



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 09:08 pm GMT

PDB ID : 6YXG  
Title : Cryogenic human adiponectin receptor 2 (ADIPOR2) with Tb-XO4 ligand determined by Serial Crystallography (SSX) using CrystalDirect  
Authors : Healey, R.D.; Basu, S.; Humm, A.S.; Leyrat, C.; Dupeux, F.; Pica, A.; Granier, S.; Marquez, J.A.  
Deposited on : 2020-05-01  
Resolution : 3.01 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 : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

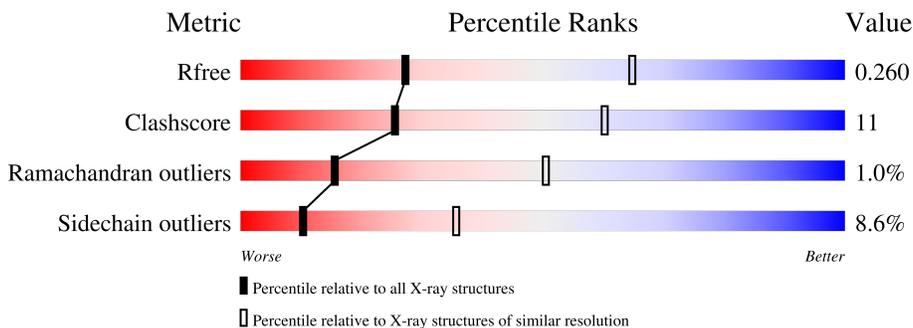
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	292	69% (green), 26% (yellow), 5% (orange), 0% (red), 0% (grey)
2	H	236	74% (green), 23% (yellow), 3% (orange), 0% (red), 0% (grey)

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 4423 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 Adiponectin receptor protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2282	1533	371	361	17	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q86V24
A	-3	GLY	-	expression tag	UNP Q86V24
A	-2	SER	-	expression tag	UNP Q86V24
A	-1	GLU	-	expression tag	UNP Q86V24
A	0	PHE	-	expression tag	UNP Q86V24

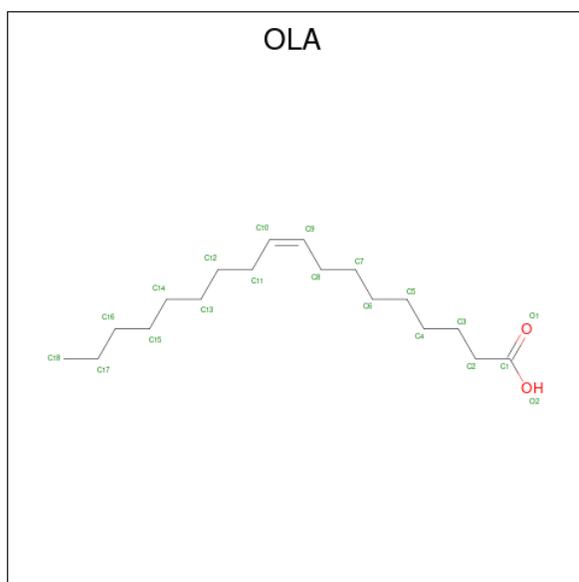
- Molecule 2 is a protein called V REGION HEAVY AND LIGHT CHAINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	236	1791	1131	296	357	7	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

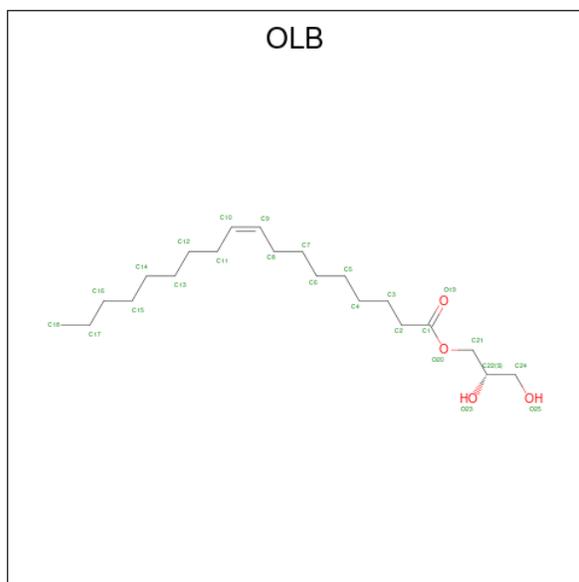
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			20	18 2		

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula:  $C_{21}H_{40}O_4$ ) (labeled as "Ligand of Interest" by depositor).



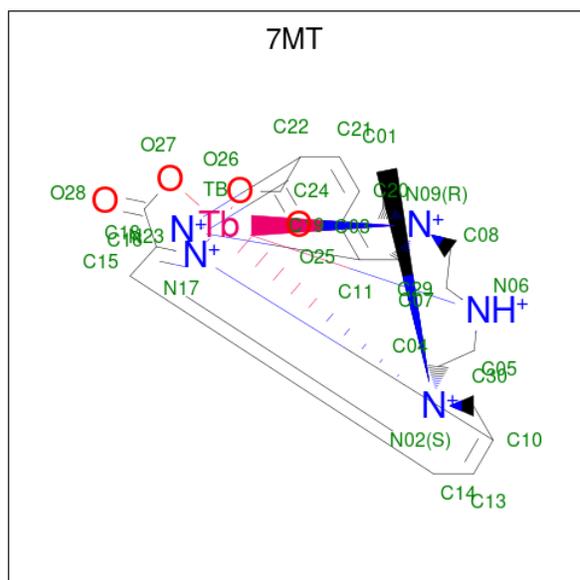
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			25	21 4		
5	A	1	Total	C O	11	0
			25	21 4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	9	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	9	0
			25	21	4		
5	H	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is Tb-Xo4 (three-letter code: 7MT) (formula:  $C_{20}H_{23}N_5O_4Tb$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	H	1	Total	C	N	O	Tb	0	0
			30	20	5	4	1		
6	H	1	Total	C	N	O	Tb	0	0
			30	20	5	4	1		

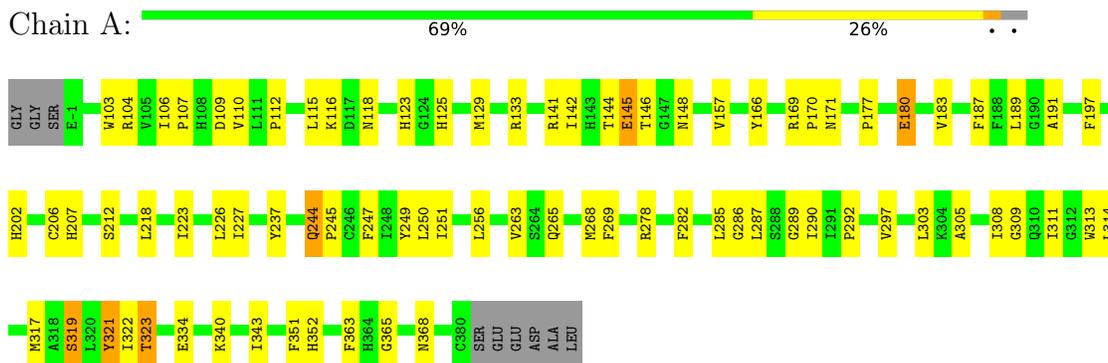
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	12	Total O 12 12	0	0
7	H	7	Total O 7 7	0	0

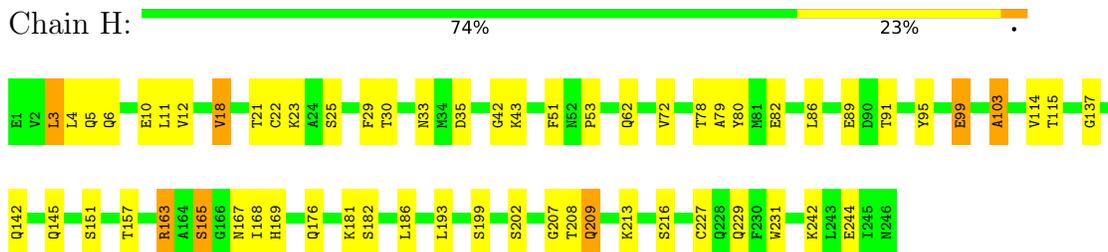
### 3 Residue-property plots [i](#)

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. 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. 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: Adiponectin receptor protein 2



- Molecule 2: V REGION HEAVY AND LIGHT CHAINS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.61Å 100.69Å 110.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 3.01 48.44 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.00-3.01) 99.9 (48.44-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, $R_{free}$	0.212 , 0.252 0.218 , 0.260	Depositor DCC
$R_{free}$ test set	971 reflections (5.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.1	Xtriage
Anisotropy	0.620	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>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: 7MT, OLB, OLA, ZN

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	0.52	0/2366	0.68	0/3216
2	H	0.53	0/1835	0.72	0/2487
All	All	0.52	0/4201	0.70	0/5703

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2260	58	0
2	H	1791	0	1701	31	0
3	A	1	0	0	0	0
4	A	20	0	33	6	0
5	A	225	0	360	20	0
5	H	25	0	40	1	0
6	H	60	0	0	5	0
7	A	12	0	0	0	0
7	H	7	0	0	0	0
All	All	4423	0	4394	93	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 11.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:GLU:HB3	2:H:103:ALA:HA	1.46	0.94
1:A:290:ILE:HD13	5:A:404:OLB:H221	1.56	0.85
1:A:319:SER:O	1:A:323:THR:HG23	1.82	0.80
1:A:290:ILE:CD1	5:A:404:OLB:H221	2.13	0.79
1:A:223:ILE:HD11	4:A:402:OLA:H22	1.65	0.78
2:H:42:GLY:O	6:H:303:7MT:C01	2.33	0.76
1:A:170:PRO:HA	5:A:406:OLB:H24	1.67	0.75
5:A:406:OLB:H3A	5:A:410:OLB:C10	2.16	0.75
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.70	0.74
2:H:176:GLN:HB2	2:H:186:LEU:HD11	1.72	0.70
2:H:167:ASN:HD21	5:H:301:OLB:H22	1.57	0.69
1:A:290:ILE:HD13	5:A:404:OLB:C9	2.24	0.67
2:H:42:GLY:O	2:H:43:LYS:HD2	1.96	0.66
2:H:91:THR:HA	2:H:114:VAL:O	1.97	0.65
2:H:22:CYS:HB3	2:H:79:ALA:HB3	1.78	0.64
1:A:351:PHE:HE1	4:A:402:OLA:H122	1.63	0.64
1:A:189:LEU:HD23	5:A:409:OLB:H38	1.79	0.63
1:A:142:ILE:HG23	1:A:343:ILE:HG21	1.81	0.62
1:A:109:ASP:HA	1:A:116:LYS:HZ1	1.65	0.61
1:A:263:VAL:HG21	5:A:411:OLB:H241	1.83	0.61
2:H:23:LYS:HA	2:H:78:THR:HG22	1.82	0.60
2:H:99:GLU:CB	2:H:103:ALA:HA	2.28	0.60
2:H:142:GLN:H	2:H:165:SER:HB3	1.68	0.58
2:H:168:ILE:HG21	2:H:229:GLN:HB2	1.86	0.57
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.87	0.56
1:A:321:TYR:HE2	5:A:404:OLB:H40	1.71	0.56
1:A:197:PHE:HE1	5:A:403:OLB:H23	1.71	0.55
1:A:227:ILE:HD12	1:A:285:LEU:HD23	1.89	0.54
1:A:308:ILE:HG13	1:A:308:ILE:O	2.08	0.54
5:A:406:OLB:H3A	5:A:410:OLB:H23	1.89	0.54
1:A:166:TYR:CE2	1:A:169:ARG:NH1	2.76	0.53
1:A:249:TYR:CD2	1:A:292:PRO:HB3	2.44	0.53
1:A:287:LEU:HA	5:A:404:OLB:H25	1.91	0.53
2:H:6:GLN:HA	2:H:21:THR:O	2.09	0.52
1:A:223:ILE:CD1	4:A:402:OLA:H22	2.37	0.52
1:A:170:PRO:HA	5:A:406:OLB:C24	2.37	0.50
1:A:247:PHE:CZ	1:A:251:ILE:HD11	2.47	0.50
2:H:157:THR:HG21	2:H:213:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:ASN:HA	2:H:208:THR:HG22	1.94	0.49
2:H:21:THR:HG23	2:H:80:TYR:CE1	2.48	0.49
2:H:169:HIS:CD2	2:H:231:TRP:CE2	3.00	0.49
1:A:202:HIS:CD2	1:A:352:HIS:HE1	2.30	0.49
1:A:289:GLY:HA3	5:A:404:OLB:H27	1.95	0.49
1:A:171:ASN:HB3	1:A:177:PRO:HG3	1.94	0.49
2:H:168:ILE:HG22	2:H:231:TRP:HB3	1.96	0.48
1:A:287:LEU:HD11	1:A:322:ILE:HG12	1.96	0.47
2:H:33:ASN:HA	2:H:53:PRO:HD3	1.95	0.47
1:A:107:PRO:HA	1:A:123:HIS:HA	1.95	0.47
2:H:95:TYR:CE1	2:H:182:SER:HB3	2.50	0.47
1:A:313:TRP:NE1	1:A:365:GLY:HA3	2.30	0.47
1:A:109:ASP:HA	1:A:116:LYS:NZ	2.28	0.47
1:A:125:HIS:CE1	1:A:144:THR:HG21	2.50	0.46
1:A:286:GLY:HA3	1:A:321:TYR:CE1	2.50	0.46
5:A:406:OLB:H5A	5:A:410:OLB:H23	1.96	0.46
1:A:314:LEU:HB3	5:A:404:OLB:H20	1.98	0.46
2:H:12:VAL:HG11	2:H:18:VAL:HG13	1.97	0.46
2:H:145:GLN:HG3	2:H:227:CYS:SG	2.56	0.45
1:A:265:GLN:OE1	5:A:408:OLB:H34	2.16	0.45
6:H:302:7MT:C07	6:H:302:7MT:N23	2.79	0.45
6:H:303:7MT:N17	6:H:303:7MT:C03	2.80	0.45
1:A:256:LEU:HD22	5:A:411:OLB:H35	1.98	0.44
1:A:180:GLU:O	1:A:183:VAL:HG22	2.17	0.44
2:H:51:PHE:CE2	2:H:72:VAL:HB	2.53	0.44
1:A:290:ILE:HD12	5:A:404:OLB:H221	1.96	0.44
1:A:305:ALA:O	1:A:308:ILE:O	2.36	0.44
1:A:244:GLN:N	1:A:245:PRO:HD2	2.33	0.44
1:A:197:PHE:CE1	5:A:403:OLB:H23	2.52	0.44
1:A:290:ILE:HD12	1:A:290:ILE:HA	1.95	0.43
1:A:106:ILE:HD12	1:A:110:VAL:HG23	1.99	0.43
1:A:313:TRP:CE2	1:A:365:GLY:HA3	2.52	0.43
2:H:3:LEU:HD22	6:H:302:7MT:C15	2.47	0.43
2:H:42:GLY:O	6:H:303:7MT:C03	2.66	0.43
1:A:218:LEU:HD23	5:A:408:OLB:H31	2.00	0.43
1:A:115:LEU:HD21	1:A:206:CYS:HA	2.01	0.43
1:A:103:TRP:CD1	1:A:129:MET:SD	3.12	0.42
1:A:118:ASN:HD21	1:A:334:GLU:HG3	1.84	0.42
2:H:29:PHE:HE2	2:H:72:VAL:CG2	2.33	0.42
1:A:202:HIS:CD2	1:A:352:HIS:CE1	3.07	0.42
2:H:163:ARG:HG2	2:H:209:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PHE:CZ	1:A:278:ARG:HG2	2.54	0.42
1:A:191:ALA:HA	1:A:226:LEU:HD13	2.01	0.42
1:A:104:ARG:NH2	2:H:30:THR:O	2.53	0.41
1:A:145:GLU:OE1	1:A:148:ASN:ND2	2.53	0.41
1:A:112:PRO:HD2	1:A:115:LEU:HB2	2.03	0.41
1:A:180:GLU:HG3	1:A:237:TYR:OH	2.20	0.41
2:H:193:LEU:HD21	2:H:199:SER:HA	2.02	0.41
1:A:129:MET:O	1:A:207:HIS:HA	2.20	0.41
1:A:282:PHE:HB2	4:A:402:OLA:H9	2.02	0.41
1:A:187:PHE:CE2	1:A:363:PHE:HB2	2.55	0.41
1:A:282:PHE:CB	4:A:402:OLA:H9	2.50	0.41
1:A:351:PHE:CE1	4:A:402:OLA:H122	2.50	0.41
2:H:91:THR:HG23	2:H:115:THR:HA	2.03	0.40
1:A:141:ARG:O	1:A:146:THR:OG1	2.32	0.40

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	281/292 (96%)	269 (96%)	11 (4%)	1 (0%)	34 71
2	H	232/236 (98%)	212 (91%)	16 (7%)	4 (2%)	9 37
All	All	513/528 (97%)	481 (94%)	27 (5%)	5 (1%)	15 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
2	H	103	ALA
2	H	216	SER
2	H	137	GLY

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Mol	Chain	Res	Type
2	H	207	GLY

### 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	240/246 (98%)	223 (93%)	17 (7%)	14	44
2	H	191/191 (100%)	171 (90%)	20 (10%)	7	26
All	All	431/437 (99%)	394 (91%)	37 (9%)	10	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	A	145	GLU
1	A	157	VAL
1	A	180	GLU
1	A	212	SER
1	A	244	GLN
1	A	250	LEU
1	A	268	MET
1	A	297	VAL
1	A	303	LEU
1	A	311	ILE
1	A	317	MET
1	A	319	SER
1	A	321	TYR
1	A	323	THR
1	A	340	LYS
1	A	368	ASN
2	H	3	LEU
2	H	4	LEU
2	H	5	GLN
2	H	10	GLU
2	H	11	LEU

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Mol	Chain	Res	Type
2	H	18	VAL
2	H	25	SER
2	H	35	ASP
2	H	62	GLN
2	H	82	GLU
2	H	89	GLU
2	H	99	GLU
2	H	151	SER
2	H	163	ARG
2	H	165	SER
2	H	181	LYS
2	H	202	SER
2	H	209	GLN
2	H	242	LYS
2	H	244	GLU

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

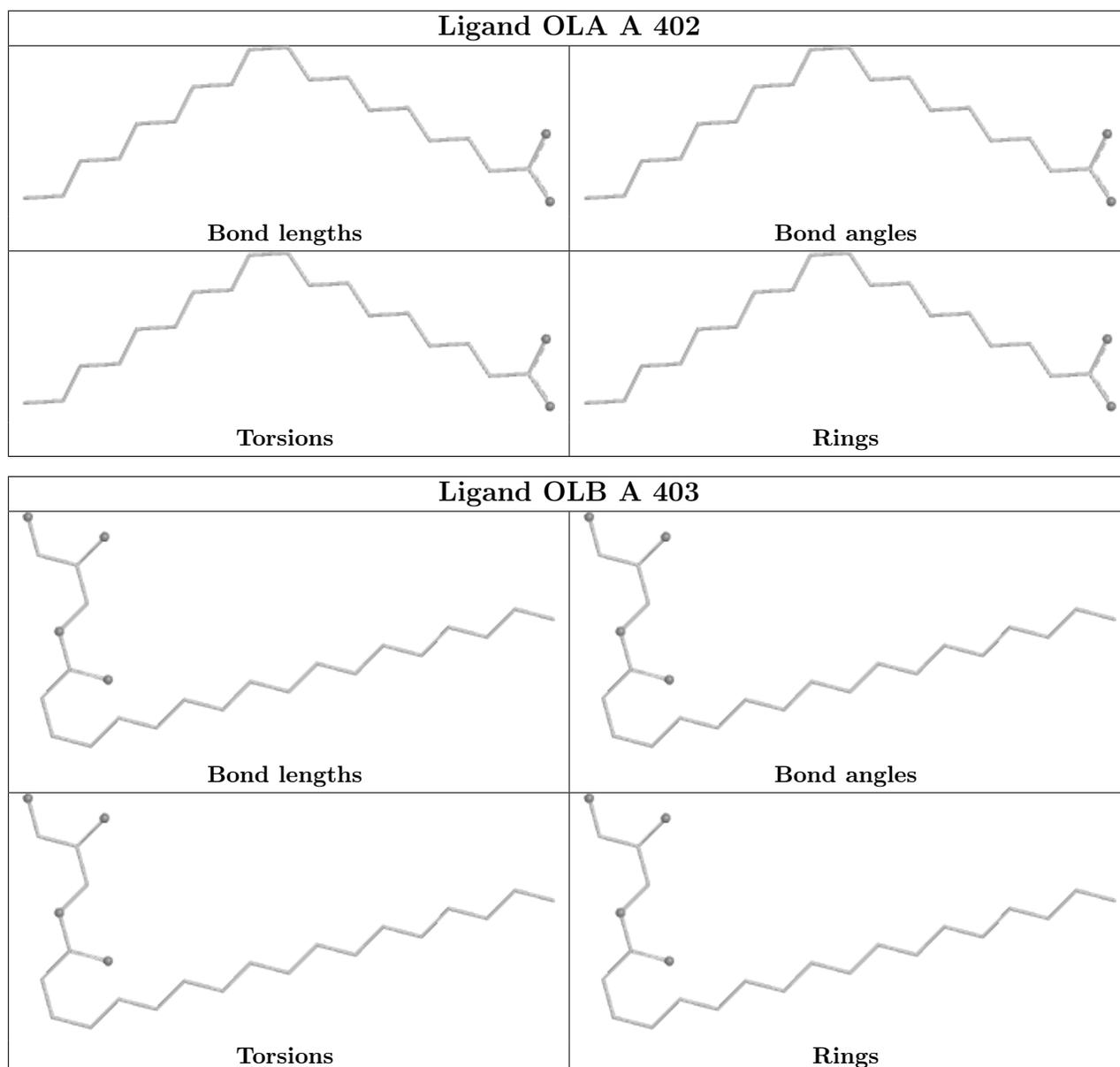
There are no chirality outliers.

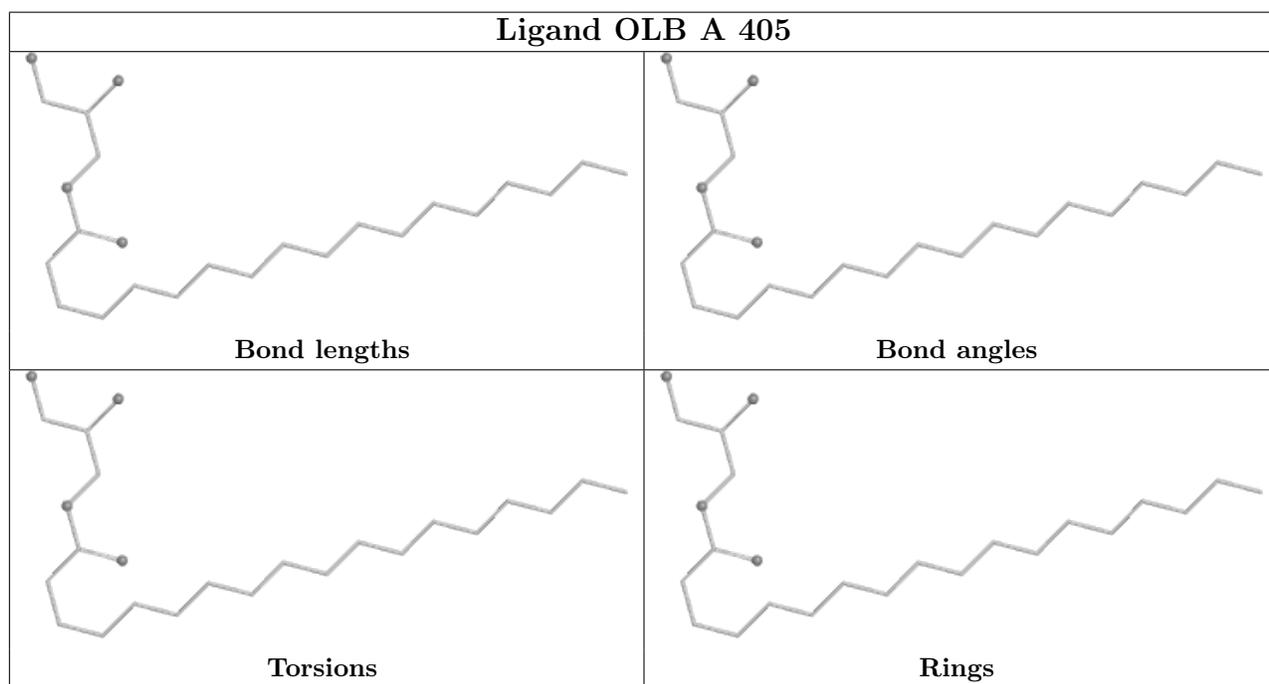
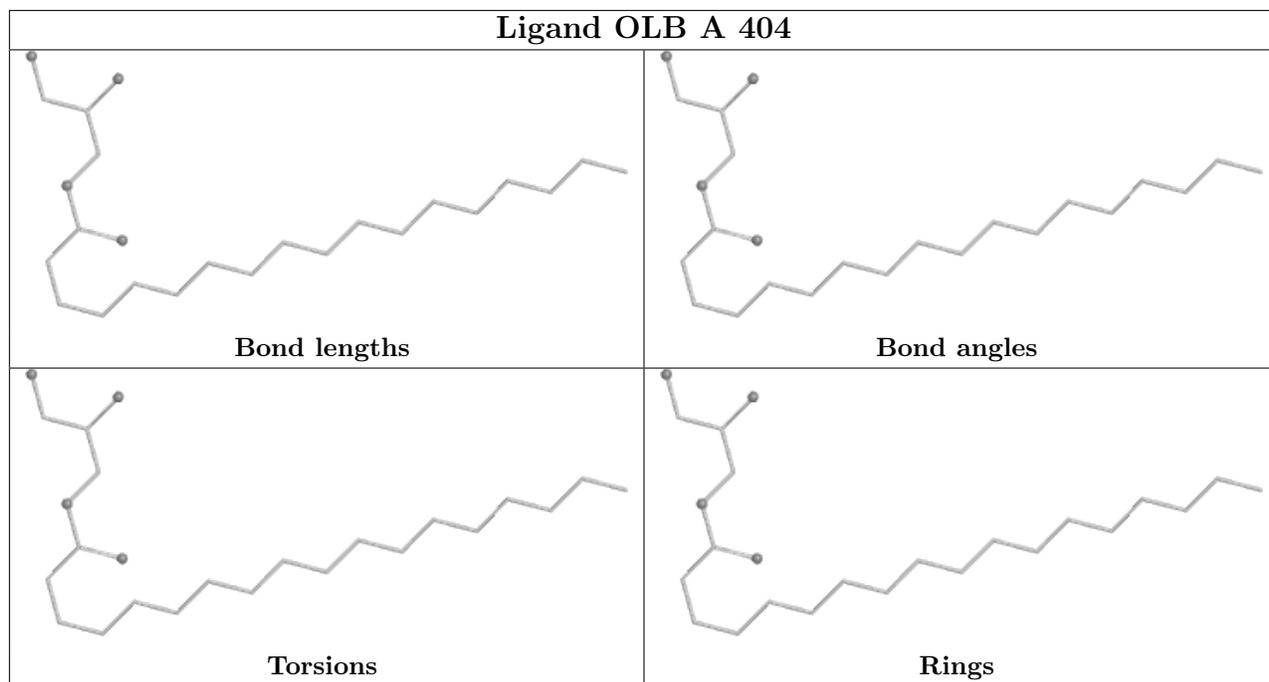
There are no torsion outliers.

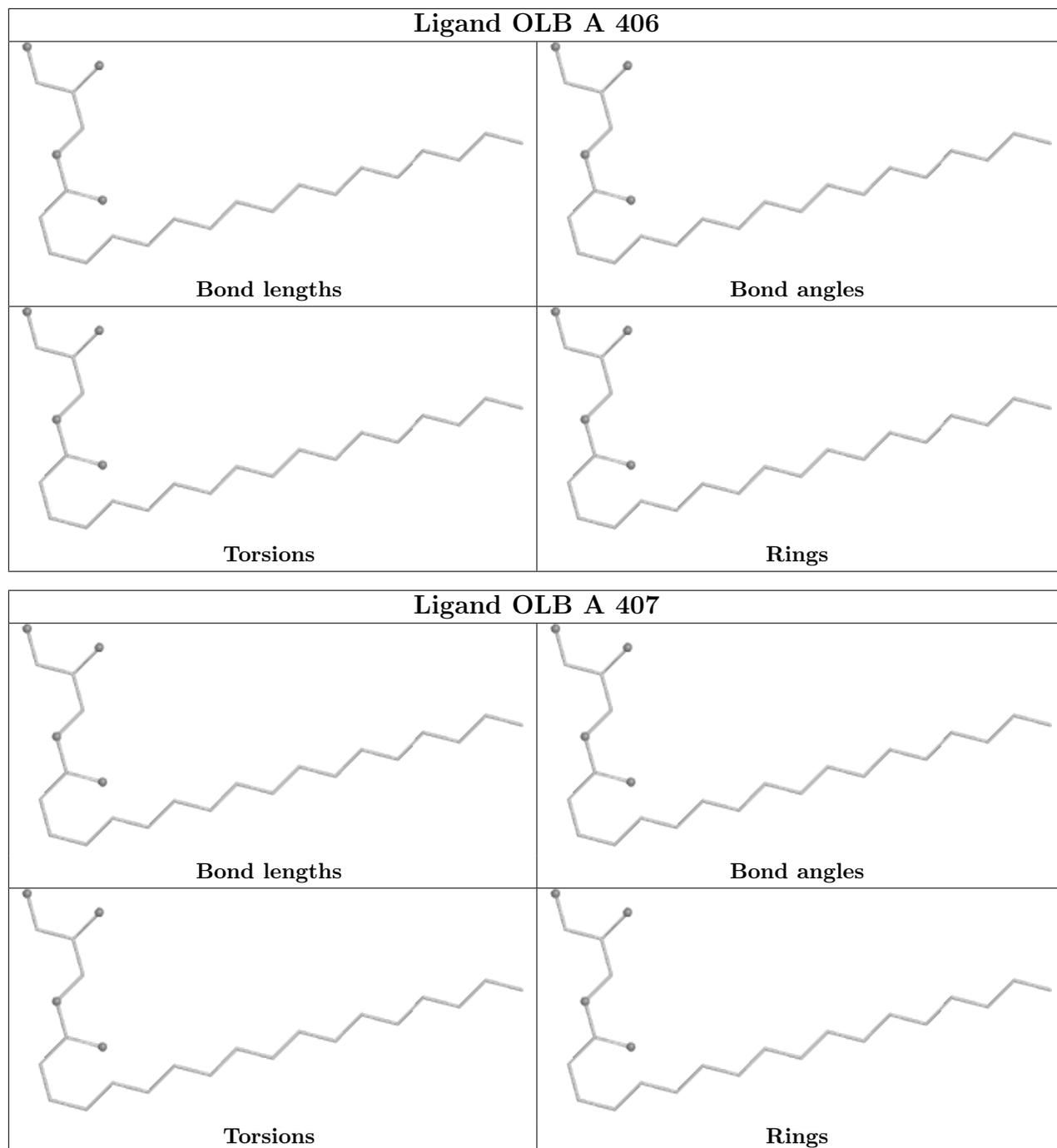
There are no ring outliers.

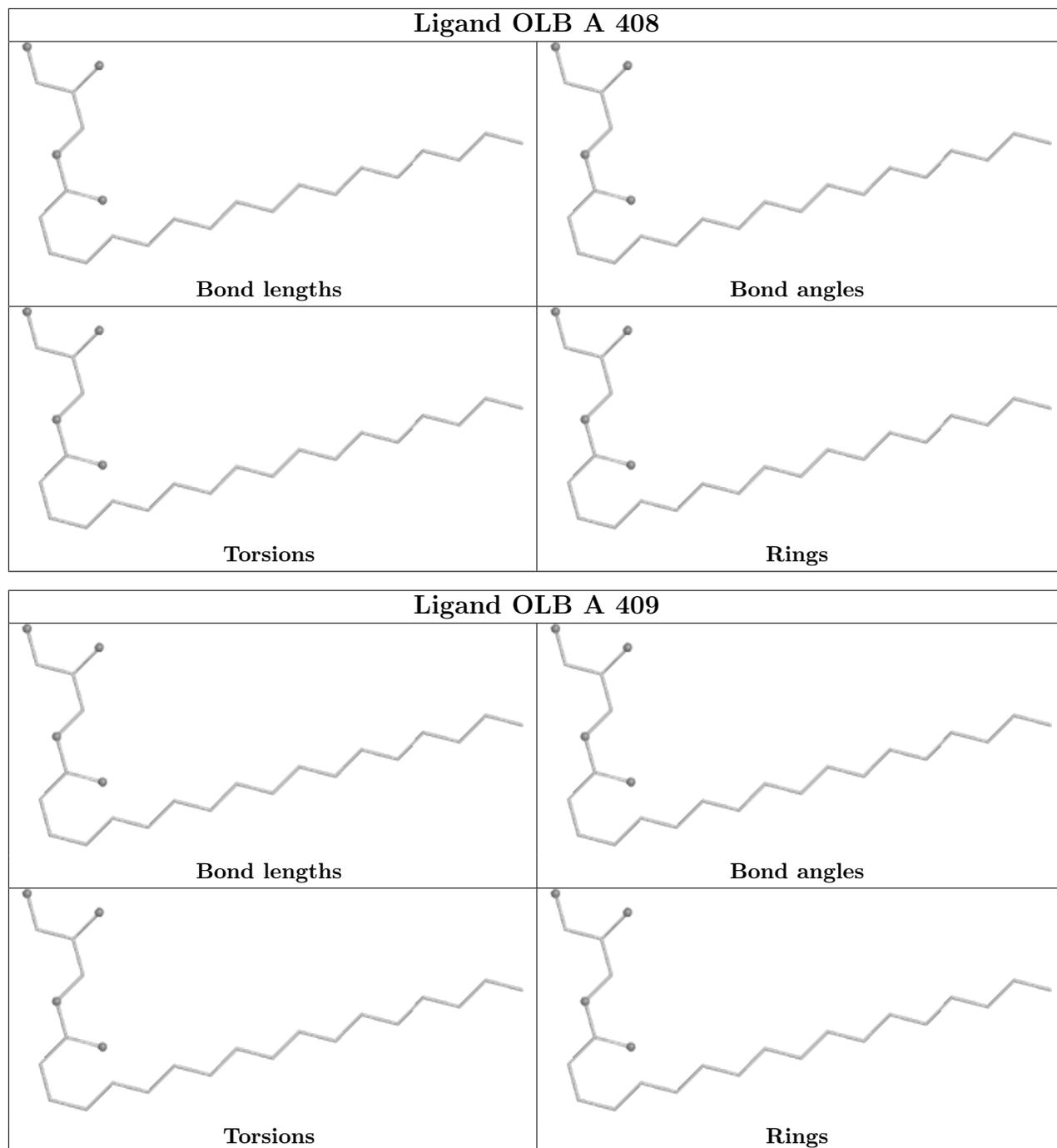
No monomer is involved in short contacts.

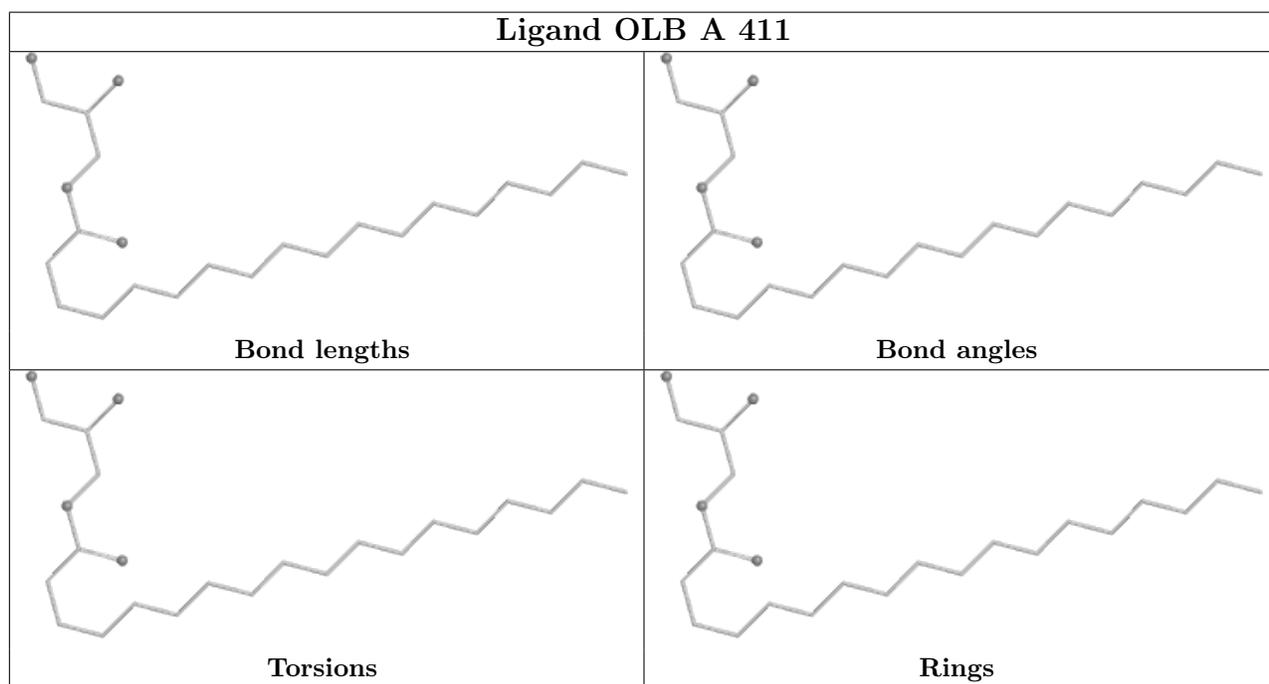
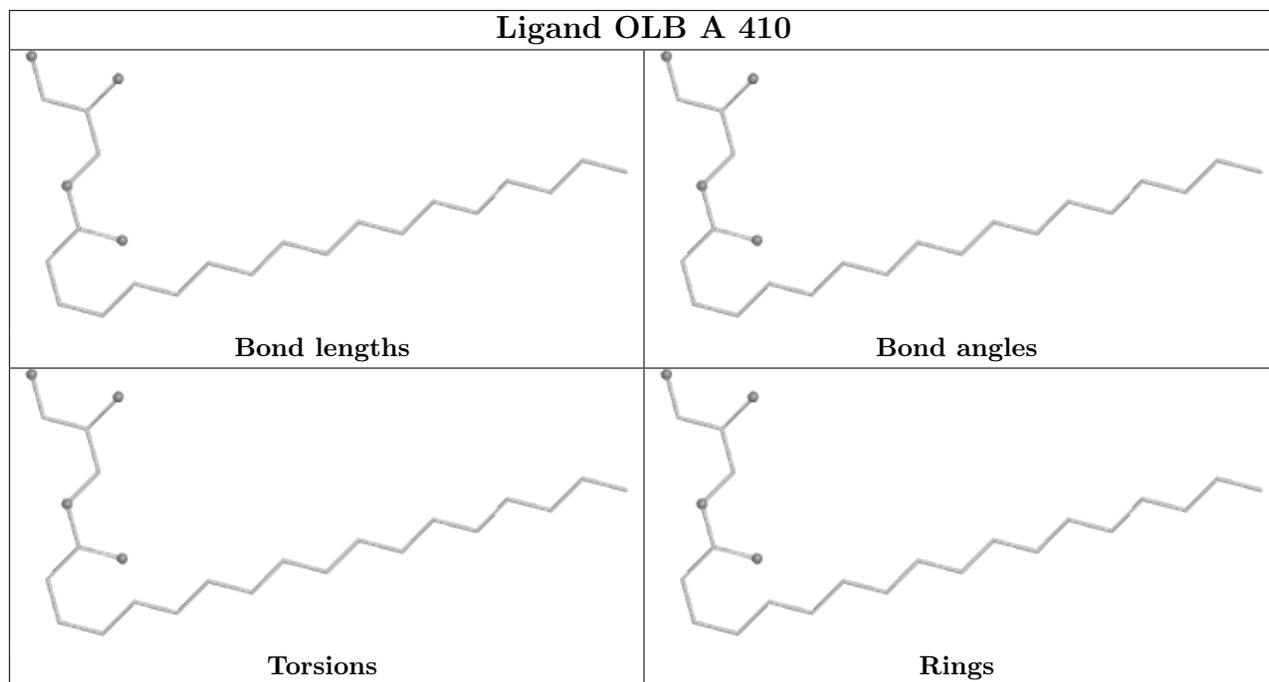
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

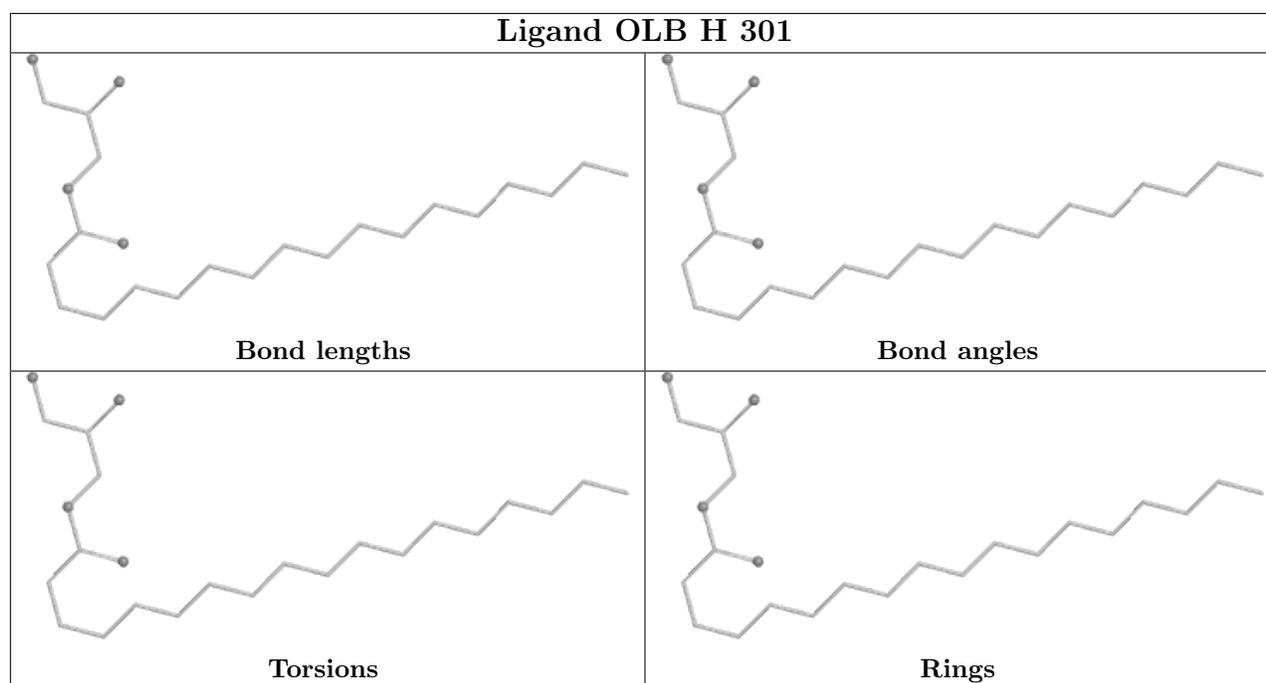












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	121:GLY	C	132:GLY	N	30.63

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

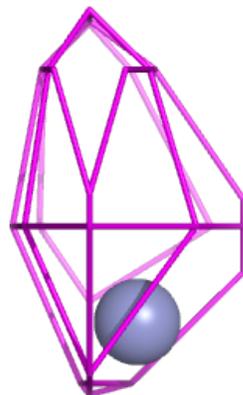
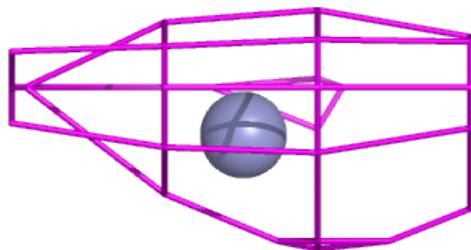
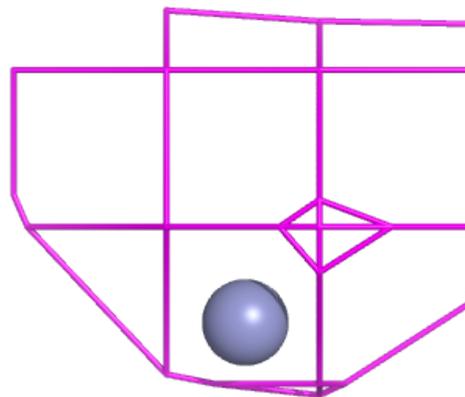
### 6.4 Ligands

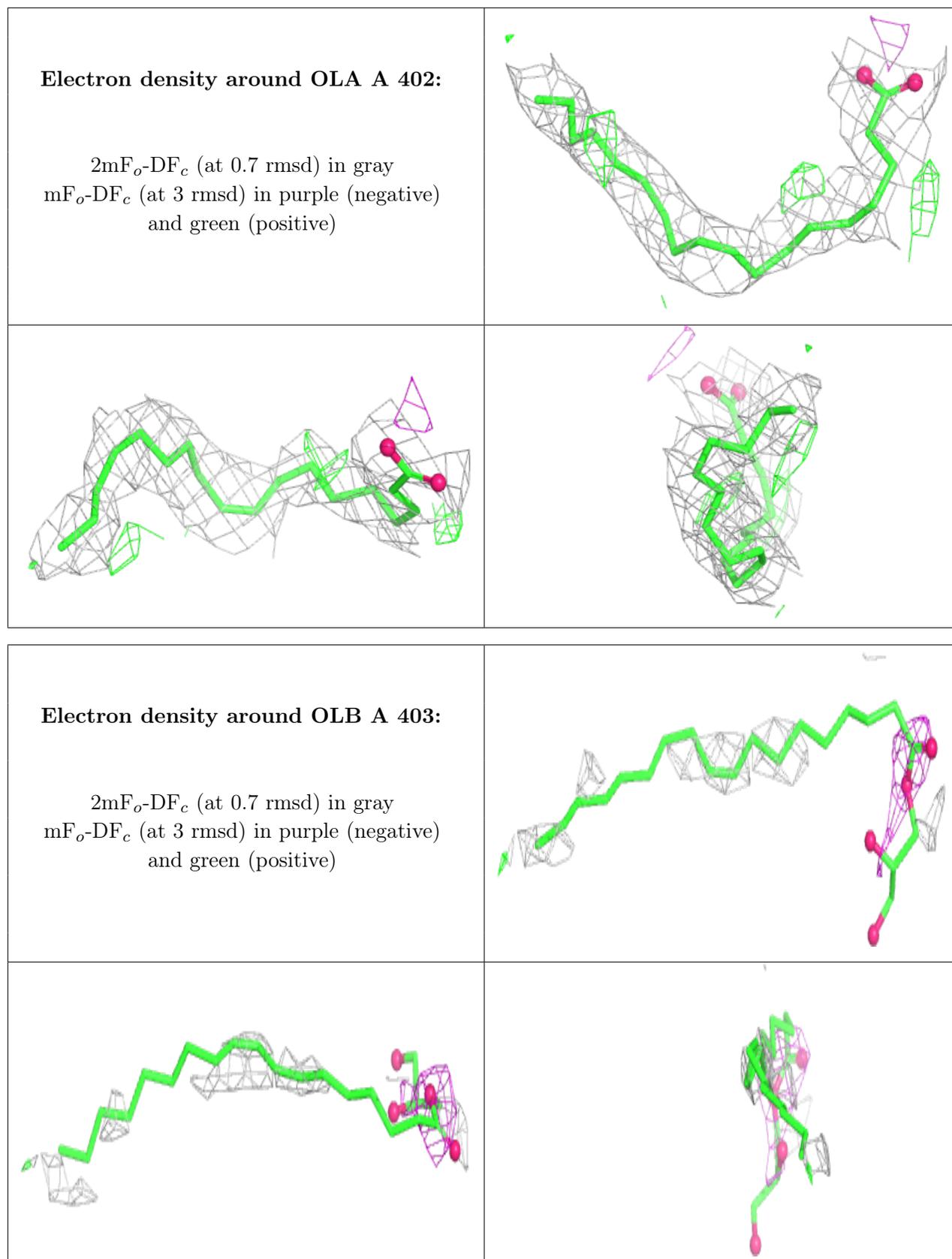
Unable to reproduce the depositors R factor - this section is therefore empty.

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 ZN A 401:**

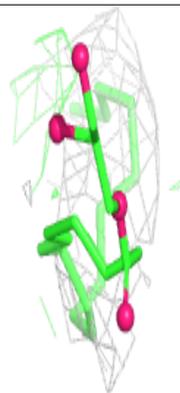
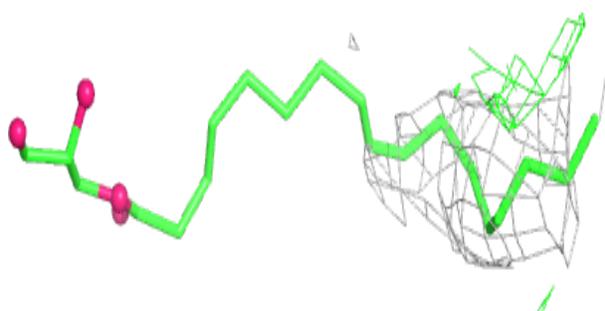
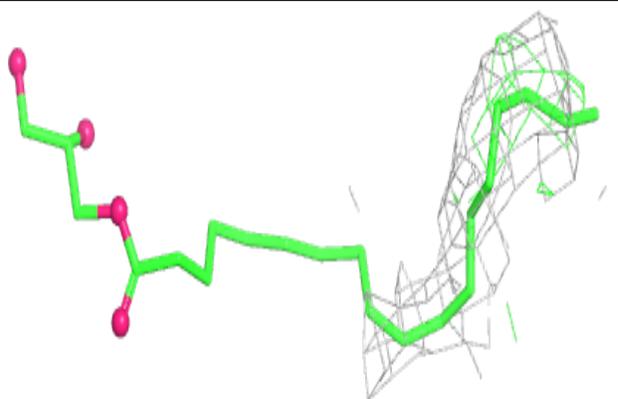
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



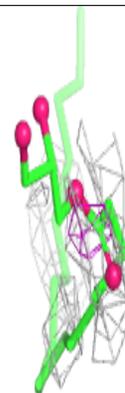
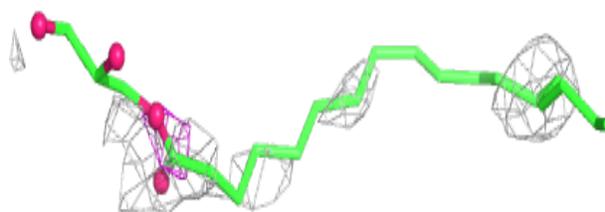
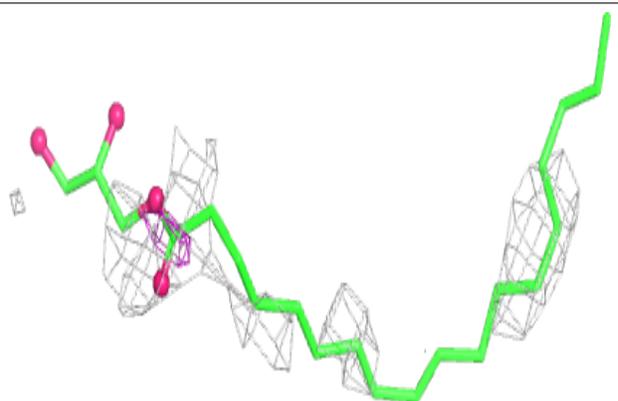


**Electron density around OLB A 404:**

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

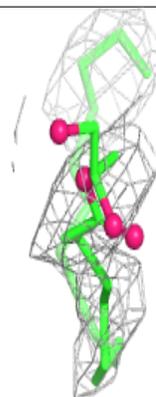
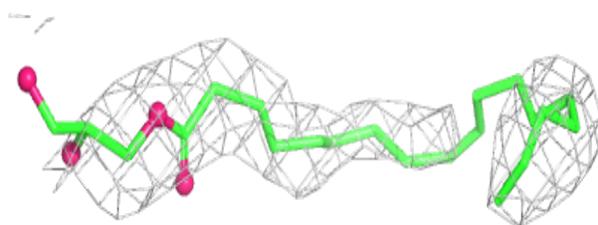
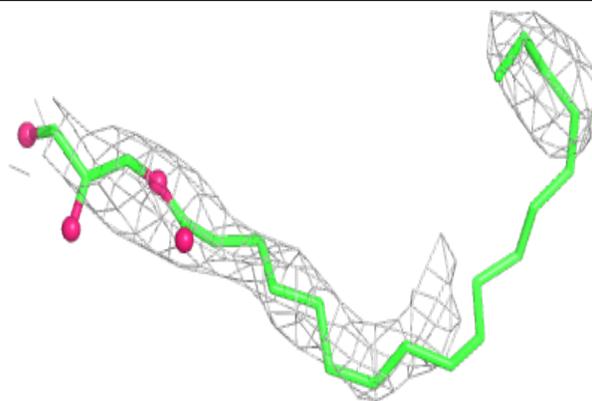
**Electron density around OLB A 405:**

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

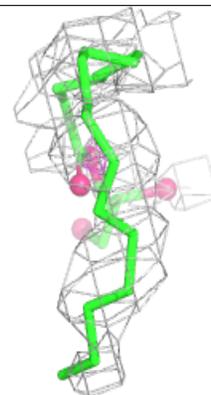
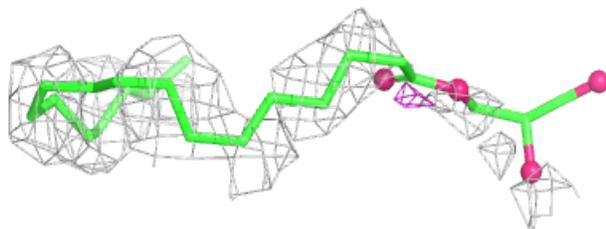
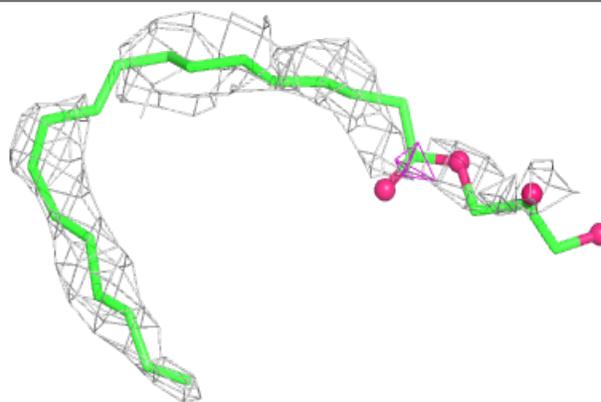


**Electron density around OLB A 406:**

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

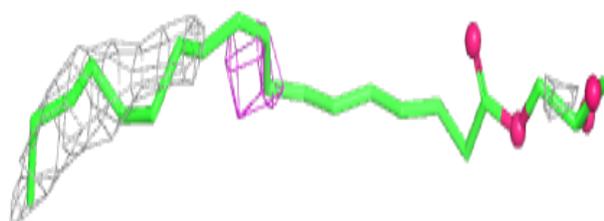
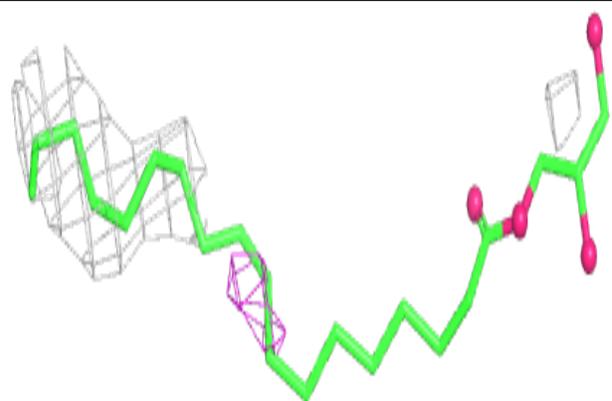
**Electron density around OLB A 407:**

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

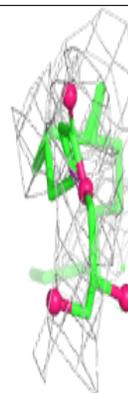
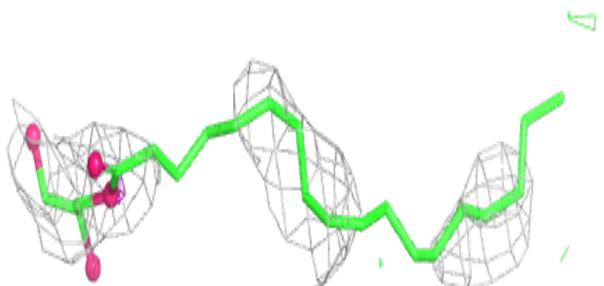
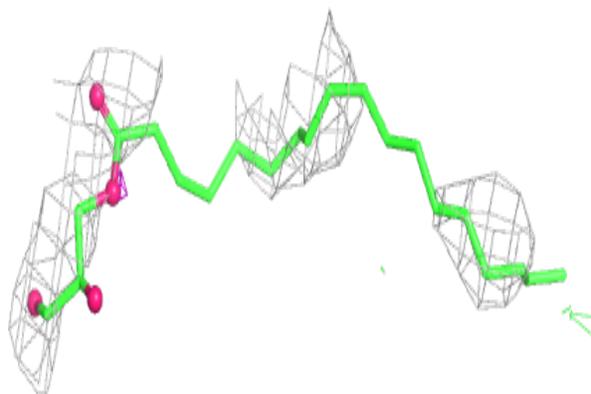


**Electron density around OLB A 408:**

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

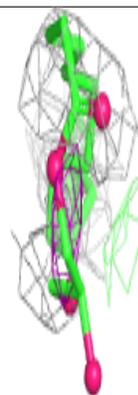
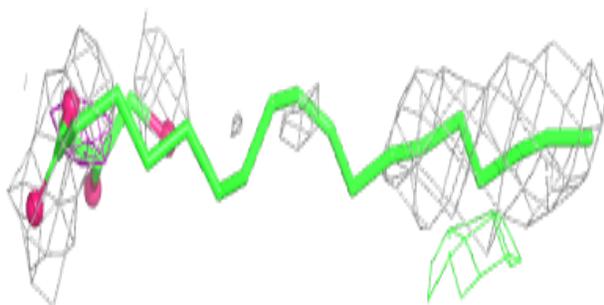
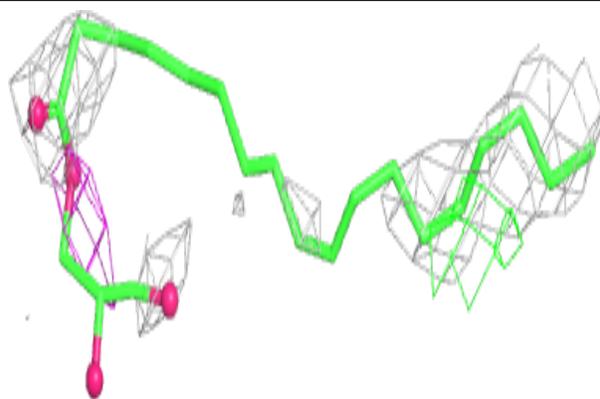
**Electron density around OLB A 409:**

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

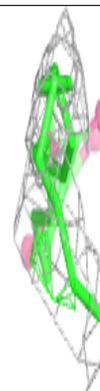
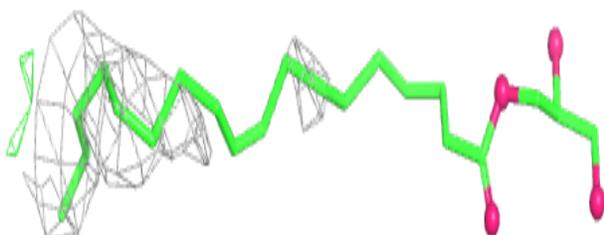
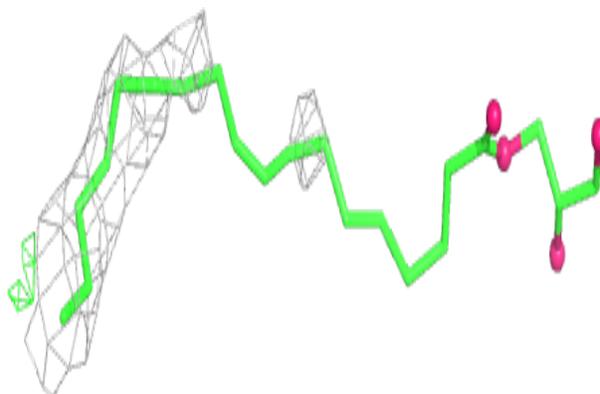


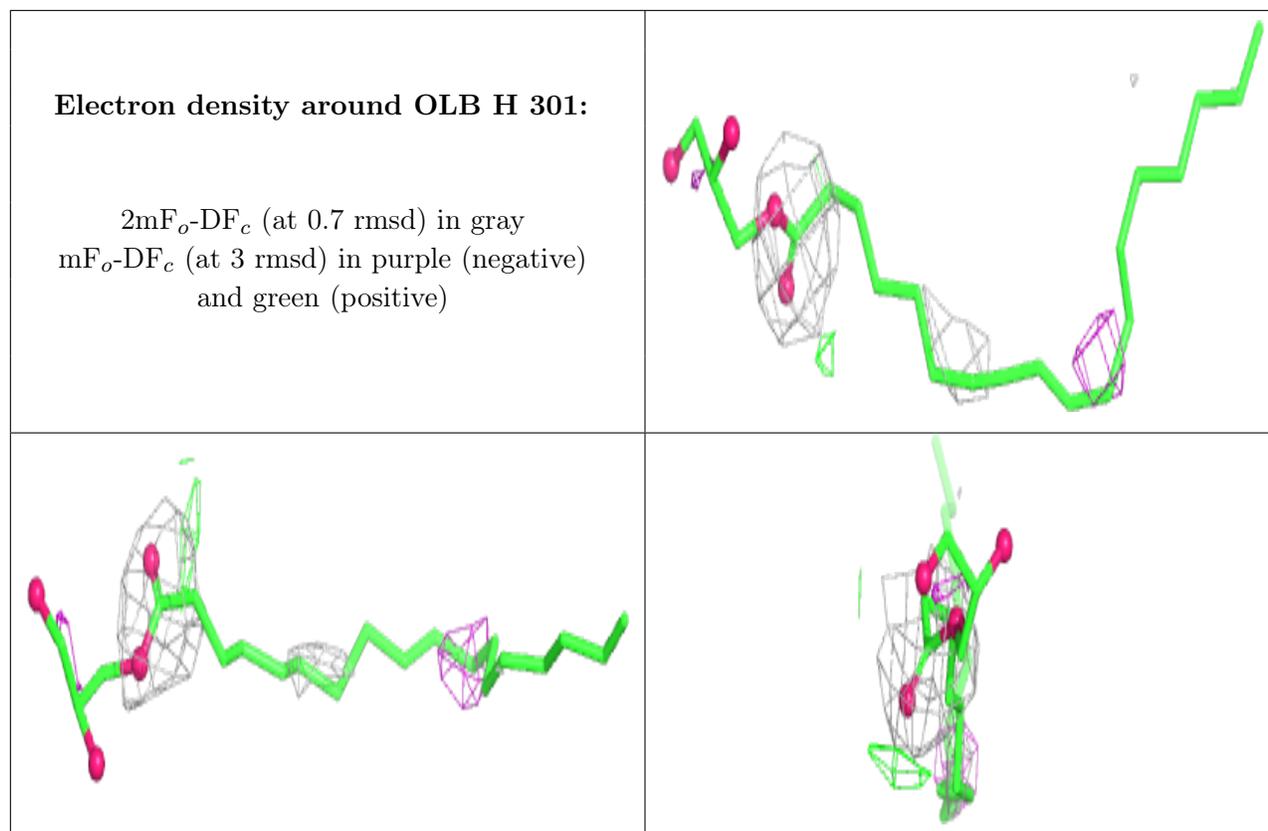
**Electron density around OLB A 410:**

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

**Electron density around OLB A 411:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.