



# wwPDB X-ray Structure Validation Summary Report

May 24, 2020 – 05:50 pm BST

PDB ID : 4Z9G  
Title : Crystal structure of human corticotropin-releasing factor receptor 1 (CRF1R) in complex with the antagonist CP-376395 in a hexagonal setting with translational non-crystallographic symmetry  
Authors : Dore, A.S.; Bortolato, A.; Hollenstein, K.; Cheng, R.K.Y.; Read, R.J.; Marshall, F.H.  
Deposited on : 2015-04-10  
Resolution : 3.18 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.

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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 : 2.11  
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) : 2.11

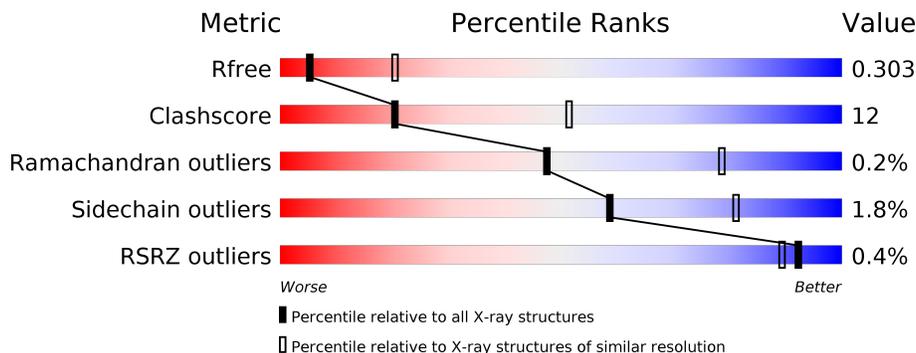
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	443	
1	B	443	
1	C	443	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLA	C	1201	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10244 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 Corticotropin-releasing factor receptor 1, Lysozyme, Corticotropin-releasing factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3385	2210	581	577	17			
1	B	415	Total	C	N	O	S	0	0	0
			3342	2185	573	567	17			
1	C	403	Total	C	N	O	S	0	0	0
			3253	2132	554	551	16			

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	GLN	expression tag	UNP P34998
A	120	ALA	VAL	engineered mutation	UNP P34998
A	144	ALA	LEU	engineered mutation	UNP P34998
A	156	ALA	TRP	engineered mutation	UNP P34998
A	160	ALA	SER	engineered mutation	UNP P34998
A	1054	SER	CYS	engineered mutation	UNP C3V2B5
A	1097	SER	CYS	engineered mutation	UNP C3V2B5
A	222	LEU	-	linker	UNP C3V2B5
A	228	ALA	LYS	engineered mutation	UNP P34998
A	260	ALA	PHE	engineered mutation	UNP P34998
A	277	ALA	ILE	engineered mutation	UNP P34998
A	309	ALA	TYR	engineered mutation	UNP P34998
A	330	ALA	PHE	engineered mutation	UNP P34998
A	349	ALA	SER	engineered mutation	UNP P34998
A	363	ALA	TYR	engineered mutation	UNP P34998
A	373	ALA	-	expression tag	UNP P34998
A	374	ALA	-	expression tag	UNP P34998
A	375	ALA	-	expression tag	UNP P34998
A	376	ALA	-	expression tag	UNP P34998
A	377	HIS	-	expression tag	UNP P34998
A	378	HIS	-	expression tag	UNP P34998
A	379	HIS	-	expression tag	UNP P34998

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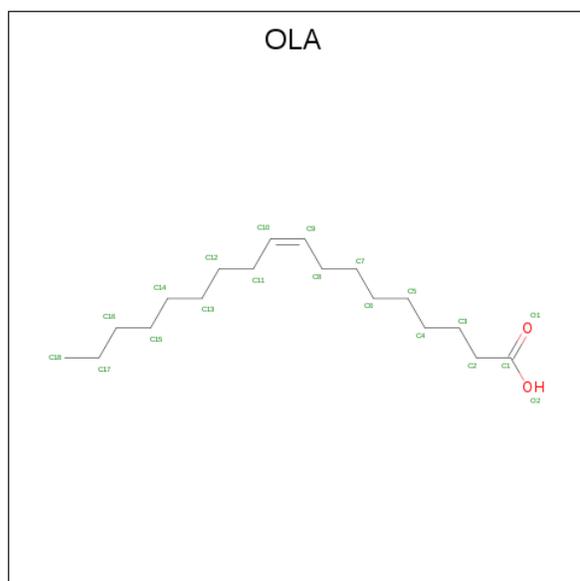
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	HIS	-	expression tag	UNP P34998
A	381	HIS	-	expression tag	UNP P34998
A	382	HIS	-	expression tag	UNP P34998
A	383	HIS	-	expression tag	UNP P34998
A	384	HIS	-	expression tag	UNP P34998
A	385	HIS	-	expression tag	UNP P34998
A	386	HIS	-	expression tag	UNP P34998
B	103	MET	GLN	expression tag	UNP P34998
B	120	ALA	VAL	engineered mutation	UNP P34998
B	144	ALA	LEU	engineered mutation	UNP P34998
B	156	ALA	TRP	engineered mutation	UNP P34998
B	160	ALA	SER	engineered mutation	UNP P34998
B	1054	SER	CYS	engineered mutation	UNP C3V2B5
B	1097	SER	CYS	engineered mutation	UNP C3V2B5
B	222	LEU	-	linker	UNP C3V2B5
B	228	ALA	LYS	engineered mutation	UNP P34998
B	260	ALA	PHE	engineered mutation	UNP P34998
B	277	ALA	ILE	engineered mutation	UNP P34998
B	309	ALA	TYR	engineered mutation	UNP P34998
B	330	ALA	PHE	engineered mutation	UNP P34998
B	349	ALA	SER	engineered mutation	UNP P34998
B	363	ALA	TYR	engineered mutation	UNP P34998
B	373	ALA	-	expression tag	UNP P34998
B	374	ALA	-	expression tag	UNP P34998
B	375	ALA	-	expression tag	UNP P34998
B	376	ALA	-	expression tag	UNP P34998
B	377	HIS	-	expression tag	UNP P34998
B	378	HIS	-	expression tag	UNP P34998
B	379	HIS	-	expression tag	UNP P34998
B	380	HIS	-	expression tag	UNP P34998
B	381	HIS	-	expression tag	UNP P34998
B	382	HIS	-	expression tag	UNP P34998
B	383	HIS	-	expression tag	UNP P34998
B	384	HIS	-	expression tag	UNP P34998
B	385	HIS	-	expression tag	UNP P34998
B	386	HIS	-	expression tag	UNP P34998
C	103	MET	GLN	expression tag	UNP P34998
C	120	ALA	VAL	engineered mutation	UNP P34998
C	144	ALA	LEU	engineered mutation	UNP P34998
C	156	ALA	TRP	engineered mutation	UNP P34998
C	160	ALA	SER	engineered mutation	UNP P34998
C	1054	SER	CYS	engineered mutation	UNP C3V2B5

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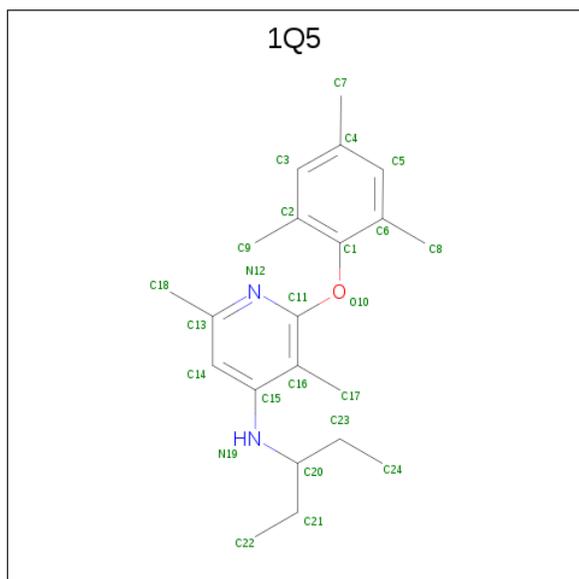
Chain	Residue	Modelled	Actual	Comment	Reference
C	1097	SER	CYS	engineered mutation	UNP C3V2B5
C	222	LEU	-	linker	UNP C3V2B5
C	228	ALA	LYS	engineered mutation	UNP P34998
C	260	ALA	PHE	engineered mutation	UNP P34998
C	277	ALA	ILE	engineered mutation	UNP P34998
C	309	ALA	TYR	engineered mutation	UNP P34998
C	330	ALA	PHE	engineered mutation	UNP P34998
C	349	ALA	SER	engineered mutation	UNP P34998
C	363	ALA	TYR	engineered mutation	UNP P34998
C	373	ALA	-	expression tag	UNP P34998
C	374	ALA	-	expression tag	UNP P34998
C	375	ALA	-	expression tag	UNP P34998
C	376	ALA	-	expression tag	UNP P34998
C	377	HIS	-	expression tag	UNP P34998
C	378	HIS	-	expression tag	UNP P34998
C	379	HIS	-	expression tag	UNP P34998
C	380	HIS	-	expression tag	UNP P34998
C	381	HIS	-	expression tag	UNP P34998
C	382	HIS	-	expression tag	UNP P34998
C	383	HIS	-	expression tag	UNP P34998
C	384	HIS	-	expression tag	UNP P34998
C	385	HIS	-	expression tag	UNP P34998
C	386	HIS	-	expression tag	UNP P34998

- Molecule 2 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
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C		0	0
			8	8			
2	B	1	Total	C	O	0	0
			18	16	2		
2	B	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			15	13	2		
2	C	1	Total	C	O	0	0
			20	18	2		
2	C	1	Total	C	O	0	0
			20	18	2		
2	C	1	Total	C	O	0	0
			16	14	2		
2	C	1	Total	C	O	0	0
			20	18	2		

- Molecule 3 is 3,6-dimethyl-N-(pentan-3-yl)-2-(2,4,6-trimethylphenoxy)pyridin-4-amine (three-letter code: 1Q5) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>2</sub>O).



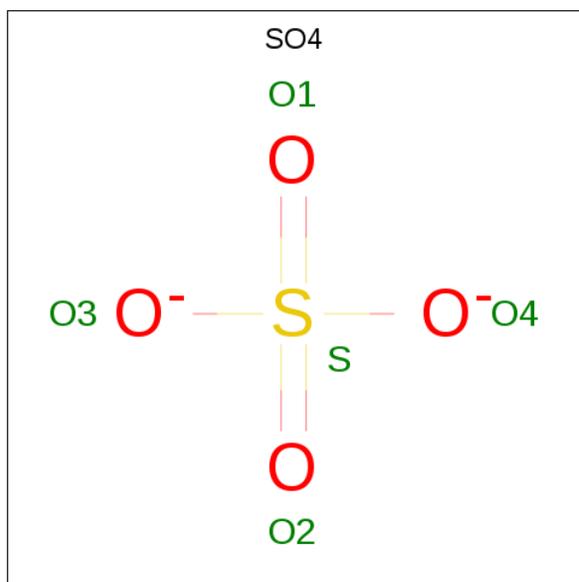
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	21	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			24	21	2	1		
3	C	1	Total	C	N	O	0	0
			24	21	2	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.36 Å 189.36 Å 88.58 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.91 – 3.18 45.48 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.91-3.18) 93.1 (45.48-3.18)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.19 Å)	Xtriage
Refinement program	PHENIX 1.8.1	Depositor
R, $R_{free}$	0.244 , 0.289 0.259 , 0.303	Depositor DCC
$R_{free}$ test set	1462 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.120 for h,-h-k,-l	Depositor
Outliers	2 of 28508 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5368e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 1Q5, OLA, SO4

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	0.34	0/3467	0.51	0/4704
1	B	0.32	0/3422	0.47	0/4642
1	C	0.32	1/3330 (0.0%)	0.47	0/4515
All	All	0.33	1/10219 (0.0%)	0.49	0/13861

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	VAL	CB-CG2	-5.82	1.40	1.52

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	3385	0	3445	102	0
1	B	3342	0	3404	80	0
1	C	3253	0	3308	74	0
2	A	48	0	81	4	0
2	B	53	0	79	7	0
2	C	76	0	121	12	0
3	A	24	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	30	4	0
3	C	24	0	30	4	0
4	A	10	0	0	0	0
4	C	5	0	0	1	0
All	All	10244	0	10528	258	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 12.

The worst 5 of 258 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:C:323:LEU:HD12	3:C:1205:1Q5:H7	1.64	0.80
1:A:199:HIS:HE2	1:A:327:TYR:HH	1.30	0.75
2:B:1201:OLA:H41	2:B:1202:OLA:H32	1.69	0.75
1:A:175:THR:OG1	1:A:175:THR:O	2.01	0.73
1:A:253:TYR:HB3	1:A:266:VAL:HG11	1.71	0.72

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	419/443 (95%)	405 (97%)	13 (3%)	1 (0%)	47 78
1	B	411/443 (93%)	396 (96%)	13 (3%)	2 (0%)	29 66
1	C	395/443 (89%)	380 (96%)	15 (4%)	0	100 100
All	All	1225/1329 (92%)	1181 (96%)	41 (3%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	B	264	PRO
1	B	1143	PRO

### 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	358/376 (95%)	351 (98%)	7 (2%)	55 79
1	B	353/376 (94%)	347 (98%)	6 (2%)	60 82
1	C	343/376 (91%)	337 (98%)	6 (2%)	60 82
All	All	1054/1128 (93%)	1035 (98%)	19 (2%)	59 81

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	B	181	HIS
1	C	1040	SER
1	B	117	HIS
1	C	284	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	C	115	HIS
1	C	155	HIS
1	C	1068	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1Q5	A	1204	-	24,25,25	1.60	3 (12%)	31,35,35	2.02	8 (25%)
2	OLA	B	1201	-	14,17,19	0.26	0	13,17,19	0.68	0
2	OLA	A	1203	-	7,7,19	0.15	0	6,6,19	0.60	0
2	OLA	C	1204	-	16,19,19	0.27	0	15,19,19	0.65	0
2	OLA	C	1203	-	12,15,19	0.27	0	11,15,19	0.72	0
4	SO4	A	1206	-	4,4,4	0.14	0	6,6,6	0.14	0
4	SO4	C	1206	-	4,4,4	0.25	0	6,6,6	0.21	0
3	1Q5	B	1204	-	24,25,25	1.59	3 (12%)	31,35,35	1.78	8 (25%)
2	OLA	B	1203	-	11,14,19	0.29	0	10,14,19	0.60	0
2	OLA	C	1201	-	16,19,19	0.22	0	15,19,19	0.77	0
2	OLA	A	1201	-	16,19,19	0.23	0	15,19,19	0.73	0
3	1Q5	C	1205	-	24,25,25	1.55	3 (12%)	31,35,35	1.80	7 (22%)
2	OLA	A	1202	-	16,19,19	0.27	0	15,19,19	0.68	0
4	SO4	A	1205	-	4,4,4	0.15	0	6,6,6	0.05	0
2	OLA	C	1202	-	16,19,19	0.29	0	15,19,19	0.73	0
2	OLA	B	1202	-	16,19,19	0.24	0	15,19,19	0.64	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
3	1Q5	A	1204	-	-	1/12/12/12	0/2/2/2
2	OLA	B	1201	-	-	8/13/15/17	-
2	OLA	A	1203	-	-	3/5/5/17	-
2	OLA	C	1204	-	-	11/15/17/17	-
2	OLA	C	1203	-	-	7/11/13/17	-
3	1Q5	B	1204	-	-	2/12/12/12	0/2/2/2
2	OLA	B	1203	-	-	6/10/12/17	-
2	OLA	C	1201	-	-	10/15/17/17	-
2	OLA	A	1201	-	-	10/15/17/17	-
3	1Q5	C	1205	-	-	3/12/12/12	0/2/2/2
2	OLA	A	1202	-	-	7/15/17/17	-
2	OLA	C	1202	-	-	9/15/17/17	-
2	OLA	B	1202	-	-	8/15/17/17	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	1Q5	C1-C6	4.58	1.48	1.40
3	B	1204	1Q5	C1-C6	4.38	1.47	1.40
3	B	1204	1Q5	C1-C2	4.20	1.47	1.40
3	C	1205	1Q5	C1-C6	4.18	1.47	1.40
3	C	1205	1Q5	C1-C2	4.14	1.47	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1204	1Q5	C1-O10-C11	6.03	123.06	116.88
3	C	1205	1Q5	C1-O10-C11	4.85	121.85	116.88
3	B	1204	1Q5	C1-O10-C11	4.19	121.18	116.88
3	A	1204	1Q5	C16-C11-N12	-4.16	119.70	125.36
3	C	1205	1Q5	C3-C4-C5	3.74	122.55	118.09

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1204	OLA	C1-C2-C3-C4
2	C	1203	OLA	C1-C2-C3-C4
2	B	1203	OLA	C1-C2-C3-C4
2	C	1201	OLA	C1-C2-C3-C4

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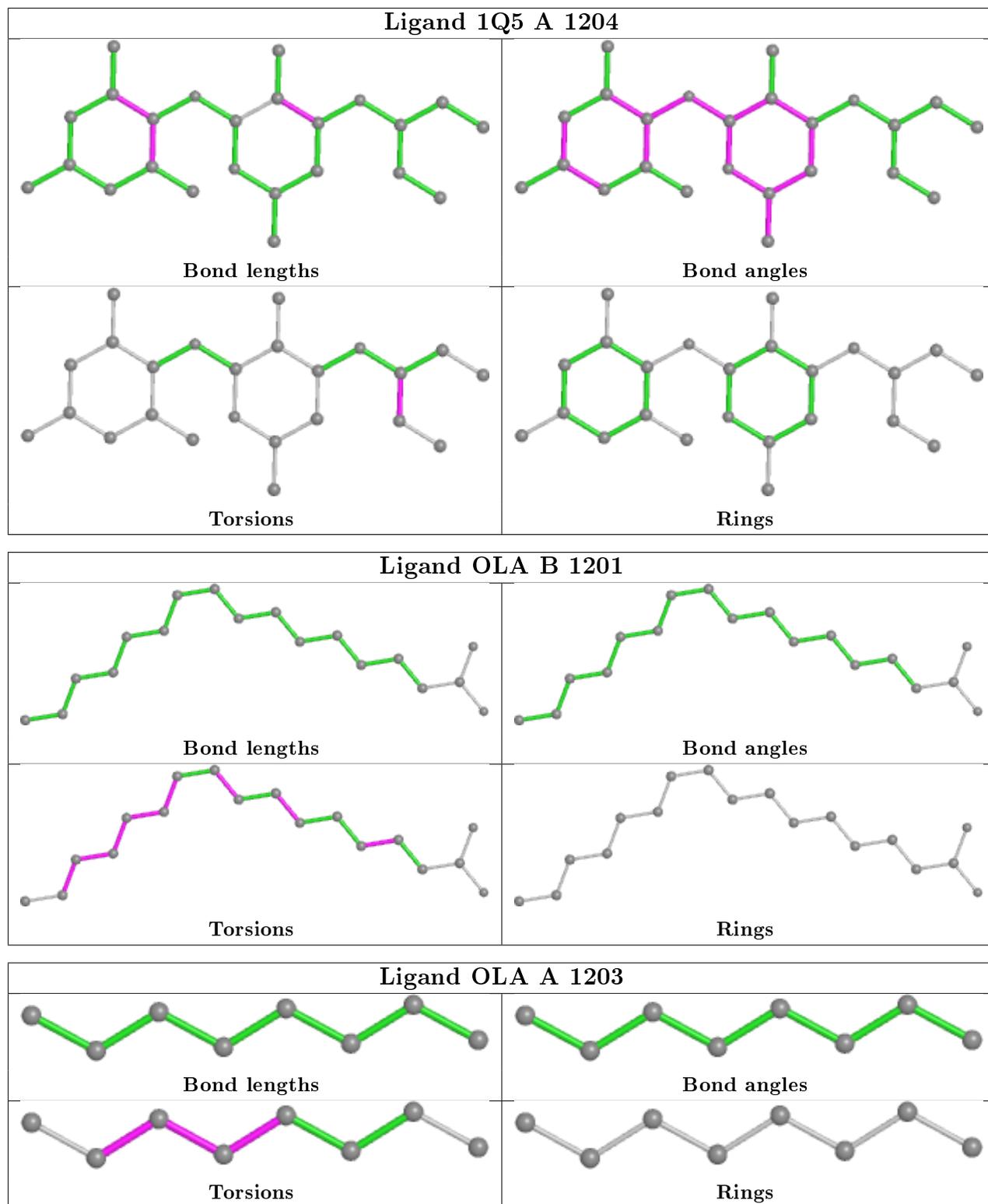
Mol	Chain	Res	Type	Atoms
3	C	1205	1Q5	N19-C20-C23-C24

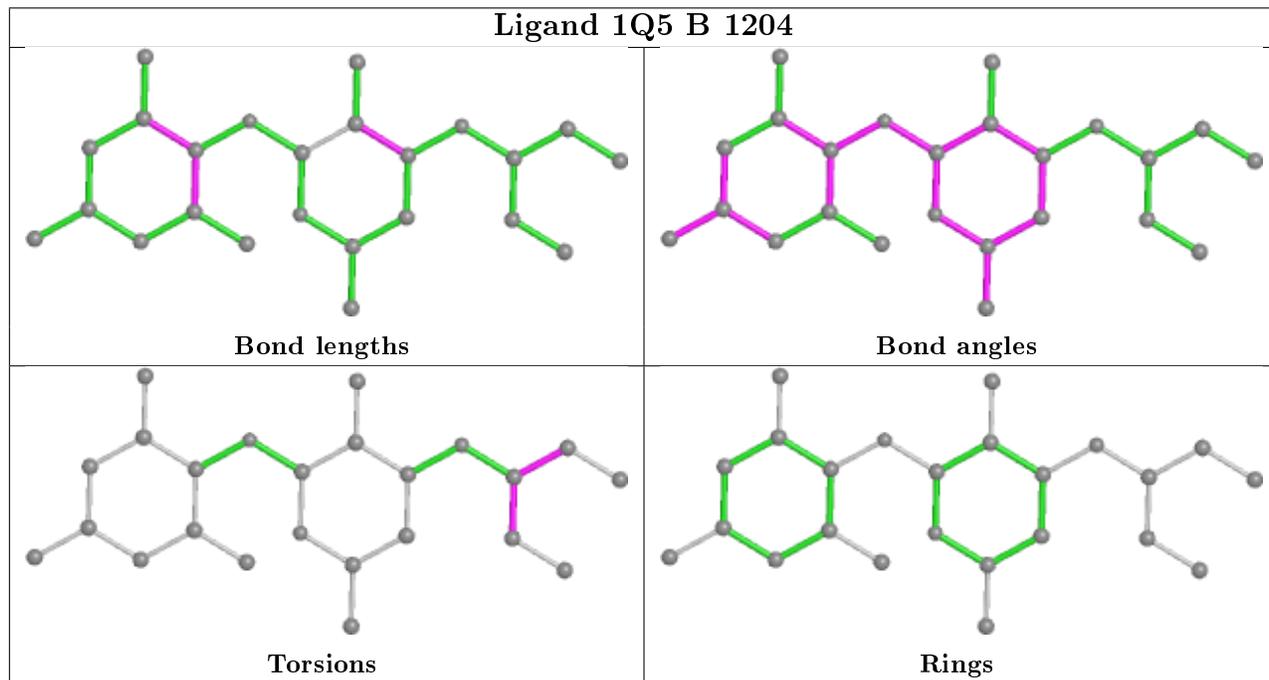
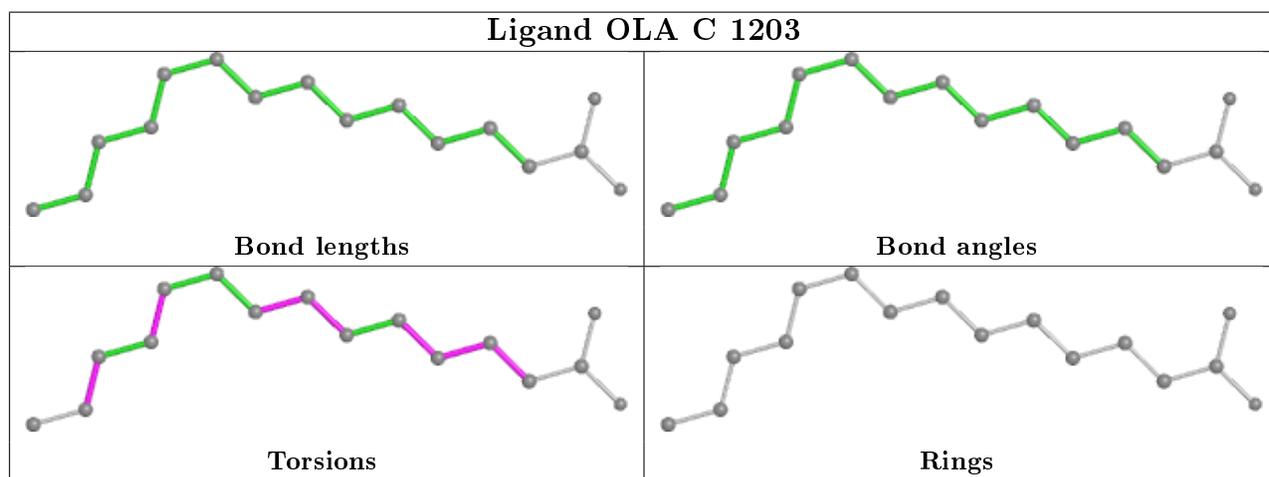
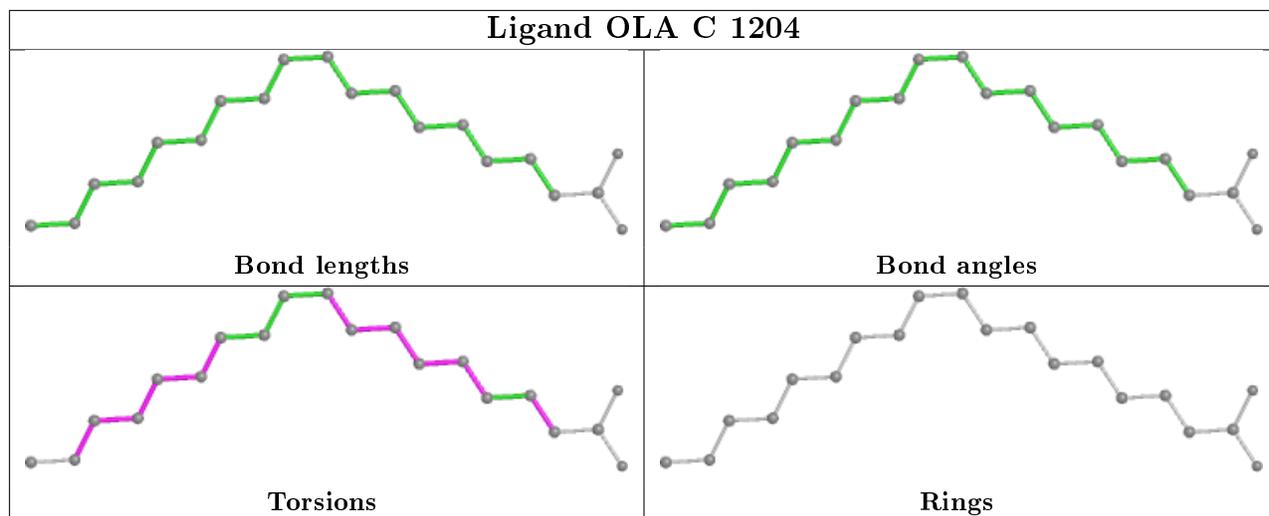
There are no ring outliers.

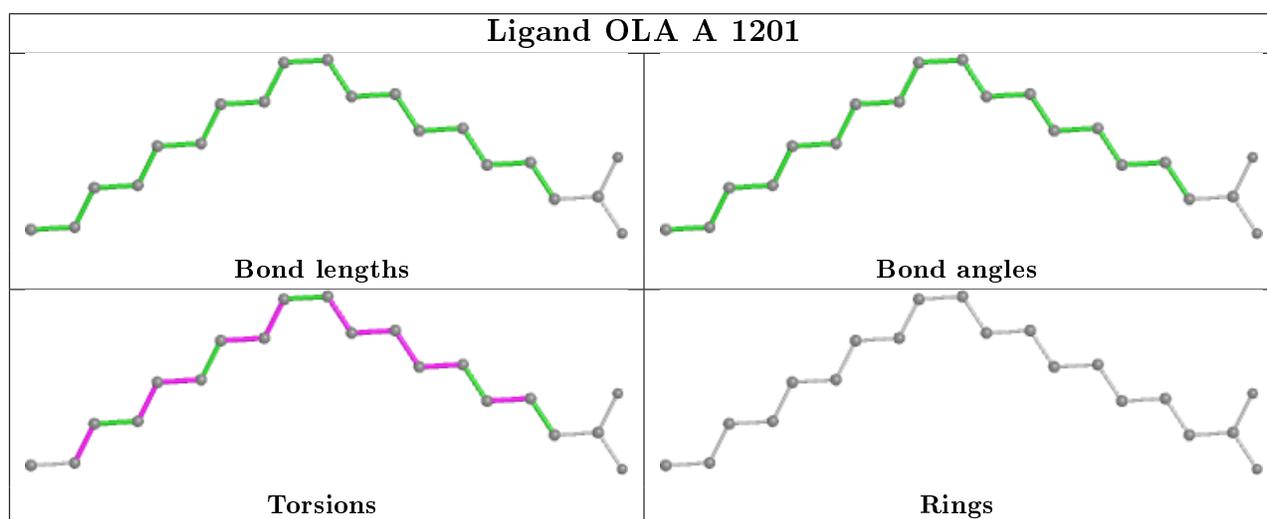
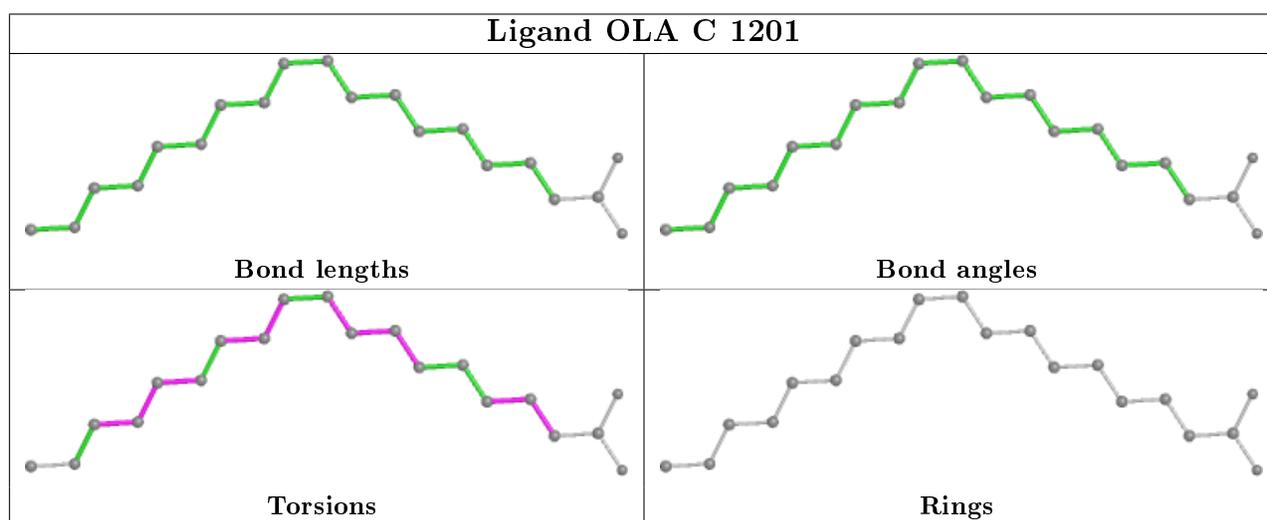
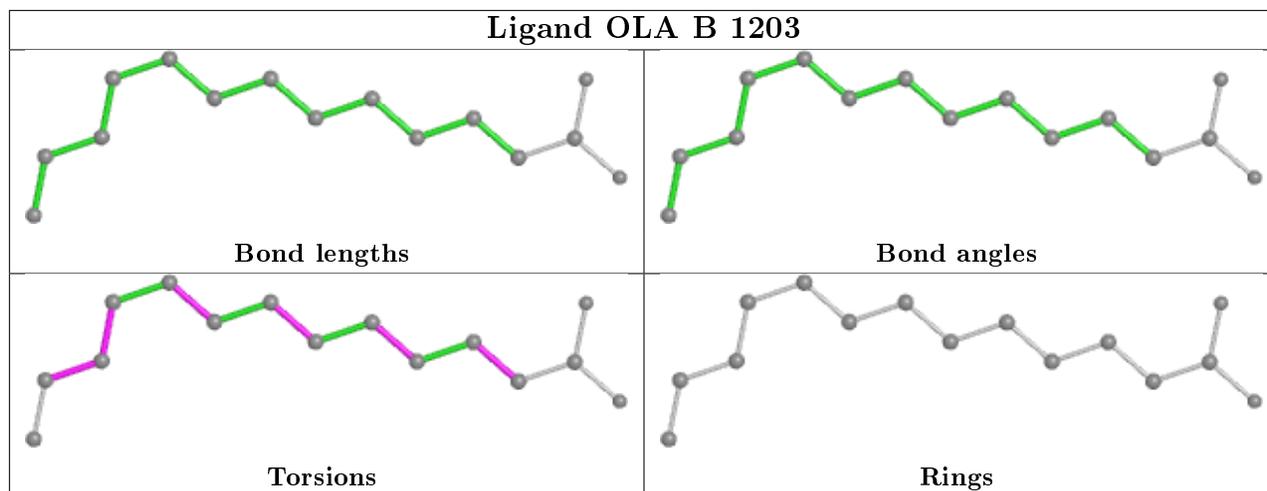
11 monomers are involved in 36 short contacts:

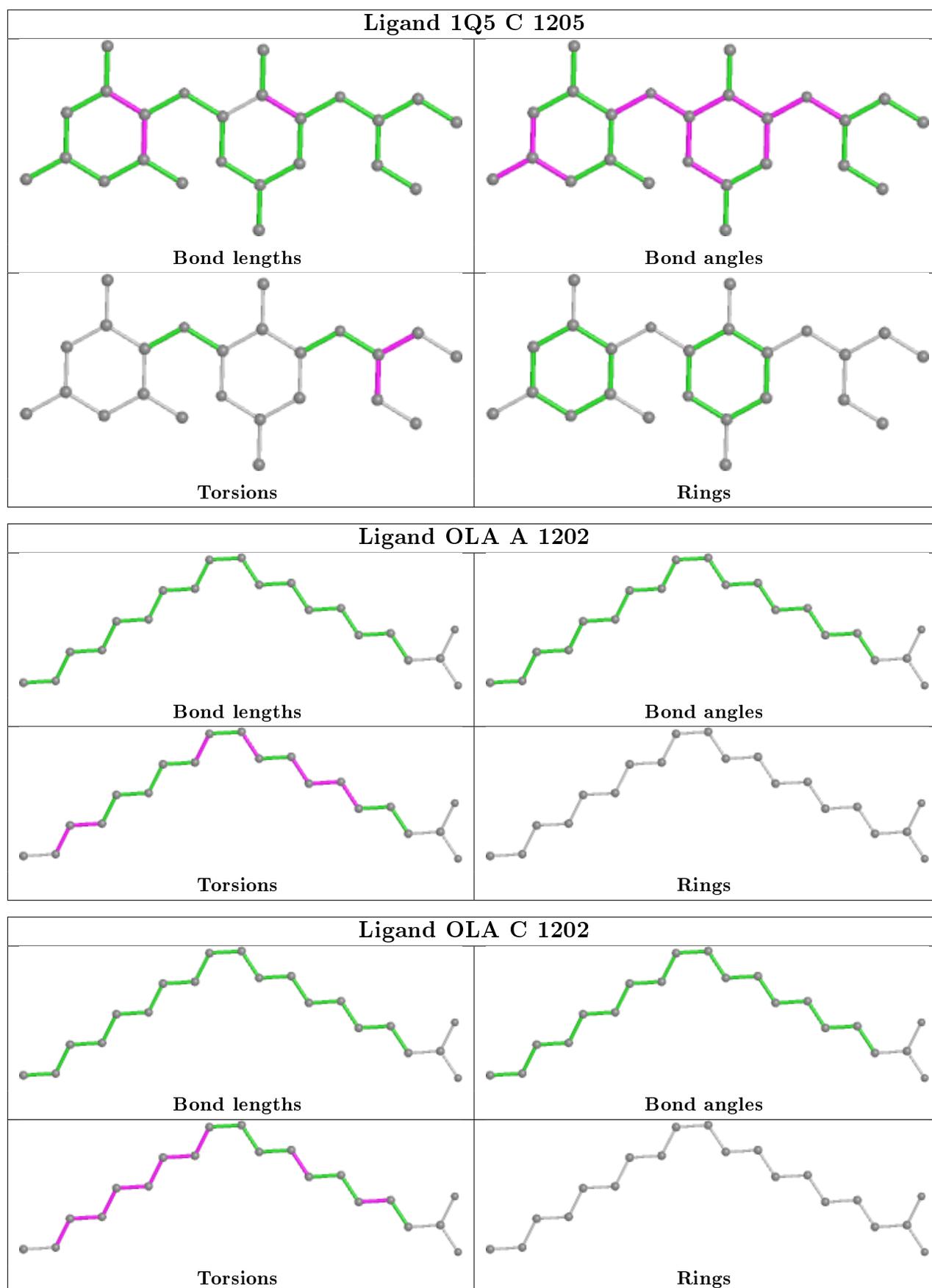
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	1Q5	4	0
2	B	1201	OLA	4	0
2	C	1203	OLA	2	0
4	C	1206	SO4	1	0
3	B	1204	1Q5	4	0
2	B	1203	OLA	2	0
2	C	1201	OLA	9	0
3	C	1205	1Q5	4	0
2	A	1202	OLA	4	0
2	C	1202	OLA	3	0
2	B	1202	OLA	5	0

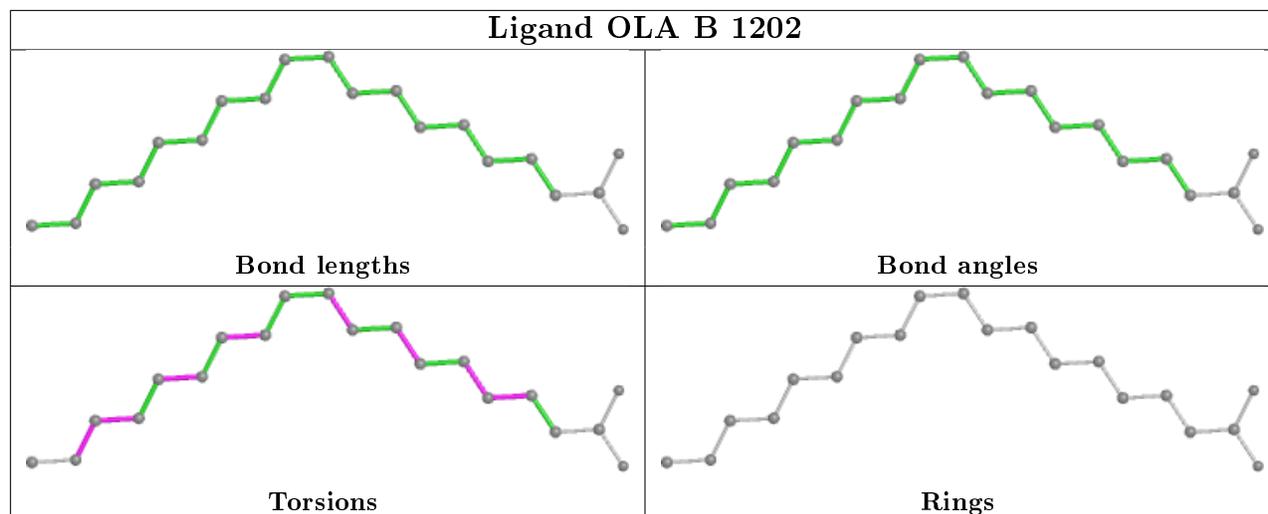
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	421/443 (95%)	-0.29	1 (0%) 95 94	34, 87, 122, 150	0
1	B	415/443 (93%)	-0.33	1 (0%) 95 94	42, 84, 131, 153	0
1	C	403/443 (90%)	-0.18	3 (0%) 87 81	24, 94, 135, 147	0
All	All	1239/1329 (93%)	-0.27	5 (0%) 92 89	24, 88, 130, 153	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	GLU	3.8
1	A	329	LEU	3.3
1	C	339	VAL	3.1
1	C	342	VAL	2.5
1	C	1057	VAL	2.2

### 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](#)

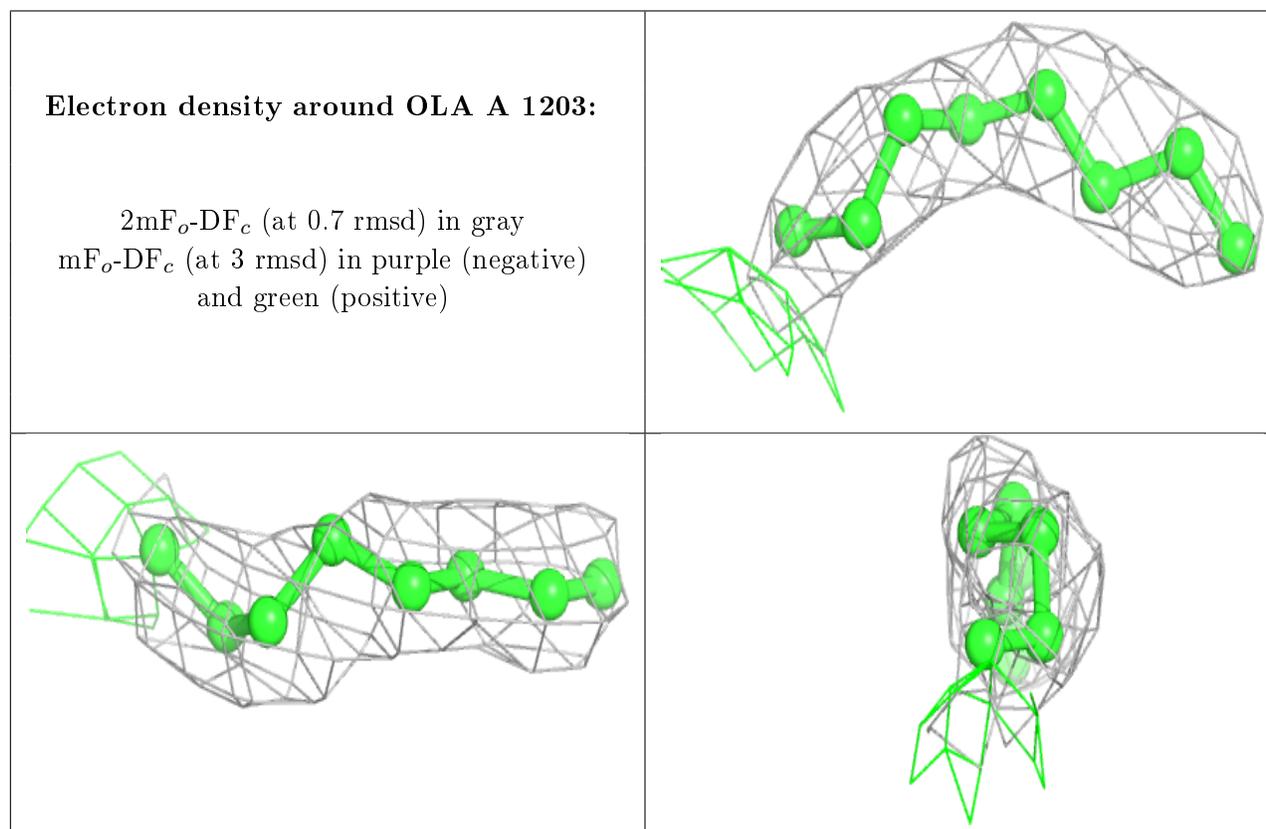
There are no carbohydrates in this entry.

### 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.

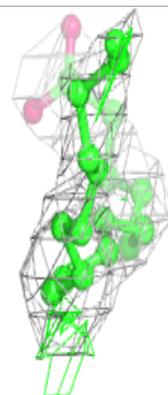
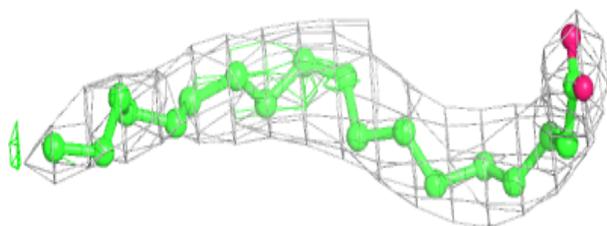
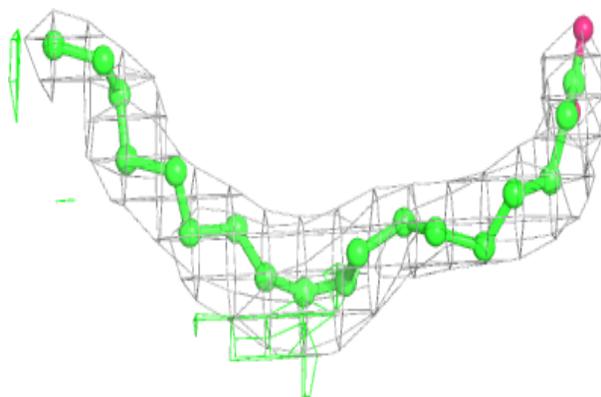
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLA	A	1203	8/20	0.84	0.29	71,75,77,77	0
2	OLA	C	1204	20/20	0.85	0.34	65,78,99,101	0
2	OLA	B	1201	18/20	0.88	0.34	70,79,85,86	0
2	OLA	C	1203	16/20	0.88	0.33	80,85,90,91	0
4	SO4	A	1206	5/5	0.88	0.16	145,146,147,147	0
2	OLA	C	1201	20/20	0.88	0.22	64,72,79,80	0
2	OLA	C	1202	20/20	0.88	0.33	63,74,84,85	0
2	OLA	B	1203	15/20	0.90	0.32	85,87,94,95	0
2	OLA	B	1202	20/20	0.91	0.45	76,82,91,93	0
2	OLA	A	1201	20/20	0.92	0.28	81,84,88,89	0
4	SO4	C	1206	5/5	0.93	0.14	131,132,133,133	0
2	OLA	A	1202	20/20	0.94	0.23	52,62,79,79	0
4	SO4	A	1205	5/5	0.94	0.12	125,125,125,126	0
3	1Q5	B	1204	24/24	0.95	0.41	82,90,95,97	0
3	1Q5	A	1204	24/24	0.95	0.26	85,89,92,93	0
3	1Q5	C	1205	24/24	0.96	0.40	86,89,99,100	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.

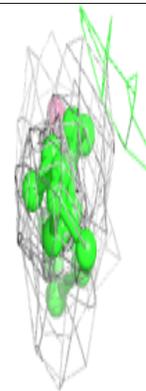
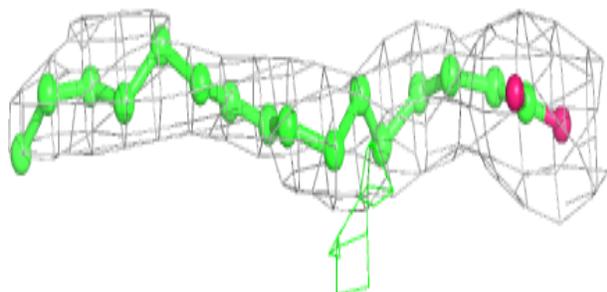
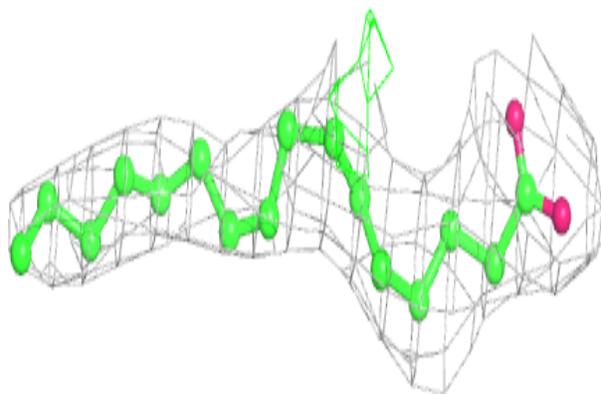


**Electron density around OLA C 1204:**

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

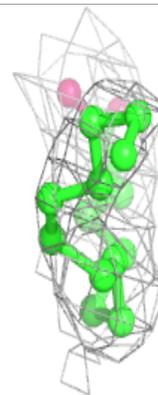
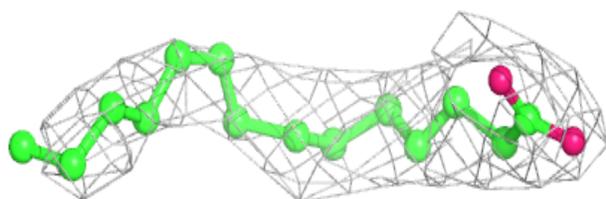
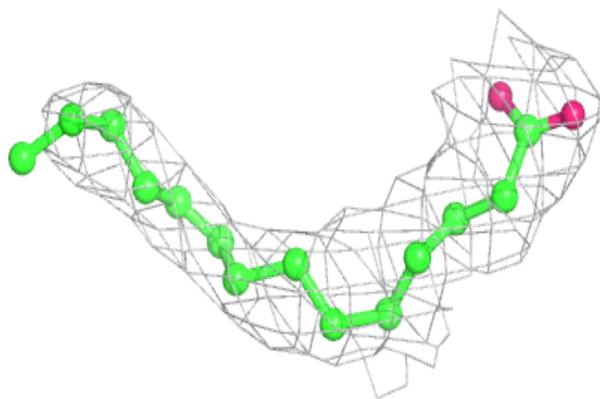
**Electron density around OLA B 1201:**

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

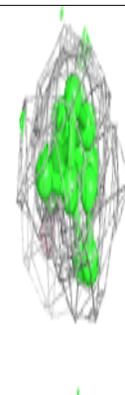
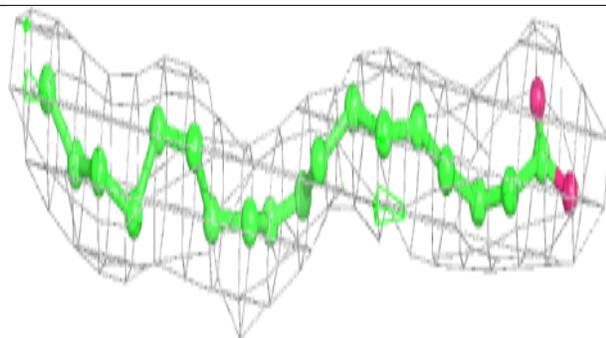
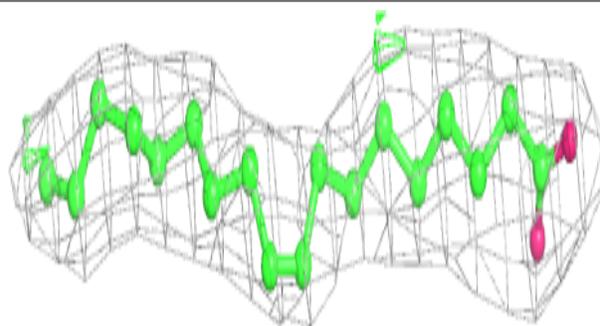


**Electron density around OLA C 1203:**

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

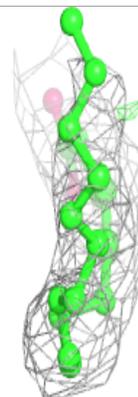
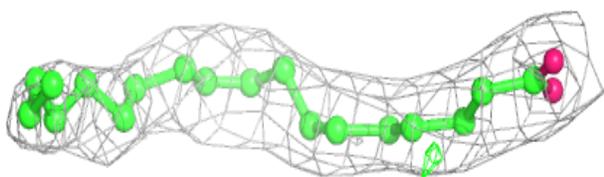
**Electron density around OLA C 1201:**

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

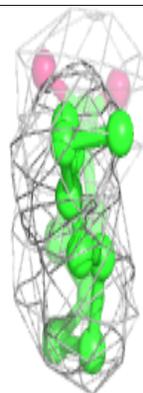
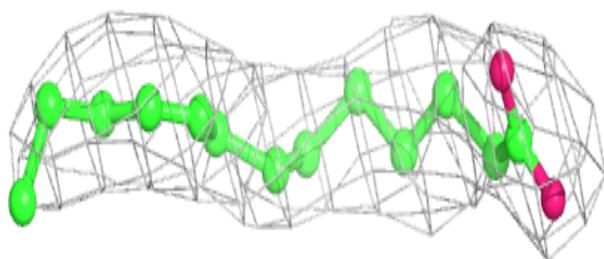
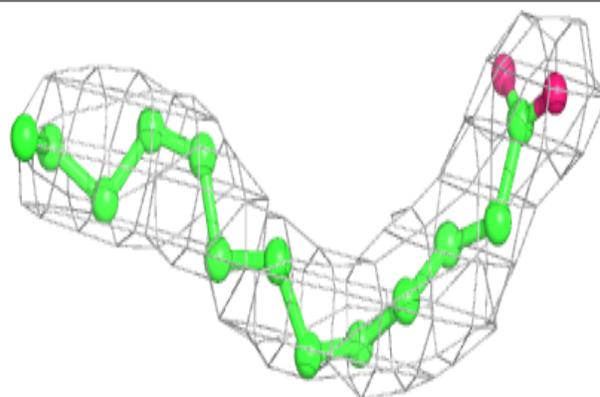


**Electron density around OLA C 1202:**

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

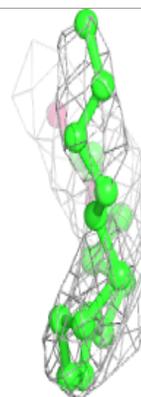
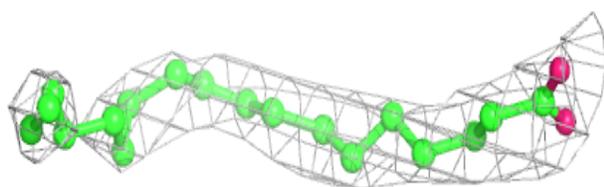
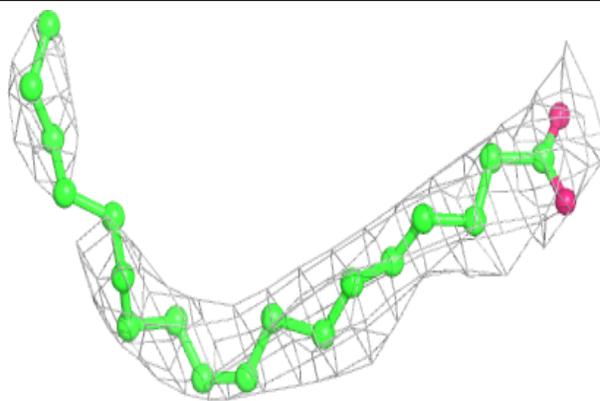
**Electron density around OLA B 1203:**

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and green (positive)

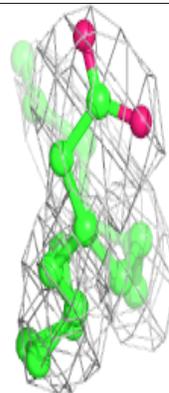
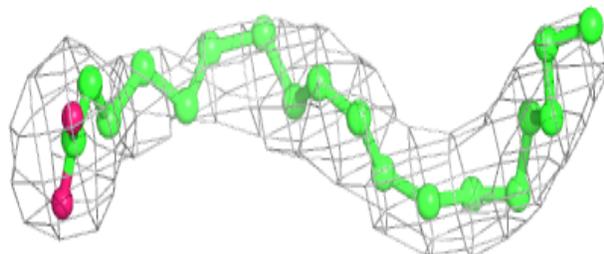
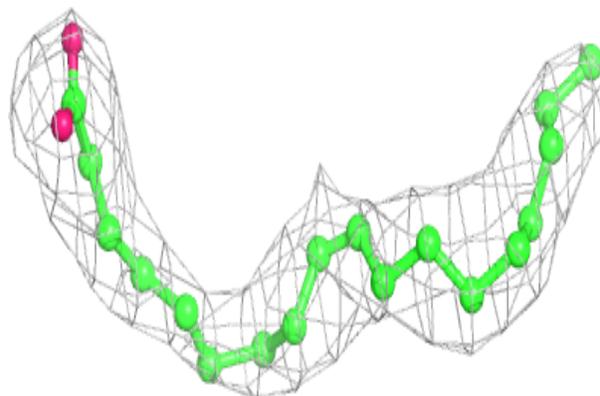


**Electron density around OLA B 1202:**

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and green (positive)

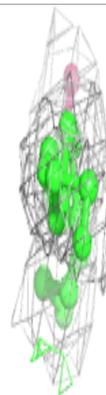
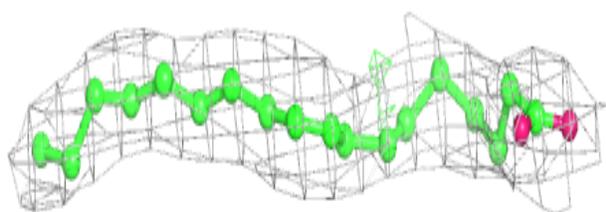
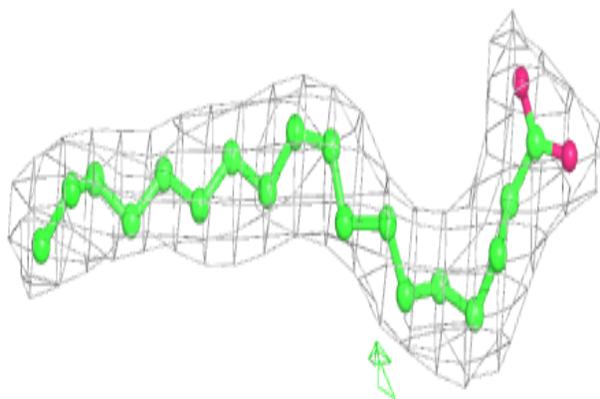
**Electron density around OLA A 1201:**

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and green (positive)

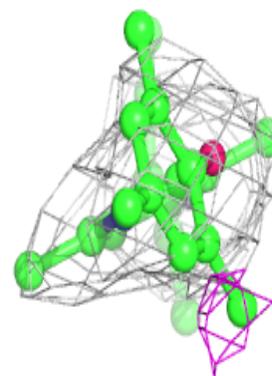
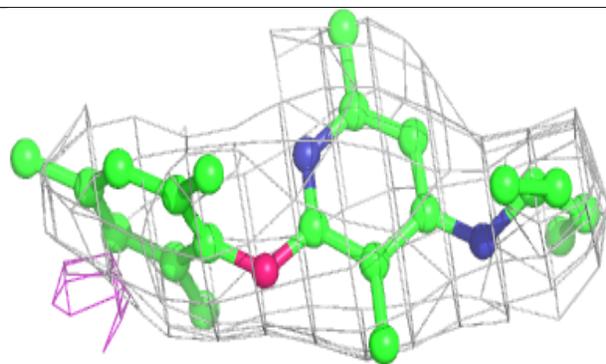
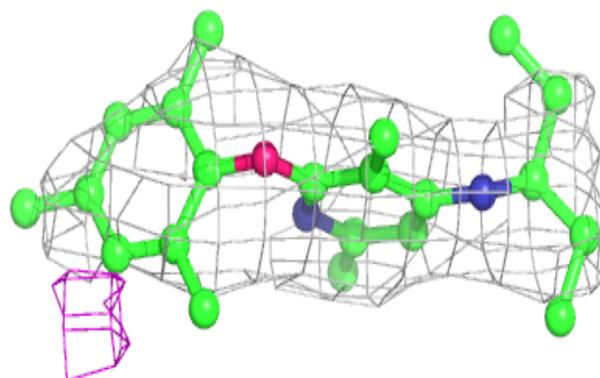


**Electron density around OLA A 1202:**

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and green (positive)

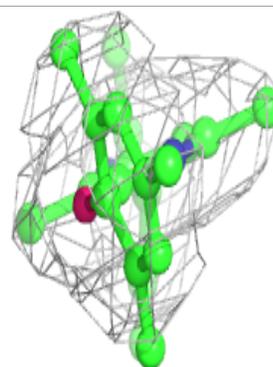
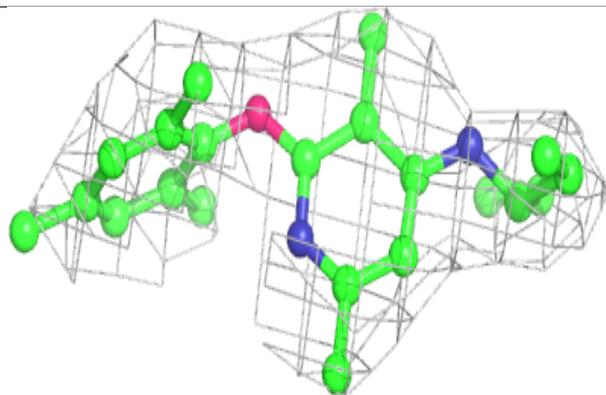
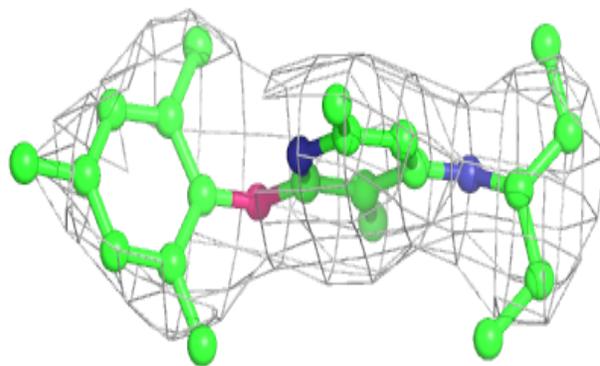
**Electron density around 1Q5 B 1204:**

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

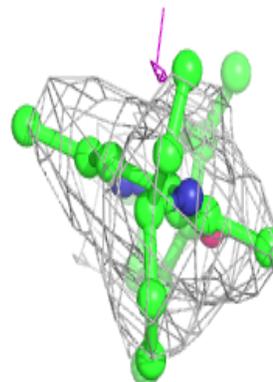
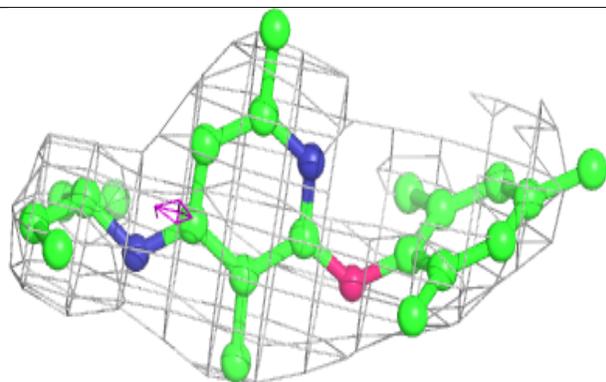
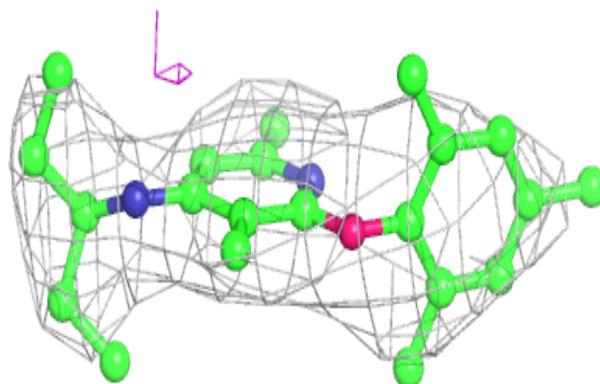


**Electron density around 1Q5 A 1204:**

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

**Electron density around 1Q5 C 1205:**

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



## 6.5 Other polymers

There are no such residues in this entry.