



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2023 – 06:20 pm GMT

PDB ID : 8A6D
Title : 10 picosecond light activated crystal structure of bovine rhodopsin in Lipidic Cubic Phase
Authors : Gruhl, T.; Weinert, T.; Rodrigues, M.J.; Milne, C.J.; Ortolani, G.; Nass, K.; Nango, E.; Sen, S.; Johnson, P.J.M.; Cirelli, C.; Furrer, A.; Mous, S.; Skopintsev, P.; James, D.; Dworkowski, F.; Baath, P.; Kekilli, D.; Oserov, D.; Tanaka, R.; Glover, H.; Bacellar, C.; Bruenle, S.; Casadei, C.M.; Diethelm, A.D.; Gashi, D.; Gotthard, G.; Guixa-Gonzalez, R.; Joti, Y.; Kabanova, V.; Knopp, G.; Lesca, E.; Ma, P.; Martiel, I.; Muehle, J.; Owada, S.; Pamula, F.; Sarabi, D.; Tejero, O.; Tsai, C.J.; Varma, N.; Wach, A.; Boutet, S.; Tono, K.; Nogly, P.; Deupi, X.; Iwata, S.; Neutze, R.; Standfuss, J.; Schertler, G.F.X.; Panneels, V.
Deposited on : 2022-06-17
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13

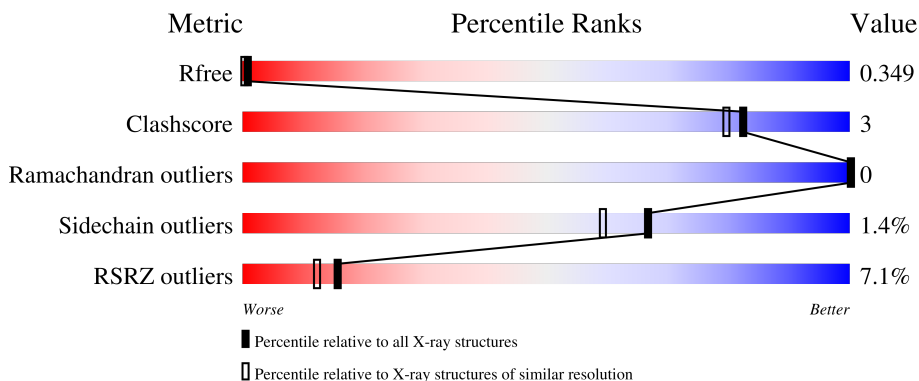
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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.

EDS : 2.32.1
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) : 2.32.1

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	
2	C	2	
2	D	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACE	A	401	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5413 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2474	1660	375	416	23	0	10	0
1	B	304	2473	1660	372	417	24	5	10	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



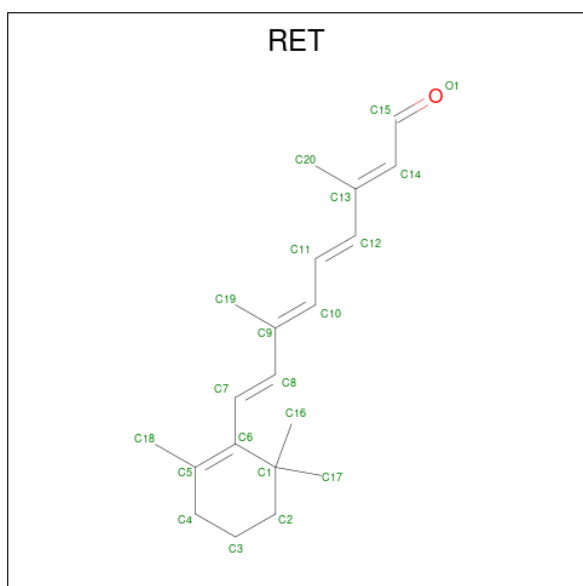
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is ACETYL GROUP (three-letter code: ACE) (formula: C₂H₄O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
3	A	1	Total	C	O	0	0
			3	2	1		
3	B	1	Total	C	O	0	0
			3	2	1		

- Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



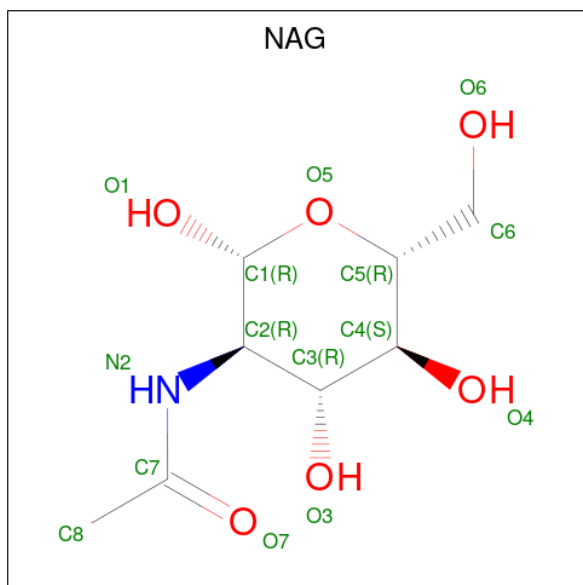
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
4	A	1	Total	C		0	0
			20	20			

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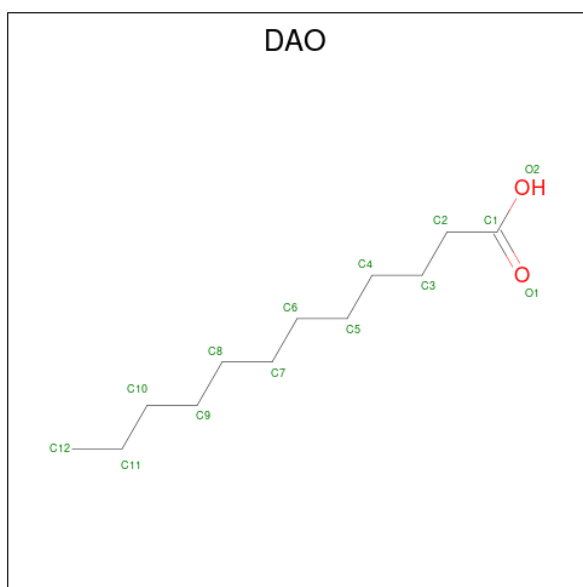
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 20 20	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



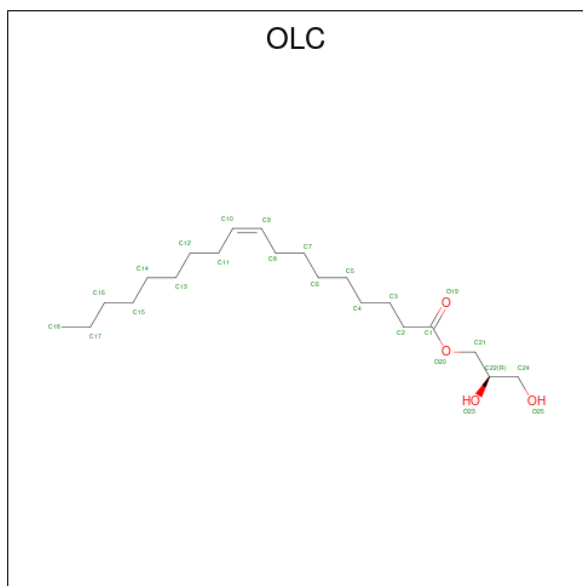
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	A	1	Total	C	O	0	0
			13	11	2		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



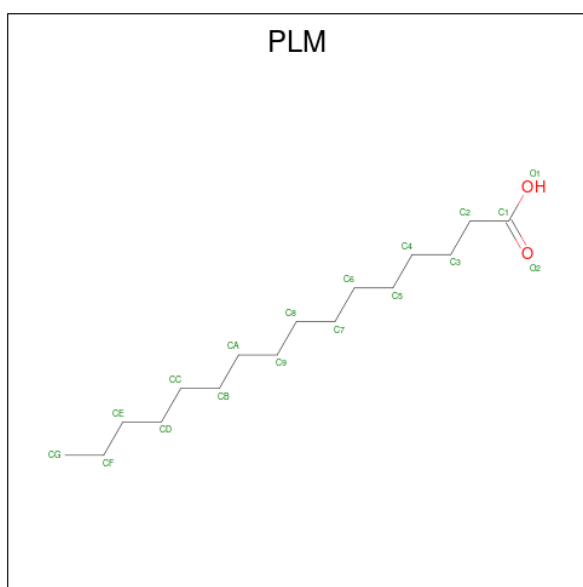
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	A	1	Total	C	O	0	0
			25	21	4		
7	A	1	Total	C	O	0	0
			17	15	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 7 7	0	0
7	A	1	Total C 10 10	0	0
7	A	1	Total C 12 12	0	0
7	A	1	Total C O 10 8 2	0	0
7	A	1	Total C O 25 21 4	0	0
7	A	1	Total C O 10 8 2	0	0
7	A	1	Total C 13 13	0	0
7	B	1	Total C O 19 17 2	0	0
7	B	1	Total C O 18 14 4	0	0
7	B	1	Total C 17 17	0	0
7	B	1	Total C 7 7	0	0

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	11	1		
8	B	1	Total	C	O	0	0
			7	6	1		

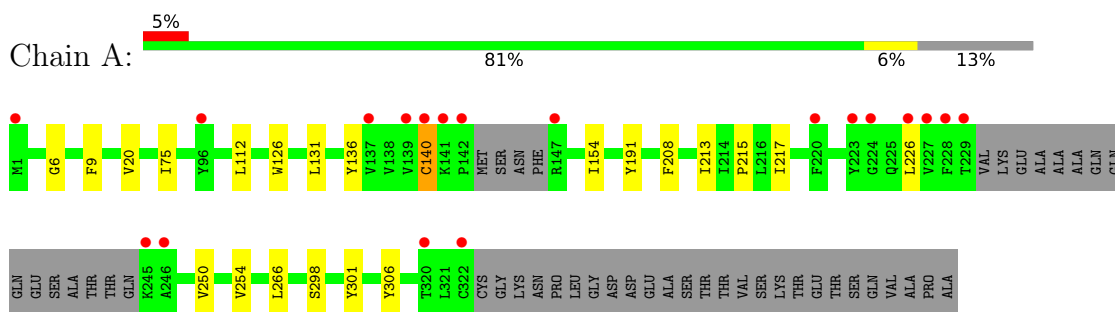
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	55	Total	O	0	0
			55	55		
9	B	59	Total	O	0	0
			59	59		

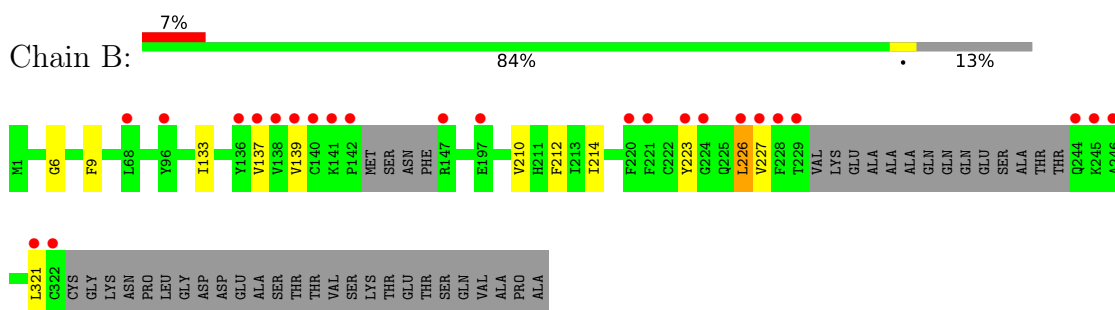
3 Residue-property plots [i](#)

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: Rhodopsin



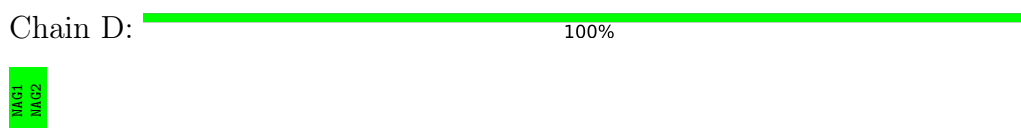
- Molecule 1: Rhodopsin



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.51Å 91.01Å 151.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 1.80 9.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.2 (9.99-1.80) 88.2 (9.99-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.314 , 0.347 0.314 , 0.349	Depositor DCC
R_{free} test set	1012 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 127.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5413	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6595e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OLC, ACE, PLM, NAG, RET, DAO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/2552	0.49	0/3486
1	B	0.32	0/2554	0.48	0/3489
All	All	0.32	0/5106	0.49	0/6975

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

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	2474	0	2432	15	0
1	B	2473	0	2416	8	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
3	A	3	0	3	0	0
3	B	3	0	3	0	0
4	A	20	0	27	3	0
4	B	20	0	27	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	129	0	188	4	0
7	B	61	0	88	3	0
8	A	12	0	18	0	0
8	B	7	0	8	0	0
9	A	55	0	0	0	0
9	B	59	0	0	0	0
All	All	5413	0	5304	27	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 3.

The worst 5 of 27 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)
4:A:402:RET:H181	4:A:402:RET:H8	1.78	0.64
1:B:139:VAL:HG11	1:B:226:LEU:HD21	1.80	0.63
1:B:210[B]:VAL:HA	1:B:214:ILE:HD12	1.81	0.62
1:B:210[A]:VAL:HA	1:B:214:ILE:HD12	1.82	0.60
1:A:208:PHE:HB3	7:A:407:OLC:H8	1.90	0.54

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	307/348 (88%)	296 (96%)	11 (4%)	0	100	100
1	B	308/348 (88%)	296 (96%)	12 (4%)	0	100	100
All	All	615/696 (88%)	592 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/296 (89%)	260 (99%)	3 (1%)	73	68
1	B	261/296 (88%)	257 (98%)	4 (2%)	65	56
All	All	524/592 (88%)	517 (99%)	7 (1%)	67	62

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	TYR
1	B	226	LEU
1	B	321	LEU
1	B	227	VAL
1	A	306	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	GLN
1	B	225	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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.36	0	17,19,21	0.49	0
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	0.44	0
2	NAG	D	1	2,1	14,14,15	0.50	0	17,19,21	0.49	0
2	NAG	D	2	2	14,14,15	0.31	0	17,19,21	0.51	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

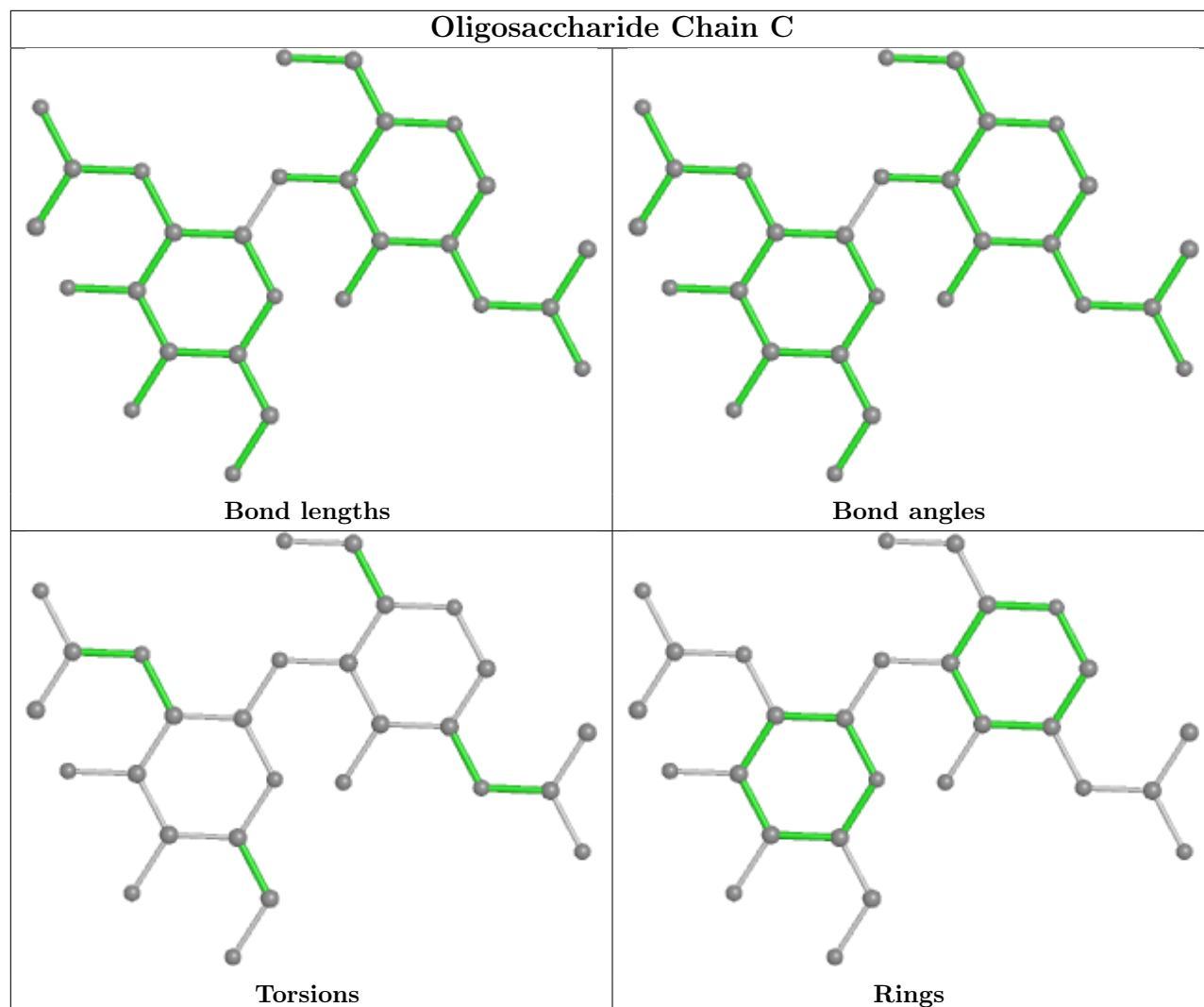
There are no torsion outliers.

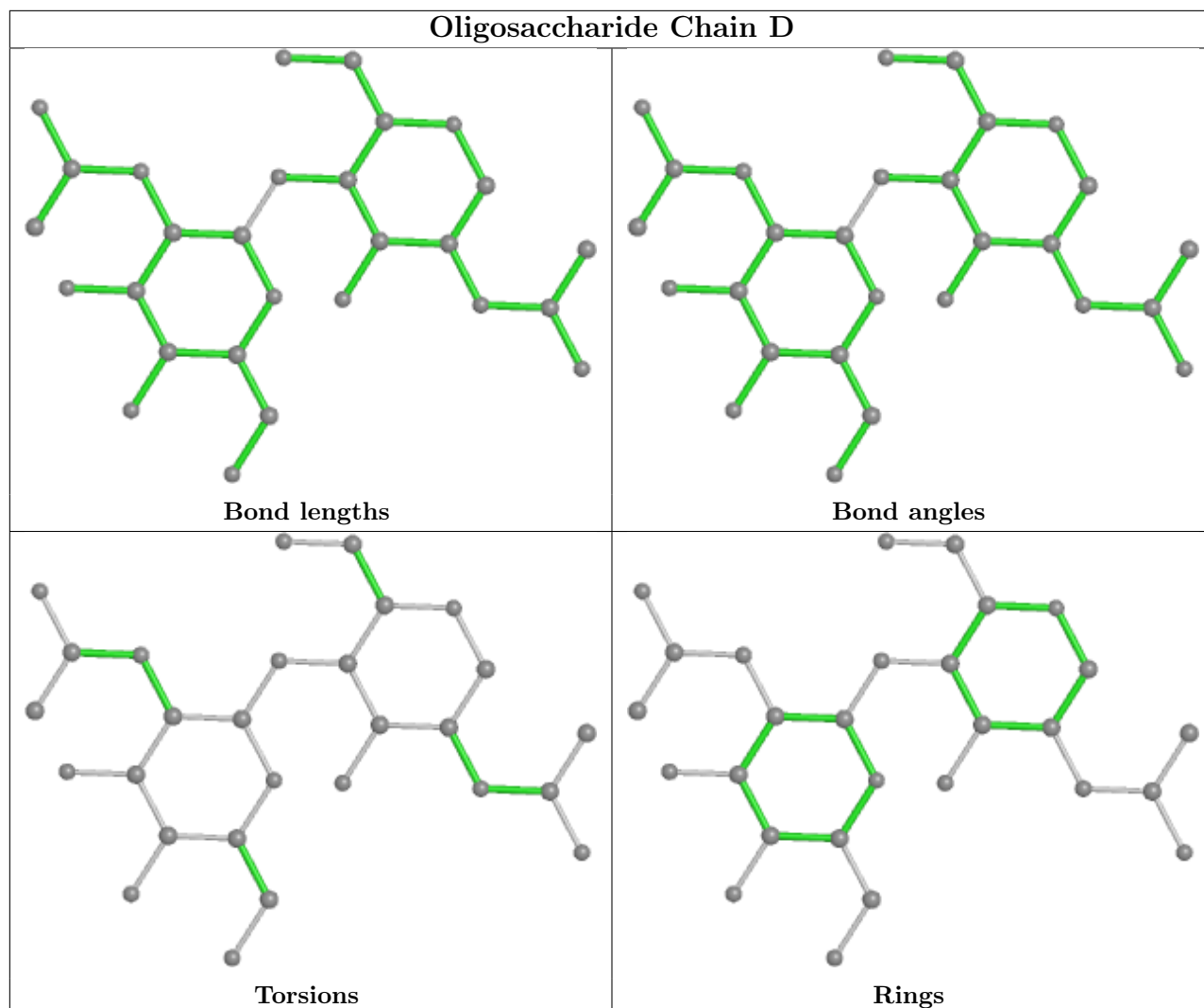
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OLC	A	413	-	9,9,24	1.51	2 (22%)	9,9,25	1.71	2 (22%)
3	ACE	A	401	1	1,2,2	0.88	0	1,1,1	0.34	0
7	OLC	B	408	-	6,6,24	0.20	0	4,5,25	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	RET	B	402	1	20,20,21	2.58	5 (25%)	27,27,28	1.36	3 (11%)
7	OLC	A	412	-	24,24,24	0.25	0	25,25,25	0.25	0
5	NAG	A	403	1	14,14,15	0.38	0	17,19,21	0.57	0
7	OLC	A	407	-	6,6,24	0.19	0	4,5,25	0.31	0
7	OLC	A	409	-	11,11,24	0.19	0	10,10,25	0.30	0
8	PLM	B	407	1	6,6,17	0.75	0	5,5,17	0.76	0
4	RET	A	402	1	20,20,21	2.34	5 (25%)	27,27,28	1.30	2 (7%)
3	ACE	B	401	1	1,2,2	0.83	0	1,1,1	0.35	0
6	DAO	A	404	-	12,12,13	0.75	0	12,12,13	0.70	0
7	OLC	A	414	-	12,12,24	0.27	0	11,11,25	0.14	0
7	OLC	A	406	-	16,16,24	0.35	0	16,16,25	0.27	0
5	NAG	B	403	1	14,14,15	0.21	0	17,19,21	0.52	0
8	PLM	A	410	1	11,11,17	0.60	0	10,10,17	0.54	0
7	OLC	A	405	-	24,24,24	0.28	0	25,25,25	0.32	0
7	OLC	B	406	-	16,16,24	0.22	0	15,15,25	0.21	0
7	OLC	A	411	-	9,9,24	1.53	2 (22%)	9,9,25	1.63	2 (22%)
7	OLC	B	405	-	17,17,24	0.26	0	18,18,25	0.37	0
7	OLC	A	408	-	9,9,24	0.27	0	8,8,25	0.21	0
7	OLC	B	404	-	18,18,24	0.35	0	18,18,25	0.23	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
7	OLC	A	413	-	-	2/7/7/24	-
7	OLC	B	408	-	-	1/4/4/24	-
4	RET	B	402	1	-	3/13/30/31	0/1/1/1
7	OLC	A	412	-	-	5/24/24/24	-
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
7	OLC	A	407	-	-	0/4/4/24	-
7	OLC	A	409	-	-	2/9/9/24	-
8	PLM	B	407	1	-	0/3/4/15	-
4	RET	A	402	1	-	4/13/30/31	0/1/1/1
6	DAO	A	404	-	-	3/10/10/11	-
7	OLC	A	414	-	-	2/10/10/24	-
7	OLC	A	406	-	-	6/14/14/24	-
5	NAG	B	403	1	-	0/6/23/26	0/1/1/1
8	PLM	A	410	1	-	1/8/9/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	405	-	-	4/24/24/24	-
7	OLC	B	406	-	-	1/14/14/24	-
7	OLC	A	411	-	-	3/7/7/24	-
7	OLC	B	405	-	-	3/17/17/24	-
7	OLC	A	408	-	-	0/7/7/24	-
7	OLC	B	404	-	-	3/17/17/24	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	RET	C14-C13	9.02	1.40	1.33
4	A	402	RET	C14-C13	7.68	1.39	1.33
4	B	402	RET	C10-C9	4.36	1.41	1.35
4	A	402	RET	C10-C9	3.91	1.41	1.35
7	A	411	OLC	O19-C1	3.41	1.33	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	RET	C19-C9-C10	-3.70	117.74	122.92
7	A	413	OLC	O19-C1-C2	-3.66	111.32	123.08
4	B	402	RET	C19-C9-C10	-3.56	117.93	122.92
7	A	413	OLC	O20-C1-C2	3.54	125.42	114.03
7	A	411	OLC	O19-C1-C2	-3.51	111.80	123.08

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	RET	C11-C10-C9-C8
4	A	402	RET	C11-C10-C9-C19
4	B	402	RET	C11-C10-C9-C8
4	B	402	RET	C11-C10-C9-C19
7	A	412	OLC	C2-C1-O20-C21

There are no ring outliers.

7 monomers are involved in 10 short contacts:

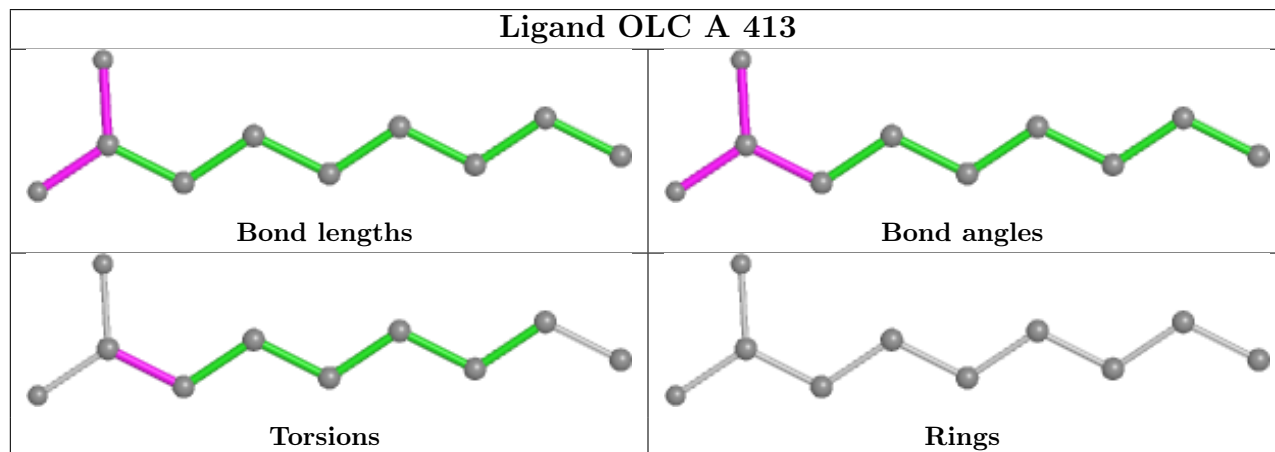
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	413	OLC	1	0

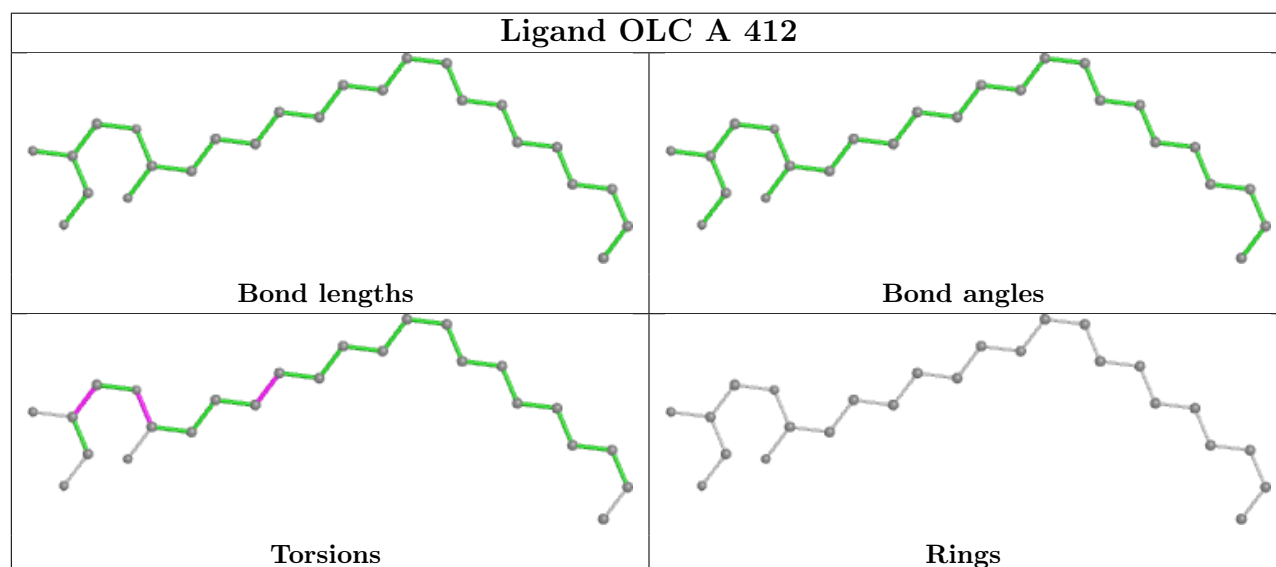
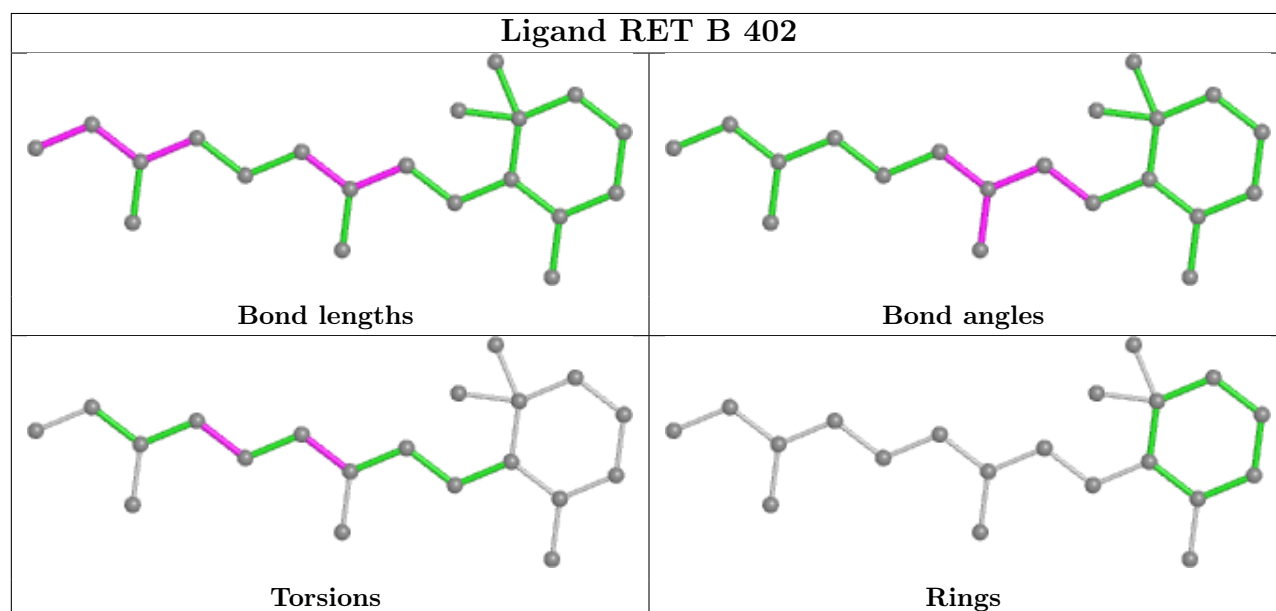
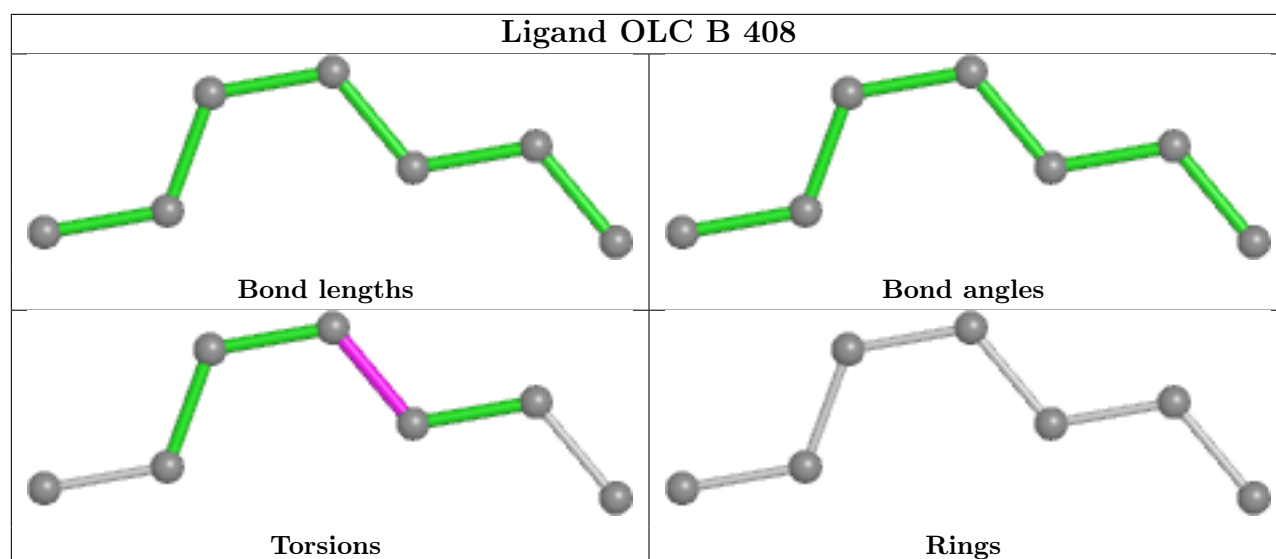
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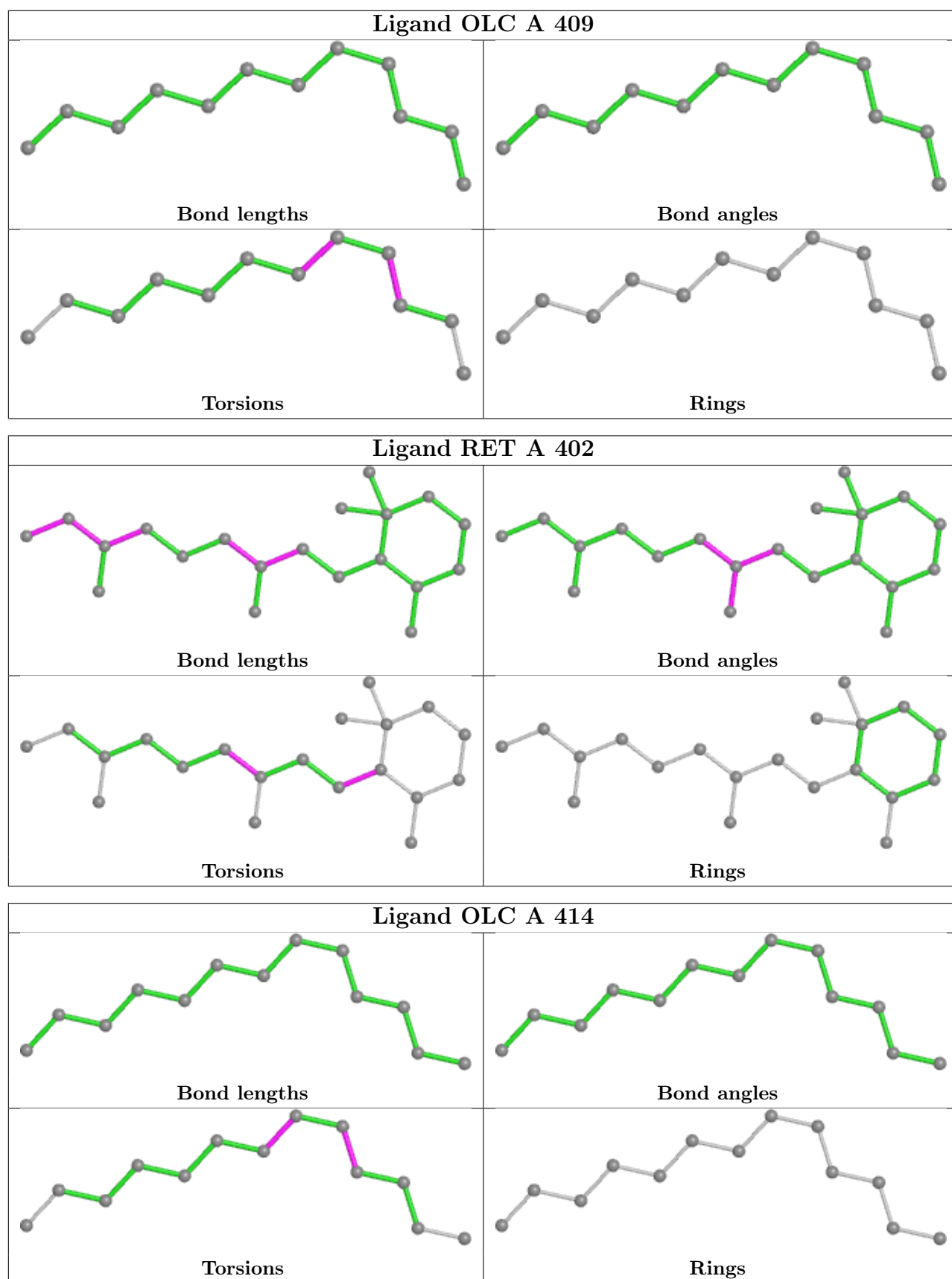
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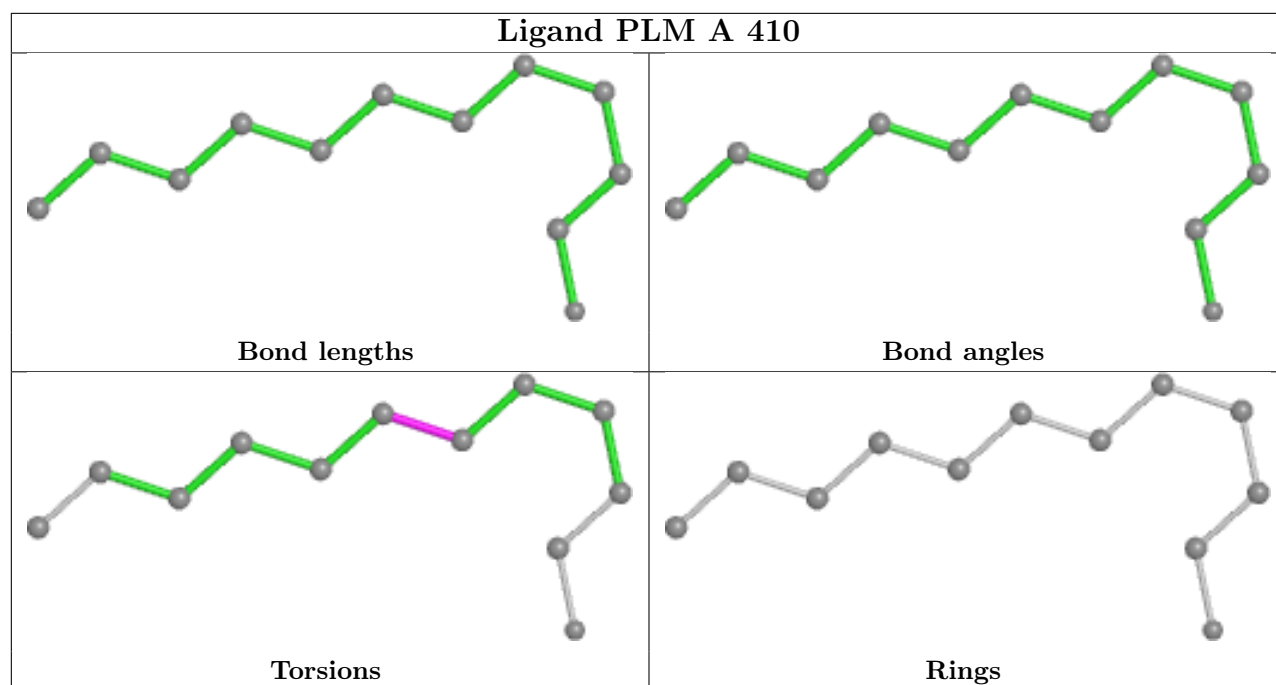
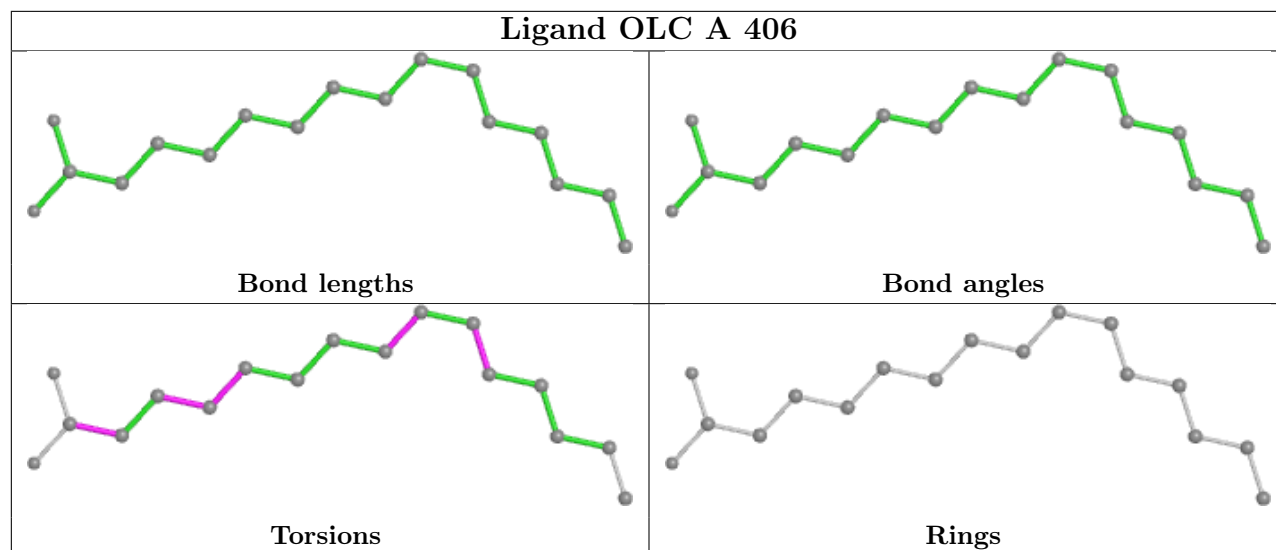
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	408	OLC	2	0
7	A	412	OLC	1	0
7	A	407	OLC	2	0
4	A	402	RET	3	0
7	A	406	OLC	1	0
7	B	405	OLC	1	0

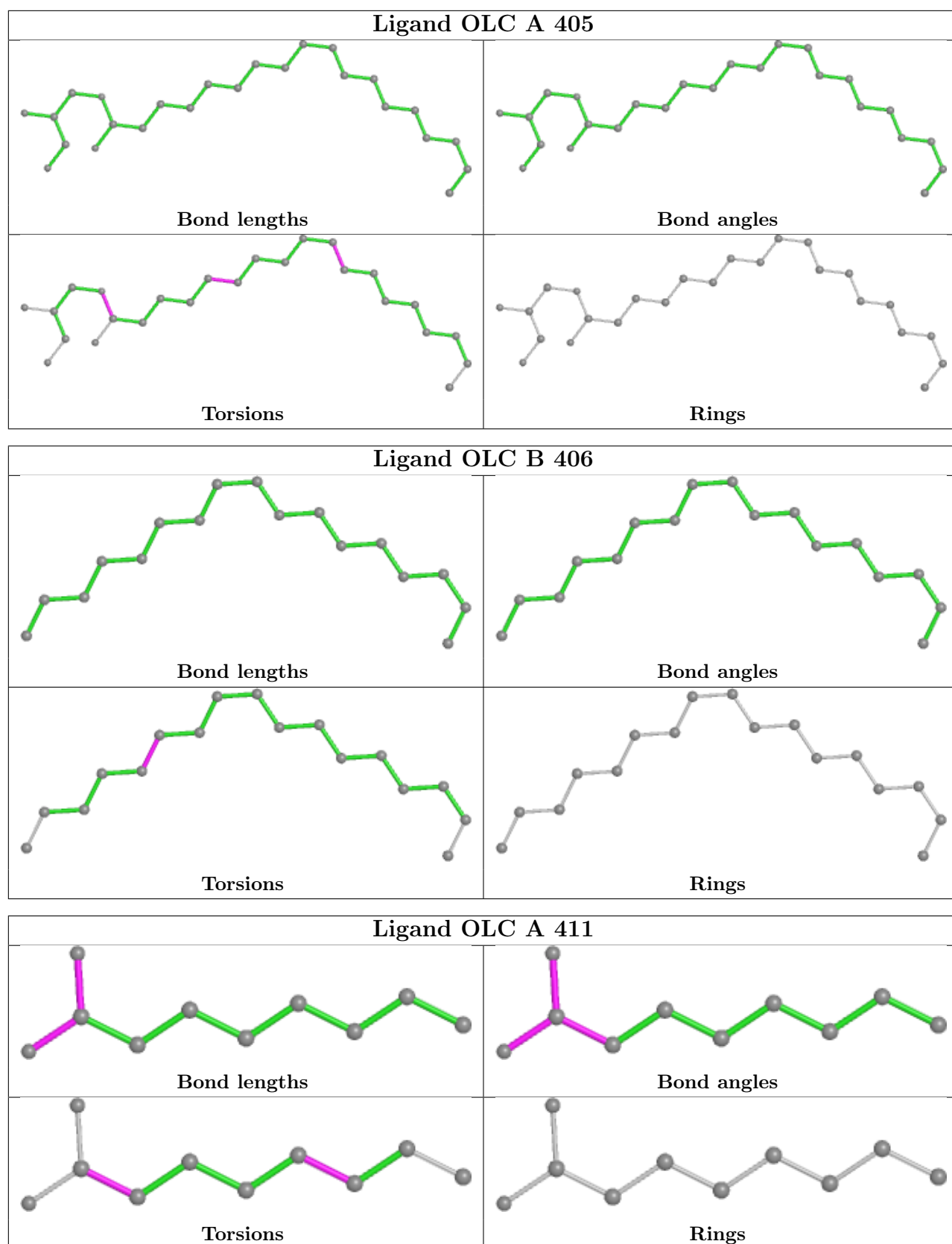
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

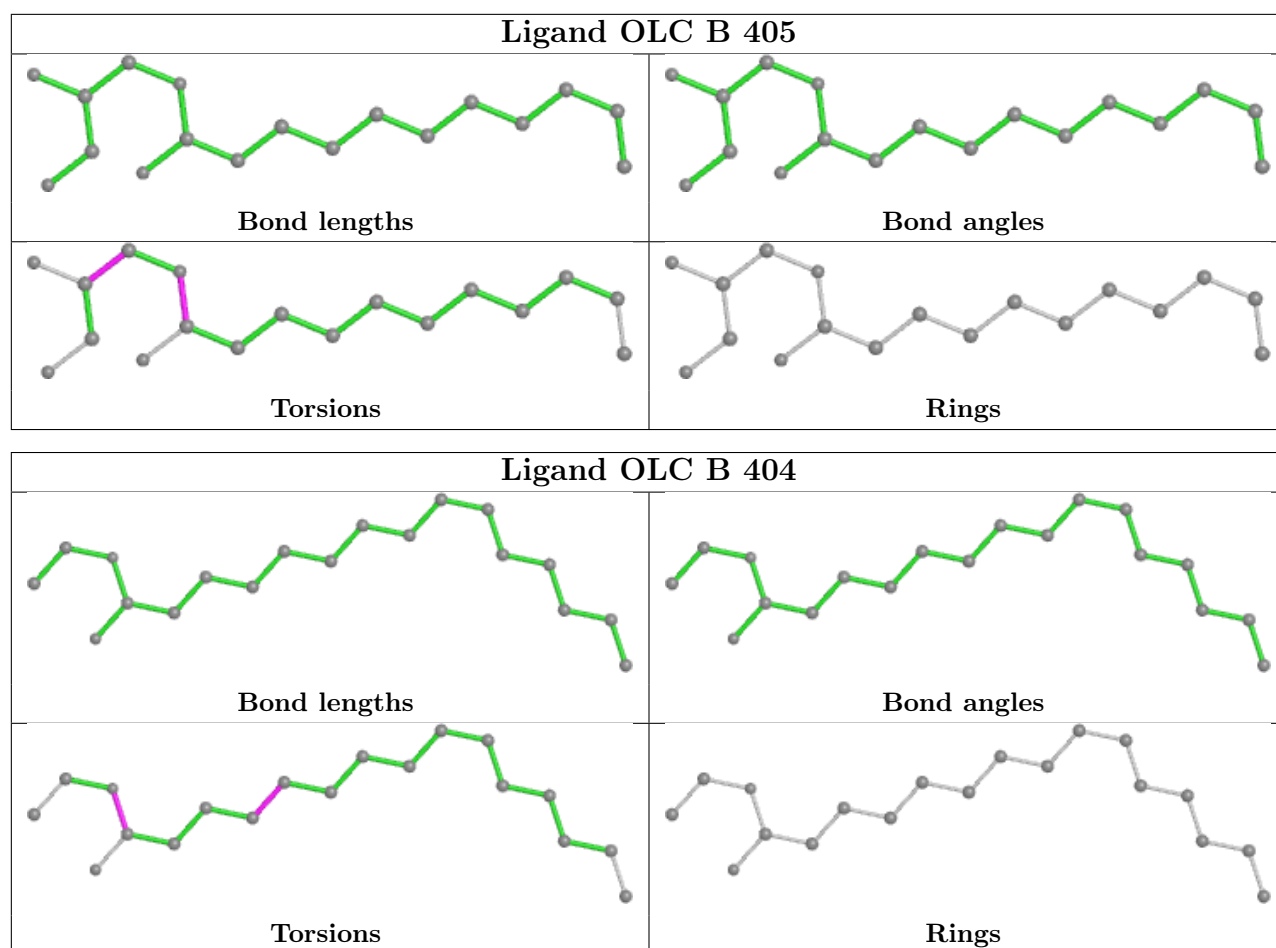












5.7 Other polymers [i](#)

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, 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	303/348 (87%)	0.38	19 (6%) 20 15	28, 38, 76, 147	0
1	B	304/348 (87%)	0.39	24 (7%) 12 9	29, 38, 81, 131	0
All	All	607/696 (87%)	0.39	43 (7%) 16 12	28, 38, 80, 147	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	CYS	16.2
1	B	142	PRO	11.3
1	B	140	CYS	10.4
1	A	142	PRO	10.1
1	B	229	THR	10.1

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

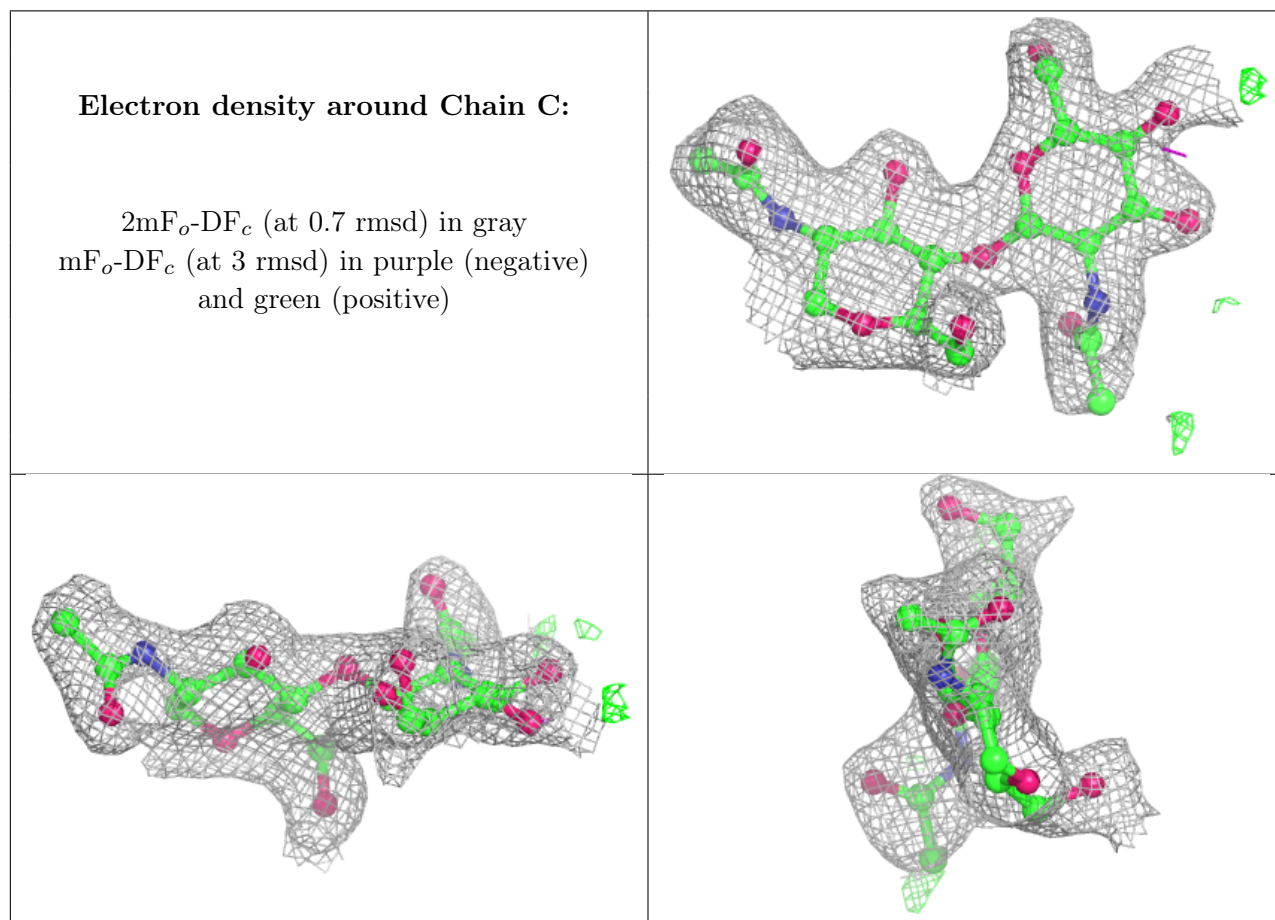
There are no non-standard protein/DNA/RNA residues in this entry.

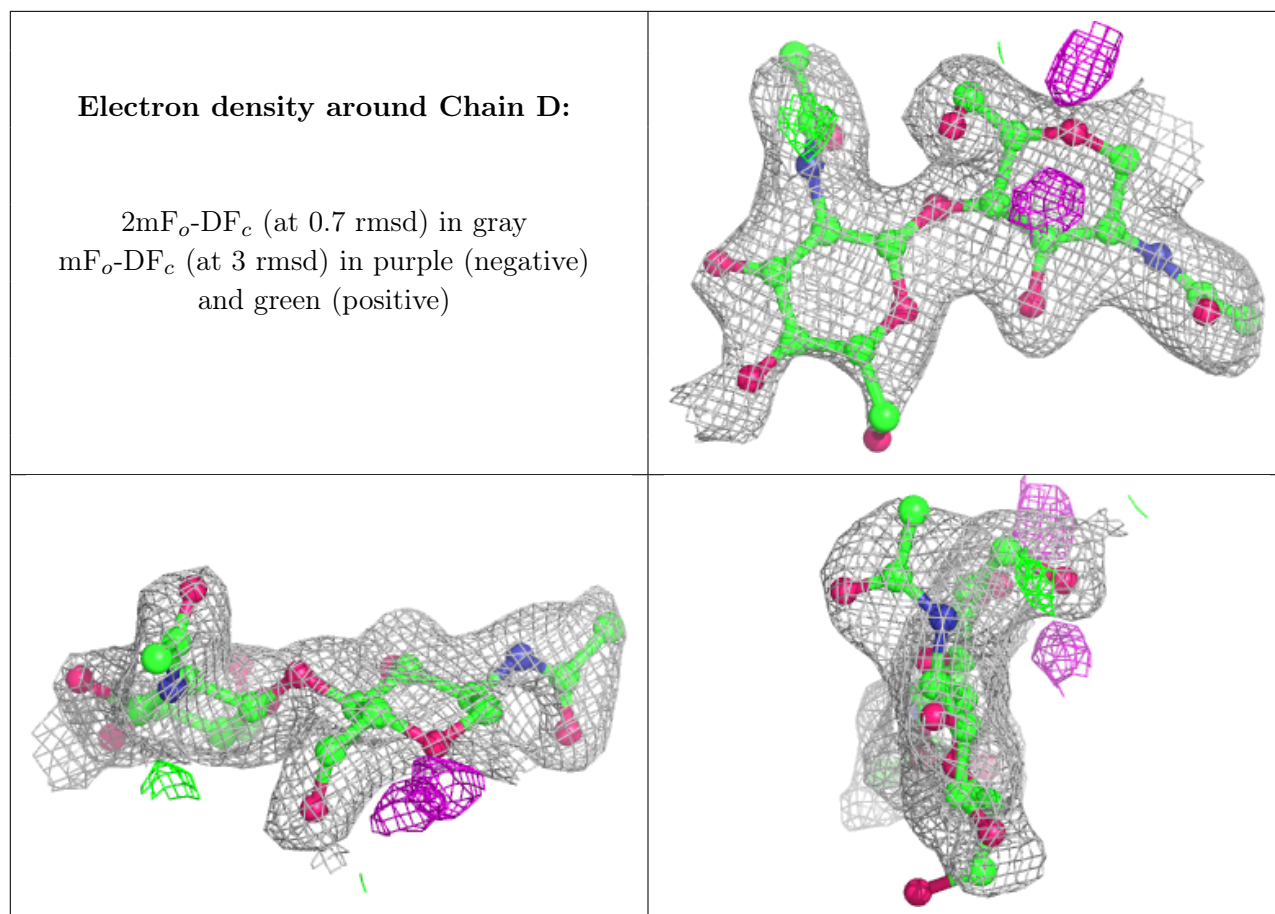
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.82	0.31	67,78,86,87	0
2	NAG	C	2	14/15	0.87	0.19	47,57,65,67	0
2	NAG	D	1	14/15	0.91	0.11	43,49,59,62	0
2	NAG	C	1	14/15	0.91	0.10	41,45,49,51	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





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.

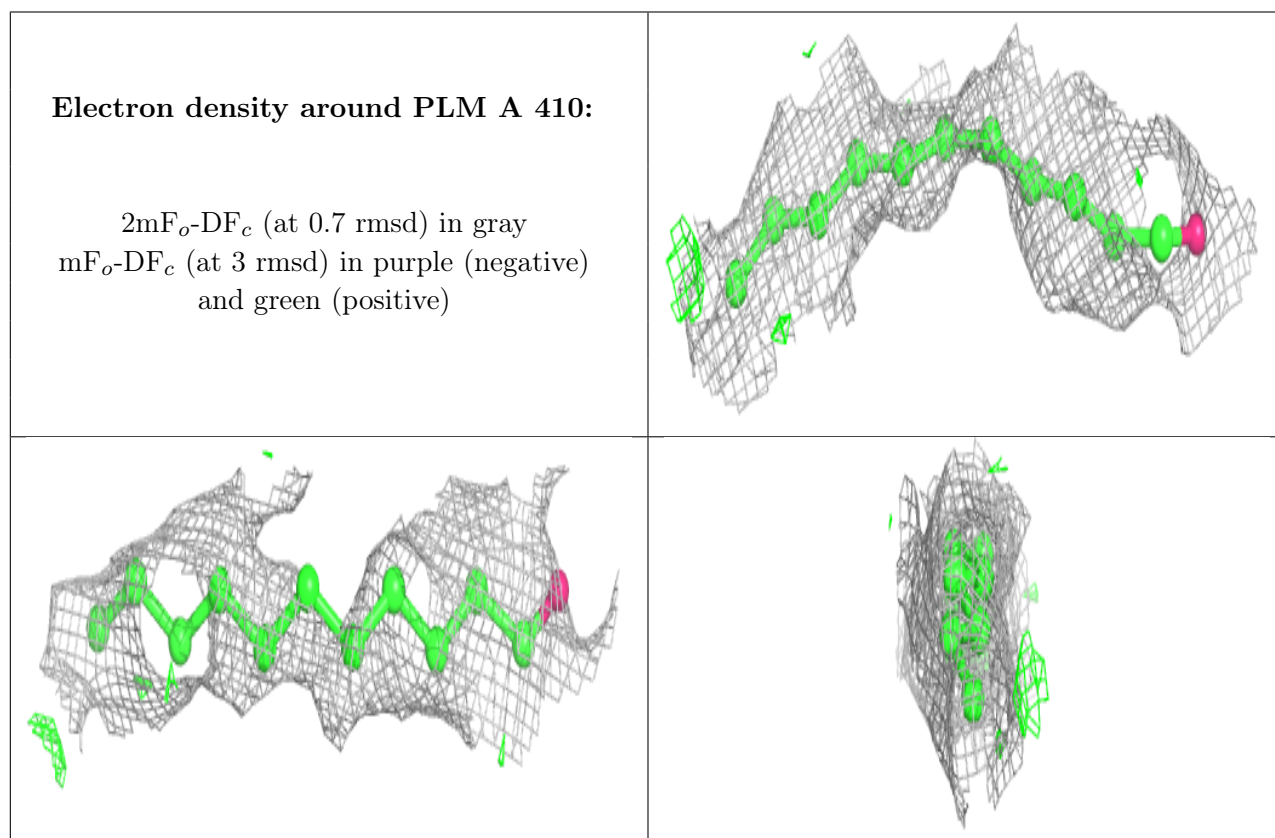
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PLM	A	410	12/18	0.61	0.19	67,74,85,97	0
8	PLM	B	407	7/18	0.62	0.17	75,77,82,84	0
7	OLC	A	405	25/25	0.68	0.17	47,65,83,87	0
7	OLC	A	406	17/25	0.69	0.20	52,66,96,127	0
7	OLC	B	406	17/25	0.71	0.15	43,54,73,73	0
7	OLC	A	409	12/25	0.73	0.17	43,60,67,75	0
7	OLC	B	404	19/25	0.74	0.17	54,59,83,98	0
7	OLC	B	408	7/25	0.76	0.18	39,51,60,64	0
7	OLC	A	412	25/25	0.76	0.14	48,58,69,85	0
7	OLC	A	414	13/25	0.76	0.20	48,59,78,81	0
5	NAG	A	403	14/15	0.78	0.25	50,65,73,80	0
3	ACE	A	401	3/3	0.79	0.50	71,71,82,87	0

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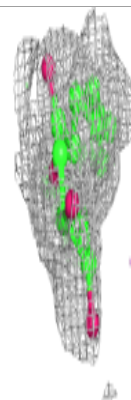
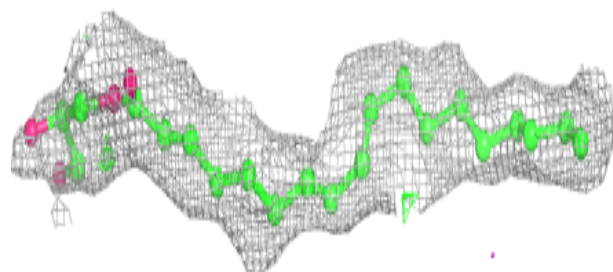
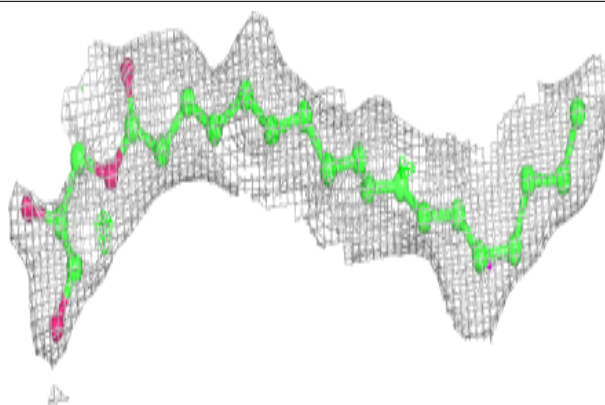
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	OLC	A	413	10/25	0.79	0.15	48,67,79,79	0
7	OLC	A	408	10/25	0.82	0.12	46,55,74,80	0
7	OLC	B	405	18/25	0.82	0.17	56,64,74,75	0
7	OLC	A	407	7/25	0.84	0.14	37,47,52,59	0
6	DAO	A	404	13/14	0.85	0.14	33,54,81,94	0
7	OLC	A	411	10/25	0.90	0.17	55,66,74,76	0
5	NAG	B	403	14/15	0.90	0.11	39,54,61,71	0
4	RET	A	402	20/21	0.93	0.08	25,33,39,42	0
4	RET	B	402	20/21	0.93	0.08	26,32,38,42	0
3	ACE	B	401	3/3	0.97	0.11	45,45,46,48	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.

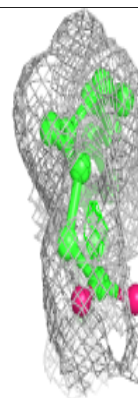
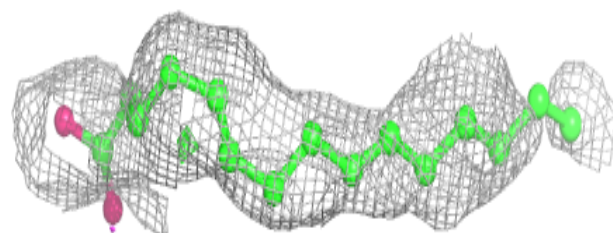
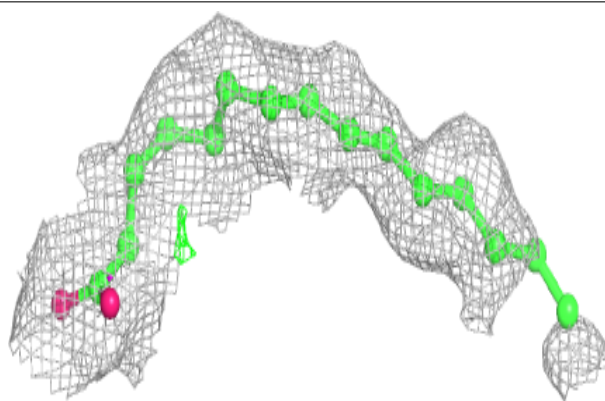


Electron density around OLC A 405:

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

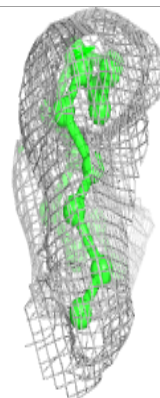
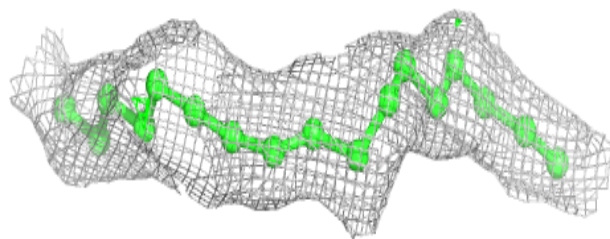
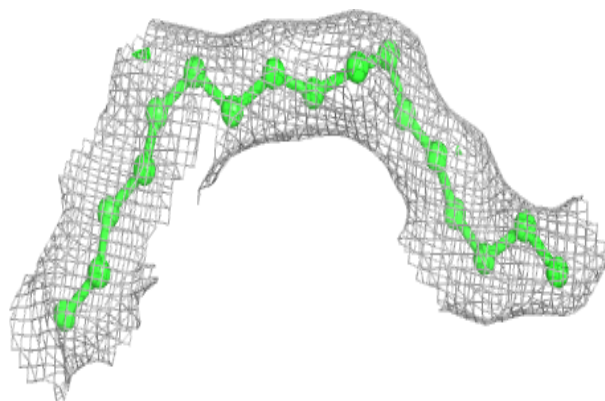
**Electron density around OLC A 406:**

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

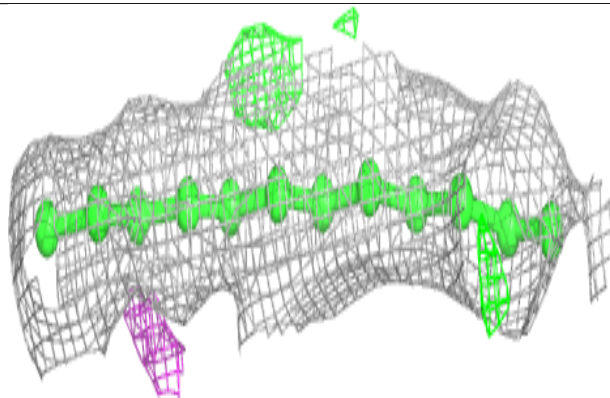
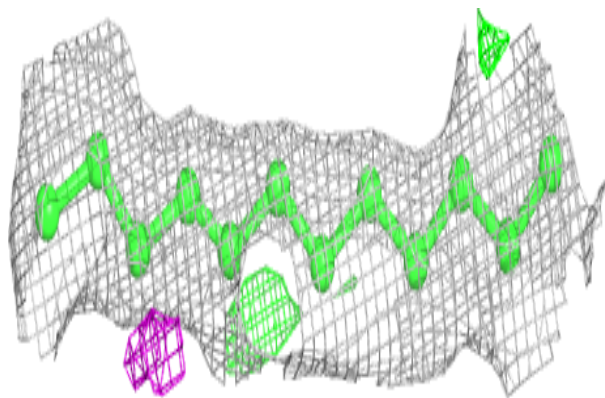


Electron density around OLC B 406:

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

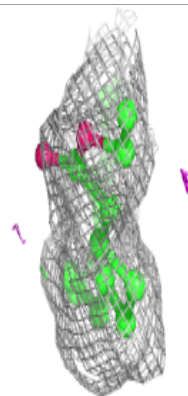
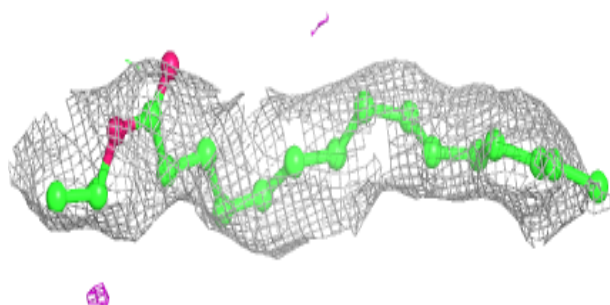
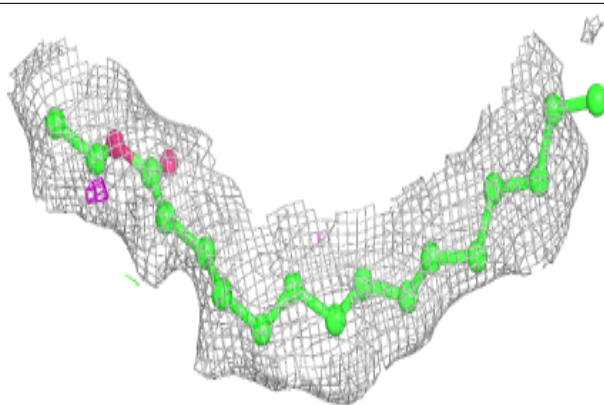
**Electron density around OLC A 409:**

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

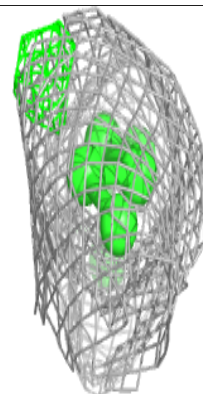
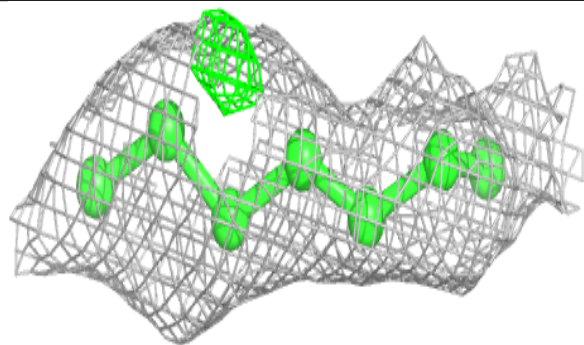
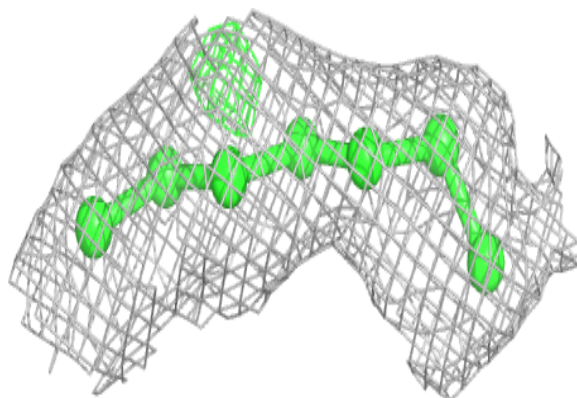


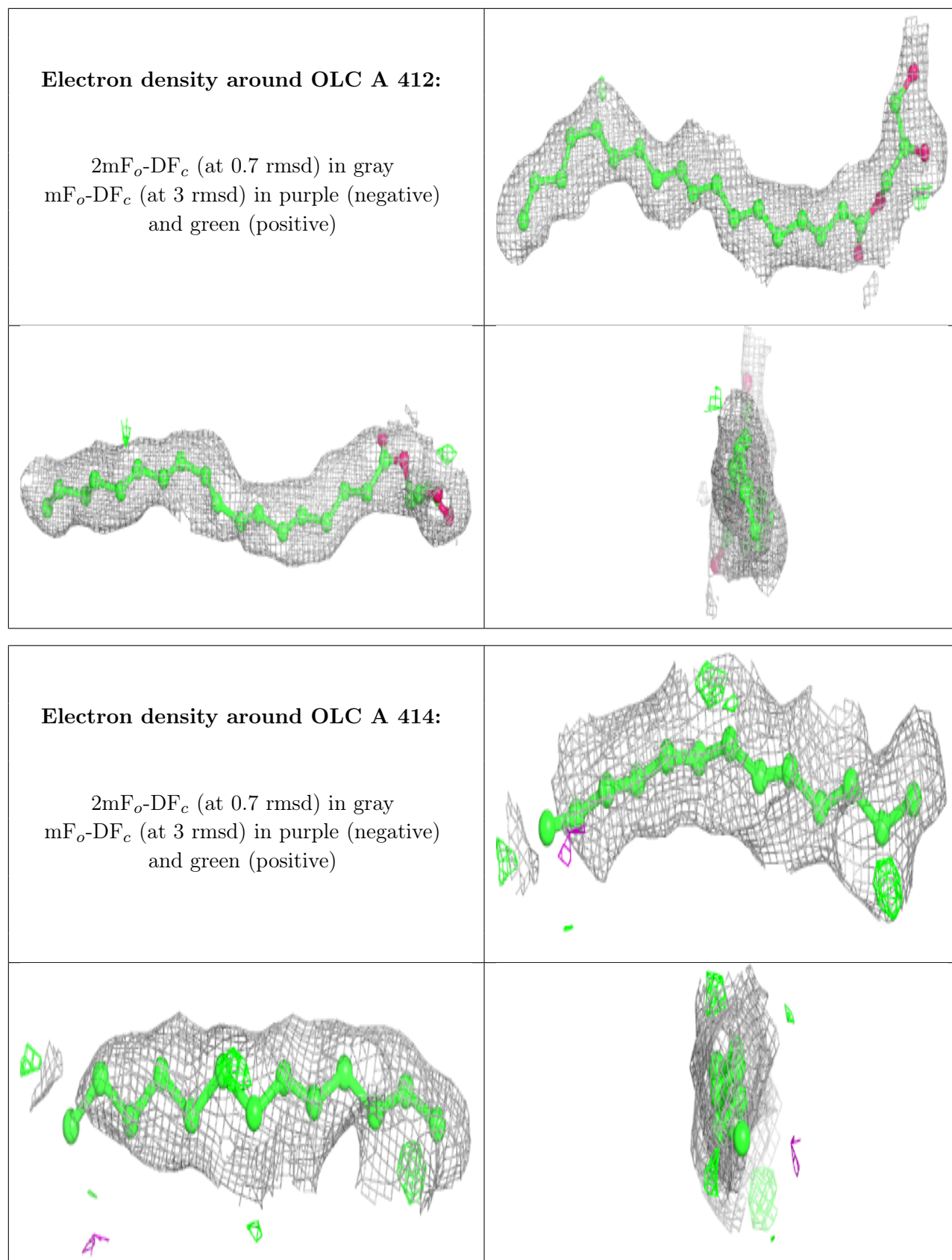
Electron density around OLC B 404:

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

**Electron density around OLC B 408:**

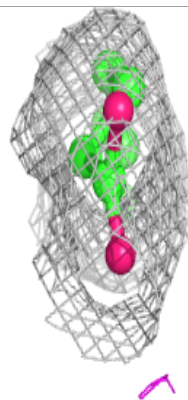
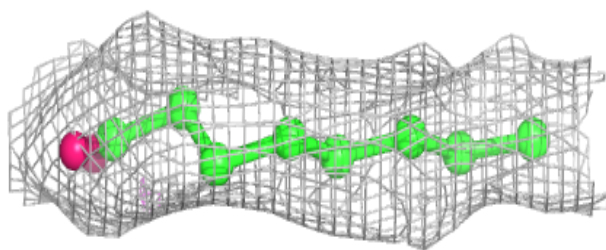
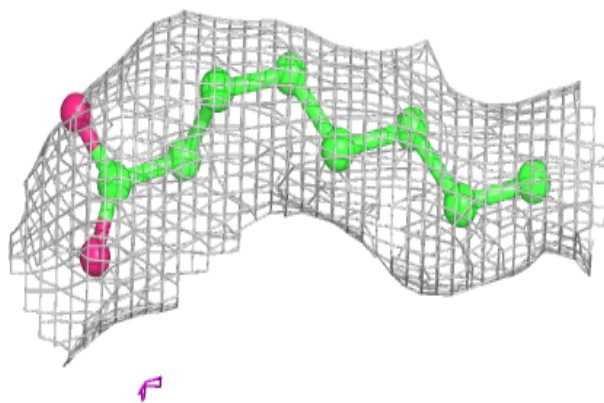
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



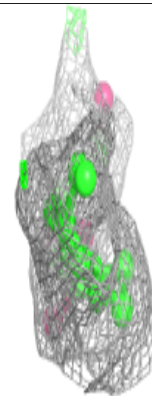
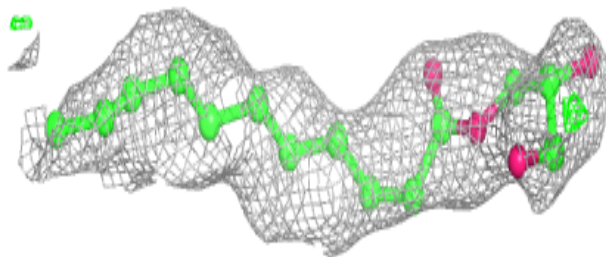
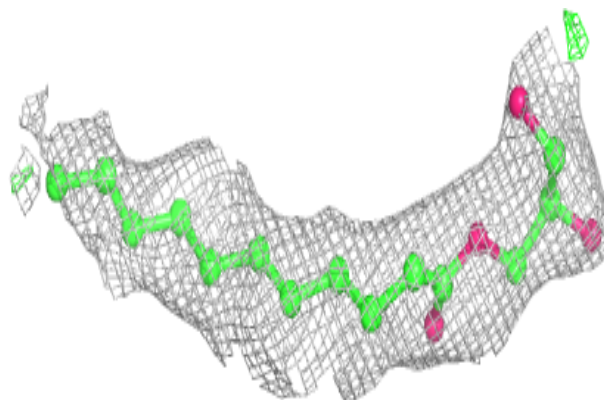


Electron density around OLC A 413:

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

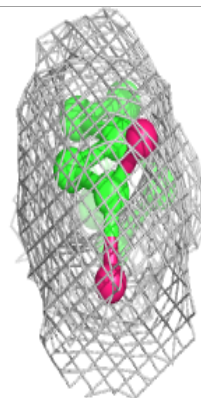
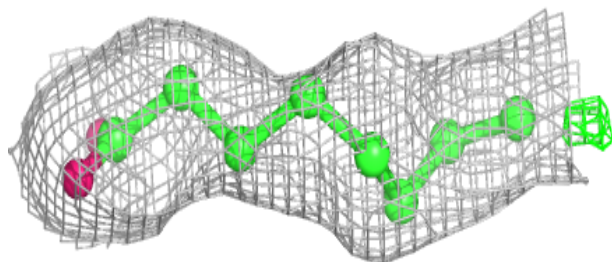
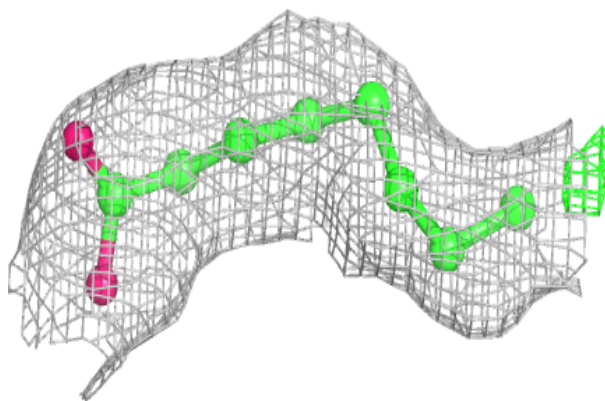
**Electron density around OLC B 405:**

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

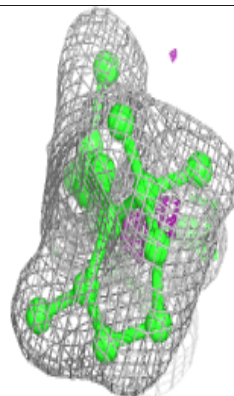
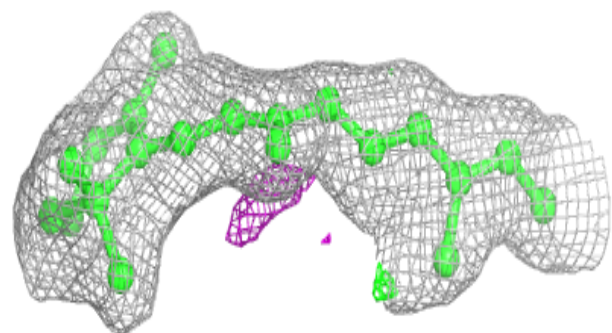
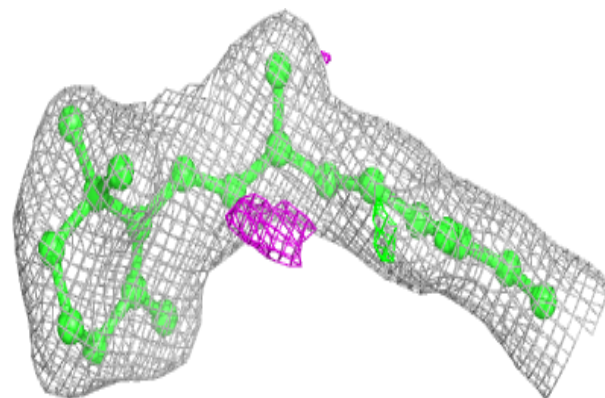


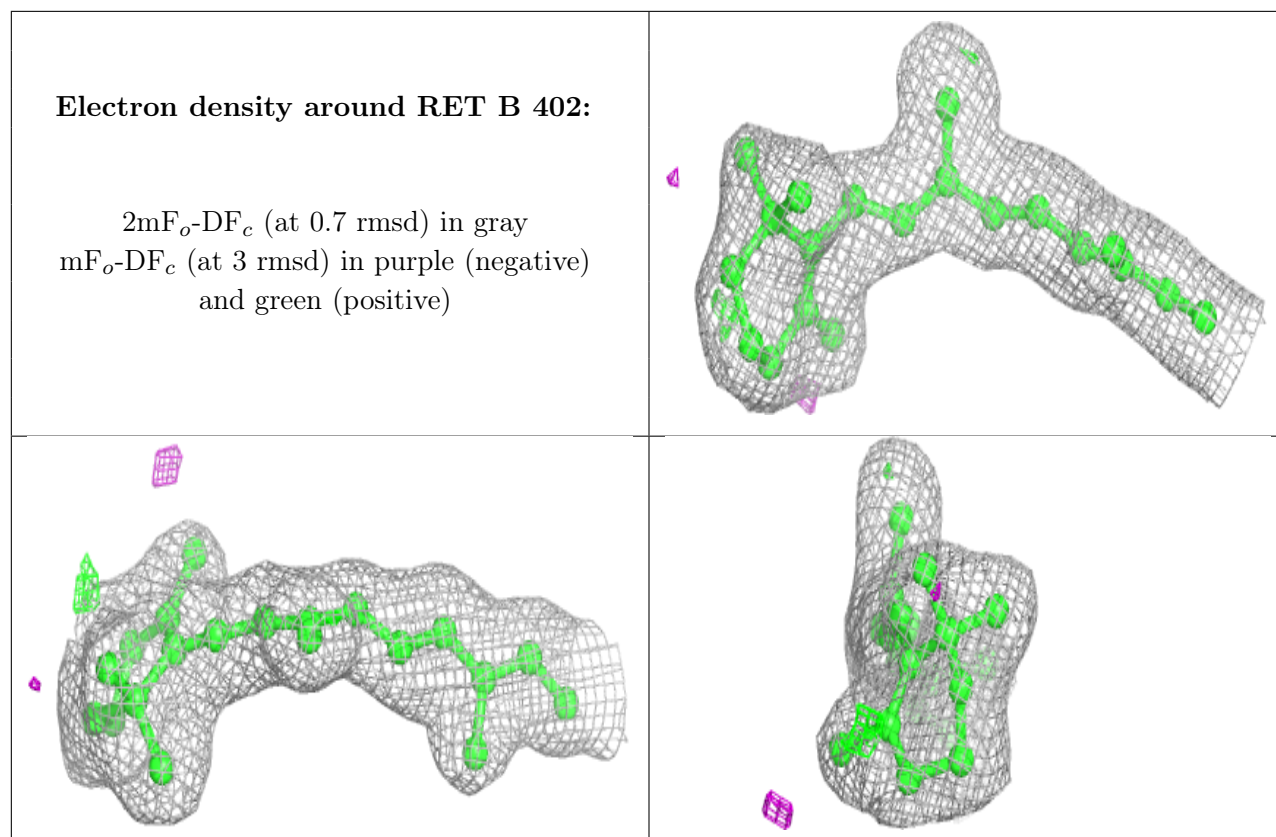
Electron density around OLC A 411:

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

**Electron density around RET 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.