Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 02:50 PM JST

PDB ID	:	7E6X
Title	:	Time-resolved serial femtosecond crystallography reveals early structural changes in channelrhodopsin: 4 ms structure
Authors	:	Oda, K.; Nomura, T.; Nakane, T.; Yamashita, K.; Inoue, K.; Ito, S.; Vierock, J.; Hirata, K.; Maturana, A.D.; Katayama, K.; Ikuta, T.; Ishigami, I.; Izume, T.; Umeda, R.; Eguma, R.; Oishi, S.; Kasuya, G.; Kato, T.; Kusakizako, T.; Shihoya, W.; Shimada, H.; Takatsuji, T.; Takemoto, M.; Taniguchi, R.; Tomita, A.; Nakamura, R.; Fukuda, M.; Miyauchi, H.; Lee, Y.; Nango, E.; Tanaka, R.; Tanaka, T.; Sugahara, M.; Kimura, T.; Shimamura, T.; Fujiwara, T.; Yamanaka, Y.; Owada, S.; Joti, Y.; Tono, K.; Ishitani, R.; Hayashi, S.; Kandori, H.; Hegemann, P.; Iwata, S.; Kubo, M.; Nishizawa, T.; Nureki, O.
Deposited on	:	2021-02-24
Resolution	:	2.50 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:

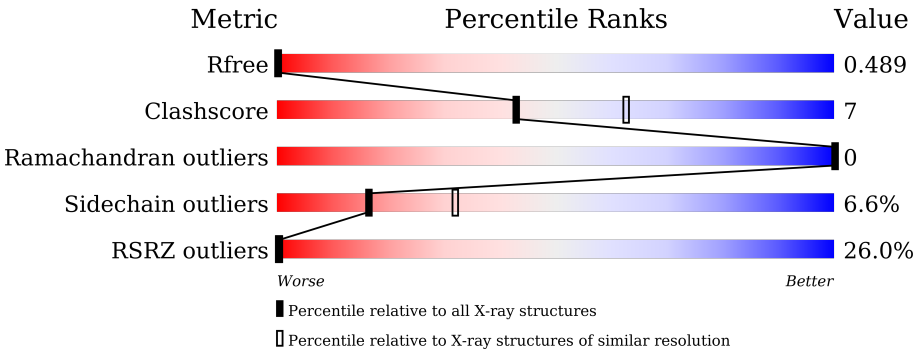
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	356	22% 70% 13% · 17%

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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)	:	2.35

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Mol	Chain	Length	Quality of chain
2	E	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	-	-	-	X
3	RET	A	401	-	-	-	X
4	OLC	A	404	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2529 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 Archaeal-type opsin 1,Archaeal-type opsin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2317	1521	369	412	15			

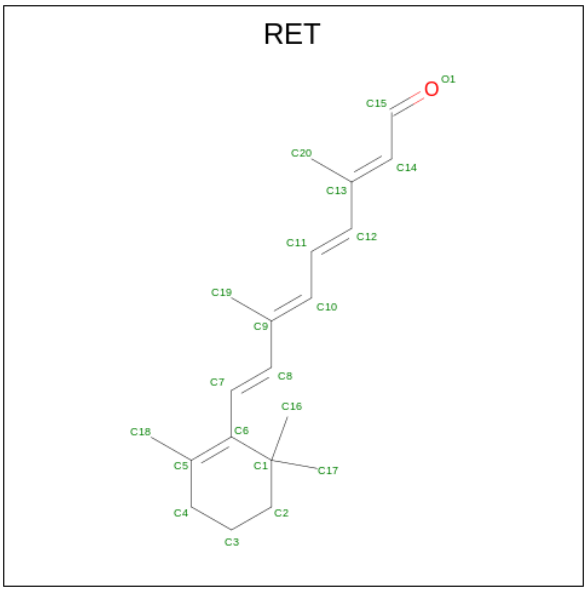
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	SER	-	expression tag	UNP Q8RUT8
A	350	SER	-	expression tag	UNP Q8RUT8
A	351	GLU	-	expression tag	UNP Q8RUT8
A	352	ASP	-	expression tag	UNP Q8RUT8
A	353	LEU	-	expression tag	UNP Q8RUT8
A	354	TYR	-	expression tag	UNP Q8RUT8
A	355	PHE	-	expression tag	UNP Q8RUT8
A	356	GLN	-	expression tag	UNP Q8RUT8

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

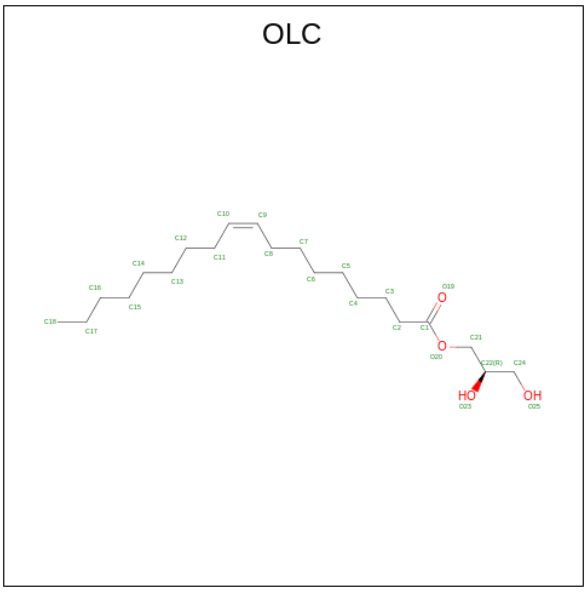
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



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

- Molecule 4 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
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 16 14 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 10 4	0	0
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	A	1	Total C O 10 8 2	0	0
4	A	1	Total C O 10 8 2	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 8 8	0	0

- Molecule 5 is water.

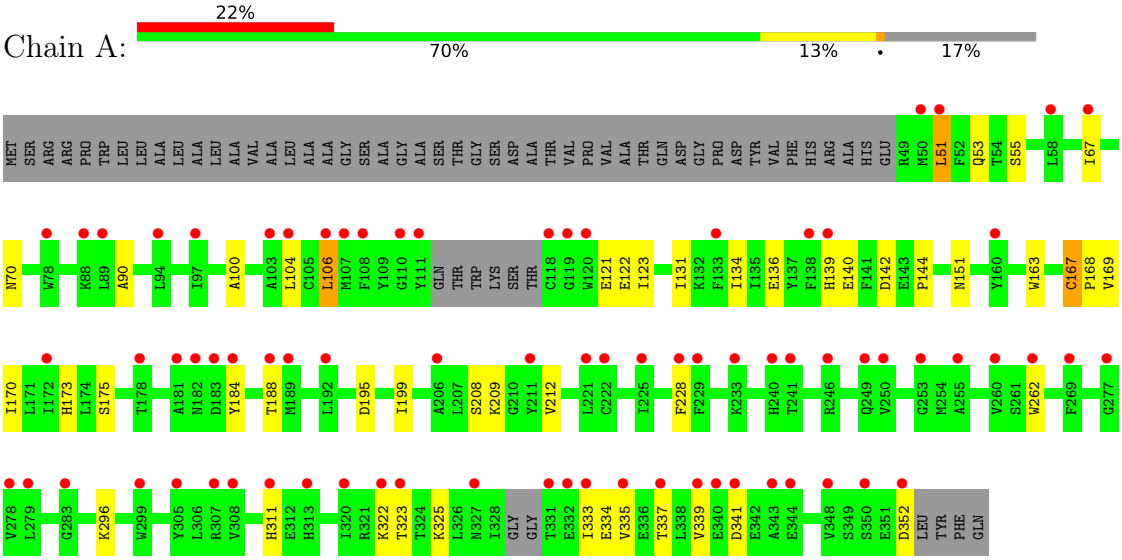
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0

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 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.

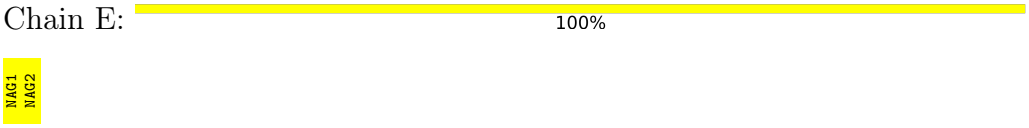
• Molecule 1: Archaeal-type opsin 1,Archaeal-type opsin 2

Chain A:



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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	61.80Å 142.20Å 94.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.96 – 2.50 14.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.0 (14.96-2.50) 81.4 (14.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.405 , 0.487 0.407 , 0.489	Depositor DCC
R_{free} test set	592 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.56$, $< L^2 > = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	2529	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NAG, RET

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	0.75	0/2377	0.83	0/3237

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	2317	0	2261	31	0
2	E	28	0	25	0	0
3	A	20	0	27	4	0
4	A	126	0	172	3	0
5	A	38	0	0	14	0
All	All	2529	0	2485	34	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 7.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HB2	5:A:506:HOH:O	1.53	1.05
1:A:168:PRO:CB	5:A:506:HOH:O	2.06	1.03
1:A:199:ILE:HG13	5:A:532:HOH:O	1.84	0.77
1:A:228:PHE:CD2	4:A:402:OLC:H18	2.19	0.77
1:A:184:TYR:HA	5:A:525:HOH:O	1.89	0.72
1:A:70:ASN:ND2	5:A:502:HOH:O	2.29	0.66
3:A:401:RET:H8	3:A:401:RET:H161	1.79	0.65
1:A:199:ILE:CG1	5:A:532:HOH:O	2.45	0.60
1:A:163:TRP:CD1	3:A:401:RET:H12	2.37	0.60
1:A:168:PRO:CG	5:A:506:HOH:O	2.39	0.59
1:A:167:CYS:SG	1:A:195:ASP:OD2	2.62	0.57
1:A:168:PRO:CD	5:A:506:HOH:O	2.52	0.57
1:A:322:LYS:HB2	1:A:337:THR:HB	1.92	0.52
1:A:169:VAL:N	5:A:506:HOH:O	2.43	0.52
1:A:212:VAL:HG21	4:A:406:OLC:C3	2.41	0.51
1:A:90:ALA:HB1	4:A:404:OLC:H6A	1.93	0.50
3:A:401:RET:H161	3:A:401:RET:C8	2.43	0.48
1:A:53:GLN:HE21	1:A:55:SER:H	1.60	0.48
1:A:121:GLU:HG3	1:A:173:HIS:CG	2.49	0.48
1:A:67:ILE:HD12	5:A:528:HOH:O	2.14	0.47
1:A:131:ILE:O	1:A:134:ILE:HG13	2.14	0.46
1:A:140:GLU:HB3	5:A:530:HOH:O	2.16	0.46
1:A:168:PRO:CA	5:A:506:HOH:O	2.50	0.45
1:A:175:SER:OG	1:A:188:THR:HG23	2.17	0.45
1:A:151:ASN:ND2	5:A:511:HOH:O	2.49	0.45
1:A:106:LEU:HD21	1:A:123:ILE:HG23	1.99	0.45
1:A:208:SER:HA	5:A:511:HOH:O	2.17	0.44
1:A:136:GLU:O	1:A:140:GLU:HB2	2.19	0.43
3:A:401:RET:H7	3:A:401:RET:H181	1.74	0.42
1:A:51:LEU:HD13	1:A:51:LEU:HA	1.81	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.77	0.41
1:A:170:ILE:HG21	1:A:262:TRP:HZ2	1.86	0.41
1:A:139:HIS:HB3	1:A:142:ASP:HB2	2.03	0.41
1:A:100:ALA:O	1:A:104:LEU:HG	2.20	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	290/356 (82%)	273 (94%)	17 (6%)	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	242/295 (82%)	226 (93%)	16 (7%)	16 32

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	106	LEU
1	A	122	GLU
1	A	144	PRO
1	A	167	CYS
1	A	209	LYS
1	A	296	LYS
1	A	311	HIS
1	A	323	THR
1	A	325	LYS
1	A	333	ILE
1	A	334	GLU
1	A	335	VAL

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Mol	Chain	Res	Type
1	A	339	VAL
1	A	341	ASP
1	A	352	ASP

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)

2 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	E	1	2,1	14,14,15	0.45	0	17,19,21	1.35	3 (17%)
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	1.59	1 (5%)

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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	4.75	118.63	112.19
2	E	1	NAG	C1-O5-C5	-3.16	107.91	112.19
2	E	1	NAG	O5-C1-C2	-2.34	107.59	111.29
2	E	1	NAG	C3-C4-C5	2.21	114.18	110.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

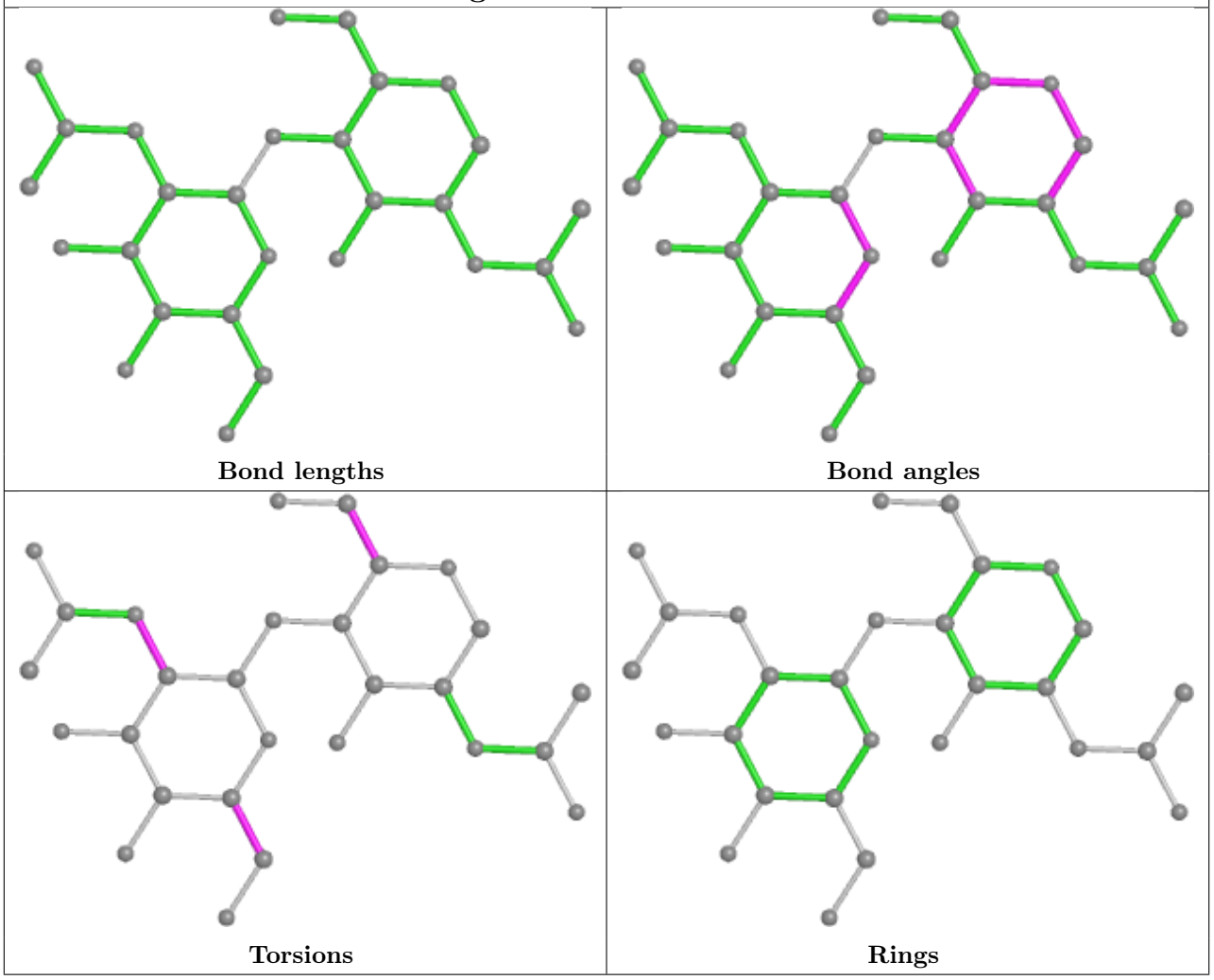
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7

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 oligosaccharide.

Oligosaccharide Chain E



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	OLC	A	406	-	17,17,24	0.29	0	18,18,25	0.36	0
4	OLC	A	409	-	8,8,24	0.31	0	7,7,25	0.26	0
4	OLC	A	407	-	9,9,24	0.38	0	9,9,25	0.28	0
4	OLC	A	410	-	7,7,24	0.35	0	6,6,25	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	RET	A	401	1	20,20,21	2.69	7 (35%)	27,27,28	2.09	9 (33%)
4	OLC	A	403	-	15,15,24	1.24	2 (13%)	15,15,25	1.48	2 (13%)
4	OLC	A	405	-	15,15,24	0.29	0	16,16,25	0.33	0
4	OLC	A	402	-	24,24,24	0.30	0	25,25,25	0.27	0
4	OLC	A	408	-	9,9,24	1.50	2 (22%)	9,9,25	1.70	2 (22%)
4	OLC	A	404	-	13,13,24	0.30	0	14,14,25	0.43	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
4	OLC	A	406	-	-	14/17/17/24	-
4	OLC	A	409	-	-	4/6/6/24	-
4	OLC	A	407	-	-	1/7/7/24	-
4	OLC	A	410	-	-	3/5/5/24	-
3	RET	A	401	1	-	0/13/30/31	0/1/1/1
4	OLC	A	403	-	-	7/13/13/24	-
4	OLC	A	405	-	-	11/15/15/24	-
4	OLC	A	402	-	-	10/24/24/24	-
4	OLC	A	408	-	-	4/7/7/24	-
4	OLC	A	404	-	-	5/13/13/24	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	RET	C14-C13	8.62	1.40	1.33
3	A	401	RET	C10-C9	4.83	1.42	1.35
3	A	401	RET	C15-C14	-3.62	1.35	1.49
4	A	403	OLC	O19-C1	3.42	1.33	1.22
4	A	408	OLC	O19-C1	3.36	1.33	1.22
3	A	401	RET	C8-C9	-3.05	1.39	1.45
4	A	403	OLC	O20-C1	-2.78	1.21	1.30
4	A	408	OLC	O20-C1	-2.68	1.21	1.30
3	A	401	RET	C11-C12	2.38	1.40	1.34
3	A	401	RET	C19-C9	-2.24	1.46	1.50
3	A	401	RET	C8-C7	2.06	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	RET	C8-C9-C10	5.80	127.84	118.94
4	A	403	OLC	O20-C1-C2	4.17	127.42	114.03
4	A	403	OLC	O19-C1-C2	-3.71	111.17	123.08
4	A	408	OLC	O20-C1-C2	3.66	125.78	114.03
3	A	401	RET	C19-C9-C10	-3.64	117.82	122.92
4	A	408	OLC	O19-C1-C2	-3.52	111.78	123.08
3	A	401	RET	C12-C13-C14	3.52	129.94	118.80
3	A	401	RET	C20-C13-C14	-3.40	113.65	123.71
3	A	401	RET	C2-C1-C6	3.39	115.70	110.48
3	A	401	RET	C10-C11-C12	2.99	132.54	123.22
3	A	401	RET	C1-C6-C7	2.48	122.80	115.78
3	A	401	RET	C1-C6-C5	-2.46	119.15	122.61
3	A	401	RET	C19-C9-C8	-2.37	114.33	118.08

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	OLC	C11-C10-C9-C8
4	A	406	OLC	C21-C22-C24-O25
4	A	406	OLC	O20-C21-C22-C24
4	A	406	OLC	O20-C21-C22-O23
4	A	405	OLC	C2-C1-O20-C21
4	A	406	OLC	C1-C2-C3-C4
4	A	404	OLC	C1-C2-C3-C4
4	A	405	OLC	O19-C1-O20-C21
4	A	403	OLC	C1-C2-C3-C4
4	A	407	OLC	C1-C2-C3-C4
4	A	406	OLC	C2-C1-O20-C21
4	A	410	OLC	C3-C4-C5-C6
4	A	402	OLC	C12-C13-C14-C15
4	A	402	OLC	C21-C22-C24-O25
4	A	404	OLC	C21-C22-C24-O25
4	A	402	OLC	C1-C2-C3-C4
4	A	403	OLC	C4-C5-C6-C7
4	A	404	OLC	C2-C1-O20-C21
4	A	404	OLC	O23-C22-C24-O25
4	A	406	OLC	O23-C22-C24-O25
4	A	402	OLC	C6-C7-C8-C9
4	A	404	OLC	O19-C1-O20-C21
4	A	406	OLC	O19-C1-O20-C21
4	A	405	OLC	C5-C6-C7-C8
4	A	403	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	A	406	OLC	C6-C7-C8-C9
4	A	405	OLC	C2-C3-C4-C5
4	A	406	OLC	C3-C4-C5-C6
4	A	406	OLC	C4-C5-C6-C7
4	A	403	OLC	C10-C11-C12-C13
4	A	405	OLC	C6-C7-C8-C9
4	A	410	OLC	C6-C7-C8-C9
4	A	405	OLC	C4-C5-C6-C7
4	A	409	OLC	C4-C5-C6-C7
4	A	405	OLC	C1-C2-C3-C4
4	A	410	OLC	C4-C5-C6-C7
4	A	402	OLC	C15-C16-C17-C18
4	A	408	OLC	C5-C6-C7-C8
4	A	402	OLC	C2-C1-O20-C21
4	A	402	OLC	O23-C22-C24-O25
4	A	402	OLC	O19-C1-O20-C21
4	A	405	OLC	O20-C21-C22-O23
4	A	409	OLC	C5-C6-C7-C8
4	A	408	OLC	C4-C5-C6-C7
4	A	403	OLC	C11-C10-C9-C8
4	A	409	OLC	C2-C3-C4-C5
4	A	408	OLC	C3-C4-C5-C6
4	A	405	OLC	O20-C21-C22-C24
4	A	402	OLC	C5-C6-C7-C8
4	A	402	OLC	C11-C12-C13-C14
4	A	409	OLC	C7-C8-C9-C10
4	A	406	OLC	O20-C1-C2-C3
4	A	403	OLC	C7-C8-C9-C10
4	A	406	OLC	O19-C1-C2-C3
4	A	403	OLC	O20-C1-C2-C3
4	A	408	OLC	O20-C1-C2-C3
4	A	405	OLC	O20-C1-C2-C3
4	A	405	OLC	O19-C1-C2-C3
4	A	406	OLC	C7-C8-C9-C10

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	OLC	1	0
3	A	401	RET	4	0
4	A	402	OLC	1	0

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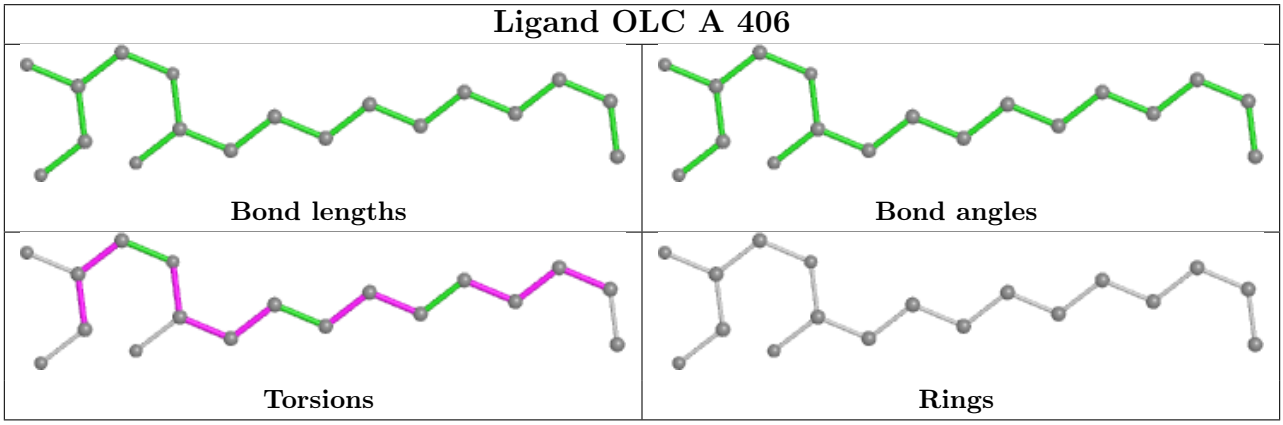
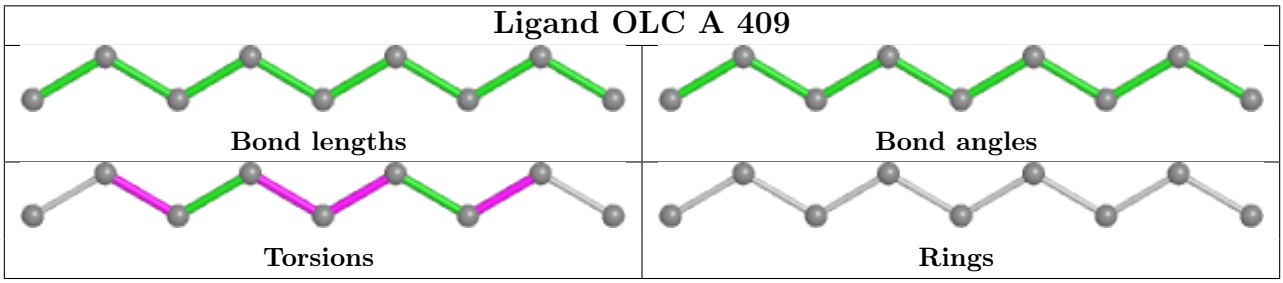
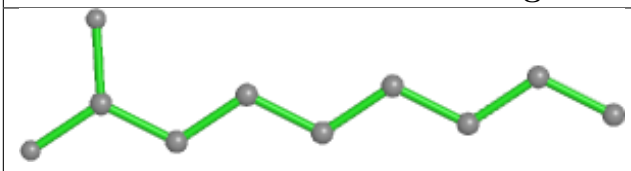
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	OLC	1	0

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 then 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.

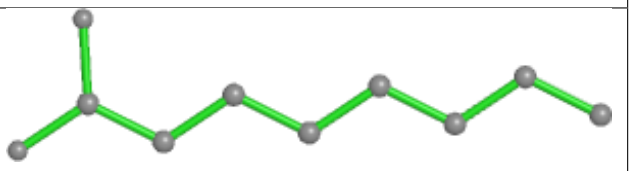




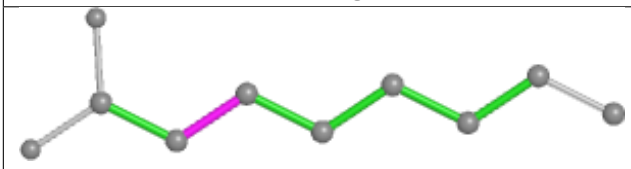
Ligand OLC A 407



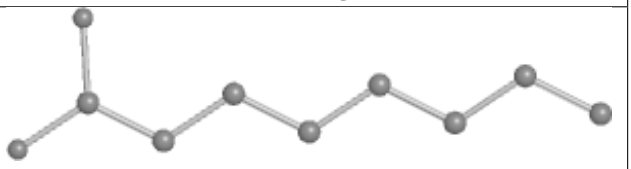
Bond lengths



Bond angles

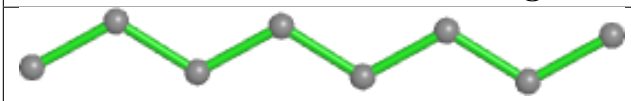


Torsions

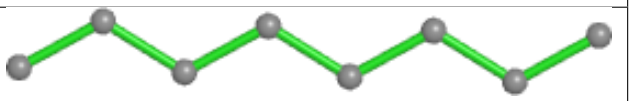


Rings

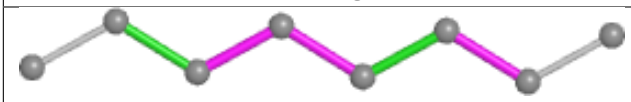
Ligand OLC A 410



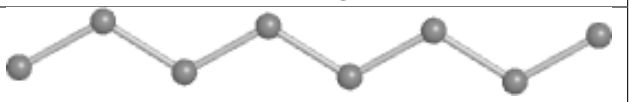
Bond lengths



Bond angles

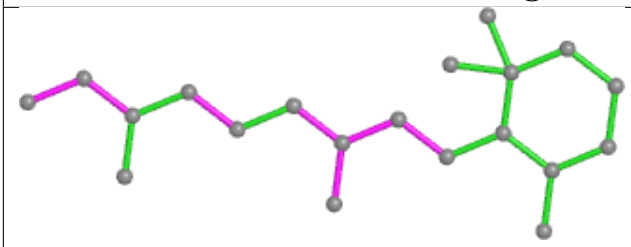


Torsions

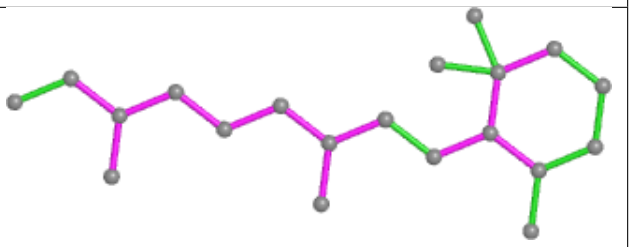


Rings

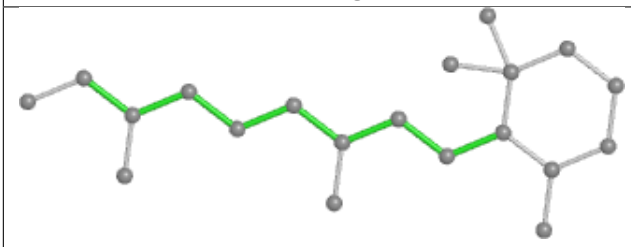
Ligand RET A 401



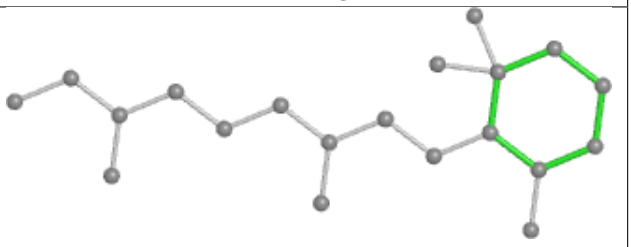
Bond lengths



Bond angles

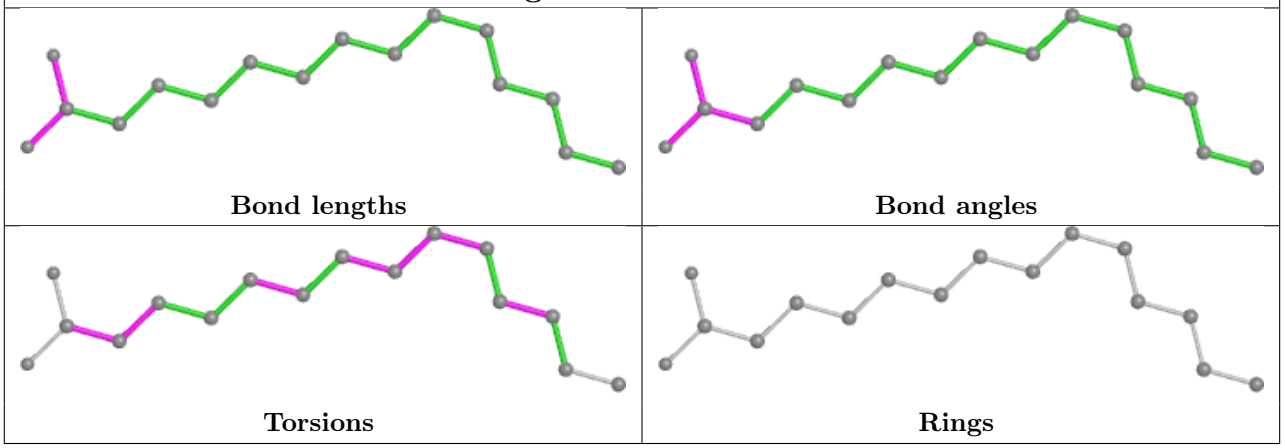


Torsions

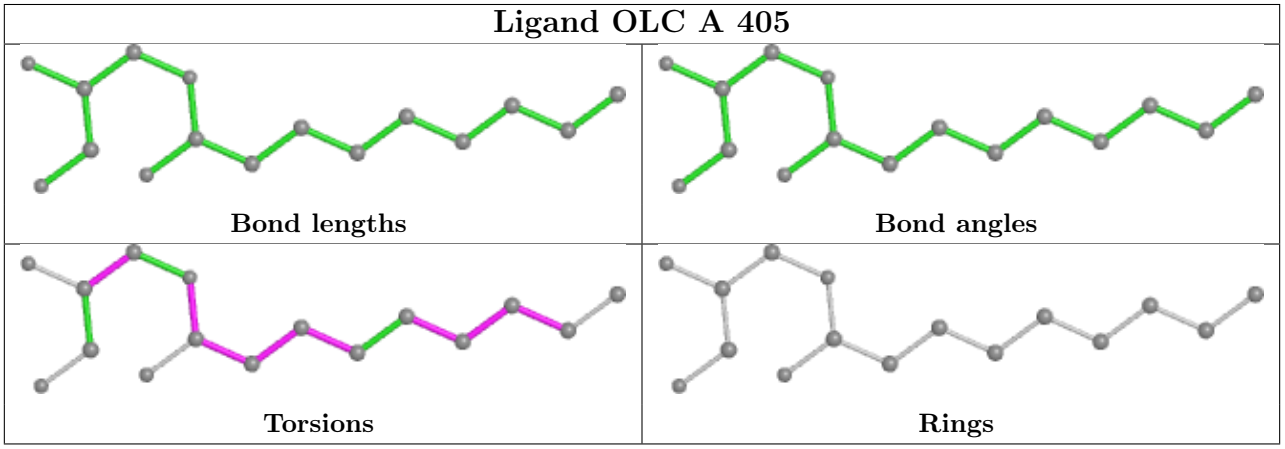


Rings

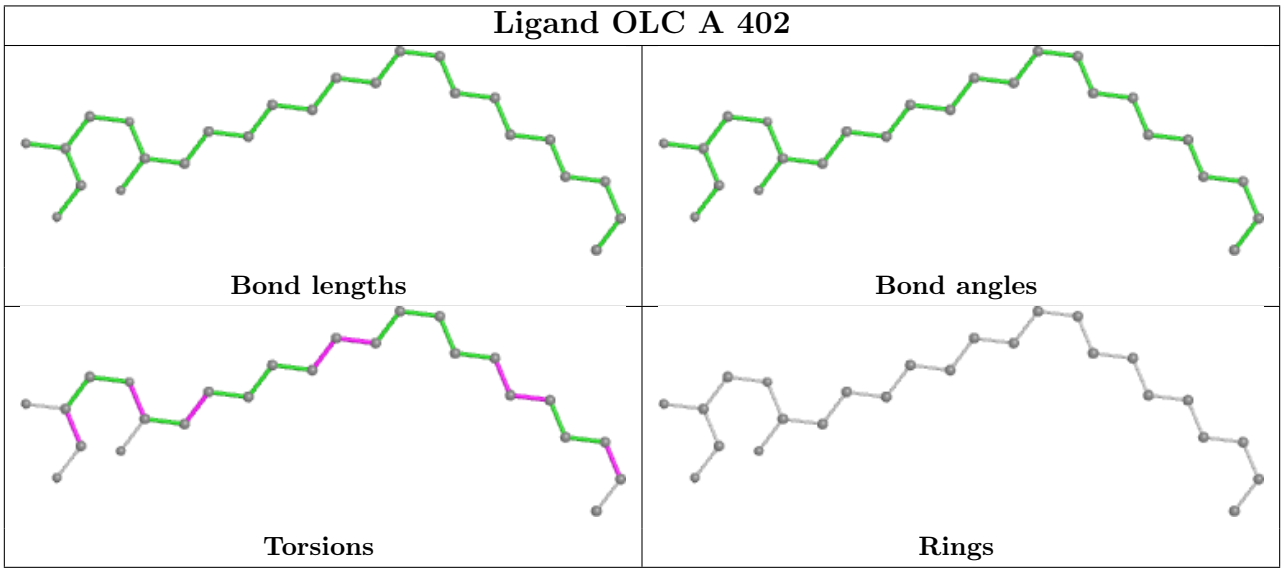
Ligand OLC A 403

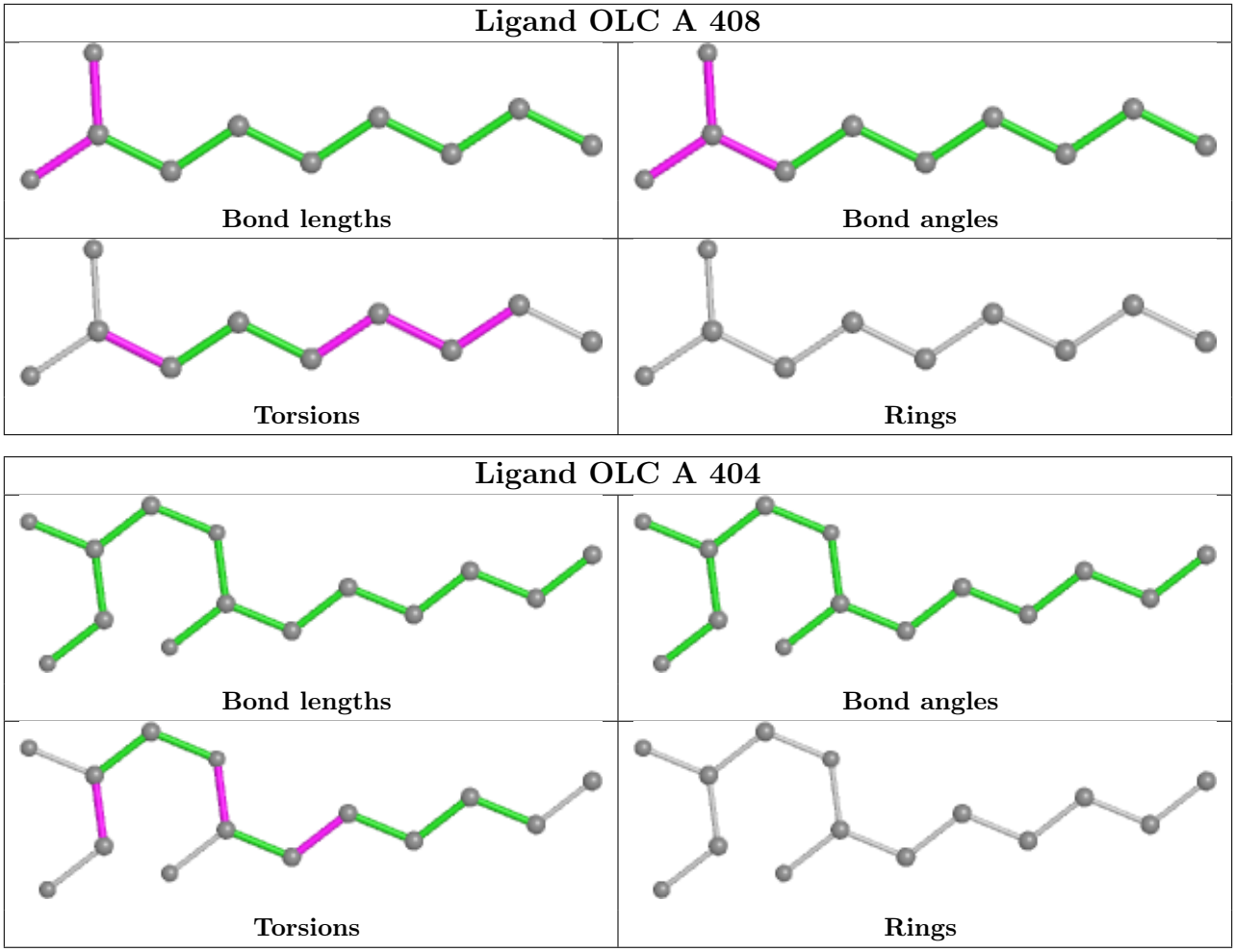


Ligand OLC A 405



Ligand OLC A 402





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, 95^{th} 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	296/356 (83%)	1.49	77 (26%)	0	0	28, 50, 88, 115	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	ALA	7.1
1	A	119	GLY	6.6
1	A	225	ILE	5.6
1	A	339	VAL	5.6
1	A	118	CYS	5.6
1	A	211	TYR	5.5
1	A	184	TYR	5.5
1	A	331	THR	5.0
1	A	332	GLU	5.0
1	A	188	THR	4.6
1	A	228	PHE	4.6
1	A	182	ASN	4.5
1	A	307	ARG	4.1
1	A	120	TRP	3.9
1	A	308	VAL	3.9
1	A	320	ILE	3.7
1	A	67	ILE	3.7
1	A	133	PHE	3.7
1	A	97	ILE	3.7
1	A	104	LEU	3.7
1	A	352	ASP	3.6
1	A	221	LEU	3.6
1	A	327	ASN	3.6
1	A	322	LYS	3.6
1	A	278	VAL	3.5
1	A	344	GLU	3.5
1	A	51	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	192	LEU	3.5
1	A	341	ASP	3.5
1	A	241	THR	3.4
1	A	348	VAL	3.4
1	A	340	GLU	3.4
1	A	323	THR	3.4
1	A	110	GLY	3.3
1	A	283	GLY	3.3
1	A	343	ALA	3.1
1	A	58	LEU	3.0
1	A	350	SER	2.9
1	A	50	MET	2.8
1	A	106	LEU	2.8
1	A	260	VAL	2.7
1	A	183	ASP	2.7
1	A	262	TRP	2.6
1	A	333	ILE	2.6
1	A	233	LYS	2.6
1	A	189	MET	2.6
1	A	206	ALA	2.6
1	A	240	HIS	2.6
1	A	160	TYR	2.5
1	A	139	HIS	2.5
1	A	172	ILE	2.5
1	A	253	GLY	2.5
1	A	78	TRP	2.4
1	A	299	TRP	2.4
1	A	89	LEU	2.4
1	A	335	VAL	2.4
1	A	305	TYR	2.4
1	A	277	GLY	2.4
1	A	311	HIS	2.3
1	A	88	LYS	2.3
1	A	279	LEU	2.3
1	A	222	CYS	2.3
1	A	178	THR	2.3
1	A	94	LEU	2.2
1	A	108	PHE	2.2
1	A	111	TYR	2.2
1	A	269	PHE	2.2
1	A	337	THR	2.2
1	A	138	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLN	2.1
1	A	313	HIS	2.1
1	A	255	ALA	2.1
1	A	229	PHE	2.1
1	A	107	MET	2.1
1	A	250	VAL	2.1
1	A	103	ALA	2.0
1	A	246	ARG	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)

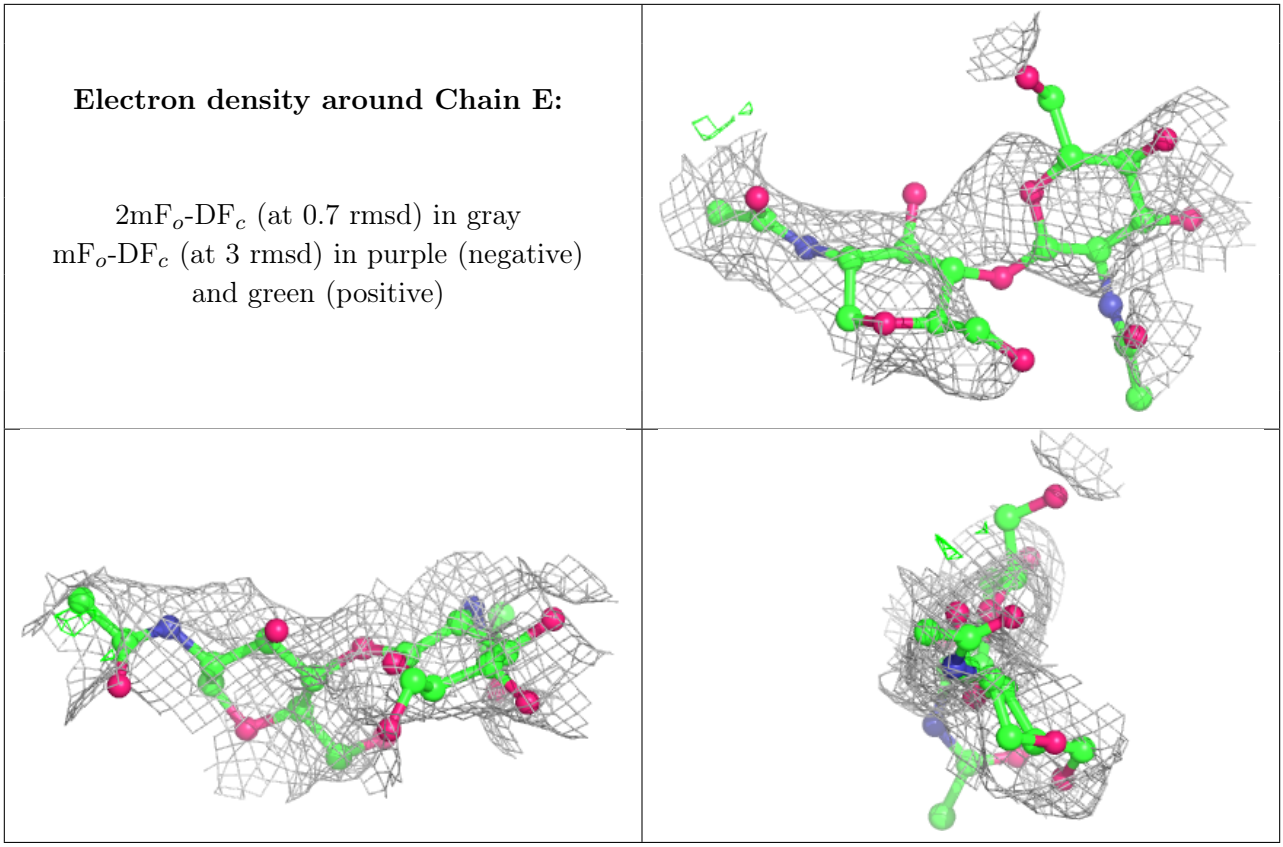
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	E	2	14/15	0.41	0.51	86,101,106,107	0
2	NAG	E	1	14/15	0.69	0.34	64,78,98,100	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.

Electron density around Chain E:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

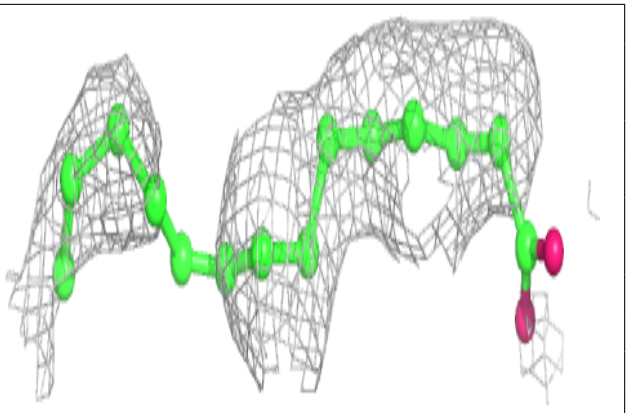
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	403	16/25	0.47	0.36	53,59,88,93	0
4	OLC	A	404	14/25	0.59	0.48	69,86,106,111	0
4	OLC	A	402	25/25	0.60	0.36	53,66,79,84	0
4	OLC	A	407	10/25	0.61	0.28	47,51,66,74	0
4	OLC	A	405	16/25	0.62	0.28	43,48,78,79	0
4	OLC	A	408	10/25	0.73	0.23	35,47,49,50	0
3	RET	A	401	20/21	0.75	0.40	37,45,66,80	0
4	OLC	A	409	9/25	0.80	0.18	46,59,62,63	0
4	OLC	A	410	8/25	0.81	0.16	42,45,47,47	0
4	OLC	A	406	18/25	0.82	0.28	38,54,65,76	0

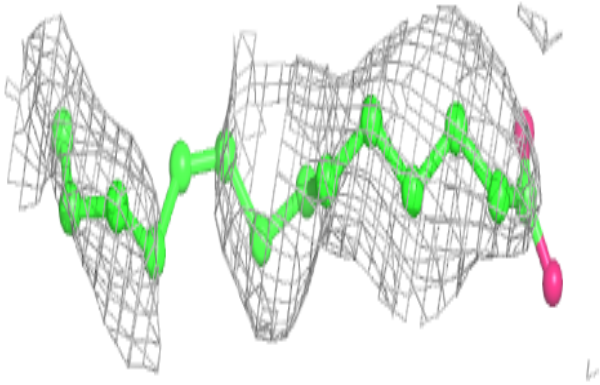
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

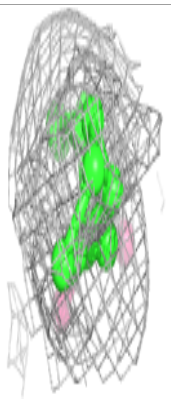
orientation to approximate a three-dimensional view.

Electron density around OLC A 403:

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

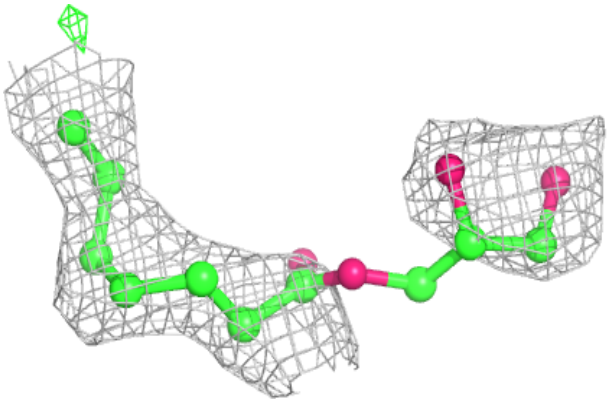


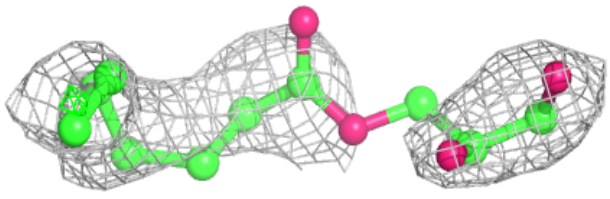


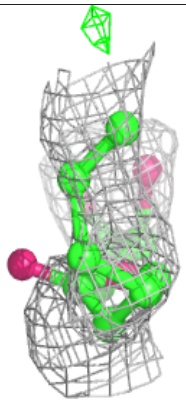


Electron density around OLC A 404:

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

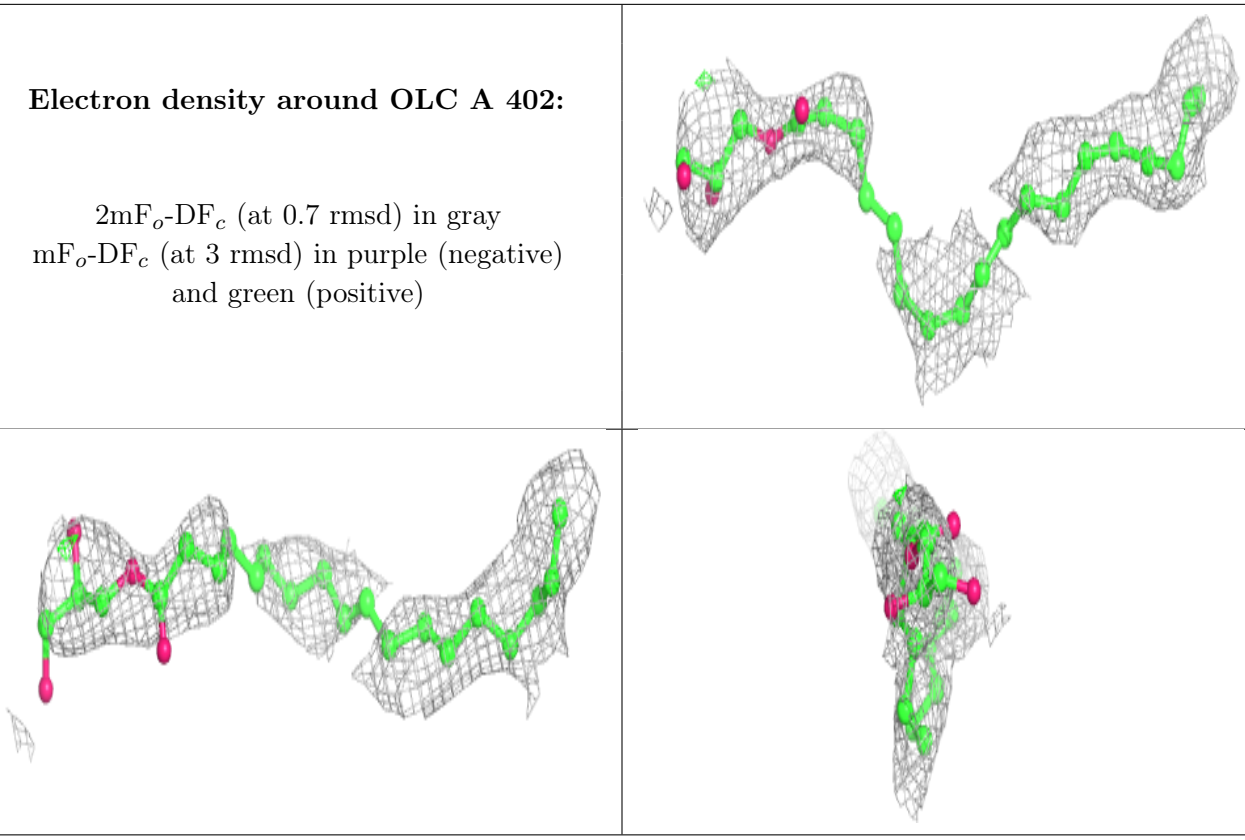






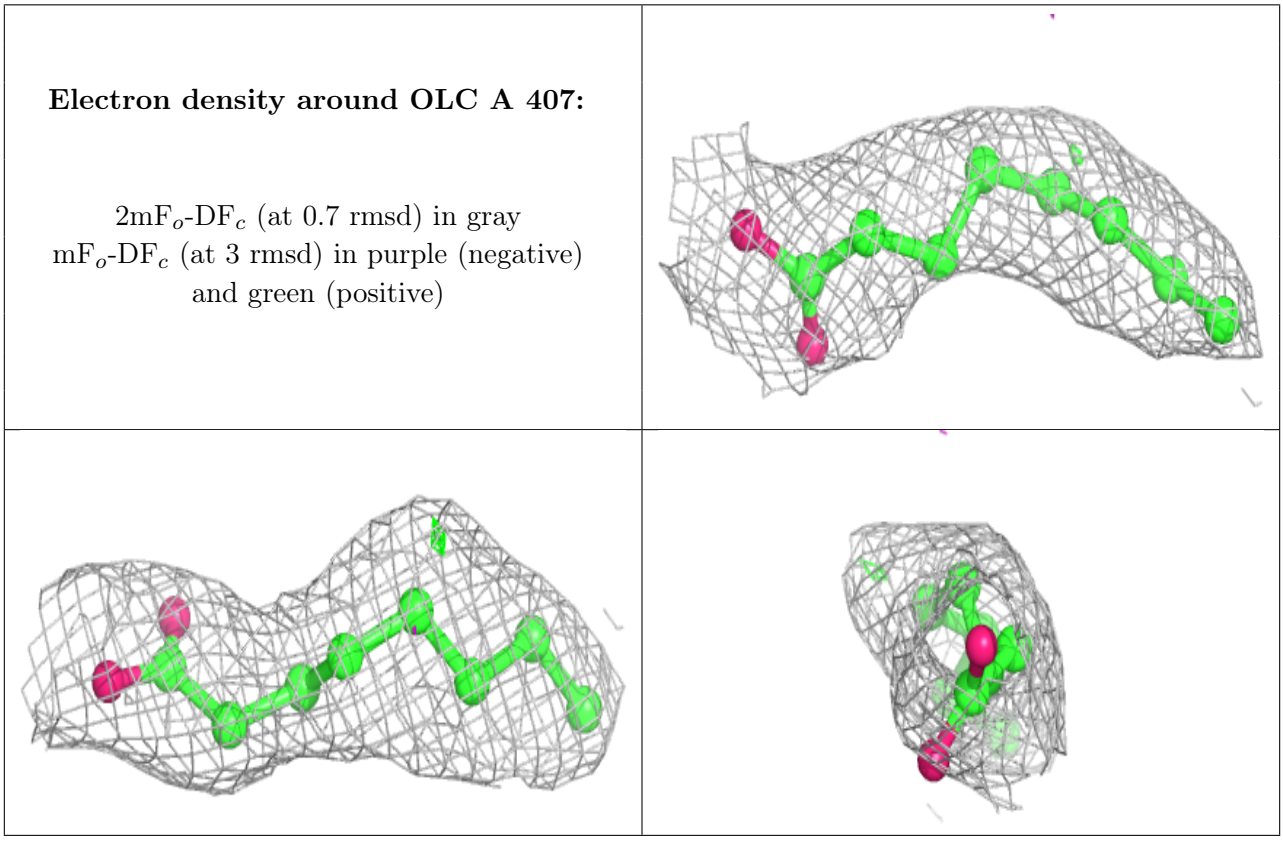
Electron density around OLC A 402:

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



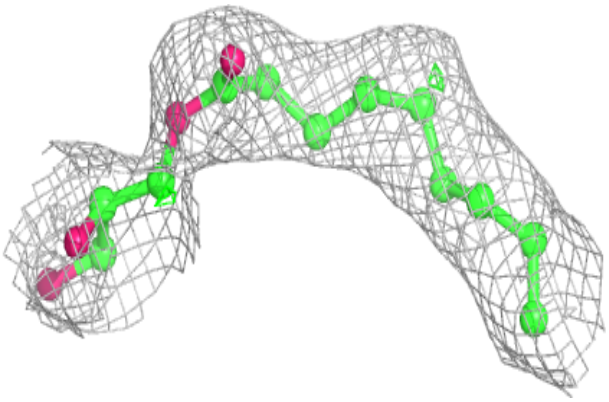
Electron density around OLC A 407:

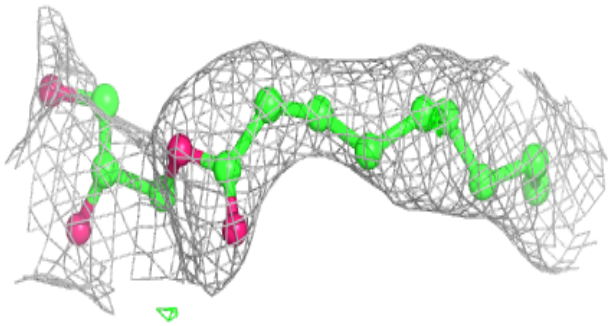
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

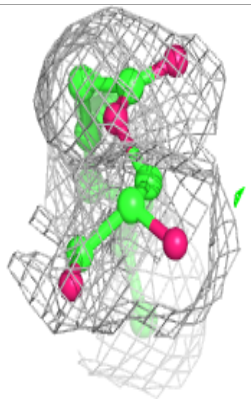


Electron density around OLC A 405:

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

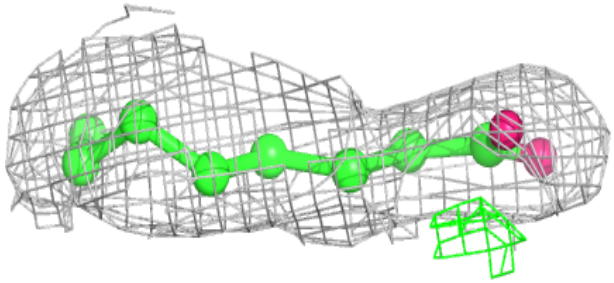


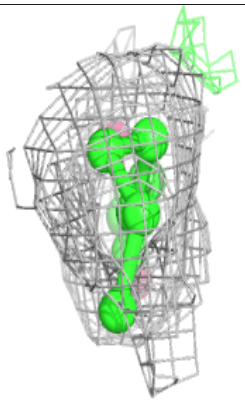




Electron density around OLC A 408:

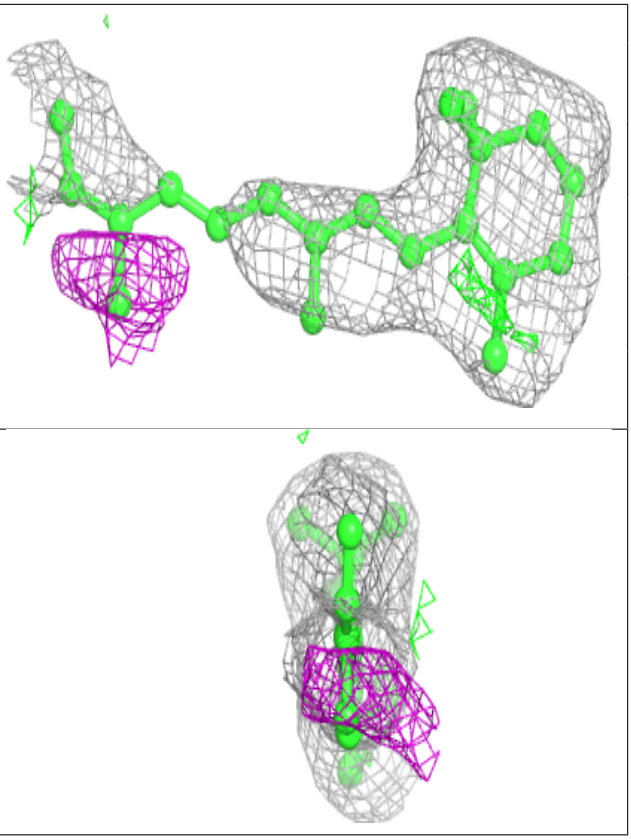
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





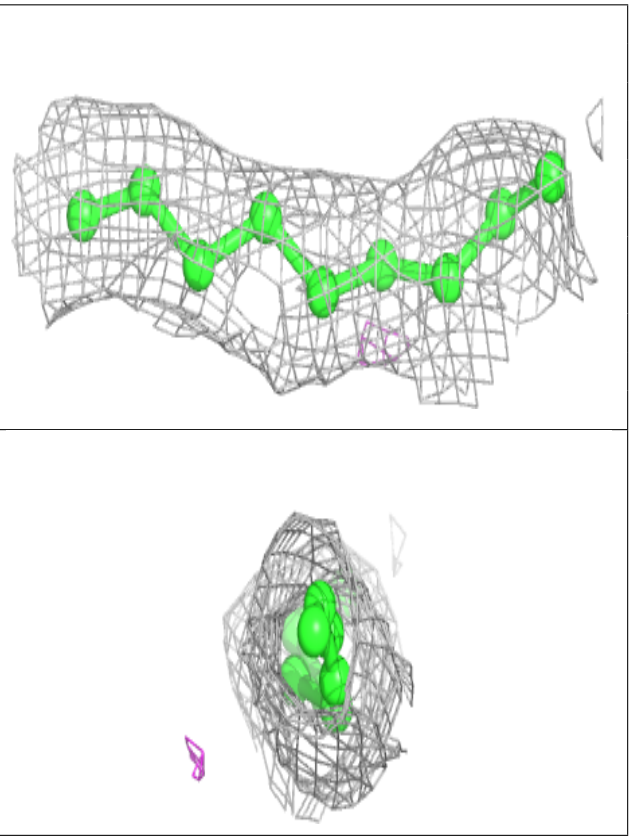
Electron density around RET A 401:

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



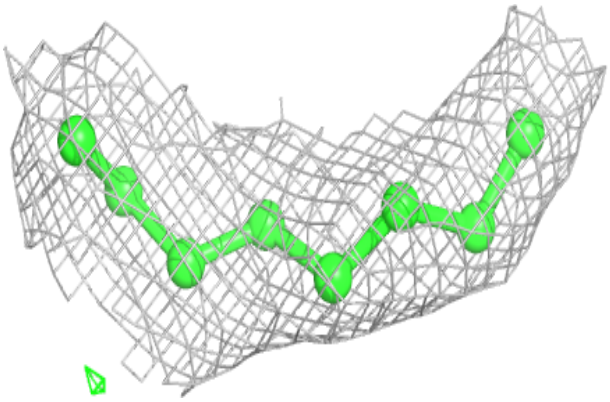
Electron density around OLC A 409:

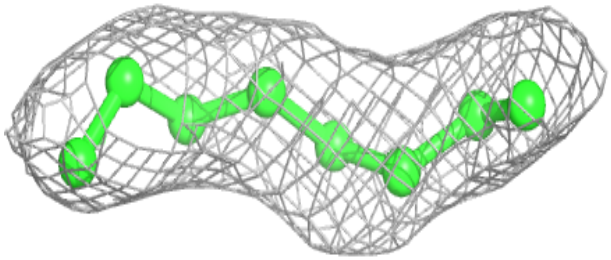
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

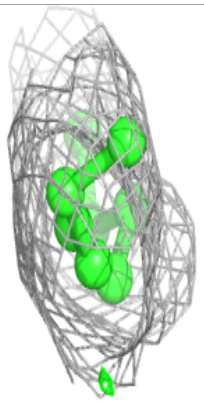


Electron density around OLC A 410:

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

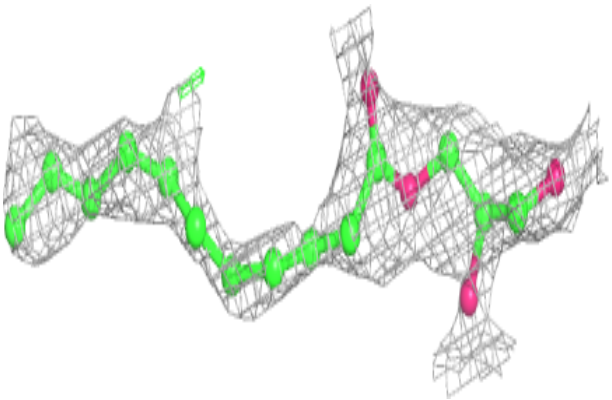


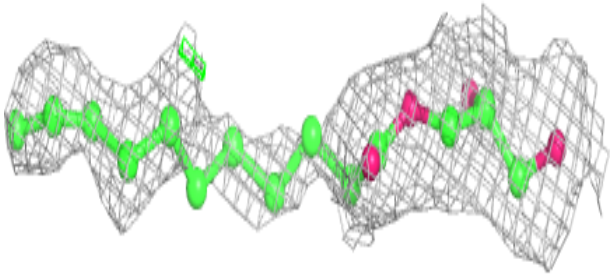


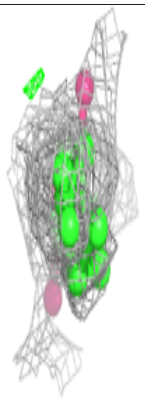


Electron density around OLC A 406:

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







6.5 Other polymers (i)

There are no such residues in this entry.