



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 8RVW / pdb_00008rvw
Title : Dark structure of the human adenosine A2A receptor bound to synthetic photoswitch "StilSwitch3" determined by serial synchrotron crystallography
Authors : Glover, H.; Bertrand, Q.
Deposited on : 2024-02-02
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

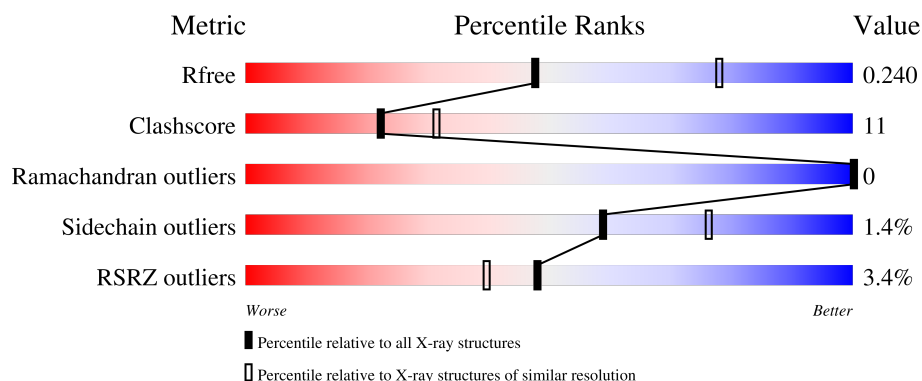
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6513 atoms, of which 3168 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, Adenosine receptor A2a, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	6	0
			5683	1902	2777	475	507	22			

There are 45 discrepancies between the modelled and reference sequences:

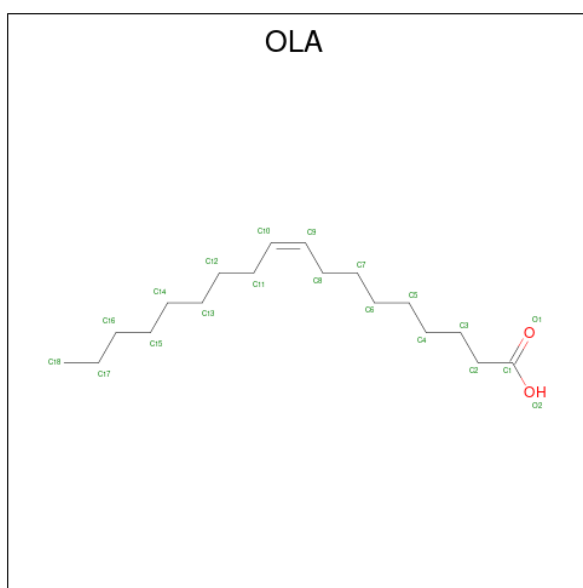
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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 OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



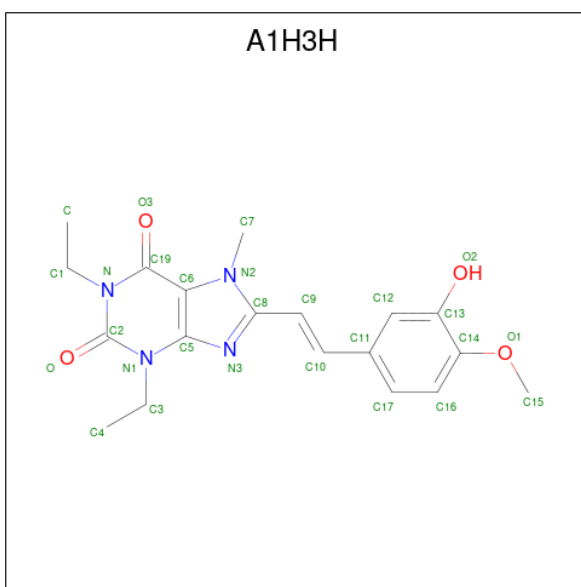
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			15	13	2		

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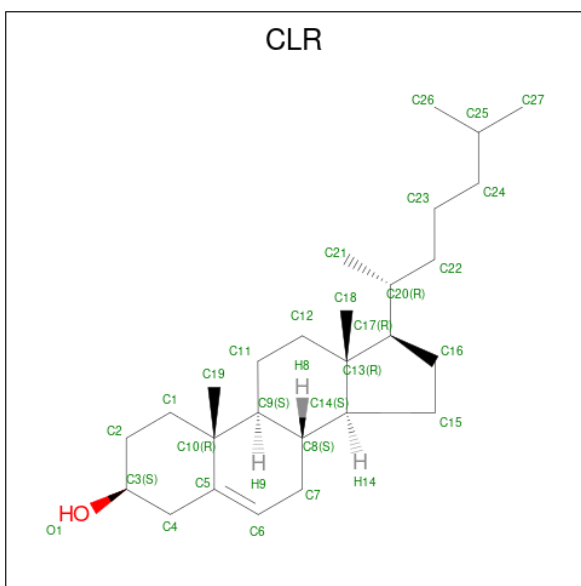
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 16 16	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C H O 28 10 16 2	0	0
2	A	1	Total C H O 43 15 26 2	0	0
2	A	1	Total C H O 40 14 24 2	0	0
2	A	1	Total C H O 40 14 24 2	0	0
2	A	1	Total C H O 53 18 33 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C H 44 15 29	0	0
2	A	1	Total C H O 26 9 15 2	0	0
2	A	1	Total C H O 21 7 12 2	0	0
2	A	1	Total C H O 18 6 10 2	0	0
2	A	1	Total C H O 43 15 26 2	0	0
2	A	1	Total C H 20 10 10	0	0
2	A	1	Total C H 26 10 16	0	0
2	A	1	Total C H O 21 7 12 2	0	0
2	A	1	Total C O 16 14 2	0	0

- Molecule 3 is 1,3-diethyl-8-[({E})-2-(4-methoxy-3-oxidanyl-phenyl)ethenyl]-7-methyl-purine-2,6-dione (CCD ID: A1H3H) (formula: C₁₉H₂₂N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	4	4		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			74	27	46	1		
4	A	1	Total	C	H	O	0	0
			74	27	46	1		
4	A	1	Total	C	H	O	0	0
			74	27	46	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total 51	O 51	0	0

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.55Å 182.54Å 143.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.65 45.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.64-2.65) 99.5 (45.64-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.192 , 0.233 0.204 , 0.240	Depositor DCC
R_{free} test set	1601 reflections (7.39%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 120.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6513	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H3H, CLR, OLA, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2995	0.65	3/4094 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1093	GLN	N-CA-C	-5.64	105.66	112.54
1	A	1092	GLU	N-CA-C	-5.22	107.08	113.50
1	A	1078	LEU	N-CA-C	-5.13	105.58	111.07

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	2906	2777	2862	67	0
2	A	276	253	388	8	0
3	A	27	0	0	0	0
4	A	84	138	138	1	0
5	A	1	0	0	0	0
6	A	51	0	0	3	0
All	All	3345	3168	3388	71	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 11.

All (71) 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:1074[B]:ASP:OD1	1:A:1075:ALA:N	2.17	0.77
1:A:236:ALA:HB1	2:A:1224:OLA:H32	1.69	0.75
1:A:174[A]:MET:SD	6:A:1344:HOH:O	2.45	0.74
1:A:108:ILE:HD12	1:A:108:ILE:O	1.91	0.69
1:A:174[B]:MET:HG2	6:A:1342:HOH:O	1.93	0.68
1:A:174[B]:MET:SD	6:A:1344:HOH:O	2.52	0.67
1:A:1007:TRP:HZ3	1:A:1102:ILE:CD1	2.08	0.67
1:A:1067:ILE:HG22	1:A:1097:THR:HG21	1.76	0.65
1:A:174[B]:MET:HE1	1:A:253:ASN:HB3	1.78	0.65
1:A:61:PRO:O	1:A:65:THR:HG23	1.98	0.62
1:A:1007:TRP:HZ3	1:A:1102:ILE:HD11	1.64	0.61
1:A:104:ILE:CG2	1:A:108:ILE:HD11	2.30	0.60
1:A:174[A]:MET:HE3	1:A:253:ASN:HB3	1.83	0.59
1:A:46:VAL:HG12	2:A:1201:OLA:H51	1.85	0.58
1:A:1011:ASN:OD1	1:A:1098:ARG:NH1	2.36	0.58
1:A:1103:GLN:OE1	1:A:1103:GLN:C	2.47	0.57
1:A:104:ILE:HG23	1:A:108:ILE:HD11	1.87	0.57
1:A:238:ILE:HD11	1:A:287:ILE:HG21	1.87	0.56
1:A:17:ALA:O	1:A:21:ILE:HD12	2.07	0.54
1:A:238:ILE:CD1	1:A:287:ILE:HG21	2.38	0.54
1:A:174[A]:MET:HE3	1:A:253:ASN:CB	2.37	0.54
1:A:95:LEU:HD21	1:A:238:ILE:HG22	1.91	0.52
1:A:1005:ASP:HA	1:A:1008:GLU:HG3	1.92	0.52
1:A:1102:ILE:C	1:A:1102:ILE:HD12	2.34	0.52
1:A:108:ILE:O	1:A:108:ILE:CD1	2.57	0.52
1:A:65:THR:HG22	2:A:1214:OLA:H9	1.93	0.51
1:A:1017:ILE:HD11	1:A:1030:LEU:HG	1.93	0.50
1:A:305:SER:HB3	1:A:306:HIS:CD2	2.47	0.50
2:A:1201:OLA:H131	2:A:1216:OLA:H122	1.93	0.49
1:A:1004:GLU:HG3	1:A:222:ARG:NH2	2.28	0.49
1:A:1008:GLU:OE2	1:A:1008:GLU:C	2.56	0.48
1:A:1011:ASN:CG	1:A:1098:ARG:HH11	2.21	0.48
1:A:1067:ILE:CG2	1:A:1097:THR:HG21	2.43	0.48
1:A:117:THR:OG1	1:A:120:ARG:HG3	2.14	0.48
1:A:234:SER:O	1:A:238:ILE:HD13	2.13	0.48
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.95	0.48
1:A:1008:GLU:OE2	1:A:1009:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:SER:HB3	1:A:306:HIS:HD2	1.79	0.47
1:A:1072:ILE:N	1:A:1072:ILE:HD13	2.28	0.47
1:A:293:ARG:HA	1:A:296:ARG:NH1	2.29	0.47
1:A:110:LEU:HG	1:A:111:ARG:H	1.80	0.47
1:A:1078:LEU:HD23	1:A:1086:GLU:HB2	1.97	0.46
1:A:110:LEU:HD23	1:A:110:LEU:H	1.81	0.45
1:A:1084:VAL:CG1	1:A:1085:LYS:N	2.79	0.45
1:A:270:MET:O	1:A:274:ILE:HG13	2.16	0.45
2:A:1204:OLA:H42	2:A:1214:OLA:H72	1.98	0.45
1:A:208:LEU:HD21	1:A:222:ARG:HH21	1.81	0.45
1:A:15:ALA:O	1:A:18[B]:VAL:HG22	2.17	0.45
1:A:1007:TRP:CE3	1:A:1106:LEU:CD2	3.00	0.45
1:A:1103:GLN:OE1	1:A:1103:GLN:O	2.34	0.44
1:A:308:LEU:HD23	1:A:308:LEU:N	2.32	0.44
1:A:1013:ASN:OD1	1:A:1032:LYS:HB2	2.18	0.44
1:A:65:THR:HG22	2:A:1214:OLA:C9	2.47	0.43
1:A:86:VAL:HG22	1:A:133:PHE:HA	1.99	0.43
1:A:150:LYS:NZ	1:A:170:ASP:OD1	2.52	0.43
1:A:1014:LEU:N	1:A:1033:MET:HE2	2.34	0.43
1:A:1014:LEU:HA	1:A:1033:MET:HE1	2.01	0.42
1:A:1105:TYR:CD2	1:A:1106:LEU:HD12	2.55	0.42
1:A:29:TRP:HD1	1:A:302:ILE:HG21	1.85	0.42
2:A:1209:OLA:H62	2:A:1209:OLA:H9	1.64	0.42
1:A:80:ILE:HD11	4:A:1207:CLR:H182	2.01	0.42
1:A:108:ILE:O	1:A:109:PRO:C	2.62	0.42
1:A:174[B]:MET:HE1	1:A:253:ASN:CB	2.47	0.42
1:A:238:ILE:HD11	1:A:287:ILE:CG2	2.51	0.41
1:A:1102:ILE:O	1:A:1105:TYR:HB3	2.21	0.41
1:A:1105:TYR:HD2	1:A:1106:LEU:CD1	2.34	0.41
1:A:70:PHE:CE2	1:A:72:ALA:HB2	2.56	0.41
1:A:108:ILE:HD12	1:A:108:ILE:C	2.46	0.41
1:A:188:VAL:HB	1:A:189:PRO:HD3	2.03	0.41
2:A:1224:OLA:H21	2:A:1224:OLA:H51	1.64	0.41
1:A:40:VAL:HG11	1:A:116:VAL:HG13	2.02	0.41

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	390/449 (87%)	382 (98%)	8 (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	291/368 (79%)	287 (99%)	4 (1%)	59	76

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

Mol	Chain	Res	Type
1	A	106	ILE
1	A	117	THR
1	A	1014	LEU
1	A	1099	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	145	ASN
1	A	181	ASN
1	A	1006	ASN

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Mol	Chain	Res	Type
1	A	1041	GLN
1	A	250	HIS
1	A	306	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLA	A	1213	-	15,15,19	0.93	1 (6%)	15,15,19	0.96	1 (6%)
2	OLA	A	1220	-	16,16,19	0.87	1 (6%)	16,16,19	0.95	1 (6%)
2	OLA	A	1218	-	8,8,19	0.70	0	8,8,19	1.25	1 (12%)
3	A1H3H	A	1205	-	29,29,29	0.27	0	40,42,42	0.62	1 (2%)
4	CLR	A	1206	-	31,31,31	0.46	0	48,48,48	0.72	0
4	CLR	A	1207	-	31,31,31	0.49	0	48,48,48	0.70	0
4	CLR	A	1208	-	31,31,31	0.51	0	48,48,48	0.87	1 (2%)
2	OLA	A	1202	-	14,14,19	0.92	1 (7%)	14,14,19	1.06	1 (7%)
2	OLA	A	1211	-	16,16,19	0.90	1 (6%)	16,16,19	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLA	A	1224	-	15,15,19	0.90	1 (6%)	15,15,19	1.04	1 (6%)
2	OLA	A	1210	-	11,11,19	1.08	1 (9%)	11,11,19	1.08	1 (9%)
2	OLA	A	1215	-	15,15,19	0.88	1 (6%)	15,15,19	0.99	0
2	OLA	A	1201	-	15,15,19	0.87	1 (6%)	15,15,19	1.01	1 (6%)
2	OLA	A	1219	-	7,7,19	0.77	0	7,7,19	1.35	1 (14%)
2	OLA	A	1214	-	19,19,19	0.80	1 (5%)	19,19,19	0.92	1 (5%)
2	OLA	A	1212	-	15,15,19	0.96	1 (6%)	15,15,19	0.95	1 (6%)
2	OLA	A	1223	-	8,8,19	0.75	0	8,8,19	1.17	1 (12%)
2	OLA	A	1204	-	10,10,19	0.91	1 (10%)	9,9,19	0.58	0
2	OLA	A	1217	-	10,10,19	0.65	0	10,10,19	1.13	1 (10%)
2	OLA	A	1221	-	9,9,19	0.97	1 (11%)	8,8,19	0.64	0
2	OLA	A	1216	-	14,14,19	0.77	1 (7%)	13,13,19	0.55	0
2	OLA	A	1209	-	15,15,19	0.88	1 (6%)	15,15,19	1.14	2 (13%)
2	OLA	A	1203	-	15,15,19	1.05	1 (6%)	14,14,19	1.11	1 (7%)
2	OLA	A	1222	-	9,9,19	1.01	1 (11%)	8,8,19	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	A	1213	-	-	8/13/13/17	-
2	OLA	A	1220	-	-	9/14/14/17	-
2	OLA	A	1218	-	-	3/6/6/17	-
3	A1H3H	A	1205	-	-	1/11/11/11	0/3/3/3
4	CLR	A	1206	-	-	3/10/68/68	0/4/4/4
4	CLR	A	1207	-	-	0/10/68/68	0/4/4/4
4	CLR	A	1208	-	-	7/10/68/68	0/4/4/4
2	OLA	A	1202	-	-	4/12/12/17	-
2	OLA	A	1211	-	-	10/14/14/17	-
2	OLA	A	1224	-	-	8/13/13/17	-
2	OLA	A	1210	-	-	5/9/9/17	-
2	OLA	A	1215	-	-	7/13/13/17	-
2	OLA	A	1201	-	-	5/13/13/17	-
2	OLA	A	1219	-	-	2/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	A	1214	-	-	10/17/17/17	-
2	OLA	A	1212	-	-	3/13/13/17	-
2	OLA	A	1223	-	-	5/6/6/17	-
2	OLA	A	1204	-	-	3/8/8/17	-
2	OLA	A	1217	-	-	2/8/8/17	-
2	OLA	A	1221	-	-	4/7/7/17	-
2	OLA	A	1216	-	-	6/12/12/17	-
2	OLA	A	1209	-	-	7/13/13/17	-
2	OLA	A	1203	-	-	8/13/13/17	-
2	OLA	A	1222	-	-	4/7/7/17	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1203	OLA	C10-C9	3.77	1.53	1.31
2	A	1212	OLA	C10-C9	2.97	1.48	1.31
2	A	1222	OLA	C10-C9	2.86	1.47	1.29
2	A	1210	OLA	C10-C9	2.86	1.47	1.29
2	A	1211	OLA	C10-C9	2.85	1.47	1.31
2	A	1213	OLA	C10-C9	2.85	1.47	1.31
2	A	1220	OLA	C10-C9	2.80	1.47	1.31
2	A	1224	OLA	C10-C9	2.79	1.47	1.31
2	A	1204	OLA	C10-C9	2.78	1.47	1.31
2	A	1221	OLA	C10-C9	2.78	1.47	1.31
2	A	1202	OLA	C10-C9	2.77	1.47	1.31
2	A	1214	OLA	C10-C9	2.75	1.47	1.31
2	A	1216	OLA	C10-C9	2.73	1.47	1.31
2	A	1215	OLA	C10-C9	2.72	1.47	1.31
2	A	1209	OLA	C10-C9	2.71	1.47	1.31
2	A	1201	OLA	C10-C9	2.69	1.47	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1208	CLR	C14-C8-C9	2.53	112.39	109.09
2	A	1209	OLA	C3-C2-C1	-2.35	108.37	114.51
2	A	1203	OLA	C8-C9-C10	-2.35	107.26	124.83
2	A	1219	OLA	O2-C1-C2	2.32	121.34	114.00
2	A	1202	OLA	C3-C2-C1	-2.31	108.47	114.51
2	A	1220	OLA	O2-C1-C2	2.31	121.31	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1213	OLA	O2-C1-C2	2.28	121.20	114.00
2	A	1214	OLA	O2-C1-C2	2.16	120.82	114.00
2	A	1209	OLA	O2-C1-C2	2.13	120.72	114.00
2	A	1223	OLA	O2-C1-C2	2.11	120.68	114.00
2	A	1211	OLA	O2-C1-C2	2.11	120.67	114.00
2	A	1224	OLA	O2-C1-C2	2.11	120.65	114.00
2	A	1217	OLA	O2-C1-C2	2.09	120.61	114.00
2	A	1210	OLA	O2-C1-C2	2.07	120.55	114.00
3	A	1205	A1H3H	O2-C13-C14	-2.05	115.31	120.13
2	A	1218	OLA	O2-C1-C2	2.05	120.46	114.00
2	A	1201	OLA	O2-C1-C2	2.02	120.38	114.00
2	A	1212	OLA	O2-C1-C2	2.01	120.36	114.00

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1209	OLA	C6-C7-C8-C9
3	A	1205	A1H3H	C4-C3-N1-C5
2	A	1209	OLA	C11-C10-C9-C8
2	A	1220	OLA	C11-C10-C9-C8
2	A	1216	OLA	C11-C10-C9-C8
2	A	1201	OLA	C4-C5-C6-C7
2	A	1202	OLA	C4-C5-C6-C7
2	A	1224	OLA	C5-C6-C7-C8
2	A	1215	OLA	C3-C4-C5-C6
2	A	1202	OLA	C1-C2-C3-C4
2	A	1209	OLA	C1-C2-C3-C4
2	A	1213	OLA	C11-C10-C9-C8
2	A	1209	OLA	C2-C3-C4-C5
2	A	1201	OLA	C1-C2-C3-C4
2	A	1213	OLA	C1-C2-C3-C4
2	A	1224	OLA	C2-C3-C4-C5
2	A	1220	OLA	C1-C2-C3-C4
2	A	1223	OLA	C1-C2-C3-C4
4	A	1208	CLR	C20-C22-C23-C24
2	A	1221	OLA	C11-C10-C9-C8
2	A	1222	OLA	C5-C6-C7-C8
4	A	1208	CLR	C23-C24-C25-C26
2	A	1211	OLA	C11-C12-C13-C14
2	A	1213	OLA	C3-C4-C5-C6
2	A	1213	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	1204	OLA	C11-C10-C9-C8
2	A	1220	OLA	C11-C12-C13-C14
2	A	1214	OLA	C1-C2-C3-C4
2	A	1215	OLA	C11-C12-C13-C14
2	A	1203	OLA	C6-C7-C8-C9
2	A	1224	OLA	C3-C4-C5-C6
2	A	1215	OLA	C5-C6-C7-C8
2	A	1210	OLA	C1-C2-C3-C4
2	A	1210	OLA	C3-C4-C5-C6
2	A	1209	OLA	C10-C11-C12-C13
2	A	1215	OLA	C4-C5-C6-C7
2	A	1223	OLA	C3-C4-C5-C6
2	A	1222	OLA	C1-C2-C3-C4
2	A	1220	OLA	C10-C11-C12-C13
2	A	1213	OLA	C5-C6-C7-C8
2	A	1203	OLA	C3-C4-C5-C6
2	A	1209	OLA	C4-C5-C6-C7
2	A	1216	OLA	C12-C13-C14-C15
2	A	1211	OLA	C3-C4-C5-C6
2	A	1201	OLA	C10-C11-C12-C13
2	A	1211	OLA	C11-C10-C9-C8
2	A	1214	OLA	C11-C10-C9-C8
2	A	1224	OLA	C11-C10-C9-C8
2	A	1203	OLA	C1-C2-C3-C4
2	A	1216	OLA	C4-C5-C6-C7
2	A	1222	OLA	C3-C4-C5-C6
2	A	1214	OLA	C10-C11-C12-C13
2	A	1209	OLA	C11-C12-C13-C14
2	A	1213	OLA	C11-C12-C13-C14
2	A	1211	OLA	C12-C13-C14-C15
2	A	1212	OLA	C5-C6-C7-C8
2	A	1204	OLA	C4-C5-C6-C7
2	A	1224	OLA	C11-C12-C13-C14
2	A	1216	OLA	C13-C14-C15-C16
2	A	1221	OLA	C11-C12-C13-C14
2	A	1211	OLA	C4-C5-C6-C7
2	A	1214	OLA	C13-C14-C15-C16
4	A	1208	CLR	C23-C24-C25-C27
2	A	1212	OLA	C4-C5-C6-C7
2	A	1203	OLA	C9-C10-C11-C12
2	A	1214	OLA	C11-C12-C13-C14
2	A	1203	OLA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	1221	OLA	C13-C14-C15-C16
2	A	1217	OLA	C3-C4-C5-C6
2	A	1214	OLA	C3-C4-C5-C6
4	A	1206	CLR	C22-C23-C24-C25
2	A	1223	OLA	C2-C3-C4-C5
2	A	1218	OLA	C3-C4-C5-C6
2	A	1211	OLA	C1-C2-C3-C4
2	A	1221	OLA	C12-C13-C14-C15
4	A	1206	CLR	C23-C24-C25-C27
2	A	1203	OLA	C13-C14-C15-C16
2	A	1215	OLA	C2-C3-C4-C5
2	A	1215	OLA	C11-C10-C9-C8
2	A	1203	OLA	C5-C6-C7-C8
4	A	1208	CLR	C13-C17-C20-C21
2	A	1224	OLA	C4-C5-C6-C7
2	A	1203	OLA	C4-C5-C6-C7
2	A	1214	OLA	C2-C3-C4-C5
2	A	1216	OLA	C14-C15-C16-C17
2	A	1217	OLA	C5-C6-C7-C8
4	A	1208	CLR	C16-C17-C20-C22
4	A	1208	CLR	C13-C17-C20-C22
2	A	1216	OLA	C15-C16-C17-C18
2	A	1211	OLA	C9-C10-C11-C12
2	A	1213	OLA	C6-C7-C8-C9
2	A	1213	OLA	C2-C3-C4-C5
4	A	1208	CLR	C16-C17-C20-C21
2	A	1211	OLA	C7-C8-C9-C10
2	A	1219	OLA	O1-C1-C2-C3
2	A	1202	OLA	C2-C3-C4-C5
2	A	1210	OLA	C4-C5-C6-C7
2	A	1223	OLA	O1-C1-C2-C3
2	A	1218	OLA	O2-C1-C2-C3
2	A	1210	OLA	C2-C3-C4-C5
2	A	1210	OLA	C7-C8-C9-C10
2	A	1218	OLA	O1-C1-C2-C3
2	A	1223	OLA	O2-C1-C2-C3
2	A	1220	OLA	O2-C1-C2-C3
2	A	1219	OLA	O2-C1-C2-C3
2	A	1204	OLA	C7-C8-C9-C10
2	A	1215	OLA	C9-C10-C11-C12
2	A	1214	OLA	C12-C13-C14-C15
2	A	1220	OLA	C7-C8-C9-C10

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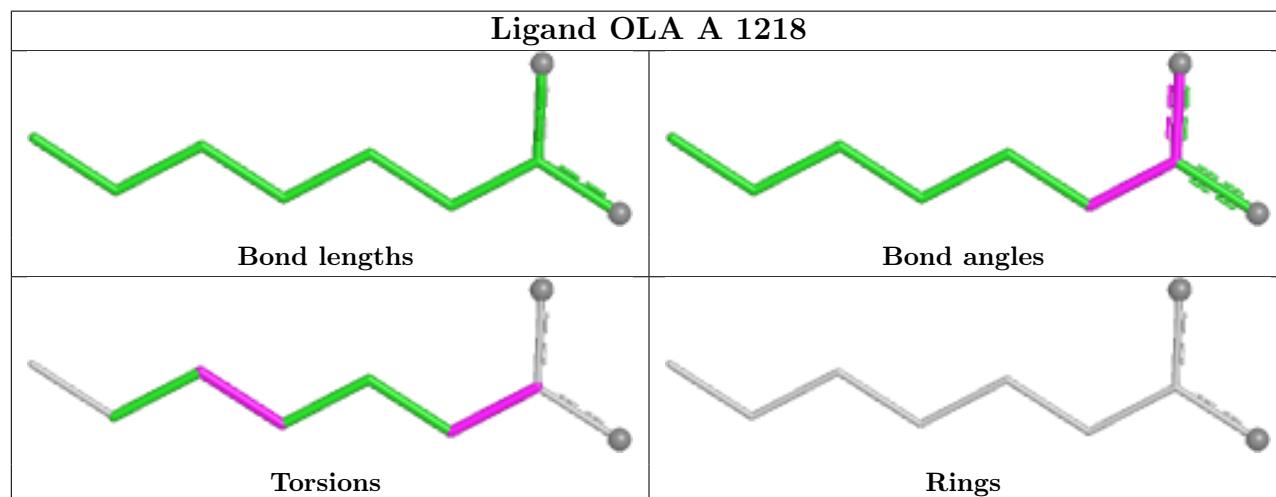
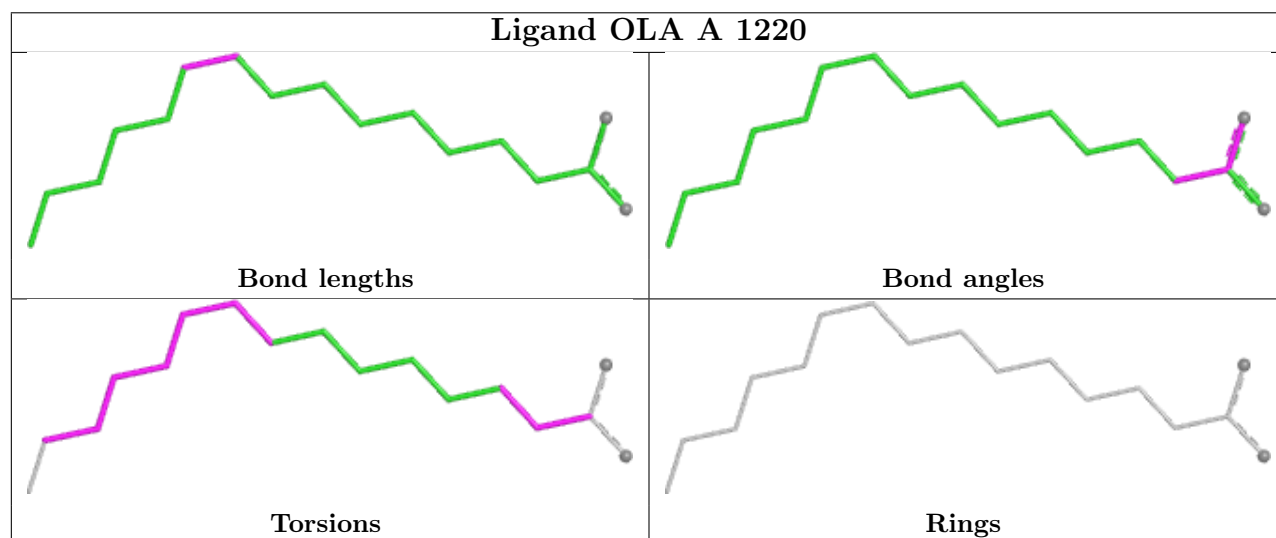
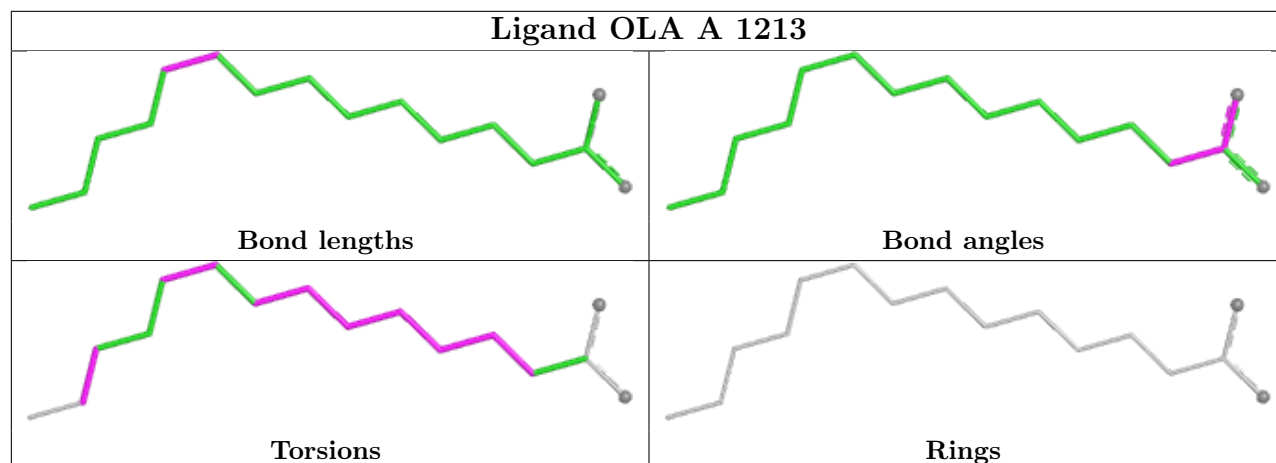
Mol	Chain	Res	Type	Atoms
2	A	1220	OLA	C9-C10-C11-C12
2	A	1220	OLA	O1-C1-C2-C3
2	A	1214	OLA	C5-C6-C7-C8
2	A	1201	OLA	C7-C8-C9-C10
2	A	1212	OLA	C9-C10-C11-C12
4	A	1206	CLR	C23-C24-C25-C26
2	A	1201	OLA	C2-C3-C4-C5
2	A	1224	OLA	C9-C10-C11-C12
2	A	1220	OLA	C12-C13-C14-C15
2	A	1202	OLA	C9-C10-C11-C12
2	A	1211	OLA	C2-C3-C4-C5
2	A	1214	OLA	C6-C7-C8-C9
2	A	1211	OLA	C5-C6-C7-C8
2	A	1224	OLA	C10-C11-C12-C13
2	A	1222	OLA	C7-C8-C9-C10

There are no ring outliers.

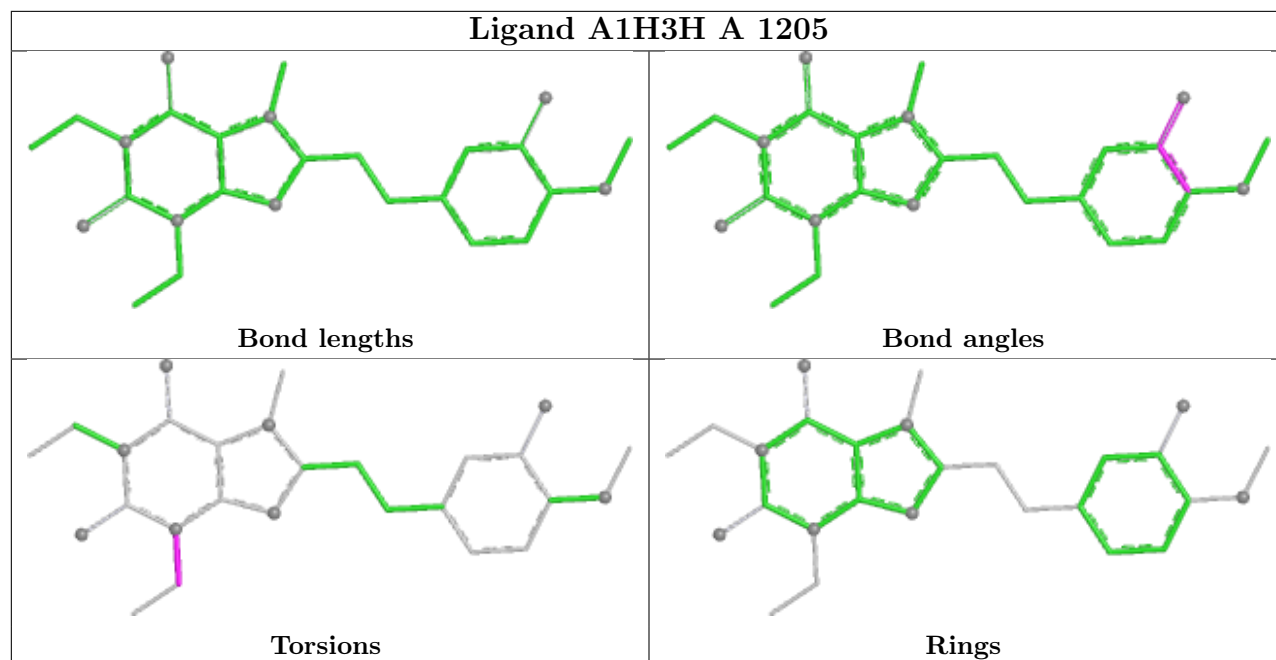
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1207	CLR	1	0
2	A	1224	OLA	2	0
2	A	1201	OLA	2	0
2	A	1214	OLA	3	0
2	A	1204	OLA	1	0
2	A	1216	OLA	1	0
2	A	1209	OLA	1	0

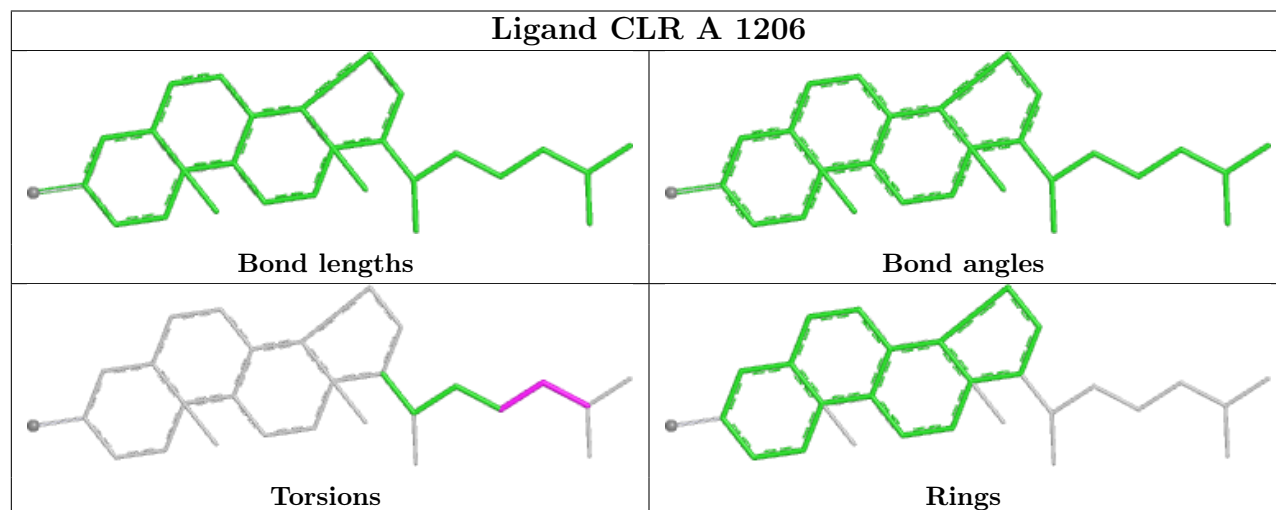
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



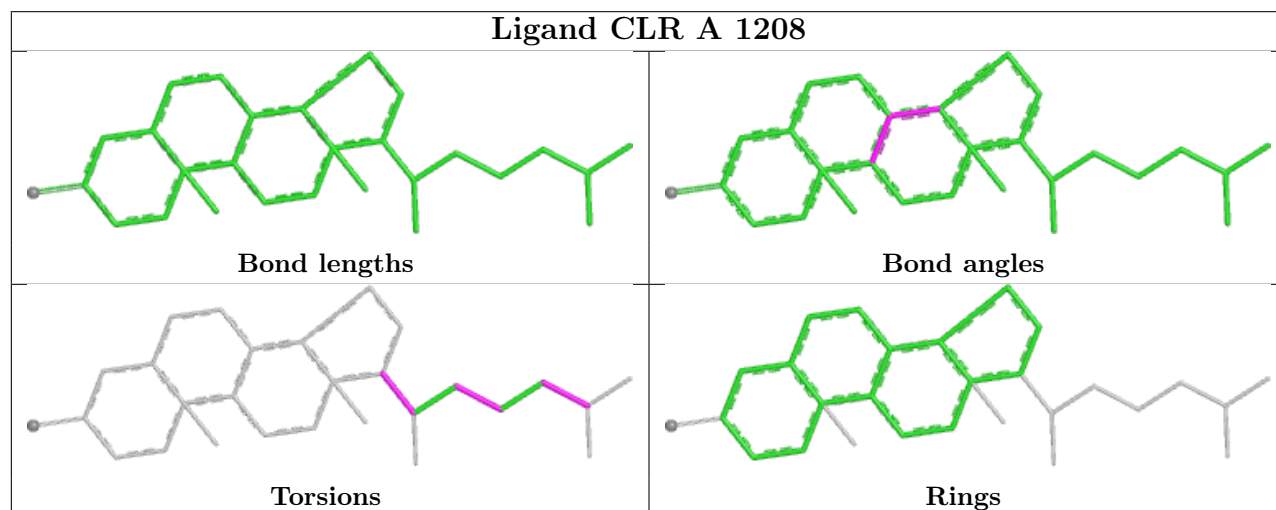
Ligand A1H3H A 1205

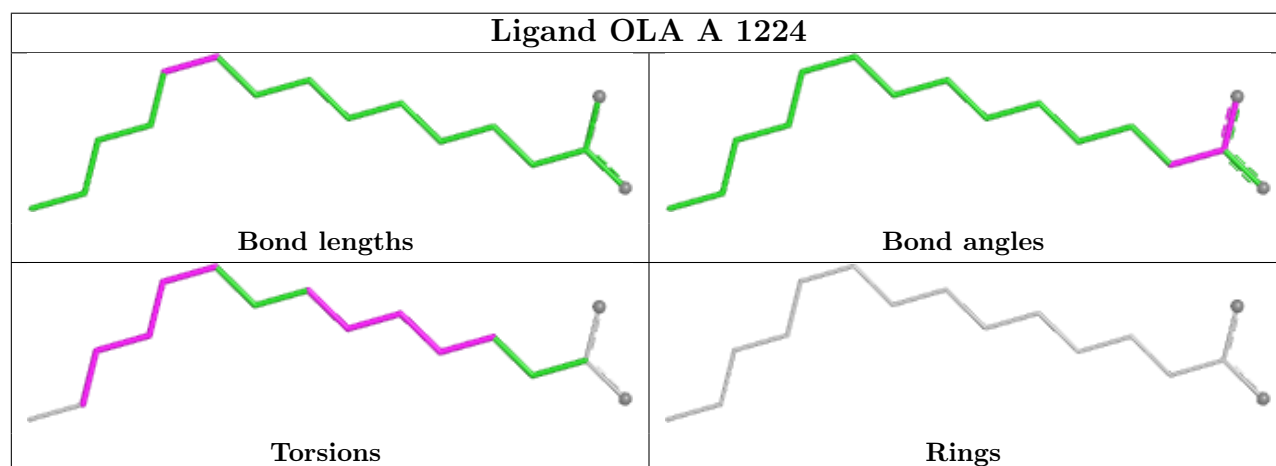
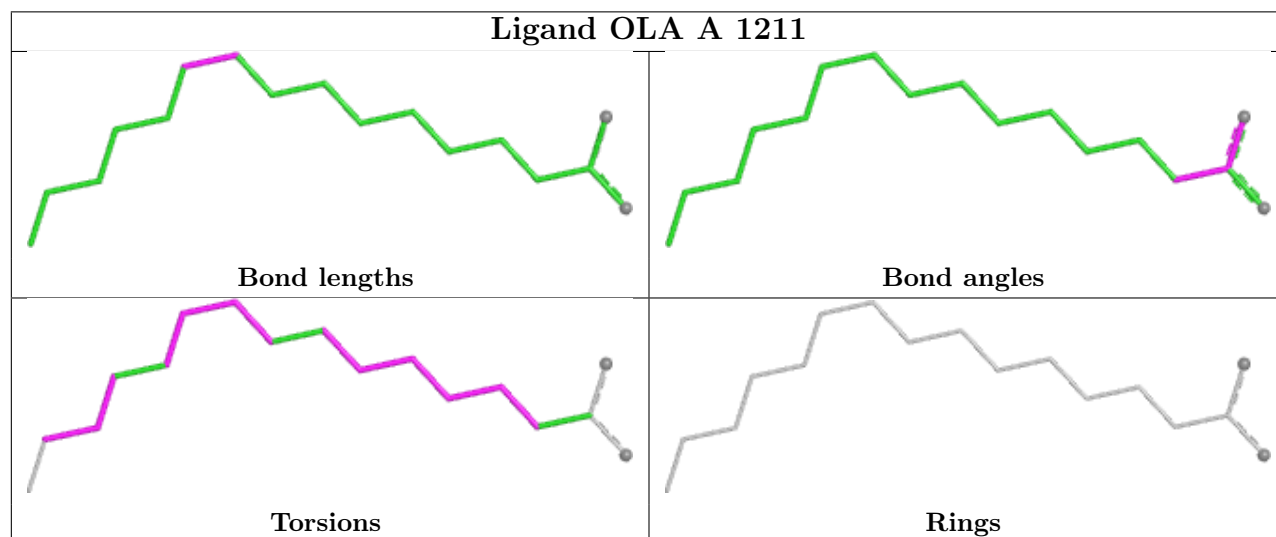
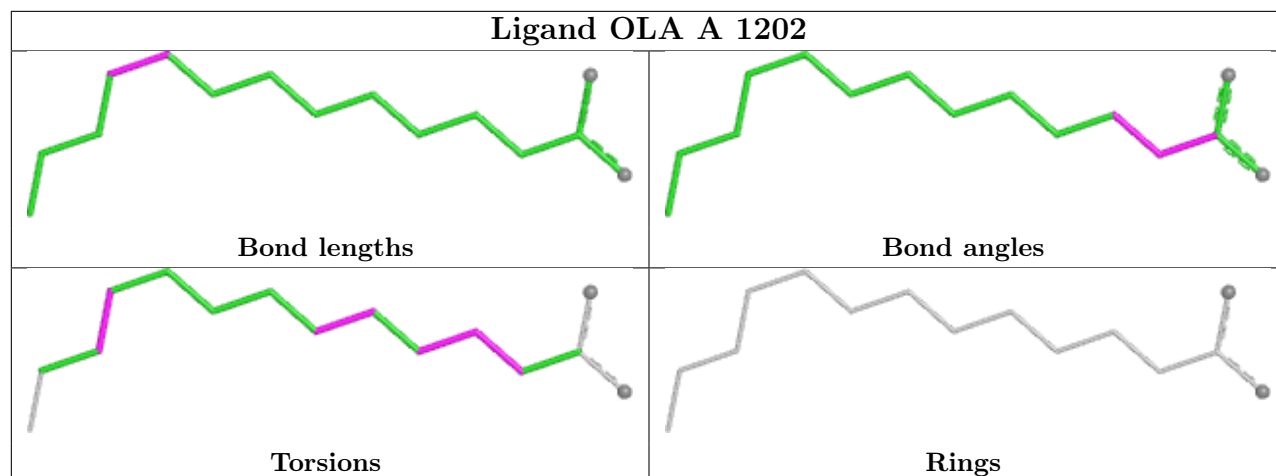


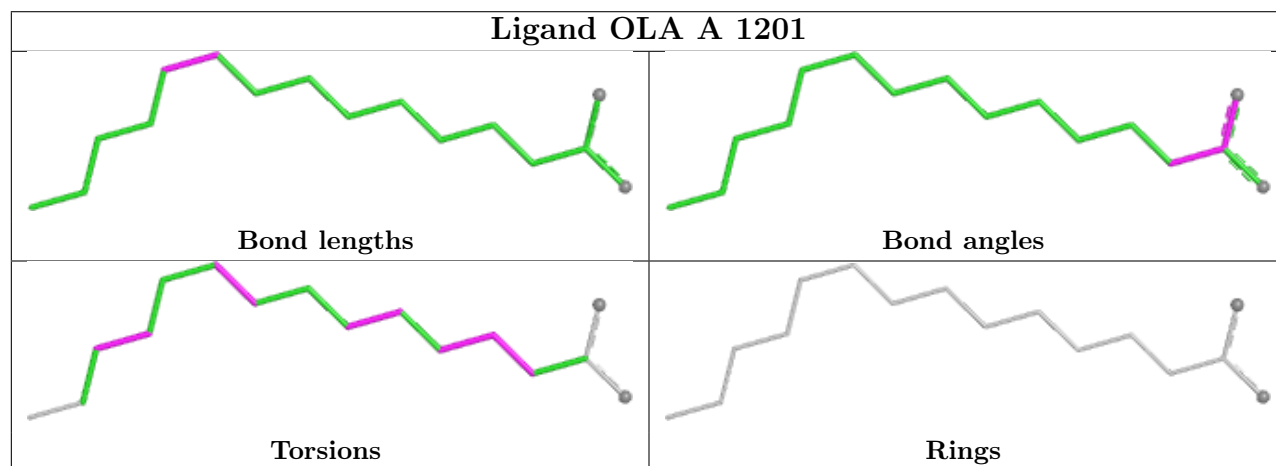
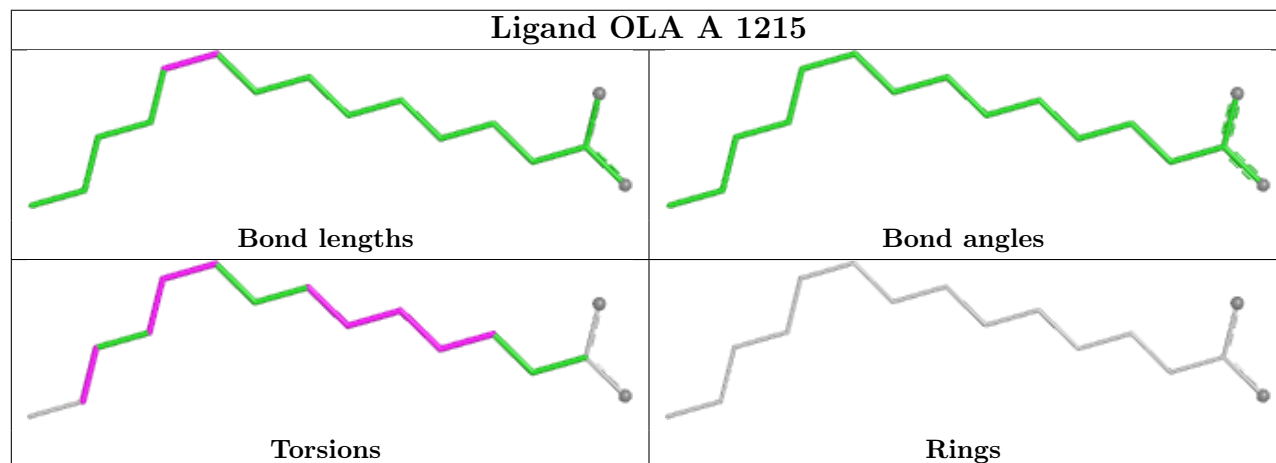
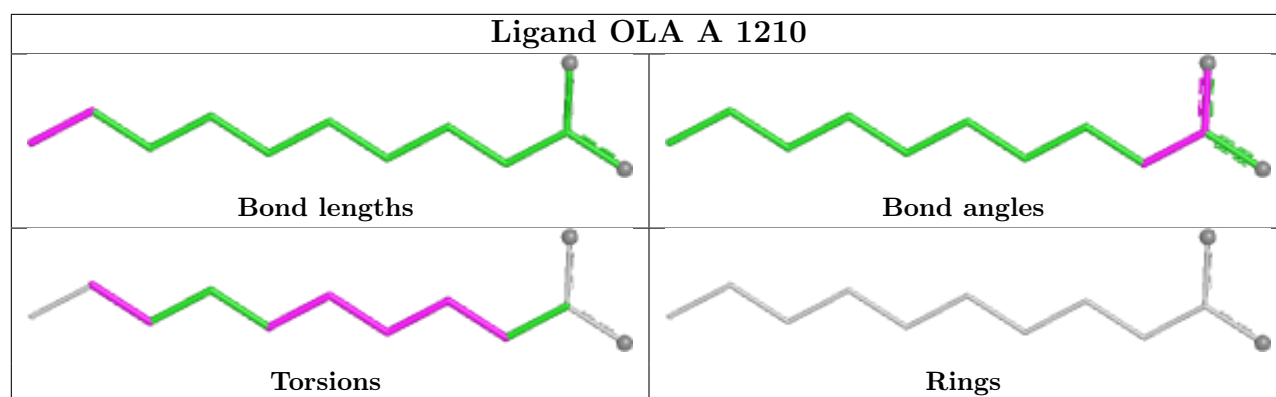
Ligand CLR A 1206

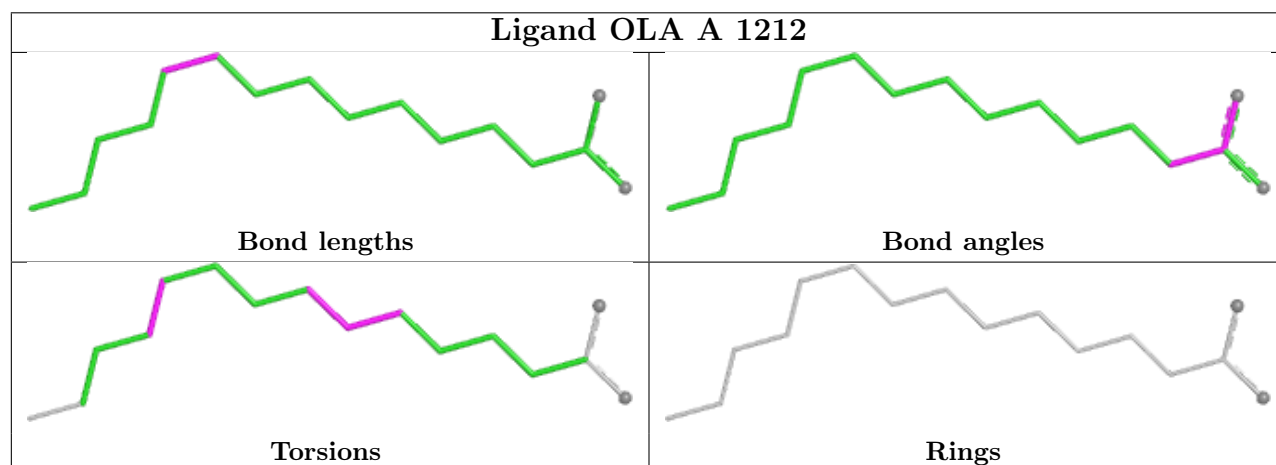
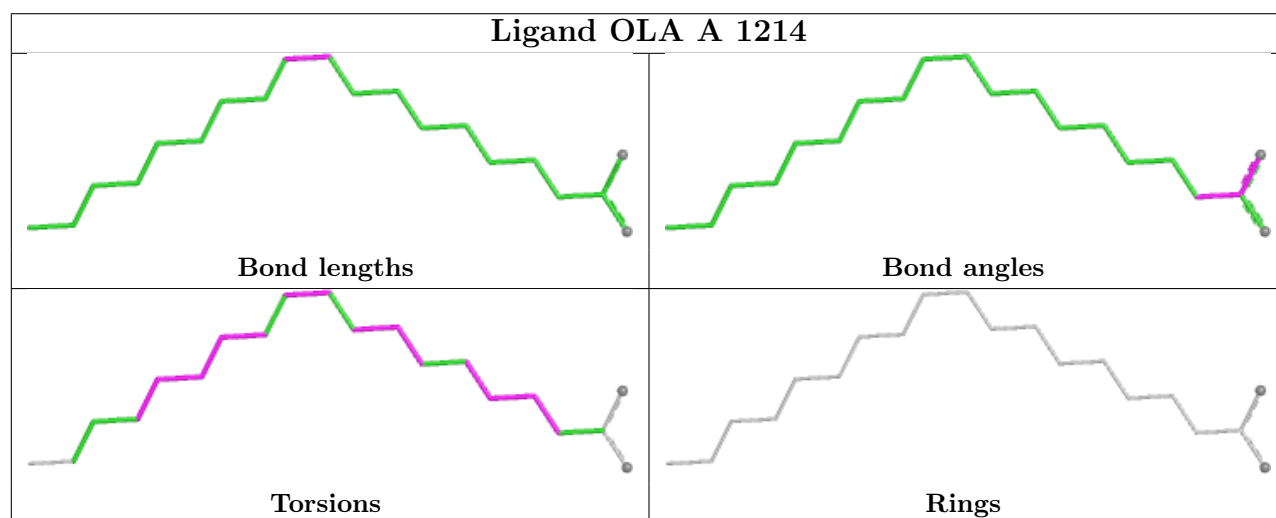
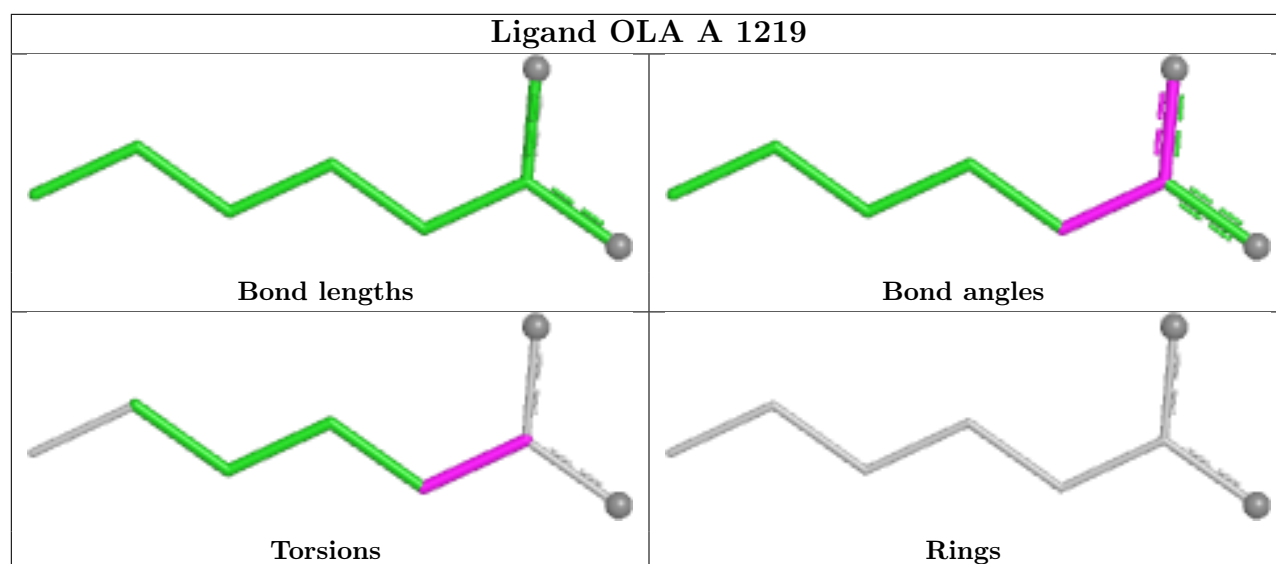


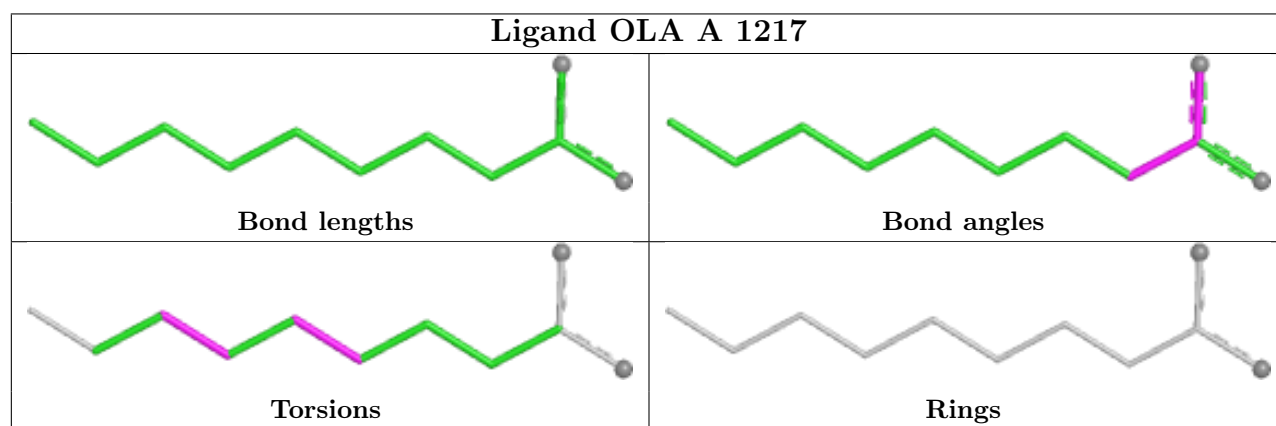
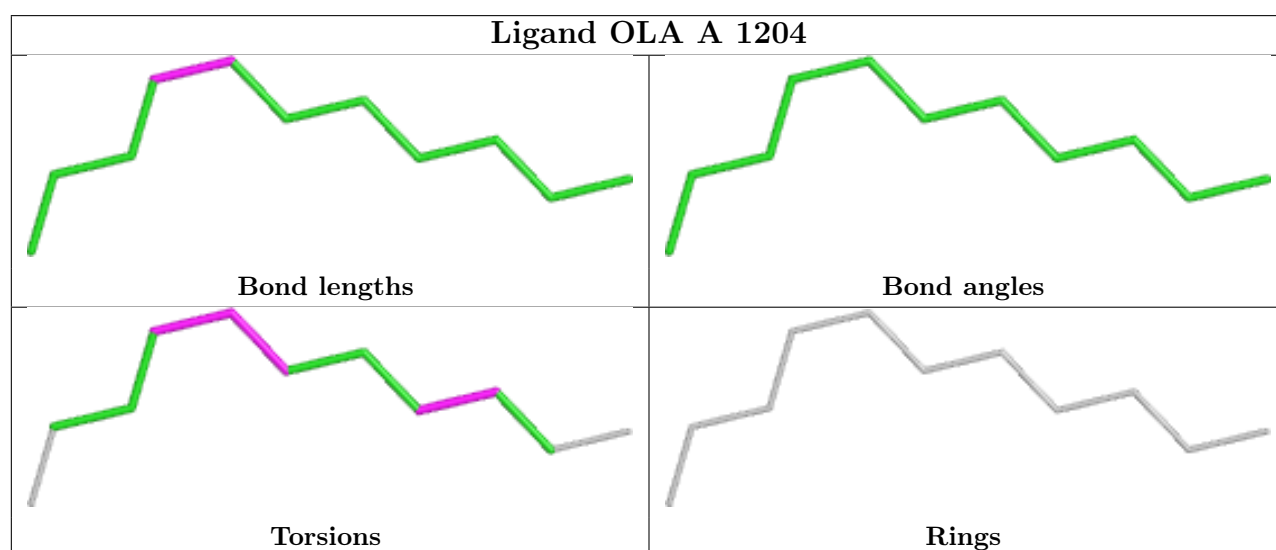
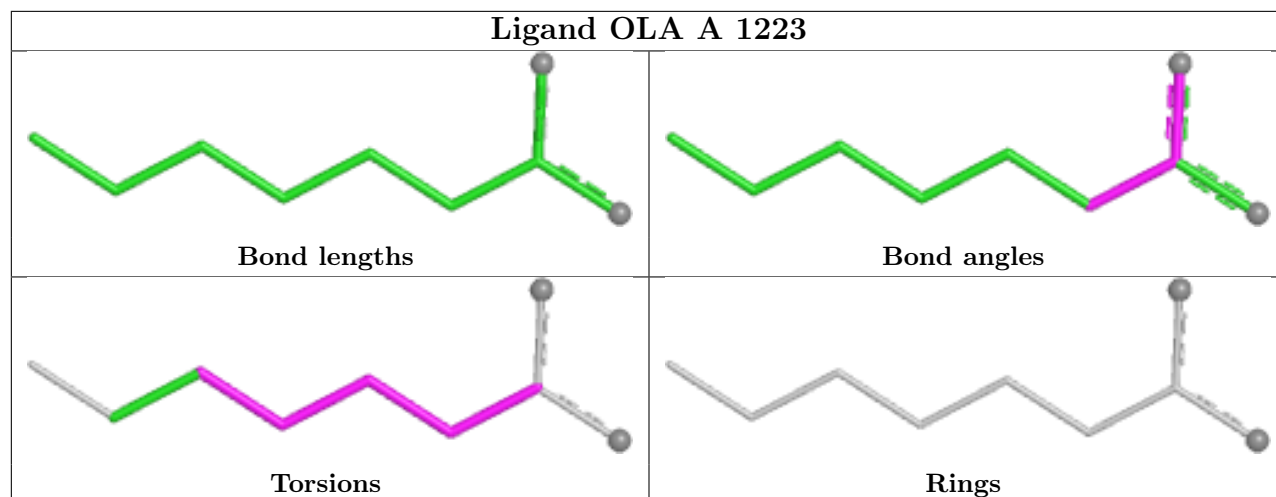
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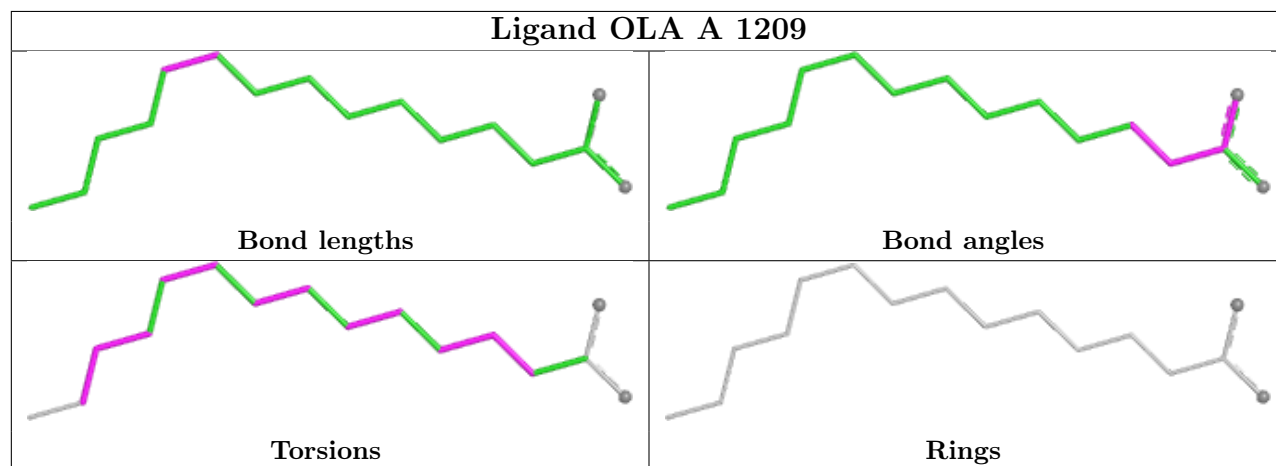
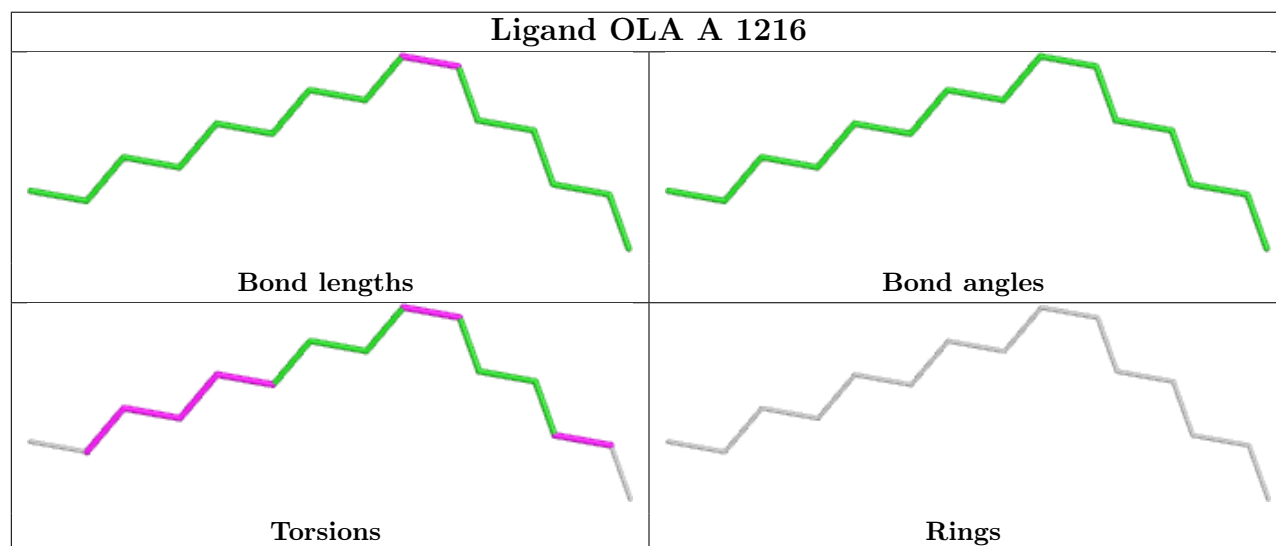
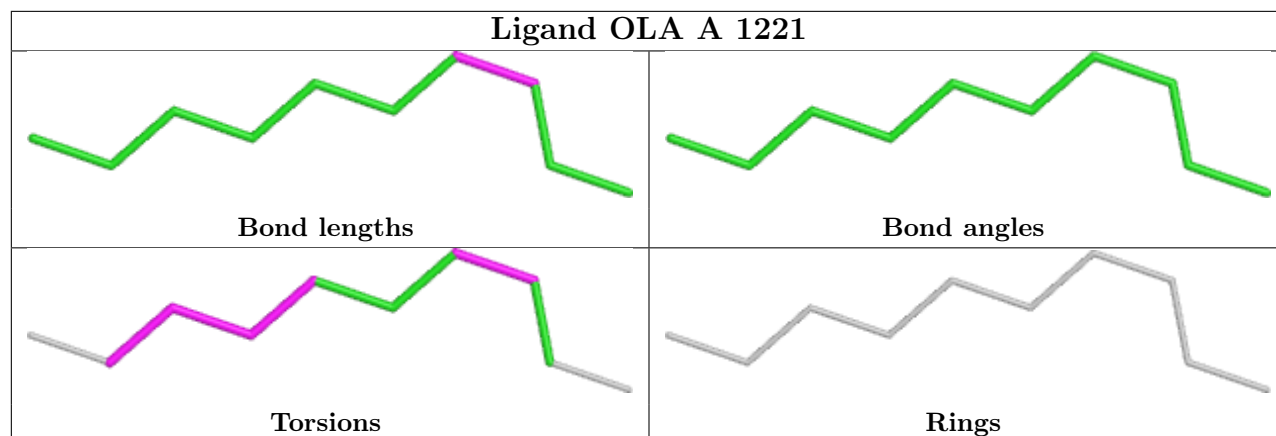


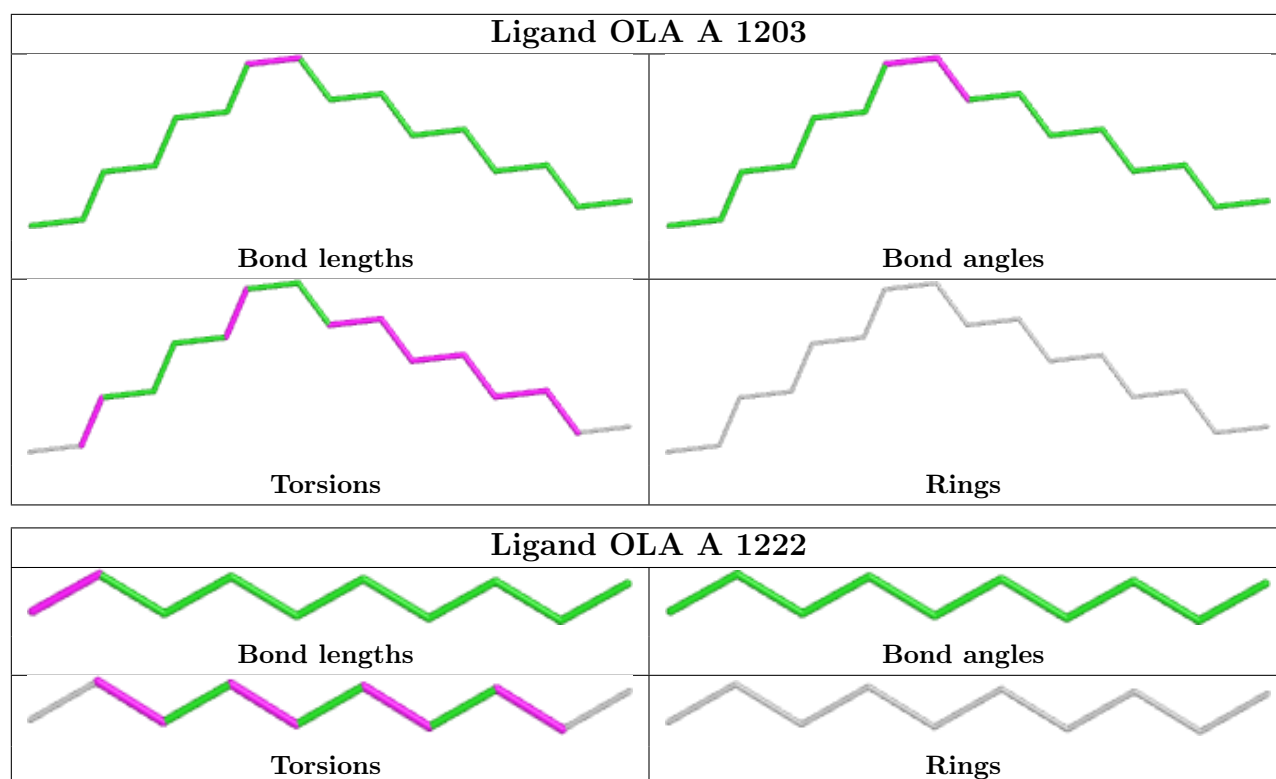












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	388/449 (86%)	-0.09	13 (3%)	48 40	36, 86, 150, 182	3 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	4.1
1	A	309	ARG	3.4
1	A	0	ALA	2.5
1	A	1100	ALA	2.3
1	A	304	ARG	2.2
1	A	1106	LEU	2.2
1	A	161	GLU	2.2
1	A	1034	ARG	2.1
1	A	1079	ALA	2.1
1	A	1026	VAL	2.1
1	A	1042	LYS	2.1
1	A	1101	TYR	2.0
1	A	1105	TYR	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 ⓘ

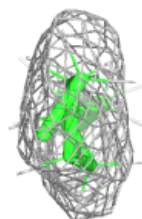
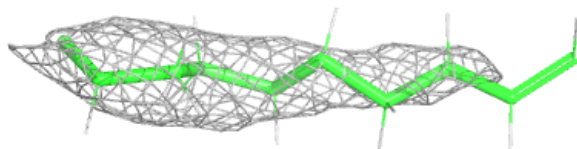
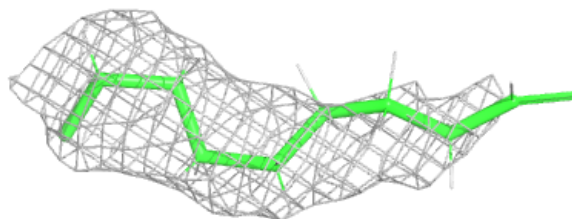
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLA	A	1222	10/20	0.76	0.22	106,128,139,140	0
2	OLA	A	1219	8/20	0.79	0.15	85,107,121,121	0
2	OLA	A	1204	11/20	0.83	0.22	86,102,117,121	0
2	OLA	A	1217	11/20	0.85	0.18	95,121,132,137	0
2	OLA	A	1215	16/20	0.86	0.16	90,96,129,139	0
2	OLA	A	1212	16/20	0.87	0.15	75,98,138,154	0
2	OLA	A	1213	16/20	0.88	0.13	78,112,121,124	0
2	OLA	A	1220	17/20	0.89	0.15	86,118,165,169	0
2	OLA	A	1203	16/20	0.89	0.24	82,97,117,117	0
2	OLA	A	1221	10/20	0.90	0.21	85,135,167,167	0
2	OLA	A	1210	12/20	0.90	0.16	103,131,146,152	0
2	OLA	A	1214	20/20	0.91	0.15	82,121,141,152	0
2	OLA	A	1201	16/20	0.92	0.16	73,90,120,124	0
2	OLA	A	1209	16/20	0.92	0.17	81,96,121,126	0
2	OLA	A	1211	17/20	0.93	0.13	78,105,125,128	0
2	OLA	A	1216	15/20	0.93	0.13	82,117,142,155	0
2	OLA	A	1202	15/20	0.93	0.13	68,85,107,116	0
2	OLA	A	1218	9/20	0.93	0.14	87,109,123,148	0
4	CLR	A	1208	28/28	0.93	0.11	79,101,126,128	0
2	OLA	A	1224	16/20	0.94	0.17	74,96,130,136	0
4	CLR	A	1207	28/28	0.94	0.10	69,101,128,139	0
2	OLA	A	1223	9/20	0.94	0.11	64,107,116,131	0
4	CLR	A	1206	28/28	0.96	0.08	69,94,116,119	0
3	A1H3H	A	1205	27/27	0.97	0.08	47,61,100,106	0
5	NA	A	1225	1/1	0.98	0.13	77,77,77,77	0

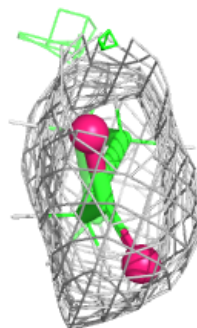
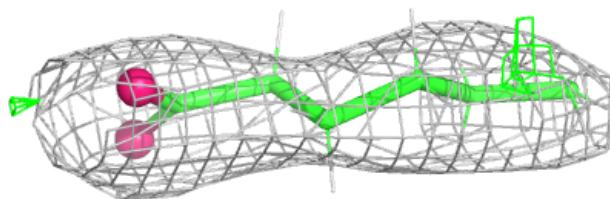
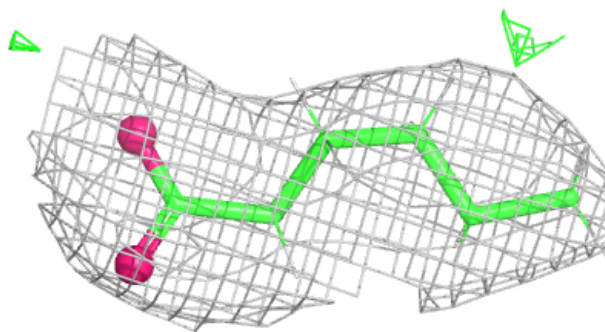
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1222:

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

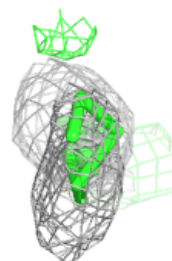
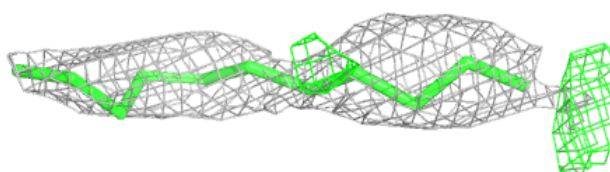
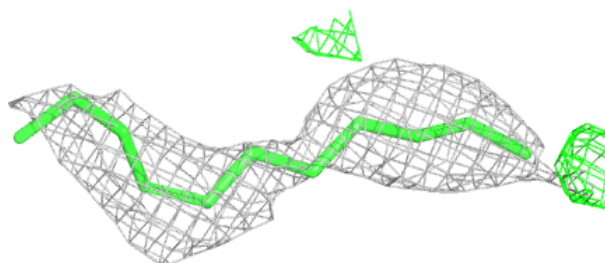
**Electron density around OLA A 1219:**

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

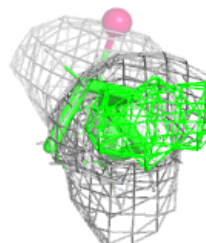
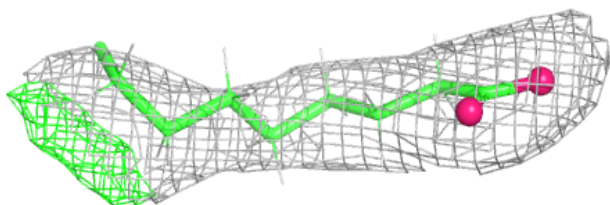
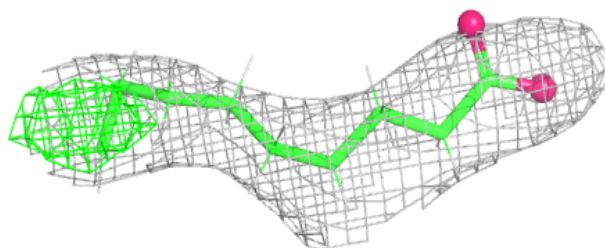


Electron density around OLA A 1204:

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

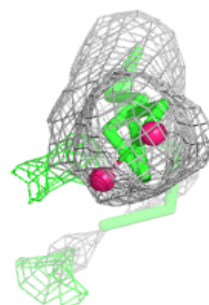
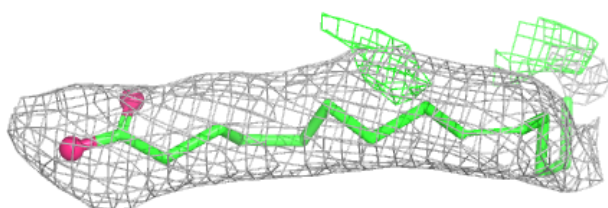
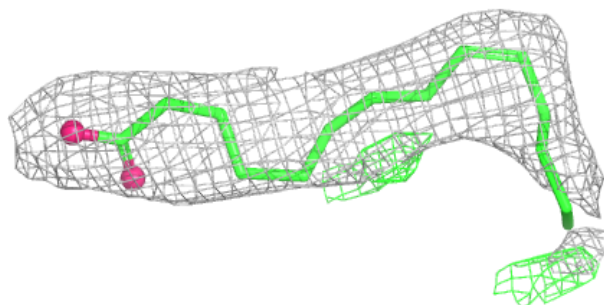
**Electron density around OLA A 1217:**

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

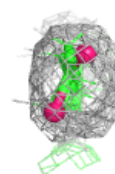
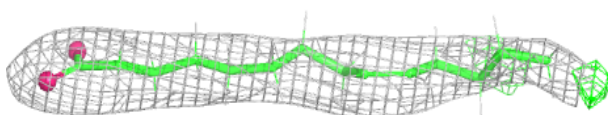
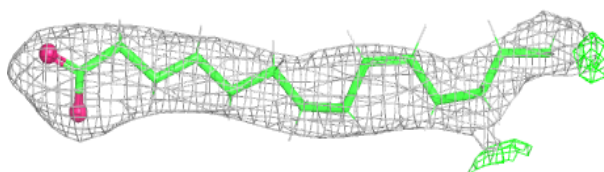


Electron density around OLA A 1215:

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

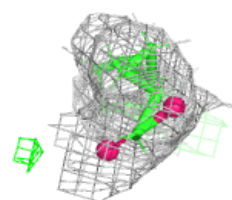
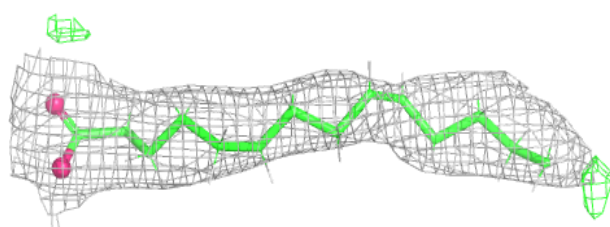
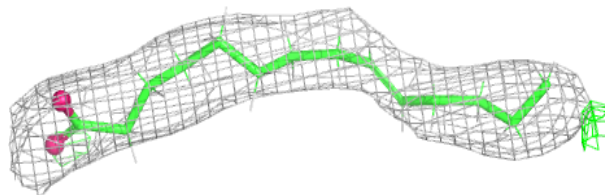
**Electron density around OLA A 1212:**

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

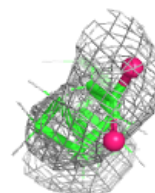
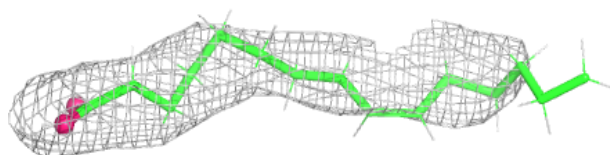
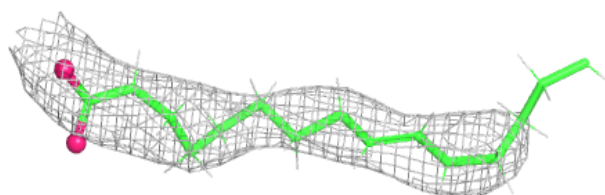


Electron density around OLA A 1213:

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

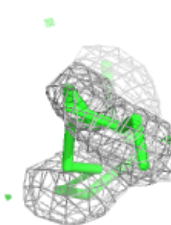
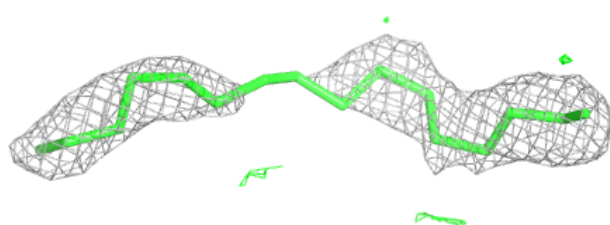
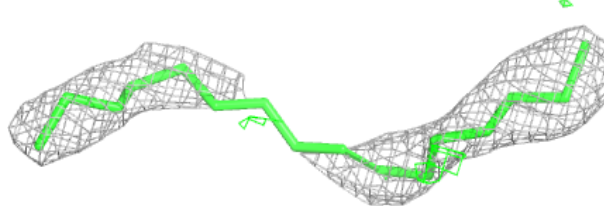
**Electron density around OLA A 1220:**

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

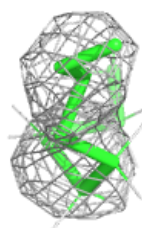
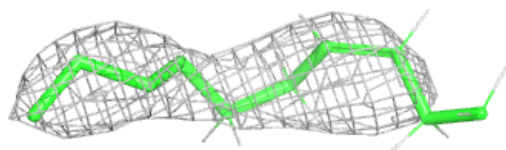
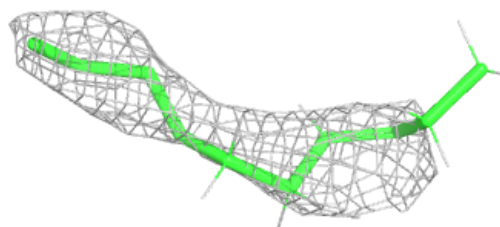


Electron density around OLA A 1203:

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

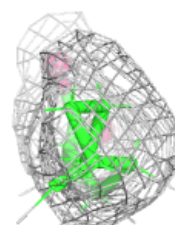
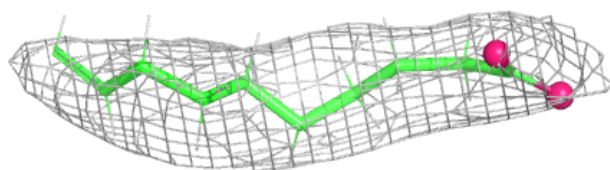
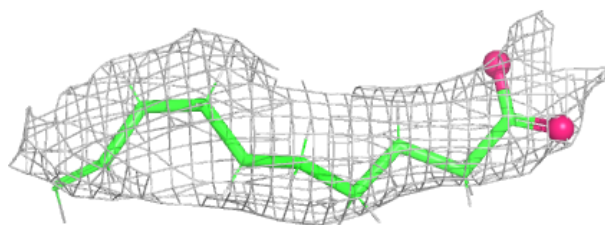
**Electron density around OLA A 1221:**

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

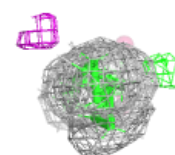
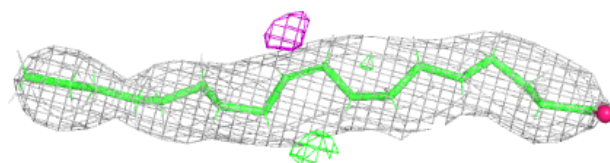
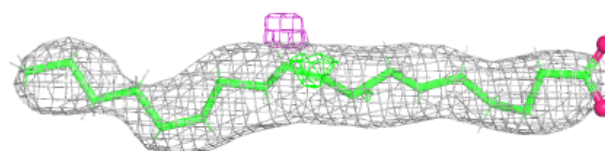


Electron density around OLA A 1210:

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

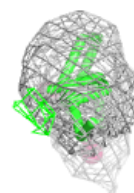
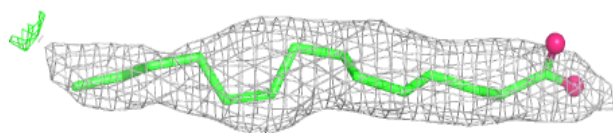
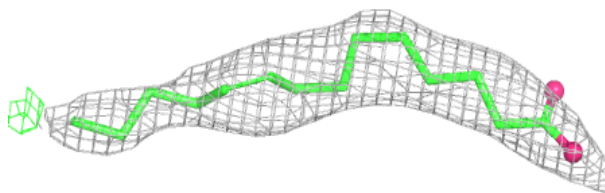
**Electron density around OLA A 1214:**

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and green (positive)

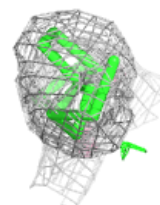
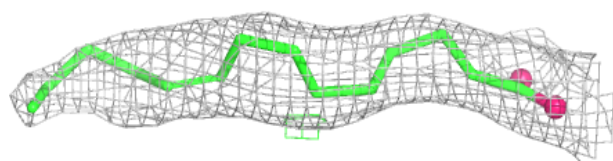
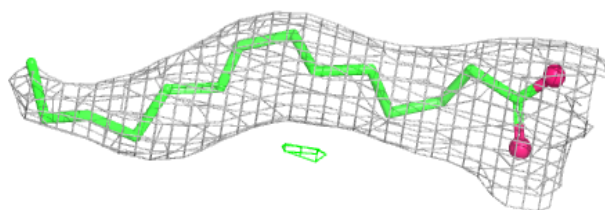


Electron density around OLA A 1201:

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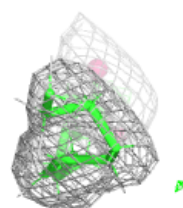
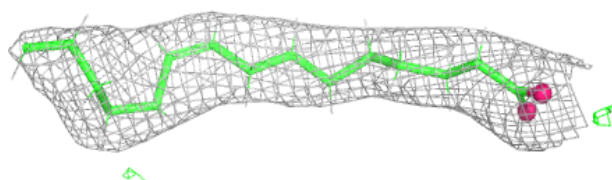
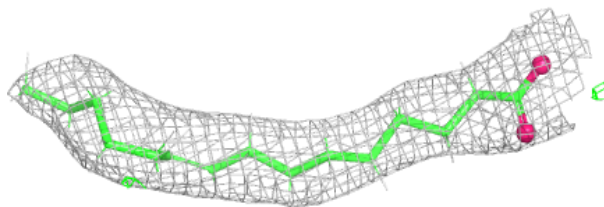
**Electron density around OLA A 1209:**

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and green (positive)

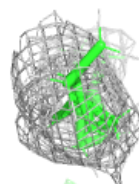
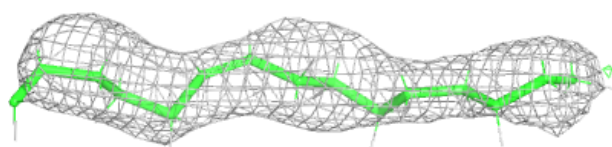
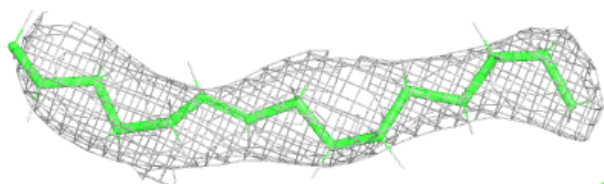


Electron density around OLA A 1211:

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and green (positive)

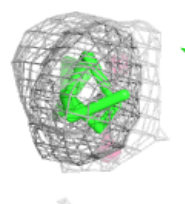
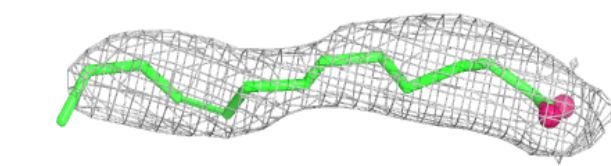
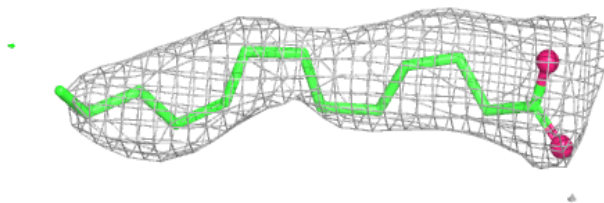
**Electron density around OLA A 1216:**

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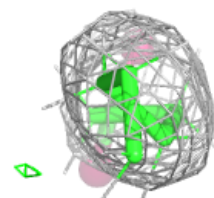
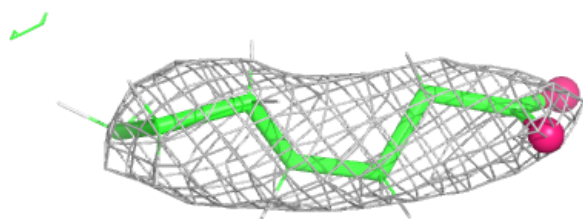
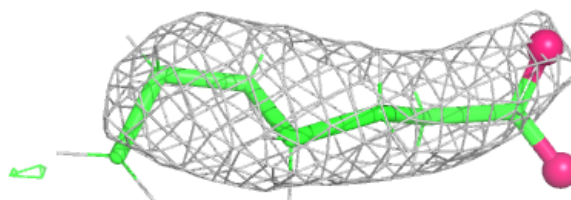


Electron density around OLA A 1202:

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and green (positive)

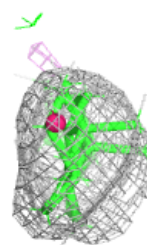
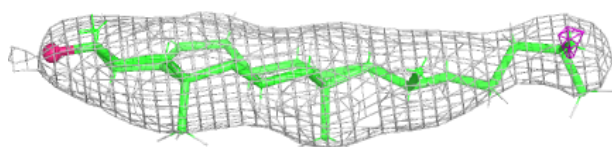
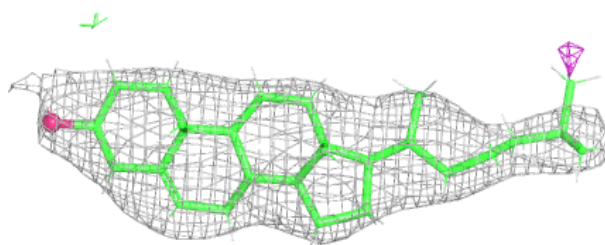
**Electron density around OLA A 1218:**

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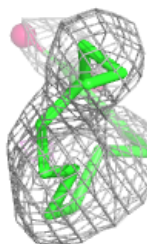
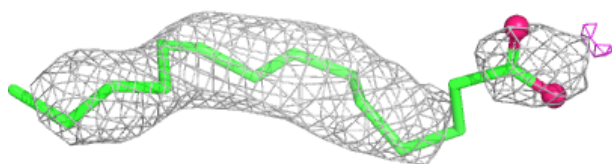
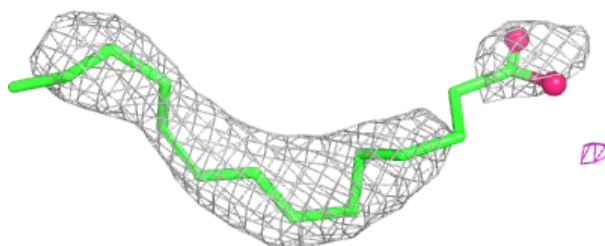


Electron density around CLR A 1208:

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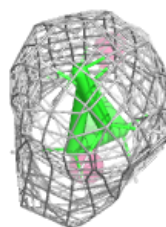
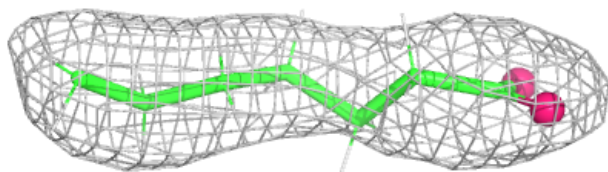
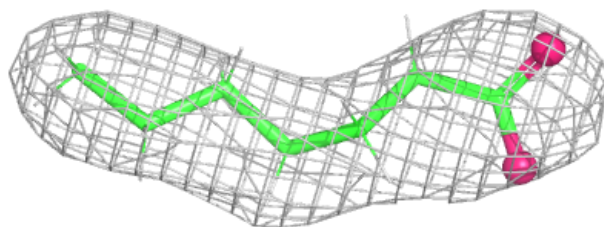
**Electron density around OLA A 1224:**

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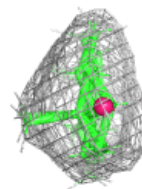
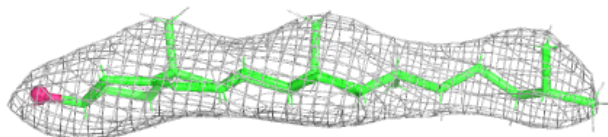
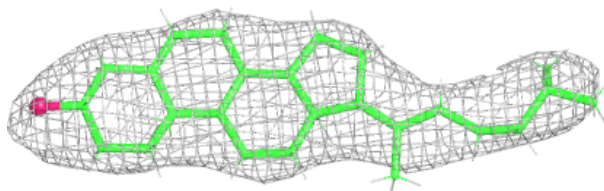


Electron density around OLA A 1223:

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

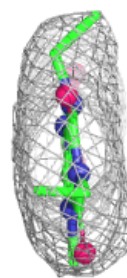
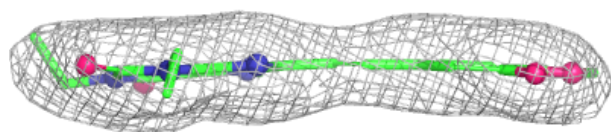
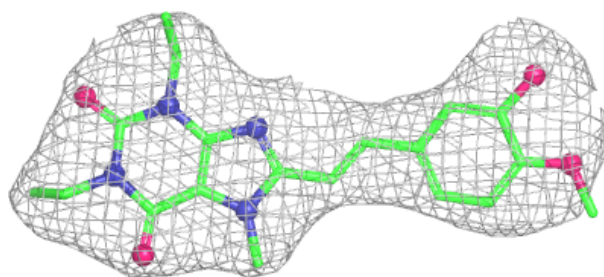
**Electron density around CLR A 1206:**

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



Electron density around A1H3H 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.