



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2020 – 12:11 PM JST

PDB ID : 7CRI  
Title : 1 ps Structure of Chloride ion pumping rhodopsin (ClR) with NTQ motif  
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Deposited on : 2020-08-13  
Resolution : 1.85 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.

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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 : 2.14.6  
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) : 2.14.6

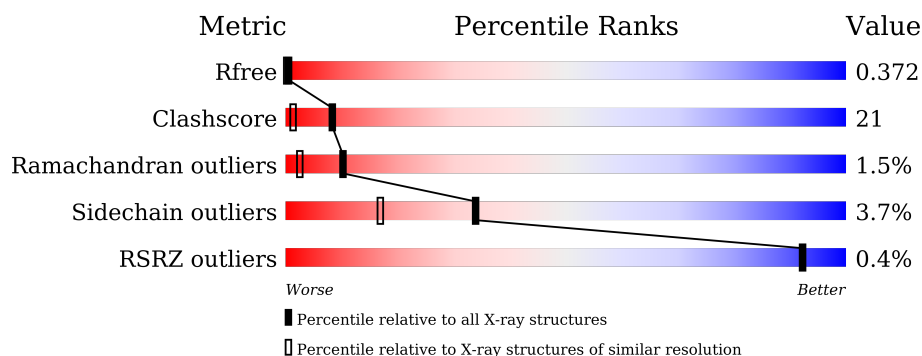
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	264	<div> <div></div> <div>59%</div> <div>34%</div> <div>6% .</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2299 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.

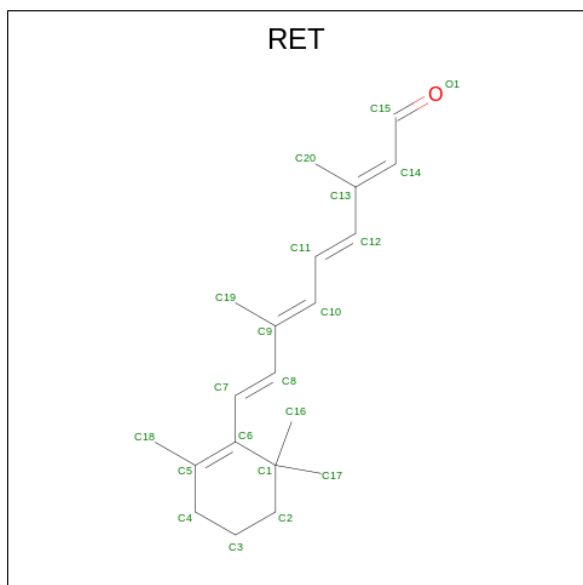
- Molecule 1 is a protein called Chloride pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2072	1378	321	359	14			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

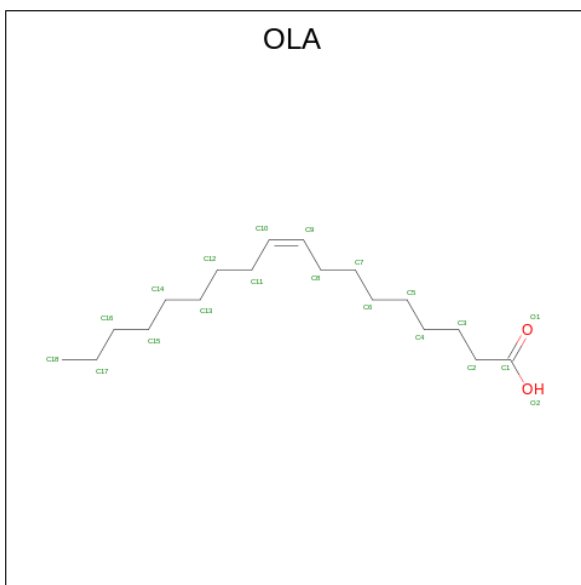
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			20	20		

- 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 14 12 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 18 16 2	0	0
4	A	1	Total C O 12 10 2	0	0
4	A	1	Total C O 20 18 2	1	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 9 9	0	0

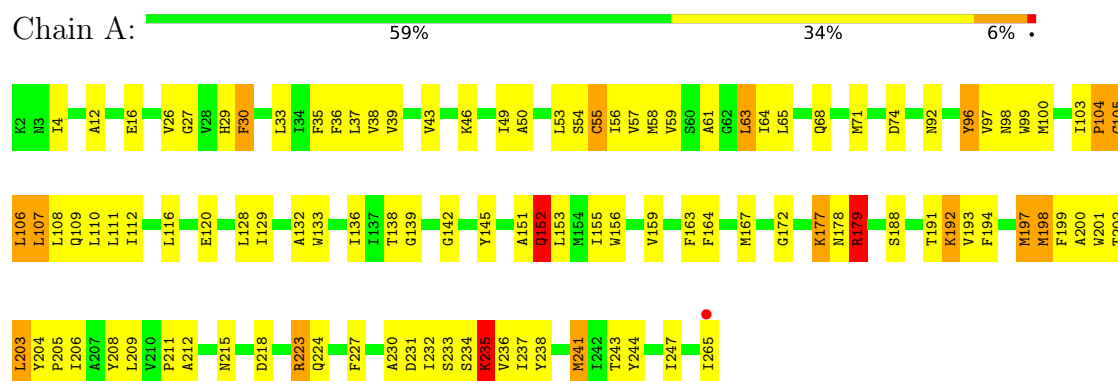
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	106	Total O 106 106	0	0

### 3 Residue-property plots

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: Chloride pumping rhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.37Å 50.09Å 69.39Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	20.64 – 1.85 20.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.64-1.85) 92.6 (20.64-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.295 , 0.372 0.295 , 0.372	Depositor DCC
$R_{free}$ test set	1720 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-2.3	Xtriage
Anisotropy	-0.726	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	2299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, RET, CL

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	1.09	10/2124 (0.5%)	1.19	18/2896 (0.6%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	CYS	CB-SG	-7.87	1.68	1.82
1	A	36	PHE	CB-CG	-6.78	1.39	1.51
1	A	30	PHE	CB-CG	6.56	1.62	1.51
1	A	206	ILE	CB-CG2	6.38	1.72	1.52
1	A	55	CYS	CB-SG	6.23	1.92	1.82
1	A	163	PHE	CE1-CZ	5.52	1.47	1.37
1	A	152	GLN	CG-CD	5.28	1.63	1.51
1	A	96	TYR	CD2-CE2	-5.12	1.31	1.39
1	A	231	ASP	CB-CG	5.10	1.62	1.51
1	A	120	GLU	CB-CG	5.07	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	MET	CB-CG-SD	8.00	136.41	112.40
1	A	231	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	203	LEU	C-N-CA	7.04	139.31	121.70
1	A	116	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	55	CYS	CA-CB-SG	6.82	126.28	114.00
1	A	106	LEU	CB-CG-CD1	-6.61	99.76	111.00
1	A	235	LYS	CB-CG-CD	6.38	128.19	111.60
1	A	65	LEU	CA-CB-CG	6.23	129.64	115.30
1	A	63	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	235	LYS	CG-CD-CE	-5.96	94.01	111.90
1	A	203	LEU	CB-CG-CD2	5.93	121.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	231	ASP	CB-CA-C	-5.32	99.77	110.40
1	A	241	MET	CB-CG-SD	5.30	128.31	112.40
1	A	241	MET	CA-CB-CG	5.23	122.19	113.30
1	A	230	ALA	C-N-CA	5.10	134.46	121.70
1	A	74	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	107	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2072	0	2105	93	1
2	A	2	0	0	1	0
3	A	20	0	27	4	0
4	A	99	0	147	5	0
5	A	106	0	0	5	2
All	All	2299	0	2279	94	3

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 21.

All (94) 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:193:VAL:HG23	1:A:241:MET:HE2	1.49	0.94
1:A:193:VAL:HG23	1:A:241:MET:CE	1.99	0.93
1:A:103:ILE:HD12	1:A:136:ILE:HD11	1.52	0.91
1:A:92:ASN:ND2	5:A:405:HOH:O	2.19	0.76
1:A:204:TYR:HB2	1:A:205:PRO:HD3	1.69	0.75
1:A:233:SER:HA	1:A:237:ILE:HB	1.69	0.73
1:A:106:LEU:HA	1:A:109:GLN:HG2	1.71	0.73
1:A:64:ILE:HG12	1:A:98:ASN:HD22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HG12	1:A:98:ASN:ND2	2.05	0.71
1:A:132:ALA:HB2	1:A:167:MET:SD	2.31	0.70
1:A:107:LEU:O	1:A:111:LEU:HG	1.94	0.66
1:A:100:MET:HG2	1:A:136:ILE:HG21	1.79	0.65
1:A:193:VAL:HG23	1:A:241:MET:HE3	1.78	0.64
1:A:201:TRP:HA	1:A:204:TYR:CD2	2.33	0.63
1:A:179:ARG:HE	1:A:191:THR:HG21	1.64	0.62
1:A:59:VAL:O	1:A:63:LEU:HD12	2.01	0.61
1:A:178:ASN:OD1	5:A:404:HOH:O	2.17	0.60
1:A:104:PRO:HG3	1:A:129:ILE:HG23	1.84	0.59
1:A:200:ALA:HB3	1:A:201:TRP:HD1	1.69	0.58
1:A:202:THR:O	1:A:205:PRO:HD2	2.05	0.57
1:A:29:HIS:CD2	1:A:61:ALA:HB3	2.40	0.56
1:A:26:VAL:HG13	1:A:30:PHE:CE2	2.40	0.56
3:A:303:RET:H8	3:A:303:RET:H161	1.88	0.56
1:A:188:SER:O	1:A:192:LYS:HE2	2.06	0.56
1:A:193:VAL:CG2	1:A:241:MET:CE	2.82	0.55
1:A:30:PHE:O	1:A:33:LEU:HB3	2.07	0.55
1:A:49:ILE:O	1:A:53:LEU:HG	2.07	0.55
1:A:138:THR:O	1:A:156:TRP:HB3	2.06	0.55
1:A:179:ARG:HE	1:A:191:THR:CG2	2.20	0.55
1:A:63:LEU:HD23	5:A:476:HOH:O	2.06	0.55
1:A:37:LEU:HD23	4:A:307:OLA:H52	1.88	0.54
1:A:194:PHE:CE1	1:A:198:MET:SD	3.00	0.54
1:A:103:ILE:O	1:A:104:PRO:C	2.46	0.53
1:A:193:VAL:O	1:A:197:MET:HG2	2.09	0.53
1:A:201:TRP:HA	1:A:204:TYR:HD2	1.74	0.52
1:A:43:VAL:HG22	1:A:247:ILE:HG12	1.92	0.51
1:A:53:LEU:O	1:A:56:ILE:HB	2.11	0.51
1:A:12:ALA:O	1:A:16:GLU:HG3	2.11	0.51
1:A:104:PRO:HG3	1:A:129:ILE:CG2	2.41	0.50
1:A:129:ILE:HG22	1:A:133:TRP:CE2	2.46	0.50
1:A:234:SER:OG	1:A:235:LYS:HE2	2.11	0.50
1:A:26:VAL:HG13	1:A:30:PHE:CD2	2.46	0.50
1:A:38:VAL:HG22	4:A:307:OLA:H31	1.95	0.49
1:A:151:ALA:O	1:A:155:ILE:HG12	2.12	0.49
1:A:107:LEU:HD13	1:A:128:LEU:HB3	1.94	0.49
1:A:208:TYR:CE2	3:A:303:RET:H31	2.48	0.49
1:A:193:VAL:CG2	1:A:241:MET:HE3	2.42	0.49
1:A:71:MET:HG2	5:A:453:HOH:O	2.12	0.49
1:A:244:TYR:HB2	4:A:310:OLA:H71	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG13	1:A:238:TYR:CE1	2.48	0.48
1:A:103:ILE:HG21	1:A:132:ALA:HB1	1.96	0.48
1:A:50:ALA:O	1:A:53:LEU:HB2	2.13	0.48
1:A:99:TRP:HD1	1:A:99:TRP:HA	1.63	0.47
1:A:100:MET:N	1:A:136:ILE:HD13	2.30	0.47
1:A:132:ALA:CB	1:A:167:MET:SD	3.01	0.47
1:A:27:GLY:HA3	4:A:308:OLA:H152	1.96	0.47
1:A:97:VAL:O	1:A:100:MET:HB2	2.14	0.47
1:A:138:THR:O	1:A:142:GLY:N	2.48	0.46
1:A:64:ILE:HD13	1:A:64:ILE:HA	1.75	0.46
1:A:64:ILE:O	1:A:68:GLN:HG2	2.15	0.46
1:A:204:TYR:CE2	3:A:303:RET:H11	2.50	0.46
1:A:224:GLN:O	1:A:227:PHE:HB2	2.16	0.46
1:A:243:THR:OG1	5:A:403:HOH:O	2.06	0.46
1:A:104:PRO:O	1:A:108:LEU:HB2	2.15	0.46
1:A:265:ILE:HD13	4:A:310:OLA:H21	1.97	0.45
1:A:211:PRO:O	1:A:215:ASN:HB2	2.15	0.45
1:A:232:ILE:HA	1:A:236:VAL:HB	1.98	0.45
1:A:53:LEU:HD13	1:A:105:CYS:O	2.17	0.45
1:A:29:HIS:HA	1:A:58:MET:SD	2.57	0.45
1:A:63:LEU:O	1:A:64:ILE:C	2.54	0.44
1:A:139:GLY:HA3	3:A:303:RET:C2	2.47	0.44
1:A:99:TRP:C	1:A:136:ILE:HD13	2.38	0.44
1:A:4:ILE:HD13	1:A:211:PRO:HG3	2.00	0.43
1:A:58:MET:HE1	1:A:235:LYS:HB2	1.99	0.43
1:A:238:TYR:O	1:A:241:MET:HB2	2.18	0.43
1:A:46:LYS:HB3	2:A:302:CL:CL	2.56	0.43
1:A:4:ILE:HG21	1:A:211:PRO:HB3	2.01	0.43
1:A:35:PHE:CE1	1:A:39:VAL:HG11	2.54	0.42
1:A:145:TYR:CZ	1:A:152:GLN:NE2	2.88	0.42
1:A:199:PHE:O	1:A:203:LEU:HG	2.19	0.42
1:A:194:PHE:CZ	1:A:198:MET:SD	3.13	0.42
1:A:110:LEU:HB2	1:A:238:TYR:OH	2.20	0.41
1:A:108:LEU:O	1:A:112:ILE:HG12	2.20	0.41
1:A:155:ILE:O	1:A:159:VAL:HG23	2.21	0.41
1:A:61:ALA:HB2	1:A:235:LYS:HD2	2.03	0.41
1:A:64:ILE:CG1	1:A:98:ASN:HD22	2.29	0.41
1:A:209:LEU:O	1:A:212:ALA:HB3	2.21	0.41
1:A:64:ILE:HD12	1:A:64:ILE:HG23	1.90	0.41
1:A:105:CYS:O	1:A:109:GLN:N	2.52	0.41
1:A:96:TYR:O	1:A:99:TRP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:HA	1:A:136:ILE:HD13	2.02	0.41
1:A:55:CYS:O	1:A:59:VAL:HG12	2.21	0.40
1:A:54:SER:HA	1:A:57:VAL:HG23	2.03	0.40
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.92	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:481:HOH:O	5:A:481:HOH:O[2_556]	1.82	0.38
5:A:406:HOH:O	5:A:430:HOH:O[2_556]	1.91	0.29
1:A:177:LYS:NZ	1:A:218:ASP:OD2[4_455]	2.08	0.12

## 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	262/264 (99%)	239 (91%)	19 (7%)	4 (2%)	<b>10</b> <b>2</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	164	PHE
1	A	172	GLY
1	A	104	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	217/217 (100%)	209 (96%)	8 (4%)	34	17

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	153	LEU
1	A	177	LYS
1	A	179	ARG
1	A	192	LYS
1	A	198	MET
1	A	223	ARG
1	A	235	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	98	ASN
1	A	143	GLN
1	A	152	GLN
1	A	168	ASN
1	A	178	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are 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
3	RET	A	303	1	20,20,21	4.26	12 (60%)	27,27,28	2.91	14 (51%)
4	OLA	A	310	-	8,8,19	0.38	0	7,7,19	0.72	0
4	OLA	A	307	-	8,11,19	1.10	1 (12%)	7,11,19	1.07	0
4	OLA	A	309	-	5,5,19	0.38	0	4,4,19	0.35	0
4	OLA	A	304	-	10,13,19	0.97	1 (10%)	8,13,19	0.73	0
4	OLA	A	305	-	16,19,19	0.67	1 (6%)	15,19,19	1.19	2 (13%)
4	OLA	A	306	-	14,17,19	0.93	1 (7%)	13,17,19	0.94	1 (7%)
4	OLA	A	308	-	16,19,19	0.81	1 (6%)	15,19,19	0.53	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	RET	A	303	1	-	3/13/30/31	0/1/1/1
4	OLA	A	310	-	-	1/6/6/17	-
4	OLA	A	307	-	-	1/7/9/17	-
4	OLA	A	309	-	-	1/3/3/17	-
4	OLA	A	304	-	-	7/9/11/17	-
4	OLA	A	305	-	-	10/15/17/17	-
4	OLA	A	306	-	-	7/13/15/17	-
4	OLA	A	308	-	-	9/15/17/17	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	RET	C14-C13	7.41	1.39	1.33
3	A	303	RET	C1-C6	6.91	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	RET	C2-C1	6.78	1.69	1.54
3	A	303	RET	C12-C13	6.41	1.59	1.45
3	A	303	RET	C7-C6	5.76	1.65	1.45
3	A	303	RET	C5-C6	-4.79	1.26	1.34
3	A	303	RET	C18-C5	4.70	1.58	1.50
3	A	303	RET	C10-C9	4.67	1.42	1.35
3	A	303	RET	C8-C9	4.56	1.55	1.45
3	A	303	RET	C11-C10	4.07	1.56	1.43
3	A	303	RET	C4-C5	-3.92	1.43	1.51
3	A	303	RET	C2-C3	3.44	1.61	1.52
4	A	307	OLA	C10-C9	3.02	1.49	1.28
4	A	308	OLA	C10-C9	2.91	1.48	1.31
4	A	306	OLA	C10-C9	2.91	1.48	1.31
4	A	304	OLA	C10-C9	2.44	1.45	1.31
4	A	305	OLA	C10-C9	2.36	1.45	1.31

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	RET	C17-C1-C6	8.00	123.27	110.30
3	A	303	RET	C18-C5-C6	-5.73	118.09	124.53
3	A	303	RET	C11-C12-C13	-4.38	114.11	126.42
3	A	303	RET	C20-C13-C14	-3.96	112.00	123.71
3	A	303	RET	C1-C6-C5	-3.66	117.45	122.61
3	A	303	RET	C2-C1-C6	-3.50	105.09	110.48
3	A	303	RET	C11-C10-C9	-3.00	123.03	127.31
3	A	303	RET	C2-C3-C4	-2.86	104.98	111.38
4	A	305	OLA	C6-C7-C8	-2.75	101.82	113.79
3	A	303	RET	C3-C2-C1	-2.63	105.19	114.60
3	A	303	RET	C12-C13-C14	2.57	126.94	118.80
4	A	305	OLA	C4-C3-C2	-2.43	104.31	113.76
3	A	303	RET	C19-C9-C10	-2.41	119.54	122.92
3	A	303	RET	C17-C1-C2	-2.27	99.85	108.91
3	A	303	RET	C7-C8-C9	2.21	129.58	126.23
4	A	306	OLA	C4-C3-C2	-2.17	105.33	113.76
3	A	303	RET	C1-C6-C7	2.01	121.47	115.78

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	RET	C11-C12-C13-C14

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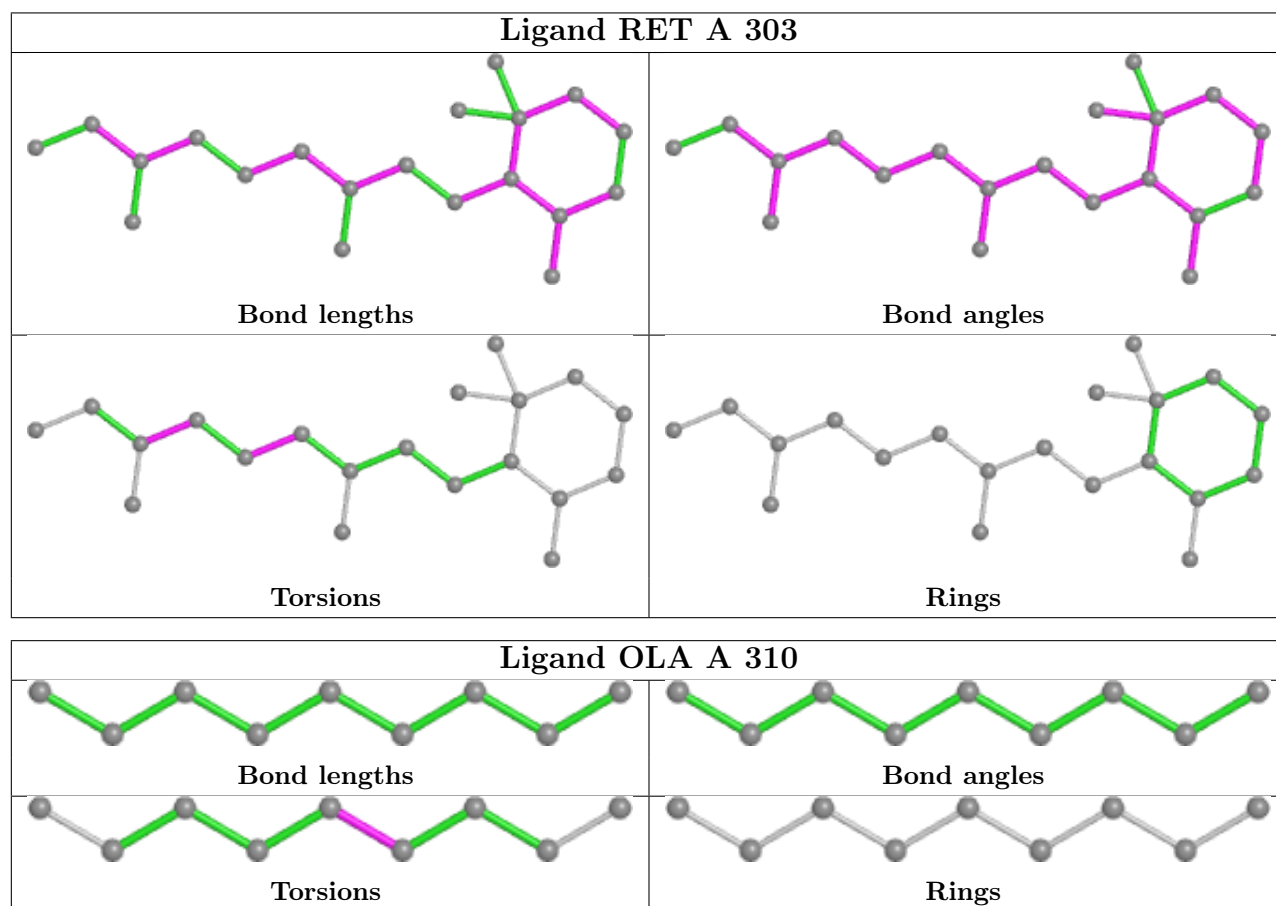
Mol	Chain	Res	Type	Atoms
3	A	303	RET	C11-C12-C13-C20
4	A	305	OLA	C1-C2-C3-C4
4	A	304	OLA	C1-C2-C3-C4
4	A	308	OLA	C1-C2-C3-C4
4	A	305	OLA	C11-C10-C9-C8
4	A	306	OLA	C11-C10-C9-C8
4	A	308	OLA	C11-C10-C9-C8
4	A	307	OLA	C4-C5-C6-C7
4	A	308	OLA	C5-C6-C7-C8
4	A	305	OLA	C5-C6-C7-C8
4	A	304	OLA	C11-C10-C9-C8
4	A	305	OLA	C2-C3-C4-C5
4	A	305	OLA	C13-C14-C15-C16
4	A	305	OLA	C3-C4-C5-C6
4	A	306	OLA	C4-C5-C6-C7
4	A	308	OLA	C4-C5-C6-C7
4	A	305	OLA	C10-C11-C12-C13
4	A	306	OLA	C10-C11-C12-C13
4	A	304	OLA	C6-C7-C8-C9
4	A	308	OLA	C11-C12-C13-C14
4	A	309	OLA	C1-C2-C3-C4
4	A	304	OLA	C4-C5-C6-C7
4	A	306	OLA	C11-C12-C13-C14
4	A	308	OLA	C13-C14-C15-C16
4	A	308	OLA	C2-C3-C4-C5
4	A	306	OLA	C13-C14-C15-C16
4	A	304	OLA	C3-C4-C5-C6
4	A	305	OLA	C4-C5-C6-C7
4	A	304	OLA	C2-C3-C4-C5
4	A	308	OLA	C12-C13-C14-C15
4	A	306	OLA	C7-C8-C9-C10
4	A	310	OLA	C3-C4-C5-C6
3	A	303	RET	C9-C10-C11-C12
4	A	304	OLA	C7-C8-C9-C10
4	A	305	OLA	C7-C8-C9-C10
4	A	308	OLA	C15-C16-C17-C18
4	A	305	OLA	C9-C10-C11-C12
4	A	306	OLA	C6-C7-C8-C9

There are no ring outliers.

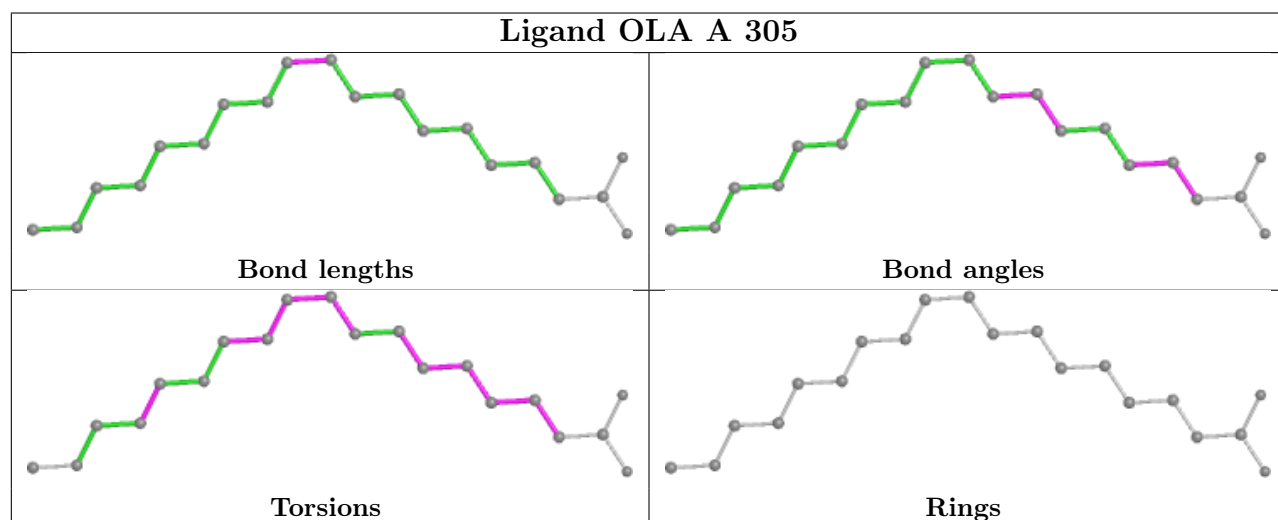
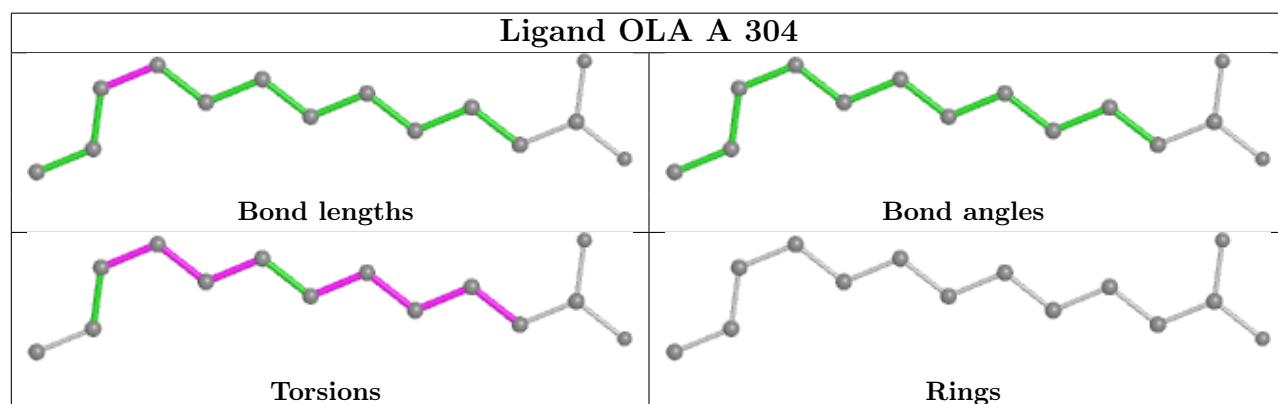
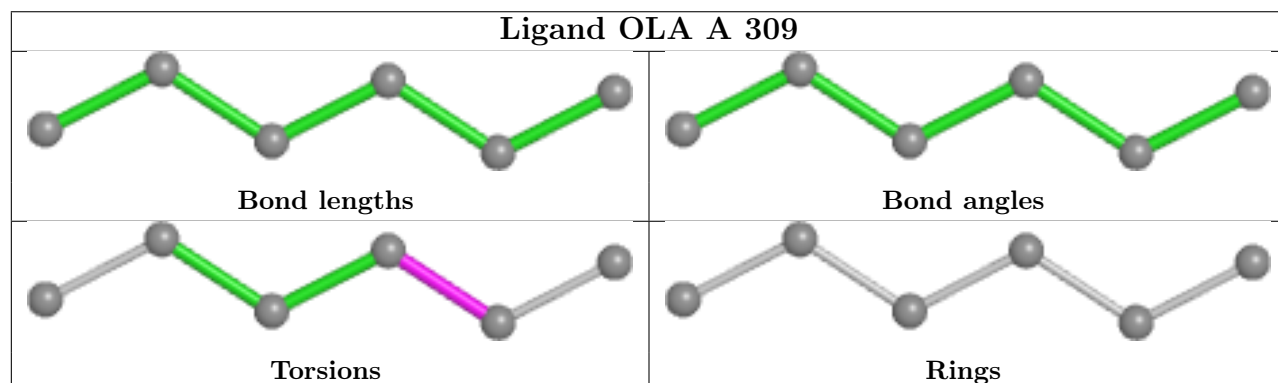
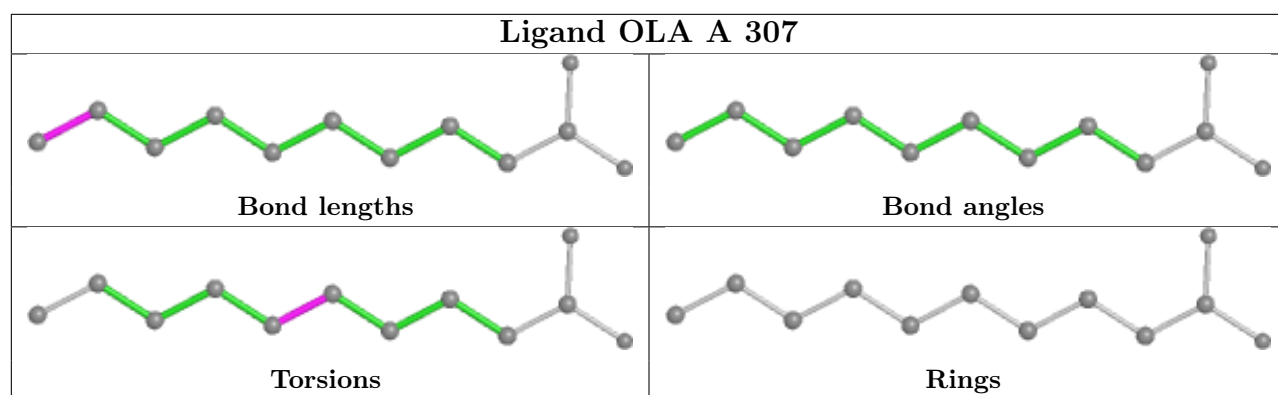
4 monomers are involved in 9 short contacts:

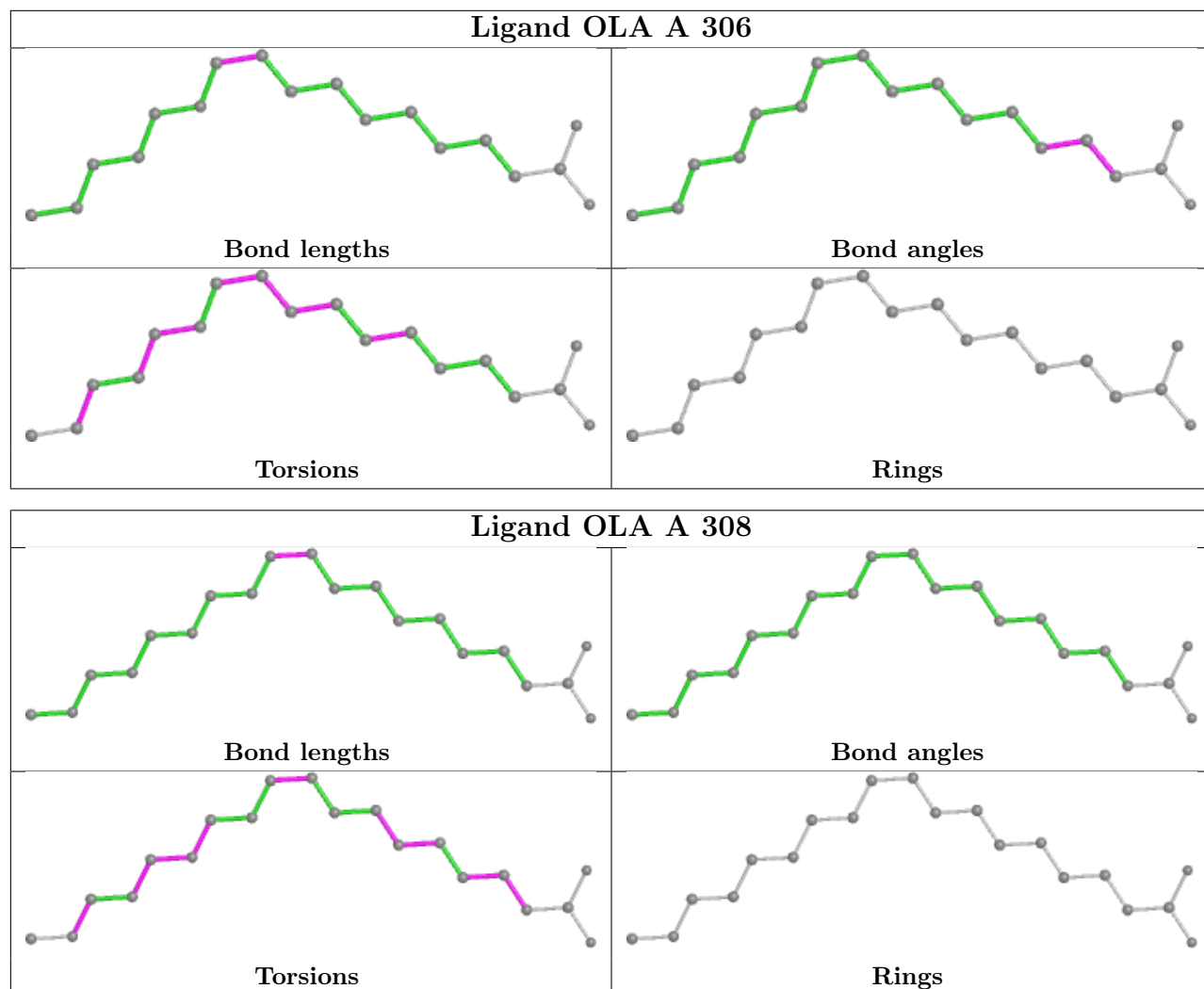
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	RET	4	0
4	A	310	OLA	2	0
4	A	307	OLA	2	0
4	A	308	OLA	1	0

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	264/264 (100%)	0.18	1 (0%) 92 92	3, 9, 19, 40	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	ILE	2.9

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

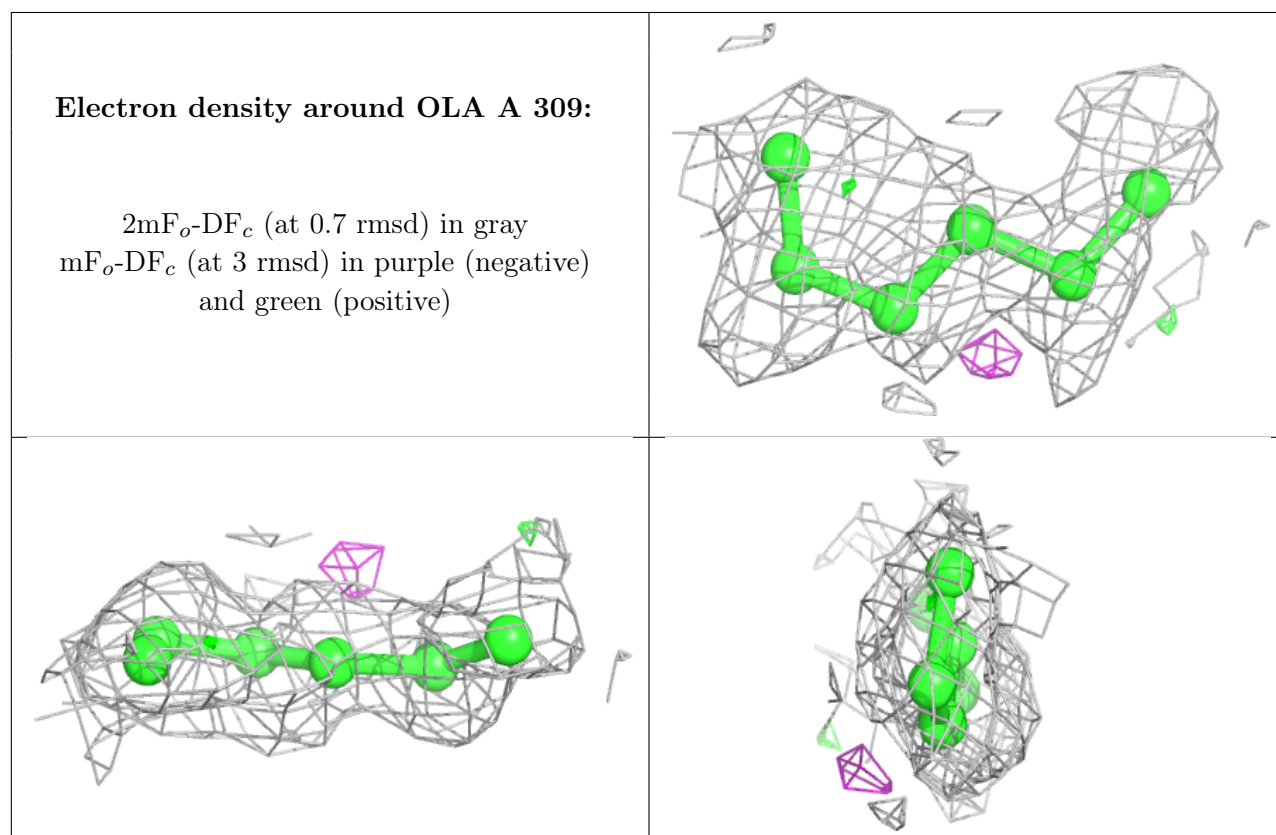
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	OLA	A	309	6/20	0.78	0.19	6,16,18,21	1
4	OLA	A	310	9/20	0.78	0.19	9,12,19,19	6
4	OLA	A	308	20/20	0.78	0.14	11,20,27,27	7
4	OLA	A	304	14/20	0.79	0.18	5,13,18,18	6
4	OLA	A	305	20/20	0.85	0.17	2,7,15,19	9
4	OLA	A	307	12/20	0.87	0.14	3,7,9,9	5

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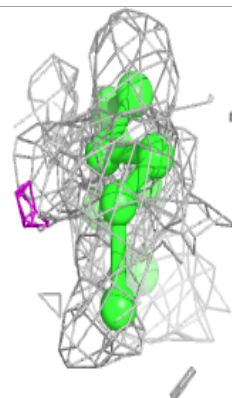
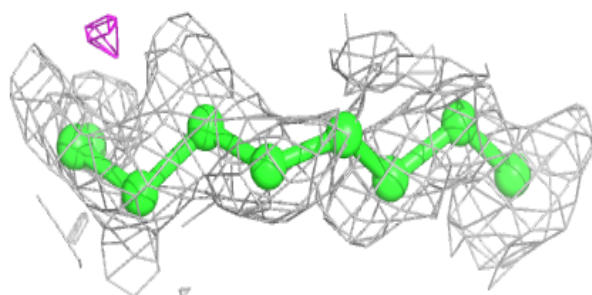
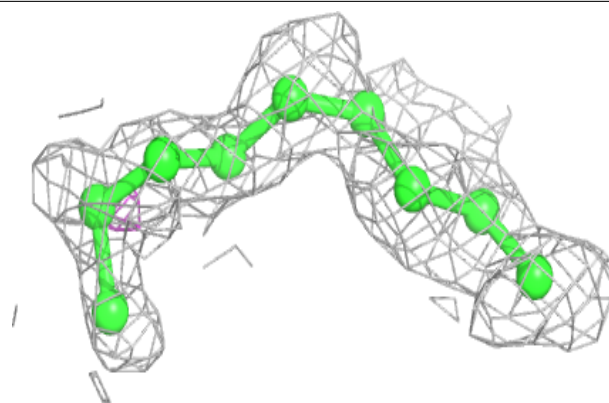
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OLA	A	306	18/20	0.88	0.13	7,11,19,22	7
2	CL	A	302	1/1	0.90	0.10	26,26,26,26	0
3	RET	A	303	20/21	0.90	0.14	0,2,7,8	0
2	CL	A	301	1/1	0.97	0.09	11,11,11,11	0

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.

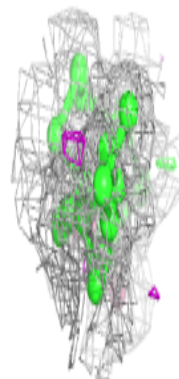
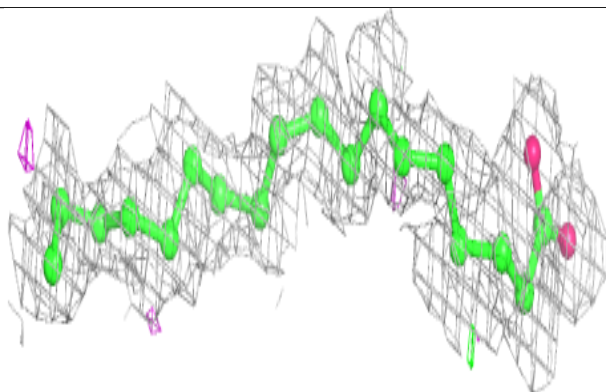
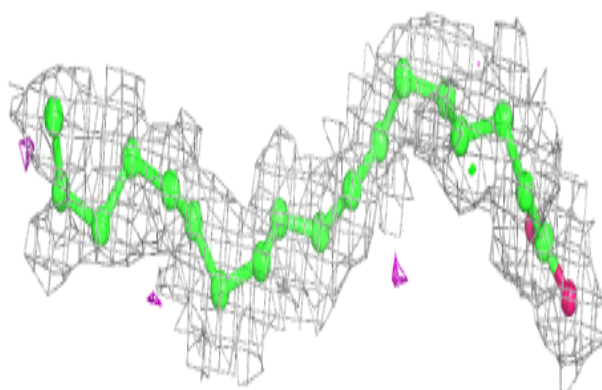


**Electron density around OLA A 310:**

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

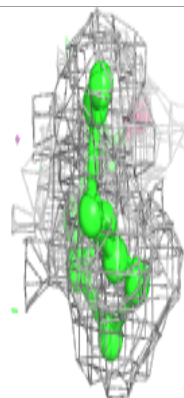
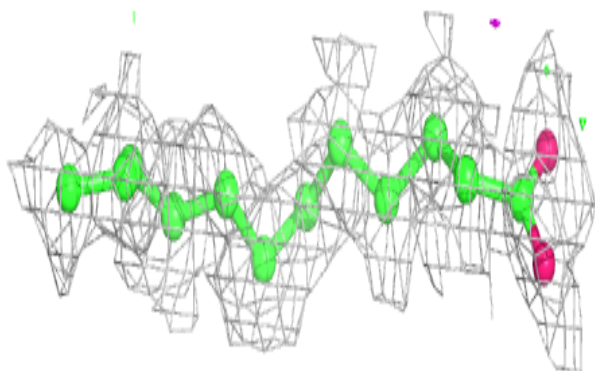
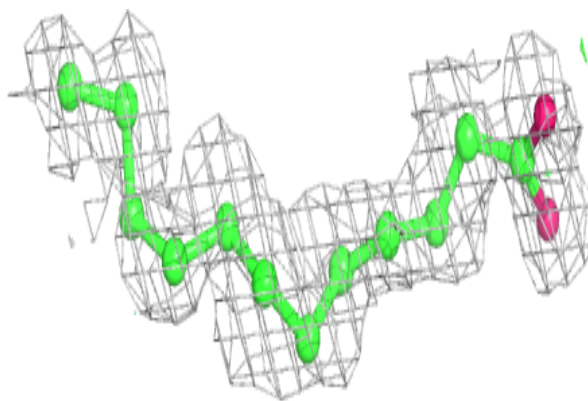
**Electron density around OLA A 308:**

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

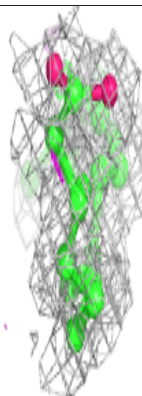
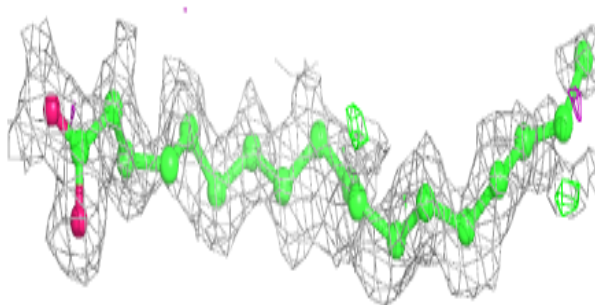
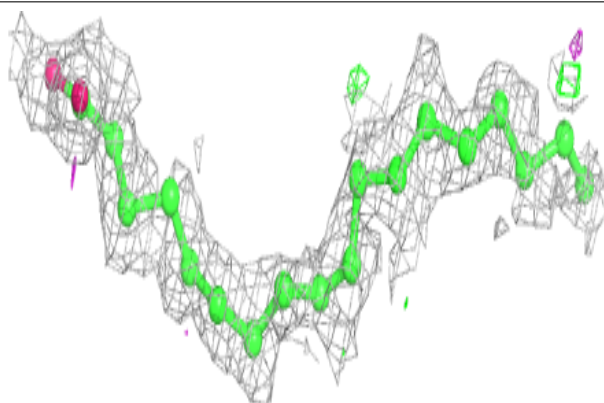


**Electron density around OLA A 304:**

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

**Electron density around OLA A 305:**

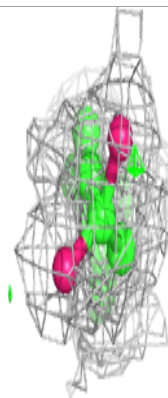
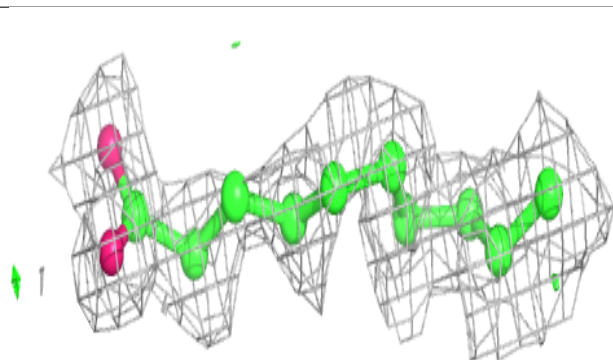
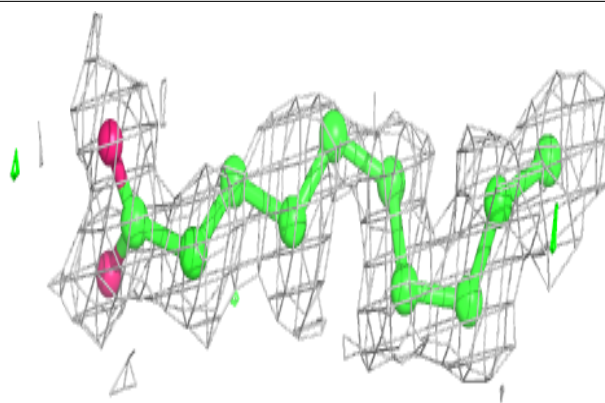
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



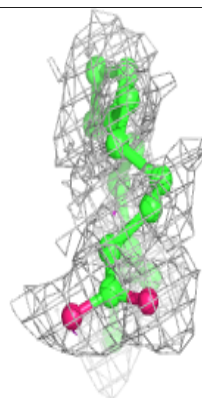
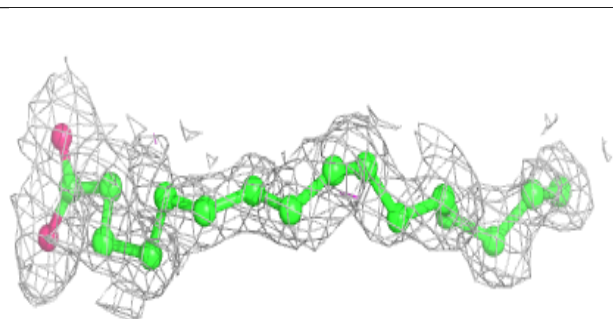
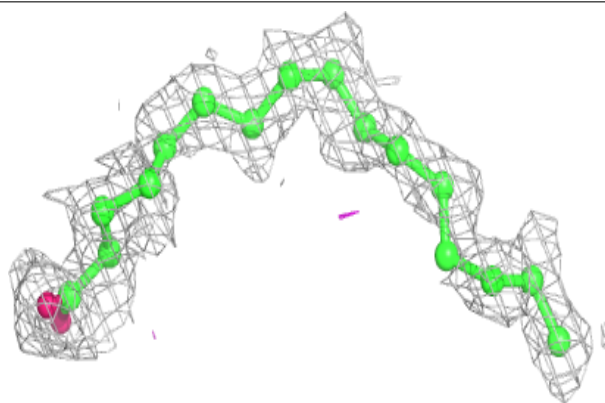


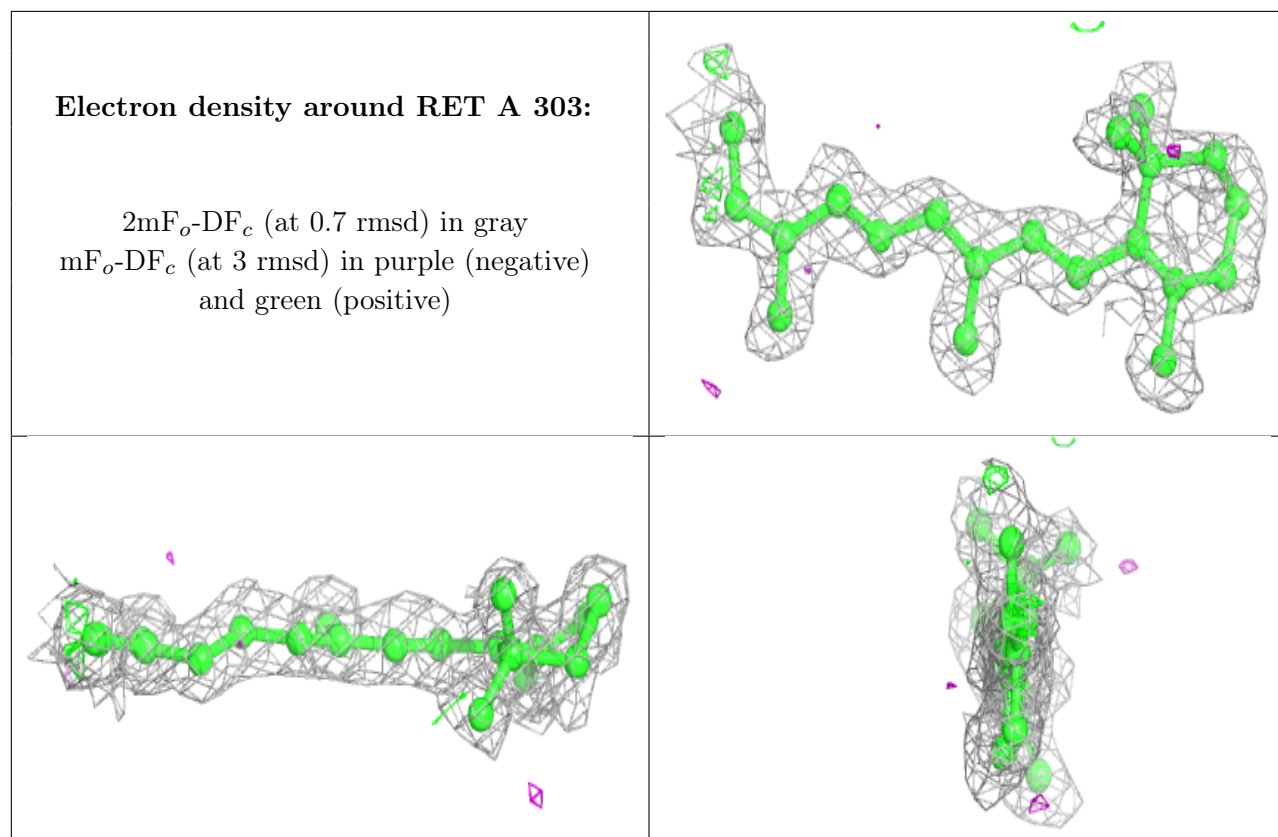
**Electron density around OLA A 307:**

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

**Electron density around OLA A 306:**

$2mF_o-DF_c$  (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.