Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 02:14 PM EDT

PDB ID	:	5UIW
Title	:	Crystal Structure of CC Chemokine Receptor 5 (CCR5) in complex with high potency HIV entry inhibitor 5P7-CCL5
Authors	:	Zheng, Y.; Qin, L.; Han, G.W.; Gustavsson, M.; Kawamura, T.; Stevens, R.C.; Cherezov, V.; Kufareva, I.; Handel, T.M.
Deposited on	:	2017-01-15
Resolution	:	2.20 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:

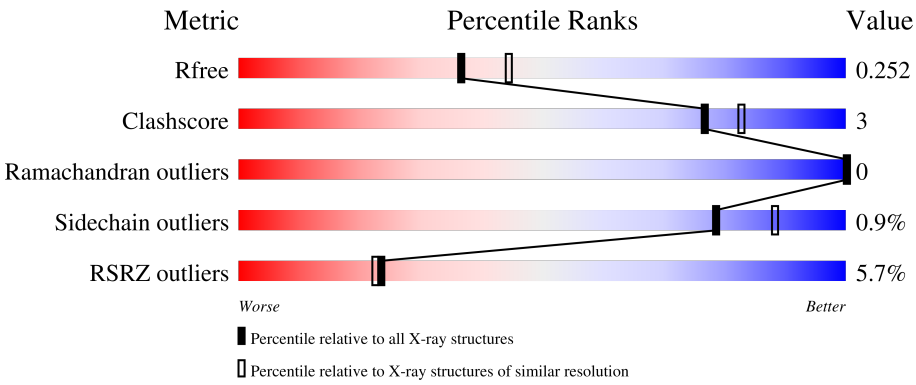
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	411	5% 81% • 14%
2	B	75	5% 73% 17% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3443 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 C-C chemokine receptor type 5,Rubredoxin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2756	1839	430	469	18	0	1	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P51681
A	0	ALA	-	expression tag	UNP P51681
A	1	PRO	-	expression tag	UNP P51681
A	58	TYR	CYS	engineered mutation	UNP P51681
A	163	ASN	GLY	engineered mutation	UNP P51681
A	233	ASP	ALA	engineered mutation	UNP P51681
A	303	GLU	LYS	engineered mutation	UNP P51681
A	?	-	ALA	deletion	UNP P51681
A	?	-	LYS	deletion	UNP P51681
A	?	-	ARG	deletion	UNP P51681
A	350	GLY	-	expression tag	UNP P51681
A	351	ARG	-	expression tag	UNP P51681
A	352	PRO	-	expression tag	UNP P51681
A	353	LEU	-	expression tag	UNP P51681
A	354	GLU	-	expression tag	UNP P51681
A	355	VAL	-	expression tag	UNP P51681
A	356	LEU	-	expression tag	UNP P51681
A	357	PHE	-	expression tag	UNP P51681
A	358	GLN	-	expression tag	UNP P51681

- Molecule 2 is a protein called C-C motif chemokine 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	68	519	336	89	89	5	0	0	0

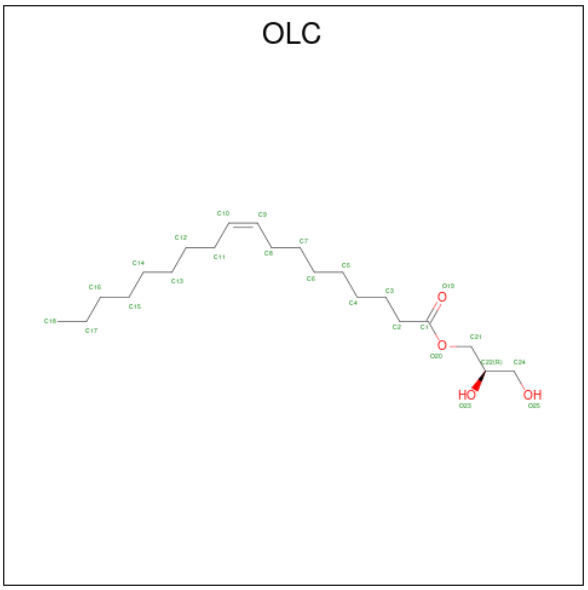
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PCA	-	expression tag	UNP P13501
B	1	GLY	-	expression tag	UNP P13501
B	2	PRO	-	expression tag	UNP P13501
B	3	PRO	-	expression tag	UNP P13501
B	4	LEU	-	expression tag	UNP P13501
B	5	MET	-	expression tag	UNP P13501
B	6	ALA	-	expression tag	UNP P13501
B	7	LEU	-	expression tag	UNP P13501
B	8	GLN	-	expression tag	UNP P13501
B	9	SER	-	expression tag	UNP P13501
B	69	LEU	-	expression tag	UNP P13501
B	70	GLU	-	expression tag	UNP P13501
B	71	VAL	-	expression tag	UNP P13501
B	72	LEU	-	expression tag	UNP P13501
B	73	PHE	-	expression tag	UNP P13501
B	74	GLN	-	expression tag	UNP P13501

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

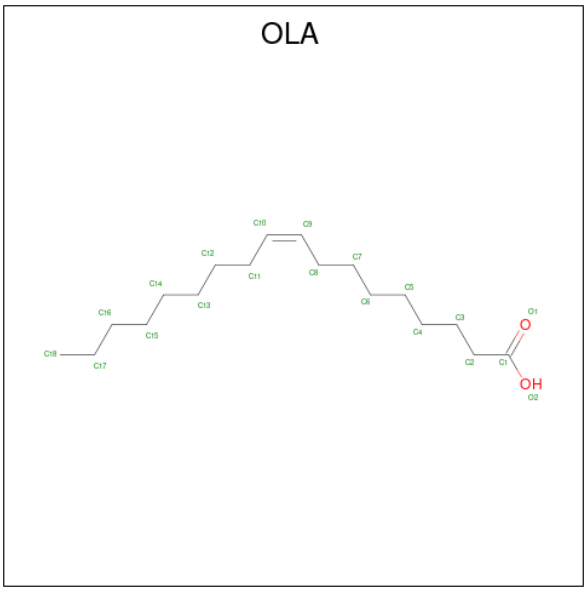
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 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		
4	A	1	16	12	4	0	0
			Total	C	O		
4	A	1	13	9	4	0	0
			Total	C	O		
4	A	1	21	17	4	0	0
			Total	C	O		
4	A	1	16	12	4	0	0
			Total	C	O		
4	A	1	13	9	4	0	0
			Total	C	O		
4	A	1	24	20	4	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



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

- Molecule 6 is water.

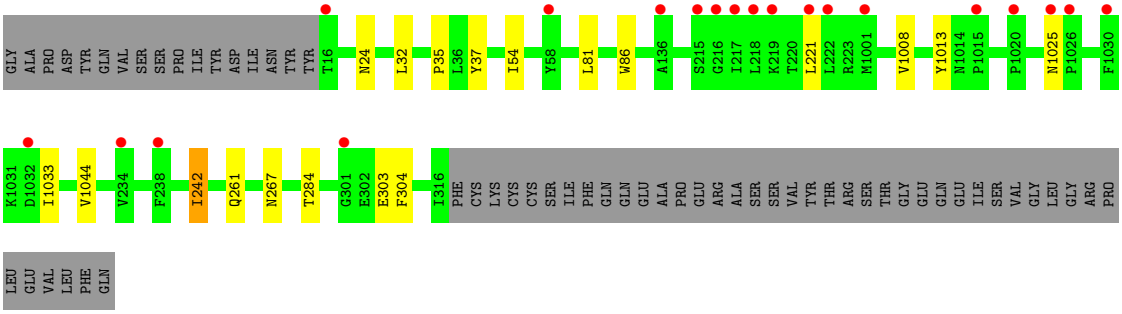
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	36	36	36	0	0
			Total	O		
6	B	8	8	8	0	0

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: C-C chemokine receptor type 5,Rubredoxin chimera

Chain A:



• Molecule 2: C-C motif chemokine 5

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	38.01Å 52.64Å 302.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.47 – 2.20 46.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	73.4 (29.47-2.20) 73.5 (46.67-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.65 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9	Depositor
R, R_{free}	0.216 , 0.250 0.221 , 0.252	Depositor DCC
R_{free} test set	1196 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3443	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% 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: ZN, PCA, OLC, 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	0.32	0/2833	0.47	0/3870
2	B	0.30	0/526	0.45	0/718
All	All	0.31	0/3359	0.47	0/4588

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	2756	0	2680	12	0
2	B	519	0	498	7	0
3	A	1	0	0	0	0
4	A	103	0	136	1	0
5	A	20	0	23	3	0
6	A	36	0	0	0	0
6	B	8	0	0	0	0
All	All	3443	0	3337	20	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 3.

All (20) 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)
2:B:25:LYS:NZ	2:B:46:ASN:OD1	2.23	0.69
1:A:1025:ASN:OD1	1:A:1025:ASN:N	2.31	0.62
5:A:1108:OLA:H61	5:A:1109:OLA:H51	1.85	0.58
5:A:1108:OLA:H31	5:A:1109:OLA:H52	1.86	0.58
1:A:261:GLN:HG3	1:A:267:ASN:HB3	1.86	0.56
1:A:86:TRP:CD2	2:B:3:PRO:HG2	2.42	0.54
1:A:1008:VAL:HG21	1:A:1044:VAL:HG11	1.89	0.53
1:A:1013:TYR:CZ	1:A:1033:ILE:HD11	2.46	0.51
1:A:242:ILE:HD11	5:A:1109:OLA:C1	2.41	0.50
1:A:303:GLU:HG2	1:A:304:PHE:N	2.27	0.50
2:B:19:LEU:HD11	2:B:49:VAL:HG11	1.94	0.49
1:A:32:LEU:O	1:A:35:PRO:HD2	2.12	0.48
1:A:24:ASN:HB3	4:A:1107:OLC:H24A	1.94	0.48
2:B:47:ARG:HD3	2:B:47:ARG:HA	1.61	0.48
1:A:37:TYR:HE1	1:A:284:THR:HG23	1.79	0.46
2:B:17:ARG:HA	2:B:17:ARG:HD2	1.79	0.45
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.77	0.44
1:A:54:ILE:HD12	1:A:304:PHE:CE1	2.52	0.44
2:B:18:PRO:HG3	2:B:57:TRP:CG	2.54	0.43
2:B:62:ILE:O	2:B:66:GLU:HG2	2.20	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	351/411 (85%)	338 (96%)	13 (4%)	0	100	100
2	B	66/75 (88%)	66 (100%)	0	0	100	100
All	All	417/486 (86%)	404 (97%)	13 (3%)	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	286/369 (78%)	284 (99%)	2 (1%)	84	91
2	B	51/66 (77%)	50 (98%)	1 (2%)	55	69
All	All	337/435 (78%)	334 (99%)	3 (1%)	78	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	242	ILE
2	B	7	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PCA	B	0	2	7,8,9	1.87	1 (14%)	9,10,12	2.03	5 (55%)

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	PCA	B	0	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	0	PCA	CD-N	4.81	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	0	PCA	OE-CD-CG	-2.94	121.63	126.76
2	B	0	PCA	CA-N-CD	-2.79	104.03	113.58
2	B	0	PCA	CB-CA-N	2.50	110.49	103.30
2	B	0	PCA	CB-CA-C	-2.47	109.31	112.70
2	B	0	PCA	CG-CD-N	2.22	114.15	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	OLC	A	1104	-	20,20,24	0.76	1 (5%)	21,21,25	0.97	1 (4%)
5	OLA	A	1108	-	11,11,19	0.67	0	11,11,19	1.27	1 (9%)
4	OLC	A	1105	-	15,15,24	0.85	1 (6%)	16,16,25	1.13	1 (6%)
5	OLA	A	1109	-	7,7,19	0.73	0	7,7,19	1.35	2 (28%)
4	OLC	A	1102	-	15,15,24	0.81	1 (6%)	16,16,25	1.01	1 (6%)
4	OLC	A	1103	-	12,12,24	0.95	1 (8%)	13,13,25	1.14	1 (7%)
4	OLC	A	1106	-	12,12,24	0.95	1 (8%)	13,13,25	1.12	1 (7%)
4	OLC	A	1107	-	23,23,24	0.68	1 (4%)	24,24,25	1.07	1 (4%)

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	OLC	A	1104	-	-	8/20/20/24	-
5	OLA	A	1108	-	-	6/9/9/17	-
4	OLC	A	1105	-	-	8/15/15/24	-
5	OLA	A	1109	-	-	1/5/5/17	-
4	OLC	A	1102	-	-	2/15/15/24	-
4	OLC	A	1103	-	-	2/12/12/24	-
4	OLC	A	1106	-	-	3/12/12/24	-
4	OLC	A	1107	-	-	8/23/23/24	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	OLC	O20-C1	2.81	1.41	1.33
4	A	1105	OLC	O20-C1	2.77	1.41	1.33
4	A	1103	OLC	O20-C1	2.72	1.41	1.33
4	A	1104	OLC	O20-C1	2.66	1.41	1.33
4	A	1107	OLC	O20-C1	2.65	1.41	1.33
4	A	1102	OLC	O20-C1	2.51	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1107	OLC	O20-C1-C2	3.21	121.99	111.91
4	A	1105	OLC	O20-C1-C2	2.99	121.29	111.91
4	A	1103	OLC	O20-C1-C2	2.98	121.25	111.91
4	A	1106	OLC	O20-C1-C2	2.86	120.89	111.91
4	A	1104	OLC	O20-C1-C2	2.66	120.25	111.91
4	A	1102	OLC	O20-C1-C2	2.57	119.98	111.91
5	A	1108	OLA	O2-C1-C2	2.04	120.59	114.03
5	A	1109	OLA	C3-C2-C1	-2.02	109.39	114.47
5	A	1109	OLA	O2-C1-C2	2.01	120.49	114.03

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	OLC	O20-C21-C22-O23
4	A	1103	OLC	O20-C21-C22-C24
4	A	1104	OLC	O20-C21-C22-C24
4	A	1106	OLC	O20-C21-C22-C24
4	A	1106	OLC	O20-C21-C22-O23
4	A	1104	OLC	C2-C1-O20-C21
4	A	1107	OLC	C2-C1-O20-C21
4	A	1103	OLC	O20-C21-C22-O23
4	A	1104	OLC	O19-C1-O20-C21
4	A	1107	OLC	O19-C1-O20-C21
4	A	1104	OLC	O20-C21-C22-O23
4	A	1105	OLC	C2-C1-O20-C21
4	A	1105	OLC	C1-C2-C3-C4
4	A	1107	OLC	C1-C2-C3-C4
5	A	1108	OLA	C1-C2-C3-C4
4	A	1105	OLC	O19-C1-O20-C21
4	A	1102	OLC	O20-C21-C22-C24
4	A	1107	OLC	C5-C6-C7-C8
4	A	1107	OLC	C4-C5-C6-C7
5	A	1108	OLA	C7-C8-C9-C10
4	A	1107	OLC	C14-C15-C16-C17
5	A	1109	OLA	C3-C4-C5-C6
4	A	1104	OLC	C3-C4-C5-C6
4	A	1105	OLC	C2-C3-C4-C5
5	A	1108	OLA	C2-C3-C4-C5
4	A	1104	OLC	C6-C7-C8-C9
4	A	1105	OLC	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1106	OLC	C2-C3-C4-C5
4	A	1105	OLC	C6-C7-C8-C9
5	A	1108	OLA	C3-C4-C5-C6
4	A	1107	OLC	C7-C8-C9-C10
5	A	1108	OLA	C4-C5-C6-C7
4	A	1104	OLC	C2-C3-C4-C5
4	A	1107	OLC	C9-C10-C11-C12
4	A	1104	OLC	C9-C10-C11-C12
5	A	1108	OLA	C5-C6-C7-C8
4	A	1105	OLC	O20-C1-C2-C3
4	A	1105	OLC	O19-C1-C2-C3

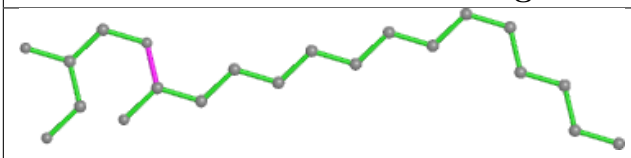
There are no ring outliers.

3 monomers are involved in 4 short contacts:

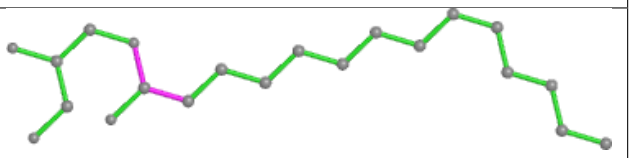
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1108	OLA	2	0
5	A	1109	OLA	3	0
4	A	1107	OLC	1	0

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

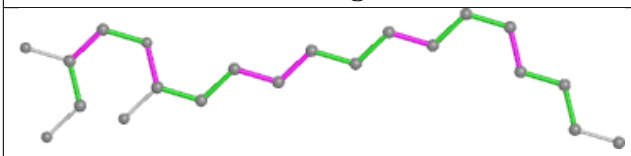
Ligand OLC A 1104



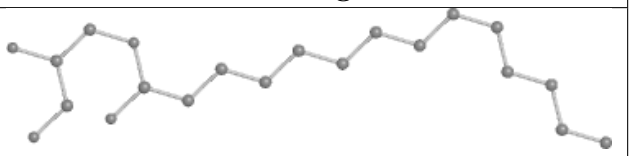
Bond lengths



Bond angles

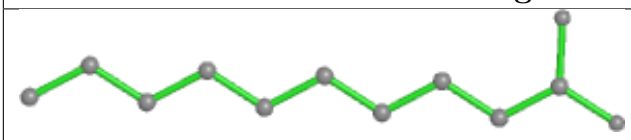


Torsions

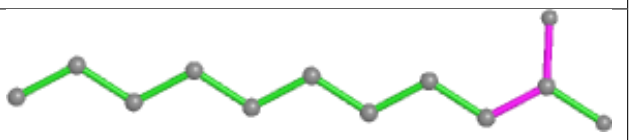


Rings

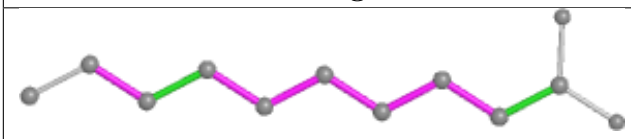
Ligand OLA A 1108



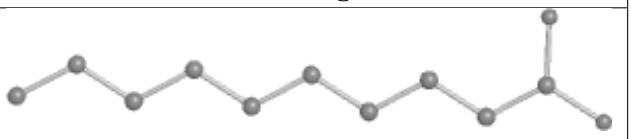
Bond lengths



Bond angles

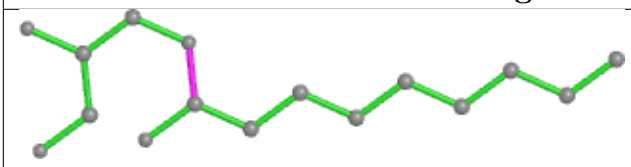


Torsions

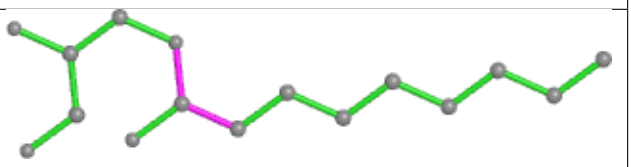


Rings

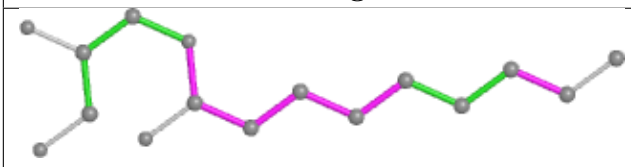
Ligand OLC A 1105



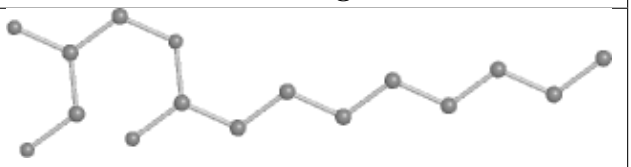
Bond lengths



Bond angles

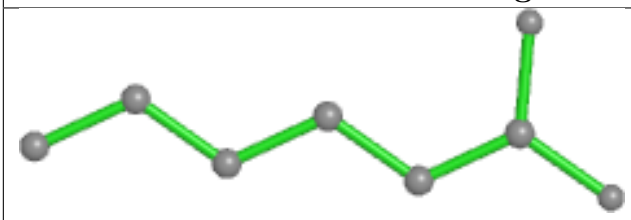


Torsions

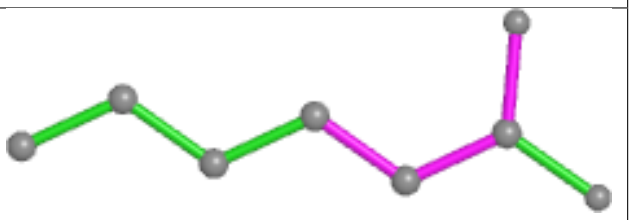


Rings

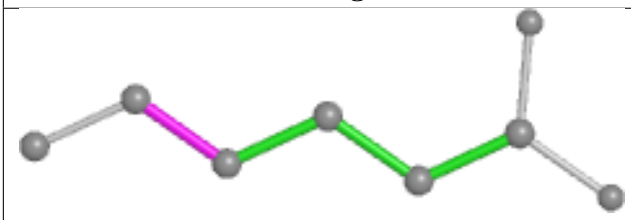
Ligand OLA A 1109



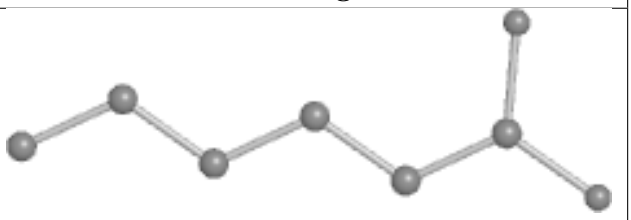
Bond lengths



Bond angles

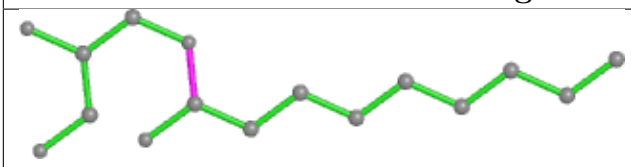


Torsions

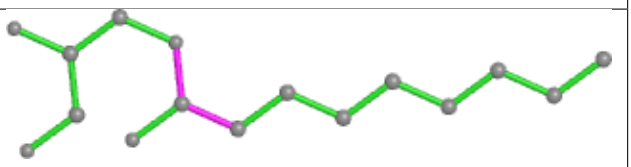


Rings

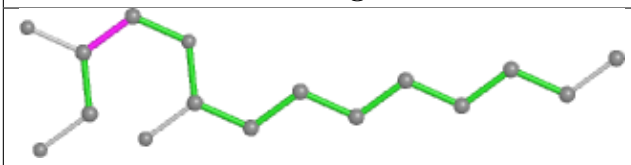
Ligand OLC A 1102



Bond lengths



Bond angles



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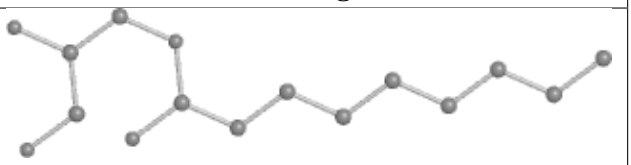
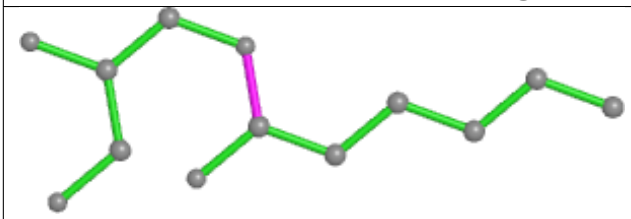
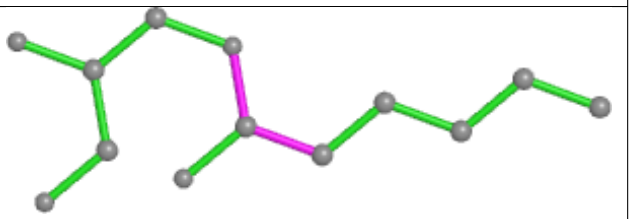


Rings

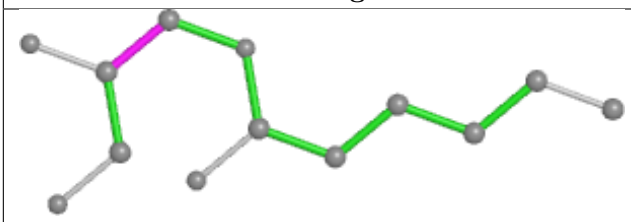
Ligand OLC A 1103



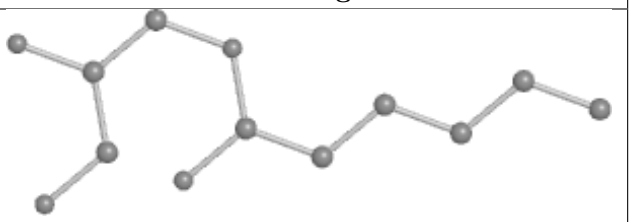
Bond lengths



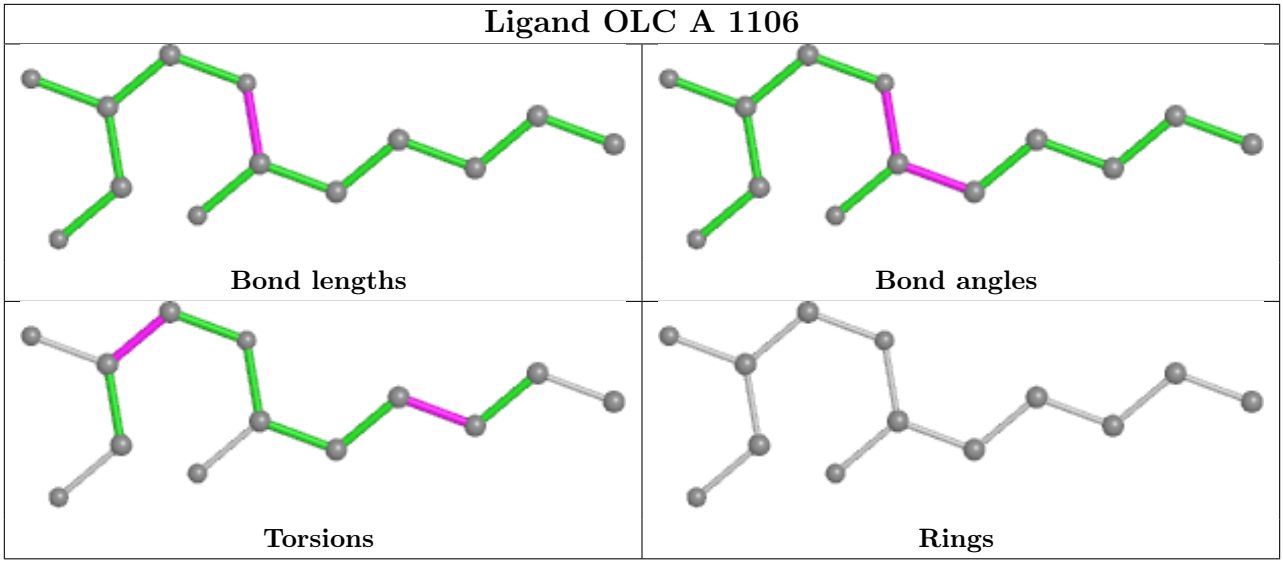
Bond angles

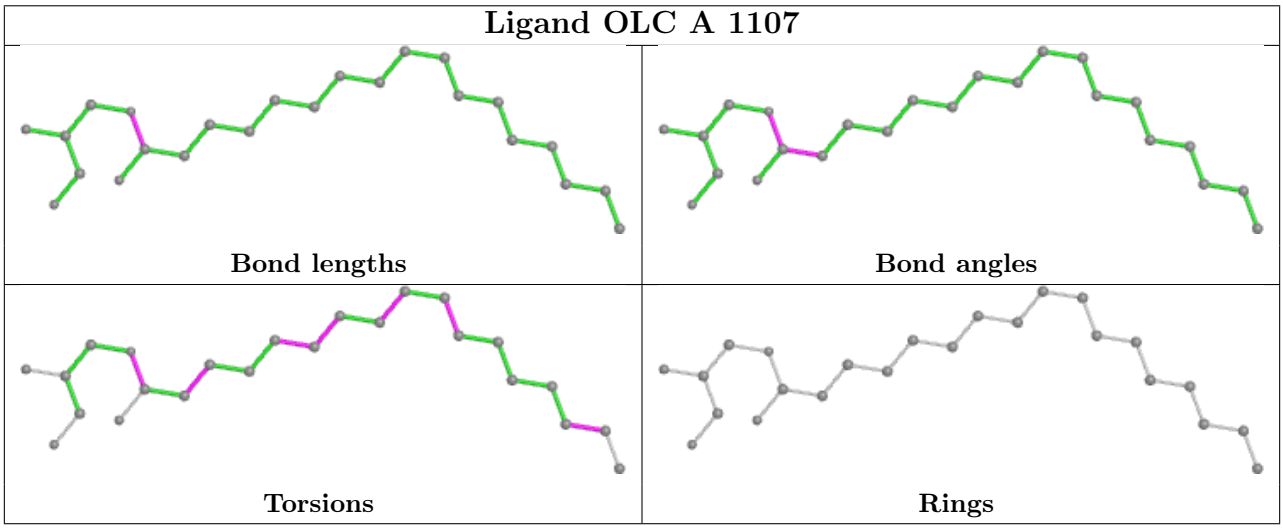


Torsions



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	352/411 (85%)	0.15	20 (5%)	23	22	16, 38, 80, 103	0
2	B	67/75 (89%)	0.28	4 (5%)	21	20	17, 38, 77, 84	0
All	All	419/486 (86%)	0.18	24 (5%)	23	22	16, 38, 80, 103	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	6.8
1	A	221	LEU	4.7
1	A	218	LEU	3.5
1	A	215	SER	3.5
1	A	1032	ASP	3.1
2	B	19	LEU	3.0
1	A	16	THR	2.9
2	B	24	ILE	2.9
1	A	216	GLY	2.8
1	A	58	TYR	2.7
2	B	22	ALA	2.7
1	A	217	ILE	2.7
1	A	1001	MET	2.6
1	A	219	LYS	2.5
2	B	61	TYR	2.4
1	A	234	VAL	2.4
1	A	1025	ASN	2.3
1	A	1030	PHE	2.3
1	A	301	GLY	2.2
1	A	238	PHE	2.1
1	A	136	ALA	2.1
1	A	1015	PRO	2.1
1	A	1020	PRO	2.1
1	A	1026	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	PCA	B	0	8/9	0.93	0.14	31,33,39,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

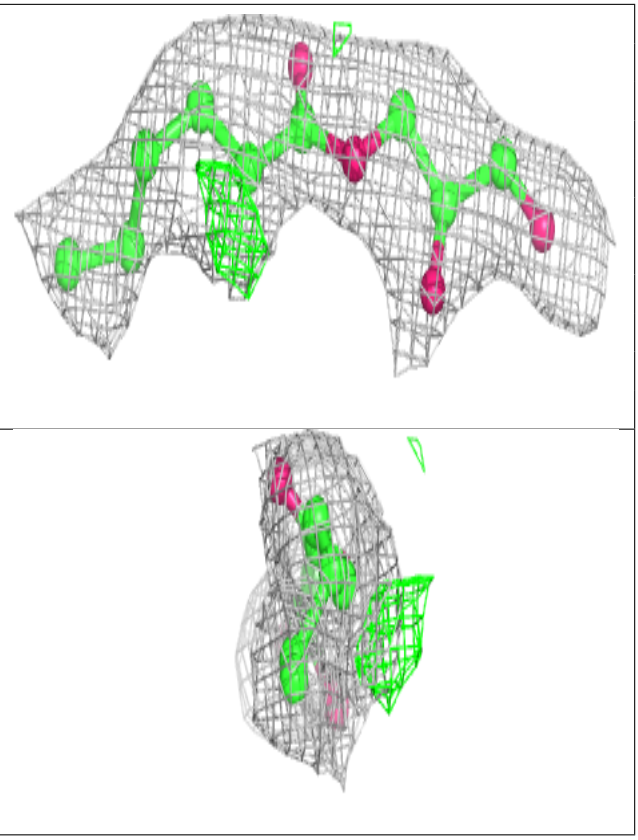
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	1106	13/25	0.63	0.22	61,69,76,76	0
5	OLA	A	1108	12/20	0.65	0.19	44,59,73,75	0
5	OLA	A	1109	8/20	0.69	0.31	75,76,77,78	0
4	OLC	A	1105	16/25	0.82	0.21	38,44,59,60	0
4	OLC	A	1103	13/25	0.83	0.28	47,64,70,74	0
4	OLC	A	1107	24/25	0.84	0.21	35,46,76,78	0
4	OLC	A	1104	21/25	0.88	0.37	45,61,65,66	0
4	OLC	A	1102	16/25	0.88	0.16	30,56,78,79	0
3	ZN	A	1101	1/1	0.98	0.12	35,35,35,35	1

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.

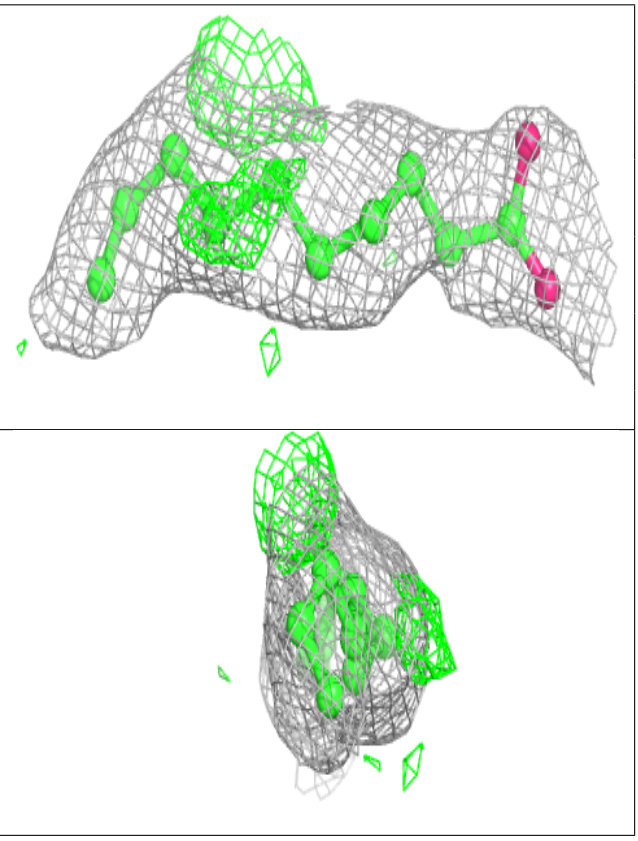
Electron density around OLC A 1106:

$2mF_o$-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 1108:

$2mF_o$-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 1109:

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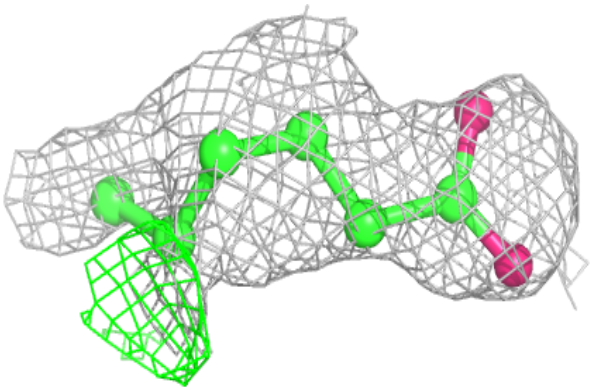
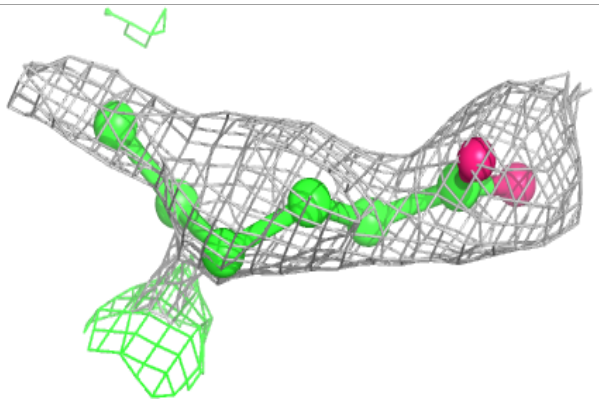
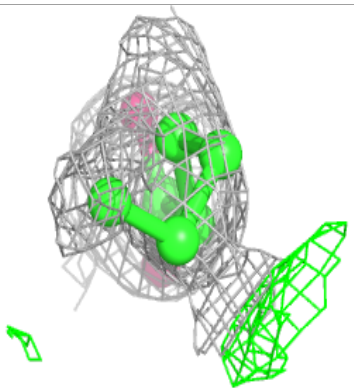
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around OLC A 1105:

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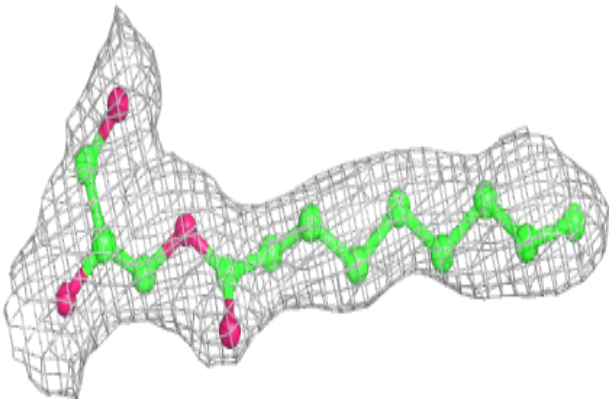
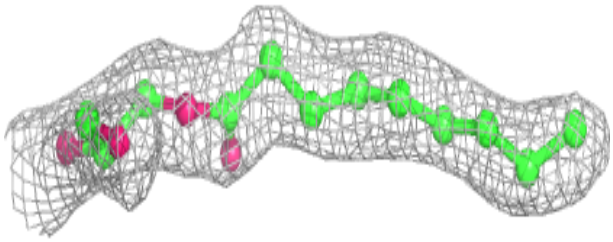
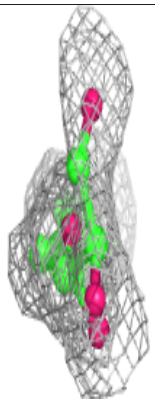
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

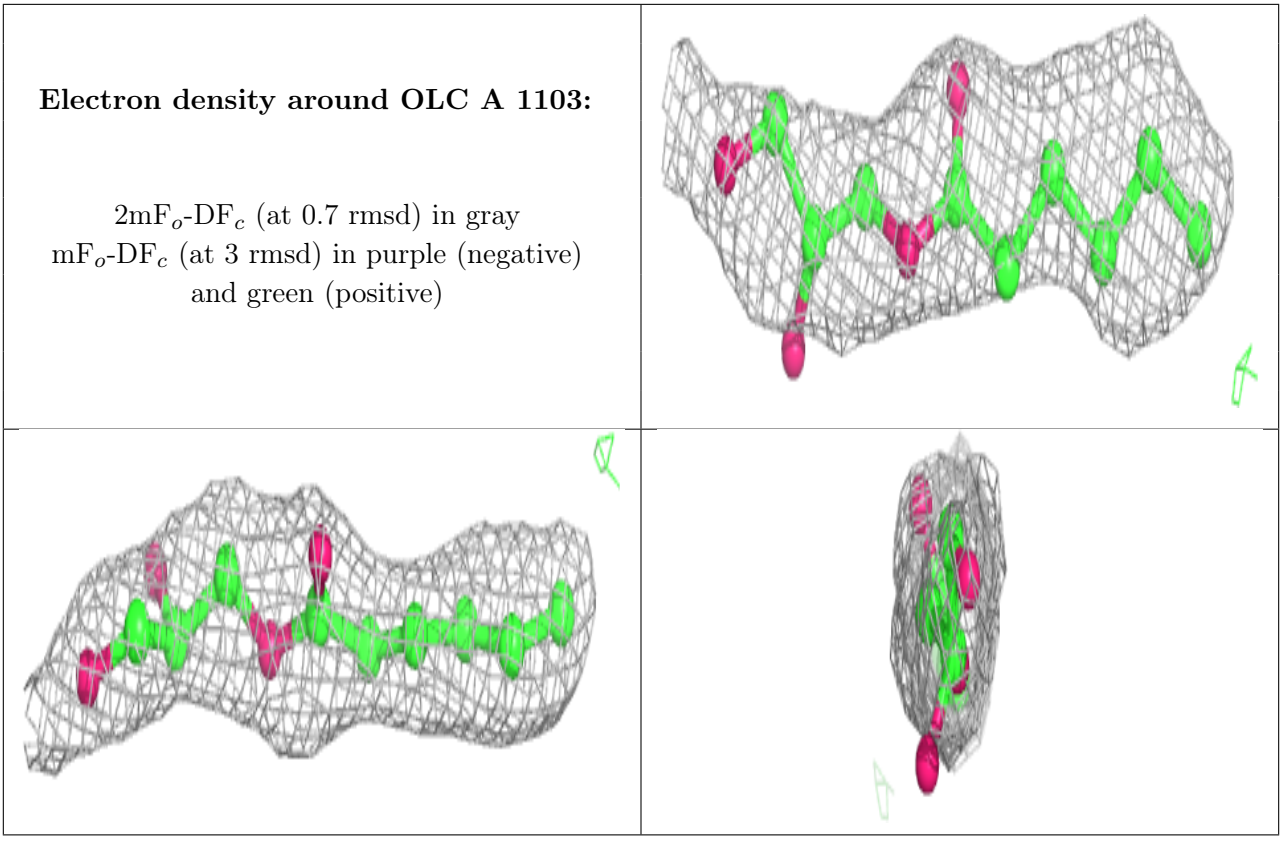






Electron density around OLC A 1103:

$2mF_o$-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 1107:

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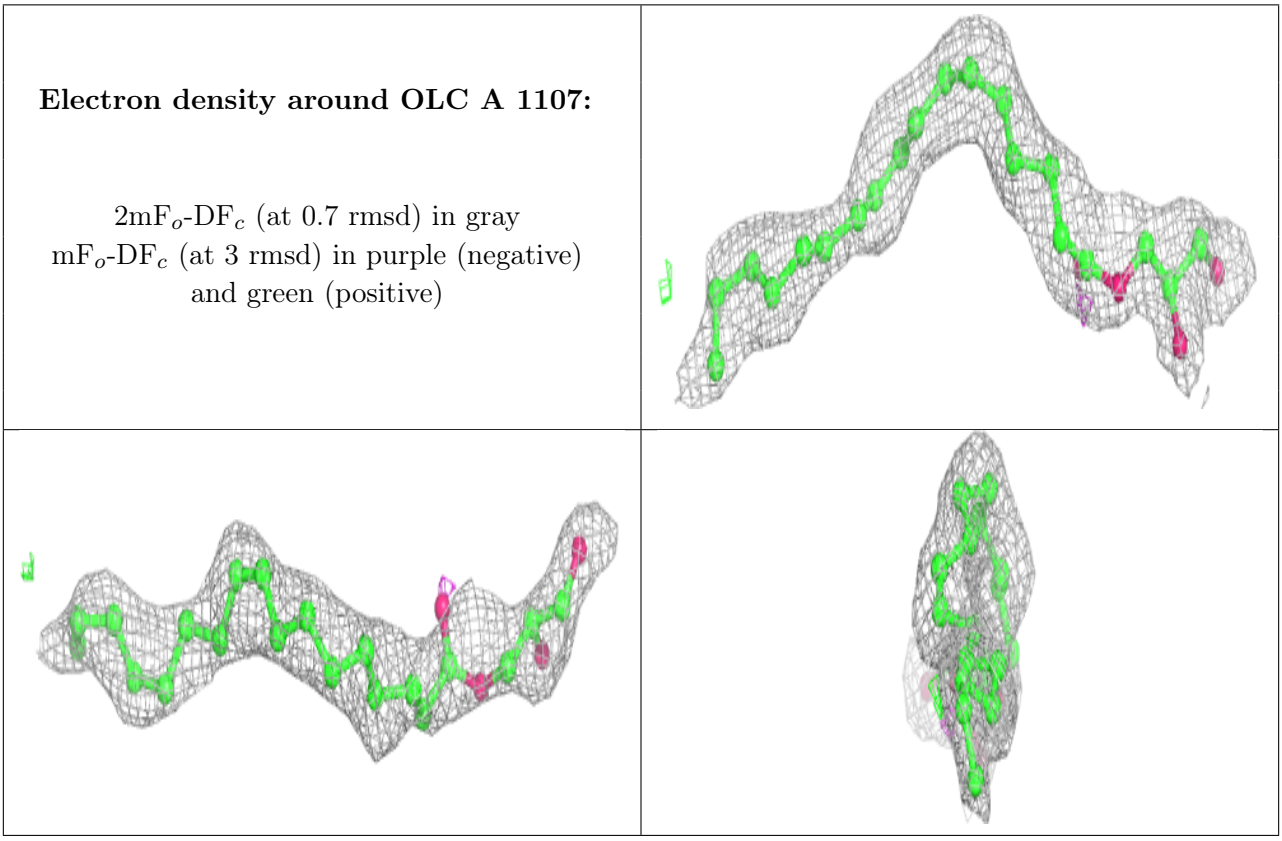
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC A 1104:

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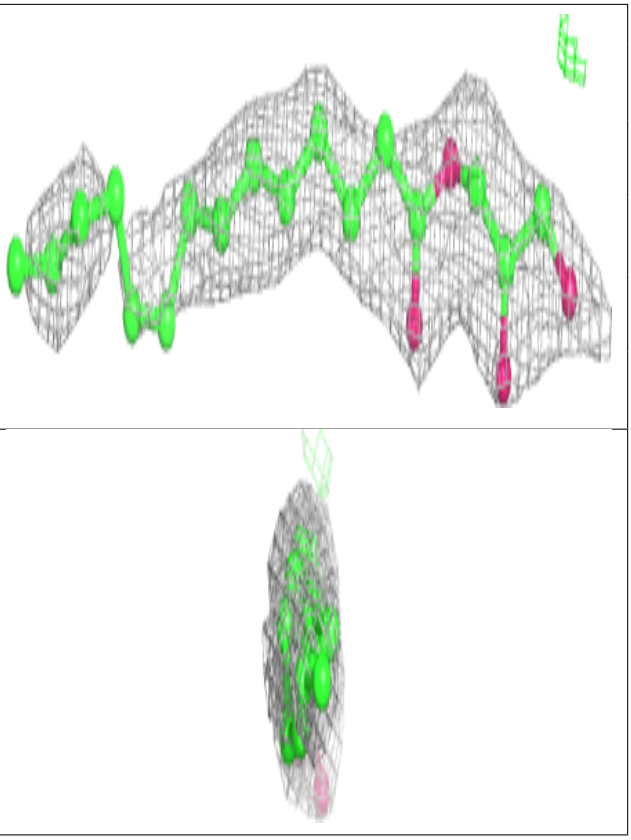
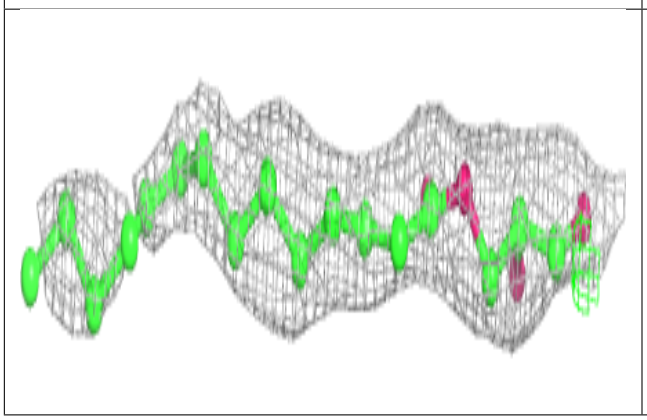
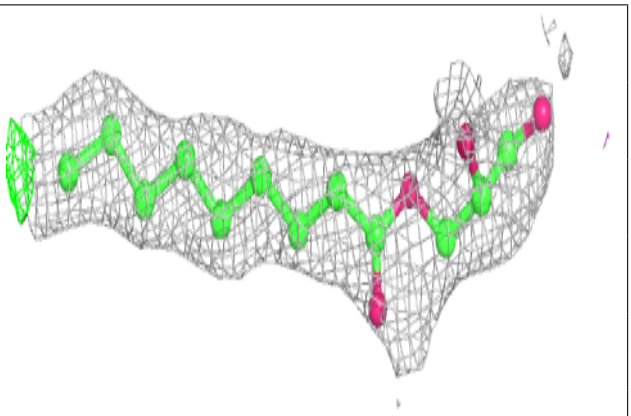
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

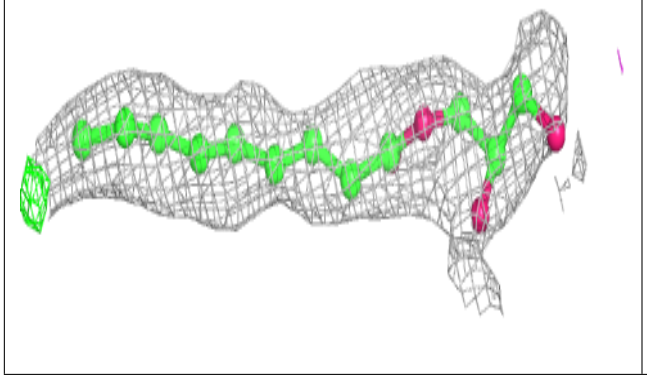


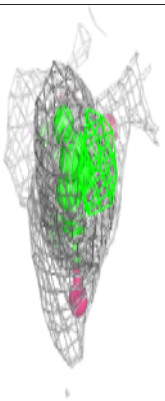


Electron density around OLC A 1102:

$2mF_o$-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.