



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 7E71 / pdb_00007e71
Title : Time-resolved serial femtosecond crystallography reveals early structural changes in channelrhodopsin: 1 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

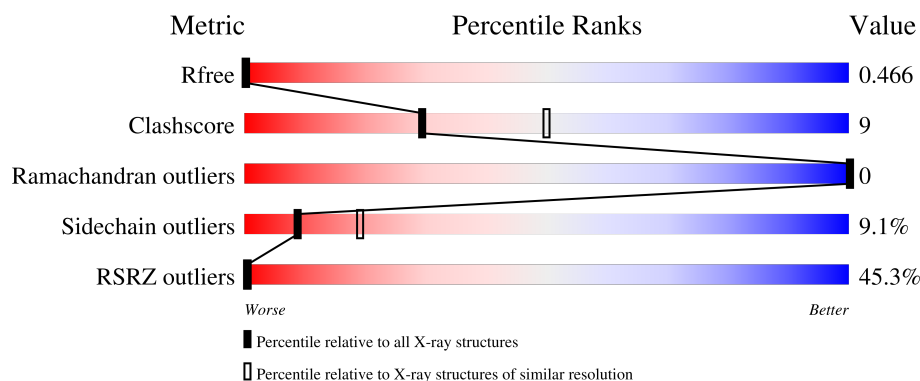
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

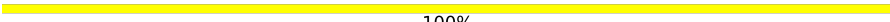
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	356	38% 66% 16% • 17%

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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

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Mol	Chain	Length	Quality of chain
2	E	2	 100%

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:

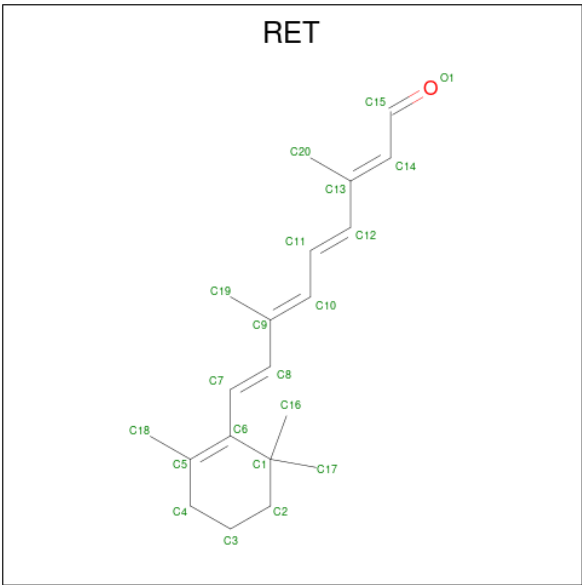
Chain	Residue	Modelled	Actual	Comment	Reference
A	349	SER	-	expression tag	UNP Q8RUT8
A	350	SER	-	expression tag	UNP Q8RUT8
A	351	GLU	-	expression tag	UNP Q8RUT8
A	352	ASP	-	expression tag	UNP Q8RUT8
A	353	LEU	-	expression tag	UNP Q8RUT8
A	354	TYR	-	expression tag	UNP Q8RUT8
A	355	PHE	-	expression tag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



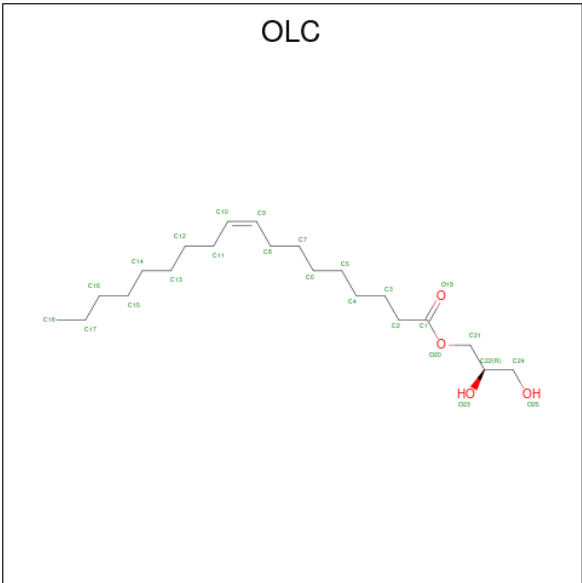
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O).



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

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			16	14	2		

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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

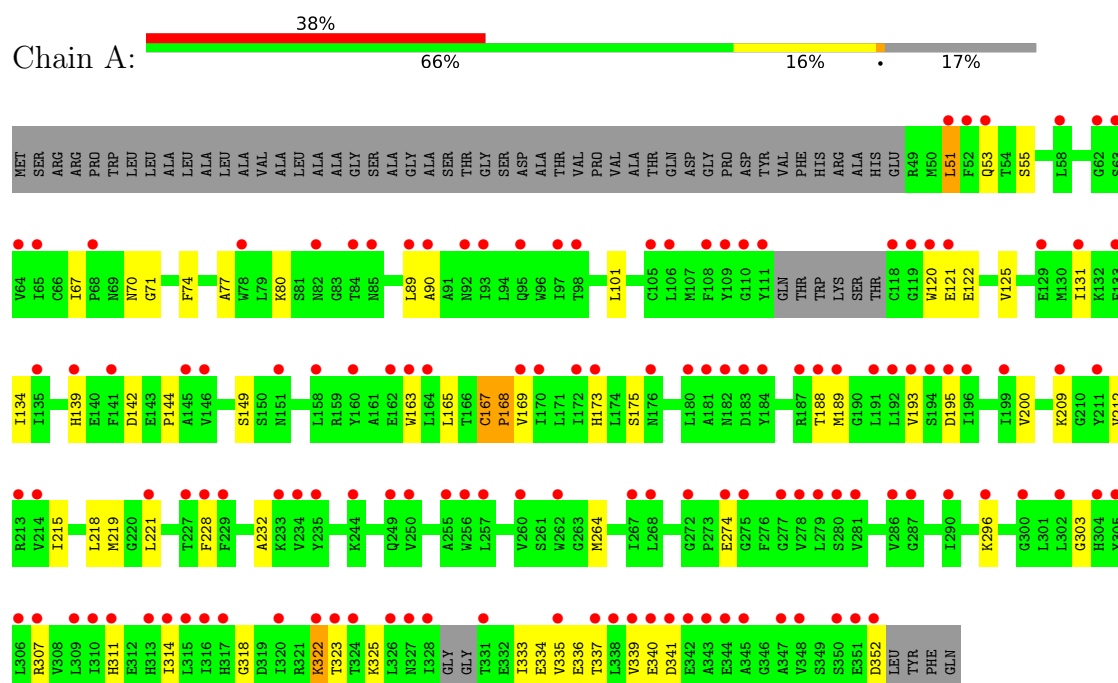
- Molecule 5 is water.

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

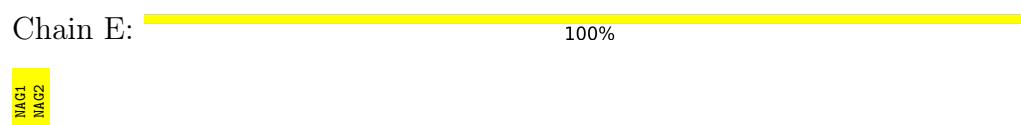
3 Residue-property plots [i](#)

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



- 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	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)	75.4 (14.96-2.50) 75.4 (14.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.411 , 0.463 0.414 , 0.466	Depositor DCC
R_{free} test set	554 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 103.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	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)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.14	0/2377	1.59	2/3237 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	318	GLY	CA-C-O	-5.24	118.38	122.52
1	A	200	VAL	CA-C-O	-5.10	115.39	121.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2317	0	2261	41	0
2	E	28	0	25	0	0
3	A	20	0	27	3	0
4	A	126	0	172	13	0
5	A	38	0	0	14	0
All	All	2529	0	2485	43	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 9.

All (43) 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:142:ASP:OD1	5:A:501:HOH:O	1.98	0.81
1:A:169:VAL:HG23	5:A:502:HOH:O	1.93	0.67
1:A:165:LEU:O	5:A:502:HOH:O	2.12	0.66
1:A:219:MET:CE	4:A:403:OLC:H7	2.27	0.65
1:A:303:GLY:HA2	5:A:514:HOH:O	2.00	0.61
1:A:303:GLY:CA	5:A:514:HOH:O	2.49	0.61
1:A:163:TRP:CD1	3:A:401:RET:H12	2.39	0.57
1:A:168:PRO:HB2	5:A:502:HOH:O	2.07	0.55
1:A:314:ILE:HD13	5:A:526:HOH:O	2.07	0.54
1:A:219:MET:HE3	4:A:403:OLC:H7	1.89	0.53
1:A:167:CYS:SG	1:A:195:ASP:OD2	2.63	0.53
1:A:322:LYS:HB2	1:A:337:THR:HB	1.91	0.52
3:A:401:RET:H8	3:A:401:RET:H161	1.92	0.50
1:A:67:ILE:HD12	5:A:506:HOH:O	2.11	0.50
1:A:53:GLN:HE21	1:A:55:SER:H	1.61	0.49
1:A:228:PHE:C	4:A:408:OLC:H6A	2.38	0.49
1:A:221:LEU:HD11	4:A:402:OLC:H12	1.95	0.48
1:A:264:MET:HE2	1:A:264:MET:HA	1.95	0.47
1:A:131:ILE:O	1:A:134:ILE:HG13	2.14	0.47
1:A:228:PHE:HB3	4:A:408:OLC:C7	2.45	0.47
1:A:121:GLU:HG3	1:A:173:HIS:CG	2.50	0.46
1:A:175:SER:OG	1:A:188:THR:HG23	2.16	0.46
1:A:51:LEU:HD13	1:A:51:LEU:HA	1.78	0.45
1:A:71:GLY:N	5:A:512:HOH:O	2.41	0.45
1:A:212:VAL:HG11	4:A:406:OLC:H3	1.99	0.45
1:A:74:PHE:CE1	5:A:510:HOH:O	2.68	0.45
1:A:215:ILE:HG21	4:A:403:OLC:C1	2.48	0.44
1:A:219:MET:SD	4:A:403:OLC:H7	2.58	0.44
1:A:228:PHE:HB3	4:A:408:OLC:C6	2.48	0.44
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.90	0.43
1:A:70:ASN:N	5:A:512:HOH:O	2.49	0.43
1:A:77:ALA:O	5:A:503:HOH:O	2.21	0.43
1:A:80:LYS:HA	5:A:537:HOH:O	2.18	0.42
1:A:90:ALA:HB2	4:A:404:OLC:O19	2.19	0.42
1:A:228:PHE:HB3	4:A:408:OLC:H7A	2.02	0.41
1:A:232:ALA:HB2	4:A:408:OLC:H5A	2.02	0.41
1:A:101:LEU:HD12	1:A:101:LEU:HA	1.91	0.41
1:A:120:TRP:CZ3	1:A:169:VAL:HG13	2.56	0.41
1:A:149:SER:OG	5:A:504:HOH:O	2.21	0.41
1:A:189:MET:O	1:A:193:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:HIS:HB3	1:A:142:ASP:HB2	2.04	0.40
3:A:401:RET:H181	3:A:401:RET:H7	1.72	0.40
1:A:89:LEU:HD23	4:A:404:OLC:H21	2.04	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%)	275 (95%)	15 (5%)	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%)	220 (91%)	22 (9%)	9	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	122	GLU
1	A	125	VAL

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Mol	Chain	Res	Type
1	A	144	PRO
1	A	167	CYS
1	A	168	PRO
1	A	209	LYS
1	A	274	GLU
1	A	296	LYS
1	A	307	ARG
1	A	311	HIS
1	A	322	LYS
1	A	323	THR
1	A	325	LYS
1	A	333	ILE
1	A	334	GLU
1	A	335	VAL
1	A	336	GLU
1	A	339	VAL
1	A	340	GLU
1	A	341	ASP
1	A	352	ASP

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

Mol	Chain	Res	Type
1	A	53	GLN
1	A	70	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	0.58	0	17,19,21	1.20	2 (11%)
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	1.75	3 (17%)

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	1,2	-	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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	4.33	117.99	112.19
2	E	2	NAG	O5-C1-C2	-3.68	105.60	111.29
2	E	2	NAG	C2-N2-C7	3.11	127.07	122.90
2	E	1	NAG	C1-O5-C5	-2.64	108.65	112.19
2	E	1	NAG	C3-C4-C5	2.42	114.62	110.23

There are no chirality outliers.

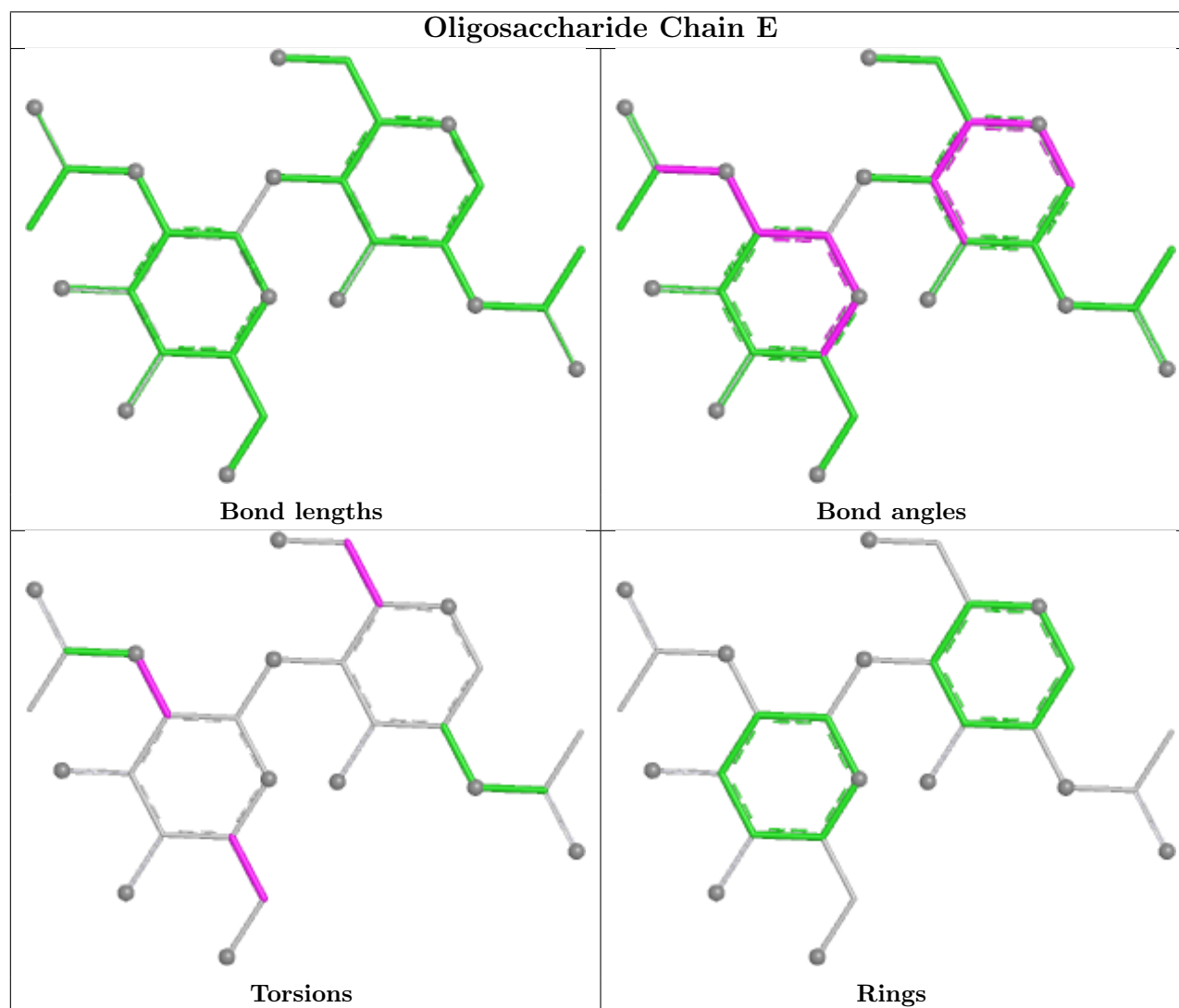
All (5) torsion outliers are listed below:

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.



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	410	-	7,7,24	0.36	0	6,6,25	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	A	402	-	24,24,24	0.42	0	25,25,25	0.40	0
3	RET	A	401	1	20,20,21	3.10	4 (20%)	27,27,28	2.28	8 (29%)
4	OLC	A	403	-	15,15,24	0.47	0	15,15,25	0.45	0
4	OLC	A	405	-	15,15,24	0.41	0	16,16,25	0.59	0
4	OLC	A	407	-	9,9,24	0.59	0	9,9,25	0.47	0
4	OLC	A	406	-	17,17,24	0.26	0	18,18,25	0.33	0
4	OLC	A	409	-	8,8,24	0.46	0	7,7,25	0.15	0
4	OLC	A	404	-	13,13,24	0.40	0	14,14,25	0.49	0
4	OLC	A	408	-	9,9,24	0.53	0	9,9,25	0.36	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	410	-	-	4/5/5/24	-
4	OLC	A	402	-	-	12/24/24/24	-
3	RET	A	401	1	-	0/13/30/31	0/1/1/1
4	OLC	A	403	-	-	6/13/13/24	-
4	OLC	A	405	-	-	8/15/15/24	-
4	OLC	A	407	-	-	1/7/7/24	-
4	OLC	A	406	-	-	14/17/17/24	-
4	OLC	A	409	-	-	5/6/6/24	-
4	OLC	A	404	-	-	6/13/13/24	-
4	OLC	A	408	-	-	2/7/7/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	RET	C14-C13	12.07	1.42	1.33
3	A	401	RET	C10-C9	3.65	1.44	1.35
3	A	401	RET	C15-C14	-3.32	1.37	1.49
3	A	401	RET	C11-C12	2.04	1.40	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	RET	C8-C9-C10	5.29	127.33	119.01
3	A	401	RET	C2-C1-C6	4.03	116.29	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	RET	C12-C13-C14	3.96	129.09	118.55
3	A	401	RET	C20-C13-C14	-3.61	113.65	123.63
3	A	401	RET	C19-C9-C10	-3.50	117.15	122.82
3	A	401	RET	C10-C11-C12	3.44	133.17	123.20
3	A	401	RET	C1-C6-C7	3.32	124.65	115.65
3	A	401	RET	C1-C6-C5	-3.28	118.16	122.64

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	404	OLC	C2-C1-O20-C21
4	A	405	OLC	C2-C1-O20-C21
4	A	405	OLC	O19-C1-O20-C21
4	A	403	OLC	C1-C2-C3-C4
4	A	402	OLC	C1-C2-C3-C4
4	A	407	OLC	C1-C2-C3-C4
4	A	404	OLC	O19-C1-O20-C21
4	A	406	OLC	C2-C1-O20-C21
4	A	402	OLC	C21-C22-C24-O25
4	A	404	OLC	C21-C22-C24-O25
4	A	402	OLC	C12-C13-C14-C15
4	A	406	OLC	O23-C22-C24-O25
4	A	406	OLC	O19-C1-O20-C21
4	A	403	OLC	C4-C5-C6-C7
4	A	408	OLC	C1-C2-C3-C4
4	A	402	OLC	C6-C7-C8-C9
4	A	403	OLC	C10-C11-C12-C13
4	A	406	OLC	C6-C7-C8-C9
4	A	403	OLC	C3-C4-C5-C6
4	A	410	OLC	C3-C4-C5-C6
4	A	409	OLC	C4-C5-C6-C7
4	A	406	OLC	C3-C4-C5-C6
4	A	410	OLC	C4-C5-C6-C7
4	A	402	OLC	C2-C1-O20-C21
4	A	402	OLC	O23-C22-C24-O25
4	A	408	OLC	C5-C6-C7-C8
4	A	402	OLC	O19-C1-O20-C21
4	A	404	OLC	O23-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	410	OLC	C6-C7-C8-C9
4	A	409	OLC	C3-C4-C5-C6
4	A	405	OLC	C1-C2-C3-C4
4	A	405	OLC	C5-C6-C7-C8
4	A	402	OLC	C5-C6-C7-C8
4	A	406	OLC	C4-C5-C6-C7
4	A	409	OLC	C5-C6-C7-C8
4	A	409	OLC	C2-C3-C4-C5
4	A	405	OLC	C6-C7-C8-C9
4	A	410	OLC	C5-C6-C7-C8
4	A	403	OLC	C2-C3-C4-C5
4	A	402	OLC	C13-C14-C15-C16
4	A	402	OLC	C15-C16-C17-C18
4	A	409	OLC	C7-C8-C9-C10
4	A	405	OLC	C4-C5-C6-C7
4	A	405	OLC	O20-C21-C22-O23
4	A	405	OLC	C2-C3-C4-C5
4	A	406	OLC	C5-C6-C7-C8
4	A	406	OLC	C7-C8-C9-C10
4	A	403	OLC	C6-C7-C8-C9
4	A	402	OLC	C10-C11-C12-C13
4	A	406	OLC	C2-C3-C4-C5
4	A	402	OLC	C14-C15-C16-C17
4	A	406	OLC	O20-C1-C2-C3
4	A	404	OLC	O20-C1-C2-C3
4	A	406	OLC	O19-C1-C2-C3
4	A	404	OLC	O19-C1-C2-C3

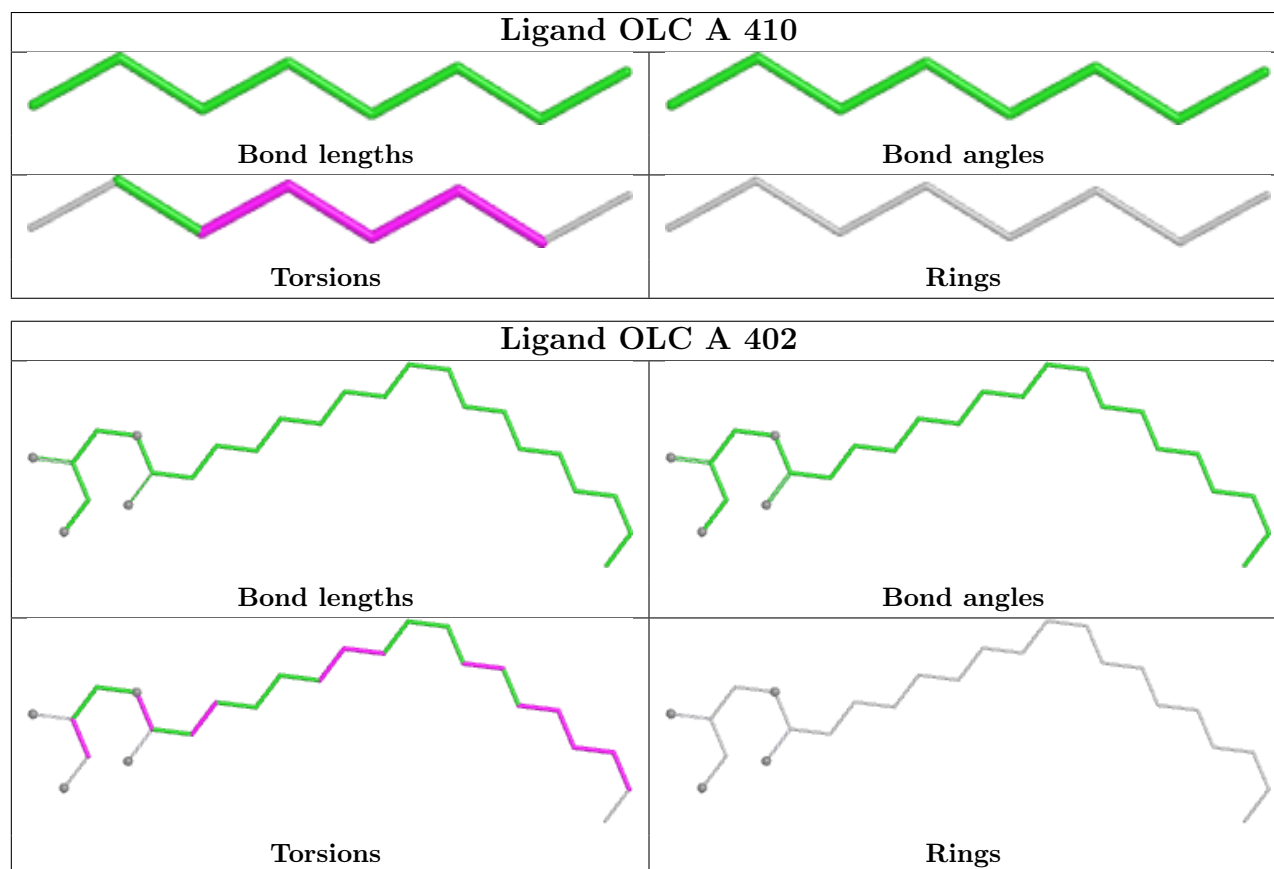
There are no ring outliers.

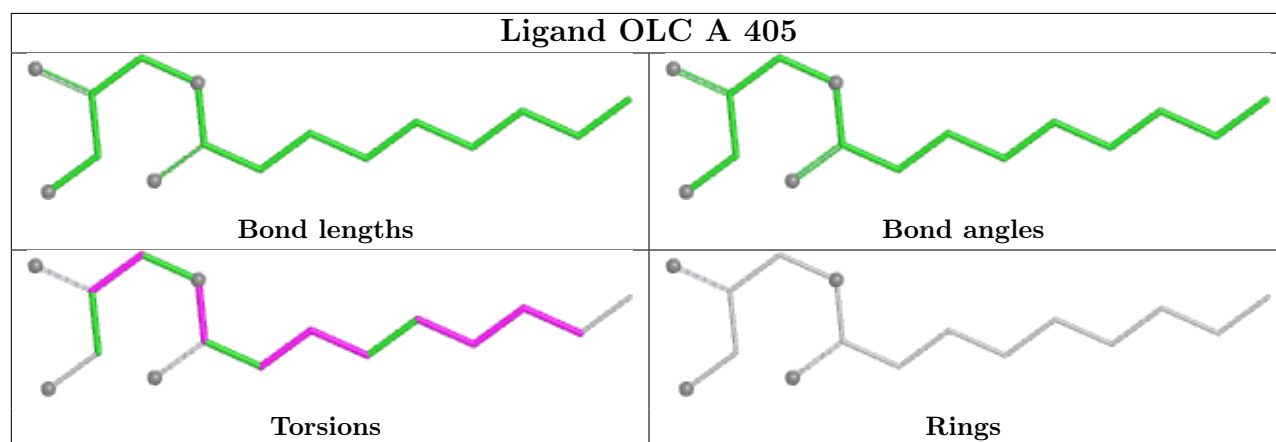
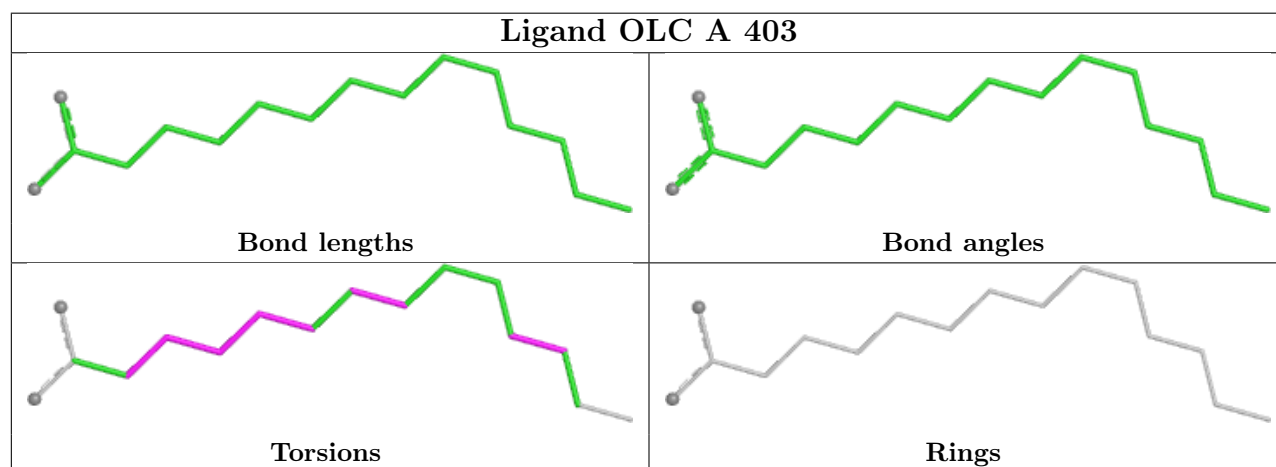
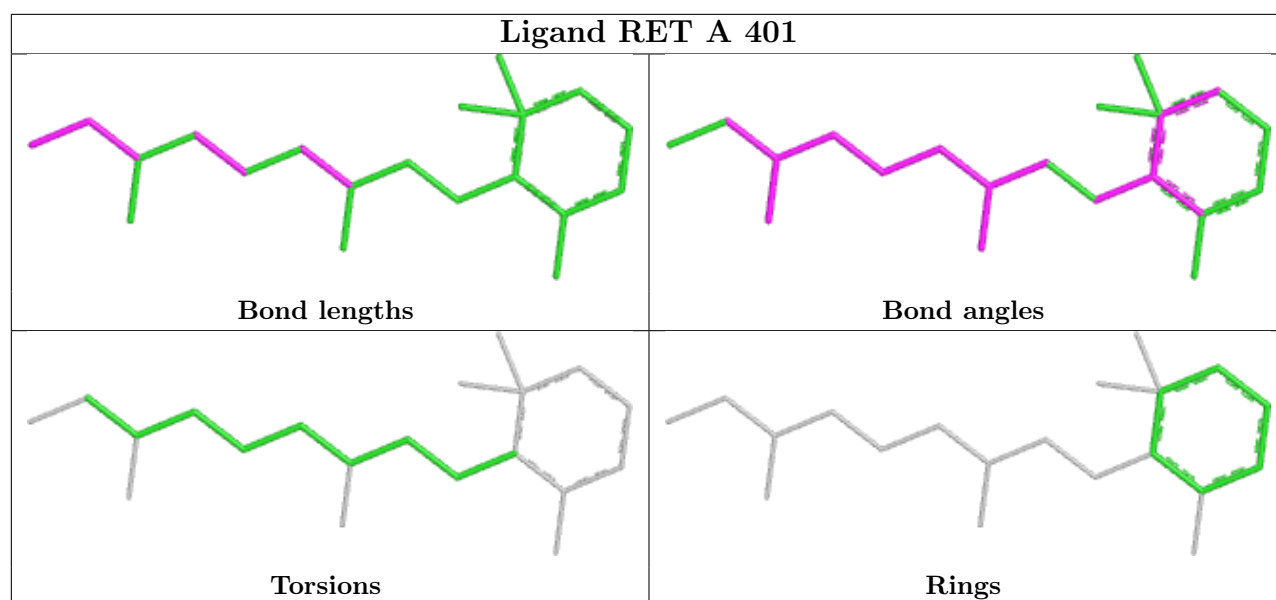
6 monomers are involved in 16 short contacts:

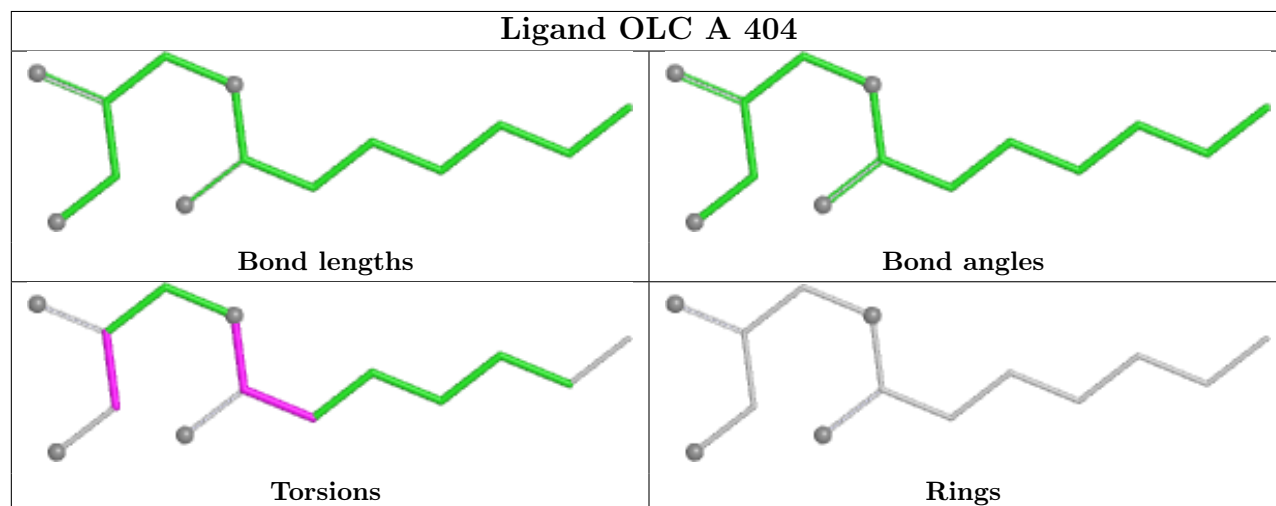
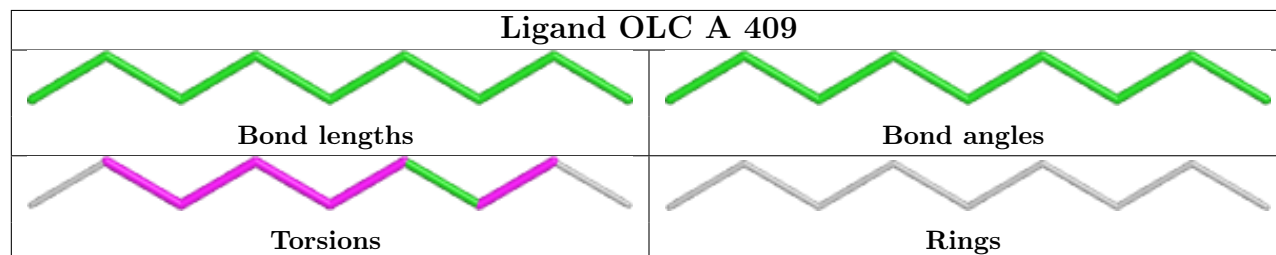
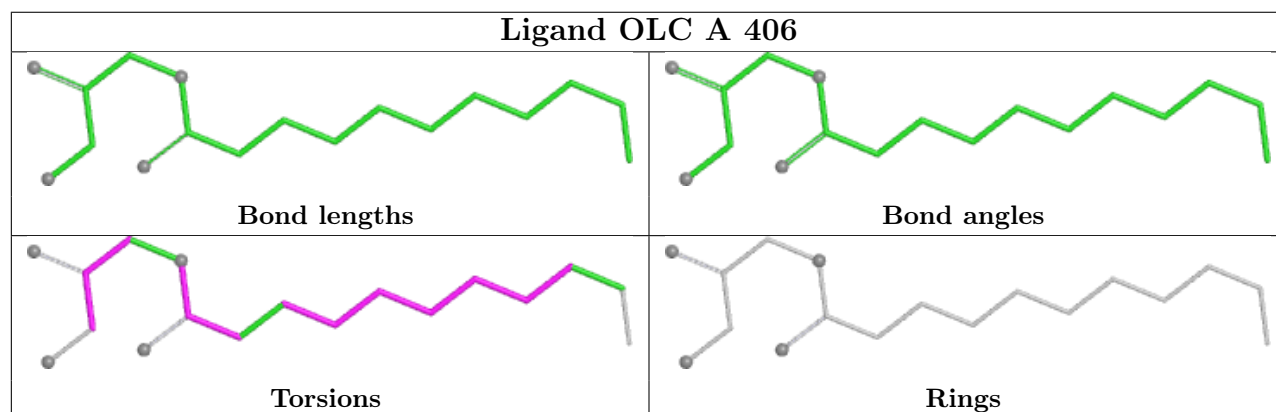
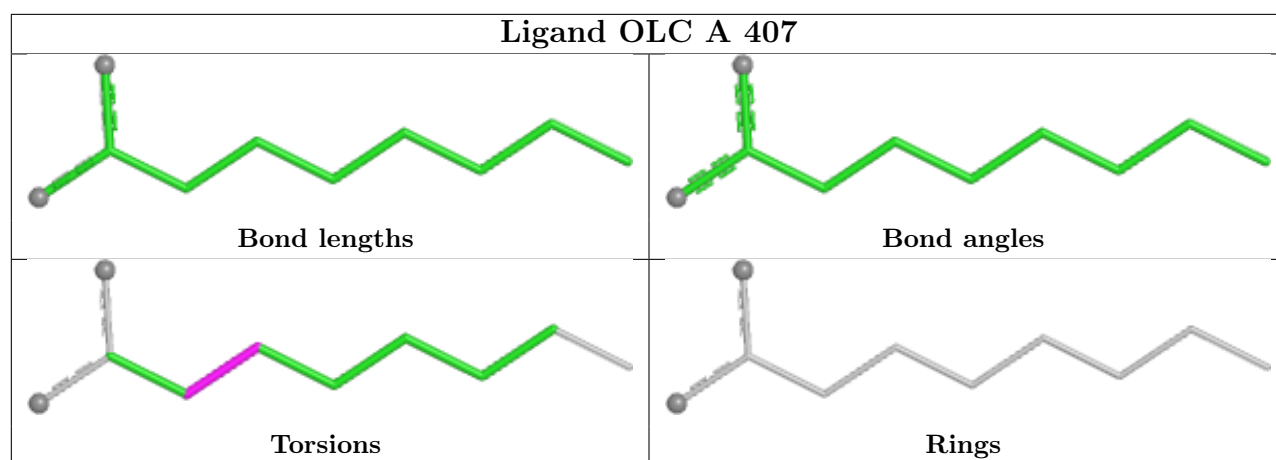
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	OLC	1	0
3	A	401	RET	3	0
4	A	403	OLC	4	0
4	A	406	OLC	1	0
4	A	404	OLC	2	0
4	A	408	OLC	5	0

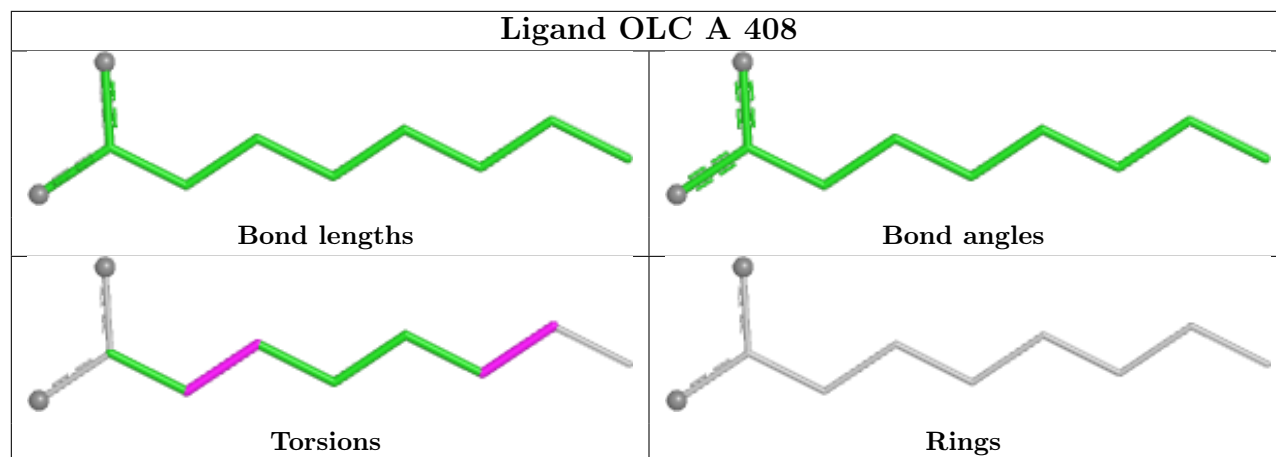
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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	296/356 (83%)	2.10	134 (45%) 0 0	39, 70, 113, 163	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	CYS	9.1
1	A	320	ILE	7.6
1	A	120	TRP	6.5
1	A	307	ARG	5.6
1	A	310	ILE	5.6
1	A	352	ASP	5.1
1	A	277	GLY	5.0
1	A	221	LEU	4.9
1	A	327	ASN	4.7
1	A	129	GLU	4.5
1	A	341	ASP	4.5
1	A	339	VAL	4.4
1	A	139	HIS	4.4
1	A	195	ASP	4.4
1	A	106	LEU	4.4
1	A	90	ALA	4.3
1	A	173	HIS	4.3
1	A	92	ASN	4.3
1	A	228	PHE	4.3
1	A	89	LEU	4.3
1	A	348	VAL	4.2
1	A	255	ALA	4.2
1	A	64	VAL	4.2
1	A	181	ALA	4.2
1	A	119	GLY	4.1
1	A	262	TRP	3.8
1	A	184	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	331	THR	3.7
1	A	199	ILE	3.7
1	A	93	ILE	3.7
1	A	342	GLU	3.6
1	A	188	THR	3.5
1	A	95	GLN	3.5
1	A	133	PHE	3.5
1	A	350	SER	3.5
1	A	158	LEU	3.5
1	A	191	LEU	3.4
1	A	211	TYR	3.4
1	A	82	ASN	3.4
1	A	151	ASN	3.4
1	A	257	LEU	3.4
1	A	326	LEU	3.4
1	A	172	ILE	3.3
1	A	121	GLU	3.3
1	A	313	HIS	3.3
1	A	328	ILE	3.3
1	A	322	LYS	3.3
1	A	78	TRP	3.2
1	A	192	LEU	3.2
1	A	296	LYS	3.2
1	A	300	GLY	3.2
1	A	316	ILE	3.2
1	A	108	PHE	3.1
1	A	275	GLY	3.1
1	A	233	LYS	3.1
1	A	131	ILE	3.1
1	A	189	MET	3.1
1	A	187	ARG	3.1
1	A	344	GLU	3.0
1	A	279	LEU	3.0
1	A	338	LEU	3.0
1	A	141	PHE	3.0
1	A	260	VAL	2.9
1	A	335	VAL	2.9
1	A	250	VAL	2.9
1	A	274	GLU	2.9
1	A	311	HIS	2.8
1	A	58	LEU	2.8
1	A	309	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	2.8
1	A	324	THR	2.8
1	A	193	VAL	2.7
1	A	145	ALA	2.7
1	A	351	GLU	2.7
1	A	317	HIS	2.7
1	A	214	VAL	2.7
1	A	52	PHE	2.7
1	A	249	GLN	2.7
1	A	183	ASP	2.7
1	A	110	GLY	2.7
1	A	244	LYS	2.6
1	A	105	CYS	2.6
1	A	229	PHE	2.6
1	A	85	ASN	2.6
1	A	278	VAL	2.6
1	A	170	ILE	2.5
1	A	340	GLU	2.5
1	A	51	LEU	2.5
1	A	286	VAL	2.5
1	A	194	SER	2.5
1	A	111	TYR	2.5
1	A	163	TRP	2.5
1	A	146	VAL	2.5
1	A	182	ASN	2.5
1	A	256	TRP	2.4
1	A	162	GLU	2.4
1	A	267	ILE	2.4
1	A	164	LEU	2.4
1	A	323	THR	2.4
1	A	97	ILE	2.4
1	A	287	GLY	2.4
1	A	84	THR	2.3
1	A	304	HIS	2.3
1	A	272	GLY	2.3
1	A	268	LEU	2.3
1	A	314	ILE	2.3
1	A	234	VAL	2.3
1	A	280	SER	2.2
1	A	305	TYR	2.2
1	A	302	LEU	2.2
1	A	176	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	209	LYS	2.2
1	A	65	ILE	2.2
1	A	63	SER	2.2
1	A	345	ALA	2.2
1	A	315	LEU	2.2
1	A	281	VAL	2.1
1	A	98	THR	2.1
1	A	109	TYR	2.1
1	A	290	ILE	2.1
1	A	213	ARG	2.1
1	A	53	GLN	2.1
1	A	62	GLY	2.1
1	A	235	TYR	2.1
1	A	68	PRO	2.1
1	A	169	VAL	2.1
1	A	180	LEU	2.1
1	A	347	ALA	2.1
1	A	227	THR	2.1
1	A	337	THR	2.1
1	A	196	ILE	2.1
1	A	343	ALA	2.0
1	A	135	ILE	2.0
1	A	160	TYR	2.0

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

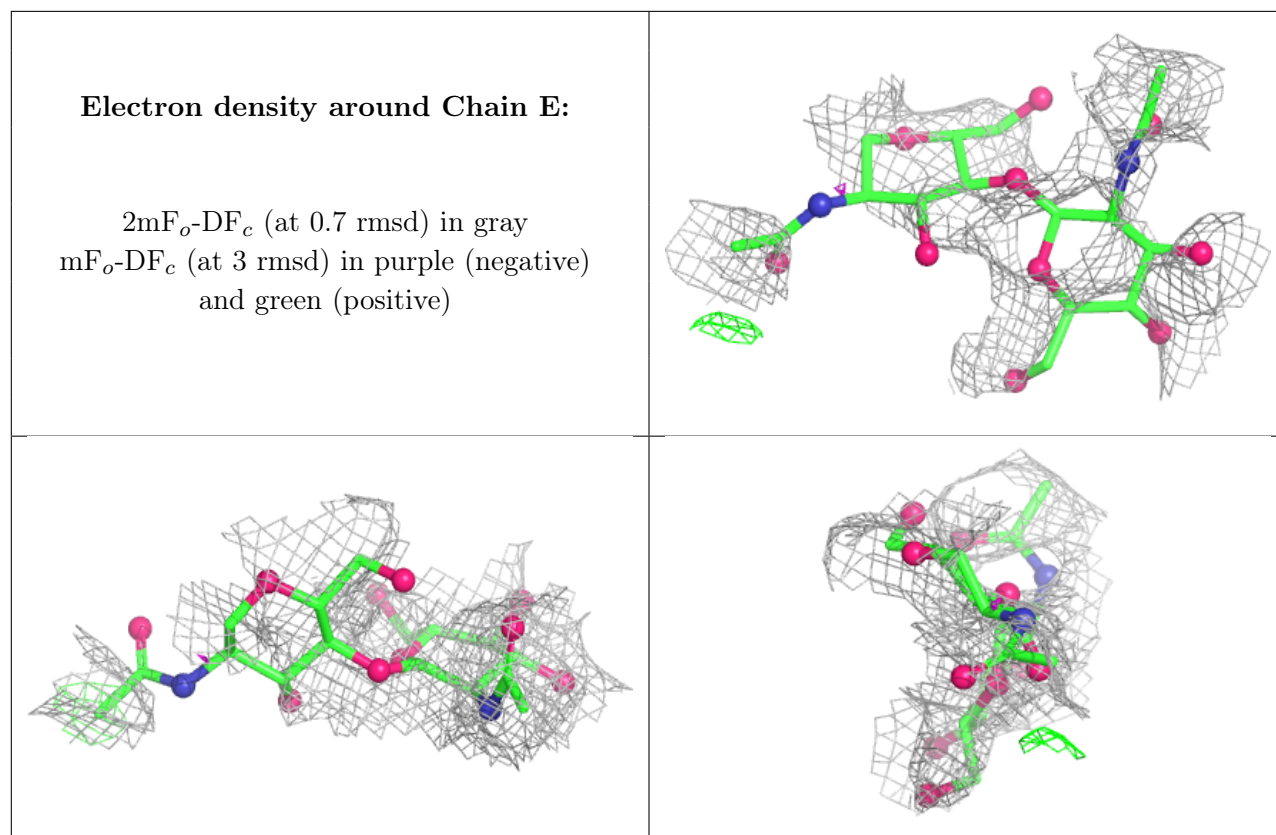
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
2	NAG	E	1	14/15	-	-	134,157,168,189	0
2	NAG	E	2	14/15	-	-	82,109,118,127	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](#)

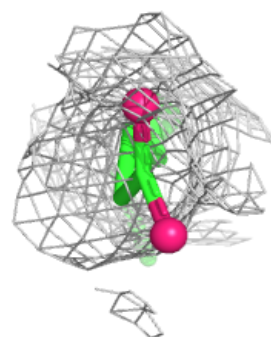
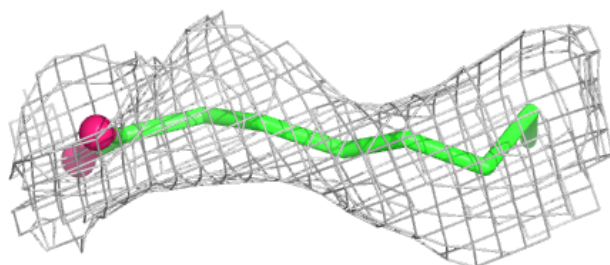
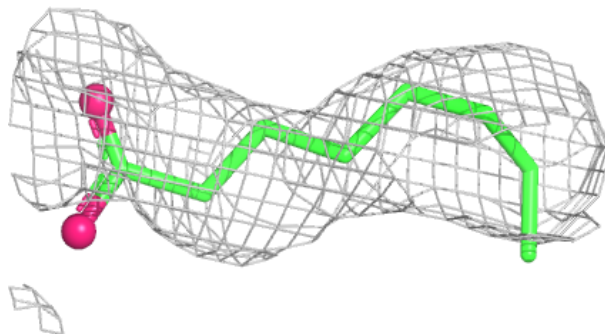
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLC	A	408	10/25	0.59	0.17	73,77,102,105	0
4	OLC	A	405	16/25	0.62	0.17	46,64,89,93	0
4	OLC	A	409	9/25	0.65	0.17	76,93,107,109	0
4	OLC	A	402	25/25	0.66	0.15	48,60,89,94	0
4	OLC	A	403	16/25	0.69	0.19	71,99,145,153	0
4	OLC	A	406	18/25	0.73	0.12	48,58,67,77	0
4	OLC	A	404	14/25	0.74	0.14	51,66,91,115	0
4	OLC	A	410	8/25	0.76	0.12	29,33,44,44	0
4	OLC	A	407	10/25	0.84	0.11	32,52,57,60	0
3	RET	A	401	20/21	0.84	0.26	34,47,100,114	0

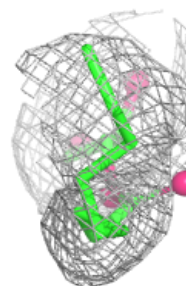
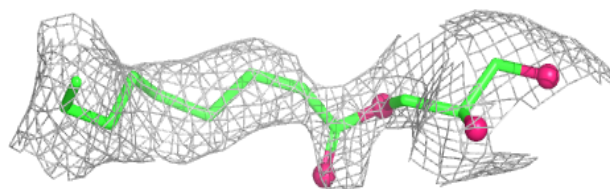
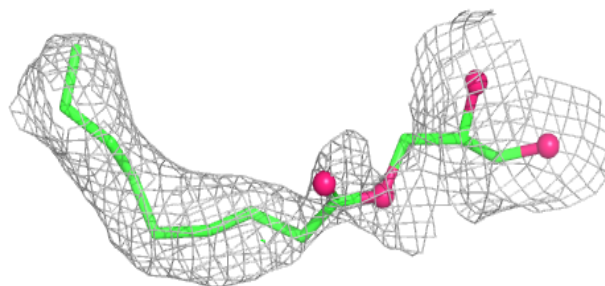
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 408:

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

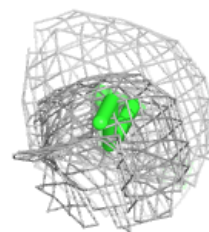
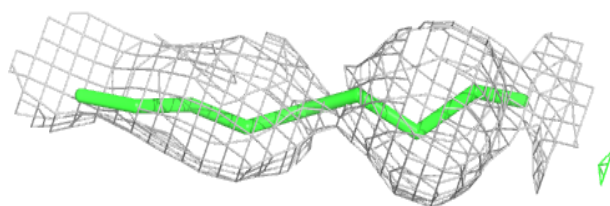
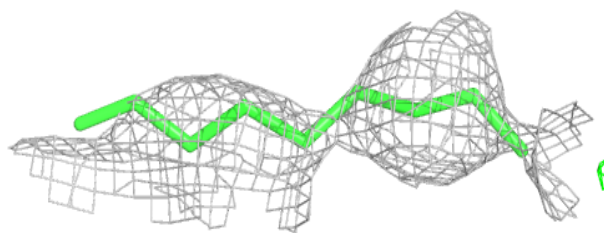
**Electron density around OLC A 405:**

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

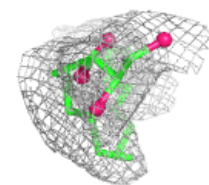
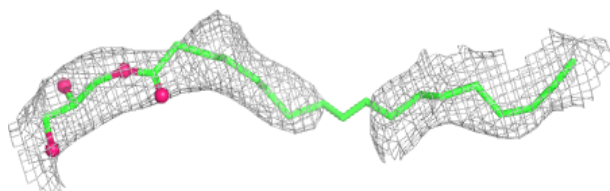
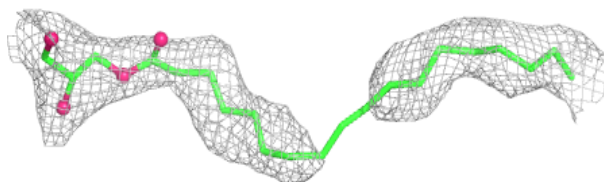


Electron density around OLC A 409:

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

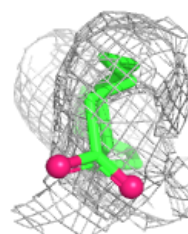
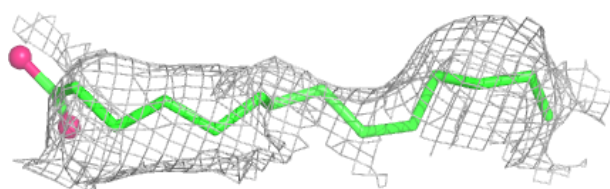
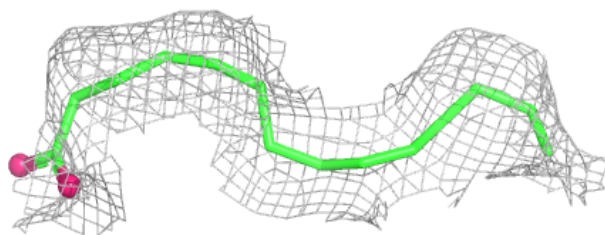
**Electron density around OLC A 402:**

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

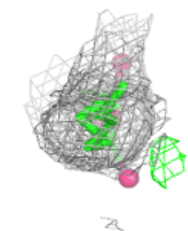
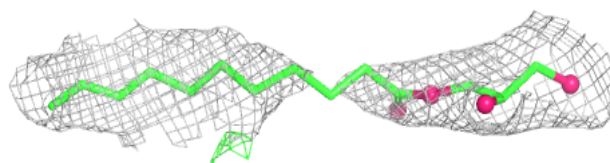
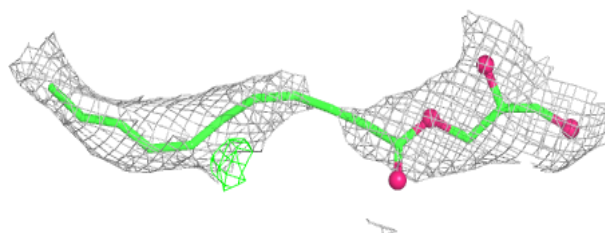


Electron density around OLC A 403:

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

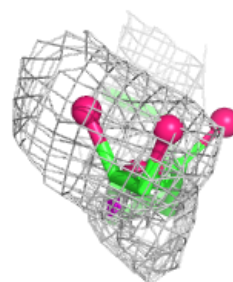
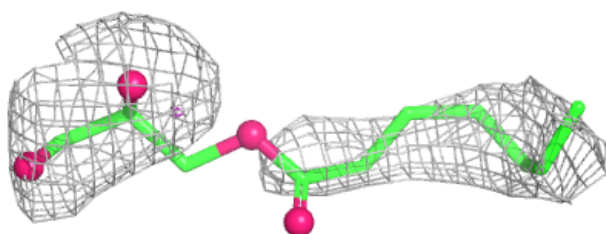
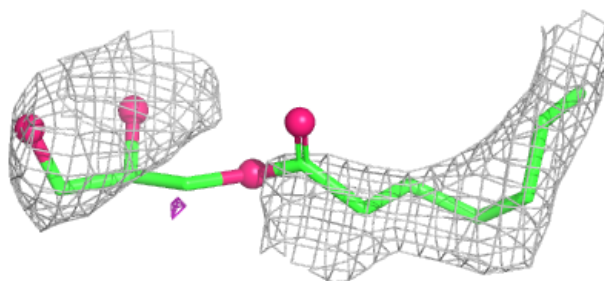
**Electron density around OLC A 406:**

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

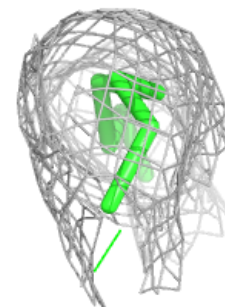
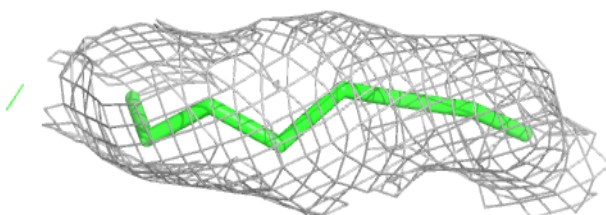
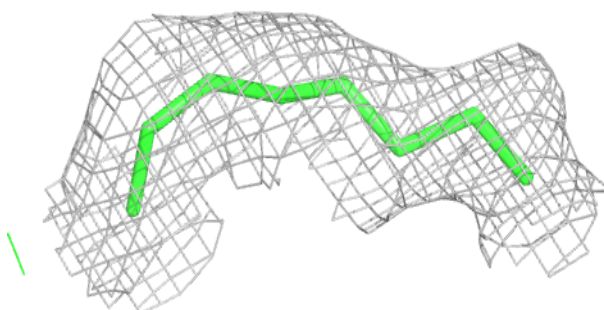


Electron density around OLC A 404:

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

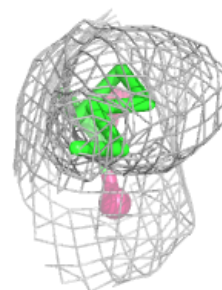
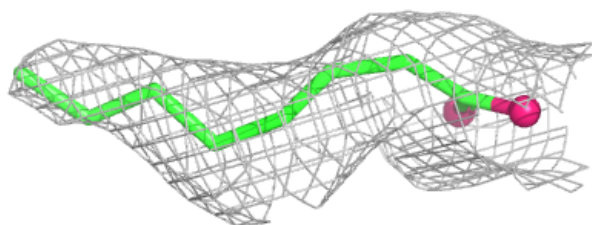
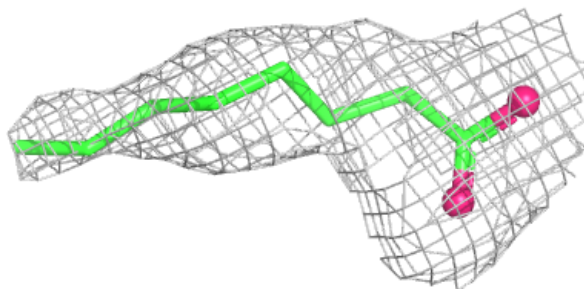
**Electron density around OLC A 410:**

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

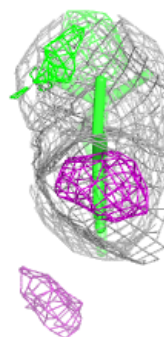
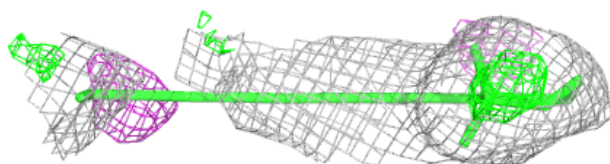
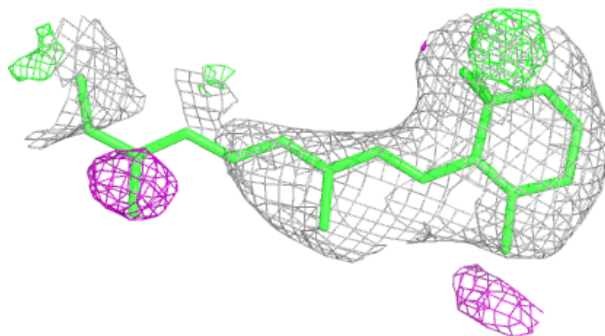


Electron density around OLC A 407:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.