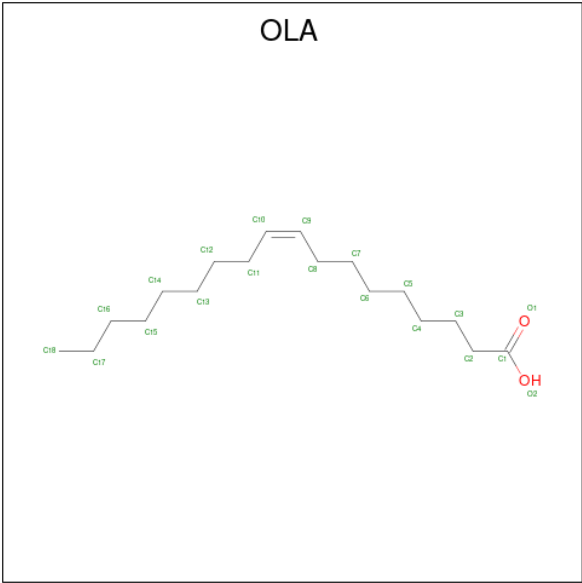
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	7	4	2		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



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

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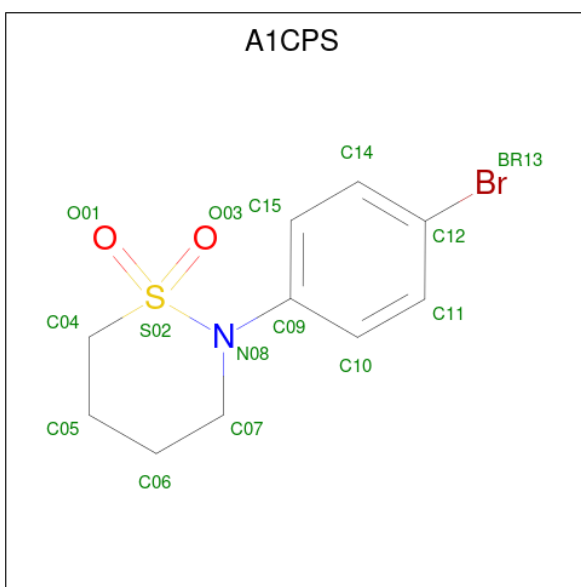
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 8 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 18 16 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 12 10 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C O 19 17 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C 10 10	0	0
5	A	1	Total C 11 11	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C 15 15	0	0
5	A	1	Total C O 13 11 2	0	0
5	A	1	Total C O 20 18 2	0	0

- 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
			16	12	4		
6	A	1	Total	C	O	0	0
			17	13	4		
6	A	1	Total	C	O	0	0
			23	19	4		
6	A	1	Total	C	O	0	0
			23	19	4		
6	A	1	Total	C	O	0	0
			23	19	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			16	12	4		

- Molecule 7 is 2-(4-bromophenyl)-1lambda 6 ,2-thiazinane-1,1-dione (CCD ID: A1CPS) (formula:  $C_{10}H_{12}BrNO_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
7	A	1	15	1	10	1	2	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	77	Total	O	0	0
			77	77		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.26Å 178.86Å 140.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.43 – 2.10 89.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	70.4 (89.43-2.10) 70.8 (89.43-2.10)	Depositor EDS
$R_{merge}$	0.76	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, $R_{free}$	0.255 , 0.281 0.256 , 0.283	Depositor DCC
$R_{free}$ test set	1063 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.6	Xtriage
Anisotropy	1.518	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	3752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, CLR, NA, TEP, A1CPS, 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	0.18	0/3184	0.34	0/4328

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3119	0	3199	25	0
2	A	1	0	0	0	0
3	A	13	0	8	0	0
4	A	84	0	138	0	0
5	A	307	0	459	20	0
6	A	136	0	186	3	0
7	A	15	0	0	0	0
8	A	77	0	0	3	0
All	All	3752	0	3990	40	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 5.

All (40) 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:298:THR:HA	1:A:301:LYS:HE2	1.66	0.78
1:A:1059:LYS:N	8:A:2501:HOH:O	2.26	0.69
1:A:1077:LYS:NZ	1:A:1081:GLU:OE2	2.32	0.63
5:A:2409:OLA:H21	5:A:2416:OLA:H32	1.81	0.62
5:A:2425:OLA:H62	6:A:2433:OLC:H3A	1.81	0.62
5:A:2422:OLA:H41	5:A:2424:OLA:H152	1.82	0.59
1:A:140[A]:MET:HE2	5:A:2425:OLA:H52	1.85	0.59
5:A:2422:OLA:H51	5:A:2426:OLA:H131	1.86	0.56
5:A:2410:OLA:H183	5:A:2421:OLA:H121	1.87	0.56
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.91	0.53
1:A:111:ARG:NH2	8:A:2505:HOH:O	2.39	0.50
1:A:140[B]:MET:HE3	5:A:2425:OLA:H71	1.94	0.50
1:A:275[B]:VAL:O	1:A:279[B]:THR:HG23	2.12	0.49
1:A:297:GLN:O	1:A:301:LYS:HG3	2.13	0.49
1:A:182:PHE:CE1	1:A:187[B]:LEU:HG	2.48	0.48
6:A:2429:OLC:H4A	6:A:2430:OLC:H2	1.95	0.48
1:A:199:ARG:HB3	8:A:2538:HOH:O	2.13	0.48
1:A:104:ILE:HG22	1:A:112:TYR:HD1	1.79	0.47
1:A:1004:GLU:OE1	1:A:222:ARG:NH2	2.47	0.47
1:A:42:ASN:HA	1:A:45:VAL:HB	1.97	0.46
1:A:1106:LEU:HD11	1:A:222:ARG:HH21	1.80	0.46
1:A:96:LEU:HB2	1:A:193:MET:HE2	1.98	0.44
5:A:2410:OLA:H111	5:A:2410:OLA:H142	1.75	0.44
5:A:2410:OLA:H82	5:A:2410:OLA:H112	1.87	0.43
1:A:75:HIS:CD2	5:A:2425:OLA:H22	2.53	0.43
1:A:127:ILE:HG12	5:A:2416:OLA:H82	2.01	0.43
5:A:2405:OLA:H71	6:A:2428:OLC:H6A	2.01	0.43
1:A:32:TRP:CE3	5:A:2415:OLA:H71	2.54	0.43
5:A:2422:OLA:C9	5:A:2425:OLA:H72	2.49	0.42
1:A:174[A]:MET:HG3	1:A:257:PHE:HB2	2.01	0.42
1:A:65:THR:HG23	5:A:2405:OLA:H41	2.02	0.42
1:A:1074:ASP:O	1:A:1077:LYS:HB3	2.20	0.41
1:A:227:LYS:HE3	1:A:227:LYS:HB3	1.82	0.41
5:A:2409:OLA:H61	5:A:2409:OLA:H9	1.81	0.41
1:A:117:THR:HG22	1:A:120:ARG:HD2	2.01	0.41
5:A:2405:OLA:H81	5:A:2405:OLA:H112	1.83	0.41
5:A:2415:OLA:H111	5:A:2415:OLA:H82	1.80	0.41
1:A:10:ILE:HG12	1:A:64:ILE:HG23	2.02	0.40
5:A:2424:OLA:H81	5:A:2424:OLA:H112	1.80	0.40
5:A:2423:OLA:H111	5:A:2423:OLA:H81	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/433 (92%)	392 (98%)	6 (2%)	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	328/354 (93%)	327 (100%)	1 (0%)	86	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLN

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	36	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	CLR	A	2402	-	31,31,31	0.30	0	48,48,48	0.49	0
5	OLA	A	2422	-	7,7,19	0.30	0	6,6,19	0.83	0
6	OLC	A	2430	-	22,22,24	1.09	1 (4%)	23,23,25	1.33	3 (13%)
6	OLC	A	2433	-	15,15,24	1.22	1 (6%)	16,16,25	1.12	1 (6%)
5	OLA	A	2413	-	14,14,19	0.64	0	14,14,19	1.15	1 (7%)
5	OLA	A	2420	-	11,11,19	0.37	0	10,10,19	0.81	0
5	OLA	A	2405	-	19,19,19	0.58	0	19,19,19	1.03	1 (5%)
5	OLA	A	2416	-	19,19,19	0.61	0	19,19,19	0.91	0
5	OLA	A	2419	-	10,10,19	0.41	0	9,9,19	0.90	0
6	OLC	A	2427	-	15,15,24	1.25	1 (6%)	16,16,25	1.30	1 (6%)
5	OLA	A	2412	-	7,7,19	0.85	0	7,7,19	1.30	1 (14%)
6	OLC	A	2432	-	17,17,24	1.27	1 (5%)	18,18,25	1.32	2 (11%)
5	OLA	A	2425	-	12,12,19	0.73	0	12,12,19	1.16	0
5	OLA	A	2410	-	19,19,19	0.57	0	19,19,19	1.09	1 (5%)
6	OLC	A	2431	-	22,22,24	1.12	1 (4%)	23,23,25	1.30	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	OLC	A	2428	-	16,16,24	1.30	1 (6%)	17,17,25	1.35	2 (11%)
3	TEP	A	2401	-	14,14,14	1.87	5 (35%)	21,21,21	3.18	12 (57%)
5	OLA	A	2421	-	8,8,19	0.30	0	7,7,19	0.81	0
5	OLA	A	2417	-	11,11,19	0.35	0	10,10,19	0.76	0
6	OLC	A	2429	-	22,22,24	1.09	1 (4%)	23,23,25	1.30	2 (8%)
5	OLA	A	2424	-	14,14,19	0.36	0	13,13,19	0.67	0
5	OLA	A	2408	-	17,17,19	0.61	0	17,17,19	1.04	1 (5%)
5	OLA	A	2414	-	10,10,19	0.72	0	10,10,19	1.28	1 (10%)
5	OLA	A	2415	-	18,18,19	0.59	0	18,18,19	1.08	1 (5%)
7	A1CPS	A	2434	-	15,16,16	2.48	6 (40%)	18,23,23	1.06	2 (11%)
5	OLA	A	2423	-	14,14,19	0.67	0	14,14,19	0.99	0
4	CLR	A	2404	-	31,31,31	0.28	0	48,48,48	0.43	0
5	OLA	A	2418	-	9,9,19	0.39	0	8,8,19	0.78	0
4	CLR	A	2403	-	31,31,31	0.29	0	48,48,48	0.42	0
5	OLA	A	2406	-	9,9,19	0.76	0	9,9,19	1.23	1 (11%)
5	OLA	A	2411	-	11,11,19	0.73	0	11,11,19	1.22	1 (9%)
5	OLA	A	2409	-	19,19,19	0.61	0	19,19,19	0.97	0
5	OLA	A	2426	-	19,19,19	0.59	0	19,19,19	1.03	1 (5%)
5	OLA	A	2407	-	8,8,19	0.82	0	8,8,19	1.27	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
4	CLR	A	2402	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2422	-	-	0/5/5/17	-
6	OLC	A	2430	-	-	11/22/22/24	-
6	OLC	A	2433	-	-	6/15/15/24	-
5	OLA	A	2413	-	-	3/12/12/17	-
5	OLA	A	2420	-	-	3/9/9/17	-
5	OLA	A	2405	-	-	10/17/17/17	-
5	OLA	A	2416	-	-	8/17/17/17	-
5	OLA	A	2419	-	-	5/8/8/17	-
6	OLC	A	2427	-	-	9/15/15/24	-
5	OLA	A	2412	-	-	1/5/5/17	-
6	OLC	A	2432	-	-	8/17/17/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	2425	-	-	6/10/10/17	-
5	OLA	A	2410	-	-	10/17/17/17	-
6	OLC	A	2431	-	-	12/22/22/24	-
6	OLC	A	2428	-	-	8/16/16/24	-
3	TEP	A	2401	-	-	-	0/2/2/2
5	OLA	A	2421	-	-	2/6/6/17	-
5	OLA	A	2417	-	-	3/9/9/17	-
6	OLC	A	2429	-	-	11/22/22/24	-
5	OLA	A	2424	-	-	2/12/12/17	-
5	OLA	A	2408	-	-	8/15/15/17	-
5	OLA	A	2414	-	-	3/8/8/17	-
5	OLA	A	2415	-	-	2/16/16/17	-
7	A1CPS	A	2434	-	-	0/4/18/18	0/2/2/2
5	OLA	A	2423	-	-	5/12/12/17	-
4	CLR	A	2404	-	-	1/10/68/68	0/4/4/4
5	OLA	A	2418	-	-	2/7/7/17	-
4	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2406	-	-	2/7/7/17	-
5	OLA	A	2411	-	-	5/9/9/17	-
5	OLA	A	2409	-	-	12/17/17/17	-
5	OLA	A	2426	-	-	12/17/17/17	-
5	OLA	A	2407	-	-	3/6/6/17	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2434	A1CPS	C05-C04	-4.78	1.47	1.52
7	A	2434	A1CPS	C07-N08	4.17	1.51	1.48
3	A	2401	TEP	C6-N1	-3.78	1.32	1.40
7	A	2434	A1CPS	C06-C07	3.64	1.63	1.51
7	A	2434	A1CPS	C04-S02	-3.54	1.71	1.76
7	A	2434	A1CPS	O01-S02	3.53	1.47	1.43
6	A	2432	OLC	O20-C1	2.98	1.42	1.33
6	A	2428	OLC	O20-C1	2.97	1.42	1.33
6	A	2431	OLC	O20-C1	2.96	1.42	1.33
6	A	2433	OLC	O20-C1	2.94	1.41	1.33
6	A	2429	OLC	O20-C1	2.91	1.41	1.33
6	A	2427	OLC	O20-C1	2.86	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2430	OLC	O20-C1	2.83	1.41	1.33
7	A	2434	A1CPS	O03-S02	2.83	1.46	1.43
3	A	2401	TEP	C5-N7	-2.57	1.34	1.38
3	A	2401	TEP	C5-C6	-2.30	1.38	1.42
3	A	2401	TEP	C5-C4	-2.26	1.34	1.37
3	A	2401	TEP	C4-N3	-2.11	1.34	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2401	TEP	C4-C5-N7	6.06	108.27	105.29
3	A	2401	TEP	C5-C6-N1	5.84	119.91	112.07
3	A	2401	TEP	C8-N9-C4	5.69	107.26	103.45
3	A	2401	TEP	C5-C4-N9	-4.77	108.28	111.63
3	A	2401	TEP	C6-C5-C4	-4.18	119.83	123.13
6	A	2431	OLC	C8-C9-C10	3.60	151.82	124.83
6	A	2429	OLC	C8-C9-C10	3.60	151.81	124.83
6	A	2428	OLC	C8-C9-C10	3.51	152.27	126.65
3	A	2401	TEP	N3-C4-N9	3.41	131.63	126.27
6	A	2430	OLC	C8-C9-C10	3.40	150.27	124.83
3	A	2401	TEP	N7-C8-N9	-3.39	109.05	112.98
6	A	2427	OLC	O20-C1-C2	3.32	121.95	111.83
3	A	2401	TEP	C6-N1-C2	-3.23	120.41	125.66
6	A	2432	OLC	C8-C9-C10	2.95	152.80	130.48
3	A	2401	TEP	C5-C4-N3	-2.91	120.09	121.73
3	A	2401	TEP	O6-C6-C5	-2.89	120.75	126.64
6	A	2428	OLC	O20-C1-C2	2.64	119.89	111.83
6	A	2430	OLC	O20-C1-C2	2.61	119.78	111.83
6	A	2432	OLC	O20-C1-C2	2.59	119.72	111.83
6	A	2433	OLC	O20-C1-C2	2.56	119.64	111.83
6	A	2431	OLC	O20-C1-C2	2.56	119.63	111.83
6	A	2429	OLC	O20-C1-C2	2.47	119.36	111.83
5	A	2410	OLA	C3-C2-C1	-2.47	108.07	114.51
7	A	2434	A1CPS	O03-S02-C04	-2.28	106.48	109.55
5	A	2406	OLA	C3-C2-C1	-2.21	108.75	114.51
7	A	2434	A1CPS	C09-N08-S02	2.20	122.55	118.66
5	A	2413	OLA	C3-C2-C1	-2.20	108.78	114.51
5	A	2414	OLA	C3-C2-C1	-2.16	108.86	114.51
3	A	2401	TEP	C3-N3-C2	2.16	121.10	117.33
6	A	2430	OLC	C11-C10-C9	-2.12	108.95	124.83
5	A	2415	OLA	C3-C2-C1	-2.10	109.02	114.51
5	A	2426	OLA	C3-C2-C1	-2.10	109.03	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2405	OLA	C3-C2-C1	-2.06	109.14	114.51
3	A	2401	TEP	N3-C2-N1	2.05	119.70	117.14
5	A	2411	OLA	O2-C1-C2	2.05	120.47	114.00
5	A	2408	OLA	C3-C2-C1	-2.04	109.18	114.51
5	A	2412	OLA	O2-C1-C2	2.01	120.35	114.00

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2410	OLA	C6-C7-C8-C9
5	A	2417	OLA	C6-C7-C8-C9
6	A	2429	OLC	C21-C22-C24-O25
6	A	2430	OLC	C21-C22-C24-O25
6	A	2430	OLC	O20-C21-C22-O23
6	A	2431	OLC	O20-C21-C22-C24
6	A	2432	OLC	O19-C1-O20-C21
6	A	2432	OLC	C2-C1-O20-C21
6	A	2431	OLC	C2-C1-O20-C21
6	A	2432	OLC	O20-C21-C22-O23
6	A	2431	OLC	C10-C11-C12-C13
6	A	2431	OLC	O19-C1-O20-C21
5	A	2425	OLA	C1-C2-C3-C4
5	A	2423	OLA	C1-C2-C3-C4
6	A	2433	OLC	C1-C2-C3-C4
6	A	2427	OLC	O20-C21-C22-O23
6	A	2431	OLC	O20-C21-C22-O23
6	A	2430	OLC	C1-C2-C3-C4
6	A	2427	OLC	O20-C21-C22-C24
6	A	2430	OLC	O20-C21-C22-C24
5	A	2426	OLA	C11-C12-C13-C14
6	A	2430	OLC	C12-C13-C14-C15
5	A	2415	OLA	C5-C6-C7-C8
6	A	2429	OLC	C3-C4-C5-C6
6	A	2429	OLC	O23-C22-C24-O25
6	A	2430	OLC	O23-C22-C24-O25
5	A	2417	OLA	C12-C13-C14-C15
4	A	2404	CLR	C20-C22-C23-C24
5	A	2419	OLA	C11-C12-C13-C14
6	A	2428	OLC	C1-C2-C3-C4
6	A	2431	OLC	C1-C2-C3-C4
6	A	2432	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	A	2429	OLC	C10-C11-C12-C13
5	A	2423	OLA	C5-C6-C7-C8
6	A	2432	OLC	C5-C6-C7-C8
5	A	2410	OLA	C1-C2-C3-C4
5	A	2414	OLA	C4-C5-C6-C7
6	A	2431	OLC	C4-C5-C6-C7
5	A	2426	OLA	C15-C16-C17-C18
5	A	2405	OLA	C14-C15-C16-C17
5	A	2423	OLA	C3-C4-C5-C6
5	A	2416	OLA	C3-C4-C5-C6
5	A	2426	OLA	C6-C7-C8-C9
6	A	2431	OLC	C6-C7-C8-C9
6	A	2432	OLC	C6-C7-C8-C9
5	A	2405	OLA	C2-C3-C4-C5
6	A	2428	OLC	C4-C5-C6-C7
5	A	2408	OLA	C4-C5-C6-C7
5	A	2416	OLA	C5-C6-C7-C8
6	A	2433	OLC	C2-C3-C4-C5
5	A	2411	OLA	C4-C5-C6-C7
5	A	2416	OLA	C11-C12-C13-C14
5	A	2408	OLA	C6-C7-C8-C9
5	A	2419	OLA	C10-C11-C12-C13
6	A	2429	OLC	C4-C5-C6-C7
5	A	2426	OLA	C1-C2-C3-C4
5	A	2424	OLA	C6-C7-C8-C9
5	A	2425	OLA	C6-C7-C8-C9
5	A	2413	OLA	C10-C11-C12-C13
5	A	2405	OLA	C11-C12-C13-C14
6	A	2429	OLC	C12-C13-C14-C15
5	A	2405	OLA	C6-C7-C8-C9
5	A	2409	OLA	C6-C7-C8-C9
5	A	2409	OLA	C10-C11-C12-C13
5	A	2410	OLA	C10-C11-C12-C13
5	A	2426	OLA	C4-C5-C6-C7
6	A	2432	OLC	C4-C5-C6-C7
5	A	2426	OLA	C12-C13-C14-C15
5	A	2405	OLA	C15-C16-C17-C18
5	A	2407	OLA	C3-C4-C5-C6
6	A	2433	OLC	C4-C5-C6-C7
6	A	2428	OLC	C7-C8-C9-C10
5	A	2409	OLA	C13-C14-C15-C16
6	A	2427	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
6	A	2433	OLC	C6-C7-C8-C9
5	A	2406	OLA	C3-C4-C5-C6
6	A	2428	OLC	C2-C1-O20-C21
6	A	2430	OLC	C2-C1-O20-C21
6	A	2428	OLC	O20-C21-C22-O23
5	A	2421	OLA	C12-C13-C14-C15
6	A	2428	OLC	C3-C4-C5-C6
5	A	2419	OLA	C12-C13-C14-C15
5	A	2425	OLA	C5-C6-C7-C8
5	A	2414	OLA	C1-C2-C3-C4
5	A	2425	OLA	C2-C3-C4-C5
6	A	2428	OLC	C2-C3-C4-C5
5	A	2410	OLA	C15-C16-C17-C18
5	A	2405	OLA	C4-C5-C6-C7
6	A	2430	OLC	C10-C11-C12-C13
5	A	2405	OLA	C12-C13-C14-C15
5	A	2409	OLA	C14-C15-C16-C17
5	A	2420	OLA	C4-C5-C6-C7
5	A	2418	OLA	C9-C10-C11-C12
6	A	2427	OLC	O23-C22-C24-O25
5	A	2417	OLA	C11-C12-C13-C14
6	A	2427	OLC	O19-C1-O20-C21
6	A	2428	OLC	O19-C1-O20-C21
6	A	2430	OLC	O19-C1-O20-C21
5	A	2408	OLA	C12-C13-C14-C15
5	A	2425	OLA	C4-C5-C6-C7
6	A	2432	OLC	O20-C21-C22-C24
5	A	2408	OLA	C3-C4-C5-C6
5	A	2409	OLA	C3-C4-C5-C6
5	A	2409	OLA	C4-C5-C6-C7
5	A	2423	OLA	C2-C3-C4-C5
5	A	2424	OLA	C12-C13-C14-C15
5	A	2409	OLA	C12-C13-C14-C15
5	A	2421	OLA	C15-C16-C17-C18
6	A	2429	OLC	O19-C1-O20-C21
6	A	2429	OLC	C2-C1-O20-C21
6	A	2431	OLC	C5-C6-C7-C8
5	A	2411	OLA	C1-C2-C3-C4
6	A	2429	OLC	C2-C3-C4-C5
5	A	2426	OLA	C14-C15-C16-C17
5	A	2419	OLA	C15-C16-C17-C18
6	A	2430	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	A	2409	OLA	C11-C12-C13-C14
5	A	2420	OLA	C9-C10-C11-C12
5	A	2410	OLA	C5-C6-C7-C8
6	A	2431	OLC	C2-C3-C4-C5
5	A	2405	OLA	C10-C11-C12-C13
6	A	2430	OLC	C4-C5-C6-C7
6	A	2431	OLC	C3-C4-C5-C6
6	A	2427	OLC	C1-C2-C3-C4
5	A	2420	OLA	C7-C8-C9-C10
5	A	2416	OLA	C6-C7-C8-C9
5	A	2412	OLA	C2-C3-C4-C5
5	A	2423	OLA	C4-C5-C6-C7
6	A	2427	OLC	C3-C4-C5-C6
6	A	2427	OLC	C6-C7-C8-C9
5	A	2408	OLA	C5-C6-C7-C8
5	A	2410	OLA	C12-C13-C14-C15
5	A	2426	OLA	C13-C14-C15-C16
5	A	2416	OLA	C7-C8-C9-C10
6	A	2429	OLC	C5-C6-C7-C8
5	A	2411	OLA	C5-C6-C7-C8
5	A	2409	OLA	O1-C1-C2-C3
5	A	2410	OLA	C4-C5-C6-C7
5	A	2416	OLA	C4-C5-C6-C7
5	A	2426	OLA	C3-C4-C5-C6
5	A	2409	OLA	O2-C1-C2-C3
5	A	2408	OLA	O2-C1-C2-C3
6	A	2429	OLC	C9-C10-C11-C12
6	A	2431	OLC	C9-C10-C11-C12
5	A	2411	OLA	C7-C8-C9-C10
5	A	2413	OLA	C9-C10-C11-C12
5	A	2411	OLA	C3-C4-C5-C6
5	A	2419	OLA	C9-C10-C11-C12
5	A	2409	OLA	C9-C10-C11-C12
5	A	2407	OLA	O2-C1-C2-C3
5	A	2408	OLA	O1-C1-C2-C3
5	A	2408	OLA	C10-C11-C12-C13
5	A	2409	OLA	C7-C8-C9-C10
5	A	2407	OLA	O1-C1-C2-C3
5	A	2416	OLA	C12-C13-C14-C15
5	A	2418	OLA	C6-C7-C8-C9
5	A	2425	OLA	C7-C8-C9-C10
5	A	2416	OLA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
5	A	2410	OLA	O2-C1-C2-C3
5	A	2413	OLA	C7-C8-C9-C10
5	A	2415	OLA	C11-C12-C13-C14
5	A	2410	OLA	C13-C14-C15-C16
5	A	2426	OLA	C2-C3-C4-C5
5	A	2410	OLA	O1-C1-C2-C3
5	A	2414	OLA	C5-C6-C7-C8
6	A	2433	OLC	C2-C1-O20-C21
5	A	2426	OLA	C7-C8-C9-C10
5	A	2405	OLA	O2-C1-C2-C3
6	A	2433	OLC	O19-C1-O20-C21
5	A	2406	OLA	O2-C1-C2-C3
6	A	2427	OLC	C5-C6-C7-C8
5	A	2405	OLA	O1-C1-C2-C3
5	A	2426	OLA	O2-C1-C2-C3

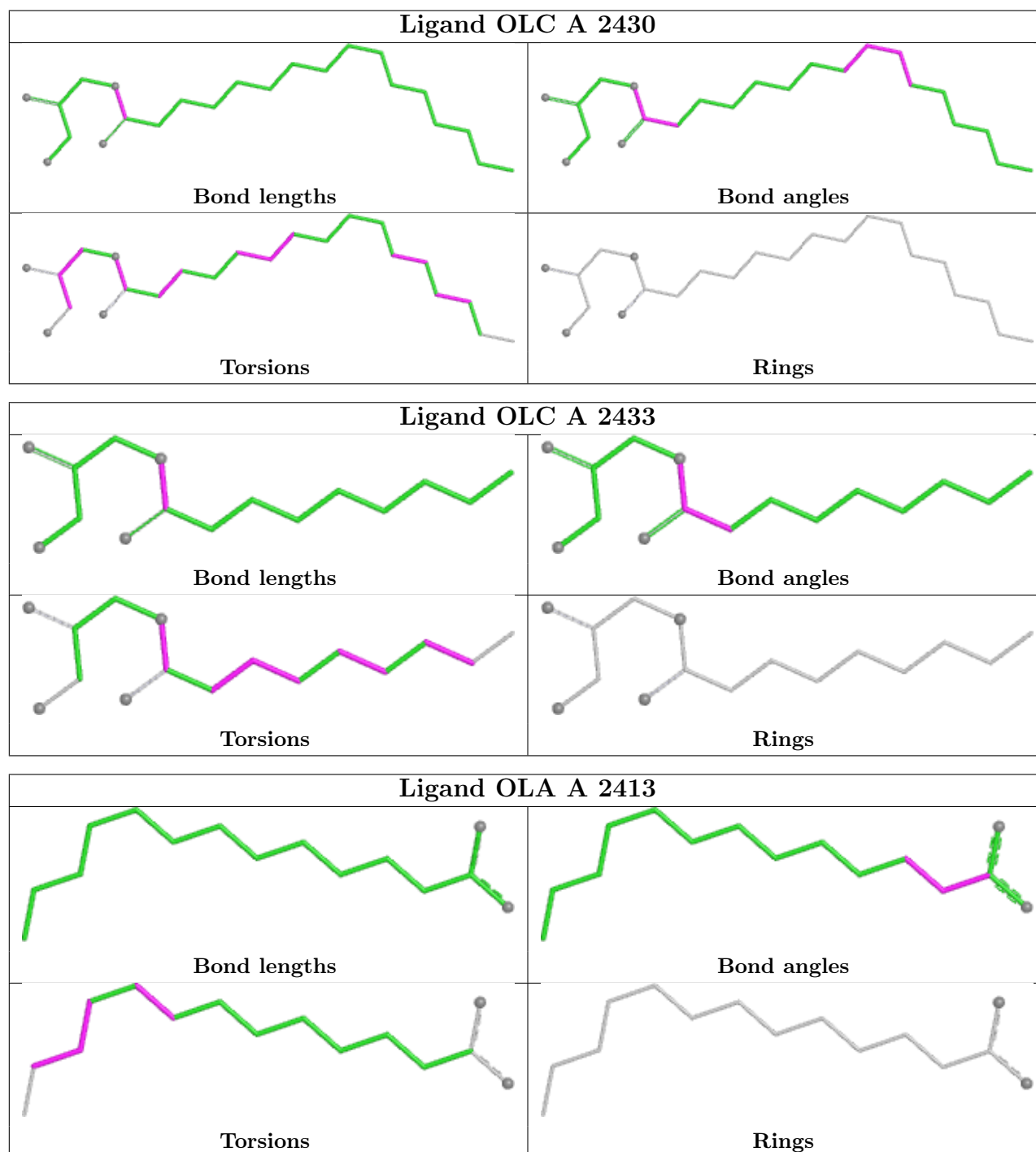
There are no ring outliers.

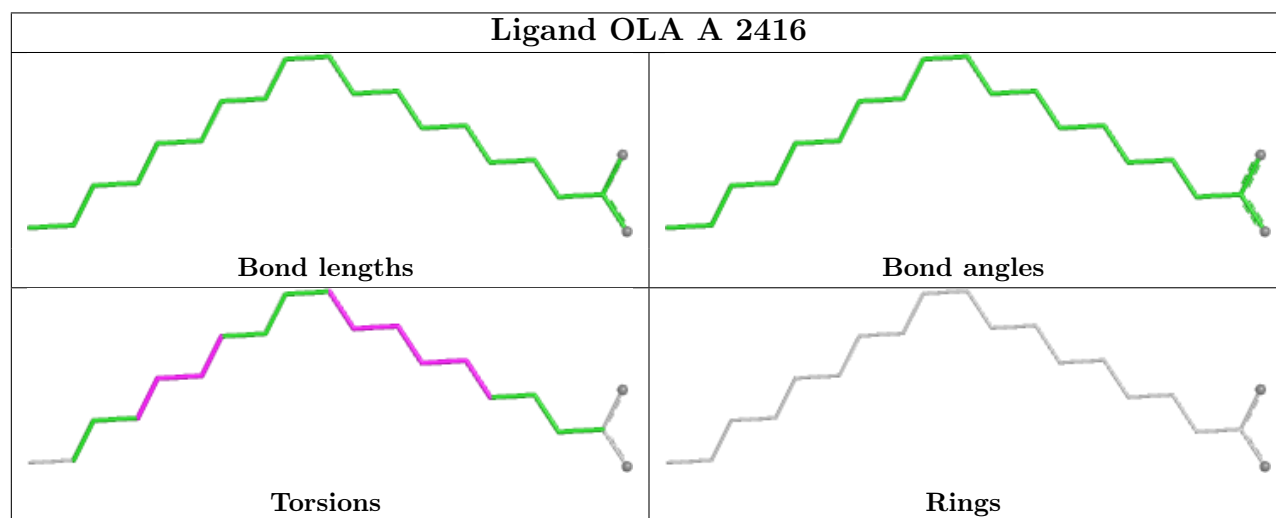
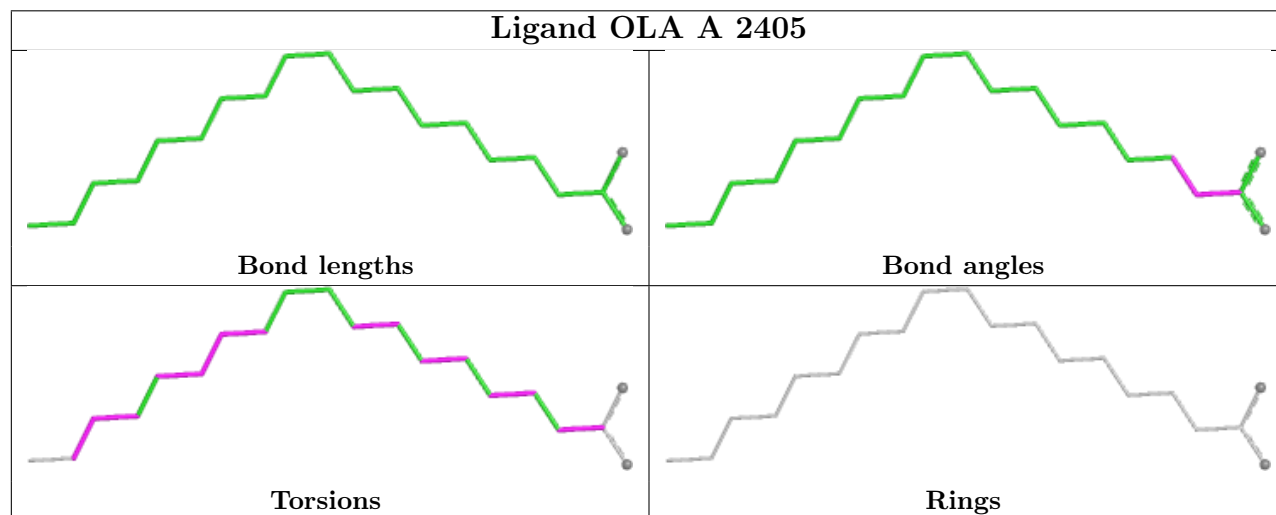
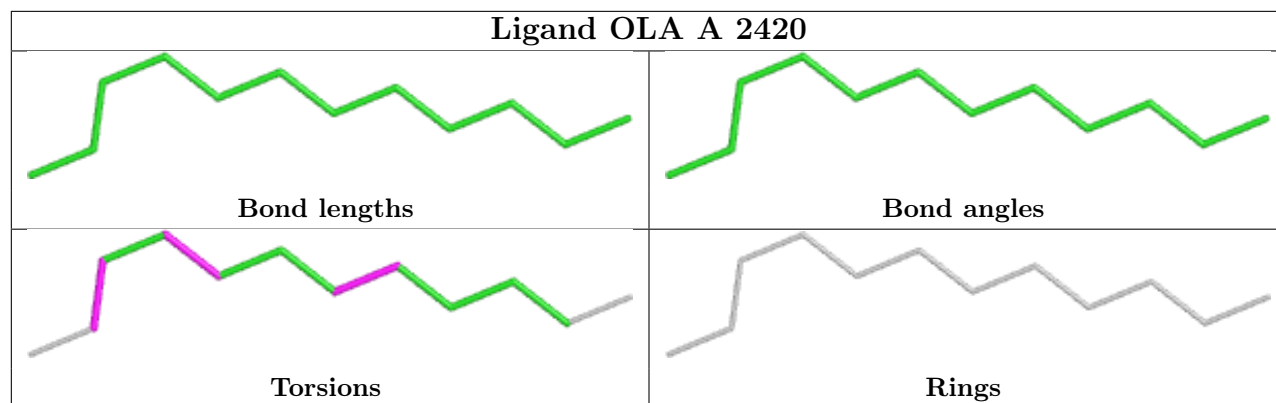
15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2422	OLA	3	0
6	A	2430	OLC	1	0
6	A	2433	OLC	1	0
5	A	2405	OLA	3	0
5	A	2416	OLA	2	0
5	A	2425	OLA	5	0
5	A	2410	OLA	3	0
6	A	2428	OLC	1	0
5	A	2421	OLA	1	0
6	A	2429	OLC	1	0
5	A	2424	OLA	2	0
5	A	2415	OLA	2	0
5	A	2423	OLA	1	0
5	A	2409	OLA	2	0
5	A	2426	OLA	1	0

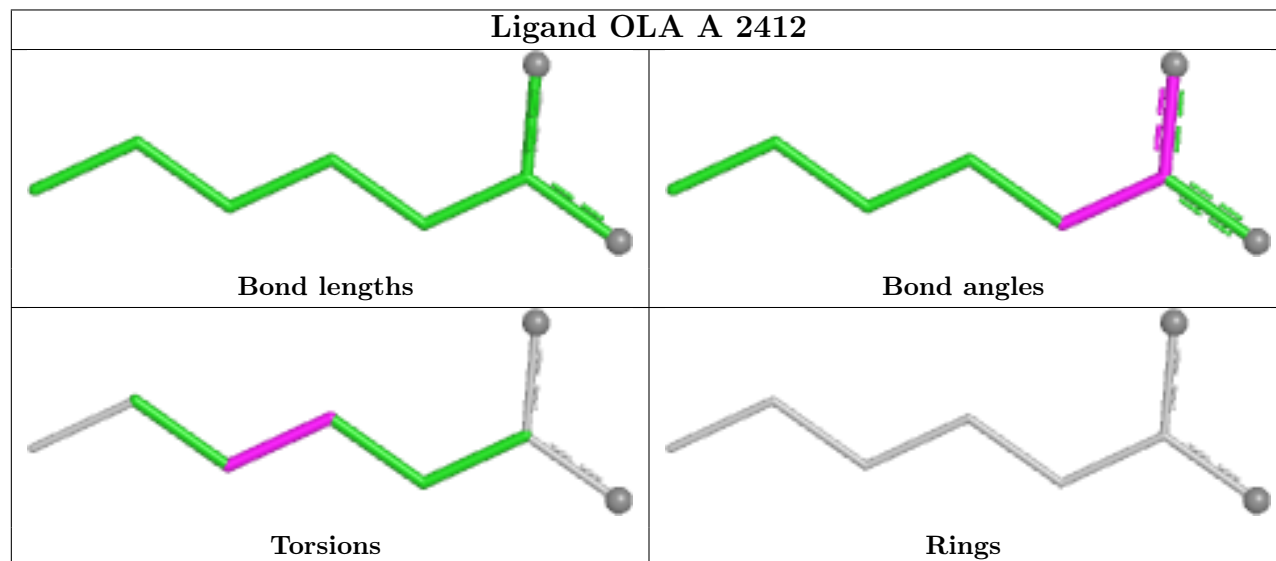
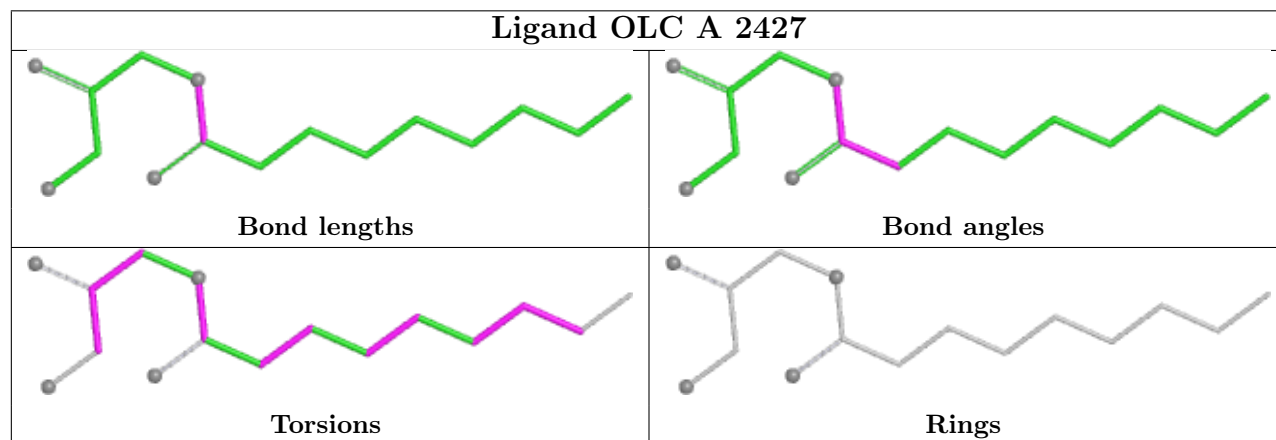
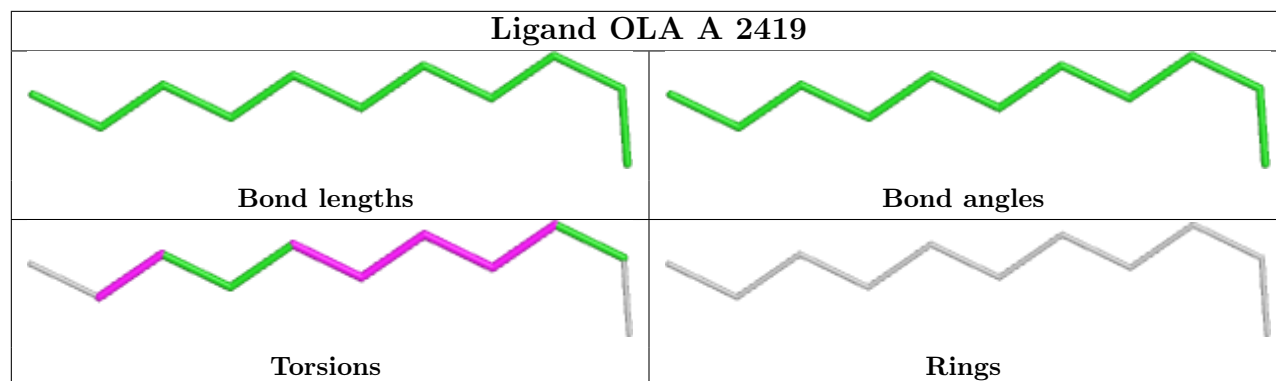
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

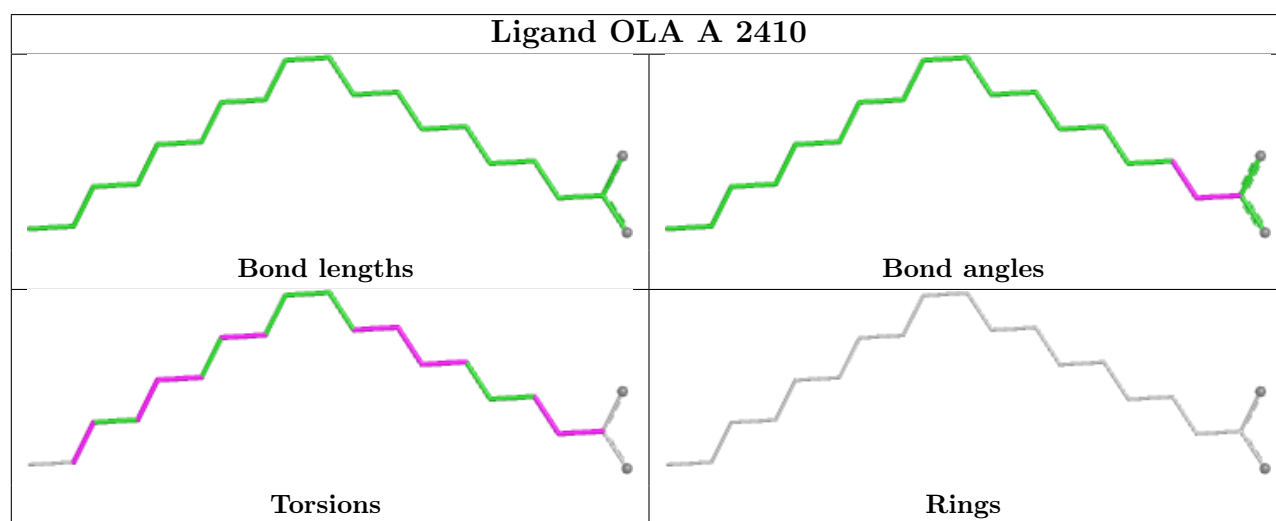
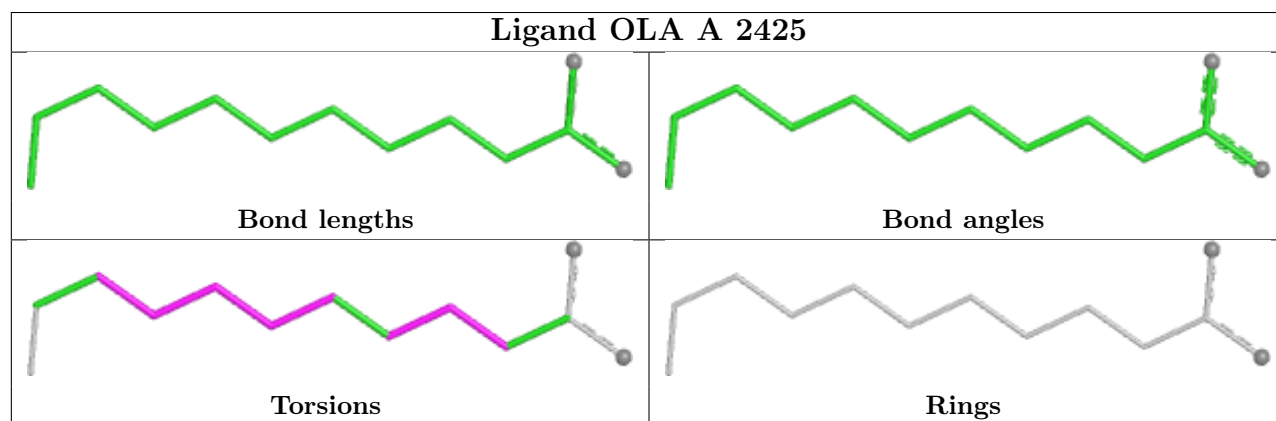
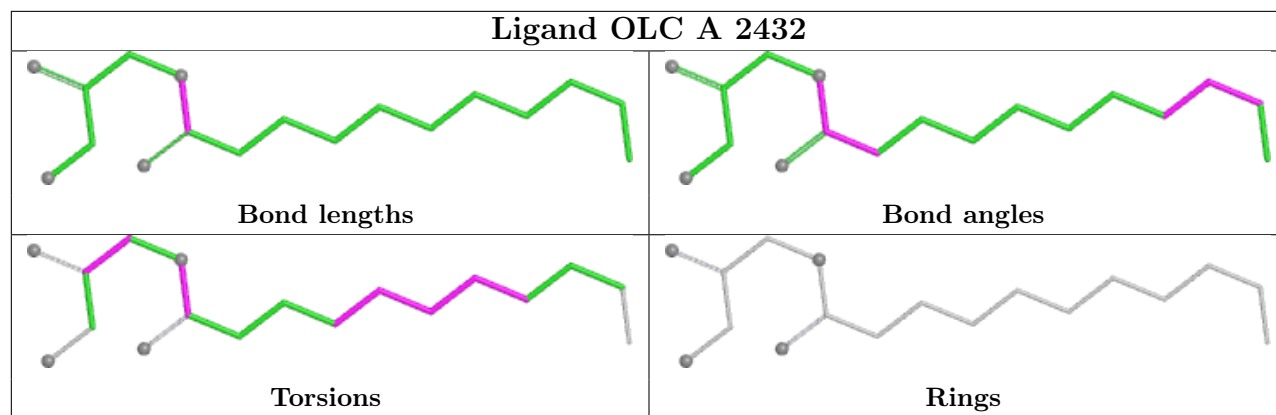
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

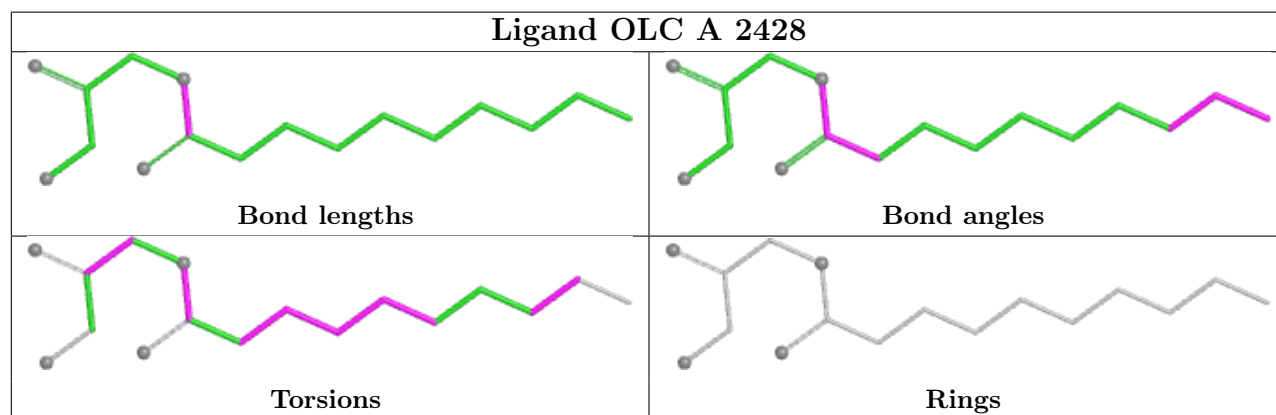
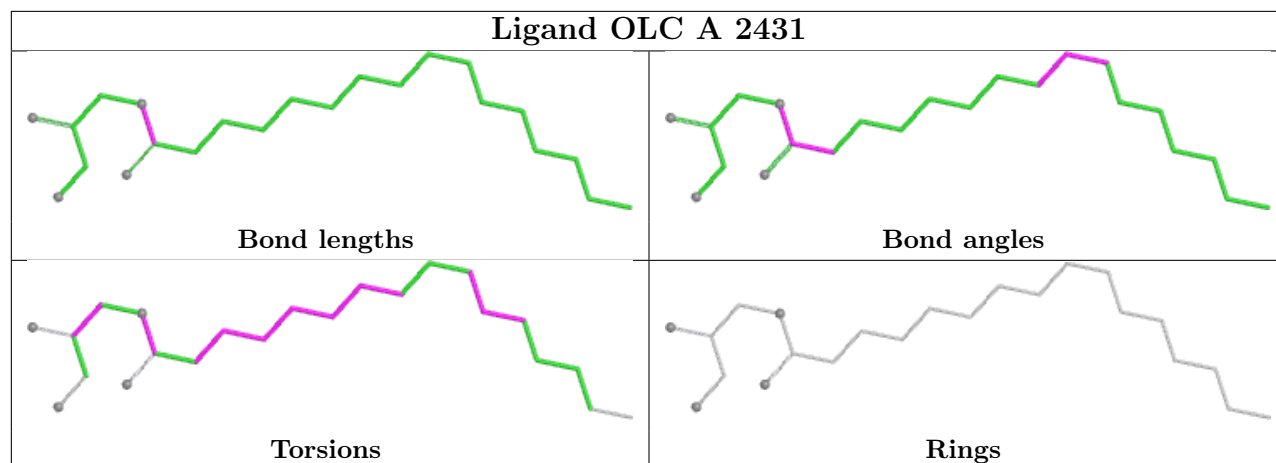


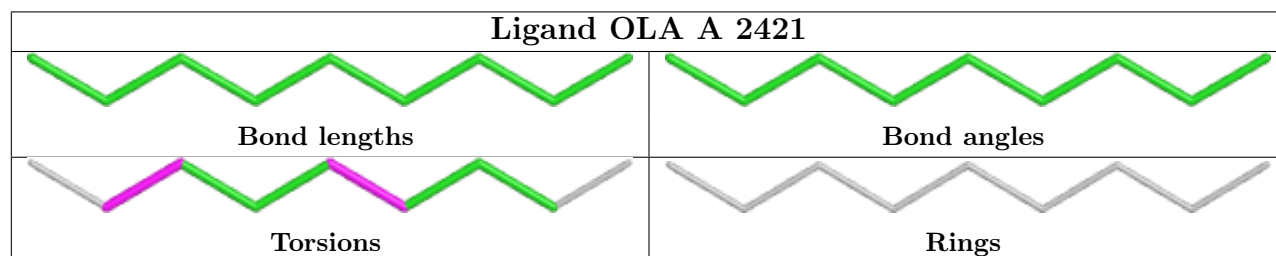
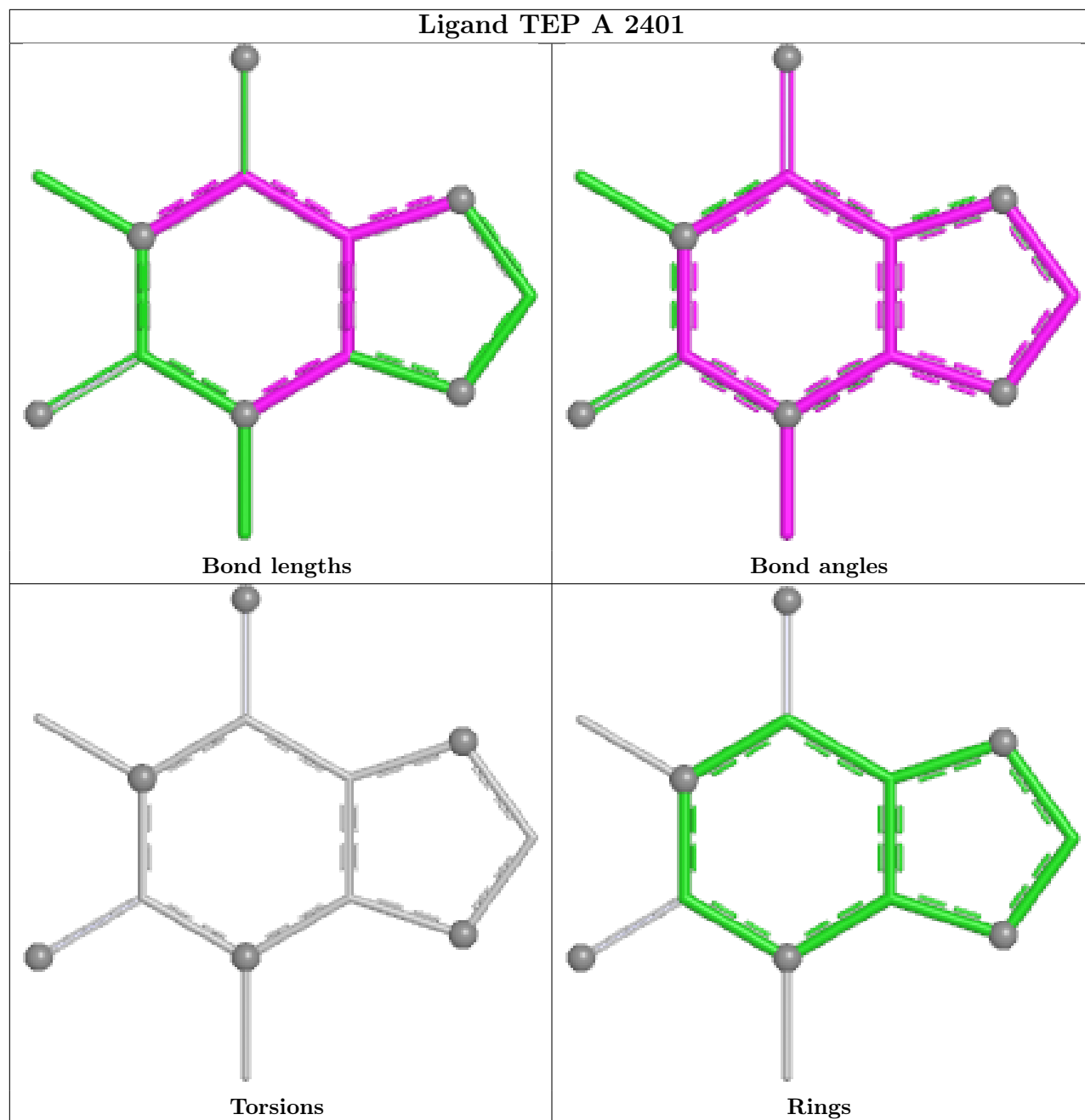


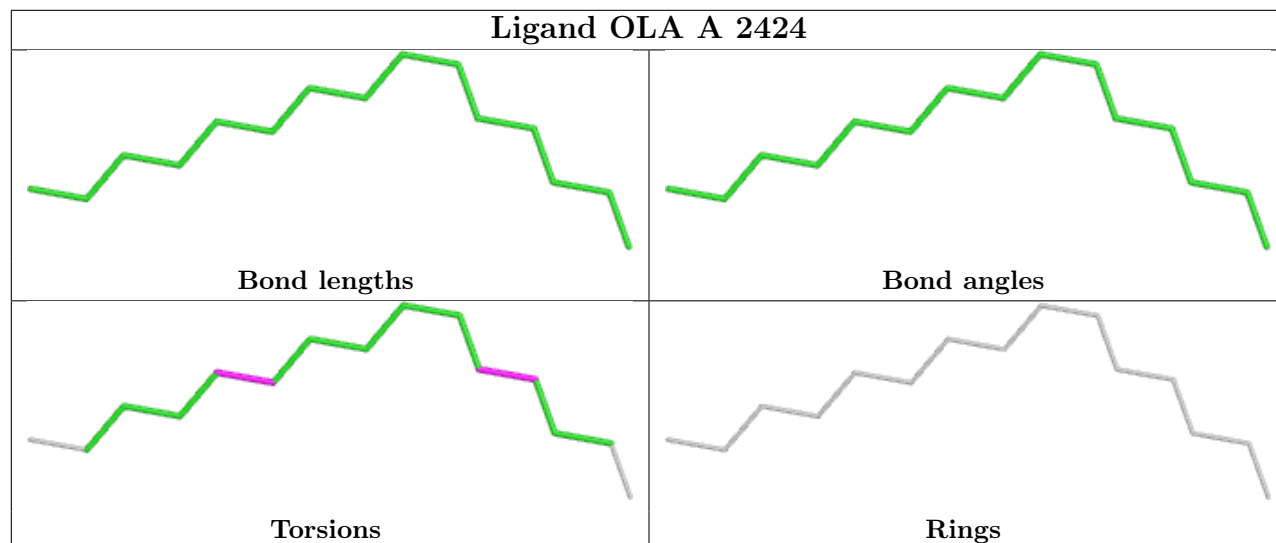
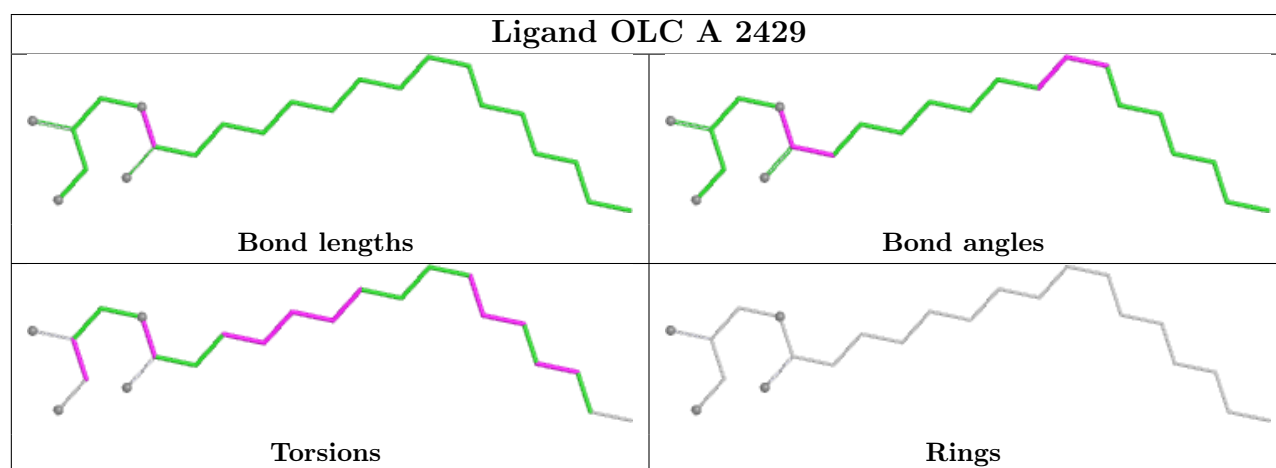
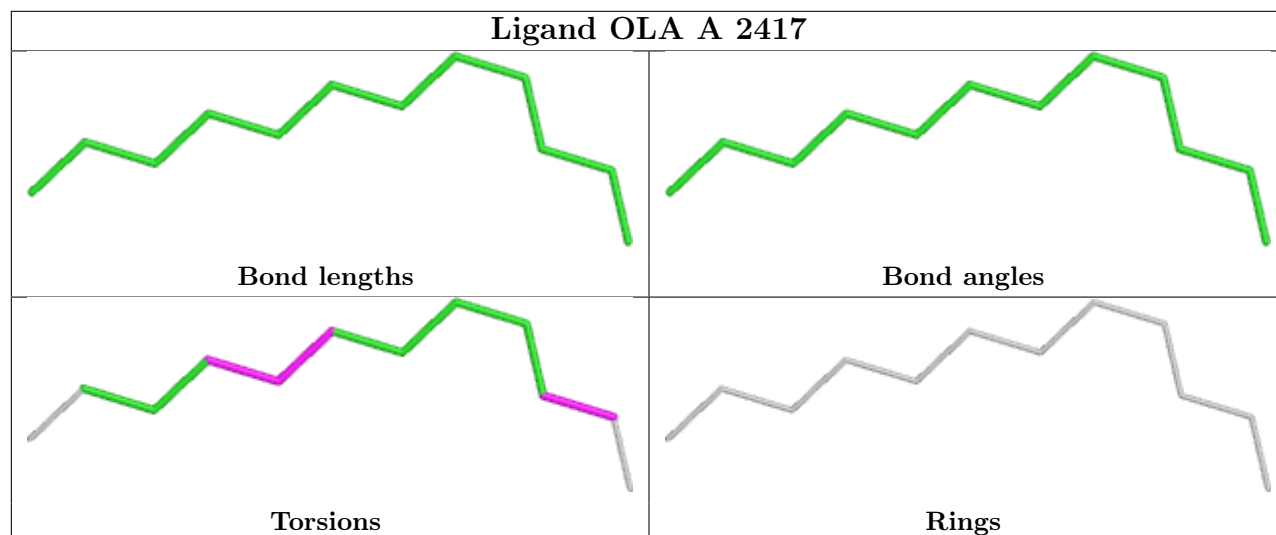


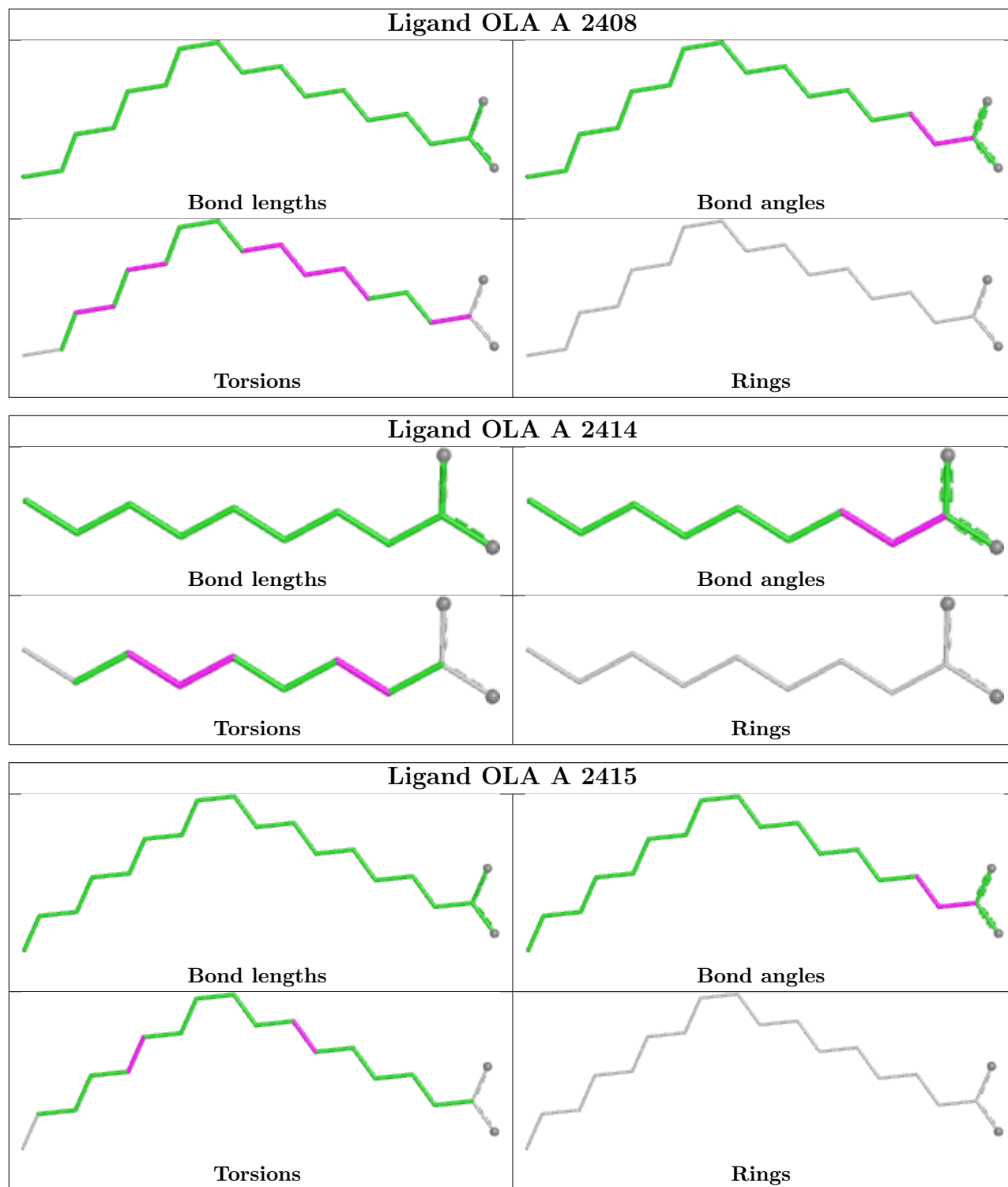




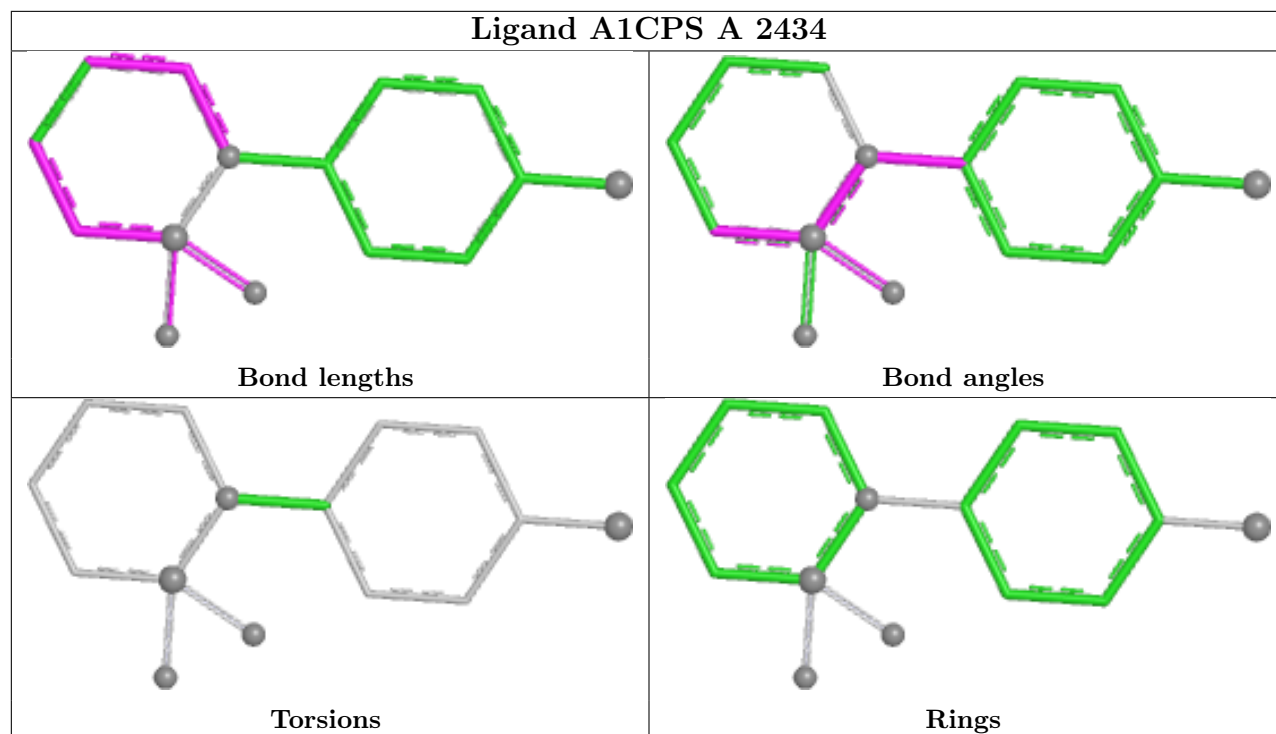




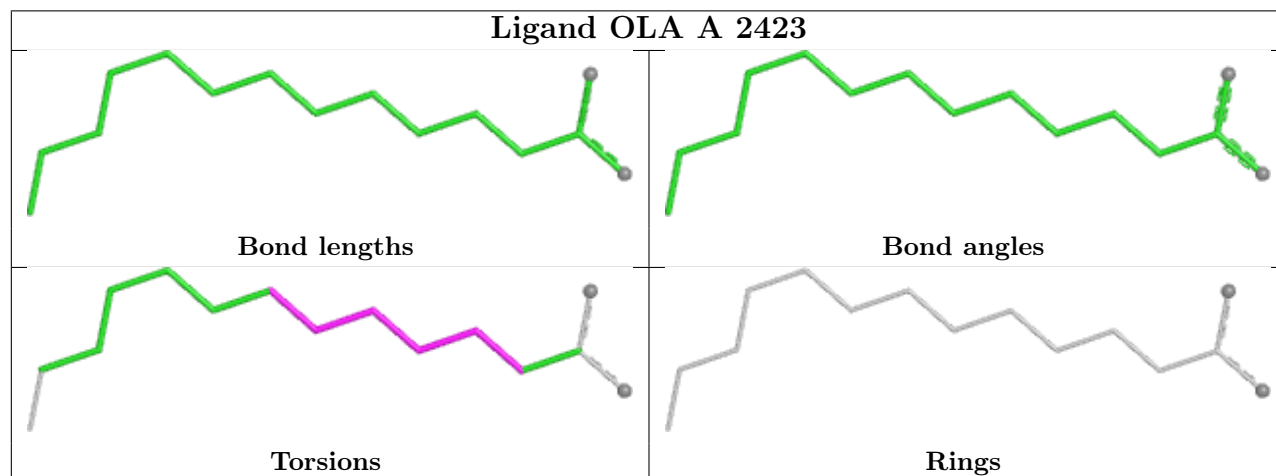




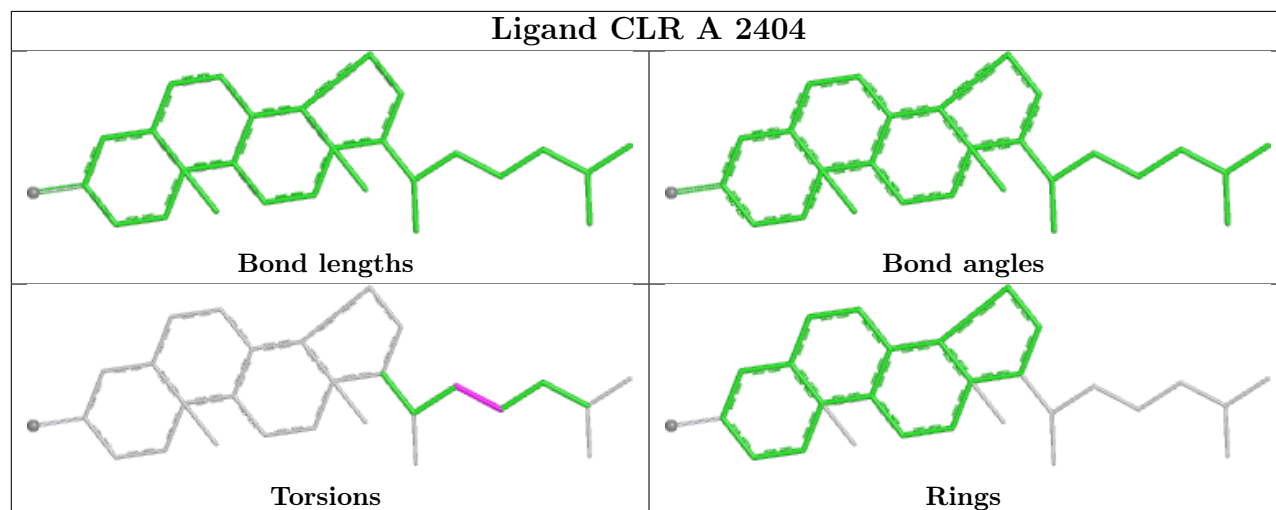
## Ligand A1CPS A 2434

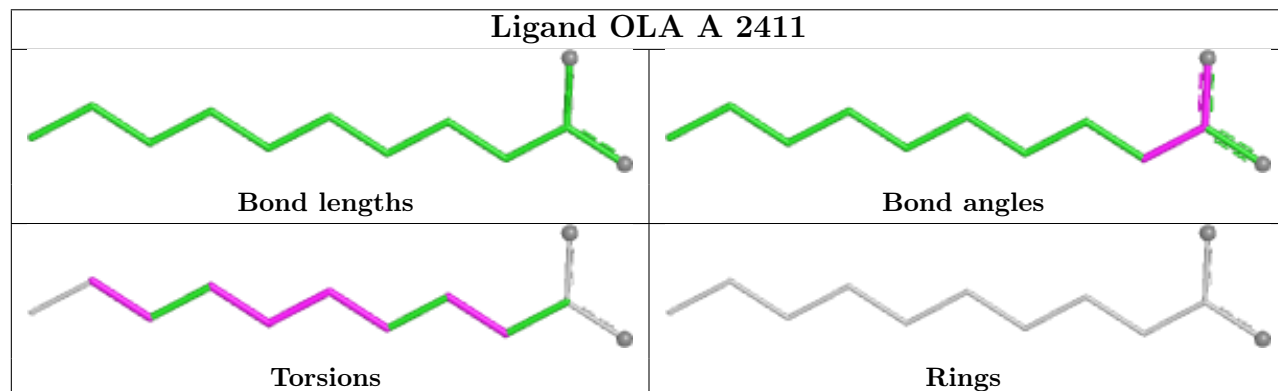
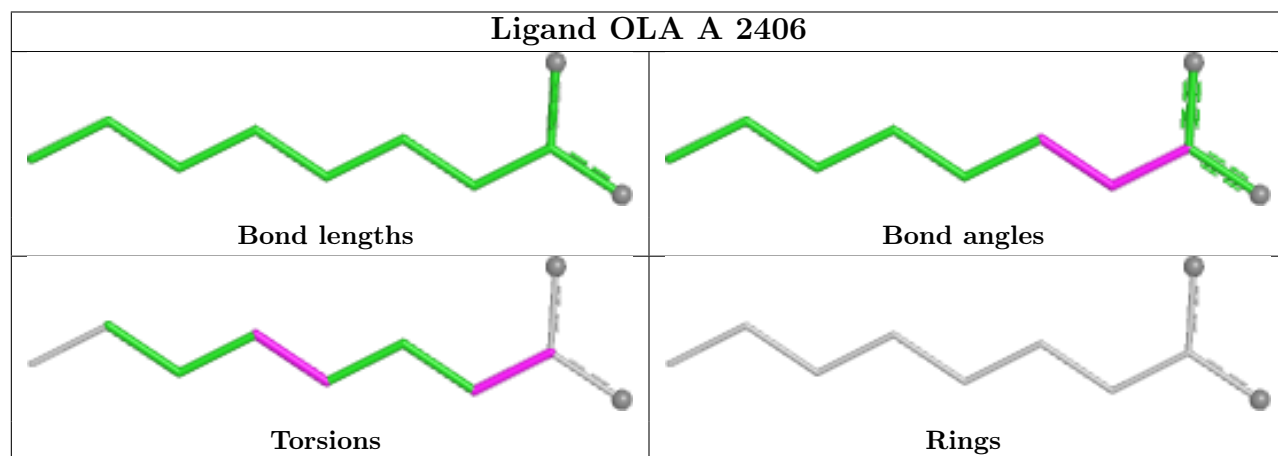
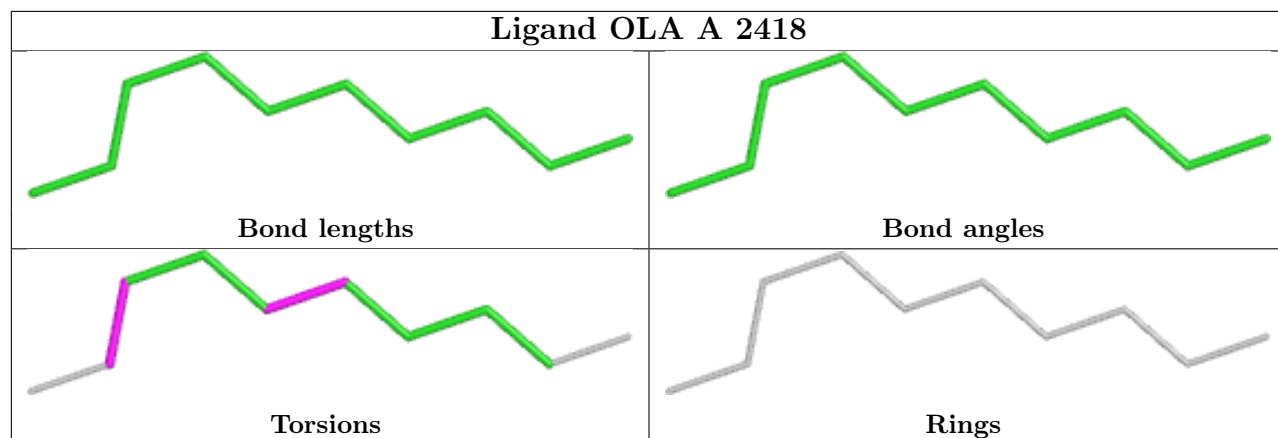


## Ligand OLA A 2423

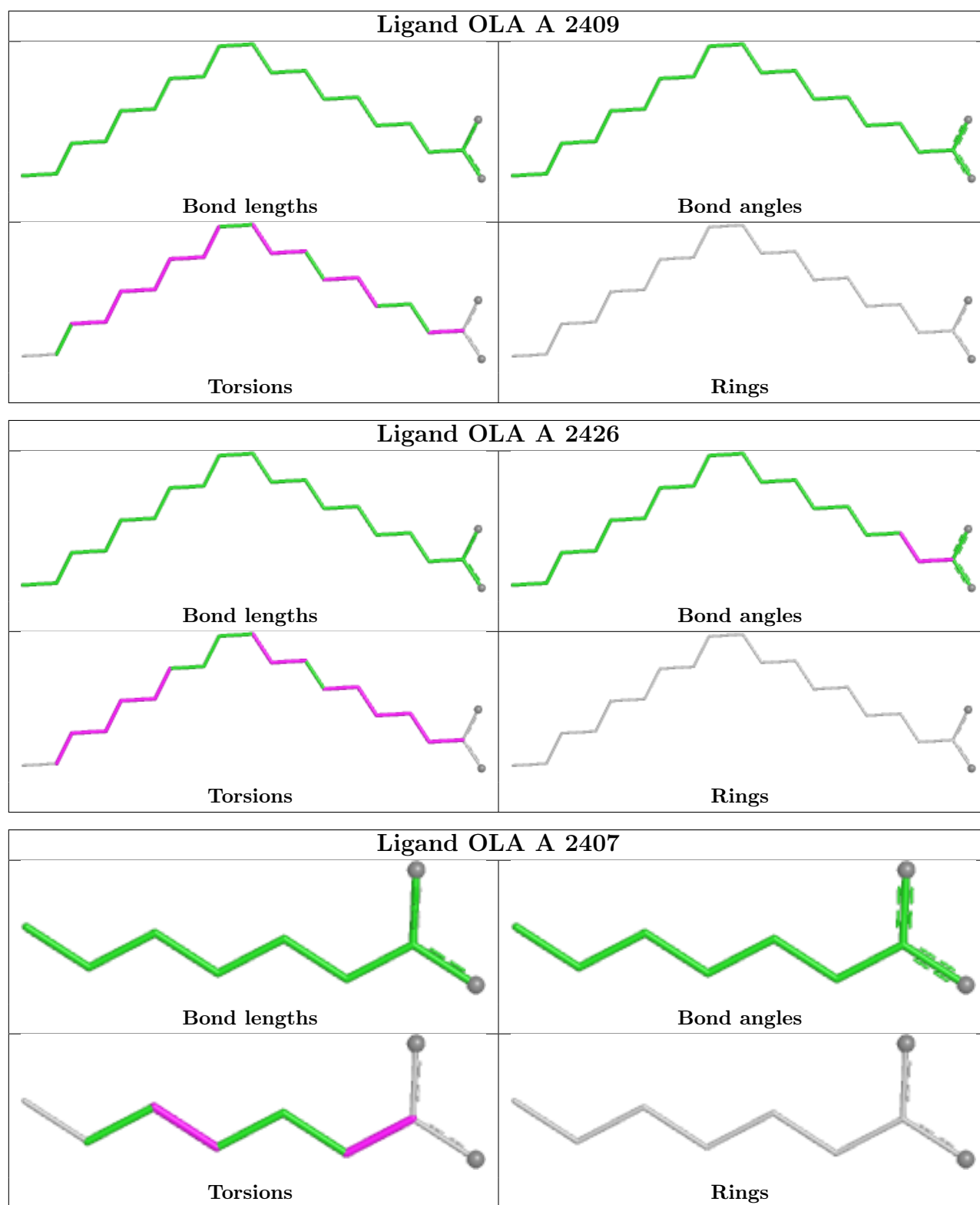


## Ligand CLR A 2404









## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	2.63	251 (64%) 0 0	2, 19, 54, 92	13 (3%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1040	ALA	8.9
1	A	1105	TYR	8.0
1	A	306	HIS	7.6
1	A	307	VAL	7.6
1	A	1061	PHE	6.9
1	A	290	TYR	6.0
1	A	1004	GLU	5.9
1	A	1028	ASP	5.8
1	A	160	GLY	5.8
1	A	308	LEU	5.7
1	A	1084	VAL	5.6
1	A	37	LEU	5.5
1	A	1094	LEU	5.5
1	A	1021	ASP	5.5
1	A	1001	ALA	5.3
1	A	1036	ALA	5.3
1	A	1003	LEU	5.1
1	A	1068	LEU	5.1
1	A	1078	LEU	5.1
1	A	161	GLU	5.1
1	A	148	GLN	5.1
1	A	1026	VAL	5.1
1	A	0	ALA	5.0
1	A	1	PRO	5.0
1	A	208	LEU	5.0
1	A	1106	LEU	4.9
1	A	1008	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1011	ASN	4.8
1	A	1022	ASN	4.8
1	A	1007	TRP	4.8
1	A	1041	GLN	4.7
1	A	114	GLY	4.7
1	A	1079	ALA	4.6
1	A	1062	ARG	4.6
1	A	206	ARG	4.6
1	A	1059	LYS	4.6
1	A	1038	LEU	4.5
1	A	1093	GLN	4.5
1	A	1064	GLY	4.5
1	A	110	LEU	4.5
1	A	29	TRP	4.5
1	A	115	LEU	4.5
1	A	1092	GLU	4.4
1	A	155	HIS	4.3
1	A	1076	LEU	4.3
1	A	303	ILE	4.3
1	A	2	PRO	4.2
1	A	305	SER	4.2
1	A	1102	ILE	4.2
1	A	152	GLY	4.2
1	A	1012	ASP	4.2
1	A	309	ARG	4.1
1	A	302	ILE	4.1
1	A	1065	PHE	4.1
1	A	32	TRP	4.1
1	A	129	TRP	4.1
1	A	1031	THR	4.1
1	A	111	ARG	4.0
1	A	1030	LEU	4.0
1	A	1063	HIS	4.0
1	A	205[A]	ARG	4.0
1	A	295	PHE	4.0
1	A	292	ILE	4.0
1	A	1082	GLY	4.0
1	A	1029	ALA	3.9
1	A	1010	LEU	3.9
1	A	147	GLY	3.9
1	A	1087	ALA	3.9
1	A	1023	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1072	ILE	3.8
1	A	1016	VAL	3.8
1	A	100	ILE	3.7
1	A	1002	ASP	3.7
1	A	1017	ILE	3.7
1	A	71	CYS	3.7
1	A	1020	ALA	3.6
1	A	19	LEU	3.6
1	A	1006	ASN	3.6
1	A	44	PHE	3.6
1	A	1100	ALA	3.6
1	A	1085	LYS	3.6
1	A	220	ARG	3.6
1	A	1101	TYR	3.5
1	A	1032	LYS	3.5
1	A	1042	LYS	3.5
1	A	301	LYS	3.5
1	A	157	GLN	3.5
1	A	187[A]	LEU	3.4
1	A	1099	ASN	3.4
1	A	1039	ASP	3.4
1	A	300[A]	ARG	3.4
1	A	1024	ALA	3.4
1	A	183	PHE	3.4
1	A	269	LEU	3.4
1	A	9	TYR	3.4
1	A	1014	LEU	3.4
1	A	151	GLU	3.3
1	A	262	CYS	3.3
1	A	162	GLY	3.3
1	A	1025	GLN	3.3
1	A	67	SER	3.3
1	A	1037	ALA	3.2
1	A	1060	ASP	3.2
1	A	1089	ALA	3.2
1	A	1066	ASP	3.2
1	A	25	VAL	3.2
1	A	1069	VAL	3.2
1	A	229	VAL	3.2
1	A	297	GLN	3.2
1	A	197	TYR	3.2
1	A	230	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	200	ILE	3.1
1	A	1015	LYS	3.1
1	A	235	ALA	3.1
1	A	271	TYR	3.1
1	A	258	PHE	3.1
1	A	1080	ASN	3.1
1	A	222	ARG	3.1
1	A	1095	LYS	3.1
1	A	201	PHE	3.1
1	A	1034	ARG	3.1
1	A	1081	GLU	3.1
1	A	1035	ALA	3.1
1	A	3	ILE	3.1
1	A	1033	MET	3.1
1	A	261	ASP	3.0
1	A	141[A]	LEU	3.0
1	A	119	THR	3.0
1	A	173	PRO	3.0
1	A	33	LEU	3.0
1	A	40	VAL	3.0
1	A	1077	LYS	3.0
1	A	225	LEU	2.9
1	A	8	VAL	2.9
1	A	223	SER	2.9
1	A	36	ASN	2.9
1	A	106	ILE	2.9
1	A	73	ALA	2.9
1	A	112	TYR	2.9
1	A	221	ALA	2.9
1	A	244[A]	LEU	2.8
1	A	274	ILE	2.8
1	A	43	TYR	2.8
1	A	103	TYR	2.8
1	A	219	GLU	2.8
1	A	304	ARG	2.8
1	A	1097	THR	2.8
1	A	1067	ILE	2.8
1	A	199	ARG	2.7
1	A	1103	GLN	2.7
1	A	49	ALA	2.7
1	A	166	CYS	2.7
1	A	6[A]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1019	LYS	2.7
1	A	1083	LYS	2.7
1	A	121	ALA	2.7
1	A	279[A]	THR	2.7
1	A	175	ASN	2.7
1	A	116	VAL	2.7
1	A	72	ALA	2.7
1	A	34	ASN	2.7
1	A	1009	THR	2.6
1	A	288	TYR	2.6
1	A	233	LYS	2.6
1	A	158	GLY	2.6
1	A	1070	GLY	2.6
1	A	107	ALA	2.6
1	A	194	LEU	2.6
1	A	150	LYS	2.6
1	A	113	ASN	2.6
1	A	167	LEU	2.6
1	A	266	PRO	2.6
1	A	257	PHE	2.6
1	A	286	PHE	2.6
1	A	27	VAL	2.6
1	A	275[A]	VAL	2.6
1	A	97	ALA	2.6
1	A	1088	GLN	2.5
1	A	60	ILE	2.5
1	A	76	GLY	2.5
1	A	249	LEU	2.5
1	A	133	PHE	2.5
1	A	259	CYS	2.5
1	A	1018	GLU	2.5
1	A	198	LEU	2.5
1	A	93	PHE	2.5
1	A	21	ILE	2.5
1	A	124	ILE	2.5
1	A	35	SER	2.5
1	A	1091	ALA	2.5
1	A	84	VAL	2.4
1	A	108	ILE	2.5
1	A	224	THR	2.4
1	A	20	ALA	2.4
1	A	289	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	75	HIS	2.4
1	A	104	ILE	2.4
1	A	172	VAL	2.4
1	A	118	GLY	2.4
1	A	18	VAL	2.4
1	A	1027	LYS	2.4
1	A	143	TRP	2.4
1	A	159	CYS	2.4
1	A	204	ALA	2.3
1	A	85	LEU	2.3
1	A	31	VAL	2.3
1	A	1071	GLN	2.3
1	A	268	TRP	2.3
1	A	203	ALA	2.3
1	A	192	LEU	2.3
1	A	38	GLN	2.3
1	A	5	GLY	2.3
1	A	293	ARG	2.3
1	A	180	PHE	2.3
1	A	171	VAL	2.3
1	A	122	ALA	2.3
1	A	1090	ALA	2.3
1	A	83	PHE	2.2
1	A	57	VAL	2.2
1	A	1098	ARG	2.2
1	A	10	ILE	2.2
1	A	61	PRO	2.2
1	A	142	GLY	2.2
1	A	291	ARG	2.2
1	A	296	ARG	2.2
1	A	30	ALA	2.2
1	A	154	ALA	2.2
1	A	231	ALA	2.2
1	A	243	ALA	2.2
1	A	265	ALA	2.2
1	A	48	LEU	2.2
1	A	77	CYS	2.2
1	A	146	CYS	2.2
1	A	234	SER	2.2
1	A	1104	LYS	2.2
1	A	1013	ASN	2.2
1	A	1075	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	7	SER	2.1
1	A	1086	GLU	2.1
1	A	117	THR	2.1
1	A	74	CYS	2.1
1	A	135	ILE	2.1
1	A	251	ILE	2.1
1	A	283	VAL	2.1
1	A	22	LEU	2.1
1	A	191	LEU	2.1
1	A	207	GLN	2.1
1	A	145	ASN	2.0
1	A	16	ILE	2.0
1	A	53	ILE	2.0
1	A	92	ILE	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
5	OLA	A	2413	15/20	0.52	0.23	30,36,41,42	0
5	OLA	A	2426	20/20	0.53	0.26	28,39,48,64	0
6	OLC	A	2428	17/25	0.53	0.22	30,39,48,51	0
5	OLA	A	2423	15/20	0.55	0.28	27,32,47,51	0
5	OLA	A	2422	8/20	0.58	0.21	26,31,32,34	0
5	OLA	A	2406	10/20	0.58	0.22	28,41,50,59	0
5	OLA	A	2408	18/20	0.59	0.23	15,27,44,47	0
5	OLA	A	2421	9/20	0.61	0.27	22,29,46,47	0
5	OLA	A	2410	20/20	0.62	0.23	24,35,48,51	0

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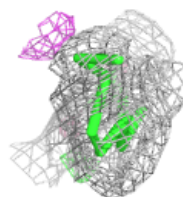
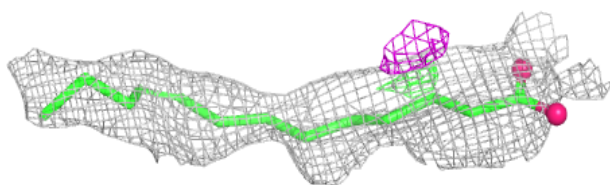
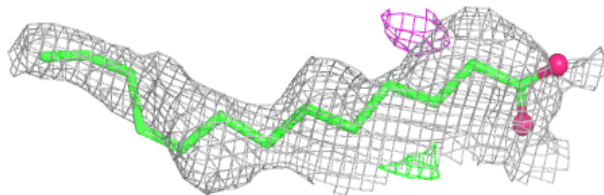
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OLA	A	2415	19/20	0.63	0.21	28,31,39,41	0
5	OLA	A	2409	20/20	0.63	0.23	12,32,42,49	0
5	OLA	A	2420	12/20	0.64	0.18	22,26,30,32	0
5	OLA	A	2416	20/20	0.64	0.22	21,35,39,42	0
6	OLC	A	2432	18/25	0.64	0.23	16,30,41,50	0
5	OLA	A	2412	8/20	0.65	0.18	28,30,34,35	0
4	CLR	A	2402	28/28	0.66	0.19	11,18,28,35	0
6	OLC	A	2427	16/25	0.68	0.20	16,22,32,34	0
5	OLA	A	2407	9/20	0.69	0.23	15,17,33,36	0
5	OLA	A	2417	12/20	0.70	0.22	14,23,33,35	0
5	OLA	A	2424	15/20	0.70	0.19	19,22,27,28	0
5	OLA	A	2414	11/20	0.71	0.18	18,24,38,47	0
5	OLA	A	2425	13/20	0.71	0.21	20,27,50,51	0
5	OLA	A	2405	20/20	0.72	0.20	17,24,34,34	0
6	OLC	A	2430	23/25	0.72	0.20	14,27,36,38	0
5	OLA	A	2418	10/20	0.72	0.22	19,33,36,36	0
6	OLC	A	2431	23/25	0.73	0.20	13,23,47,55	0
6	OLC	A	2429	23/25	0.74	0.21	18,27,46,49	0
6	OLC	A	2433	16/25	0.75	0.18	12,22,30,34	0
5	OLA	A	2411	12/20	0.79	0.18	10,28,36,42	0
4	CLR	A	2403	28/28	0.80	0.17	12,19,24,26	0
4	CLR	A	2404	28/28	0.80	0.14	9,15,22,30	0
7	A1CPS	A	2434	15/15	0.80	0.20	16,22,29,37	0
5	OLA	A	2419	11/20	0.81	0.17	12,21,34,37	0
3	TEP	A	2401	13/13	0.86	0.13	4,6,10,11	0
2	NA	A	2400	1/1	0.89	0.12	16,16,16,16	0

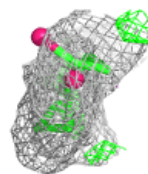
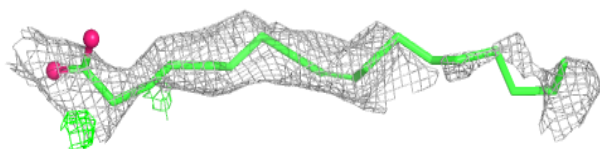
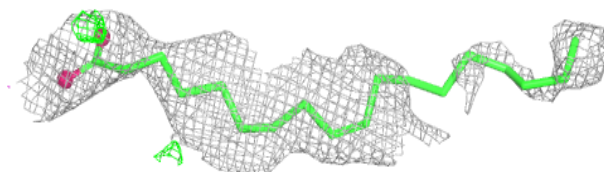
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLA A 2413:**

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

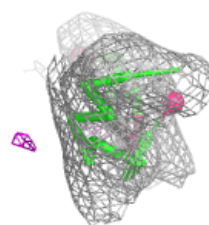
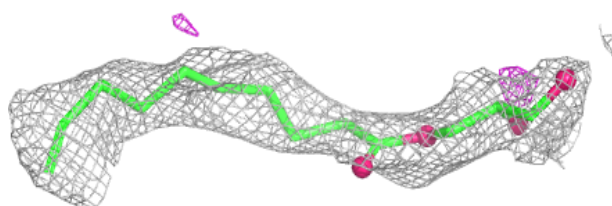
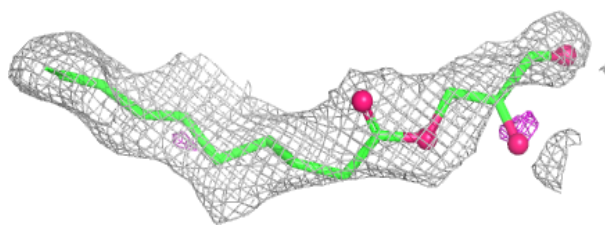
**Electron density around OLA A 2426:**

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

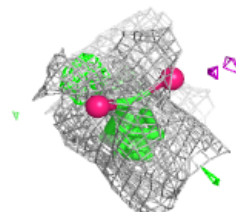
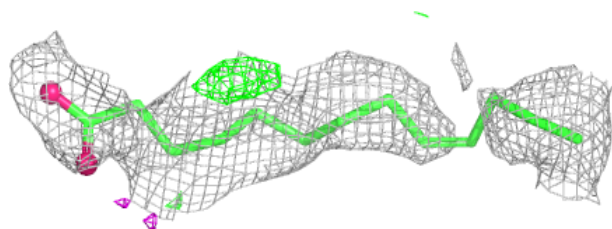
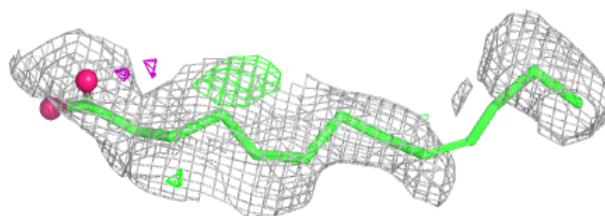


**Electron density around OLC A 2428:**

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

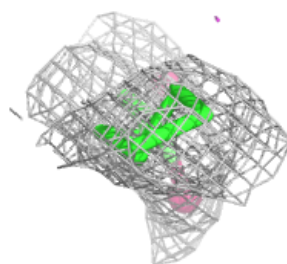
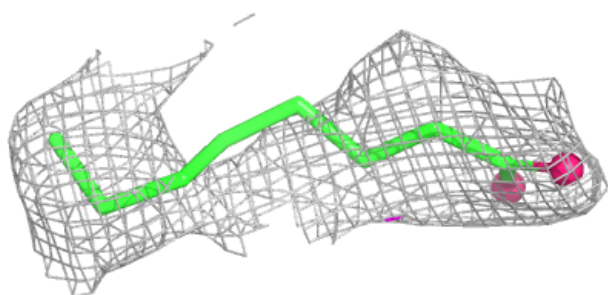
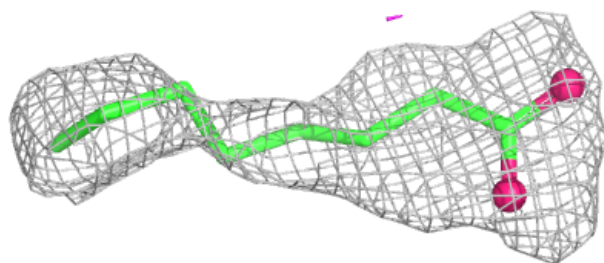
**Electron density around OLA A 2423:**

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

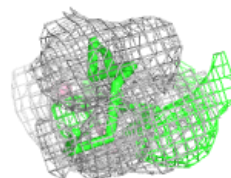
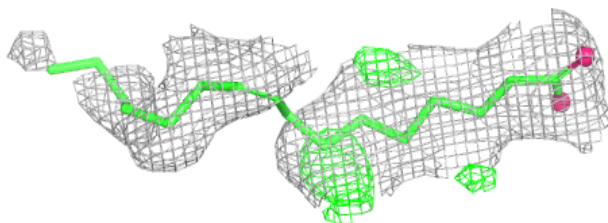
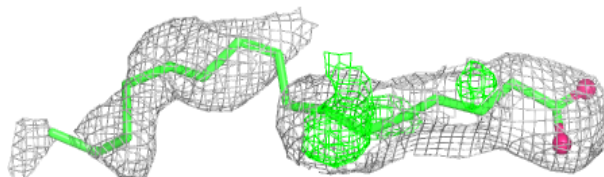


**Electron density around OLA A 2406:**

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

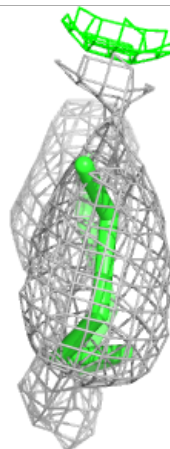
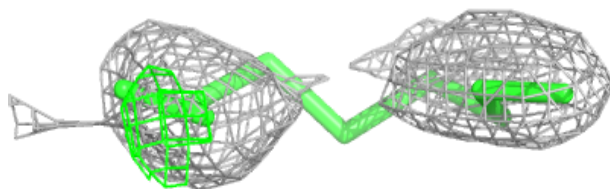
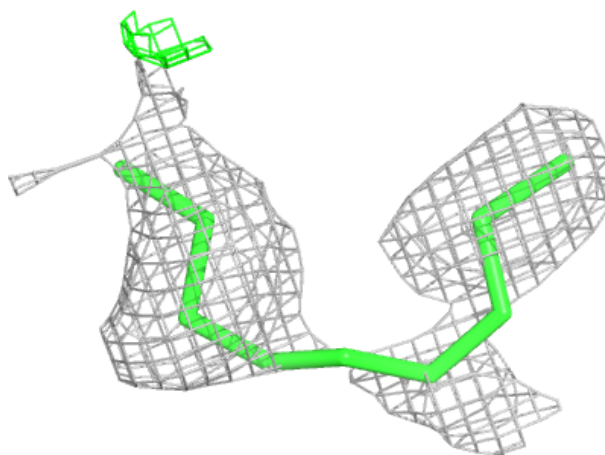
**Electron density around OLA A 2408:**

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



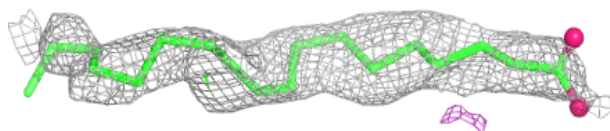
**Electron density around OLA A 2421:**

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

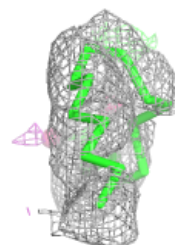
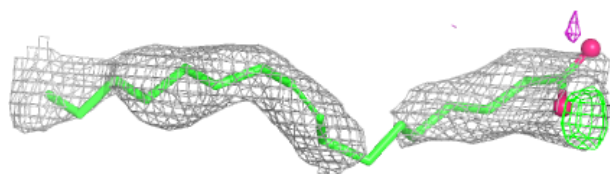
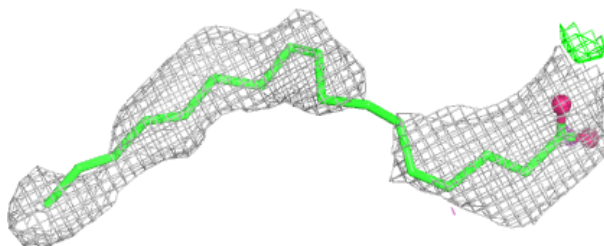


**Electron density around OLA A 2410:**

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

**Electron density around OLA A 2415:**

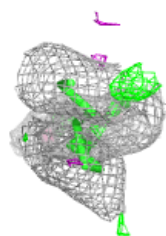
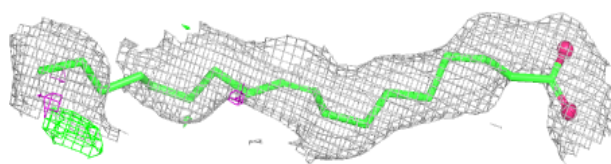
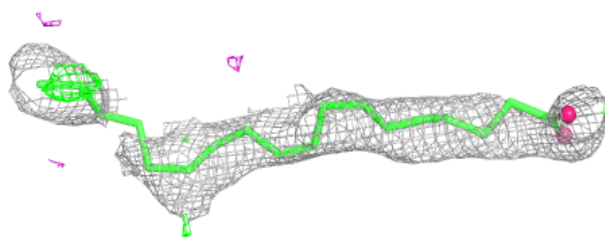
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



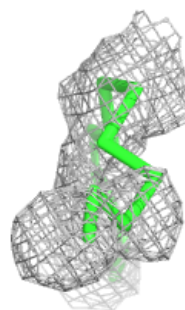
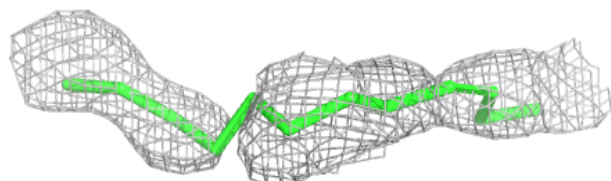
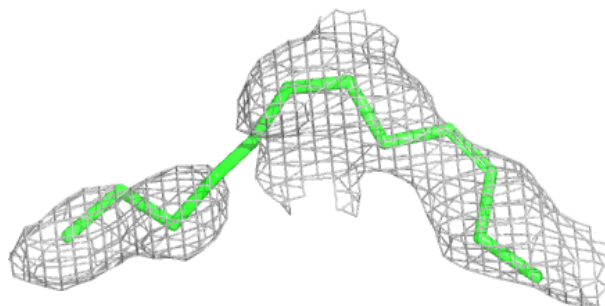


**Electron density around OLA A 2409:**

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

**Electron density around OLA A 2420:**

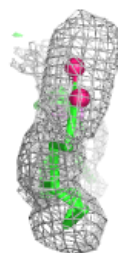
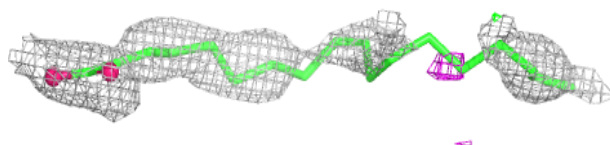
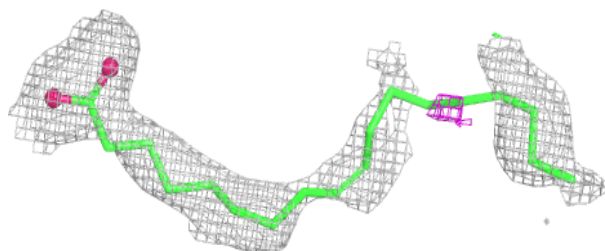
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



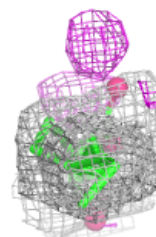
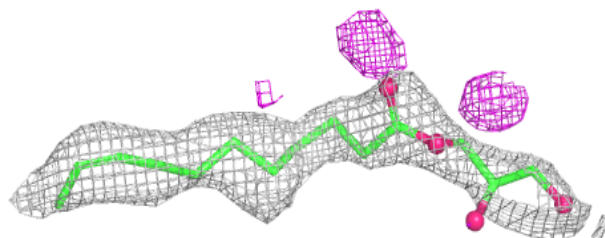


**Electron density around OLA A 2416:**

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

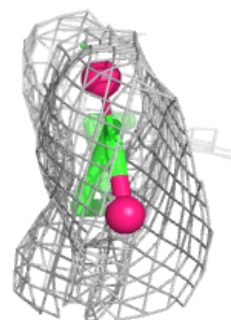
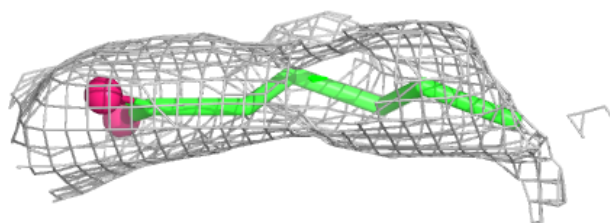
**Electron density around OLC A 2432:**

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

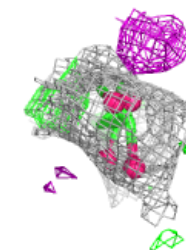
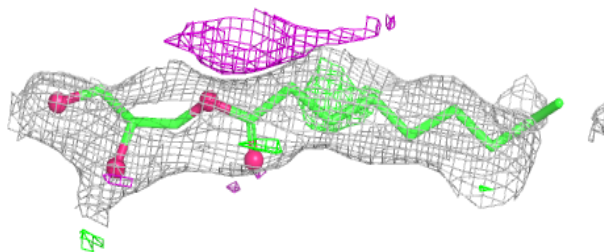


**Electron density around OLA A 2412:**

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

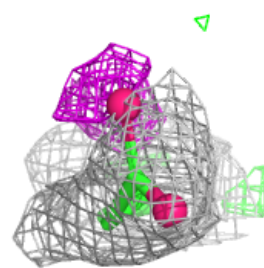
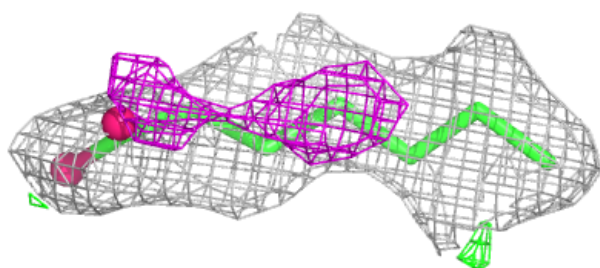
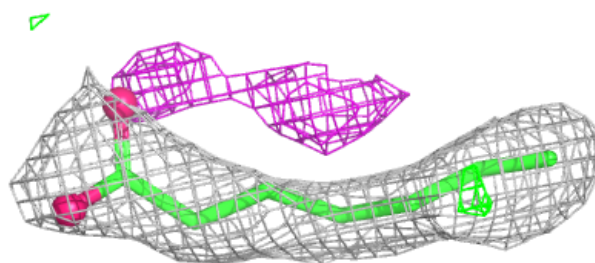
**Electron density around OLC A 2427:**

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

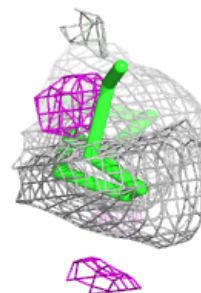
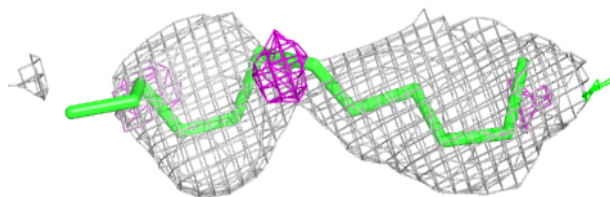
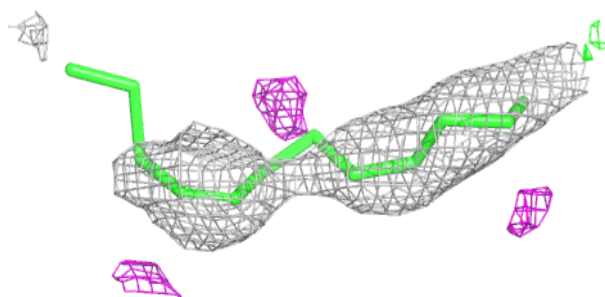


**Electron density around OLA A 2407:**

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

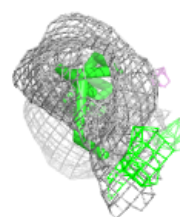
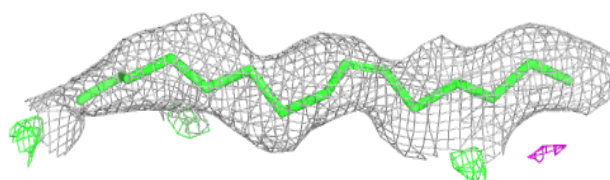
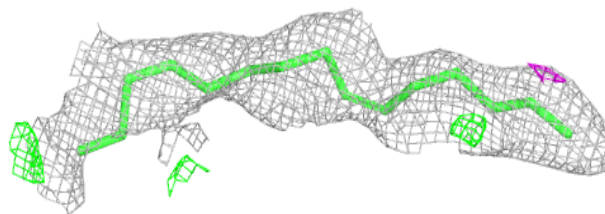
**Electron density around OLA A 2417:**

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

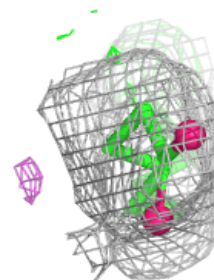
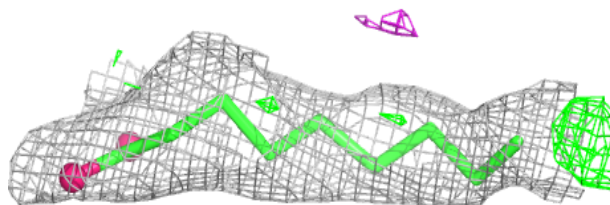


**Electron density around OLA A 2424:**

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

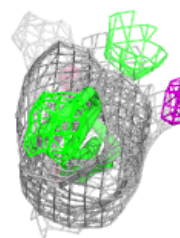
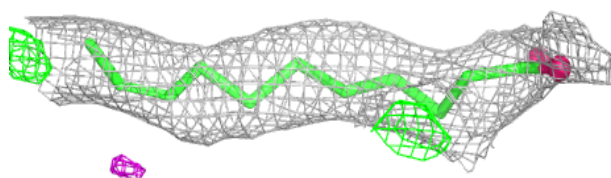
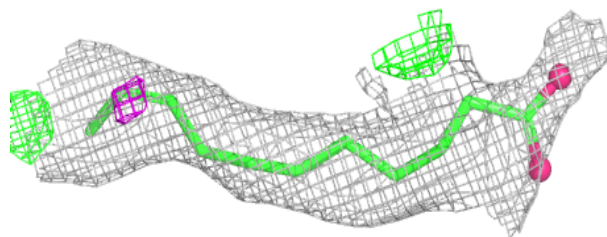
**Electron density around OLA A 2414:**

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

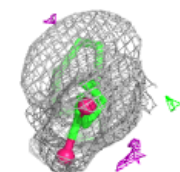
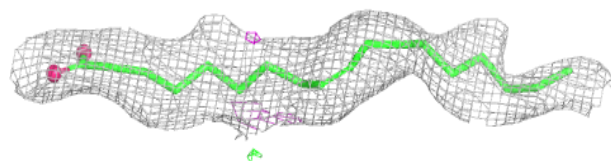
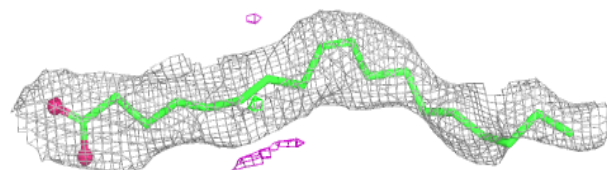


**Electron density around OLA A 2425:**

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

**Electron density around OLA A 2405:**

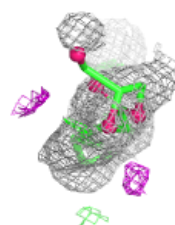
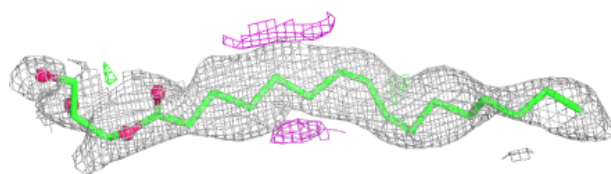
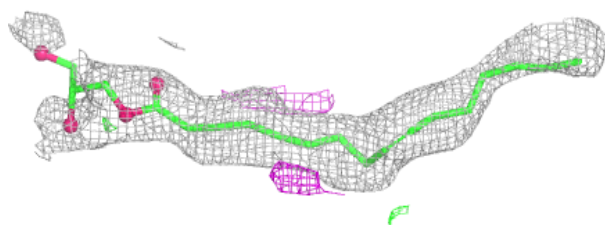
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



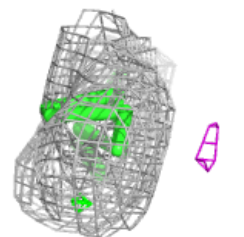
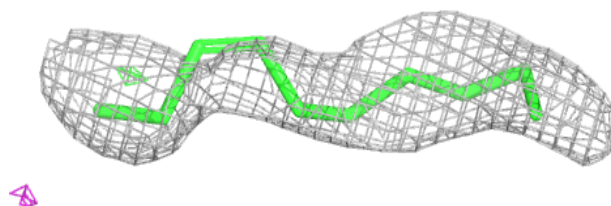
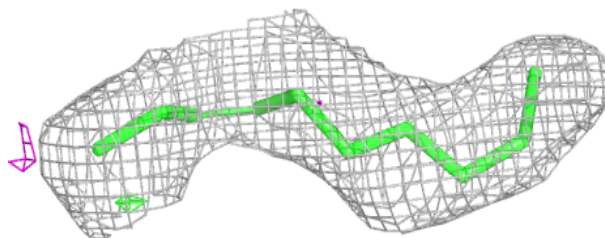


**Electron density around OLC A 2430:**

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

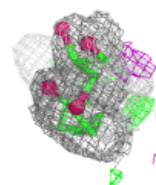
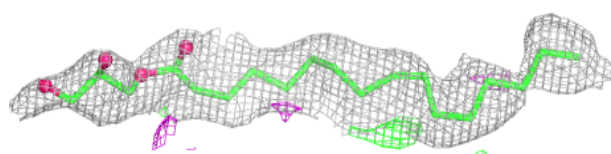
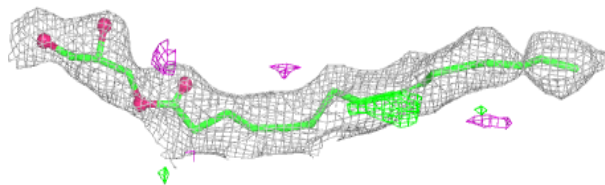
**Electron density around OLA A 2418:**

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

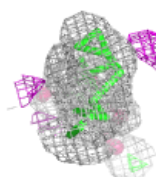
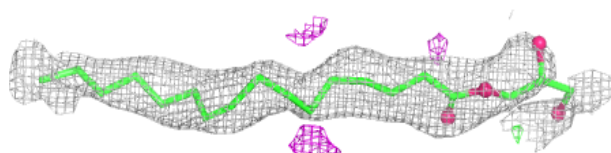
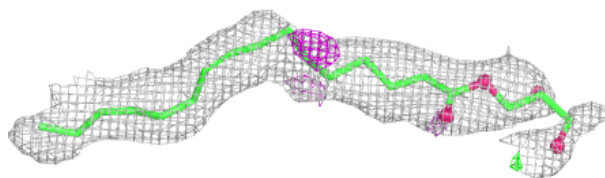


**Electron density around OLC A 2431:**

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

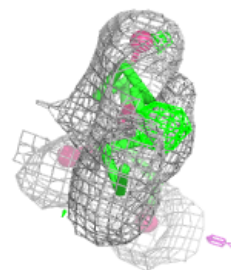
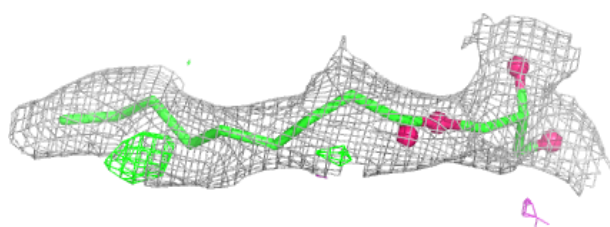
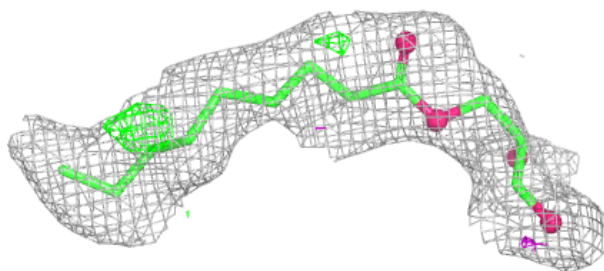
**Electron density around OLC A 2429:**

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

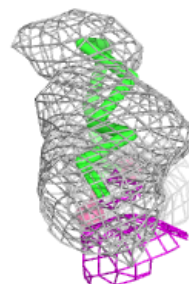
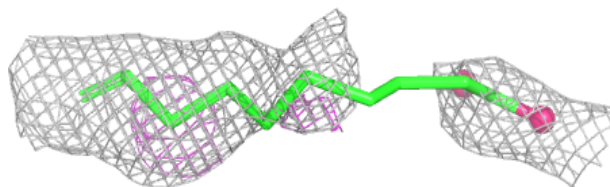
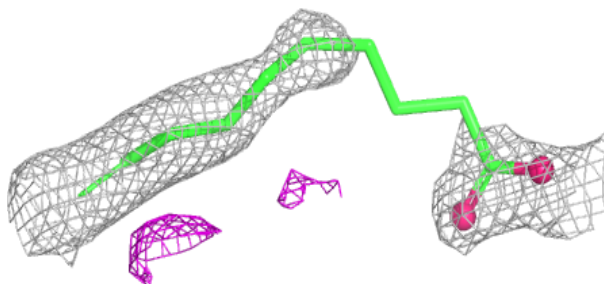


**Electron density around OLC A 2433:**

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

**Electron density around OLA A 2411:**

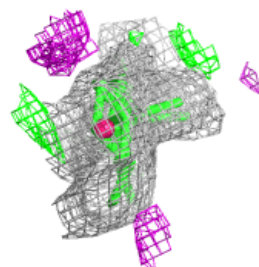
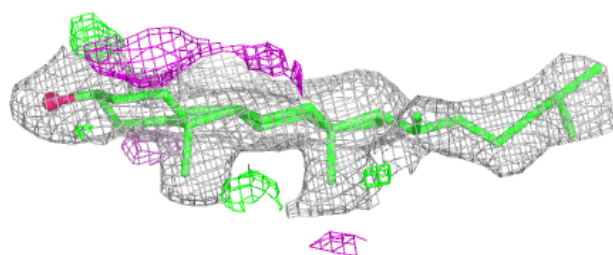
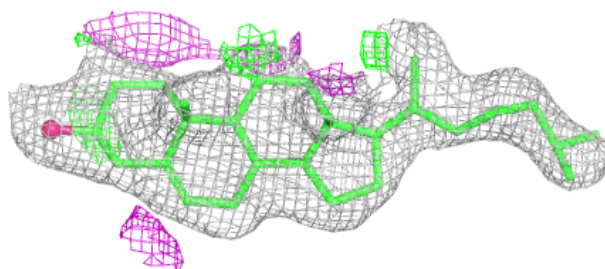
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



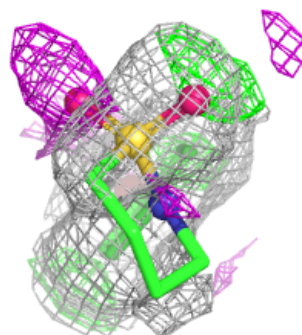
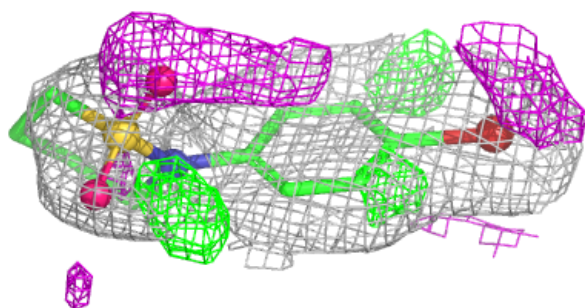
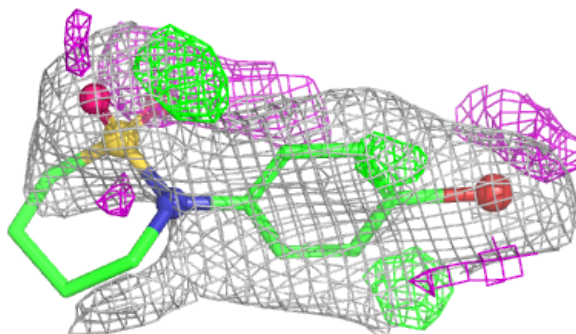


**Electron density around CLR A 2404:**

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

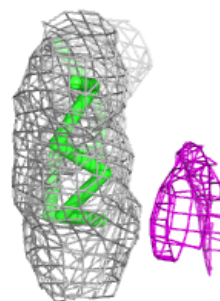
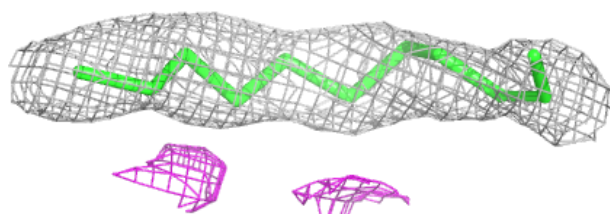
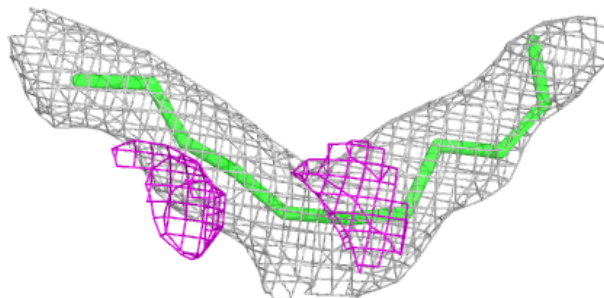
**Electron density around A1CPS A 2434:**

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



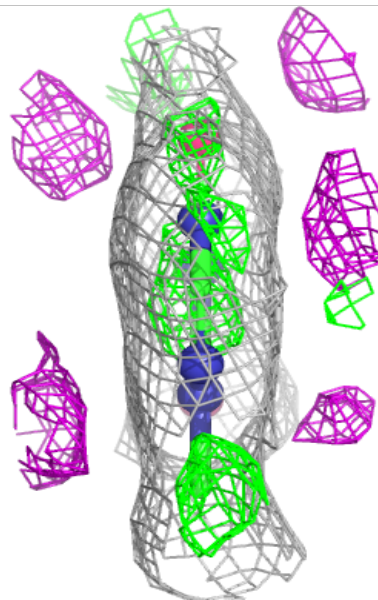
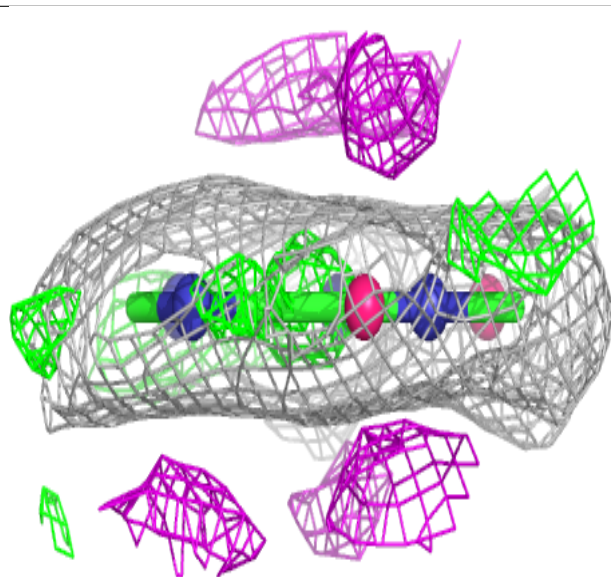
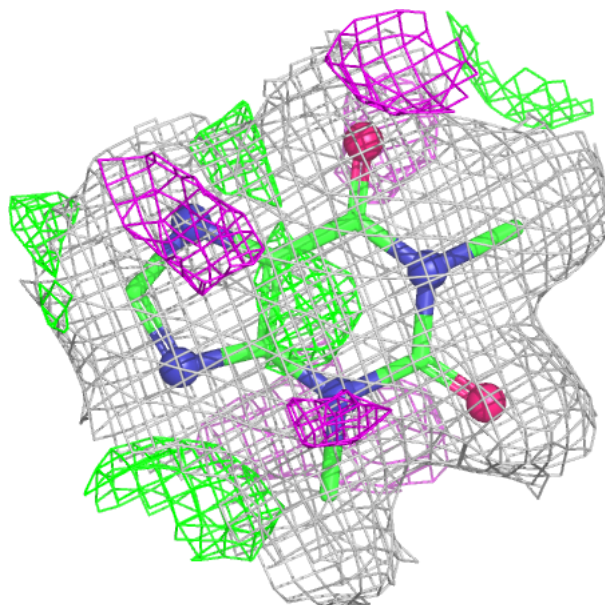
**Electron density around OLA A 2419:**

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



**Electron density around TEP A 2401:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.