Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:16 AM EDT

PDB ID	:	6PS3
Title	:	XFEL beta2 AR structure by ligand exchange from Timolol to Carvedilol.
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Deposited on	:	2019-07-12
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

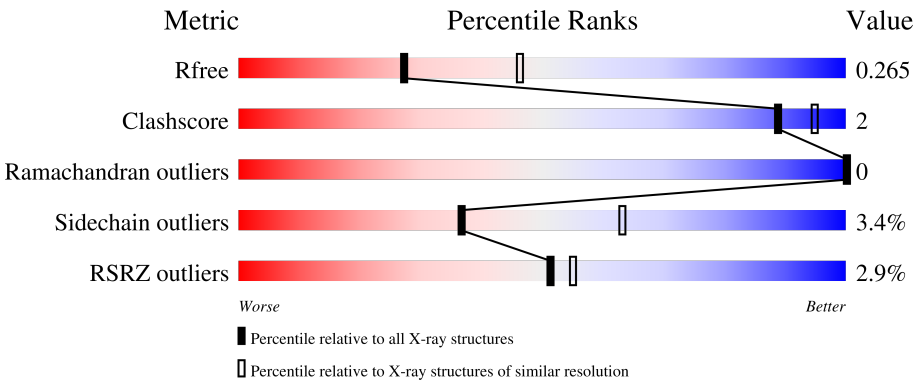
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	506	3% 81% 5% • 13%

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
5	OLC	A	1209	-	-	-	X
6	OLA	A	1216	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3713 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 Fusion protein of Beta-2 adrenergic receptor and T4 Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3497	2296	571	604	26	0	7	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP P07550
A	-22	LYS	-	expression tag	UNP P07550
A	-21	THR	-	expression tag	UNP P07550
A	-20	ILE	-	expression tag	UNP P07550
A	-19	ILE	-	expression tag	UNP P07550
A	-18	ALA	-	expression tag	UNP P07550
A	-17	LEU	-	expression tag	UNP P07550
A	-16	SER	-	expression tag	UNP P07550
A	-15	TYR	-	expression tag	UNP P07550
A	-14	ILE	-	expression tag	UNP P07550
A	-13	PHE	-	expression tag	UNP P07550
A	-12	CYS	-	expression tag	UNP P07550
A	-11	LEU	-	expression tag	UNP P07550
A	-10	VAL	-	expression tag	UNP P07550
A	-9	PHE	-	expression tag	UNP P07550
A	-8	ALA	-	expression tag	UNP P07550
A	-7	ASP	-	expression tag	UNP P07550
A	-6	TYR	-	expression tag	UNP P07550
A	-5	LYS	-	expression tag	UNP P07550
A	-4	ASP	-	expression tag	UNP P07550
A	-3	ASP	-	expression tag	UNP P07550
A	-2	ASP	-	expression tag	UNP P07550
A	-1	ASP	-	expression tag	UNP P07550
A	0	ALA	-	expression tag	UNP P07550
A	16	ARG	GLY	variant	UNP P07550
A	27	GLN	GLU	variant	UNP P07550
A	122	TRP	GLU	engineered mutation	UNP P07550

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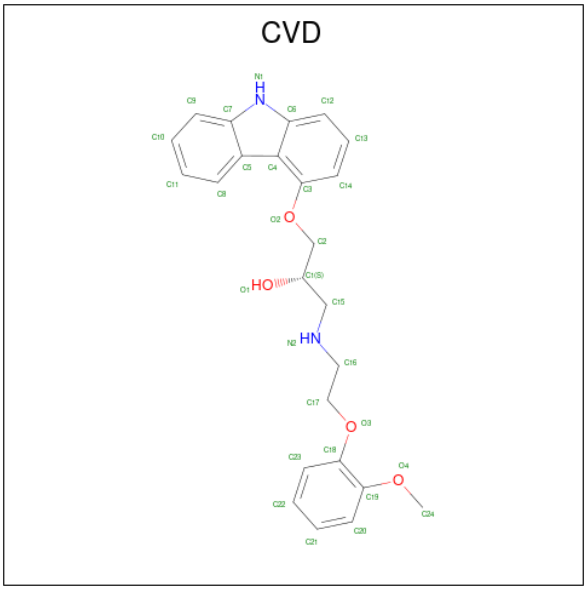
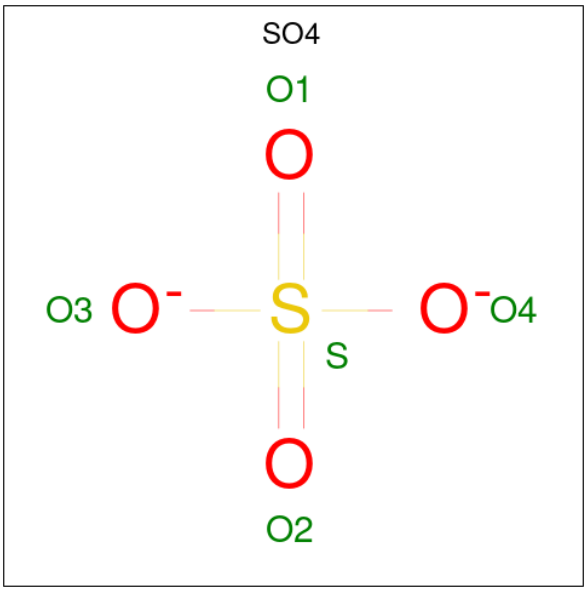
Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLU	ASN	engineered mutation	UNP P07550
A	1054	THR	CYS	engineered mutation	UNP D9IEF7
A	1097	ALA	CYS	engineered mutation	UNP D9IEF7
A	349	HIS	-	expression tag	UNP P07550
A	350	HIS	-	expression tag	UNP P07550
A	351	HIS	-	expression tag	UNP P07550
A	352	HIS	-	expression tag	UNP P07550
A	353	HIS	-	expression tag	UNP P07550
A	354	HIS	-	expression tag	UNP P07550

- Molecule 2 is (2S)-1-(8H-CARBAZOL-4-YLOXY)-3-[2-(2-METHOXYPHENOXY)ETHYLAMINO]PROPAN-2-OL (three-letter code: CVD) (formula: $C_{24}H_{26}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



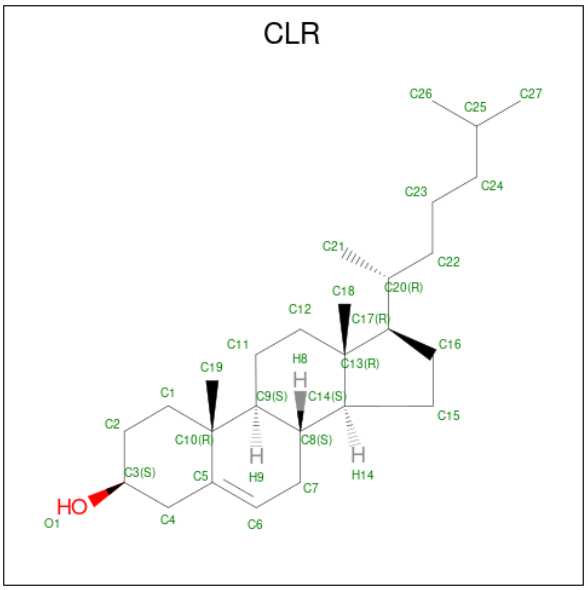
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	24	2	4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



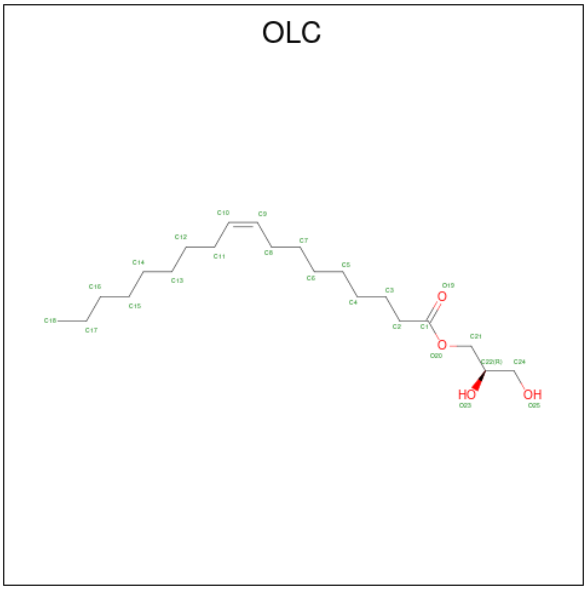
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



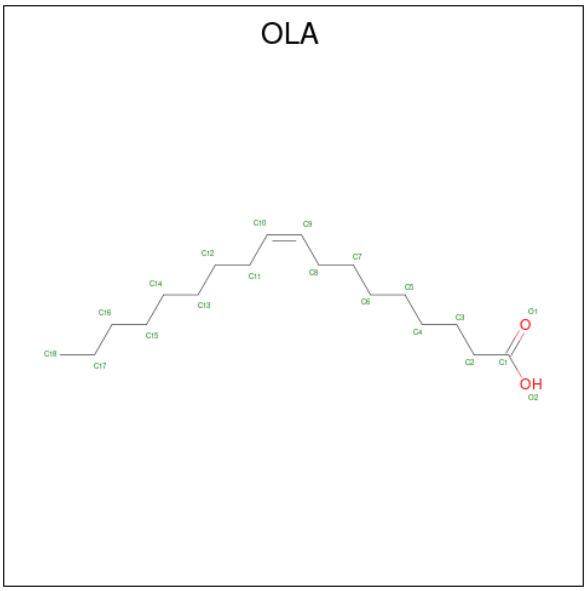
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	28	27	1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	16	12	4	0	0
			Total	C	O		
5	A	1	18	14	4	0	0
			Total	C	O		
5	A	1	12	8	4	0	0
			Total	C	O		
5	A	1	13	9	4	0	0
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C			
5	A	1	5	5		0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	14	12	2	0	0
			Total	C	O		
6	A	1	10	8	2	0	0
			Total	C	O		
6	A	1	13	11	2	0	0
			Total	C	O		
6	A	1	14	12	2	0	0

- Molecule 7 is water.

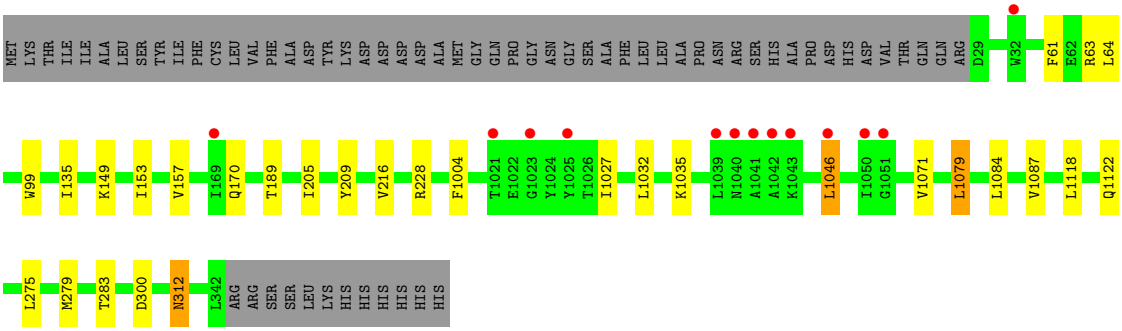
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	13	13	13	0	0

3 Residue-property plots (i)

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

• Molecule 1: Fusion protein of Beta-2 adrenergic receptor and T4 Lysozyme

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.55Å 77.44Å 173.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.40 – 2.50 46.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.40-2.50) 99.1 (46.40-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.203 , 0.242 0.217 , 0.265	Depositor DCC
R_{free} test set	1022 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	81.7	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 109.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3713	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, OLC, CVD, CLR, OLA

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	0.52	0/3594	0.64	0/4896

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	3497	0	3488	14	0
2	A	30	0	26	0	0
3	A	20	0	0	0	0
4	A	28	0	46	0	0
5	A	74	0	85	0	0
6	A	51	0	64	1	0
7	A	13	0	0	0	0
All	All	3713	0	3709	14	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 2.

All (14) 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:279:MET:O	1:A:283:THR:HG23	1.98	0.63
1:A:205[A]:ILE:HA	1:A:209:TYR:HB2	1.88	0.56
1:A:1027:ILE:HD13	1:A:1046:LEU:HD21	1.86	0.55
1:A:1087:VAL:HG11	1:A:1118:LEU:HD22	1.89	0.55
1:A:216:VAL:HG12	6:A:1215:OLA:H61	1.90	0.54
1:A:205[B]:ILE:HA	1:A:209:TYR:HB2	1.92	0.51
1:A:153:ILE:O	1:A:157:VAL:HG13	2.11	0.51
1:A:1084:LEU:O	1:A:1087:VAL:HG12	2.13	0.49
1:A:312:ASN:HD22	1:A:312:ASN:C	2.23	0.42
1:A:1004:PHE:CE1	1:A:1071:VAL:HG11	2.55	0.42
1:A:149:LYS:O	1:A:153:ILE:HG12	2.20	0.42
1:A:61:PHE:HB2	1:A:64:LEU:HD12	2.02	0.41
1:A:1079:LEU:H	1:A:1079:LEU:HG	1.74	0.41
1:A:99:TRP:O	1:A:189:THR:HA	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	447/506 (88%)	439 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	364/438 (83%)	352 (97%)	12 (3%)	38 64

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	135	ILE
1	A	170	GLN
1	A	228	ARG
1	A	1032	LEU
1	A	1035	LYS
1	A	1046	LEU
1	A	1079	LEU
1	A	1122	GLN
1	A	275	LEU
1	A	300	ASP
1	A	312	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	142	GLN
1	A	1031	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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	CVD	A	1201	-	31,33,33	3.86	13 (41%)	41,44,44	1.30	6 (14%)
3	SO4	A	1203	-	4,4,4	0.15	0	6,6,6	0.13	0
5	OLC	A	1212	-	4,4,24	0.49	0	2,3,25	0.64	0
3	SO4	A	1205	-	4,4,4	0.14	0	6,6,6	0.08	0
5	OLC	A	1210	-	12,12,24	0.39	0	13,13,25	1.00	1 (7%)
6	OLA	A	1216	-	13,13,19	0.61	0	12,13,19	1.07	1 (8%)
6	OLA	A	1213	-	13,13,19	0.62	0	12,13,19	1.05	2 (16%)
5	OLC	A	1209	-	11,11,24	0.46	0	12,12,25	1.10	2 (16%)
3	SO4	A	1204	-	4,4,4	0.22	0	6,6,6	0.13	0
6	OLA	A	1214	-	9,9,19	0.75	0	9,9,19	1.23	2 (22%)
4	CLR	A	1206	-	31,31,31	0.66	0	48,48,48	1.34	4 (8%)
5	OLC	A	1207	-	15,15,24	0.34	0	16,16,25	1.08	1 (6%)
6	OLA	A	1215	-	12,12,19	0.69	0	12,12,19	1.05	1 (8%)
5	OLC	A	1211	-	9,9,24	0.39	0	10,10,25	1.38	1 (10%)
5	OLC	A	1208	-	17,17,24	0.39	0	18,18,25	0.95	1 (5%)
3	SO4	A	1202	-	4,4,4	0.27	0	6,6,6	0.19	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	CVD	A	1201	-	-	7/15/15/15	0/4/4/4
6	OLA	A	1216	-	-	7/11/11/17	-
5	OLC	A	1212	-	-	1/2/2/24	-
5	OLC	A	1210	-	-	6/12/12/24	-
6	OLA	A	1213	-	-	9/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	1209	-	-	6/11/11/24	-
6	OLA	A	1214	-	-	6/7/7/17	-
5	OLC	A	1207	-	-	6/15/15/24	-
4	CLR	A	1206	-	-	6/10/68/68	0/4/4/4
6	OLA	A	1215	-	-	7/10/10/17	-
5	OLC	A	1211	-	-	8/9/9/24	-
5	OLC	A	1208	-	-	6/17/17/24	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	CVD	C13-C14	7.43	1.54	1.38
2	A	1201	CVD	C21-C20	7.25	1.54	1.38
2	A	1201	CVD	C22-C23	7.16	1.54	1.38
2	A	1201	CVD	C19-C18	6.92	1.55	1.40
2	A	1201	CVD	C9-C7	6.51	1.53	1.41
2	A	1201	CVD	C12-C6	6.48	1.53	1.41
2	A	1201	CVD	C8-C5	6.17	1.53	1.41
2	A	1201	CVD	C10-C11	6.12	1.54	1.38
2	A	1201	CVD	C3-C4	5.88	1.53	1.41
2	A	1201	CVD	O4-C19	3.16	1.42	1.37
2	A	1201	CVD	C5-C7	-2.97	1.34	1.42
2	A	1201	CVD	C20-C19	-2.89	1.33	1.39
2	A	1201	CVD	C23-C18	-2.84	1.33	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1206	CLR	C4-C5-C10	4.65	122.60	116.42
2	A	1201	CVD	O4-C19-C18	4.49	121.67	115.41
5	A	1211	OLC	O20-C1-C2	3.46	120.44	111.38
2	A	1201	CVD	C6-N1-C7	3.40	114.08	107.09
4	A	1206	CLR	C4-C5-C6	-3.11	116.12	120.61
2	A	1201	CVD	O4-C19-C20	-2.91	119.37	124.37
5	A	1207	OLC	O20-C1-C2	2.73	120.47	111.91
6	A	1214	OLA	O2-C1-C2	2.54	122.18	114.03
4	A	1206	CLR	C21-C20-C22	-2.51	106.43	110.36
6	A	1214	OLA	O2-C1-O1	-2.45	117.20	123.30
5	A	1209	OLC	O20-C1-C2	2.45	119.58	111.91
2	A	1201	CVD	O3-C18-C19	2.39	120.67	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1206	CLR	C21-C20-C17	2.37	116.54	112.92
2	A	1201	CVD	C14-C3-C4	-2.30	118.78	121.58
6	A	1213	OLA	O2-C1-C2	2.25	121.27	114.03
5	A	1210	OLC	O20-C1-C2	2.24	118.94	111.91
2	A	1201	CVD	O3-C18-C23	-2.22	119.17	123.97
5	A	1208	OLC	O20-C1-C2	2.14	118.62	111.91
6	A	1216	OLA	O2-C1-C2	2.11	120.81	114.03
5	A	1209	OLC	O20-C1-O19	-2.09	118.31	123.59
6	A	1213	OLA	O2-C1-O1	-2.07	118.14	123.30
6	A	1215	OLA	O2-C1-O1	-2.02	118.25	123.30

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1210	OLC	C21-C22-C24-O25
5	A	1210	OLC	O20-C21-C22-C24
5	A	1211	OLC	C21-C22-C24-O25
5	A	1212	OLC	C7-C8-C9-C10
6	A	1213	OLA	C9-C10-C11-C12
6	A	1216	OLA	C9-C10-C11-C12
5	A	1209	OLC	C2-C1-O20-C21
5	A	1211	OLC	C2-C1-O20-C21
5	A	1209	OLC	O19-C1-O20-C21
4	A	1206	CLR	C17-C20-C22-C23
5	A	1211	OLC	O19-C1-O20-C21
5	A	1210	OLC	O20-C21-C22-O23
4	A	1206	CLR	C21-C20-C22-C23
5	A	1208	OLC	C2-C1-O20-C21
5	A	1210	OLC	O23-C22-C24-O25
5	A	1211	OLC	O23-C22-C24-O25
5	A	1209	OLC	C1-C2-C3-C4
5	A	1207	OLC	C2-C1-O20-C21
2	A	1201	CVD	C15-C1-C2-O2
6	A	1213	OLA	C1-C2-C3-C4
5	A	1208	OLC	O19-C1-O20-C21
2	A	1201	CVD	O1-C1-C2-O2
5	A	1211	OLC	O20-C21-C22-O23
2	A	1201	CVD	C20-C19-O4-C24
6	A	1213	OLA	C3-C4-C5-C6
6	A	1213	OLA	C5-C6-C7-C8
5	A	1211	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
6	A	1215	OLA	C3-C4-C5-C6
6	A	1215	OLA	C4-C5-C6-C7
6	A	1215	OLA	C5-C6-C7-C8
6	A	1213	OLA	C4-C5-C6-C7
5	A	1207	OLC	O19-C1-O20-C21
5	A	1207	OLC	C4-C5-C6-C7
5	A	1207	OLC	C3-C4-C5-C6
4	A	1206	CLR	C23-C24-C25-C26
5	A	1207	OLC	C2-C3-C4-C5
6	A	1213	OLA	C2-C3-C4-C5
6	A	1216	OLA	C3-C4-C5-C6
5	A	1208	OLC	C4-C5-C6-C7
6	A	1214	OLA	C4-C5-C6-C7
5	A	1207	OLC	C1-C2-C3-C4
6	A	1215	OLA	C1-C2-C3-C4
2	A	1201	CVD	C18-C19-O4-C24
6	A	1214	OLA	C3-C4-C5-C6
4	A	1206	CLR	C23-C24-C25-C27
5	A	1208	OLC	C2-C3-C4-C5
5	A	1210	OLC	C3-C4-C5-C6
6	A	1215	OLA	C6-C7-C8-C9
6	A	1216	OLA	C6-C7-C8-C9
6	A	1216	OLA	C1-C2-C3-C4
5	A	1209	OLC	O20-C21-C22-C24
2	A	1201	CVD	C23-C18-O3-C17
5	A	1208	OLC	C1-C2-C3-C4
6	A	1214	OLA	C2-C3-C4-C5
5	A	1208	OLC	C3-C4-C5-C6
2	A	1201	CVD	C19-C18-O3-C17
5	A	1209	OLC	C21-C22-C24-O25
4	A	1206	CLR	C20-C22-C23-C24
6	A	1213	OLA	C6-C7-C8-C9
6	A	1213	OLA	O1-C1-C2-C3
2	A	1201	CVD	C14-C3-O2-C2
6	A	1215	OLA	O2-C1-C2-C3
6	A	1213	OLA	O2-C1-C2-C3
6	A	1215	OLA	O1-C1-C2-C3
6	A	1216	OLA	O2-C1-C2-C3
5	A	1209	OLC	O20-C21-C22-O23
6	A	1216	OLA	O1-C1-C2-C3
5	A	1211	OLC	O19-C1-C2-C3
6	A	1214	OLA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	1210	OLC	C2-C3-C4-C5
4	A	1206	CLR	C22-C23-C24-C25
5	A	1211	OLC	O20-C1-C2-C3
6	A	1214	OLA	O2-C1-C2-C3
6	A	1216	OLA	C5-C6-C7-C8
6	A	1214	OLA	C1-C2-C3-C4

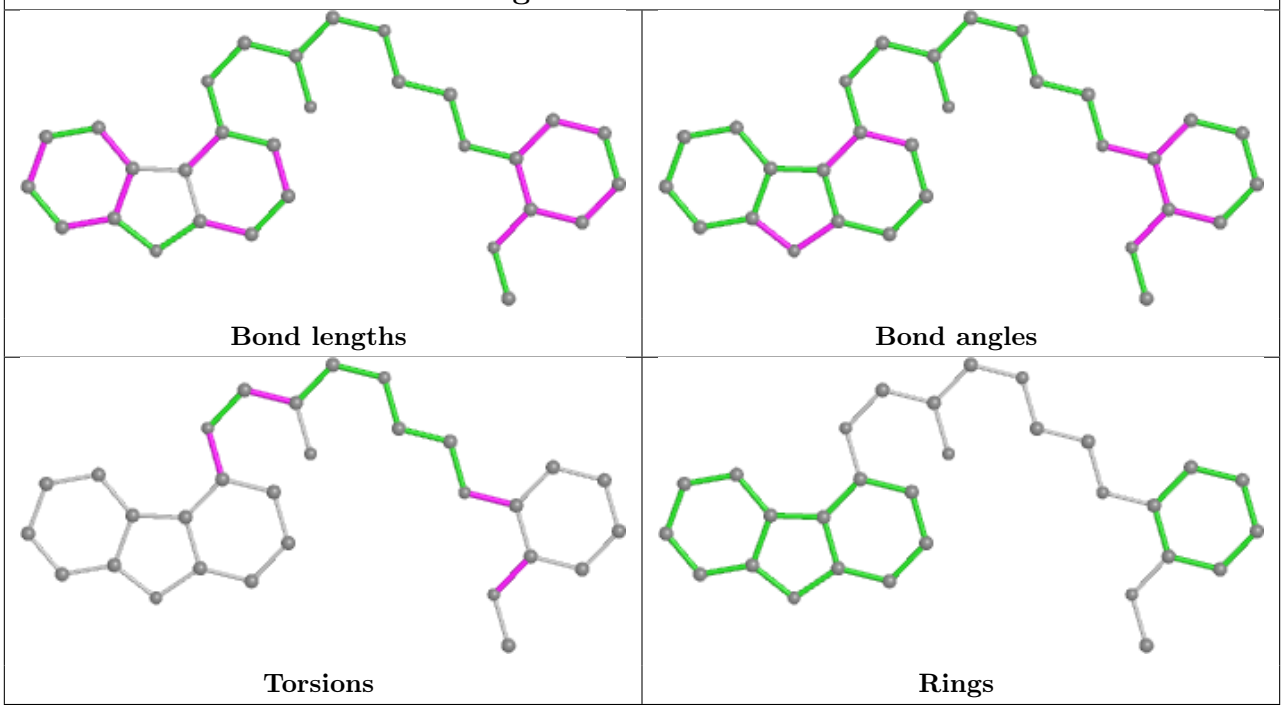
There are no ring outliers.

1 monomer is involved in 1 short contact:

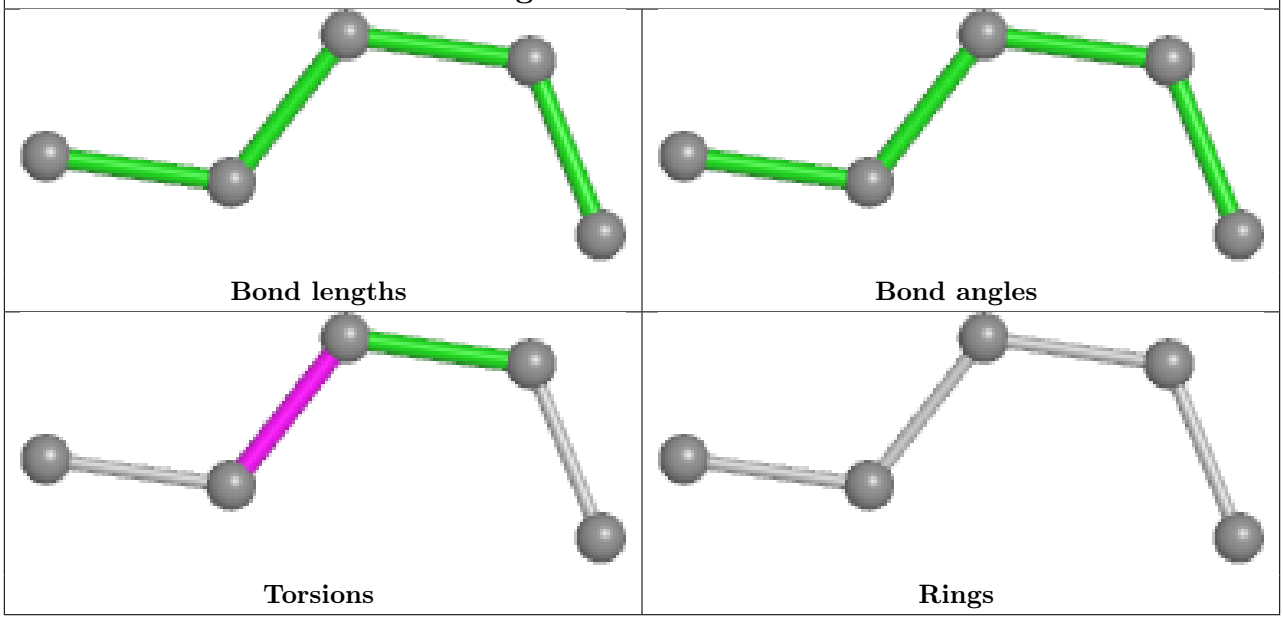
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1215	OLA	1	0

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 then 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.

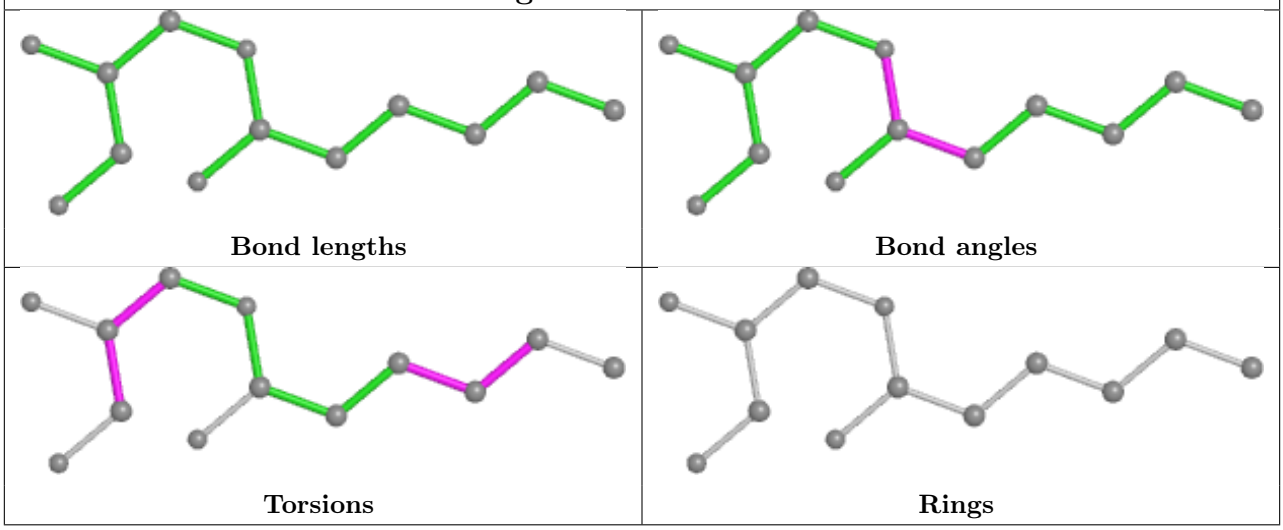
Ligand CVD A 1201



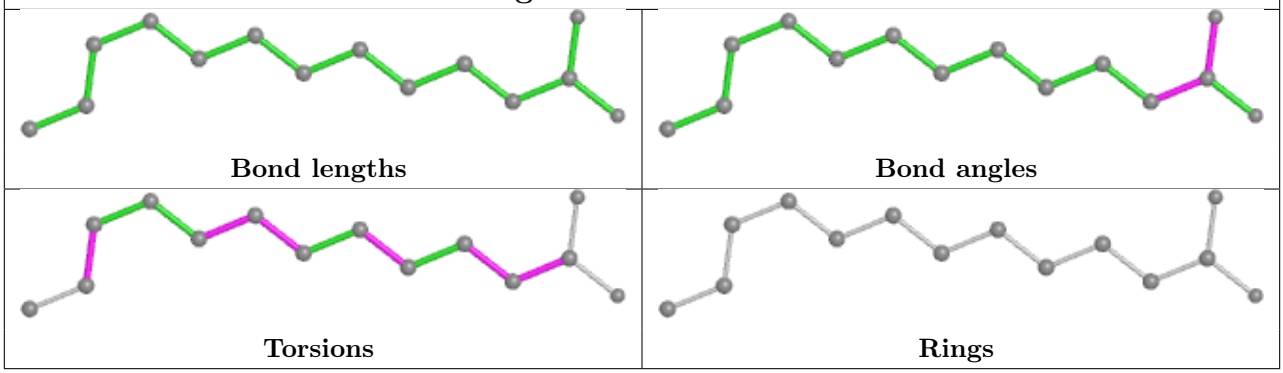
Ligand OLC A 1212



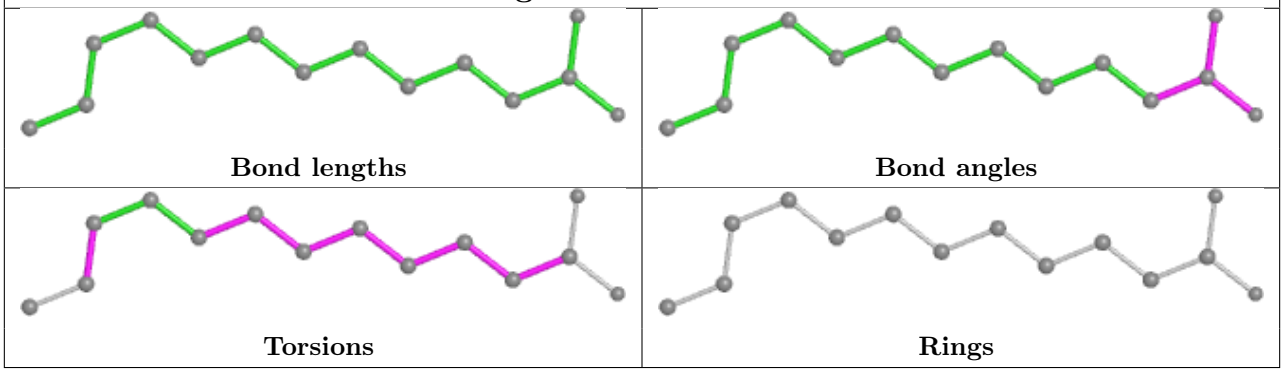
Ligand OLC A 1210



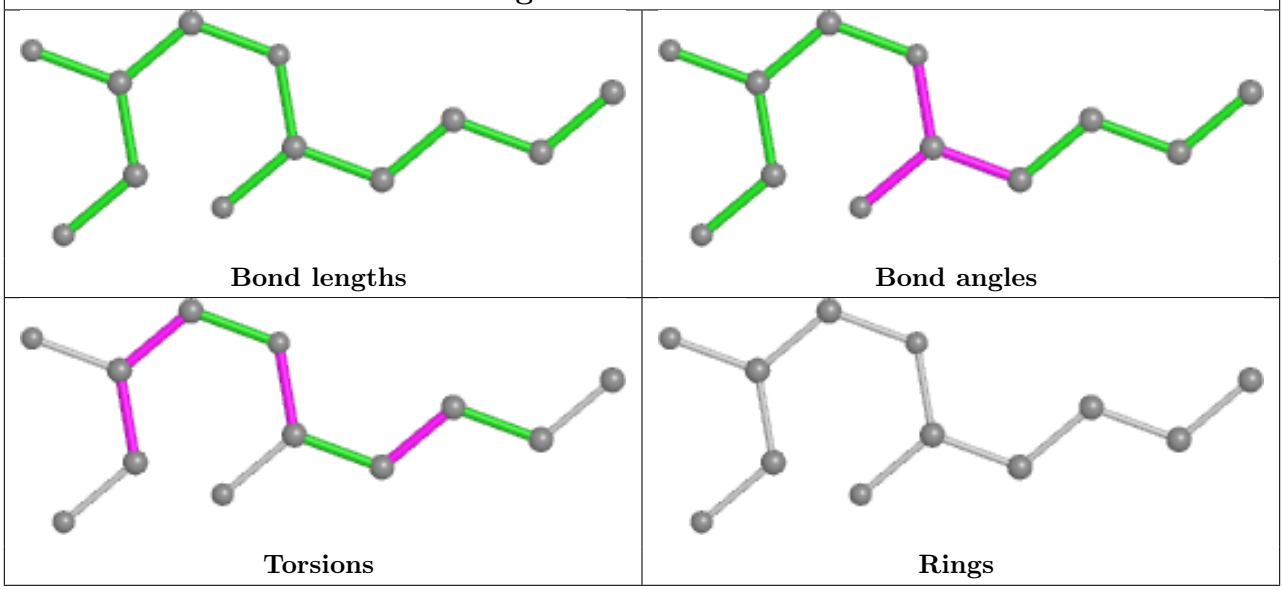
Ligand OLA A 1216



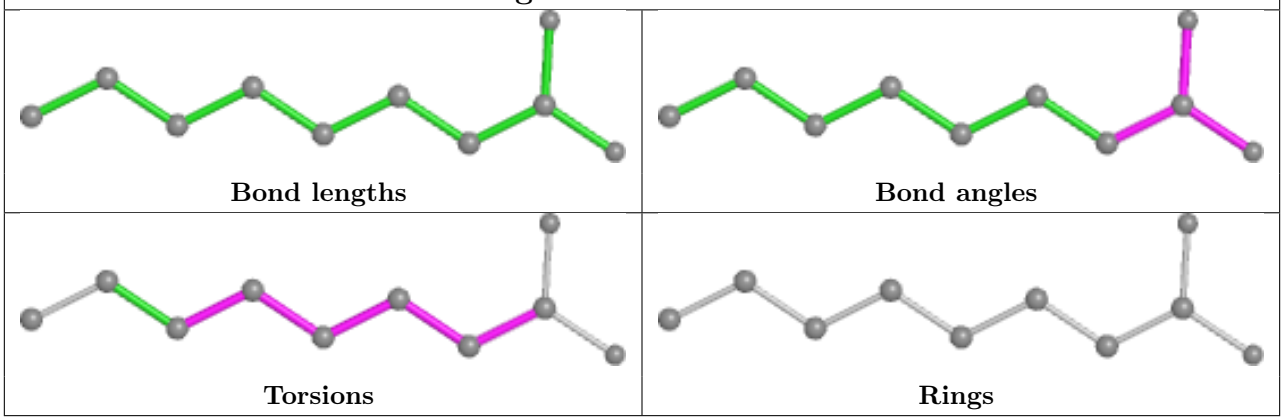
Ligand OLA A 1213



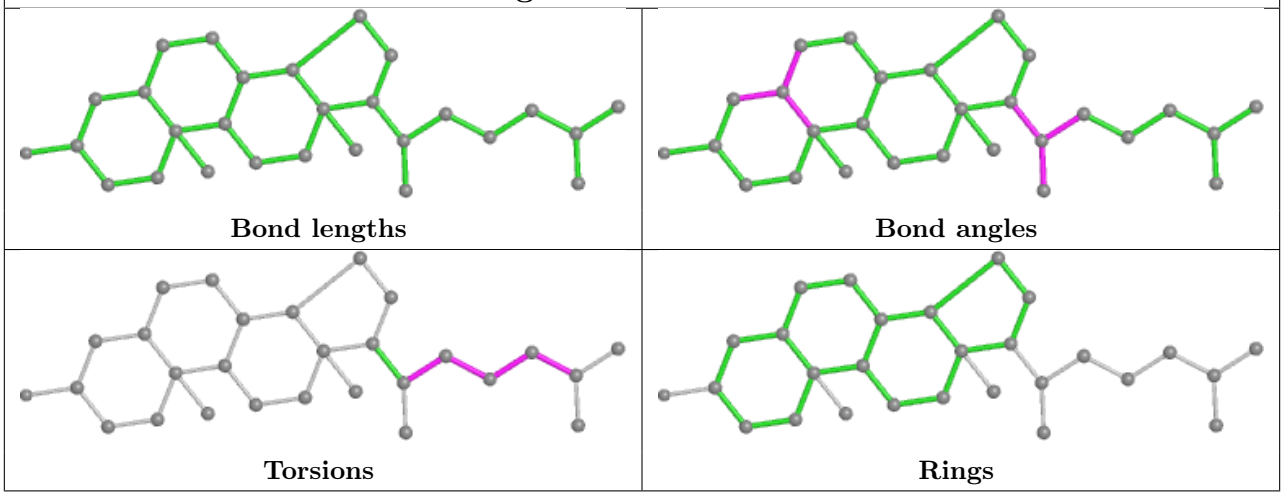
Ligand OLC A 1209



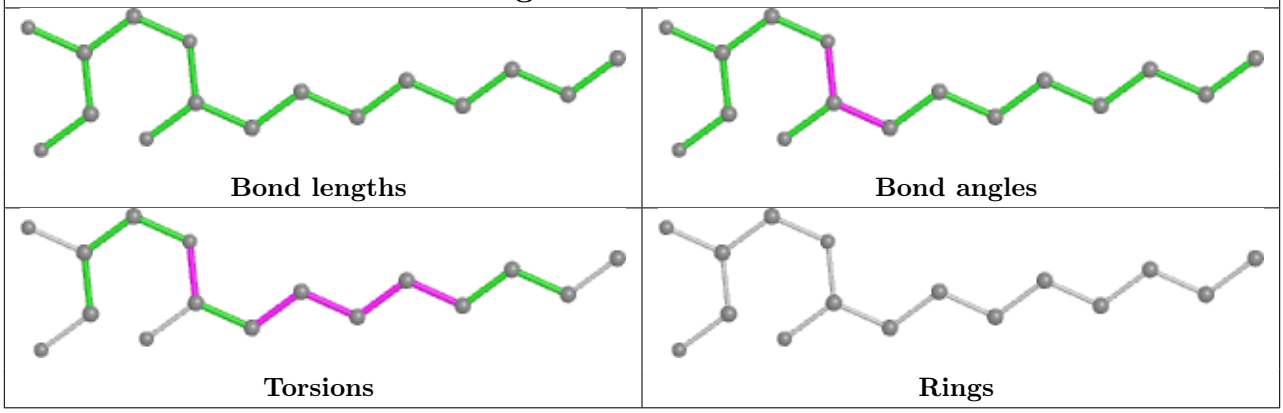
Ligand OLA A 1214



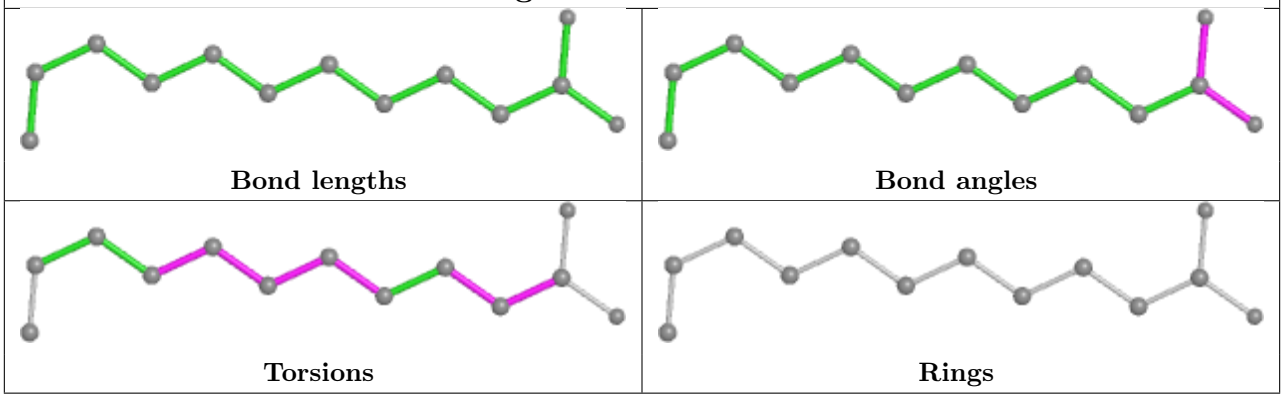
Ligand CLR A 1206



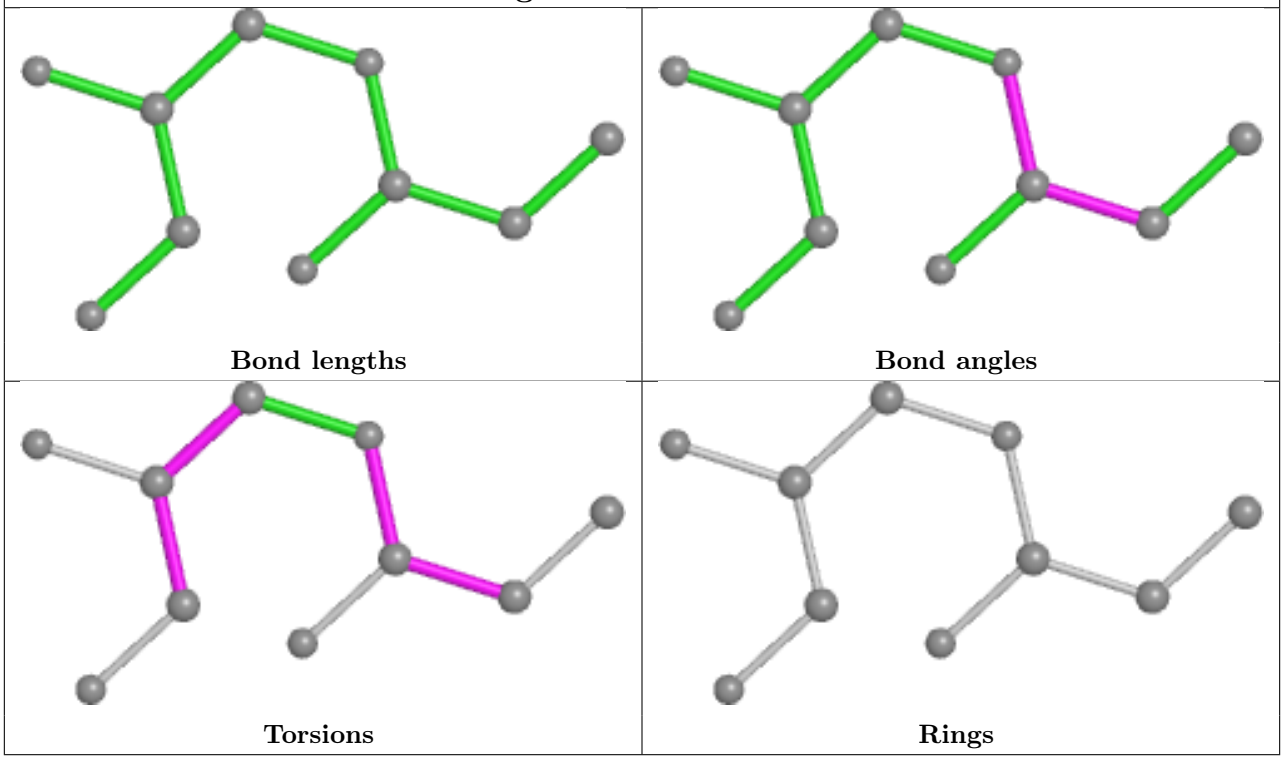
Ligand OLC A 1207

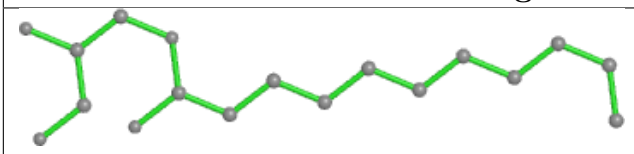
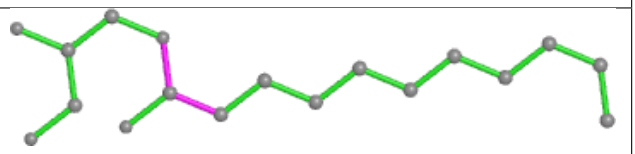
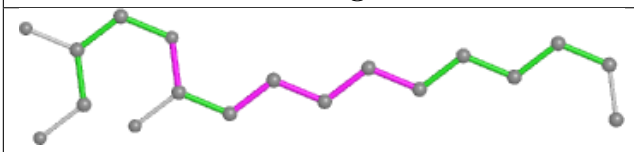
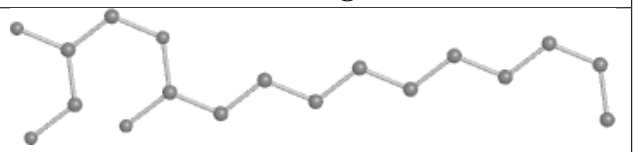


Ligand OLA A 1215



Ligand OLC A 1211



Ligand OLC A 1208	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	442/506 (87%)	0.40	13 (2%) 51 55	69, 89, 132, 178	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1051	GLY	5.5
1	A	1050	ILE	4.4
1	A	1039	LEU	4.4
1	A	1046	LEU	3.5
1	A	1040	ASN	3.5
1	A	1023	GLY	3.0
1	A	1025	TYR	2.8
1	A	32	TRP	2.8
1	A	1021	THR	2.6
1	A	1043	LYS	2.6
1	A	1042	ALA	2.6
1	A	169	ILE	2.1
1	A	1041	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

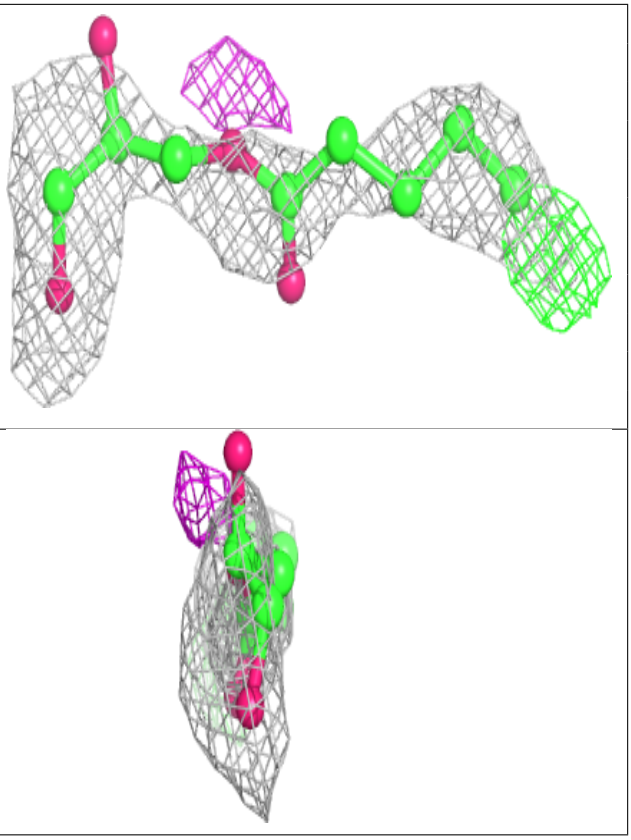
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

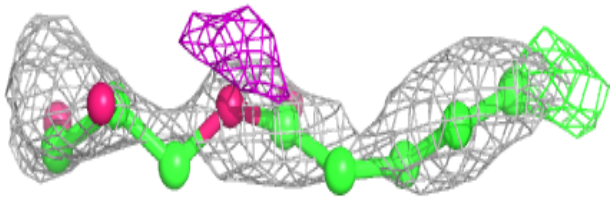
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OLC	A	1209	12/25	0.35	0.50	121,126,127,128	0
5	OLC	A	1210	13/25	0.48	0.30	99,115,119,121	0
5	OLC	A	1212	5/25	0.52	0.36	102,103,104,105	0
5	OLC	A	1208	18/25	0.54	0.31	108,121,134,135	0
6	OLA	A	1213	14/20	0.63	0.23	112,113,116,118	0
6	OLA	A	1216	14/20	0.67	0.44	118,122,125,125	0
6	OLA	A	1215	13/20	0.69	0.29	112,115,124,125	0
5	OLC	A	1207	16/25	0.71	0.24	112,122,127,127	0
6	OLA	A	1214	10/20	0.74	0.30	96,98,100,101	0
5	OLC	A	1211	10/25	0.76	0.31	106,110,112,113	0
3	SO4	A	1203	5/5	0.84	0.19	154,155,155,155	0
3	SO4	A	1204	5/5	0.90	0.20	144,144,145,146	0
3	SO4	A	1205	5/5	0.93	0.12	174,174,174,174	0
4	CLR	A	1206	28/28	0.93	0.19	100,105,107,108	0
2	CVD	A	1201	30/30	0.93	0.25	75,82,107,109	0
3	SO4	A	1202	5/5	0.93	0.22	94,95,98,98	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 OLC A 1209:

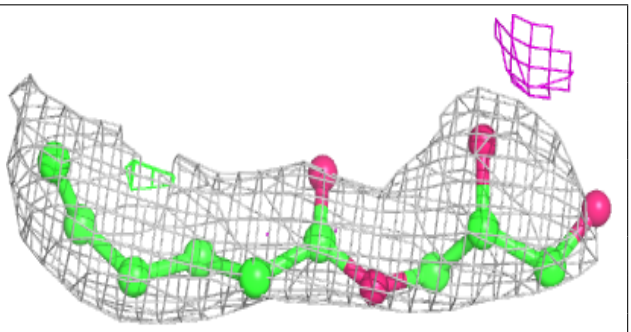
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

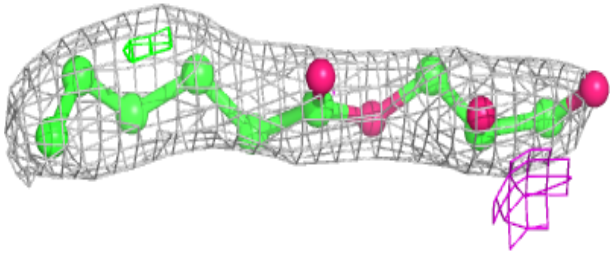


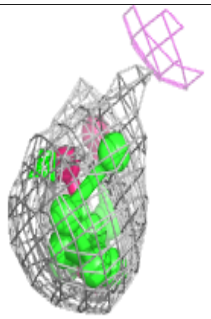


Electron density around OLC A 1210:

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







Electron density around OLC A 1212:

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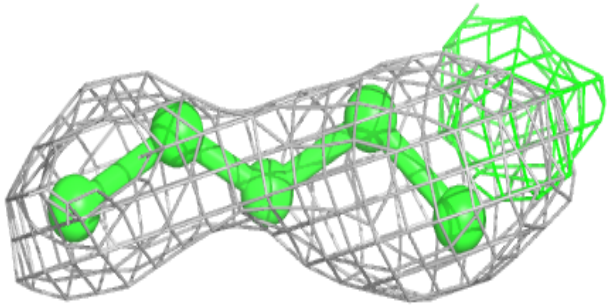
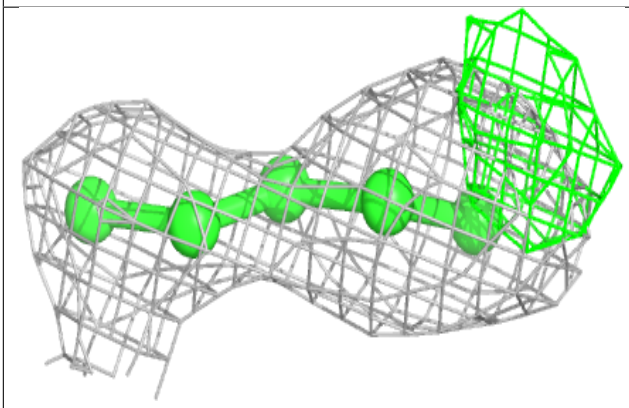
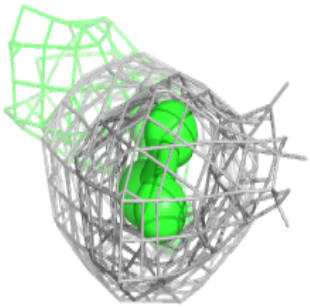
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around OLC A 1208:

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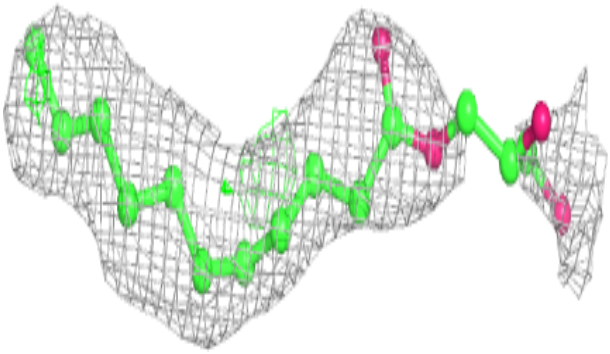
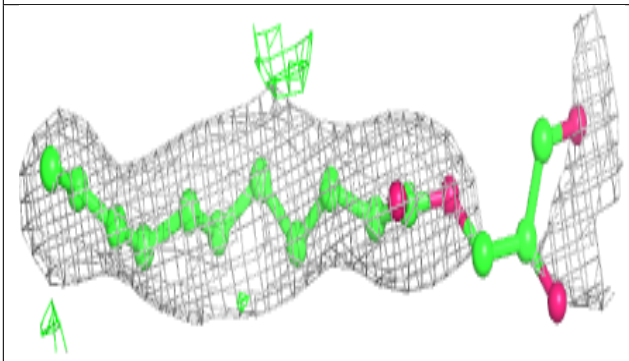
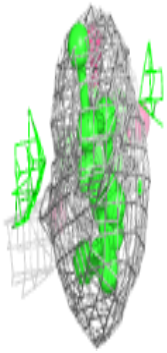
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

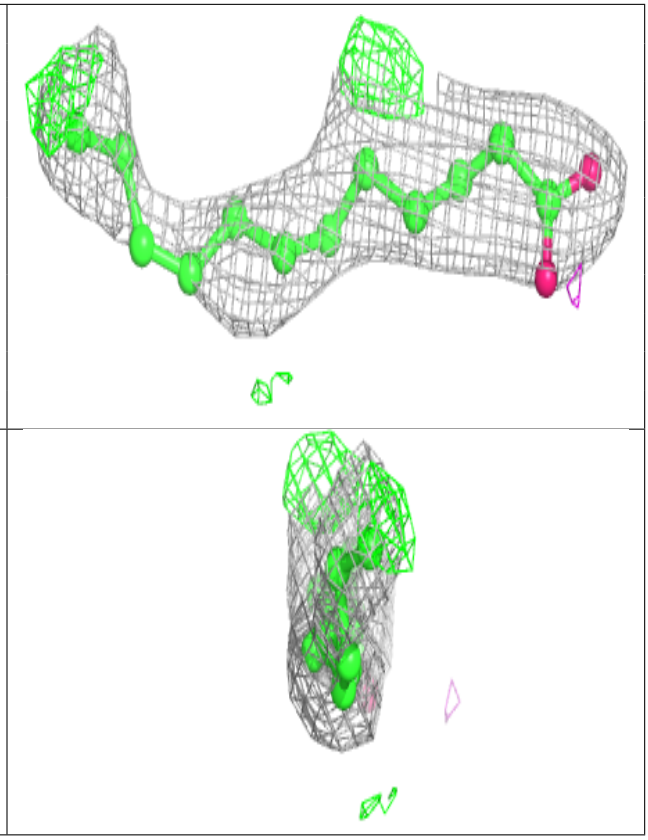






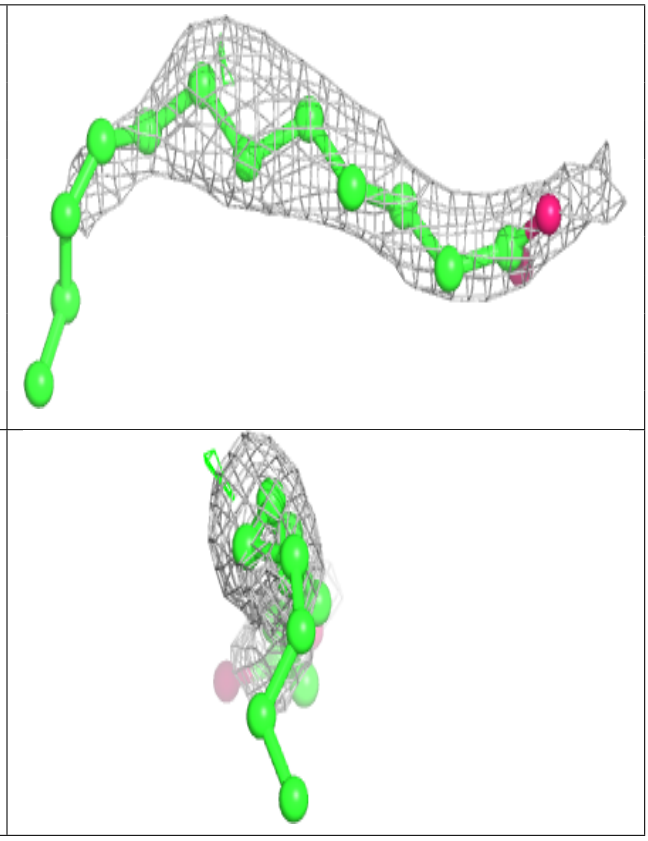
Electron density around OLA A 1213:

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



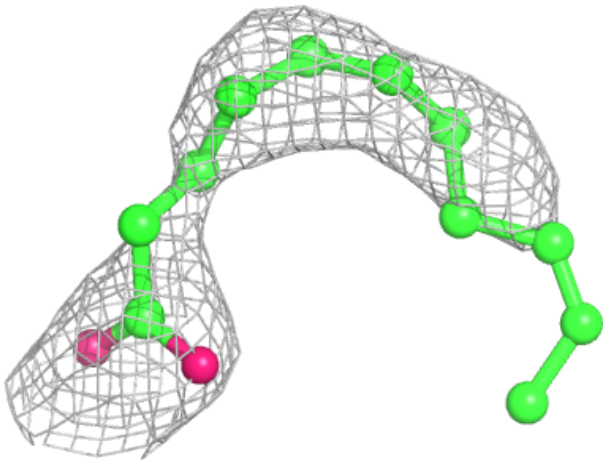
Electron density around OLA A 1216:

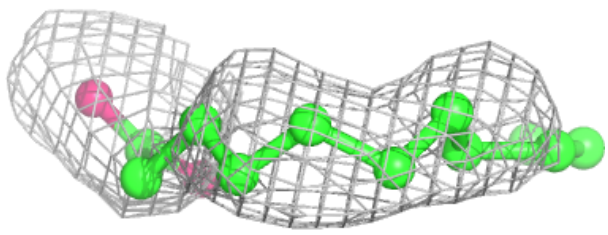
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

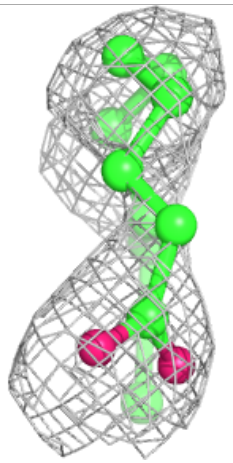


Electron density around OLA A 1215:

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

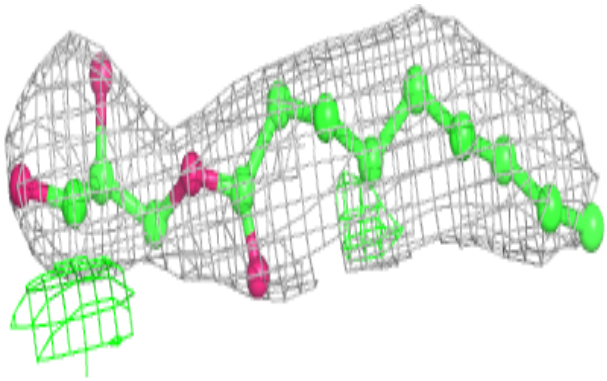


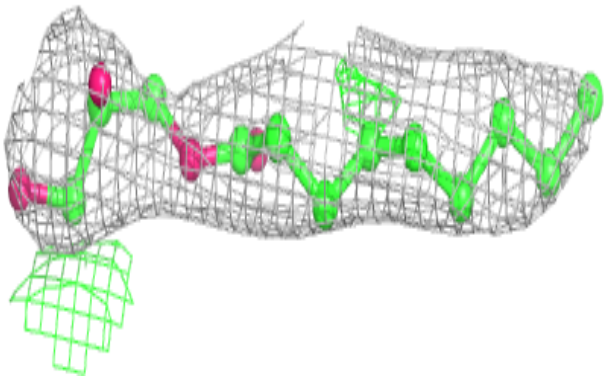


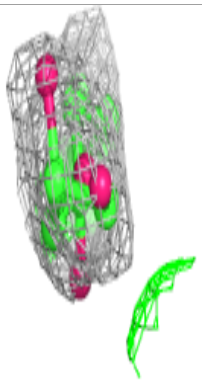


Electron density around OLC A 1207:

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

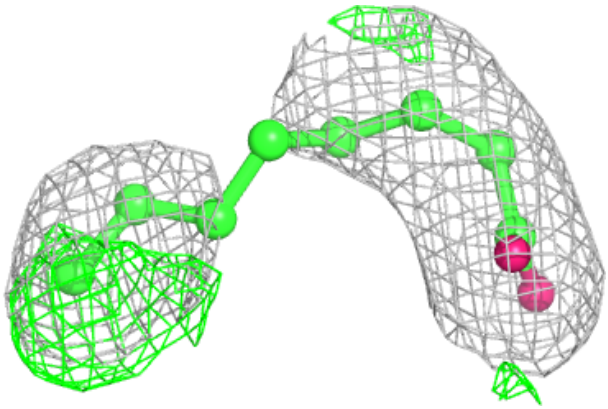


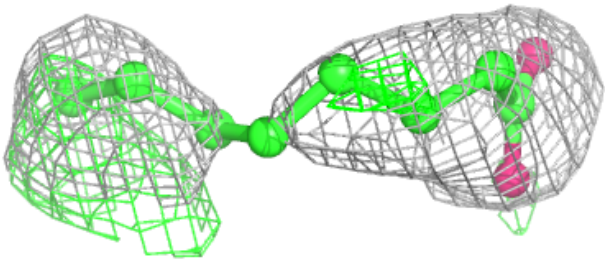


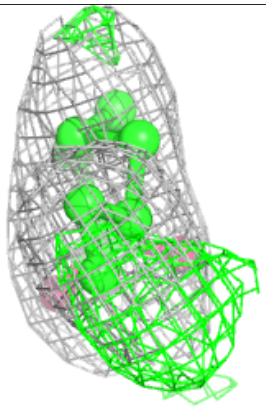


Electron density around OLA A 1214:

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

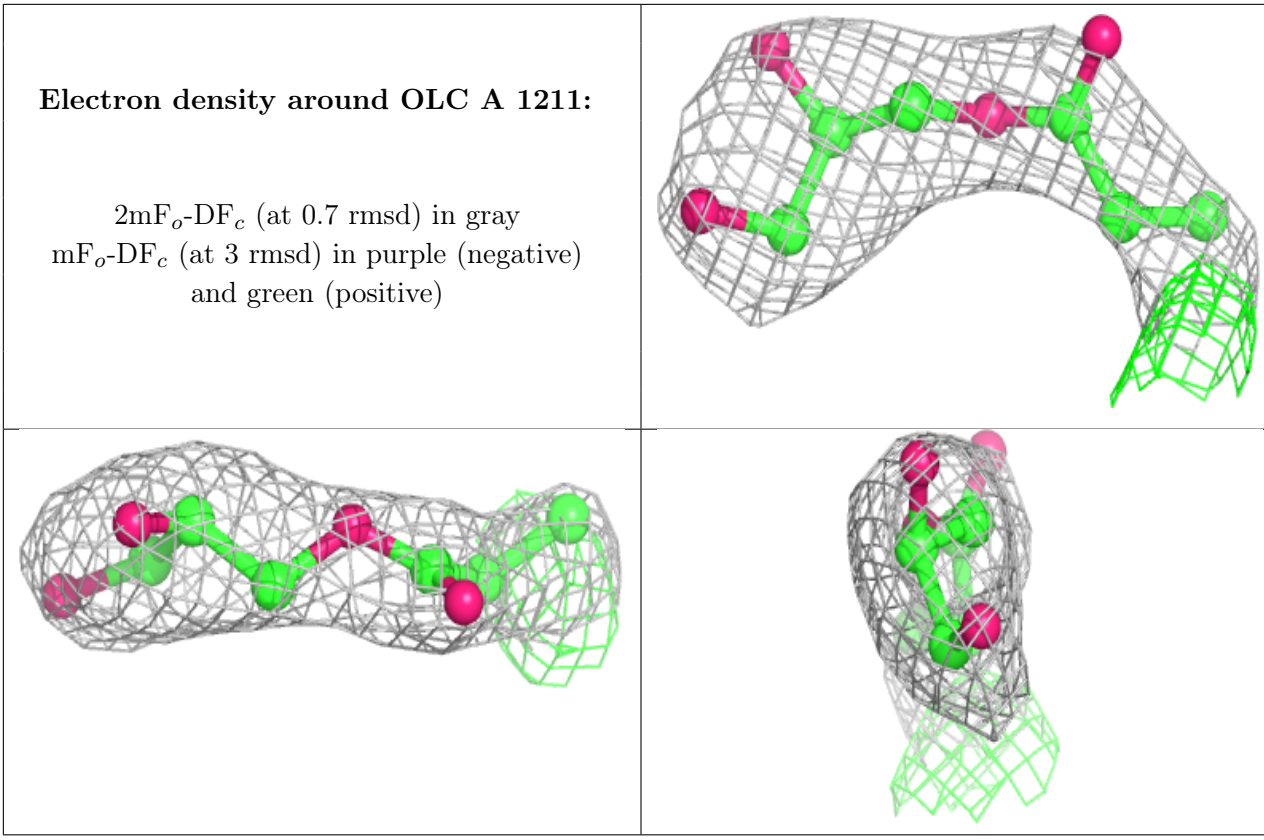






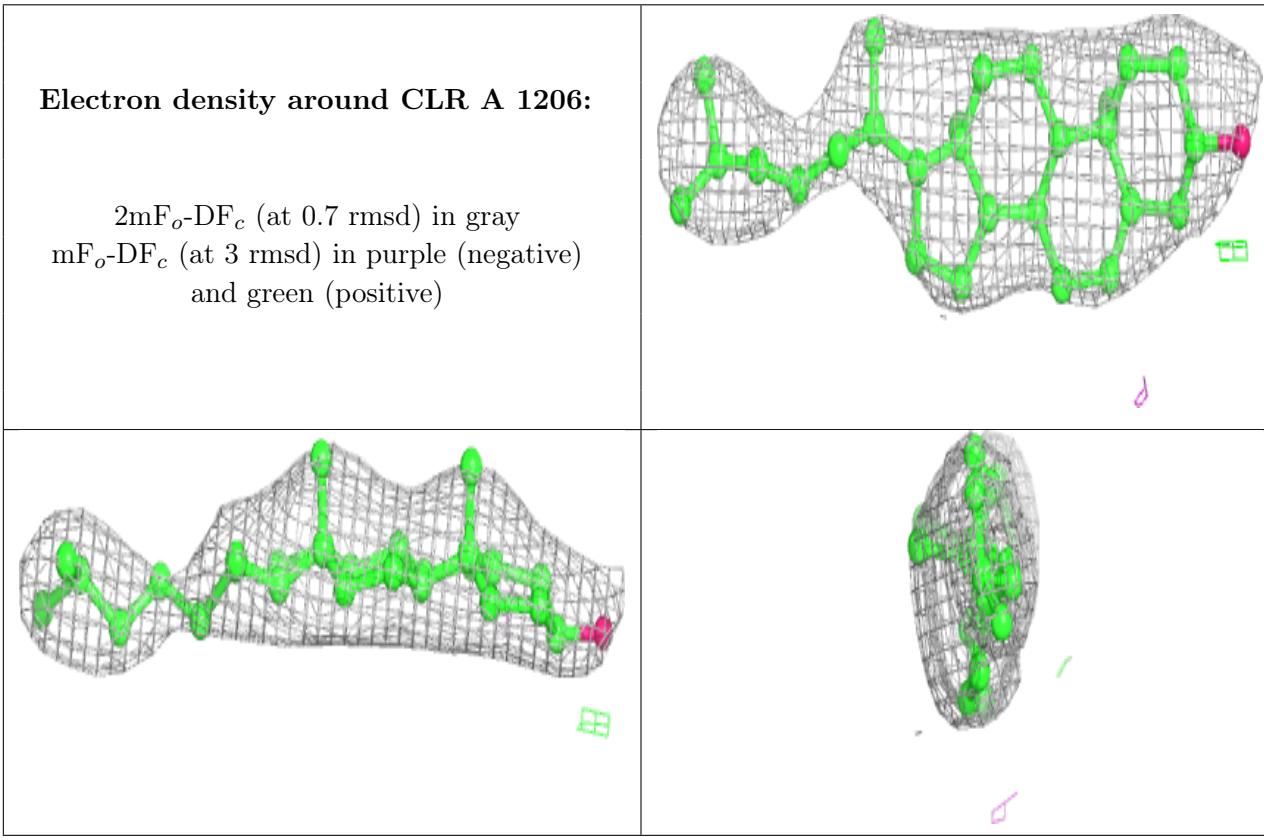
Electron density around OLC A 1211:

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



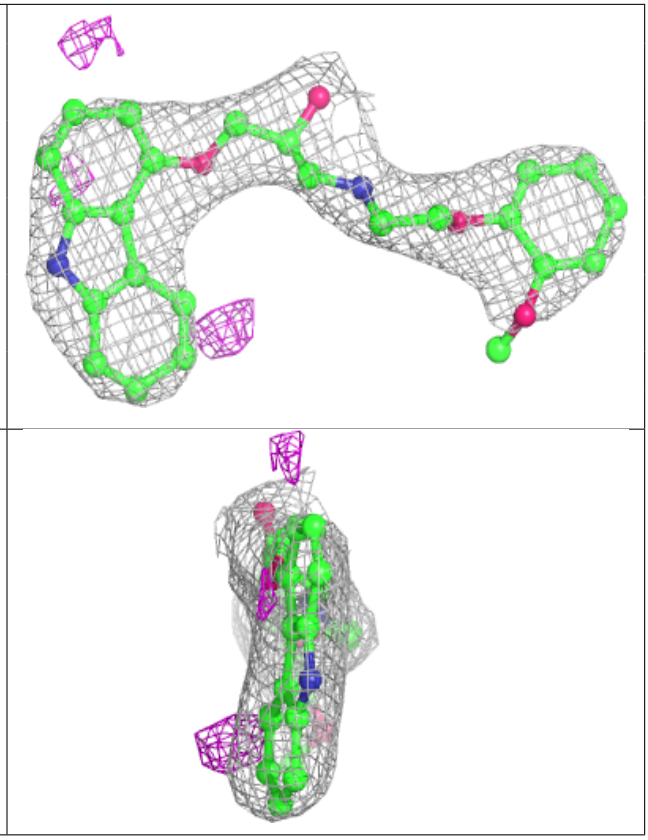
Electron density around CLR A 1206:

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



Electron density around CVD A 1201:

$2mF_o$-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.