



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:48 PM BST

PDB ID : 6W25  
Title : Crystal structure of the Melanocortin-4 Receptor (MC4R) in complex with SHU9119  
Authors : Yu, J.; Gimenez, L.E.; Hernandez, C.C.; Wu, Y.; Wein, A.H.; Han, G.W.; McClary, K.; Mittal, S.R.; Burdsall, K.; Stauch, B.; Wu, L.; Stevens, S.N.; Peisley, A.; Williams, S.Y.; Chen, V.; Millhauser, G.L.; Zhao, S.; Cone, R.D.; Stevens, R.C.  
Deposited on : 2020-03-04  
Resolution : 2.75 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.2  
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) : 2.14.2

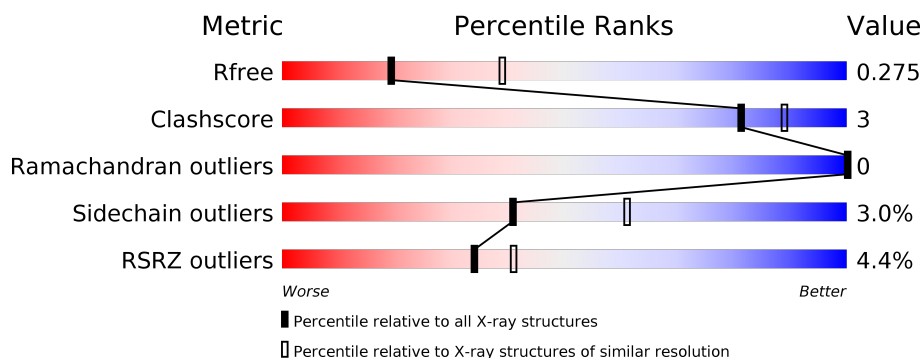
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>13%</div> </div> </div>
2	B	9	<div> <div>56%</div> <div>44%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3821 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 Melanocortin receptor 4, GlgA glycogen synthase, Melanocortin receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	1	0
			3628	2370	580	645	33			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P32245
A	-10	LYS	-	expression tag	UNP P32245
A	-9	THR	-	expression tag	UNP P32245
A	-8	ILE	-	expression tag	UNP P32245
A	-7	ILE	-	expression tag	UNP P32245
A	-6	ALA	-	expression tag	UNP P32245
A	-5	LEU	-	expression tag	UNP P32245
A	-4	SER	-	expression tag	UNP P32245
A	-3	TYR	-	expression tag	UNP P32245
A	-2	ILE	-	expression tag	UNP P32245
A	-1	PHE	-	expression tag	UNP P32245
A	0	CYS	-	expression tag	UNP P32245
A	1	LEU	-	expression tag	UNP P32245
A	2	VAL	-	expression tag	UNP P32245
A	3	PHE	-	expression tag	UNP P32245
A	4	ALA	-	expression tag	UNP P32245
A	5	ASP	-	expression tag	UNP P32245
A	6	TYR	-	expression tag	UNP P32245
A	7	LYS	-	expression tag	UNP P32245
A	8	ASP	-	expression tag	UNP P32245
A	9	ASP	-	expression tag	UNP P32245
A	10	ASP	-	expression tag	UNP P32245
A	11	ASP	-	expression tag	UNP P32245
A	12	ALA	-	expression tag	UNP P32245
A	13	GLY	-	expression tag	UNP P32245
A	14	ARG	-	expression tag	UNP P32245

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	-	expression tag	UNP P32245
A	49	VAL	GLU	engineered mutation	UNP P32245
A	97	LEU	ASN	engineered mutation	UNP P32245
A	99	PHE	SER	engineered mutation	UNP P32245
A	131	ALA	SER	engineered mutation	UNP P32245
A	298	ASN	ASP	engineered mutation	UNP P32245
A	2000	GLU	-	expression tag	UNP P32245
A	2001	PHE	-	expression tag	UNP P32245
A	2002	LEU	-	expression tag	UNP P32245
A	2003	GLU	-	expression tag	UNP P32245
A	2004	VAL	-	expression tag	UNP P32245
A	2005	LEU	-	expression tag	UNP P32245
A	2006	PHE	-	expression tag	UNP P32245
A	2007	GLN	-	expression tag	UNP P32245
A	2008	GLY	-	expression tag	UNP P32245
A	2009	PRO	-	expression tag	UNP P32245
A	2010	HIS	-	expression tag	UNP P32245
A	2011	HIS	-	expression tag	UNP P32245
A	2012	HIS	-	expression tag	UNP P32245
A	2013	HIS	-	expression tag	UNP P32245
A	2014	HIS	-	expression tag	UNP P32245
A	2015	HIS	-	expression tag	UNP P32245
A	2016	HIS	-	expression tag	UNP P32245
A	2017	HIS	-	expression tag	UNP P32245
A	2018	HIS	-	expression tag	UNP P32245
A	2019	HIS	-	expression tag	UNP P32245

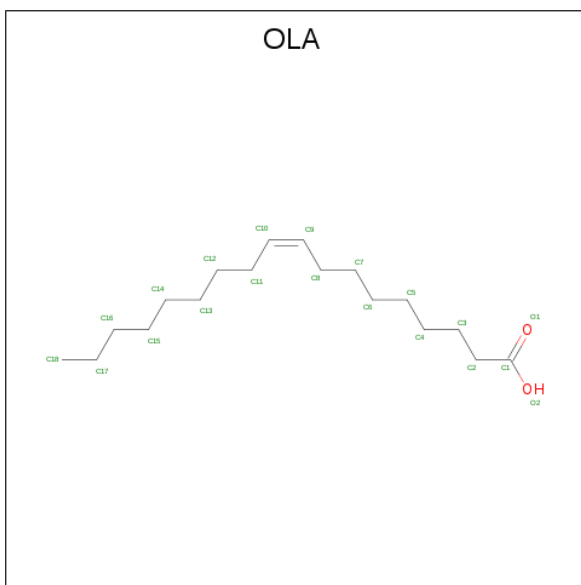
- Molecule 2 is a protein called SHU9119.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	1
			78	54	15	9			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			10	8	2		
4	A	1	Total	C	O	0	0
			7	5	2		
4	A	1	Total	C	O	0	0
			18	16	2		
4	A	1	Total	C	O	0	0
			12	10	2		
4	A	1	Total	C	O	0	0
			17	15	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			15	13	2		

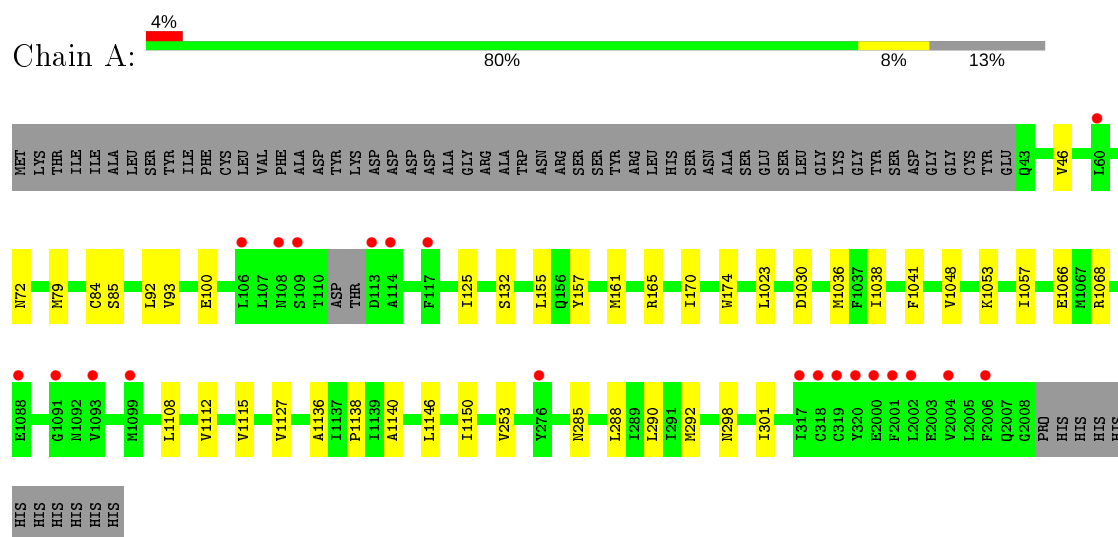
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	5	Total	O	0	0
			5	5		

### 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: Melanocortin receptor 4, GlgA glycogen synthase, Melanocortin receptor 4



- Molecule 2: SHU9119



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.91 Å   44.49 Å   88.05 Å 90.00°   97.47°   90.00°	Depositor
Resolution (Å)	43.65 – 2.75 42.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.65-2.75) 100.0 (42.91-2.75)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.77 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.233   ,   0.259 0.241   ,   0.275	Depositor DCC
$R_{free}$ test set	815 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.3	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, ACE, CA, 4J2, NLE, YCM, NH2

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	0.40	0/3687	0.58	0/4990
2	B	1.62	2/52 (3.8%)	1.49	0/66
All	All	0.44	2/3739 (0.1%)	0.60	0/5056

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	TRP	CG-CD2	-5.64	1.34	1.43
2	B	6	TRP	CD2-CE2	-5.09	1.35	1.41

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	3628	0	3685	19	0
2	B	78	0	69	0	0
3	A	1	0	0	0	0
4	A	93	0	115	2	0
5	A	16	0	0	0	0
5	B	5	0	0	0	0
All	All	3821	0	3869	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)
1:A:1030:ASP:HB3	1:A:1068:ARG:HH11	1.62	0.65
1:A:253:VAL:HG21	1:A:301:ILE:HD11	1.82	0.60
1:A:1036:MET:HB2	1:A:1112:VAL:HG11	1.89	0.53
1:A:157:TYR:CZ	1:A:161:MET:HG3	2.44	0.52
1:A:170:ILE:HG21	4:A:2107:OLA:H52	1.92	0.51
1:A:157:TYR:CE1	1:A:161:MET:HG3	2.48	0.49
1:A:1053:LYS:O	1:A:1057:ILE:HG12	2.13	0.48
1:A:85:SER:HB2	1:A:174:TRP:HE1	1.79	0.48
1:A:1023:LEU:HD21	1:A:1108:LEU:HD23	1.97	0.47
1:A:93:VAL:HG23	1:A:132:SER:HB2	1.96	0.45
1:A:1140:ALA:HB1	1:A:1146:LEU:HD13	1.97	0.45
1:A:46:VAL:HG22	1:A:285:ASN:HB3	1.98	0.45
1:A:46:VAL:CG2	1:A:285:ASN:HB3	2.47	0.44
1:A:298:ASN:HA	1:A:301:ILE:HD12	2.00	0.44
1:A:288:LEU:O	1:A:292:MET:HG2	2.19	0.43
1:A:1138:PRO:HG2	1:A:1150:ILE:HG12	2.02	0.41
4:A:2104:OLA:H21	4:A:2109:OLA:H41	2.03	0.41
1:A:1115:VAL:HG23	1:A:1136:ALA:HB1	2.02	0.41
1:A:100:GLU:HB2	1:A:125:ILE:HG21	2.02	0.41
1:A:1041:PHE:HA	1:A:1048:VAL:HG11	2.03	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	464/535 (87%)	453 (98%)	11 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	5/9 (56%)	5 (100%)	0	0	100	100
All	All	469/544 (86%)	458 (98%)	11 (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	396/466 (85%)	386 (98%)	10 (2%)	47	67
2	B	5/5 (100%)	3 (60%)	2 (40%)	0	0
All	All	401/471 (85%)	389 (97%)	12 (3%)	41	61

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

Mol	Chain	Res	Type
1	A	72	ASN
1	A	79	MET
1	A	84	CYS
1	A	92	LEU
1	A	155	LEU
1	A	165	ARG
1	A	1038	ILE
1	A	1066	GLU
1	A	1127	VAL
1	A	290	LEU
2	B	5	ARG
2	B	7	LYS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	YCM	A	1004	1	7,9,10	0.40	0	4,10,12	0.34	0
2	NLE	B	1	2	6,7,8	0.67	0	2,7,9	0.68	0
2	4J2	B	4	3,2	15,16,17	1.52	1 (6%)	18,21,23	0.71	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
1	YCM	A	1004	1	-	1/6/8/10	-
2	NLE	B	1	2	-	2/5/6/8	-
2	4J2	B	4	3,2	-	0/5/6/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	4J2	CB-CG	-4.48	1.40	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NLE	CA-CB-CG-CD

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1	NLE	CE-CD-CG-CB
1	A	1004	YCM	SG-CD-CE-NZ2

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	OLA	A	2108	-	4,7,19	0.26	0	3,7,19	0.56	0
4	OLA	A	2107	-	13,16,19	0.27	0	12,16,19	0.55	0
4	OLA	A	2104	-	3,6,19	0.25	0	2,6,19	0.53	0
4	OLA	A	2103	-	6,9,19	0.25	0	5,9,19	0.54	0
4	OLA	A	2109	-	11,14,19	0.31	0	10,14,19	0.40	0
4	OLA	A	2105	-	14,17,19	0.28	0	13,17,19	0.51	0
4	OLA	A	2106	-	8,11,19	0.35	0	7,11,19	0.76	0
4	OLA	A	2102	-	2,5,19	0.37	0	2,5,19	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	2108	-	-	2/3/5/17	-
4	OLA	A	2107	-	-	7/12/14/17	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	2104	-	-	1/2/4/17	-
4	OLA	A	2103	-	-	2/5/7/17	-
4	OLA	A	2109	-	-	7/10/12/17	-
4	OLA	A	2105	-	-	7/13/15/17	-
4	OLA	A	2106	-	-	3/7/9/17	-
4	OLA	A	2102	-	-	0/1/3/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2108	OLA	C1-C2-C3-C4
4	A	2107	OLA	C1-C2-C3-C4
4	A	2109	OLA	C1-C2-C3-C4
4	A	2105	OLA	C1-C2-C3-C4
4	A	2103	OLA	C2-C3-C4-C5
4	A	2105	OLA	C12-C13-C14-C15
4	A	2109	OLA	C4-C5-C6-C7
4	A	2105	OLA	C10-C11-C12-C13
4	A	2105	OLA	C4-C5-C6-C7
4	A	2109	OLA	C2-C3-C4-C5
4	A	2107	OLA	C3-C4-C5-C6
4	A	2107	OLA	C6-C7-C8-C9
4	A	2109	OLA	C5-C6-C7-C8
4	A	2109	OLA	C6-C7-C8-C9
4	A	2104	OLA	C2-C3-C4-C5
4	A	2106	OLA	C6-C7-C8-C9
4	A	2103	OLA	C5-C6-C7-C8
4	A	2109	OLA	C10-C11-C12-C13
4	A	2105	OLA	C13-C14-C15-C16
4	A	2108	OLA	C3-C4-C5-C6
4	A	2105	OLA	C3-C4-C5-C6
4	A	2107	OLA	C12-C13-C14-C15
4	A	2107	OLA	C2-C3-C4-C5
4	A	2106	OLA	C4-C5-C6-C7
4	A	2107	OLA	C7-C8-C9-C10
4	A	2105	OLA	C7-C8-C9-C10
4	A	2107	OLA	C4-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

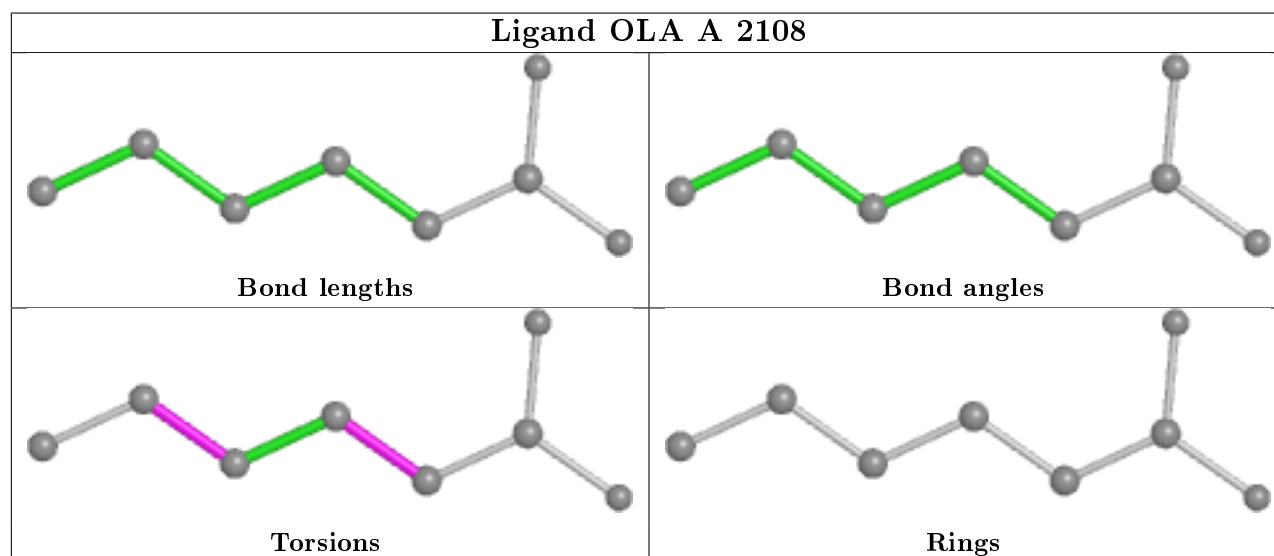
Mol	Chain	Res	Type	Atoms
4	A	2106	OLA	C7-C8-C9-C10
4	A	2109	OLA	C3-C4-C5-C6

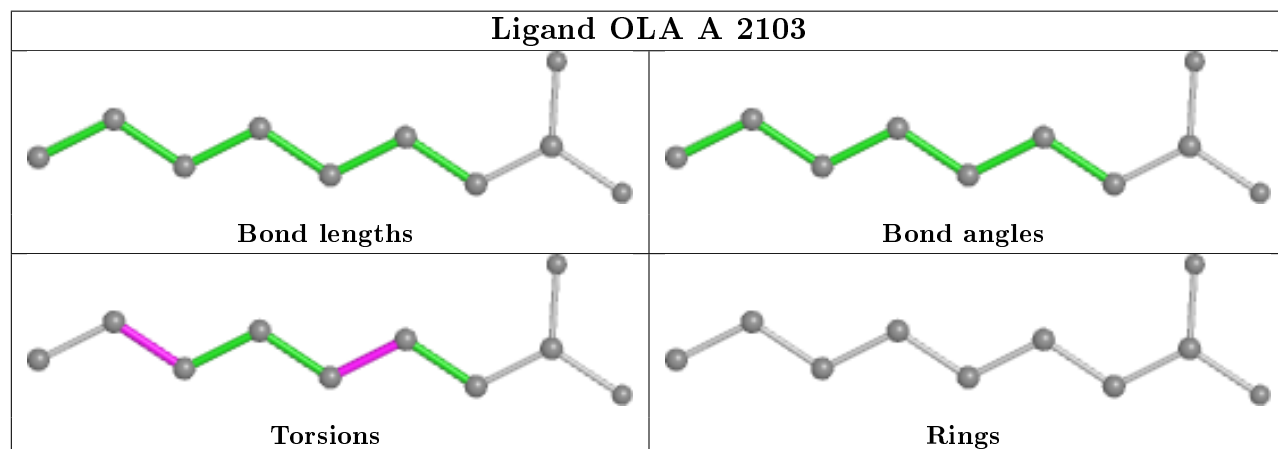
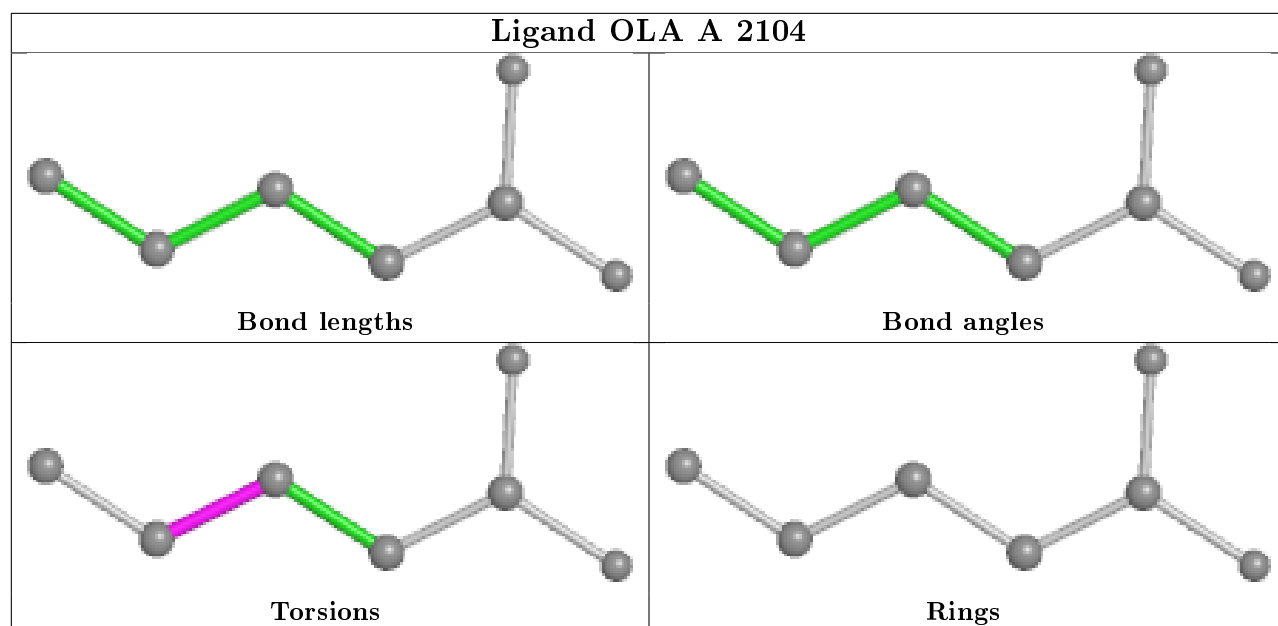
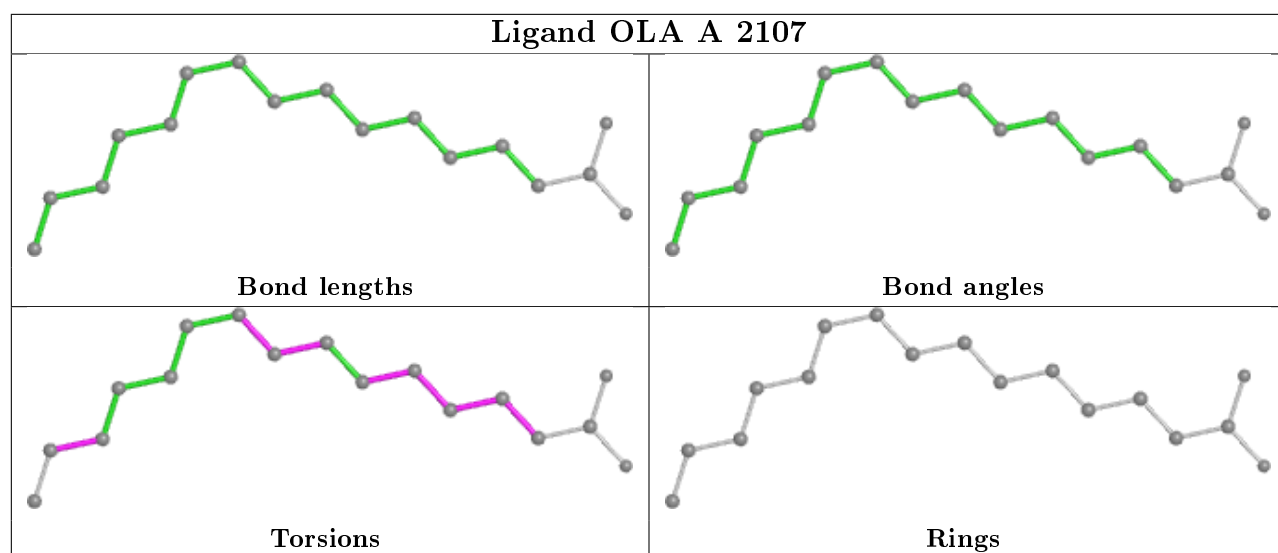
There are no ring outliers.

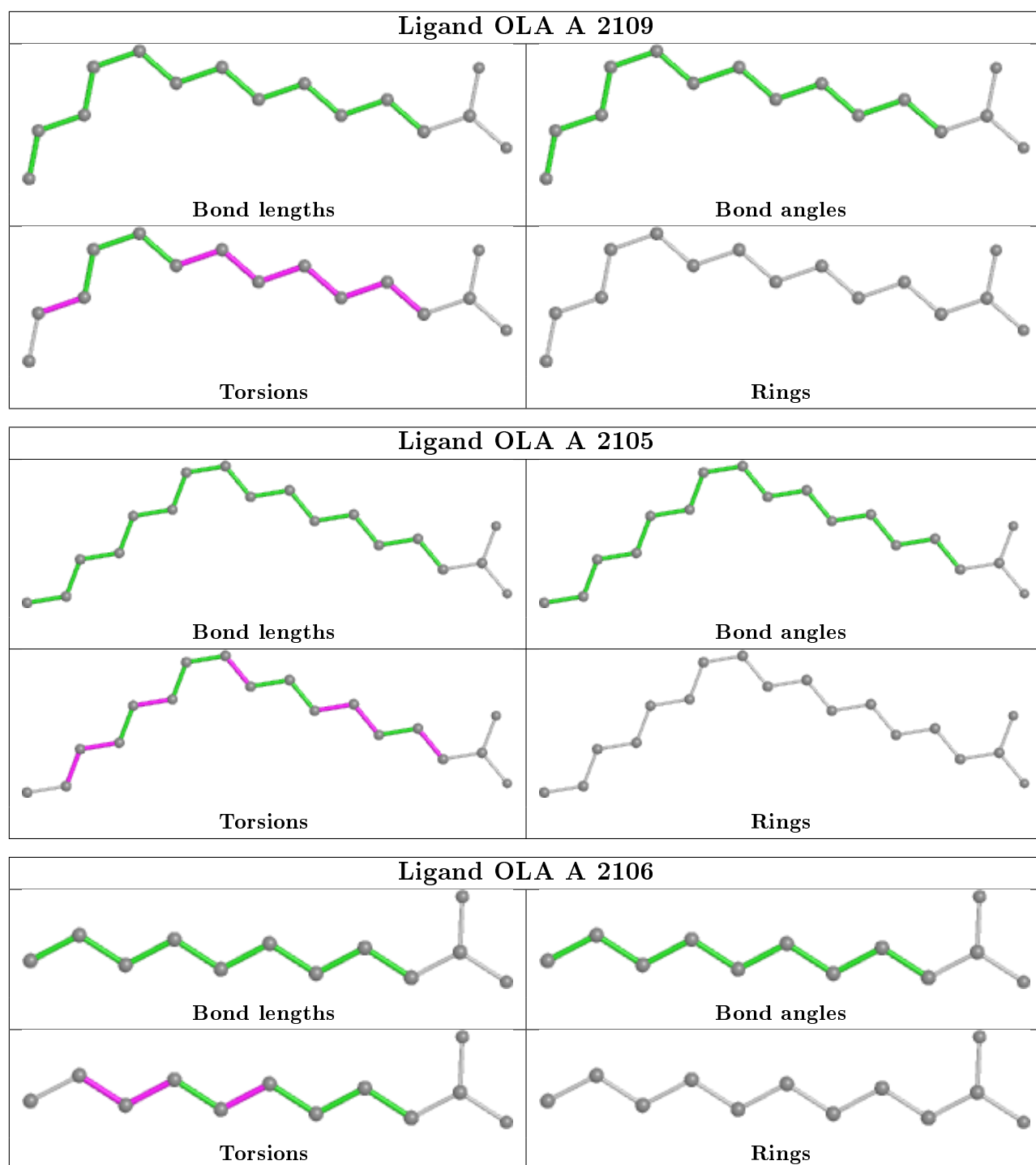
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2107	OLA	1	0
4	A	2104	OLA	1	0
4	A	2109	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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	467/535 (87%)	0.51	21 (4%) 33 39	58, 76, 114, 162	0
2	B	5/9 (55%)	0.07	0 100 100	69, 72, 79, 80	0
All	All	472/544 (86%)	0.50	21 (4%) 34 41	58, 76, 114, 162	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	SER	8.7
1	A	320	TYR	8.3
1	A	108	ASN	5.2
1	A	2001	PHE	5.1
1	A	319	CYS	5.1
1	A	2002	LEU	4.5
1	A	117	PHE	3.8
1	A	2006	PHE	3.7
1	A	2004	VAL	3.7
1	A	1099	MET	3.3
1	A	318	CYS	3.2
1	A	106	LEU	2.9
1	A	1093	VAL	2.8
1	A	113	ASP	2.8
1	A	1091	GLY	2.4
1	A	276	TYR	2.3
1	A	2000	GLU	2.1
1	A	317	ILE	2.0
1	A	1088	GLU	2.0
1	A	114	ALA	2.0
1	A	60	LEU	2.0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NLE	B	1	8/9	0.89	0.20	84,84,85,87	0
2	4J2	B	4	15/16	0.96	0.17	62,64,70,72	0
1	YCM	A	1004	10/11	0.97	0.17	70,74,75,75	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

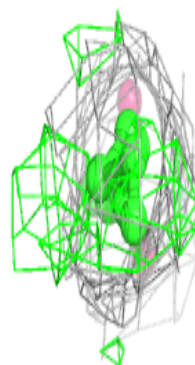
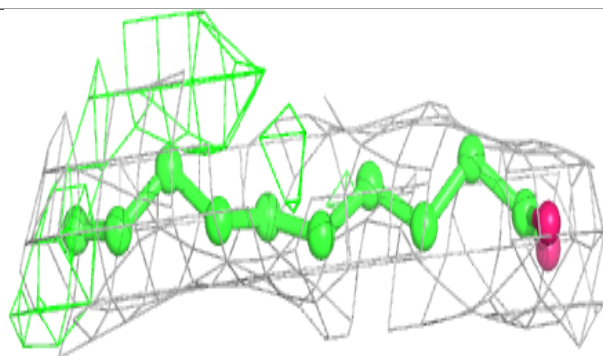
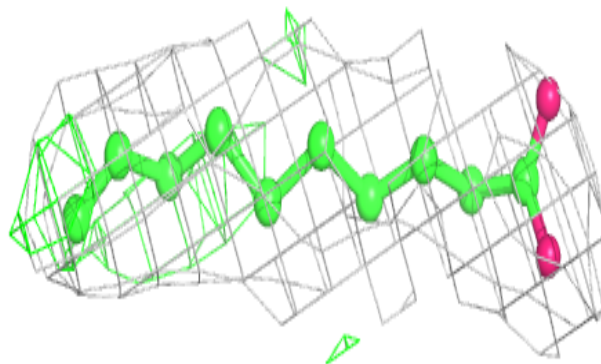
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OLA	A	2106	12/20	0.72	0.17	104,107,110,110	0
4	OLA	A	2108	8/20	0.73	0.34	83,84,86,86	0
4	OLA	A	2109	15/20	0.74	0.22	100,103,107,107	0
4	OLA	A	2102	6/20	0.77	0.26	93,94,95,96	0
4	OLA	A	2105	18/20	0.79	0.35	79,83,90,90	0
4	OLA	A	2107	17/20	0.81	0.32	87,89,93,93	0
4	OLA	A	2104	7/20	0.83	0.33	92,93,94,95	0
4	OLA	A	2103	10/20	0.91	0.38	67,72,75,76	0
3	CA	A	2101	1/1	0.95	0.14	84,84,84,84	0

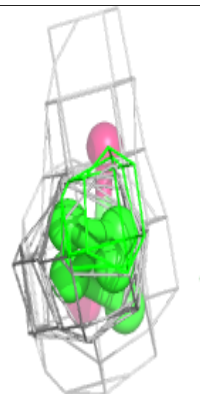
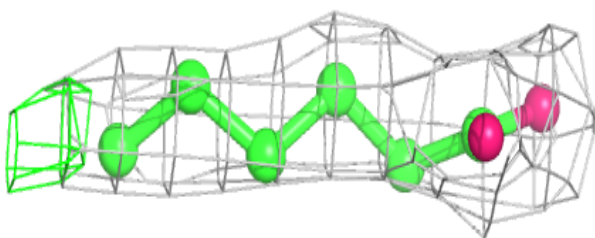
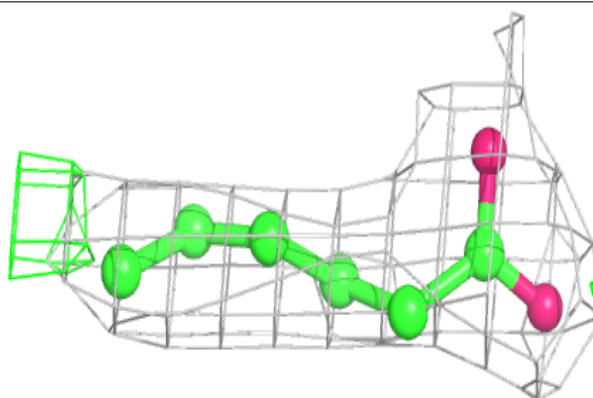
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLA A 2106:**

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

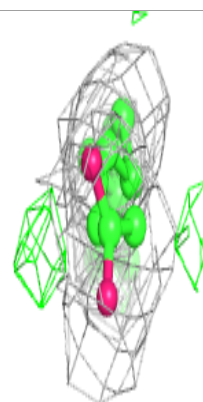
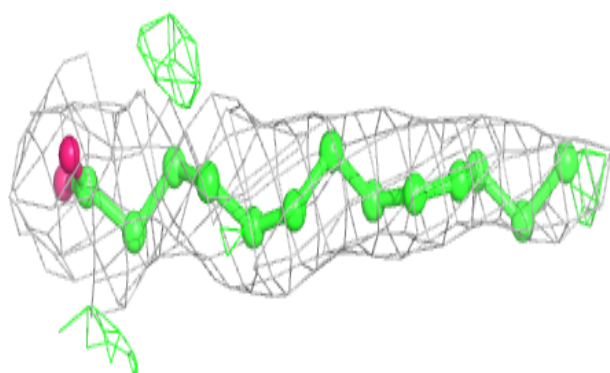
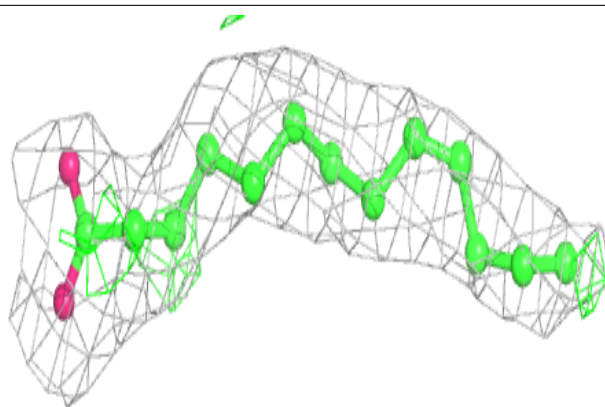
**Electron density around OLA A 2108:**

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

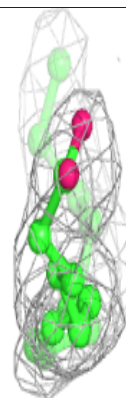
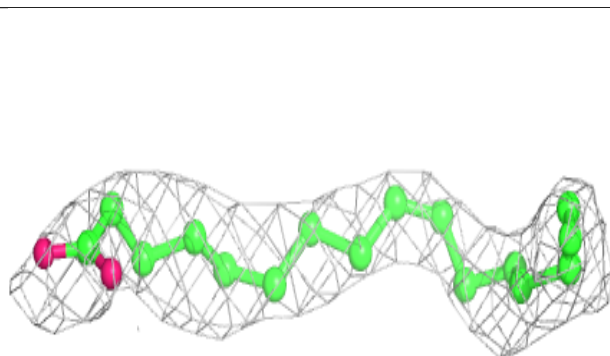
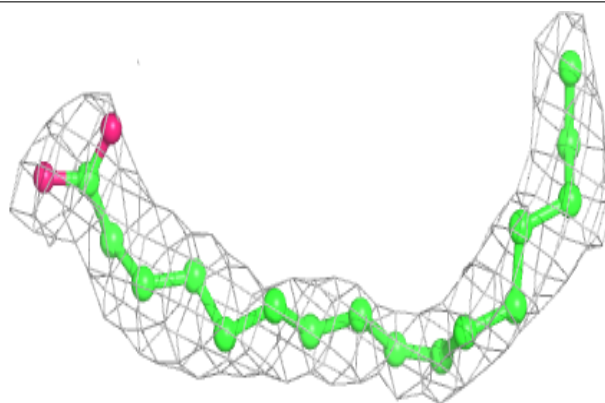


**Electron density around OLA A 2109:**

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

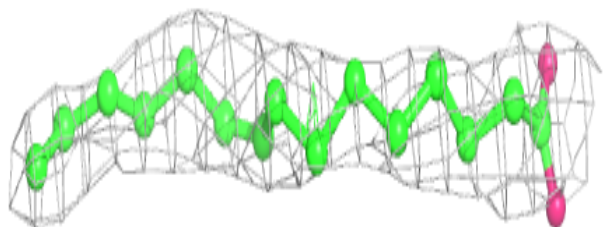
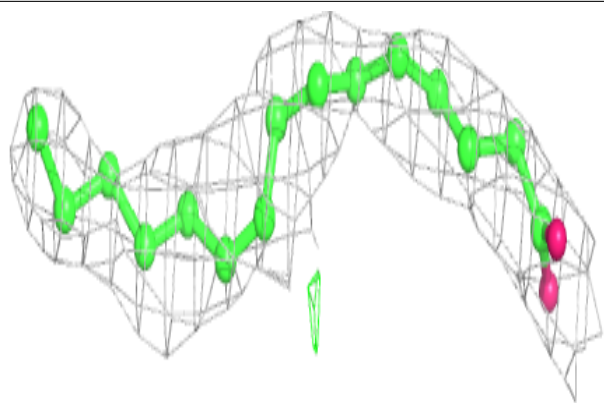
**Electron density around OLA A 2105:**

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

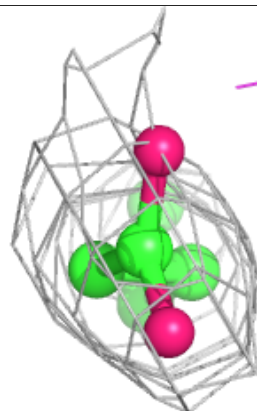
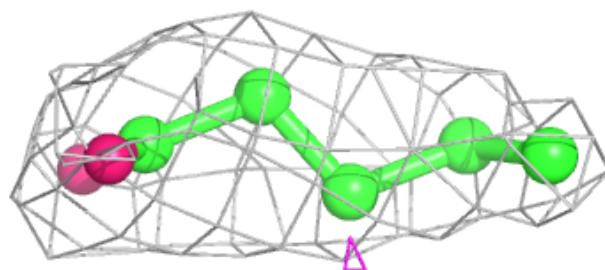
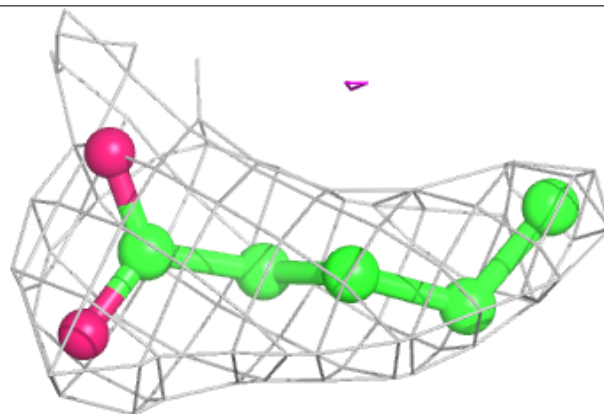


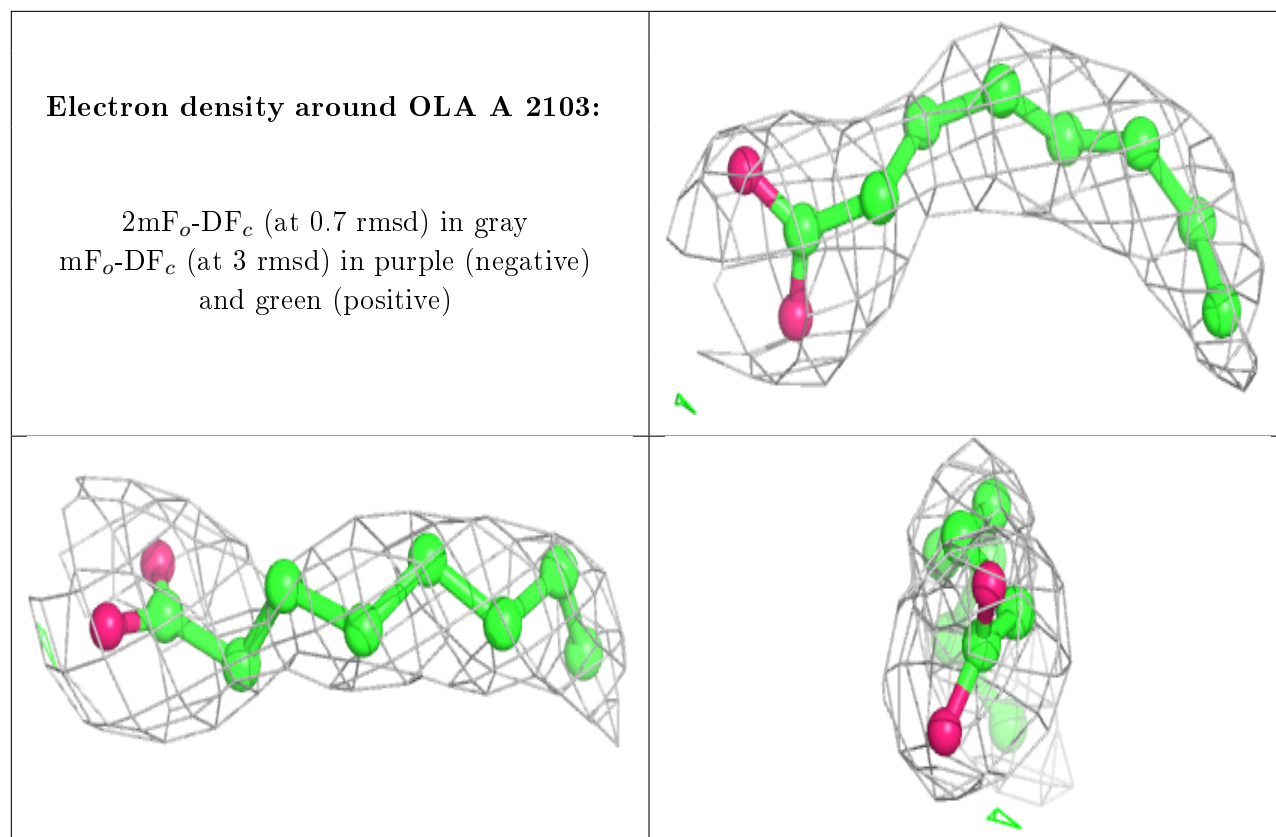
**Electron density around OLA A 2107:**

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

**Electron density around OLA A 2104:**

$2mF_o-DF_c$  (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.