



# wwPDB X-ray Structure Validation Summary Report

Mar 10, 2026 – 12:18 PM UTC

PDB ID : 5EE7 / pdb\_00005ee7  
Title : Crystal structure of the human glucagon receptor (GCGR) in complex with the antagonist MK-0893  
Authors : Jazayeri, A.; Dore, A.S.; Lamb, D.; Krishnamurthy, H.; Southall, S.M.; Baig, A.H.; Bortolato, A.; Koglin, M.; Robertson, N.J.; Errey, J.C.; Andrews, S.P.; Brown, A.J.H.; Cooke, R.M.; Weir, M.; Marshall, F.H.  
Deposited on : 2015-10-22  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

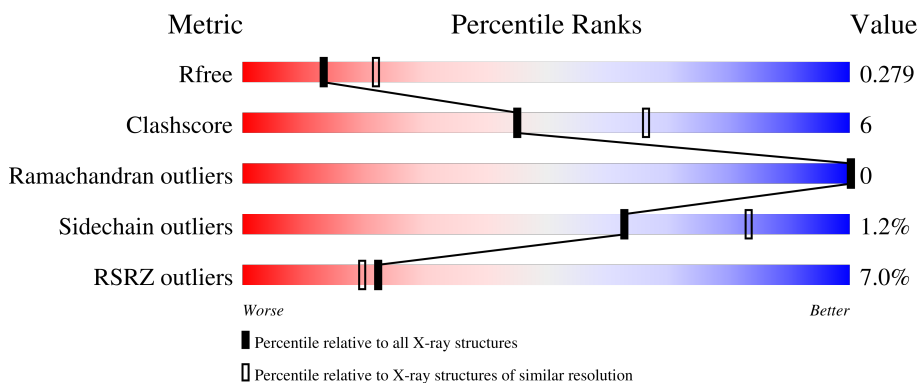
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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  $\geq 3$ , 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	452	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3619 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 Glucagon receptor,Endolysin,Glucagon receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3331	2184	573	560	14	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

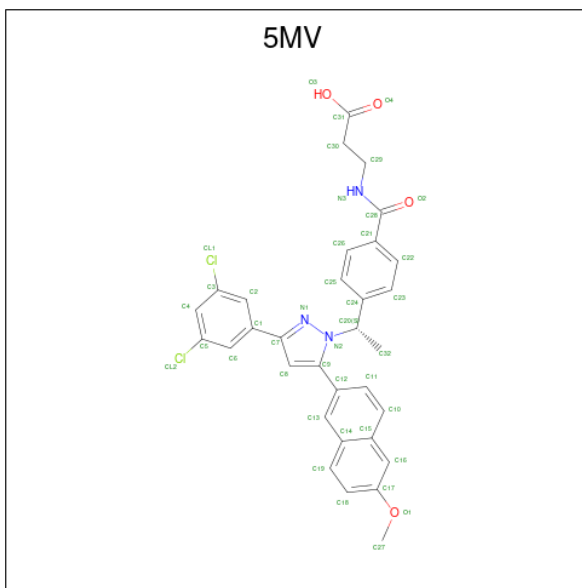
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	MET	engineered mutation	UNP P47871
A	154	ALA	GLY	engineered mutation	UNP P47871
A	173	ALA	ARG	engineered mutation	UNP P47871
A	182	LEU	ALA	engineered mutation	UNP P47871
A	190	ALA	SER	engineered mutation	UNP P47871
A	193	PHE	VAL	engineered mutation	UNP P47871
A	207	GLU	GLY	engineered mutation	UNP P47871
A	223	ALA	GLY	engineered mutation	UNP P47871
A	255	LEU	MET	linker	UNP P00720
A	1010	GLY	ARG	engineered mutation	UNP P00720
A	1052	THR	CYS	engineered mutation	UNP P00720
A	1095	ALA	CYS	engineered mutation	UNP P00720
A	1135	ARG	ILE	engineered mutation	UNP P00720
A	1159	TYR	-	linker	UNP P00720
A	276	ALA	MET	engineered mutation	UNP P47871
A	344	ALA	LYS	engineered mutation	UNP P47871
A	362	PHE	GLU	engineered mutation	UNP P47871
A	387	ALA	PHE	engineered mutation	UNP P47871
A	418	ALA	-	expression tag	UNP P47871
A	419	ALA	-	expression tag	UNP P47871
A	420	ALA	-	expression tag	UNP P47871
A	421	HIS	-	expression tag	UNP P47871
A	422	HIS	-	expression tag	UNP P47871
A	423	HIS	-	expression tag	UNP P47871
A	424	HIS	-	expression tag	UNP P47871
A	425	HIS	-	expression tag	UNP P47871
A	426	HIS	-	expression tag	UNP P47871

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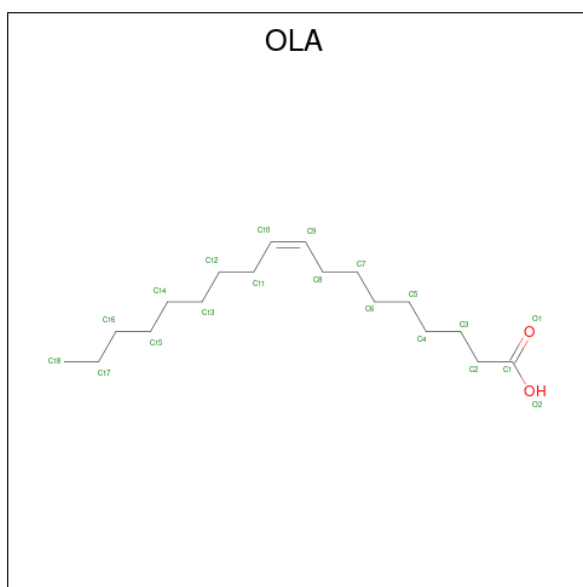
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP P47871
A	428	HIS	-	expression tag	UNP P47871
A	429	HIS	-	expression tag	UNP P47871
A	430	HIS	-	expression tag	UNP P47871

- Molecule 2 is 3-[[4-[(1 {S})-1-[3-[3,5-bis(chloranyl)phenyl]-5-(6-methoxynaphthalen-2-yl)pyrazol-1-yl]ethyl]phenyl]carbonylamino]propanoic acid (CCD ID: 5MV) (formula: C<sub>32</sub>H<sub>27</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>4</sub>).



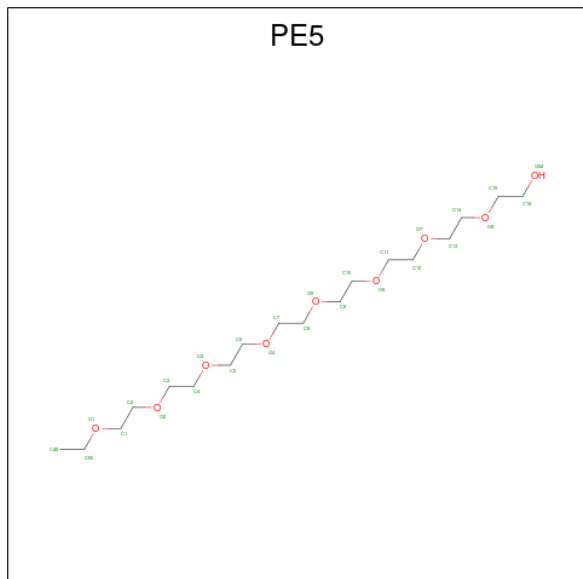
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	41	32	2	3	4	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



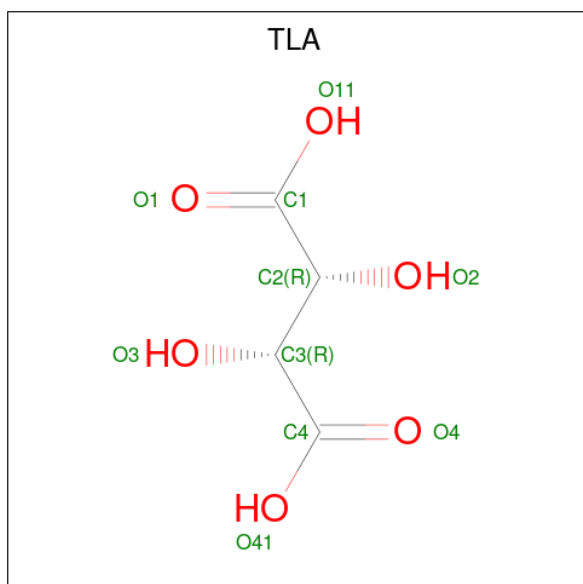
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 8 2	0	0
3	A	1	Total C O 15 13 2	0	0
3	A	1	Total C O 15 13 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 11 9 2	0	0

- Molecule 4 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula:  $C_{18}H_{38}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	24	16	8	0	0

- Molecule 5 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	4	6	0	0

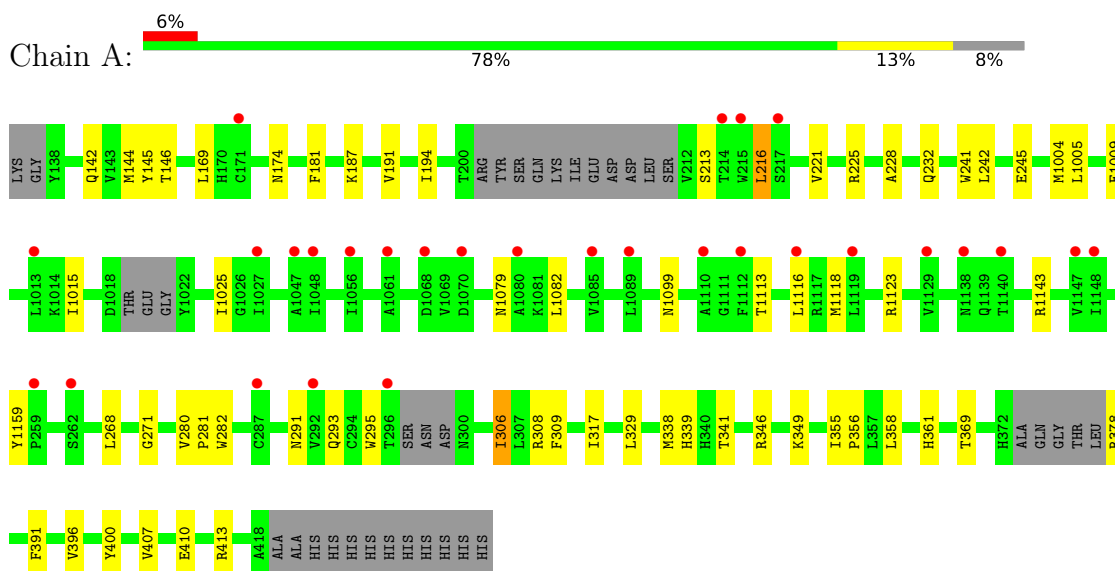
- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	24	Total 24	O 24	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: Glucagon receptor,Endolysin,Glucagon receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.58Å 71.48Å 183.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (19.97-2.50) 89.5 (19.97-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.226 , 0.263 (Not available) , 0.279	Depositor DCC
$R_{free}$ test set	777 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% 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: 5MV, OLA, TLA, PE5

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	0/3408	0.68	2/4618 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	PHE	CA-C-N	-5.10	113.39	119.05
1	A	309	PHE	C-N-CA	-5.10	113.39	119.05

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	3331	0	3403	39	0
2	A	41	0	0	2	0
3	A	189	0	271	6	0
4	A	24	0	33	7	0
5	A	10	0	4	1	0
6	A	24	0	0	0	0
All	All	3619	0	3711	43	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 6.

The worst 5 of 43 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:306:ILE:H	1:A:306:ILE:HD12	1.42	0.84
1:A:391:PHE:HB3	3:A:1204:OLA:H9	1.69	0.74
1:A:1118:MET:HG2	1:A:1123:ARG:HH21	1.54	0.71
1:A:308:ARG:NH2	1:A:369:THR:OG1	2.25	0.68
1:A:242:LEU:HD21	1:A:355:ILE:HA	1.77	0.67

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	406/452 (90%)	397 (98%)	9 (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	321/378 (85%)	317 (99%)	4 (1%)	63 83

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

Mol	Chain	Res	Type
1	A	144	MET
1	A	216	LEU
1	A	268	LEU
1	A	306	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1139	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
5	TLA	A	1217	-	9,9,9	1.04	0	12,12,12	1.32	2 (16%)
4	PE5	A	1216	-	23,23,26	0.63	0	22,22,25	0.41	0
3	OLA	A	1214	-	13,13,19	0.59	0	13,13,19	0.79	0
3	OLA	A	1211	-	6,6,19	0.12	0	5,5,19	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OLA	A	1205	-	10,10,19	0.63	0	10,10,19	0.85	0
3	OLA	A	1208	-	19,19,19	0.49	0	19,19,19	0.68	0
3	OLA	A	1202	-	9,9,19	0.65	0	9,9,19	0.92	0
3	OLA	A	1212	-	10,10,19	0.28	0	9,9,19	0.45	0
3	OLA	A	1215	-	10,10,19	0.62	0	10,10,19	0.86	0
3	OLA	A	1206	-	10,10,19	0.62	0	10,10,19	0.87	0
3	OLA	A	1209	-	19,19,19	0.49	0	19,19,19	0.69	0
3	OLA	A	1204	-	14,14,19	0.57	0	14,14,19	0.75	0
3	OLA	A	1203	-	14,14,19	0.57	0	14,14,19	0.76	0
2	5MV	A	1201	-	45,45,45	1.33	5 (11%)	63,64,64	0.98	1 (1%)
3	OLA	A	1213	-	6,6,19	0.12	0	5,5,19	0.29	0
3	OLA	A	1210	-	16,16,19	0.52	0	16,16,19	0.72	0
3	OLA	A	1207	-	19,19,19	0.48	0	19,19,19	0.68	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
5	TLA	A	1217	-	-	8/12/12/12	-
4	PE5	A	1216	-	-	10/21/21/24	-
3	OLA	A	1214	-	-	3/11/11/17	-
3	OLA	A	1211	-	-	2/4/4/17	-
3	OLA	A	1205	-	-	2/8/8/17	-
3	OLA	A	1208	-	-	5/17/17/17	-
3	OLA	A	1202	-	-	6/7/7/17	-
3	OLA	A	1212	-	-	4/8/8/17	-
3	OLA	A	1215	-	-	5/8/8/17	-
3	OLA	A	1206	-	-	6/8/8/17	-
3	OLA	A	1209	-	-	7/17/17/17	-
3	OLA	A	1204	-	-	7/12/12/17	-
3	OLA	A	1203	-	-	5/12/12/17	-
2	5MV	A	1201	-	-	5/28/28/28	0/5/5/5
3	OLA	A	1213	-	-	0/4/4/17	-
3	OLA	A	1210	-	-	4/14/14/17	-
3	OLA	A	1207	-	-	9/17/17/17	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	5MV	C16-C17	2.91	1.42	1.37
2	A	1201	5MV	C9-N2	2.58	1.39	1.36
2	A	1201	5MV	C13-C12	2.35	1.41	1.37
2	A	1201	5MV	C19-C18	2.15	1.41	1.36
2	A	1201	5MV	C25-C24	2.08	1.42	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	1217	TLA	O41-C4-C3	2.52	120.33	113.31
5	A	1217	TLA	O11-C1-C2	2.40	119.97	113.31
2	A	1201	5MV	C7-N1-N2	2.17	105.86	104.61

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	OLA	C10-C11-C12-C13
5	A	1217	TLA	O3-C3-C4-O4
5	A	1217	TLA	O3-C3-C4-O41
3	A	1215	OLA	C1-C2-C3-C4
3	A	1209	OLA	C1-C2-C3-C4

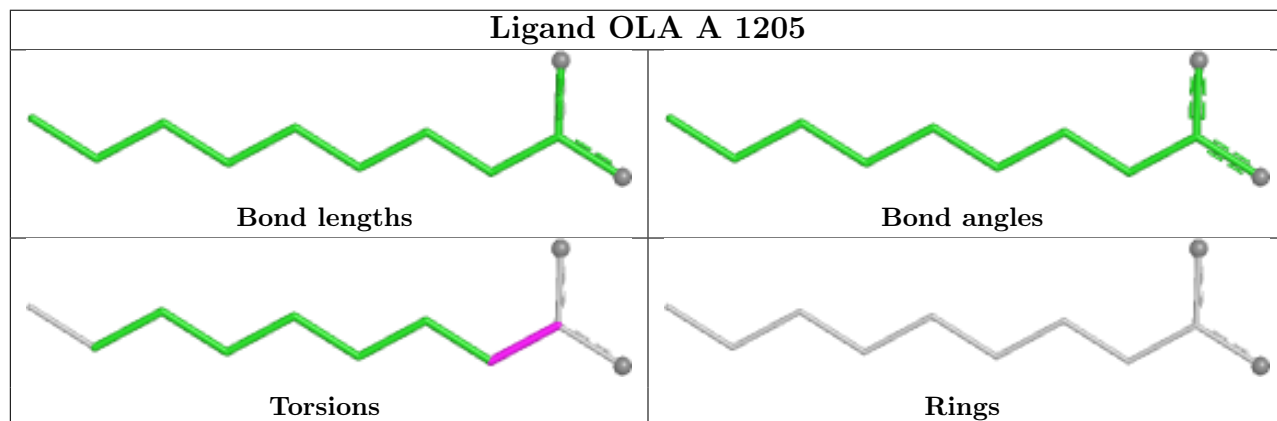
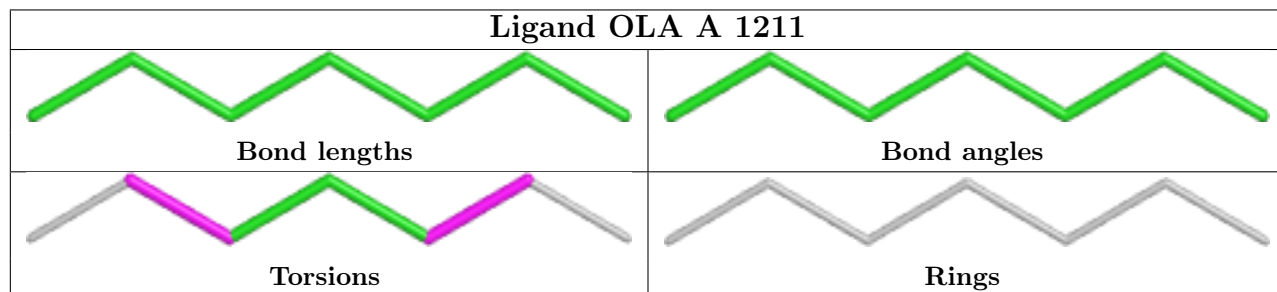
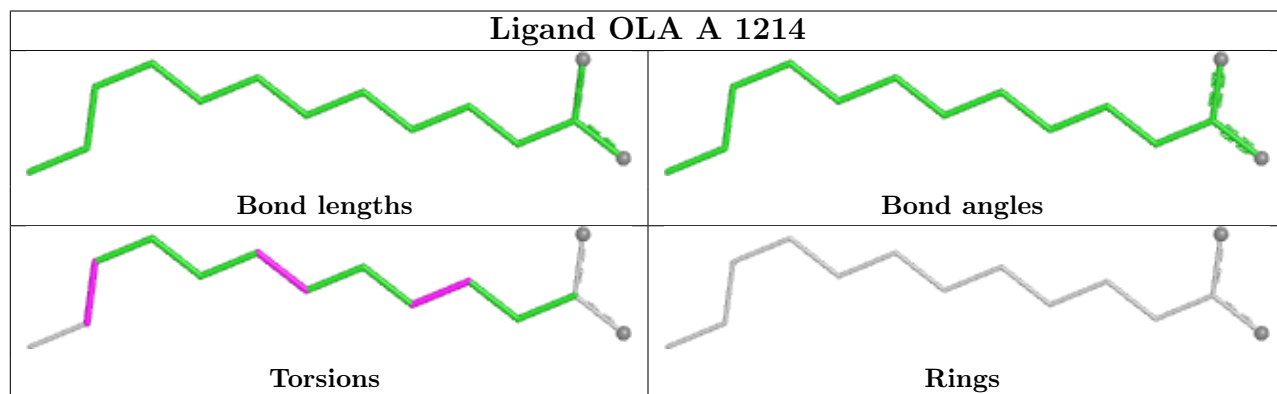
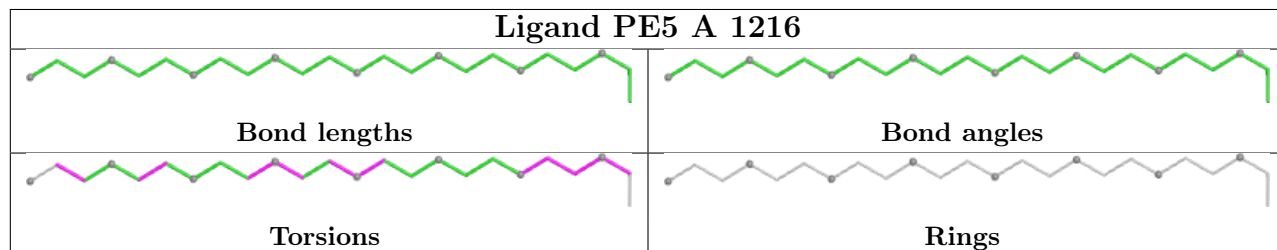
There are no ring outliers.

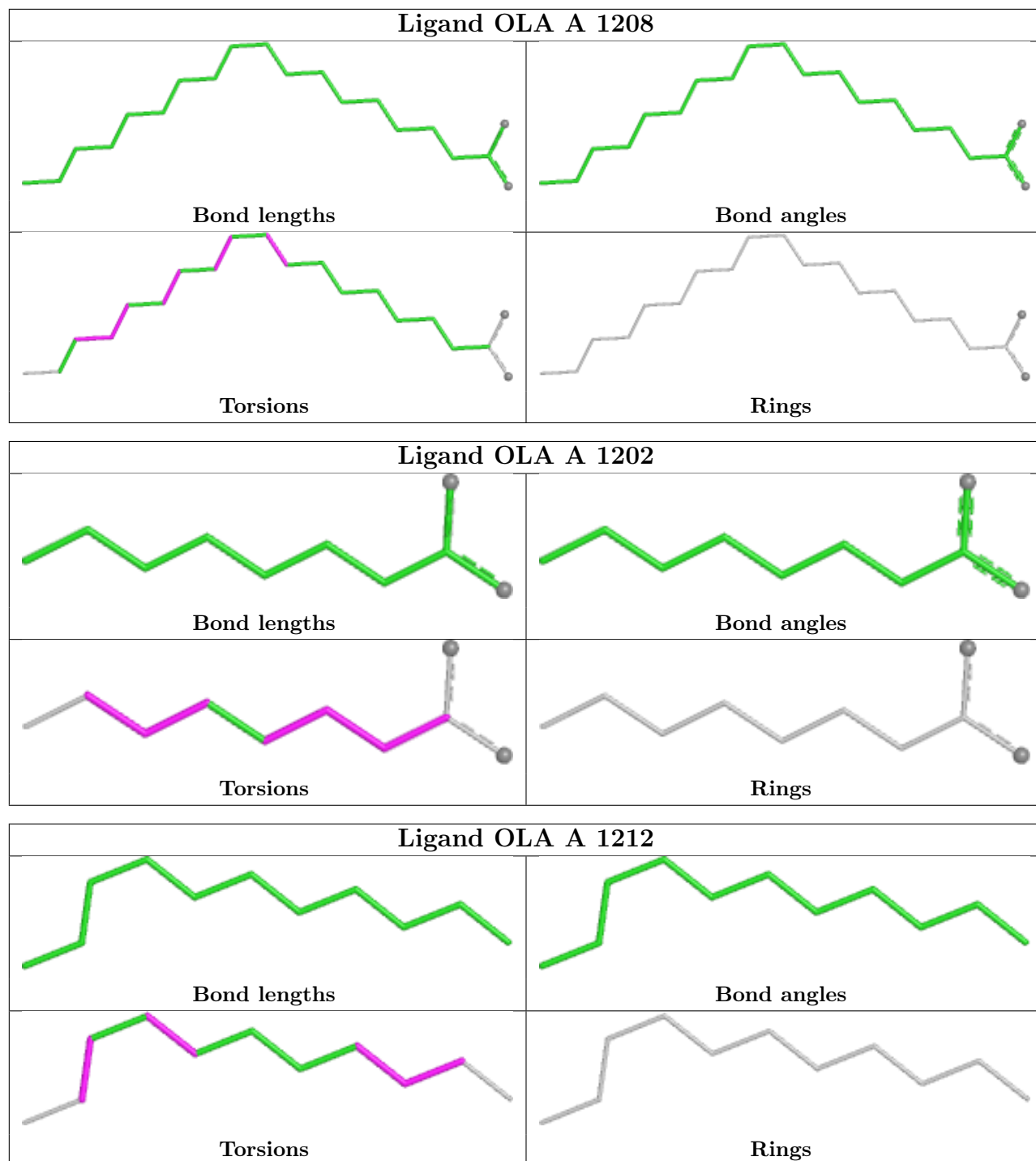
9 monomers are involved in 14 short contacts:

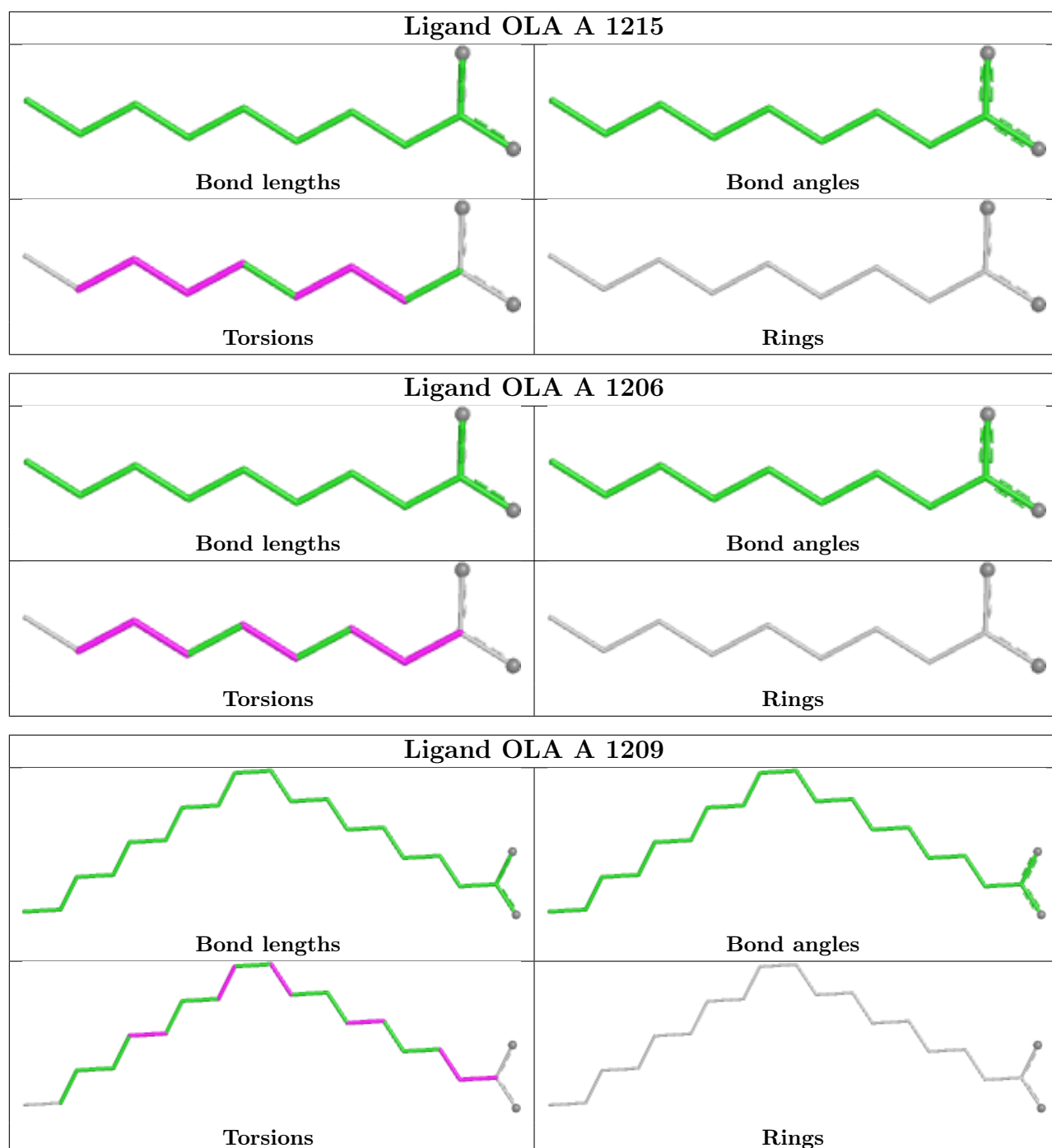
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1217	TLA	1	0
4	A	1216	PE5	7	0
3	A	1214	OLA	2	0
3	A	1212	OLA	1	0
3	A	1206	OLA	1	0
3	A	1209	OLA	1	0
3	A	1204	OLA	1	0
2	A	1201	5MV	2	0
3	A	1213	OLA	1	0

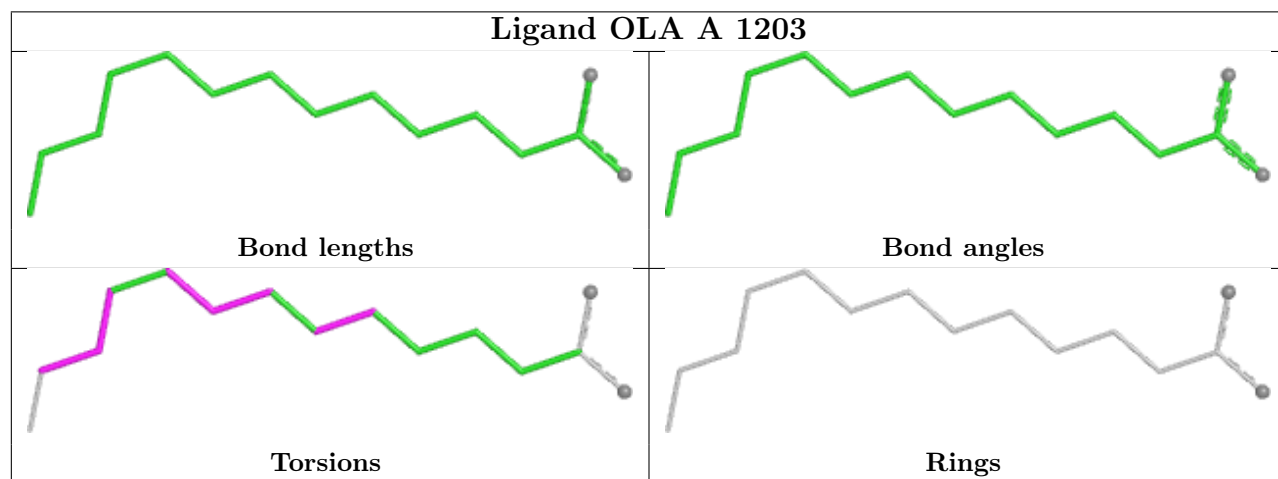
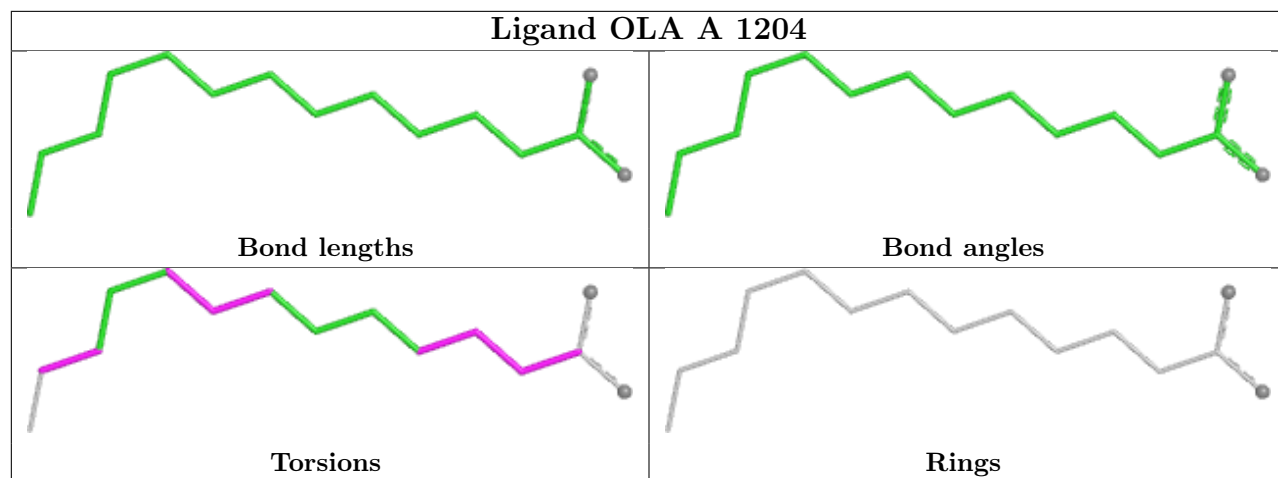
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

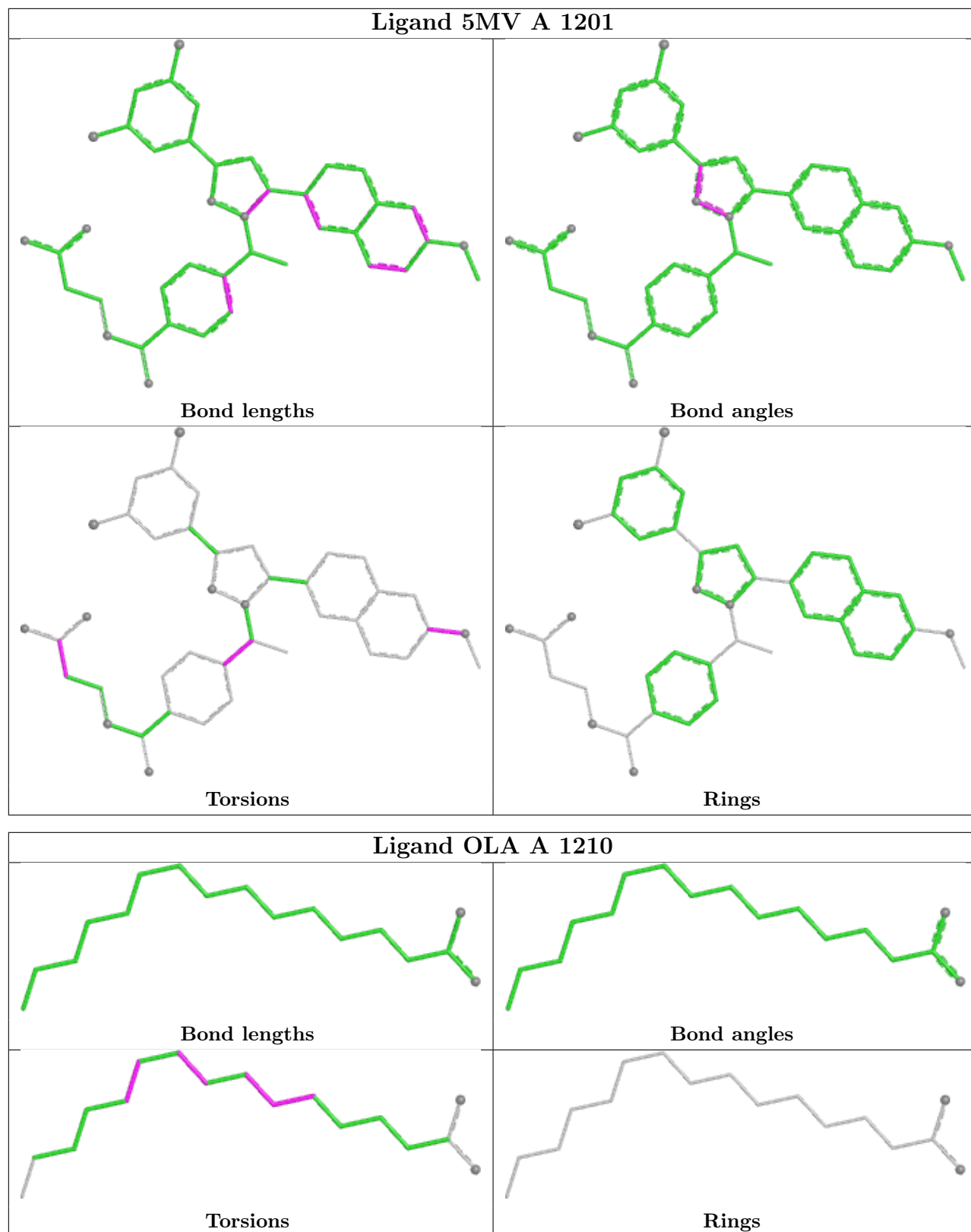
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

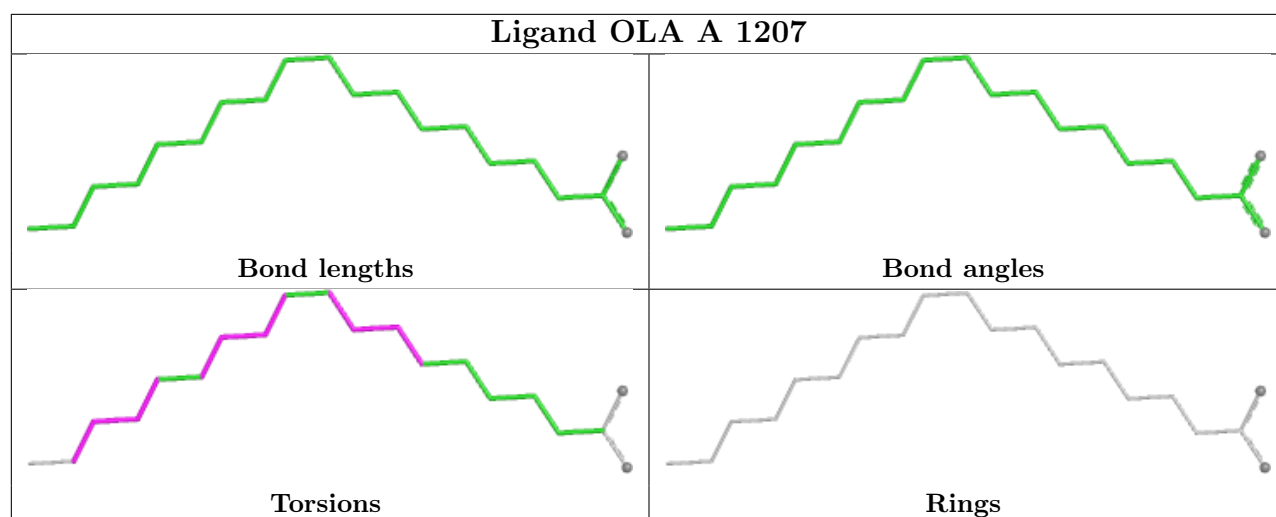












## 5.7 Other polymers [i](#)

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 [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, 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	416/452 (92%)	0.47	29 (6%) <b>22</b> <b>20</b>	25, 60, 127, 144	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1119	LEU	4.7
1	A	1047	ALA	3.7
1	A	1070	ASP	3.5
1	A	1013	LEU	3.3
1	A	1110	ALA	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

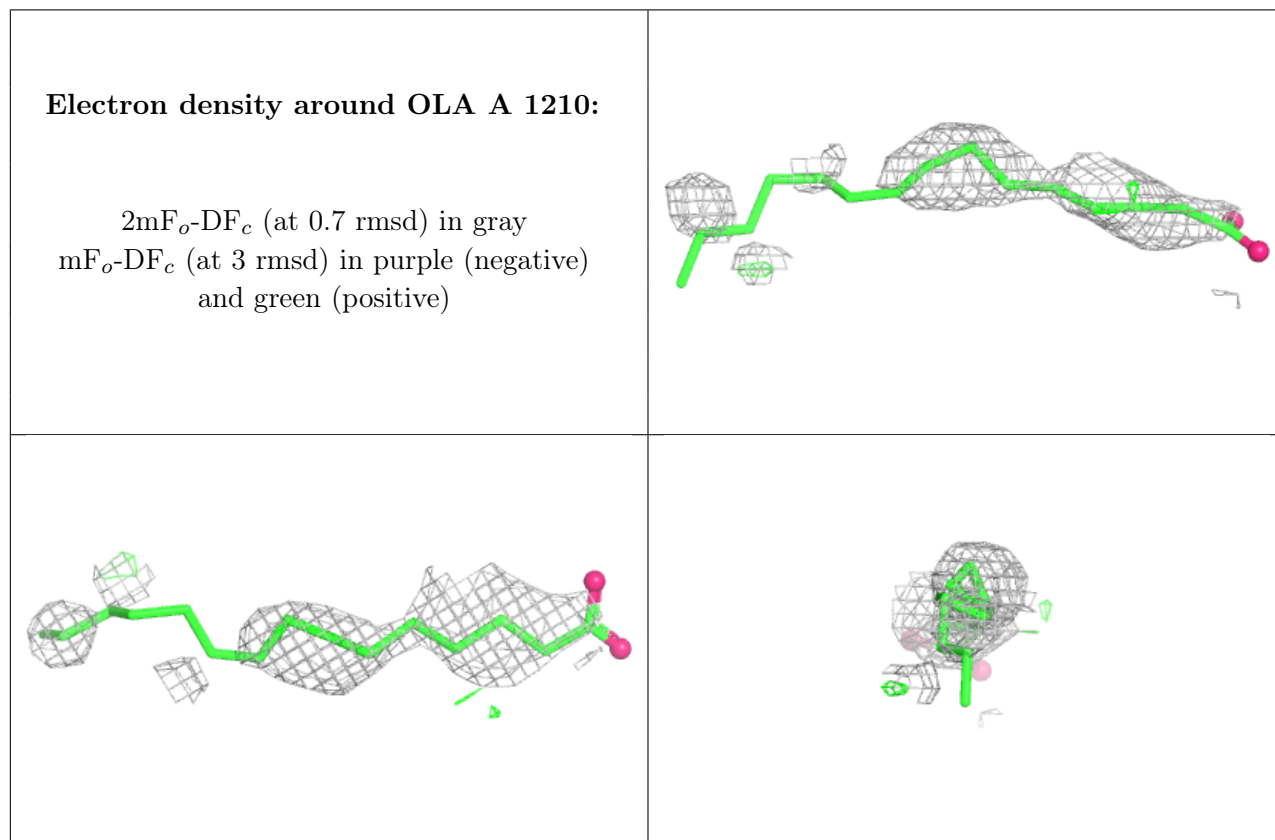
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	OLA	A	1210	17/20	0.74	0.18	54,66,91,93	0
3	OLA	A	1208	20/20	0.80	0.14	43,51,63,65	0

*Continued on next page...*

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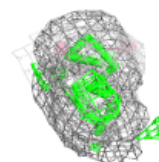
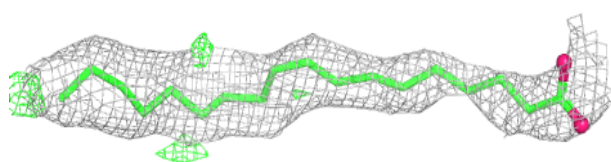
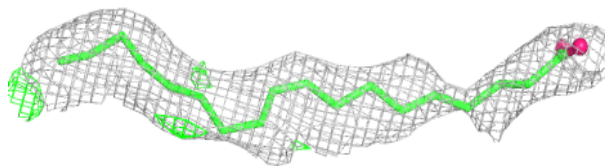
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OLA	A	1205	11/20	0.81	0.12	33,39,45,57	0
3	OLA	A	1204	15/20	0.82	0.10	40,42,62,64	0
3	OLA	A	1214	14/20	0.82	0.12	46,52,57,63	0
3	OLA	A	1211	7/20	0.84	0.11	45,48,55,58	0
3	OLA	A	1207	20/20	0.84	0.12	33,45,54,54	0
3	OLA	A	1215	11/20	0.84	0.13	59,63,68,68	0
3	OLA	A	1212	11/20	0.85	0.10	50,52,55,55	0
3	OLA	A	1202	10/20	0.86	0.10	45,51,61,61	0
3	OLA	A	1203	15/20	0.86	0.12	46,51,68,76	0
3	OLA	A	1209	20/20	0.86	0.10	40,49,66,73	0
3	OLA	A	1206	11/20	0.86	0.11	39,49,62,72	0
5	TLA	A	1217	10/10	0.87	0.14	43,52,58,61	0
4	PE5	A	1216	24/27	0.88	0.11	42,52,70,77	0
3	OLA	A	1213	7/20	0.88	0.08	35,44,48,49	0
2	5MV	A	1201	41/41	0.92	0.09	24,37,49,63	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.

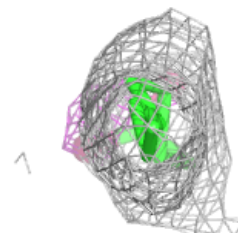
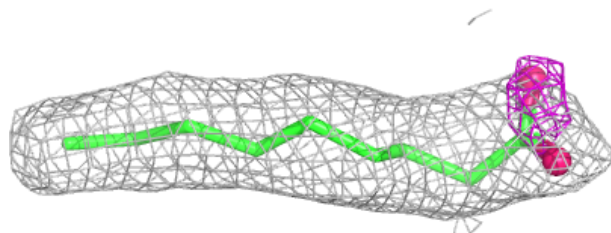
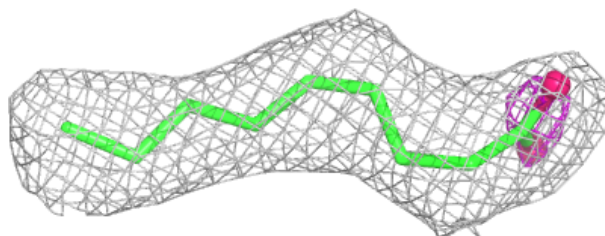


**Electron density around OLA A 1208:**

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

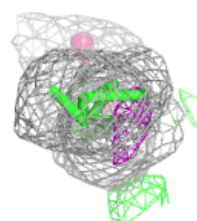
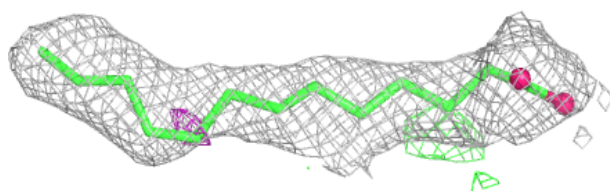
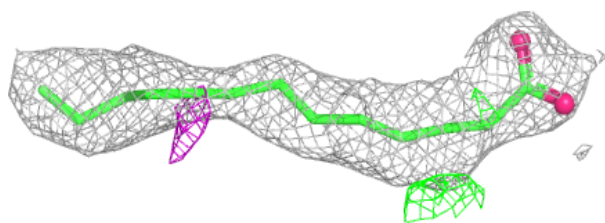
**Electron density around OLA A 1205:**

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

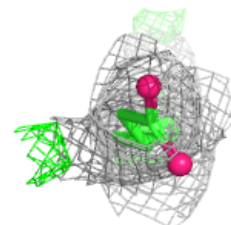
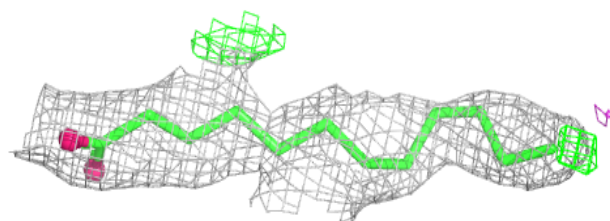
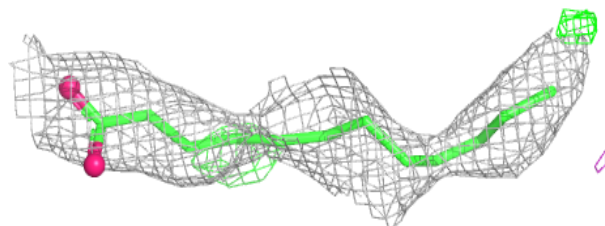


**Electron density around OLA A 1204:**

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

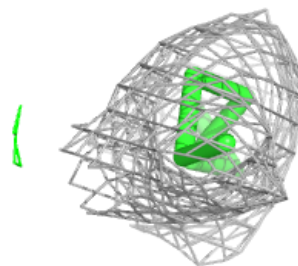
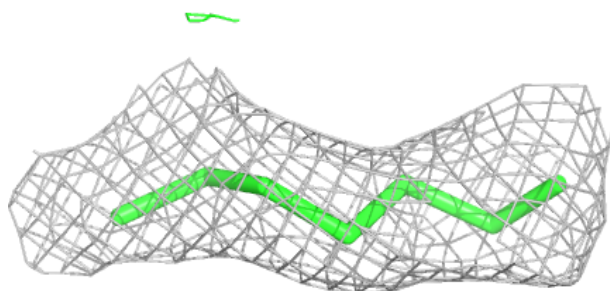
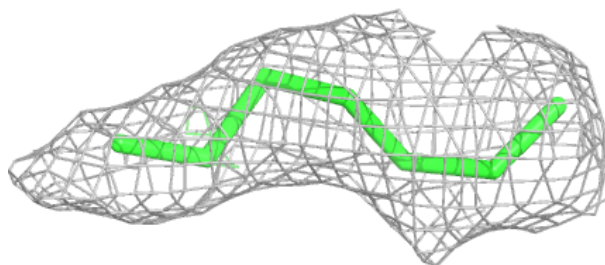
**Electron density around OLA A 1214:**

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

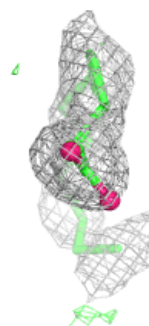
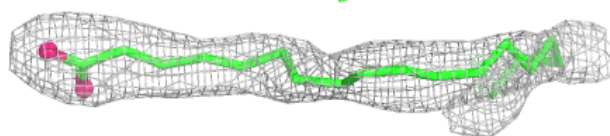
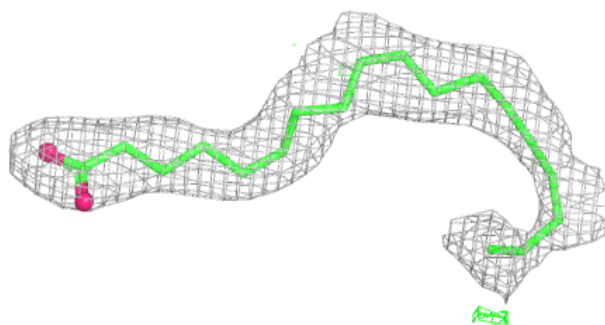


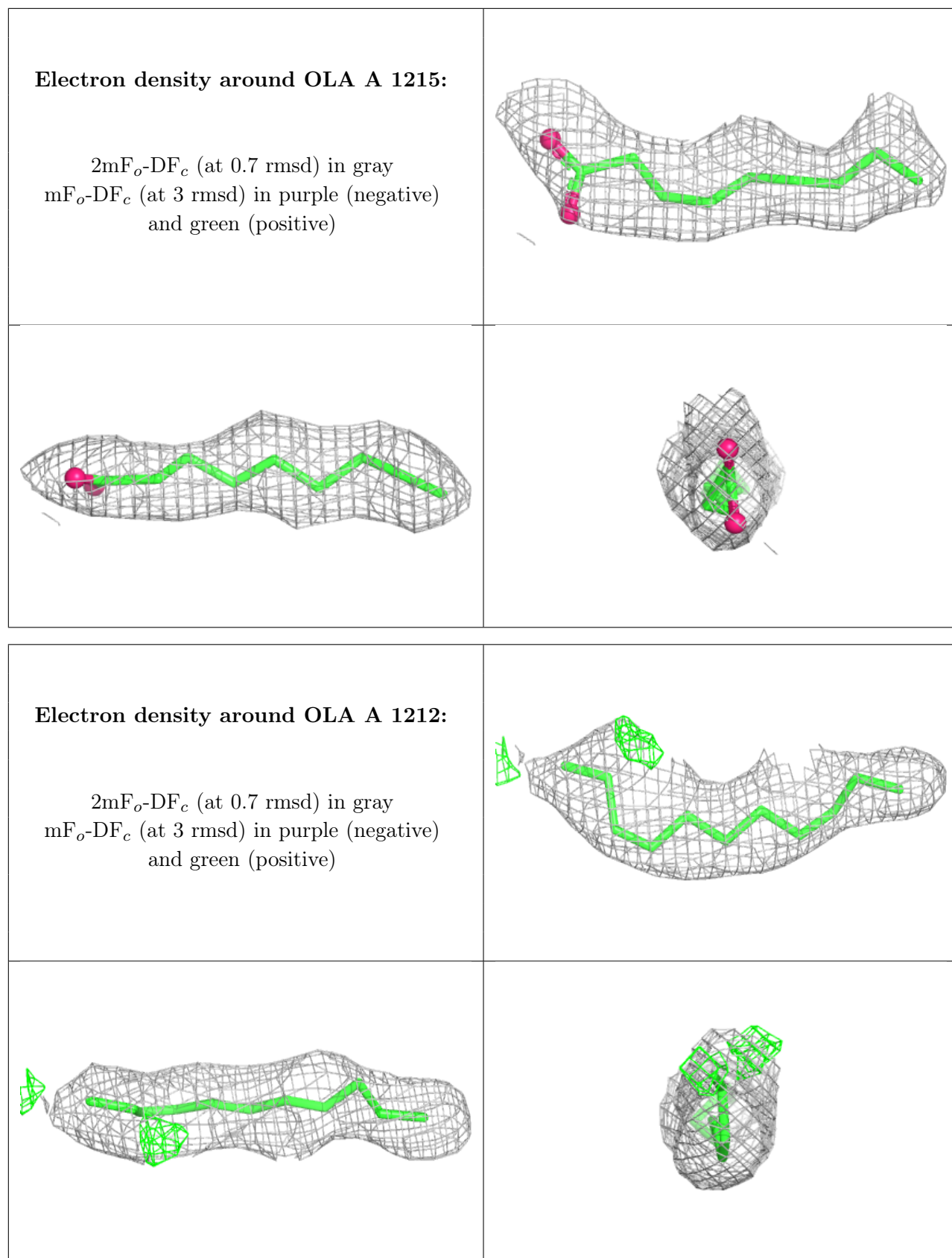
**Electron density around OLA A 1211:**

$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
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and green (positive)

**Electron density around OLA A 1207:**

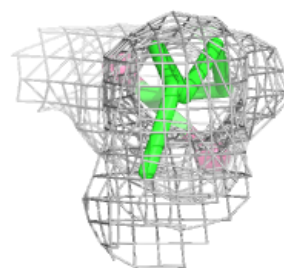
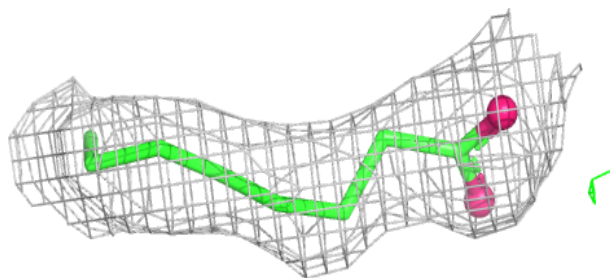
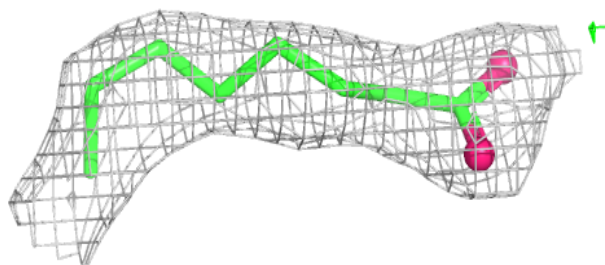
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



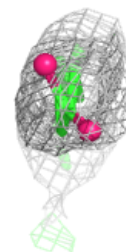
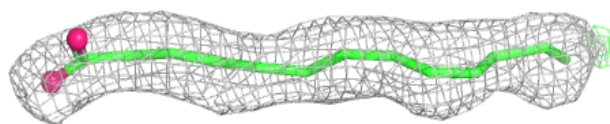
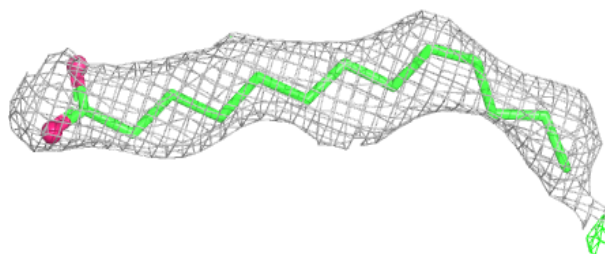


**Electron density around OLA A 1202:**

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

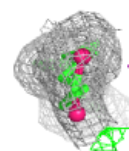
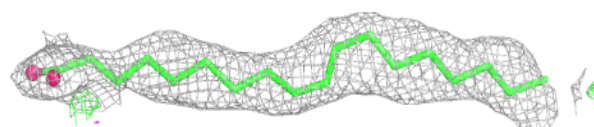
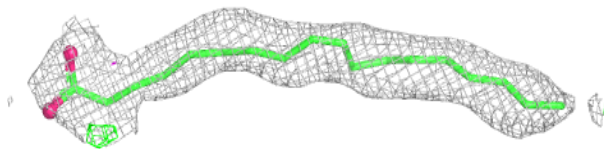
**Electron density around OLA A 1203:**

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

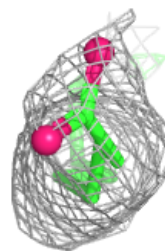
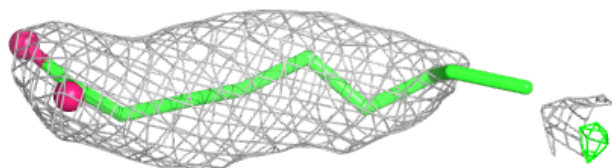
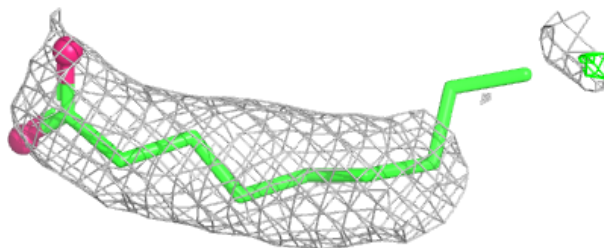


**Electron density around OLA A 1209:**

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

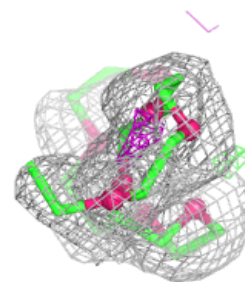
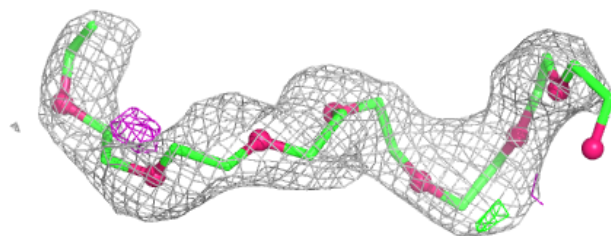
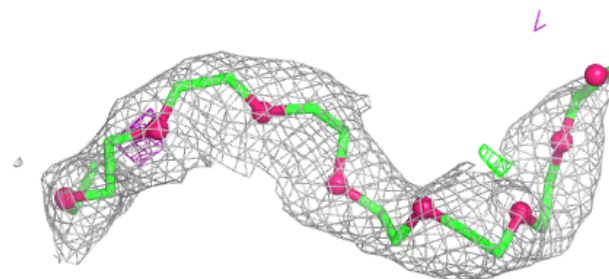
**Electron density around OLA A 1206:**

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

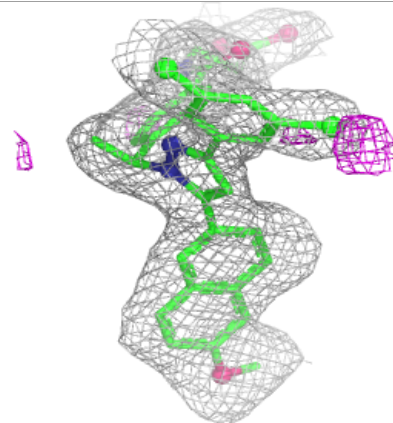
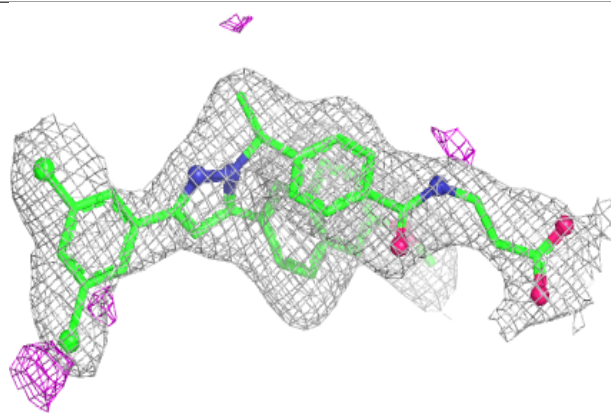
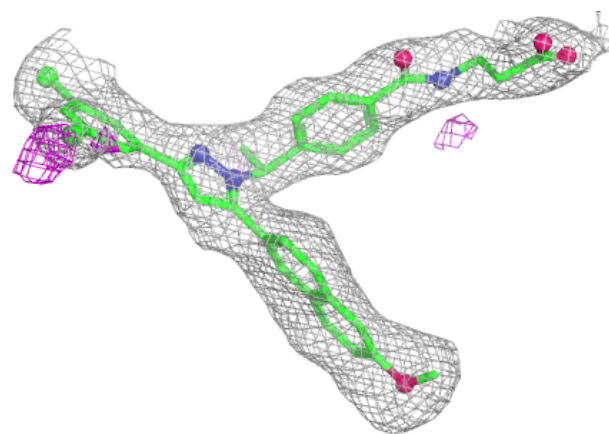


**Electron density around PE5 A 1216:**

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

**Electron density around 5MV 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.