



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:06 PM UTC

PDB ID : 5LX9 / pdb_00005lx9
Title : CRYSTAL STRUCTURE OF HUMAN ADIPONECTIN RECEPTOR 2 IN COMPLEX WITH A C18 FREE FATTY ACID AT 2.4 ANGSTROM RESOLUTION
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Deposited on : 2016-09-20
Resolution : 2.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

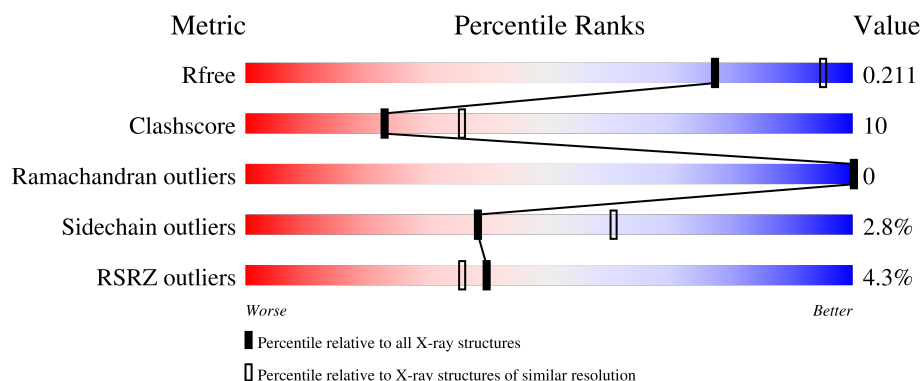
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 ≥ 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	307	5% 76% 15% 8%
2	H	284	2% 72% 7% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4885 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 HUMAN ADIPONECTIN RECEPTOR 2.

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

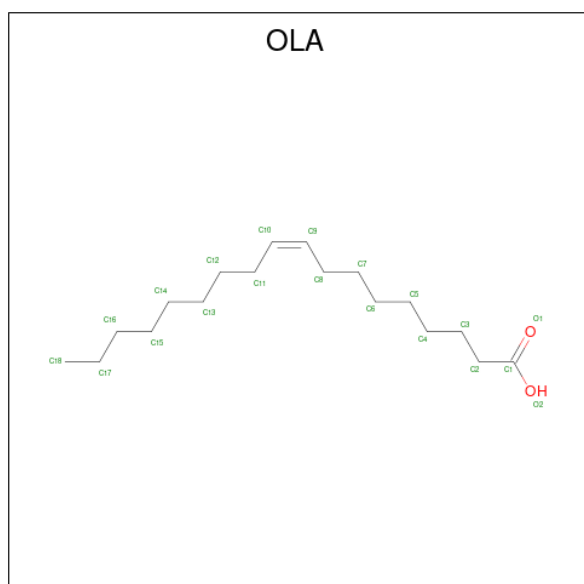
- Molecule 2 is a protein called single-chain variable fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1755	1113	288	347	7			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

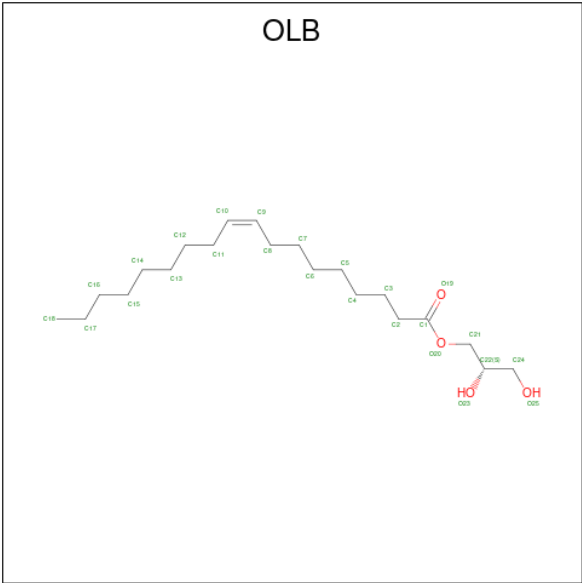
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



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 (CCD ID: OLB) (formula: C₂₁H₄₀O₄).



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		
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	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		

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

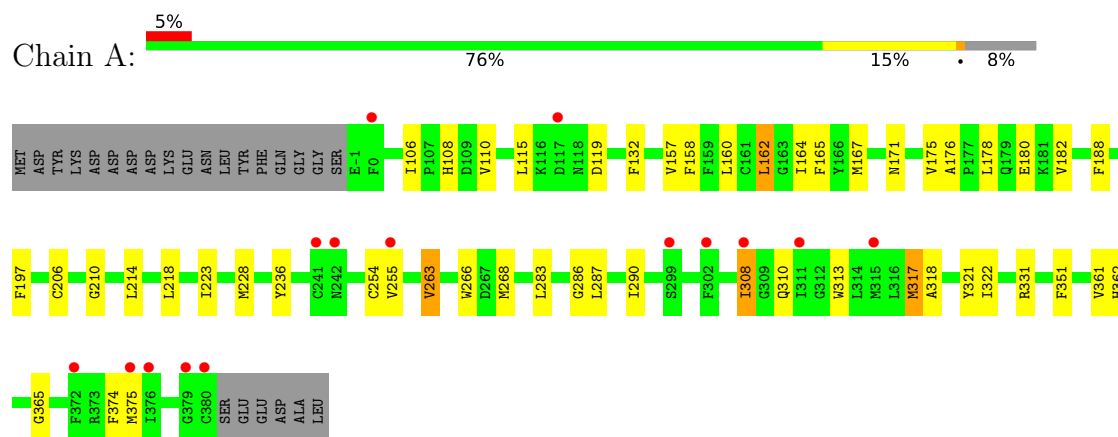
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	0
			220	220		
6	H	307	Total	O	0	0
			307	307		

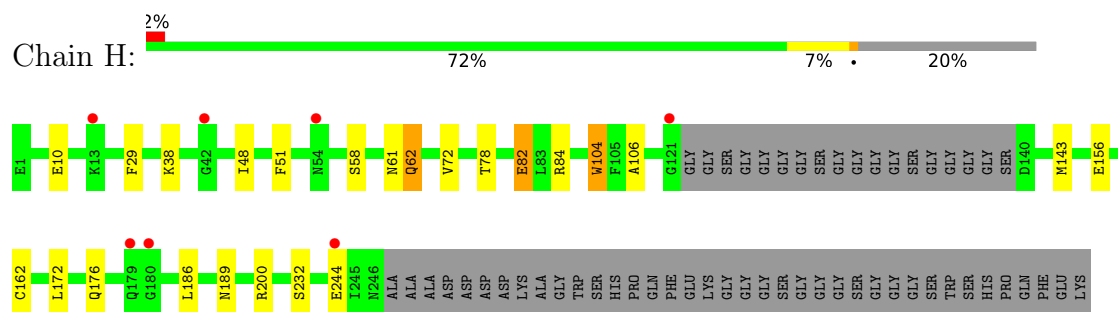
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HUMAN ADIPONECTIN RECEPTOR 2



- Molecule 2: single-chain variable fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 101.13Å 111.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.13 – 2.40 101.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (101.13-2.40) 99.9 (101.13-2.40)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.181 , 0.205 0.190 , 0.211	Depositor DCC
R_{free} test set	1626 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4885	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, OLB, 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	0.81	1/2366 (0.0%)	1.35	2/3216 (0.1%)
2	H	0.74	0/1799	1.09	5/2441 (0.2%)
All	All	0.78	1/4165 (0.0%)	1.25	7/5657 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	MET	SD-CE	-5.22	1.66	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ILE	N-CA-C	-10.40	96.17	109.58
2	H	61	ASN	N-CA-C	-6.23	100.61	109.96
1	A	119	ASP	CA-CB-CG	6.00	118.60	112.60
2	H	189	ASN	CA-C-N	5.37	131.79	121.54
2	H	189	ASN	C-N-CA	5.37	131.79	121.54
2	H	104	TRP	N-CA-C	-5.25	101.13	109.59
2	H	61	ASN	CA-CB-CG	5.01	117.61	112.60

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	2282	0	2260	47	0
2	H	1755	0	1677	14	0
3	A	1	0	0	0	0
4	A	20	0	33	6	0
5	A	250	0	400	39	4
5	H	50	0	80	18	1
6	A	220	0	0	5	0
6	H	307	0	0	5	0
All	All	4885	0	4450	89	4

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 10.

All (89) 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)
5:A:403:OLB:H2	5:H:302:OLB:H20	1.29	1.12
5:A:405:OLB:O19	5:A:412:OLB:H3A	1.70	0.92
5:A:405:OLB:O19	5:A:412:OLB:C3	2.19	0.91
5:A:403:OLB:C2	5:H:302:OLB:H20	2.00	0.90
1:A:165:PHE:HB3	5:A:407:OLB:H20	1.56	0.87
1:A:321:TYR:OH	5:A:404:OLB:H40	1.76	0.85
1:A:317:MET:HG3	5:A:404:OLB:H32	1.62	0.79
1:A:210:GLY:HA3	5:H:302:OLB:H2	1.62	0.78
1:A:317:MET:HE1	1:A:361:VAL:HB	1.67	0.75
2:H:62:GLN:HB2	6:H:587:HOH:O	1.86	0.74
2:H:84:ARG:HH11	2:H:84:ARG:HG2	1.51	0.74
5:A:403:OLB:H4A	5:H:302:OLB:C8	2.21	0.70
1:A:321:TYR:OH	5:A:404:OLB:C18	2.40	0.69
1:A:218:LEU:HD23	5:A:409:OLB:H30	1.76	0.67
5:A:403:OLB:O23	5:A:403:OLB:H3A	1.96	0.66
2:H:143:MET:HE3	2:H:162:CYS:SG	2.36	0.66
1:A:351:PHE:HE1	4:A:402:OLA:H122	1.61	0.64
5:A:403:OLB:H35	5:H:301:OLB:H39	1.79	0.64
1:A:362:HIS:ND1	5:A:404:OLB:H34	2.14	0.61
2:H:84:ARG:HG2	2:H:84:ARG:NH1	2.12	0.61
5:A:403:OLB:H4A	5:H:302:OLB:H211	1.82	0.60
1:A:287:LEU:O	1:A:290:ILE:HG22	2.00	0.60
5:H:301:OLB:H33	5:H:302:OLB:H37	1.85	0.59
2:H:244:GLU:HG3	6:H:494:HOH:O	2.03	0.57
1:A:236:TYR:HE1	5:A:410:OLB:H21	1.69	0.57
1:A:108:HIS:HB3	6:A:585:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HD11	1:A:310:GLN:HG3	1.86	0.56
5:A:405:OLB:H4	5:A:412:OLB:H4A	1.87	0.56
5:H:301:OLB:H33	5:H:302:OLB:C17	2.35	0.56
1:A:351:PHE:CZ	4:A:402:OLA:H72	2.40	0.56
5:A:403:OLB:H4A	5:H:302:OLB:H23	1.89	0.55
1:A:236:TYR:CE1	5:A:410:OLB:H21	2.42	0.54
5:A:407:OLB:H211	6:A:525:HOH:O	2.06	0.53
5:A:405:OLB:O19	5:A:412:OLB:H4A	2.09	0.53
1:A:223:ILE:HD11	4:A:402:OLA:H21	1.91	0.53
5:A:405:OLB:O19	5:A:412:OLB:C4	2.56	0.52
1:A:287:LEU:HD11	1:A:322:ILE:HD11	1.91	0.52
2:H:51:PHE:CE2	2:H:72:VAL:HB	2.45	0.52
1:A:317:MET:HE3	1:A:361:VAL:HG12	1.91	0.51
1:A:197:PHE:HE1	5:A:403:OLB:H23	1.74	0.51
2:H:200:ARG:HG3	6:H:580:HOH:O	2.09	0.51
5:A:411:OLB:H18	5:A:411:OLB:O25	2.11	0.51
5:A:403:OLB:H2	5:H:302:OLB:C8	2.21	0.51
1:A:321:TYR:CD1	4:A:402:OLA:H111	2.46	0.51
2:H:78:THR:HG21	6:H:638:HOH:O	2.11	0.50
1:A:214:LEU:HD21	5:A:403:OLB:H4	1.93	0.50
1:A:351:PHE:CE1	4:A:402:OLA:H122	2.46	0.50
2:H:104:TRP:CZ3	2:H:106:ALA:HB2	2.47	0.49
1:A:165:PHE:O	5:A:407:OLB:H23	2.12	0.49
2:H:156:GLU:HG2	6:H:576:HOH:O	2.11	0.49
1:A:266:TRP:CE2	1:A:268:MET:HB2	2.48	0.49
5:A:404:OLB:C12	5:A:404:OLB:H36	2.43	0.48
1:A:158:PHE:HA	5:A:407:OLB:H21	1.95	0.48
1:A:263:VAL:HG21	5:A:412:OLB:H241	1.94	0.48
5:H:301:OLB:C15	5:H:302:OLB:H39	2.43	0.48
1:A:313:TRP:CE2	1:A:365:GLY:HA3	2.48	0.47
5:H:301:OLB:H33	5:H:302:OLB:H39	1.95	0.47
1:A:162:LEU:HD23	1:A:188:PHE:HE1	1.79	0.47
5:H:301:OLB:H33	5:H:302:OLB:C18	2.45	0.47
1:A:165:PHE:CD2	5:A:407:OLB:H31	2.49	0.47
1:A:171:ASN:ND2	5:A:411:OLB:H22	2.30	0.47
1:A:308:ILE:CD1	1:A:310:GLN:HG3	2.46	0.46
1:A:286:GLY:HA3	1:A:321:TYR:CE1	2.50	0.46
2:H:176:GLN:HB2	2:H:186:LEU:HD11	1.97	0.46
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.98	0.46
2:H:29:PHE:HE2	2:H:72:VAL:CG2	2.29	0.46
1:A:132:PHE:HB2	5:H:301:OLB:H4A	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:407:OLB:H4A	6:A:662:HOH:O	2.15	0.45
1:A:228:MET:HE3	1:A:254:CYS:HA	1.99	0.45
1:A:283:LEU:HD11	1:A:322:ILE:HD13	1.99	0.44
1:A:318:ALA:O	1:A:322:ILE:HG12	2.17	0.44
1:A:178:LEU:O	1:A:182:VAL:HG23	2.18	0.44
1:A:197:PHE:CE1	5:A:403:OLB:H23	2.52	0.44
5:A:403:OLB:H4A	5:H:302:OLB:C10	2.47	0.44
1:A:331:ARG:HD3	6:A:527:HOH:O	2.18	0.43
1:A:176:ALA:O	1:A:180:GLU:HG3	2.18	0.43
1:A:106:ILE:HD12	1:A:110:VAL:HG23	2.00	0.43
1:A:317:MET:CG	5:A:404:OLB:H32	2.43	0.42
1:A:115:LEU:HD21	1:A:206:CYS:HA	2.00	0.42
1:A:160:LEU:O	1:A:164:ILE:HG12	2.20	0.42
1:A:171:ASN:ND2	5:A:411:OLB:H2	2.35	0.41
5:A:403:OLB:H2	5:H:302:OLB:H17	2.02	0.41
5:A:404:OLB:H36	5:A:404:OLB:H26	2.01	0.41
2:H:82:GLU:OE2	2:H:84:ARG:NH1	2.53	0.41
1:A:132:PHE:HB2	5:H:301:OLB:C4	2.51	0.41
6:A:504:HOH:O	5:H:302:OLB:H2A	2.21	0.41
4:A:402:OLA:H161	4:A:402:OLA:H132	1.77	0.40
5:A:405:OLB:C4	5:A:412:OLB:H4A	2.51	0.40
1:A:175:VAL:HG23	1:A:374:PHE:HA	2.03	0.40

All (4) 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:405:OLB:O23	5:A:406:OLB:O25[3_454]	1.97	0.23
5:A:403:OLB:C17	5:A:408:OLB:C18[3_554]	2.02	0.18
5:A:405:OLB:O23	5:A:406:OLB:C24[3_454]	2.10	0.10
5:A:408:OLB:C17	5:H:301:OLB:C18[3_454]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/307 (92%)	279 (99%)	2 (1%)	0	100	100
2	H	224/284 (79%)	220 (98%)	4 (2%)	0	100	100
All	All	505/591 (85%)	499 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/261 (92%)	234 (98%)	6 (2%)	42	64
2	H	189/217 (87%)	183 (97%)	6 (3%)	34	56
All	All	429/478 (90%)	417 (97%)	12 (3%)	38	60

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

Mol	Chain	Res	Type
1	A	157	VAL
1	A	162	LEU
1	A	167	MET
1	A	255	VAL
1	A	263	VAL
1	A	375	MET
2	H	10	GLU
2	H	58	SER
2	H	62	GLN
2	H	82	GLU
2	H	172	LEU
2	H	232	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	273	GLN
1	A	370	GLN
2	H	39	GLN
2	H	54	ASN
2	H	170	ASN
2	H	177	GLN
2	H	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\# Z > 2$
5	OLB	A	404	-	24,24,24	0.35	0	25,25,25	0.45	0
5	OLB	A	407	-	24,24,24	0.14	0	25,25,25	0.22	0
5	OLB	A	408	-	24,24,24	0.35	0	25,25,25	0.33	0
5	OLB	H	301	-	24,24,24	0.32	0	25,25,25	0.42	0
4	OLA	A	402	-	19,19,19	0.28	0	19,19,19	0.41	0
5	OLB	H	302	-	24,24,24	0.29	0	25,25,25	0.29	0
5	OLB	A	410	-	24,24,24	0.16	0	25,25,25	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLB	A	405	-	24,24,24	0.43	0	25,25,25	0.66	1 (4%)
5	OLB	A	406	-	24,24,24	0.27	0	25,25,25	0.59	0
5	OLB	A	411	-	24,24,24	0.21	0	25,25,25	0.31	0
5	OLB	A	409	-	24,24,24	0.20	0	25,25,25	0.30	0
5	OLB	A	403	-	24,24,24	0.30	0	25,25,25	0.49	0
5	OLB	A	412	-	24,24,24	0.25	0	25,25,25	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLB	A	404	-	-	15/24/24/24	-
5	OLB	A	407	-	-	11/24/24/24	-
5	OLB	A	408	-	-	7/24/24/24	-
5	OLB	H	301	-	-	12/24/24/24	-
4	OLA	A	402	-	-	8/17/17/17	-
5	OLB	H	302	-	-	7/24/24/24	-
5	OLB	A	410	-	-	13/24/24/24	-
5	OLB	A	405	-	-	12/24/24/24	-
5	OLB	A	406	-	-	9/24/24/24	-
5	OLB	A	411	-	-	8/24/24/24	-
5	OLB	A	409	-	-	8/24/24/24	-
5	OLB	A	403	-	-	16/24/24/24	-
5	OLB	A	412	-	-	15/24/24/24	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	OLB	O20-C21-C22	-2.32	94.92	105.85

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	OLB	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
5	A	403	OLB	O20-C21-C22-C24
5	A	403	OLB	C21-C22-C24-O25
5	A	405	OLB	O20-C21-C22-C24
5	A	407	OLB	C21-C22-C24-O25
5	A	409	OLB	C21-C22-C24-O25
5	A	412	OLB	O20-C21-C22-C24
5	A	410	OLB	O19-C1-O20-C21
5	A	403	OLB	C22-C21-O20-C1
5	A	405	OLB	O19-C1-O20-C21
5	A	403	OLB	C2-C1-O20-C21
5	A	410	OLB	C2-C1-O20-C21
5	A	405	OLB	C2-C1-O20-C21
5	H	301	OLB	C2-C1-O20-C21
5	H	301	OLB	O19-C1-O20-C21
5	A	403	OLB	O20-C21-C22-O23
5	A	405	OLB	O20-C21-C22-O23
5	A	412	OLB	O20-C21-C22-O23
4	A	402	OLA	C13-C14-C15-C16
5	A	408	OLB	C2-C1-O20-C21
5	A	411	OLB	C2-C1-O20-C21
5	A	404	OLB	O20-C21-C22-C24
5	A	404	OLB	O20-C21-C22-O23
5	A	412	OLB	C2-C1-O20-C21
5	H	301	OLB	O23-C22-C24-O25
4	A	402	OLA	C1-C2-C3-C4
5	A	411	OLB	C1-C2-C3-C4
5	A	412	OLB	C1-C2-C3-C4
5	A	408	OLB	O19-C1-O20-C21
5	A	411	OLB	O19-C1-O20-C21
5	A	404	OLB	C2-C1-O20-C21
5	A	412	OLB	O19-C1-O20-C21
5	A	404	OLB	C21-C22-C24-O25
5	A	405	OLB	C21-C22-C24-O25
5	A	406	OLB	C21-C22-C24-O25
5	A	412	OLB	C21-C22-C24-O25
5	H	301	OLB	C21-C22-C24-O25
5	A	407	OLB	C14-C15-C16-C17
5	A	404	OLB	O23-C22-C24-O25
5	A	407	OLB	O23-C22-C24-O25
5	A	409	OLB	O23-C22-C24-O25
5	A	409	OLB	C5-C6-C7-C8
5	A	409	OLB	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
5	A	410	OLB	C4-C5-C6-C7
5	H	302	OLB	C3-C4-C5-C6
5	A	404	OLB	C12-C13-C14-C15
5	A	412	OLB	C5-C6-C7-C8
5	A	407	OLB	C5-C6-C7-C8
5	A	407	OLB	C2-C1-O20-C21
5	H	302	OLB	C5-C6-C7-C8
5	A	407	OLB	C11-C12-C13-C14
5	A	412	OLB	C13-C14-C15-C16
5	A	404	OLB	O19-C1-O20-C21
4	A	402	OLA	C2-C3-C4-C5
5	A	405	OLB	C2-C3-C4-C5
5	A	411	OLB	C12-C13-C14-C15
5	H	301	OLB	C11-C12-C13-C14
5	A	407	OLB	C13-C14-C15-C16
5	A	403	OLB	C6-C7-C8-C9
5	A	410	OLB	C6-C7-C8-C9
5	A	411	OLB	C10-C11-C12-C13
5	A	411	OLB	C14-C15-C16-C17
5	A	405	OLB	C14-C15-C16-C17
5	A	410	OLB	C5-C6-C7-C8
5	A	403	OLB	C12-C13-C14-C15
5	A	404	OLB	C10-C11-C12-C13
5	A	412	OLB	C10-C11-C12-C13
5	A	412	OLB	C3-C4-C5-C6
5	A	404	OLB	C11-C12-C13-C14
5	A	403	OLB	O23-C22-C24-O25
5	A	406	OLB	O20-C21-C22-O23
5	A	408	OLB	O20-C21-C22-O23
5	A	408	OLB	O20-C21-C22-C24
5	A	404	OLB	C3-C4-C5-C6
5	H	301	OLB	C13-C14-C15-C16
5	A	405	OLB	C1-C2-C3-C4
5	A	410	OLB	C14-C15-C16-C17
5	A	403	OLB	C3-C4-C5-C6
5	A	407	OLB	O19-C1-O20-C21
5	A	411	OLB	C5-C6-C7-C8
5	A	406	OLB	C11-C12-C13-C14
5	H	301	OLB	C4-C5-C6-C7
5	A	406	OLB	C2-C3-C4-C5
5	H	302	OLB	C12-C13-C14-C15
5	A	406	OLB	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	H	302	OLB	C15-C16-C17-C18
4	A	402	OLA	C11-C12-C13-C14
5	A	409	OLB	C15-C16-C17-C18
5	A	406	OLB	C15-C16-C17-C18
5	A	408	OLB	C12-C13-C14-C15
5	A	406	OLB	O23-C22-C24-O25
5	H	301	OLB	C1-C2-C3-C4
4	A	402	OLA	C12-C13-C14-C15
5	A	408	OLB	C15-C16-C17-C18
5	A	408	OLB	C14-C15-C16-C17
5	A	412	OLB	C12-C13-C14-C15
5	A	406	OLB	C14-C15-C16-C17
5	A	410	OLB	C2-C3-C4-C5
5	A	404	OLB	C14-C15-C16-C17
5	A	410	OLB	C1-C2-C3-C4
5	A	410	OLB	C10-C11-C12-C13
5	H	302	OLB	C6-C7-C8-C9
5	A	405	OLB	C11-C12-C13-C14
5	A	403	OLB	C1-C2-C3-C4
5	A	409	OLB	C2-C1-O20-C21
5	A	409	OLB	C14-C15-C16-C17
5	H	302	OLB	C14-C15-C16-C17
5	A	412	OLB	O23-C22-C24-O25
5	A	410	OLB	C7-C8-C9-C10
5	A	407	OLB	C15-C16-C17-C18
5	A	403	OLB	C2-C3-C4-C5
5	A	406	OLB	C5-C6-C7-C8
5	A	403	OLB	C5-C6-C7-C8
5	A	412	OLB	C14-C15-C16-C17
5	A	404	OLB	C9-C10-C11-C12
5	A	412	OLB	C2-C3-C4-C5
4	A	402	OLA	O1-C1-C2-C3
5	A	407	OLB	C3-C4-C5-C6
5	A	403	OLB	C13-C14-C15-C16
4	A	402	OLA	C14-C15-C16-C17
5	H	302	OLB	C9-C10-C11-C12
4	A	402	OLA	O2-C1-C2-C3
5	A	405	OLB	C9-C10-C11-C12
5	A	405	OLB	C12-C13-C14-C15
5	A	404	OLB	C6-C7-C8-C9
5	A	405	OLB	O23-C22-C24-O25
5	A	409	OLB	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
5	A	412	OLB	C4-C5-C6-C7
5	A	404	OLB	C7-C8-C9-C10
5	A	407	OLB	C12-C13-C14-C15
5	A	403	OLB	C9-C10-C11-C12
5	H	301	OLB	C10-C11-C12-C13
5	A	404	OLB	C4-C5-C6-C7
5	A	410	OLB	O20-C1-C2-C3
5	H	301	OLB	O20-C1-C2-C3
5	A	410	OLB	O20-C21-C22-O23
5	H	301	OLB	C14-C15-C16-C17
5	H	301	OLB	O19-C1-C2-C3
5	A	410	OLB	O19-C1-C2-C3
5	A	411	OLB	C2-C3-C4-C5
5	A	403	OLB	C14-C15-C16-C17

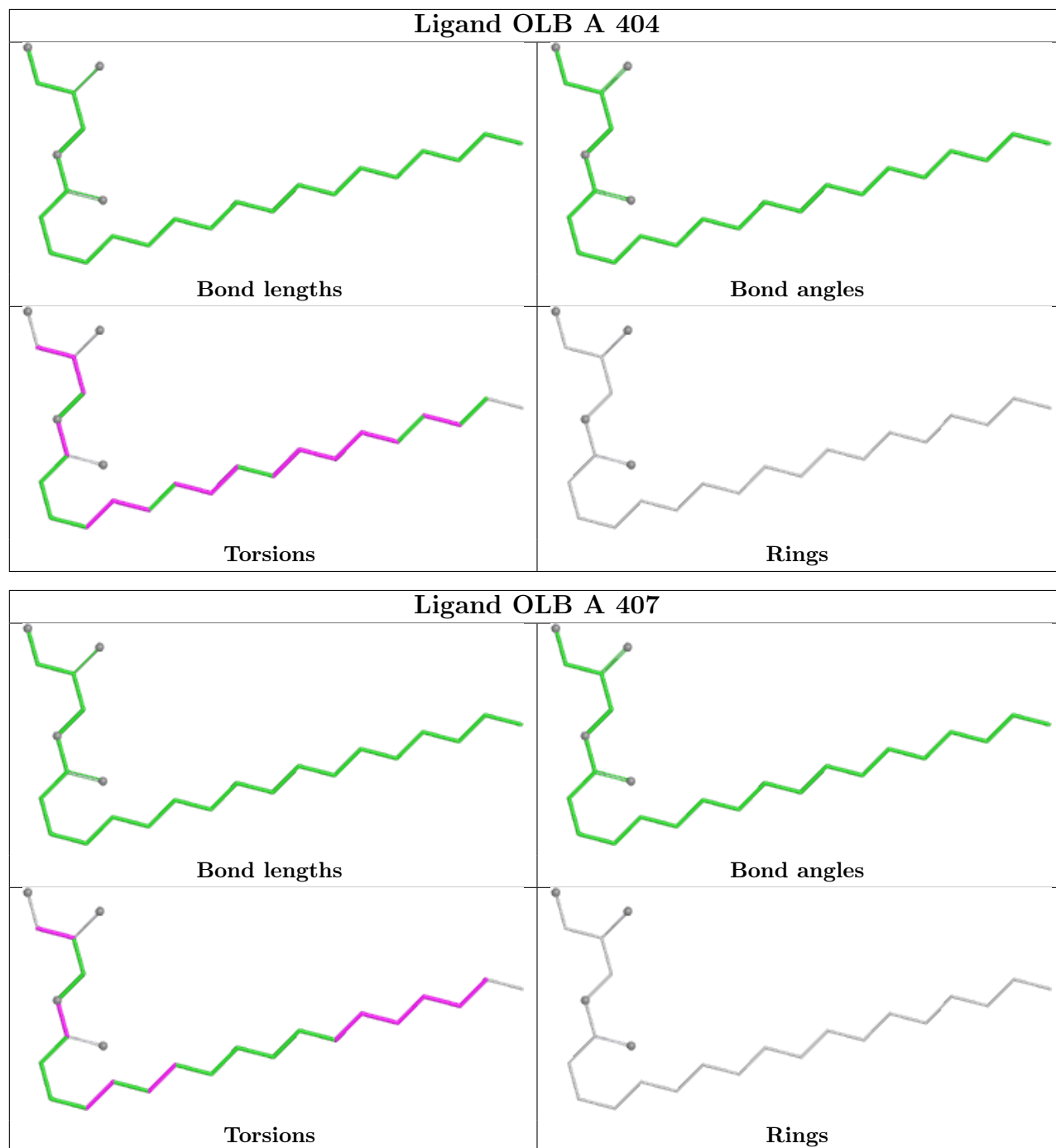
There are no ring outliers.

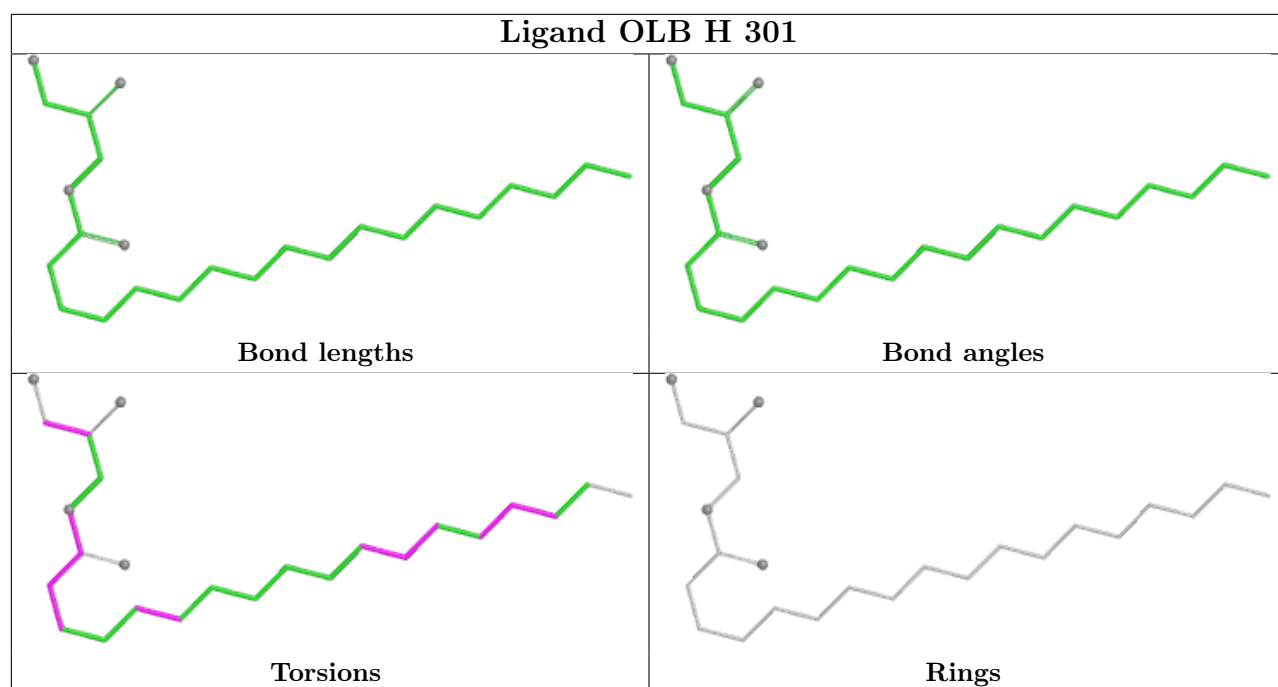
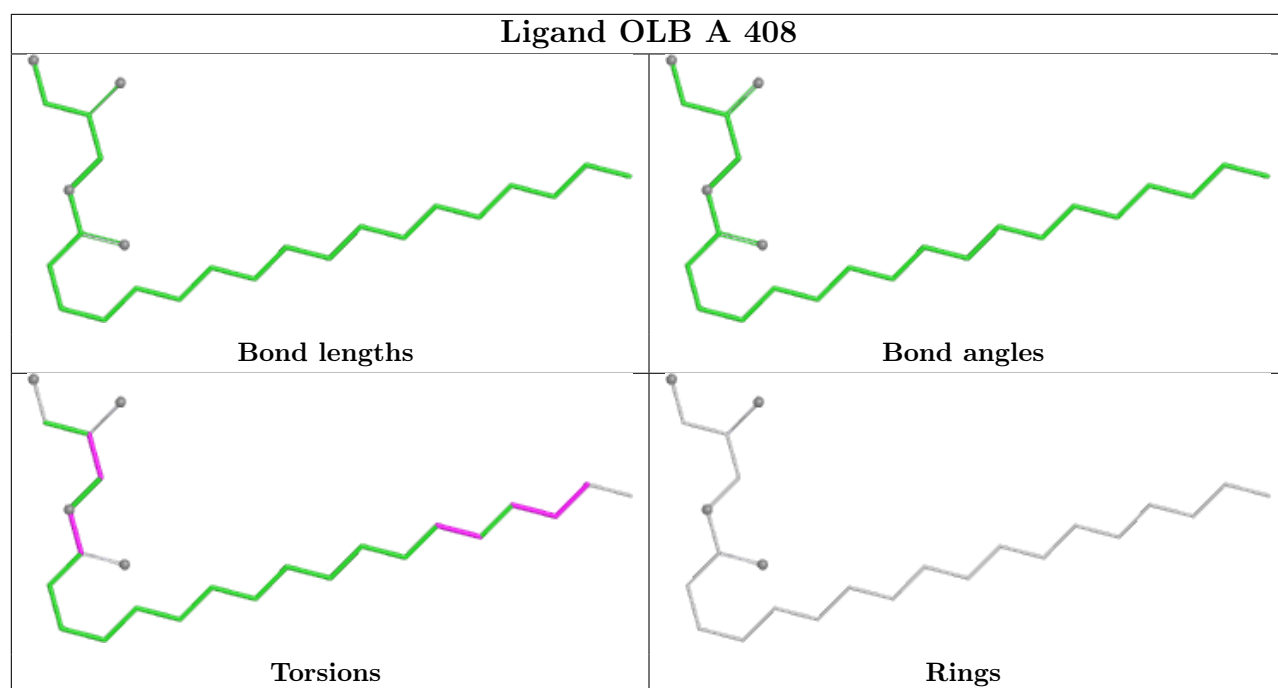
13 monomers are involved in 58 short contacts:

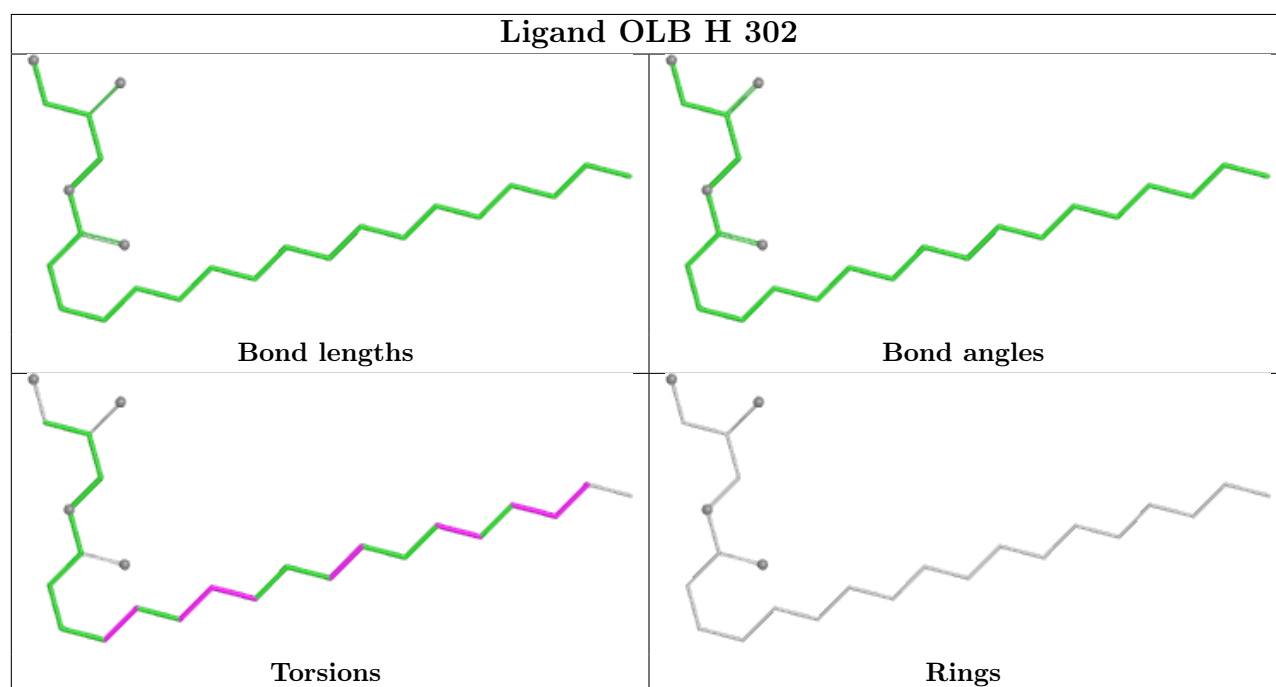
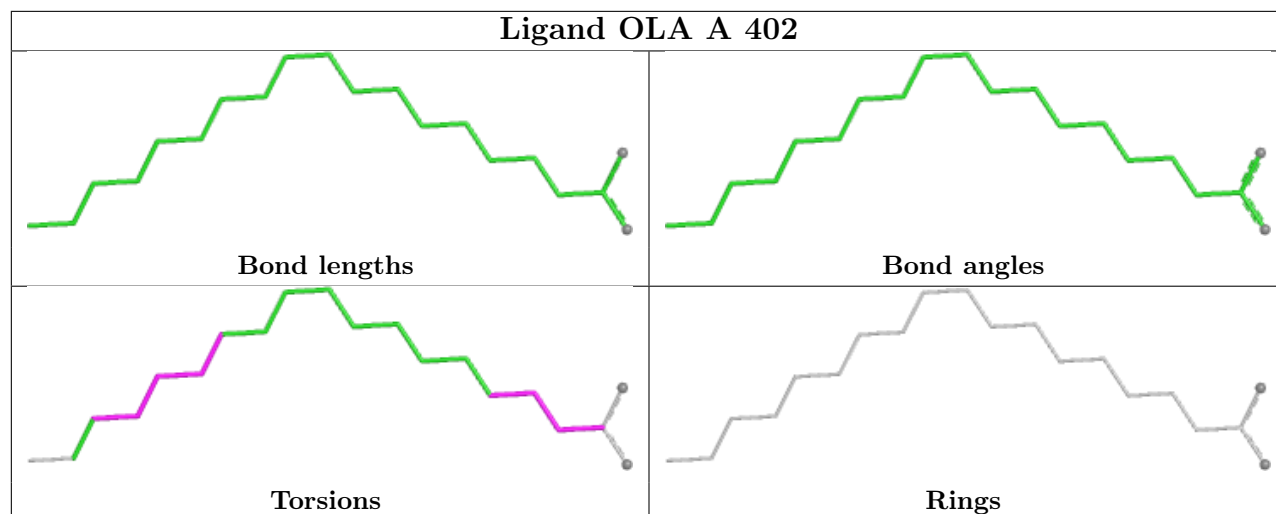
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	OLB	7	0
5	A	407	OLB	6	0
5	A	408	OLB	0	2
5	H	301	OLB	8	1
4	A	402	OLA	6	0
5	H	302	OLB	15	0
5	A	410	OLB	2	0
5	A	405	OLB	6	2
5	A	406	OLB	0	2
5	A	411	OLB	3	0
5	A	409	OLB	1	0
5	A	403	OLB	13	1
5	A	412	OLB	7	0

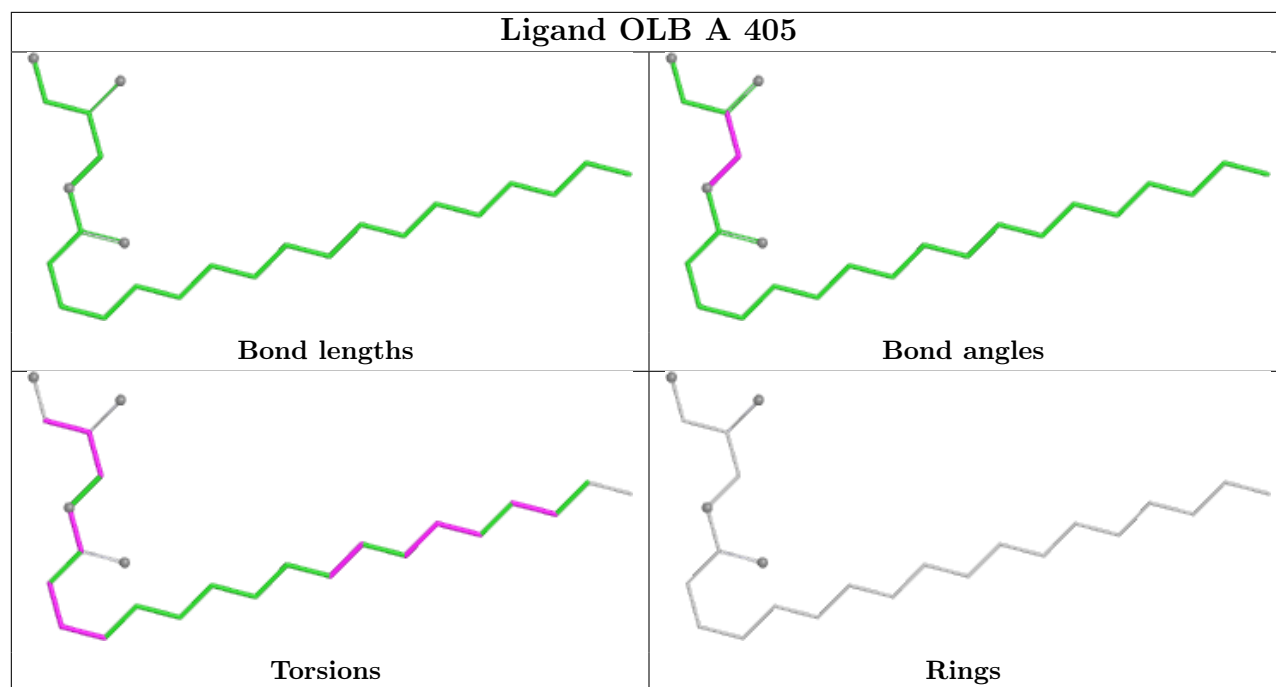
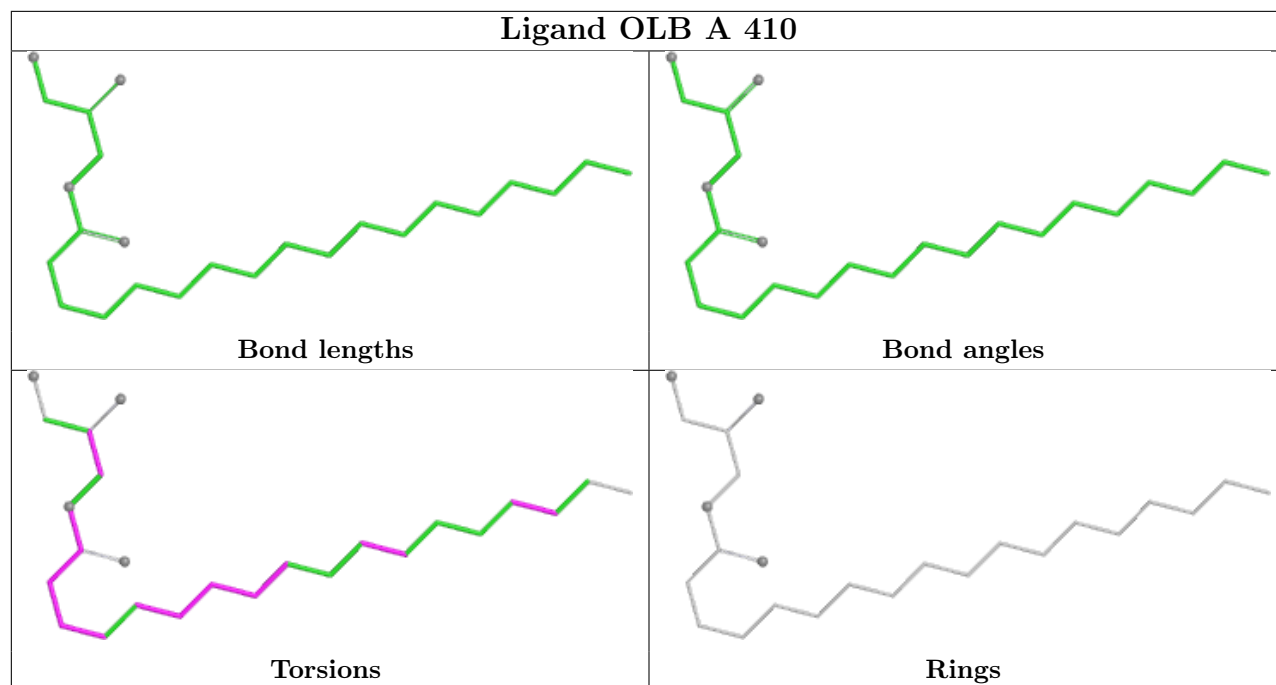
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

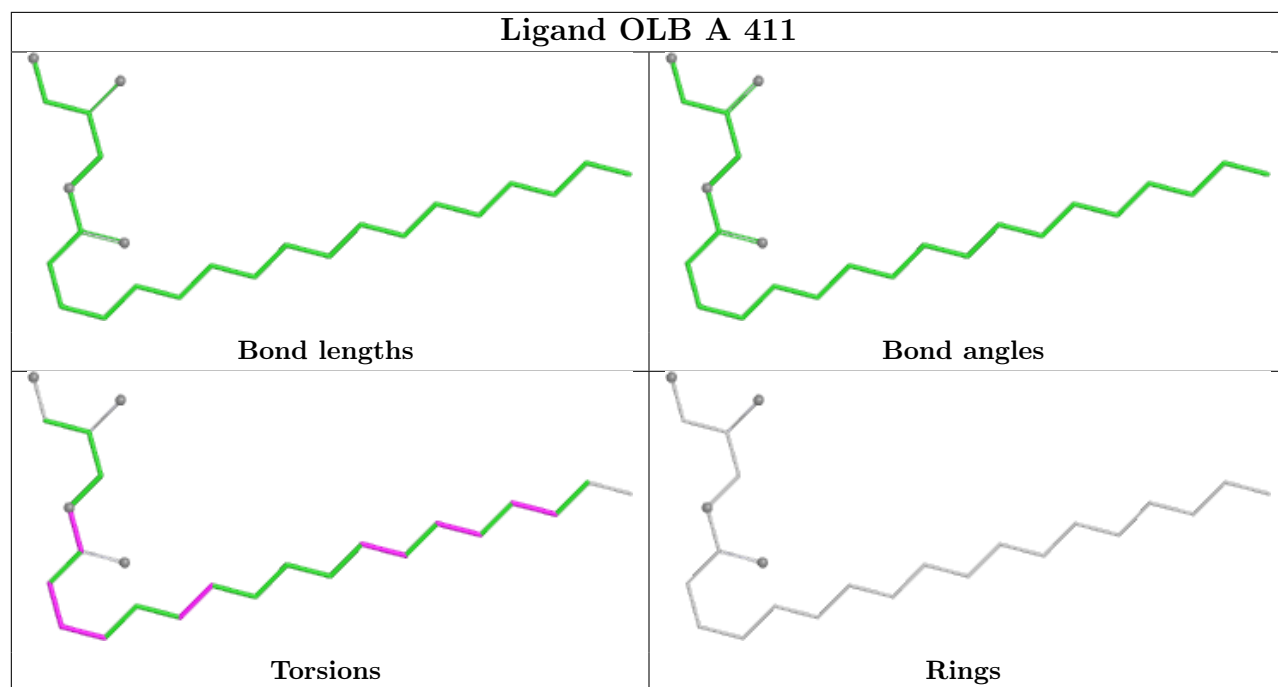
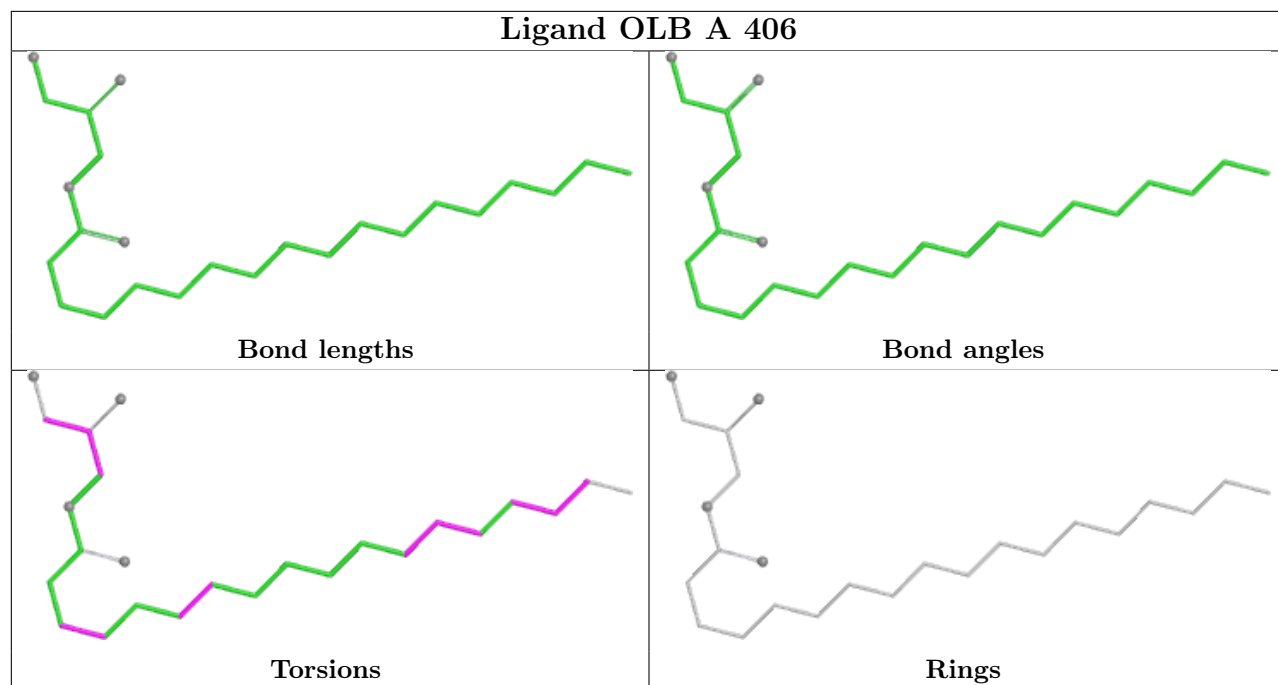
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

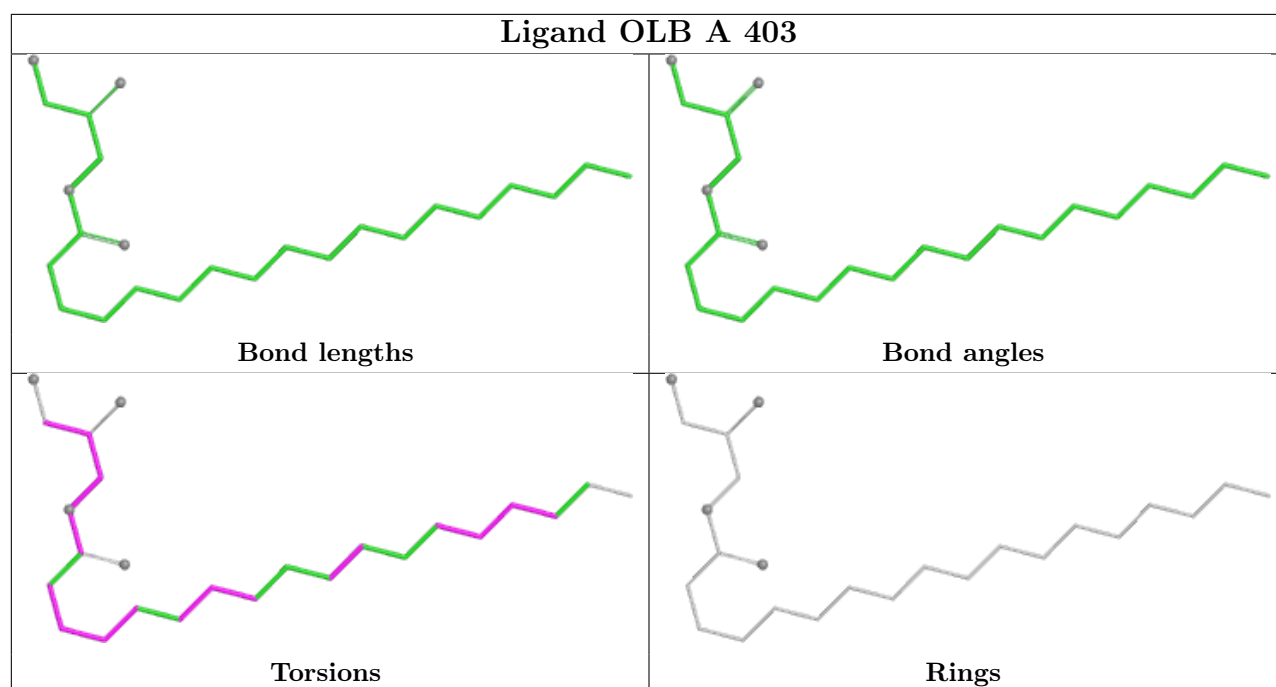
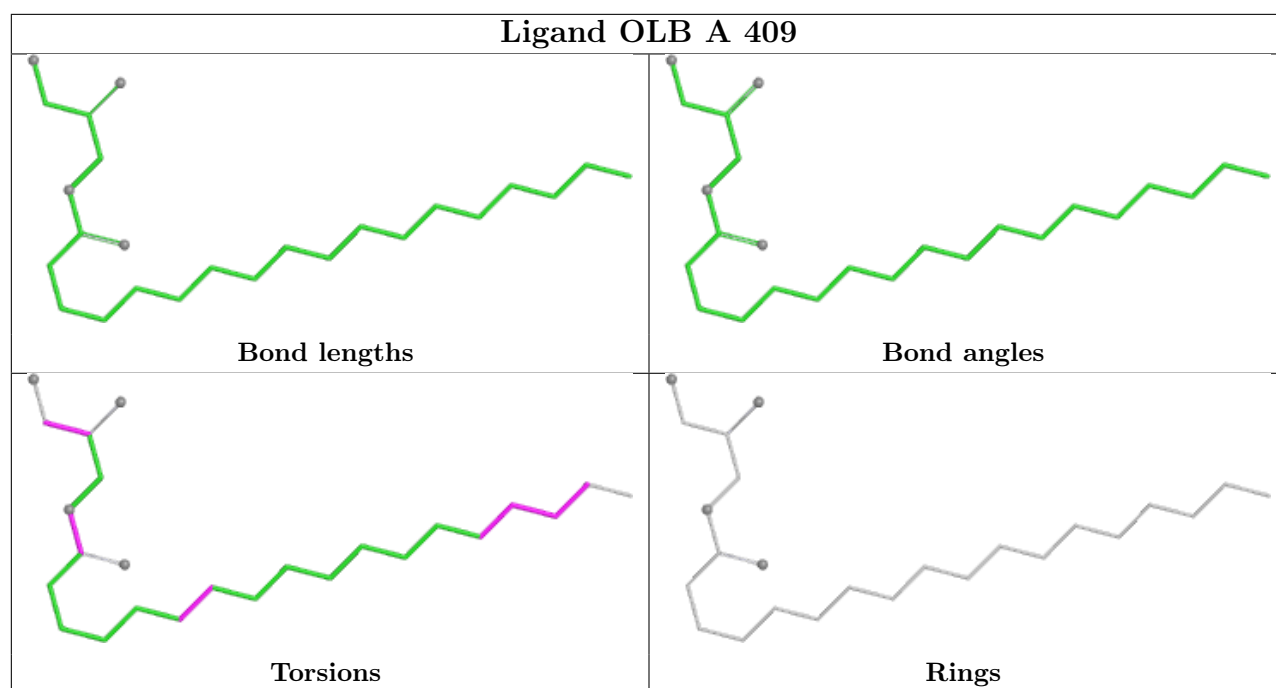


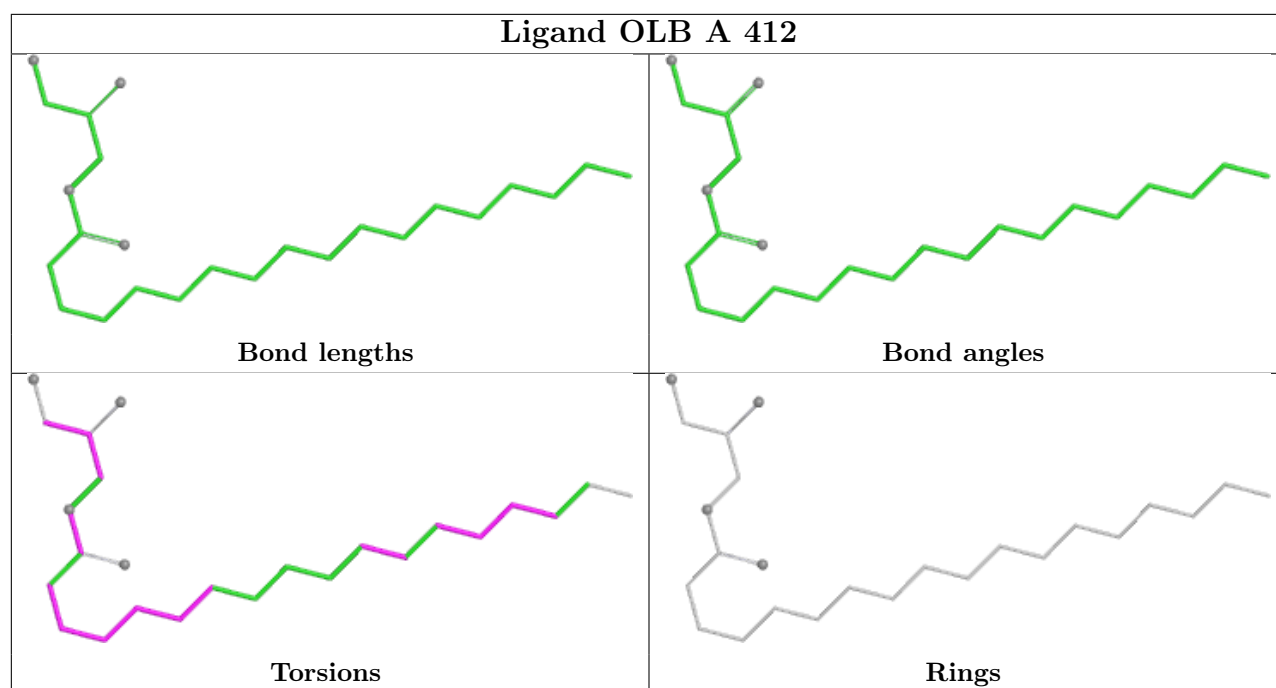












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	283/307 (92%)	0.33	15 (5%) 32 28	29, 46, 76, 116	2 (0%)
2	H	228/284 (80%)	-0.05	7 (3%) 51 47	23, 41, 65, 83	0
All	All	511/591 (86%)	0.16	22 (4%) 40 36	23, 44, 73, 116	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	179	GLN	6.6
1	A	380	CYS	6.2
2	H	42	GLY	3.3
2	H	180	GLY	3.3
1	A	375	MET	3.1
1	A	242	ASN	2.9
1	A	241	CYS	2.9
2	H	121	GLY	2.9
2	H	54	ASN	2.7
2	H	13	LYS	2.6
1	A	308	ILE	2.6
1	A	302	PHE	2.5
1	A	255	VAL	2.4
2	H	244	GLU	2.4
1	A	376	ILE	2.3
1	A	0	PHE	2.2
1	A	372	PHE	2.2
1	A	117	ASP	2.2
1	A	311	ILE	2.1
1	A	379	GLY	2.0
1	A	315	MET	2.0
1	A	299	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

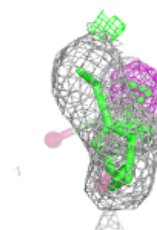
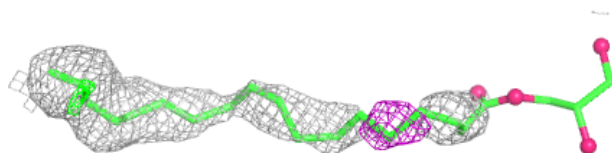
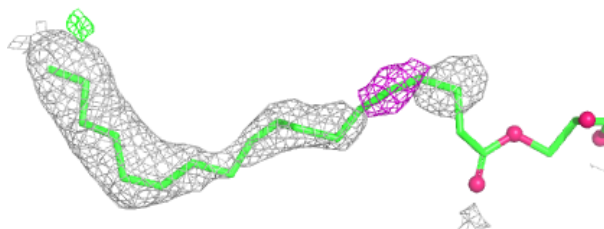
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	OLB	A	412	25/25	0.75	0.23	59,63,66,69	9
5	OLB	A	406	25/25	0.78	0.26	61,76,89,95	0
5	OLB	A	405	25/25	0.81	0.25	77,86,126,128	0
5	OLB	A	407	25/25	0.83	0.20	66,94,108,109	0
5	OLB	A	411	25/25	0.84	0.24	60,82,122,123	0
5	OLB	A	410	25/25	0.84	0.21	60,81,104,104	0
5	OLB	H	302	25/25	0.84	0.19	63,86,128,130	0
5	OLB	H	301	25/25	0.85	0.20	55,65,75,76	0
5	OLB	A	403	25/25	0.86	0.17	64,78,104,104	0
5	OLB	A	404	25/25	0.87	0.21	48,63,74,76	11
5	OLB	A	409	25/25	0.88	0.18	60,67,70,71	9
4	OLA	A	402	20/20	0.88	0.15	40,46,53,56	0
5	OLB	A	408	25/25	0.89	0.22	67,76,85,87	9
3	ZN	A	401	1/1	0.99	0.04	35,35,35,35	0

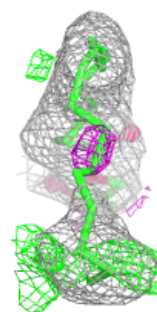
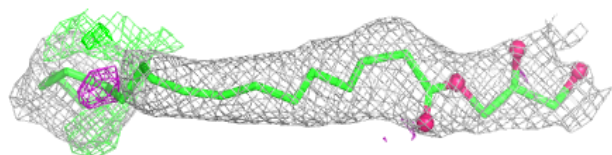
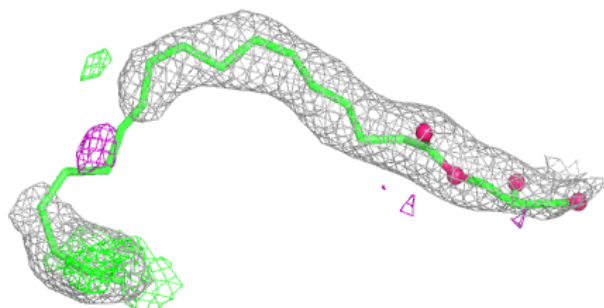
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLB A 412:

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

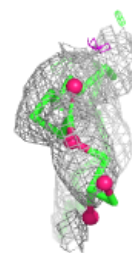
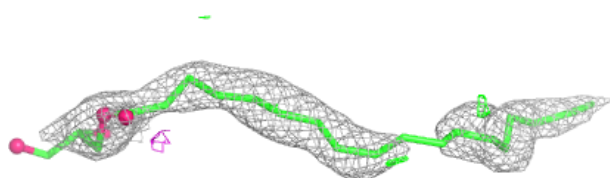
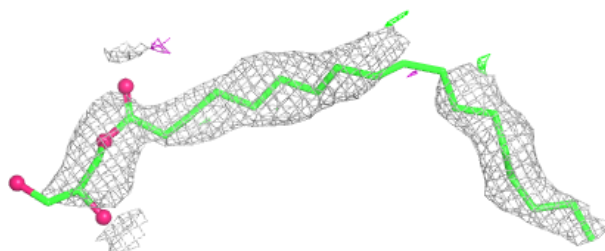
**Electron density around OLB A 406:**

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

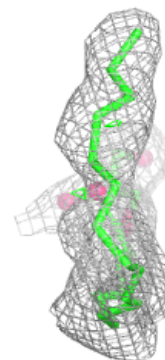
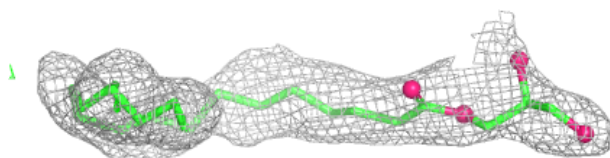
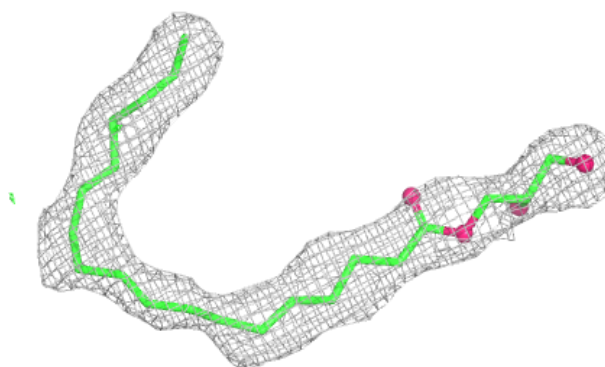


Electron density around OLB A 405:

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

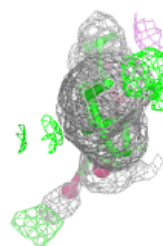
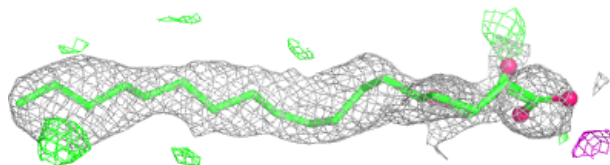
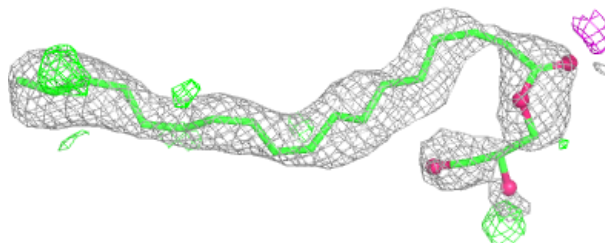
**Electron density around OLB A 407:**

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

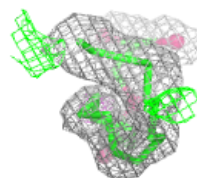
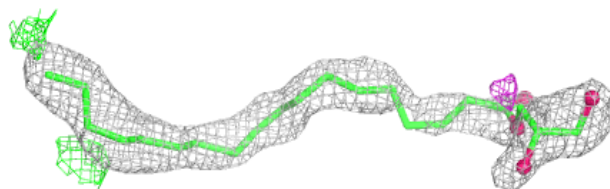
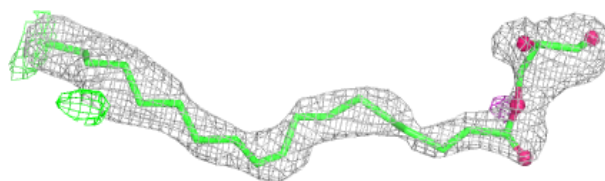


Electron density around OLB A 411:

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

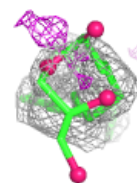
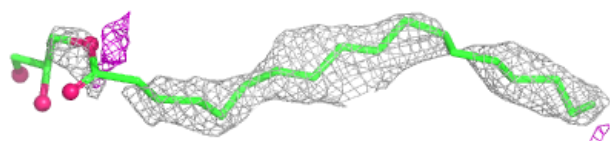
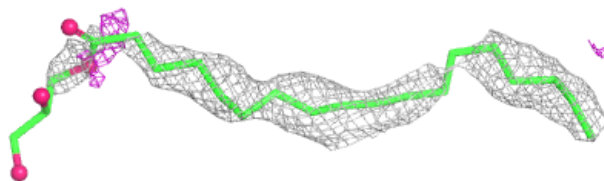
**Electron density around OLB A 410:**

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

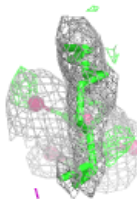
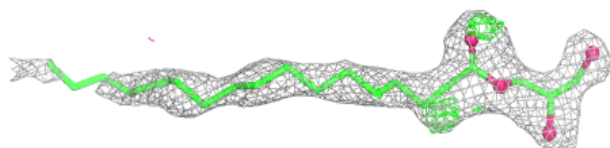
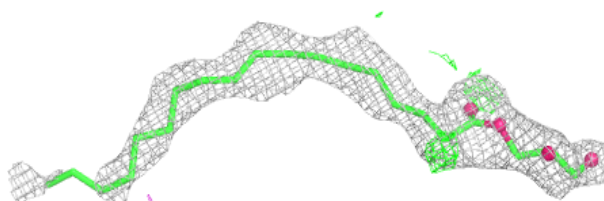


Electron density around OLB H 302:

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

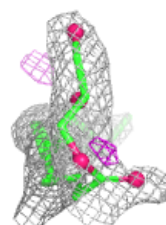
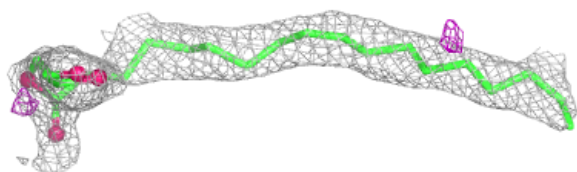
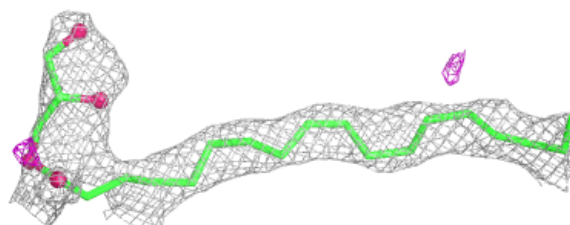
**Electron density around OLB H 301:**

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

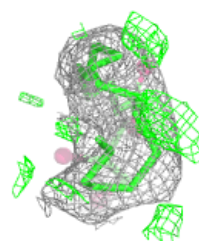
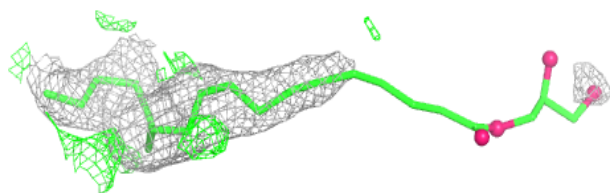
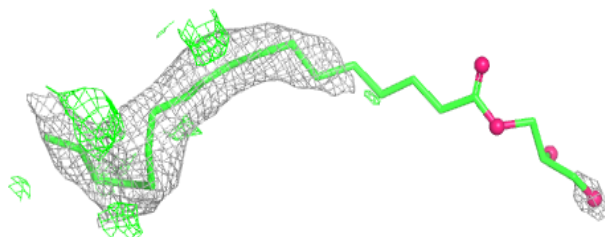


Electron density around OLB A 403:

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

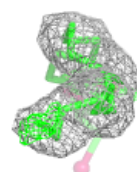
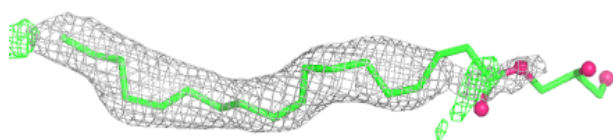
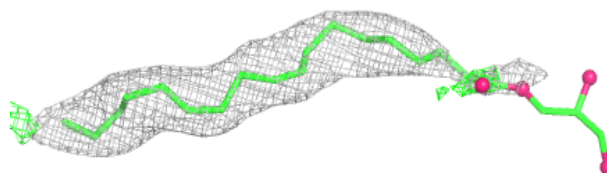
**Electron density around OLB A 404:**

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

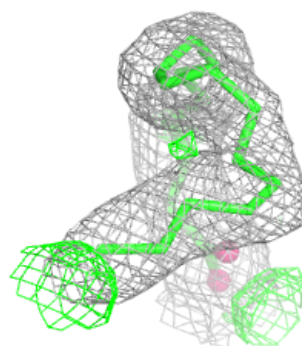
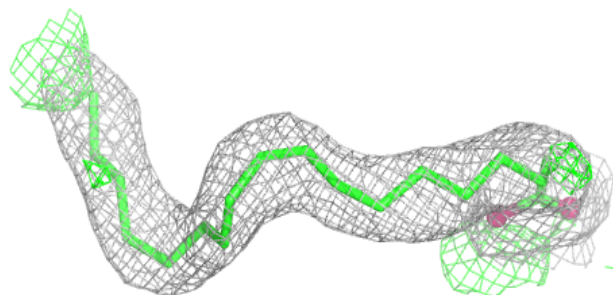
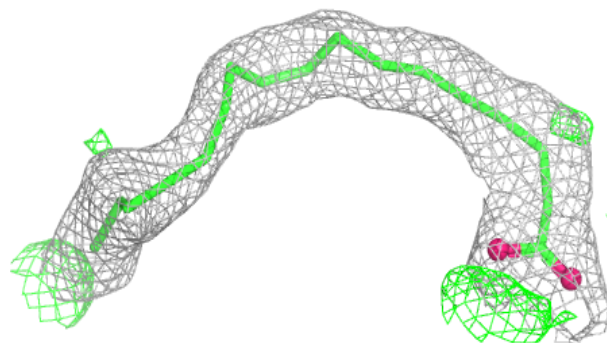


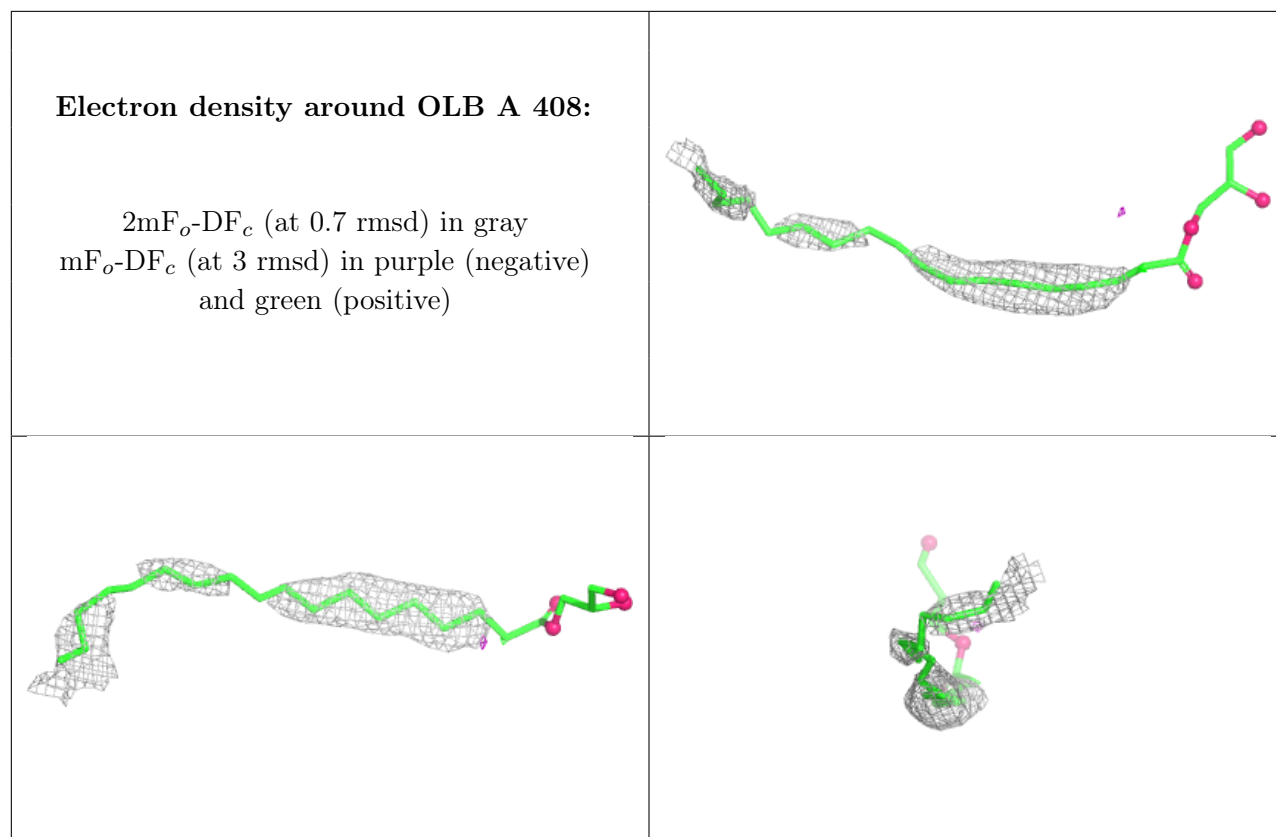
Electron density around OLB A 409:

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

**Electron density around OLA A 402:**

$2mF_o-DF_c$ (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.