



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:04 PM EDT

PDB ID : 7E6Y / pdb_00007e6y
Title : Time-resolved serial femtosecond crystallography reveals early structural changes in channelrhodopsin: 1 microsecond 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

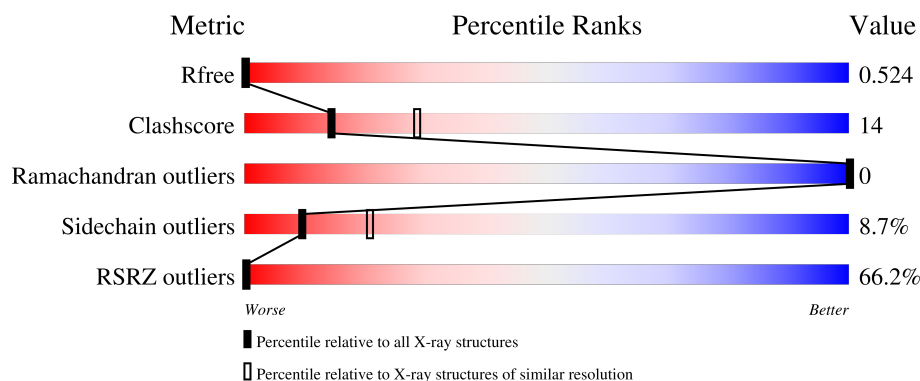
1 Overall quality at a glance

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)

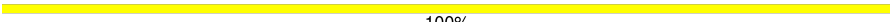
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	55% 61% 21% • 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 [i](#)

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:

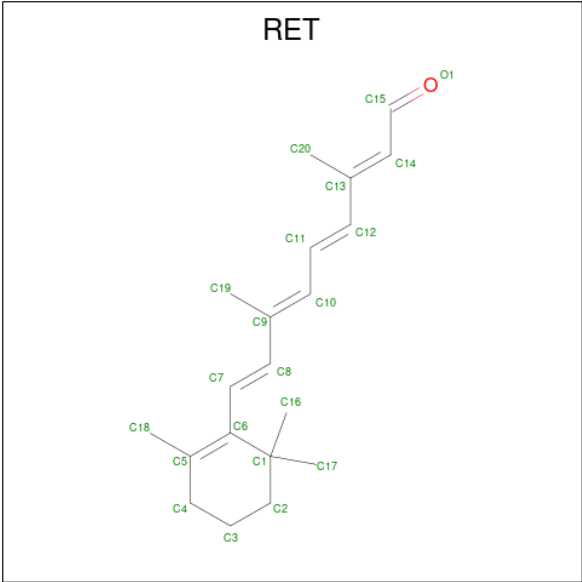
Chain	Residue	Modelled	Actual	Comment	Reference
A	349	SER	-	expression tag	UNP Q8RUT8
A	350	SER	-	expression tag	UNP Q8RUT8
A	351	GLU	-	expression tag	UNP Q8RUT8
A	352	ASP	-	expression tag	UNP Q8RUT8
A	353	LEU	-	expression tag	UNP Q8RUT8
A	354	TYR	-	expression tag	UNP Q8RUT8
A	355	PHE	-	expression tag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



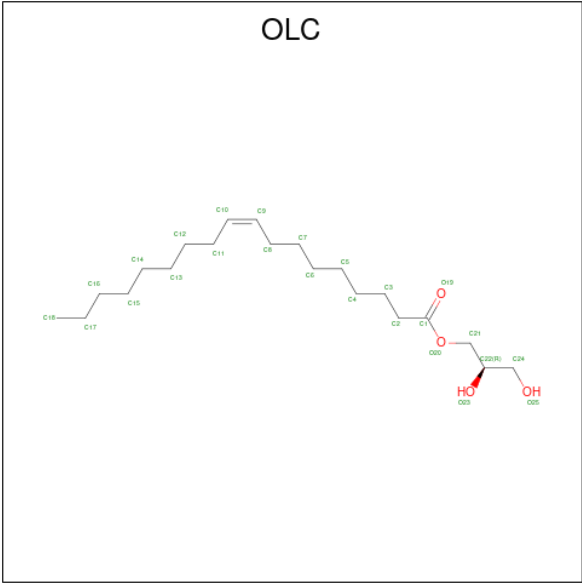
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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

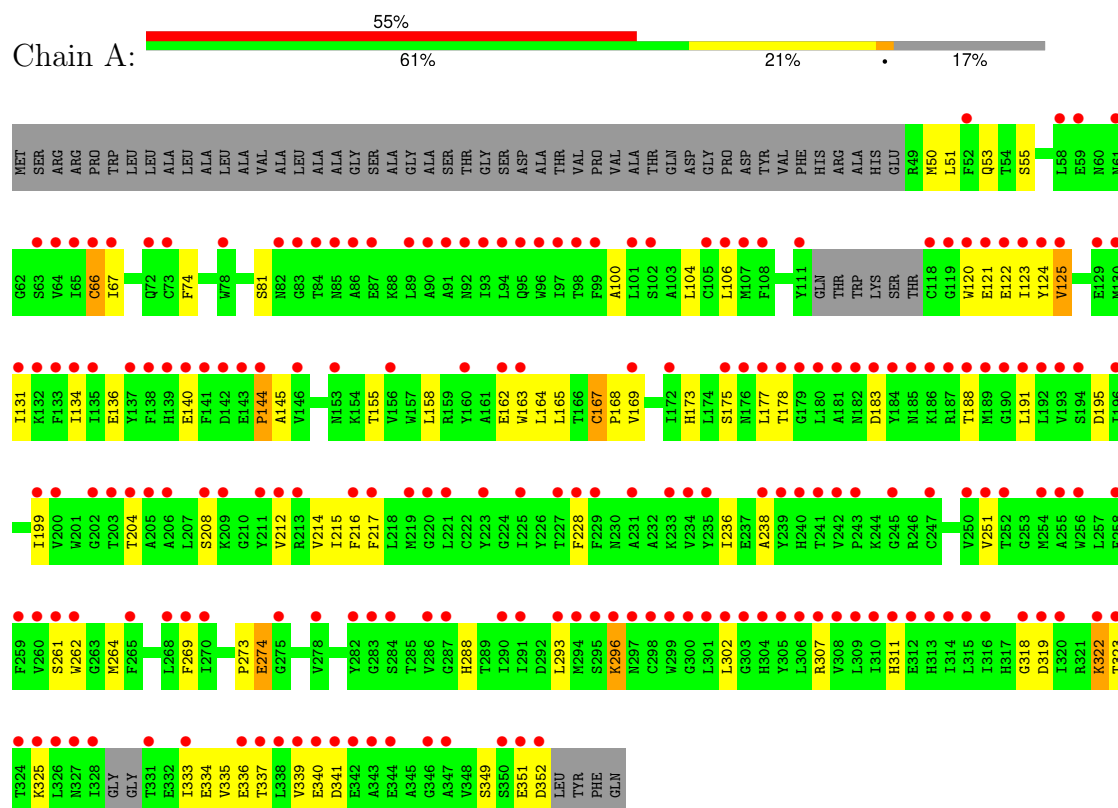
- Molecule 5 is water.

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

3 Residue-property plots

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)	74.1 (14.96-2.50) 74.1 (14.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.445 , 0.515 0.448 , 0.524	Depositor DCC
R_{free} test set	542 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 99.1	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	0.77	EDS
Total number of atoms	2529	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.19	6/2377 (0.3%)	1.56	3/3237 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	SER	C-O	5.84	1.30	1.24
1	A	296	LYS	C-O	5.50	1.30	1.24
1	A	293	LEU	C-O	5.41	1.30	1.24
1	A	50	MET	N-CA	5.38	1.52	1.46
1	A	125	VAL	C-O	5.09	1.30	1.24
1	A	66	CYS	C-O	5.05	1.30	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	GLY	CA-C-O	-5.50	118.17	122.52
1	A	251	VAL	O-C-N	5.15	126.96	121.91
1	A	144	PRO	N-CA-CB	-5.00	97.10	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2317	0	2261	68	3
2	E	28	0	25	0	0
3	A	20	0	27	3	0
4	A	126	0	172	24	0
5	A	38	0	0	28	0
All	All	2529	0	2485	70	3

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 14.

All (70) 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:215:ILE:HD13	4:A:403:OLC:C1	1.85	1.07
1:A:215:ILE:HD13	4:A:403:OLC:O20	1.53	1.07
1:A:74:PHE:HA	5:A:524:HOH:O	1.60	1.02
1:A:215:ILE:CD1	4:A:403:OLC:O20	2.13	0.97
1:A:208:SER:HA	5:A:528:HOH:O	1.71	0.90
1:A:274:GLU:HG2	5:A:514:HOH:O	1.72	0.90
1:A:215:ILE:CD1	4:A:403:OLC:C1	2.55	0.84
1:A:274:GLU:CG	5:A:514:HOH:O	2.25	0.84
1:A:262:TRP:CZ3	5:A:506:HOH:O	2.30	0.83
1:A:262:TRP:HZ3	5:A:506:HOH:O	1.61	0.82
1:A:165:LEU:O	5:A:502:HOH:O	1.99	0.80
1:A:228:PHE:CD2	4:A:402:OLC:H18	2.17	0.79
1:A:162:GLU:OE1	5:A:503:HOH:O	2.03	0.77
1:A:215:ILE:HG21	4:A:403:OLC:C1	2.14	0.76
1:A:215:ILE:HG21	4:A:403:OLC:O19	1.89	0.73
1:A:145:ALA:HB1	5:A:504:HOH:O	1.90	0.71
1:A:81:SER:N	5:A:507:HOH:O	2.25	0.70
1:A:140:GLU:O	5:A:504:HOH:O	2.10	0.69
1:A:140:GLU:HA	5:A:504:HOH:O	1.93	0.67
1:A:204:THR:HG21	4:A:406:OLC:C10	2.25	0.67
1:A:155:THR:OG1	5:A:505:HOH:O	2.13	0.66
1:A:195:ASP:OD1	5:A:506:HOH:O	2.16	0.62
1:A:288:HIS:NE2	5:A:501:HOH:O	1.82	0.62
1:A:319:ASP:N	5:A:513:HOH:O	2.34	0.60
1:A:163:TRP:CD1	3:A:401:RET:H12	2.38	0.58
1:A:215:ILE:CG2	4:A:403:OLC:O19	2.53	0.56
1:A:216:PHE:CZ	4:A:406:OLC:H9	2.41	0.55
1:A:167:CYS:SG	1:A:195:ASP:OD2	2.63	0.55
1:A:124:TYR:HD1	4:A:409:OLC:C2	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD21	1:A:123:ILE:HG23	1.91	0.53
1:A:214:VAL:HG22	4:A:402:OLC:O20	2.08	0.53
1:A:168:PRO:HB2	5:A:518:HOH:O	2.08	0.53
3:A:401:RET:H8	3:A:401:RET:H161	1.90	0.53
1:A:274:GLU:HG3	5:A:514:HOH:O	2.02	0.52
1:A:175:SER:OG	1:A:188:THR:HG23	2.10	0.52
1:A:264:MET:HE2	1:A:264:MET:HA	1.91	0.51
1:A:215:ILE:CD1	4:A:403:OLC:O19	2.59	0.51
1:A:238:ALA:HB2	5:A:526:HOH:O	2.10	0.50
1:A:212:VAL:HG21	4:A:406:OLC:H3A	1.94	0.50
1:A:236:ILE:HA	4:A:407:OLC:H4A	1.93	0.50
1:A:322:LYS:HB2	1:A:337:THR:HB	1.94	0.50
1:A:158:LEU:HD22	5:A:504:HOH:O	2.12	0.49
1:A:136:GLU:O	1:A:140:GLU:HB2	2.12	0.49
1:A:121:GLU:HG3	1:A:173:HIS:HB2	1.94	0.48
1:A:217:PHE:CD2	4:A:402:OLC:H4A	2.50	0.47
1:A:131:ILE:O	1:A:134:ILE:HG13	2.14	0.47
1:A:121:GLU:HG3	1:A:173:HIS:CG	2.50	0.47
1:A:204:THR:CG2	4:A:406:OLC:C10	2.93	0.47
1:A:228:PHE:CG	4:A:402:OLC:H18	2.49	0.46
1:A:215:ILE:HD12	4:A:403:OLC:O20	2.12	0.46
1:A:262:TRP:CE3	5:A:506:HOH:O	2.65	0.45
1:A:53:GLN:HE21	1:A:55:SER:H	1.64	0.44
3:A:401:RET:H7	3:A:401:RET:H181	1.72	0.44
1:A:215:ILE:CB	4:A:403:OLC:O19	2.65	0.44
1:A:269:PHE:HD2	5:A:532:HOH:O	1.98	0.44
1:A:124:TYR:CD1	4:A:409:OLC:C2	3.01	0.44
1:A:155:THR:N	5:A:505:HOH:O	2.51	0.44
1:A:67:ILE:HD12	5:A:533:HOH:O	2.16	0.44
1:A:164:LEU:HG	1:A:199:ILE:HG21	1.99	0.44
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.80	0.43
1:A:120:TRP:CZ3	1:A:169:VAL:HG13	2.53	0.43
1:A:169:VAL:HG23	5:A:518:HOH:O	2.19	0.43
1:A:215:ILE:HB	4:A:403:OLC:O19	2.19	0.42
1:A:228:PHE:CE2	4:A:402:OLC:C17	3.02	0.42
1:A:177:LEU:N	5:A:510:HOH:O	2.52	0.42
1:A:178:THR:HG23	5:A:510:HOH:O	2.19	0.42
1:A:204:THR:HG21	4:A:406:OLC:C11	2.50	0.41
1:A:188:THR:O	1:A:191:LEU:HB2	2.20	0.41
1:A:273:PRO:HB2	5:A:523:HOH:O	2.21	0.41
1:A:100:ALA:O	1:A:104:LEU:HG	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:CYS:SG	1:A:66:CYS:SG[3_555]	1.65	0.55
1:A:351:GLU:OE1	1:A:351:GLU:OE1[4_565]	2.04	0.16
1:A:349:SER:O	1:A:349:SER:O[4_565]	2.05	0.15

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%)	274 (94%)	16 (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%)	221 (91%)	21 (9%)	9	21

All (21) 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
1	A	144	PRO

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Mol	Chain	Res	Type
1	A	167	CYS
1	A	183	ASP
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	70	ASN
1	A	173	HIS

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	2,1	14,14,15	0.71	0	17,19,21	1.16	2 (11%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	2.12	4 (23%)

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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	5.91	120.11	112.19
2	E	2	NAG	O5-C1-C2	-5.10	103.40	111.29
2	E	1	NAG	C2-N2-C7	2.53	126.29	122.90
2	E	1	NAG	C4-C3-C2	2.14	114.15	111.02
2	E	2	NAG	C2-N2-C7	2.09	125.70	122.90
2	E	2	NAG	O7-C7-N2	2.06	125.63	121.98

There are no chirality outliers.

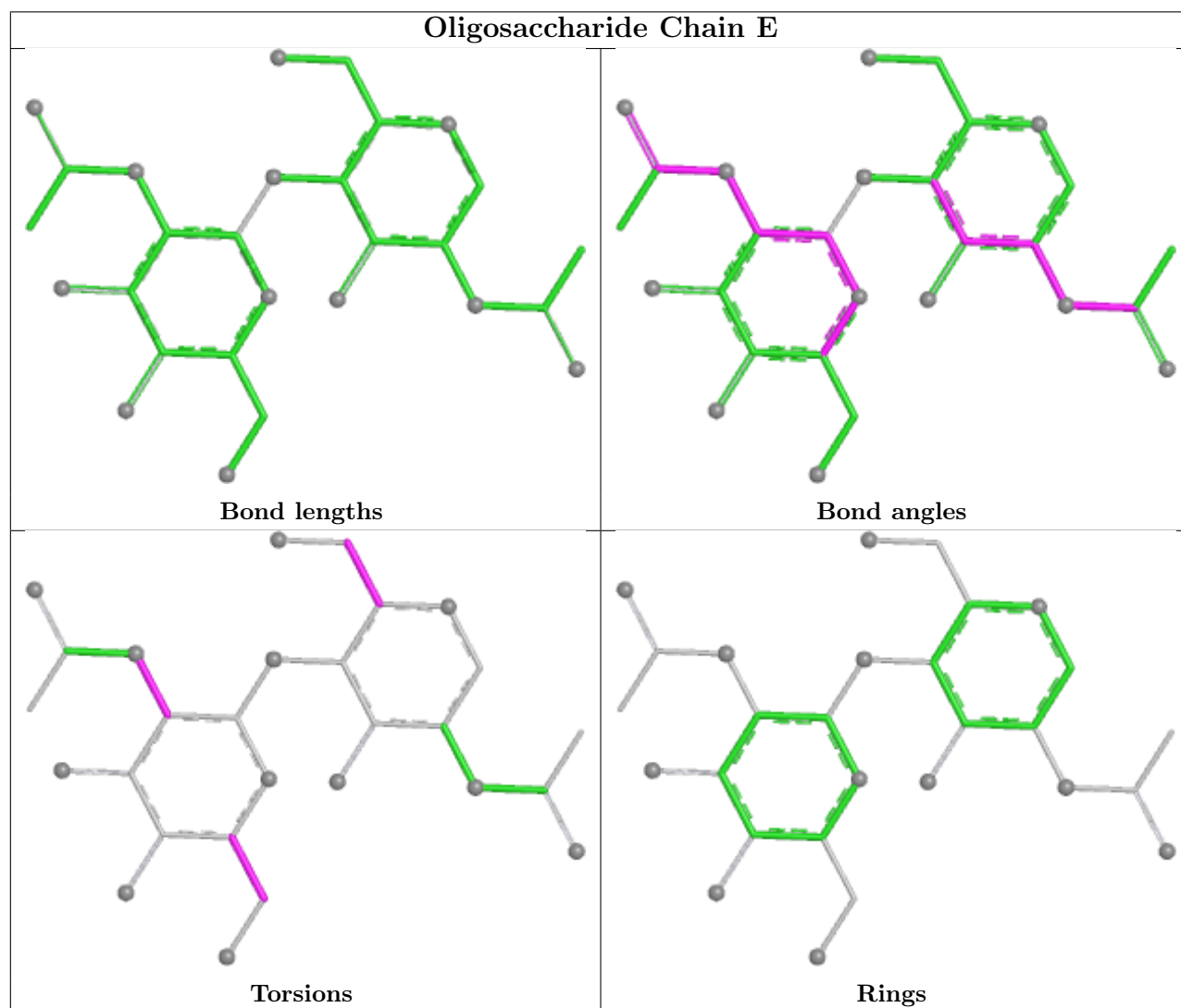
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-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	404	-	13,13,24	0.76	0	14,14,25	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	A	406	-	17,17,24	0.51	0	18,18,25	0.67	0
3	RET	A	401	1	20,20,21	3.05	4 (20%)	27,27,28	1.96	9 (33%)
4	OLC	A	410	-	7,7,24	0.69	0	6,6,25	0.32	0
4	OLC	A	407	-	9,9,24	0.83	0	9,9,25	0.56	0
4	OLC	A	408	-	9,9,24	0.84	0	9,9,25	0.62	0
4	OLC	A	403	-	15,15,24	0.99	2 (13%)	15,15,25	0.35	0
4	OLC	A	409	-	8,8,24	0.72	0	7,7,25	0.28	0
4	OLC	A	402	-	24,24,24	0.56	0	25,25,25	0.75	0
4	OLC	A	405	-	15,15,24	0.60	0	16,16,25	0.65	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	404	-	-	7/13/13/24	-
4	OLC	A	406	-	-	10/17/17/24	-
3	RET	A	401	1	-	0/13/30/31	0/1/1/1
4	OLC	A	410	-	-	5/5/5/24	-
4	OLC	A	407	-	-	2/7/7/24	-
4	OLC	A	408	-	-	4/7/7/24	-
4	OLC	A	403	-	-	7/13/13/24	-
4	OLC	A	409	-	-	4/6/6/24	-
4	OLC	A	402	-	-	12/24/24/24	-
4	OLC	A	405	-	-	10/15/15/24	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	RET	C14-C13	11.76	1.41	1.33
3	A	401	RET	C10-C9	3.37	1.43	1.35
3	A	401	RET	C15-C14	-3.29	1.37	1.49
3	A	401	RET	C8-C9	-2.66	1.40	1.46
4	A	403	OLC	C3-C2	2.17	1.60	1.52
4	A	403	OLC	C2-C1	2.17	1.55	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	RET	C12-C13-C14	4.18	129.67	118.55
3	A	401	RET	C8-C9-C10	3.91	125.16	119.01
3	A	401	RET	C2-C1-C6	3.84	116.01	110.44
3	A	401	RET	C20-C13-C14	-3.61	113.67	123.63
3	A	401	RET	C19-C9-C10	-3.28	117.50	122.82
3	A	401	RET	C10-C11-C12	2.98	131.82	123.20
3	A	401	RET	C1-C6-C7	2.78	123.19	115.65
3	A	401	RET	C1-C6-C5	-2.03	119.86	122.64
3	A	401	RET	C7-C6-C5	-2.00	116.95	121.56

There are no chirality outliers.

All (61) 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	404	OLC	C1-C2-C3-C4
4	A	404	OLC	O19-C1-O20-C21
4	A	407	OLC	C1-C2-C3-C4
4	A	402	OLC	C1-C2-C3-C4
4	A	405	OLC	O20-C21-C22-O23
4	A	404	OLC	C21-C22-C24-O25
4	A	406	OLC	O23-C22-C24-O25
4	A	403	OLC	C4-C5-C6-C7
4	A	409	OLC	C4-C5-C6-C7
4	A	406	OLC	C4-C5-C6-C7
4	A	405	OLC	C2-C3-C4-C5
4	A	410	OLC	C3-C4-C5-C6
4	A	403	OLC	C11-C10-C9-C8
4	A	402	OLC	C2-C3-C4-C5
4	A	410	OLC	C4-C5-C6-C7
4	A	408	OLC	C3-C4-C5-C6
4	A	402	OLC	C6-C7-C8-C9
4	A	406	OLC	C6-C7-C8-C9
4	A	405	OLC	C5-C6-C7-C8
4	A	404	OLC	O23-C22-C24-O25
4	A	403	OLC	C2-C3-C4-C5
4	A	405	OLC	C1-C2-C3-C4
4	A	402	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
4	A	410	OLC	C6-C7-C8-C9
4	A	402	OLC	C3-C4-C5-C6
4	A	405	OLC	C6-C7-C8-C9
4	A	405	OLC	O20-C21-C22-C24
4	A	409	OLC	C3-C4-C5-C6
4	A	403	OLC	C3-C4-C5-C6
4	A	409	OLC	C2-C3-C4-C5
4	A	408	OLC	C5-C6-C7-C8
4	A	406	OLC	C3-C4-C5-C6
4	A	407	OLC	C4-C5-C6-C7
4	A	403	OLC	C10-C11-C12-C13
4	A	402	OLC	O19-C1-O20-C21
4	A	402	OLC	C15-C16-C17-C18
4	A	402	OLC	C12-C13-C14-C15
4	A	408	OLC	C2-C3-C4-C5
4	A	410	OLC	C5-C6-C7-C8
4	A	408	OLC	C1-C2-C3-C4
4	A	405	OLC	C4-C5-C6-C7
4	A	406	OLC	C2-C1-O20-C21
4	A	402	OLC	C14-C15-C16-C17
4	A	402	OLC	C7-C8-C9-C10
4	A	402	OLC	C4-C5-C6-C7
4	A	403	OLC	C9-C10-C11-C12
4	A	409	OLC	C7-C8-C9-C10
4	A	410	OLC	C2-C3-C4-C5
4	A	402	OLC	C11-C12-C13-C14
4	A	405	OLC	C3-C4-C5-C6
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	403	OLC	C7-C8-C9-C10
4	A	404	OLC	O19-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 27 short contacts:

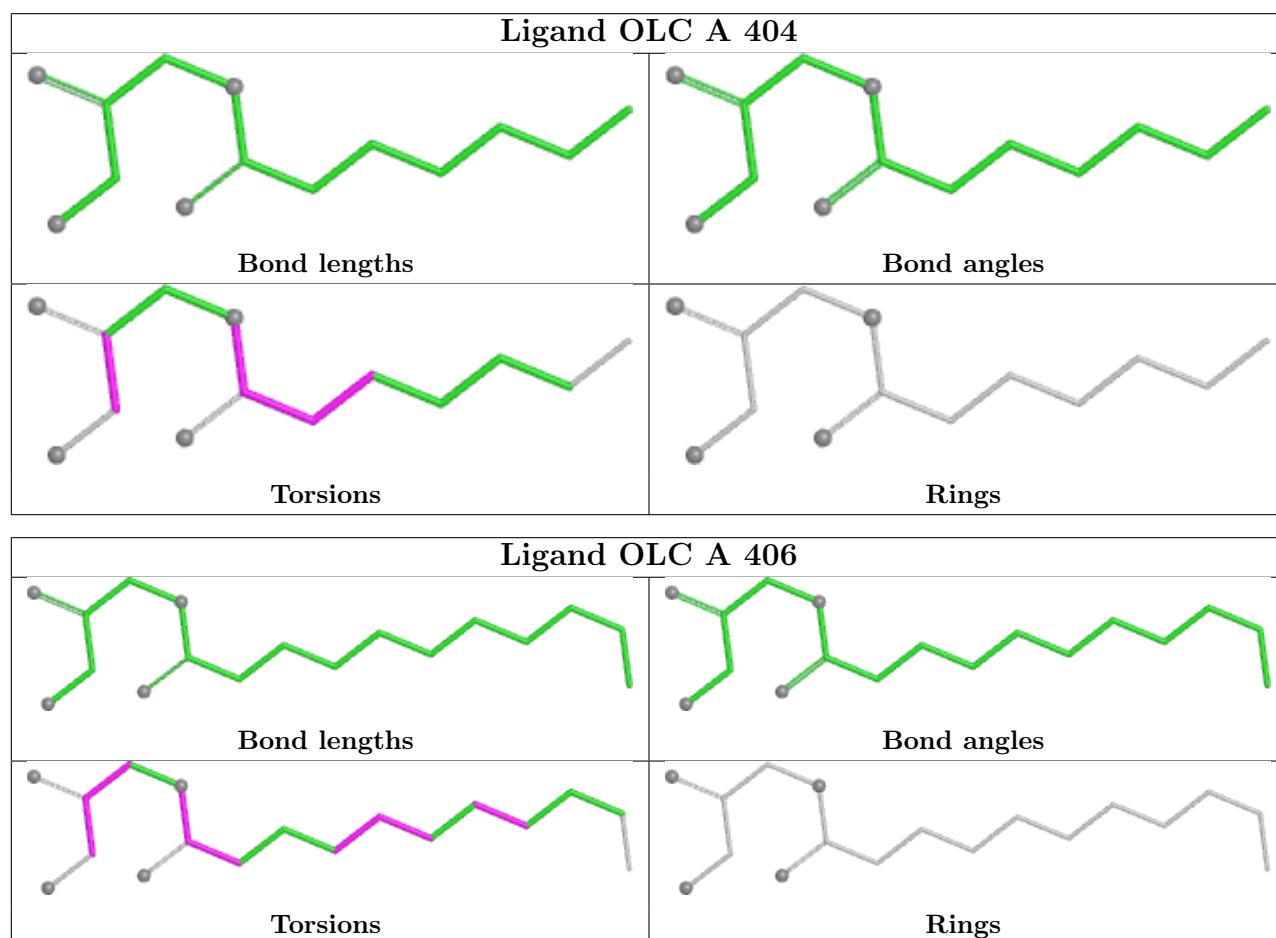
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	OLC	5	0
3	A	401	RET	3	0
4	A	407	OLC	1	0
4	A	403	OLC	11	0
4	A	409	OLC	2	0

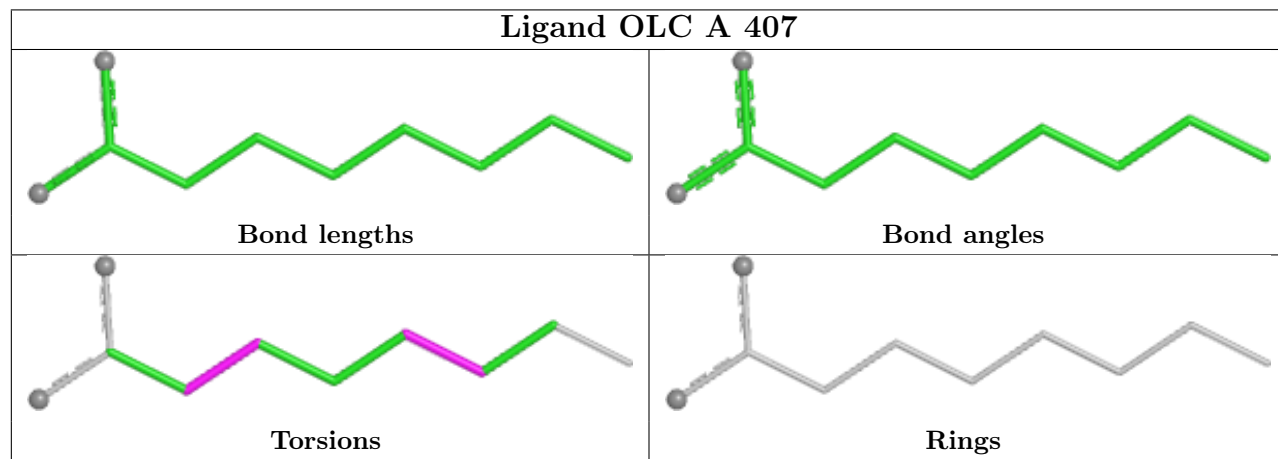
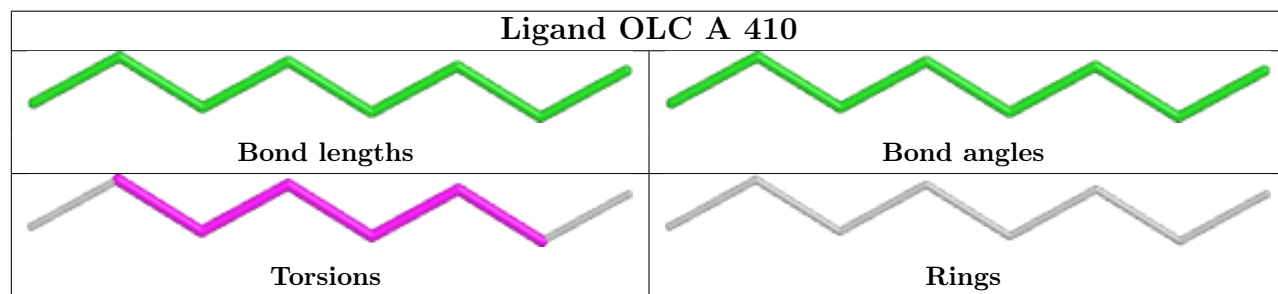
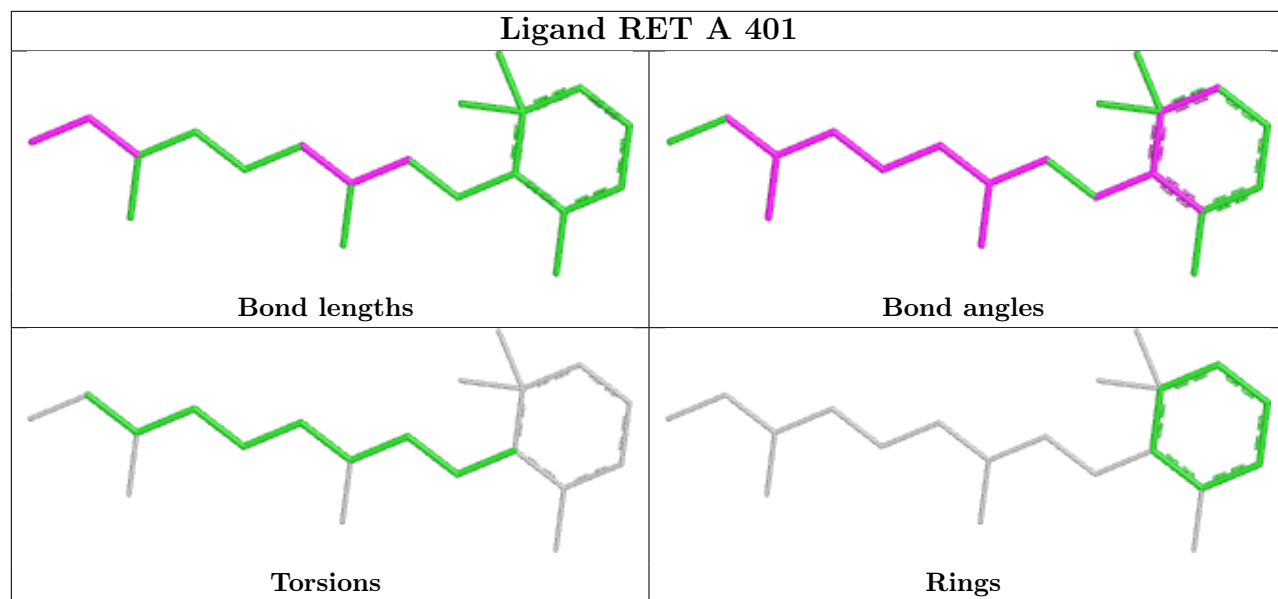
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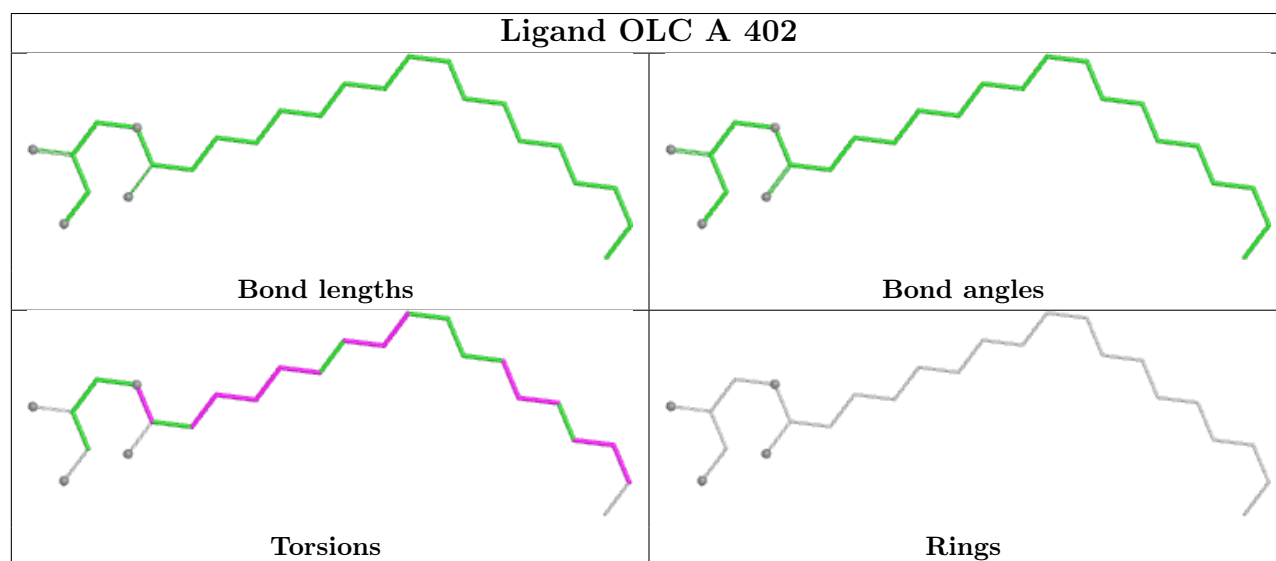
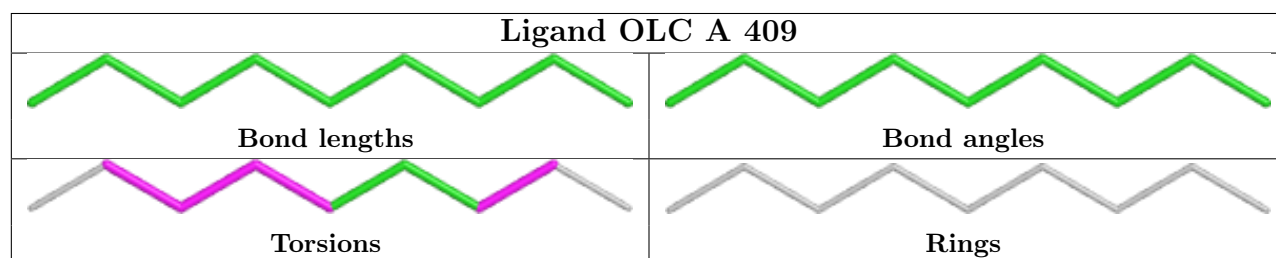
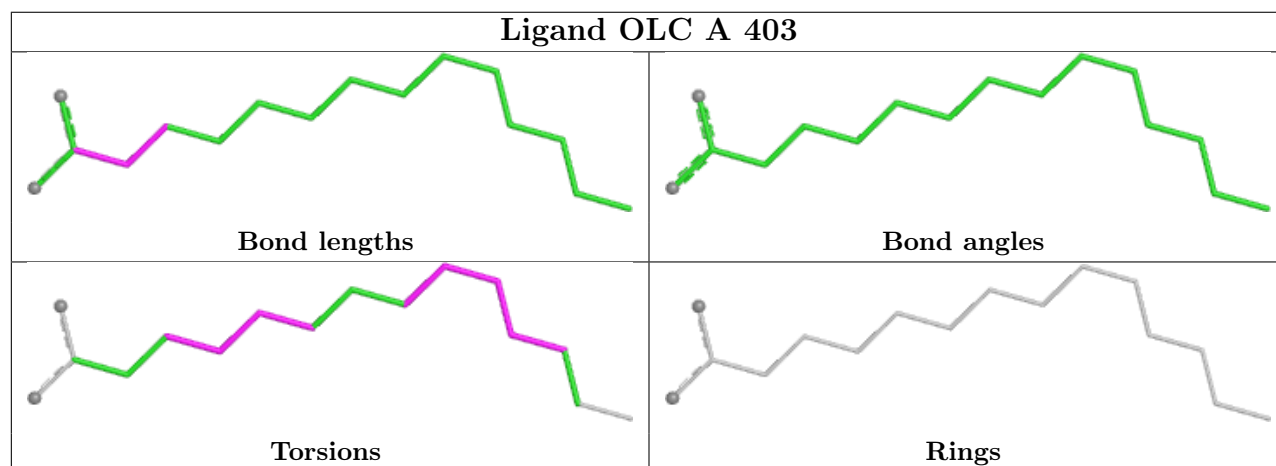
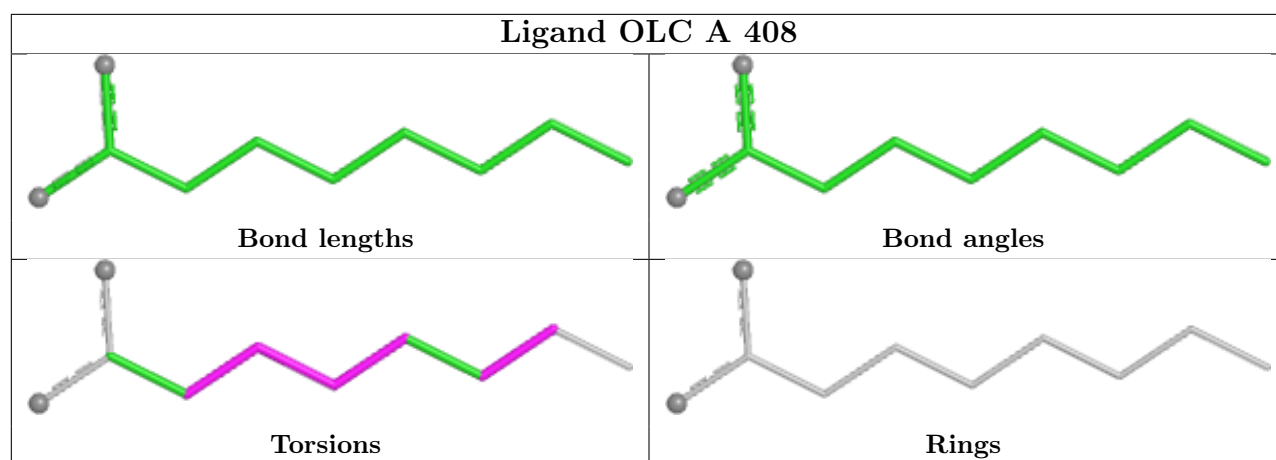
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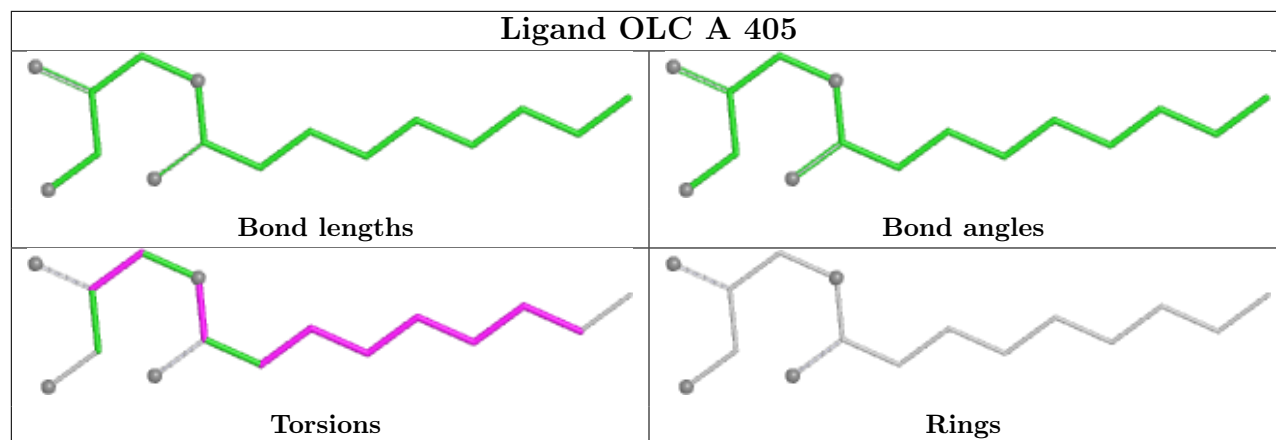
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	OLC	5	0

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%)	2.70	196 (66%) 0 0	37, 72, 118, 173	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	THR	8.3
1	A	229	PHE	7.9
1	A	350	SER	7.5
1	A	300	GLY	7.0
1	A	58	LEU	6.7
1	A	221	LEU	6.6
1	A	181	ALA	6.5
1	A	320	ILE	6.3
1	A	310	ILE	6.3
1	A	93	ILE	6.3
1	A	352	ASP	6.1
1	A	313	HIS	6.0
1	A	199	ILE	5.9
1	A	287	GLY	5.7
1	A	192	LEU	5.5
1	A	282	TYR	5.4
1	A	291	ILE	5.4
1	A	172	ILE	5.3
1	A	132	LYS	5.3
1	A	178	THR	5.1
1	A	196	ILE	5.1
1	A	179	GLY	5.0
1	A	325	LYS	5.0
1	A	89	LEU	4.9
1	A	293	LEU	4.7
1	A	123	ILE	4.7
1	A	129	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	194	SER	4.6
1	A	191	LEU	4.6
1	A	139	HIS	4.6
1	A	333	ILE	4.6
1	A	106	LEU	4.6
1	A	182	ASN	4.5
1	A	189	MET	4.5
1	A	131	ILE	4.5
1	A	338	LEU	4.4
1	A	108	PHE	4.4
1	A	78	TRP	4.4
1	A	86	ALA	4.4
1	A	142	ASP	4.4
1	A	84	THR	4.3
1	A	211	TYR	4.3
1	A	322	LYS	4.3
1	A	255	ALA	4.2
1	A	92	ASN	4.2
1	A	140	GLU	4.2
1	A	340	GLU	4.1
1	A	235	TYR	4.0
1	A	190	GLY	4.0
1	A	241	THR	4.0
1	A	284	SER	4.0
1	A	256	TRP	3.9
1	A	225	ILE	3.9
1	A	341	ASP	3.9
1	A	90	ALA	3.9
1	A	315	LEU	3.8
1	A	299	TRP	3.8
1	A	268	LEU	3.8
1	A	138	PHE	3.7
1	A	52	PHE	3.7
1	A	343	ALA	3.7
1	A	326	LEU	3.7
1	A	306	LEU	3.7
1	A	96	TRP	3.6
1	A	260	VAL	3.6
1	A	188	THR	3.6
1	A	307	ARG	3.5
1	A	245	GLY	3.5
1	A	97	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	339	VAL	3.5
1	A	133	PHE	3.5
1	A	177	LEU	3.4
1	A	175	SER	3.4
1	A	87	GLU	3.3
1	A	169	VAL	3.3
1	A	250	VAL	3.3
1	A	297	ASN	3.3
1	A	67	ILE	3.3
1	A	234	VAL	3.3
1	A	83	GLY	3.3
1	A	220	GLY	3.3
1	A	240	HIS	3.2
1	A	183	ASP	3.2
1	A	85	ASN	3.2
1	A	121	GLU	3.2
1	A	278	VAL	3.2
1	A	308	VAL	3.2
1	A	316	ILE	3.2
1	A	305	TYR	3.2
1	A	223	TYR	3.1
1	A	323	THR	3.1
1	A	212	VAL	3.1
1	A	217	PHE	3.1
1	A	219	MET	3.0
1	A	342	GLU	3.0
1	A	102	SER	3.0
1	A	208	SER	3.0
1	A	312	GLU	3.0
1	A	295	SER	3.0
1	A	122	GLU	3.0
1	A	228	PHE	3.0
1	A	66	CYS	3.0
1	A	105	CYS	3.0
1	A	95	GLN	3.0
1	A	119	GLY	2.9
1	A	185	ASN	2.9
1	A	98	THR	2.9
1	A	187	ARG	2.9
1	A	101	LEU	2.9
1	A	275	GLY	2.9
1	A	118	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	94	LEU	2.9
1	A	254	MET	2.9
1	A	205	ALA	2.8
1	A	99	PHE	2.8
1	A	141	PHE	2.8
1	A	314	ILE	2.8
1	A	227	THR	2.8
1	A	134	ILE	2.8
1	A	247	CYS	2.8
1	A	336	GLU	2.8
1	A	294	MET	2.7
1	A	269	PHE	2.7
1	A	65	ILE	2.7
1	A	124	TYR	2.7
1	A	180	LEU	2.7
1	A	252	THR	2.7
1	A	242	VAL	2.7
1	A	324	THR	2.7
1	A	311	HIS	2.7
1	A	233	LYS	2.7
1	A	204	THR	2.6
1	A	163	TRP	2.6
1	A	82	ASN	2.6
1	A	184	TYR	2.6
1	A	213	ARG	2.6
1	A	351	GLU	2.6
1	A	162	GLU	2.5
1	A	72	GLN	2.5
1	A	156	VAL	2.5
1	A	251	VAL	2.5
1	A	135	ILE	2.5
1	A	130	MET	2.5
1	A	111	TYR	2.5
1	A	262	TRP	2.5
1	A	243	PRO	2.4
1	A	296	LYS	2.4
1	A	186	LYS	2.4
1	A	160	TYR	2.4
1	A	261	SER	2.4
1	A	290	ILE	2.4
1	A	63	SER	2.4
1	A	202	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	176	ASN	2.4
1	A	347	ALA	2.4
1	A	298	CYS	2.3
1	A	146	VAL	2.3
1	A	143	GLU	2.3
1	A	216	PHE	2.3
1	A	200	VAL	2.3
1	A	61	ASN	2.3
1	A	203	THR	2.3
1	A	283	GLY	2.3
1	A	238	ALA	2.3
1	A	303	GLY	2.3
1	A	120	TRP	2.3
1	A	258	PHE	2.3
1	A	259	PHE	2.3
1	A	153	ASN	2.2
1	A	346	GLY	2.2
1	A	193	VAL	2.2
1	A	91	ALA	2.2
1	A	327	ASN	2.2
1	A	309	LEU	2.2
1	A	64	VAL	2.2
1	A	206	ALA	2.2
1	A	59	GLU	2.2
1	A	125	VAL	2.2
1	A	331	THR	2.2
1	A	239	TYR	2.1
1	A	344	GLU	2.1
1	A	286	VAL	2.1
1	A	304	HIS	2.1
1	A	301	LEU	2.1
1	A	270	ILE	2.1
1	A	231	ALA	2.1
1	A	318	GLY	2.1
1	A	73	CYS	2.1
1	A	319	ASP	2.1
1	A	265	PHE	2.1
1	A	328	ILE	2.1
1	A	209	LYS	2.1
1	A	137	TYR	2.1
1	A	144	PRO	2.1
1	A	302	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	107	MET	2.0

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

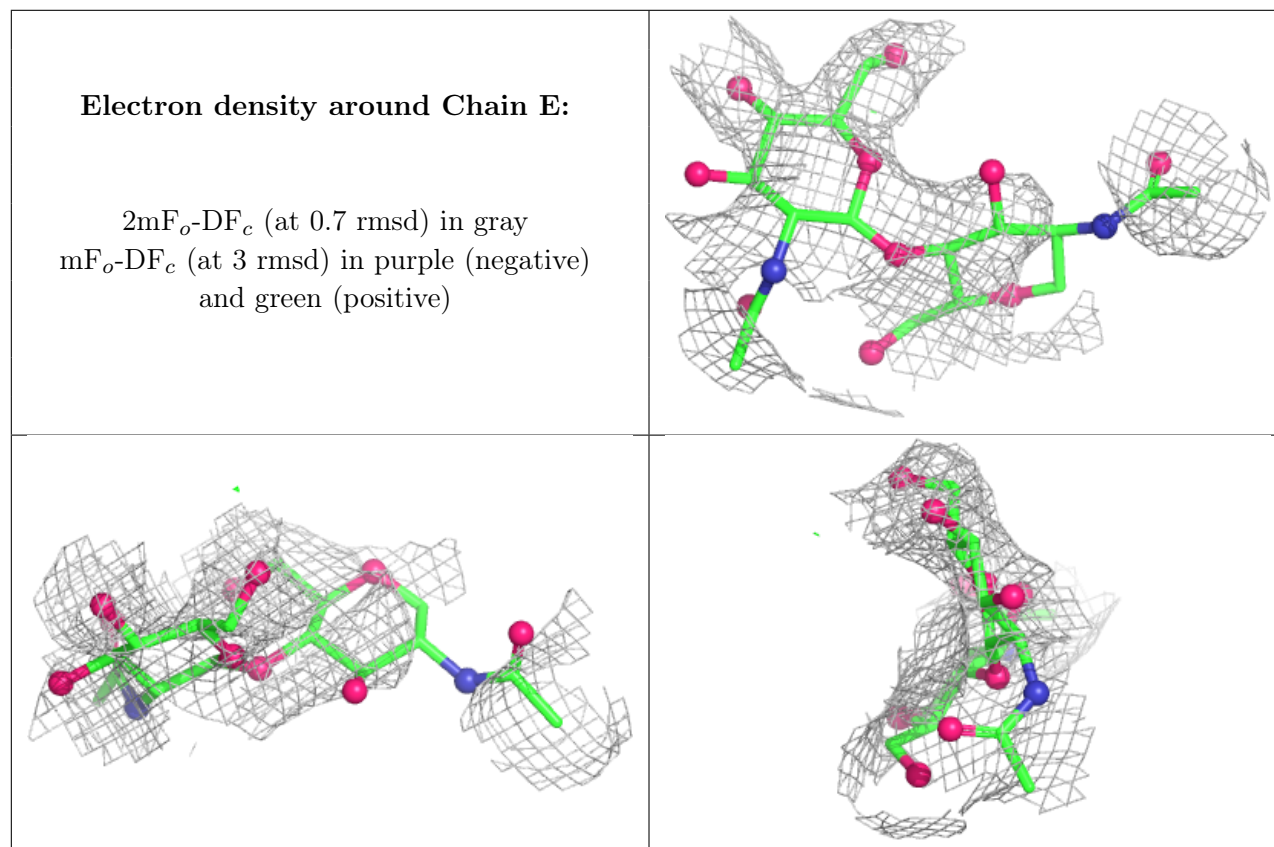
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	NAG	E	1	14/15	-	-	48,95,125,135	0
2	NAG	E	2	14/15	-	-	54,77,90,121	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.

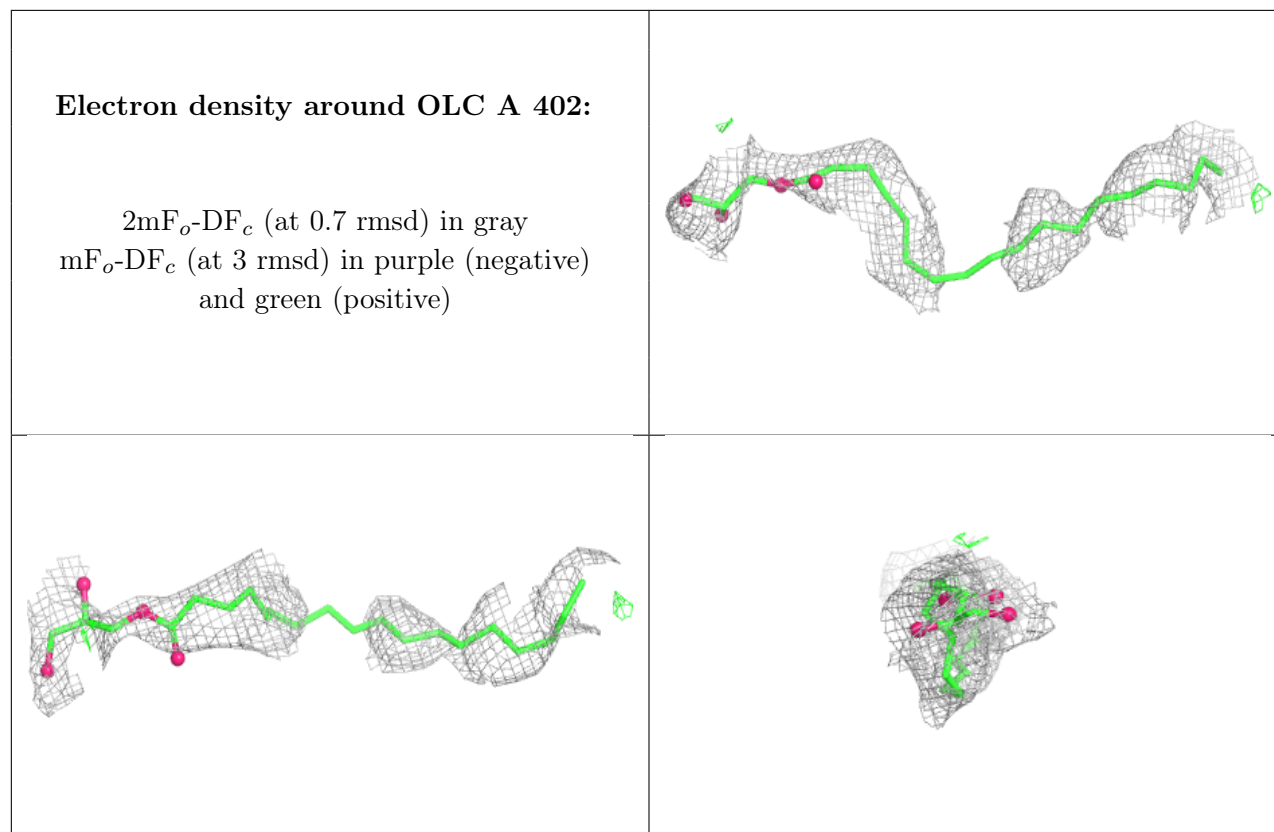


6.4 Ligands ⓘ

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.

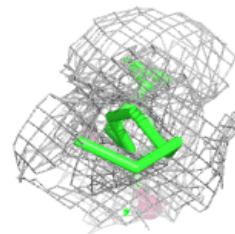
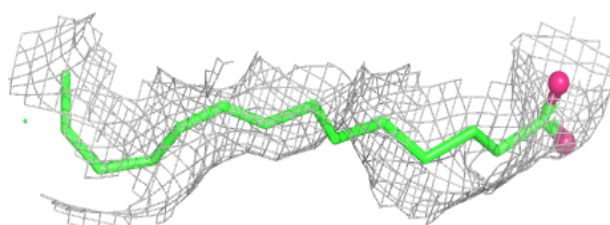
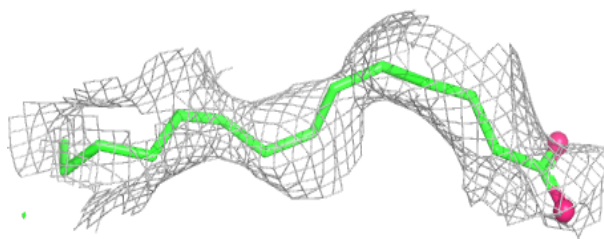
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLC	A	402	25/25	0.29	0.24	58,79,100,104	0
4	OLC	A	403	16/25	0.36	0.19	53,63,85,89	0
4	OLC	A	410	8/25	0.42	0.32	67,84,98,105	0
4	OLC	A	409	9/25	0.45	0.16	58,65,76,83	0
4	OLC	A	404	14/25	0.45	0.18	46,76,101,107	0
4	OLC	A	406	18/25	0.53	0.17	48,59,77,78	0
4	OLC	A	407	10/25	0.60	0.17	54,66,72,74	0
3	RET	A	401	20/21	0.71	0.26	45,68,93,97	0
4	OLC	A	405	16/25	0.75	0.12	42,53,82,97	0
4	OLC	A	408	10/25	0.76	0.12	54,73,78,79	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.

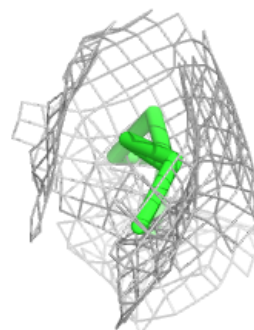
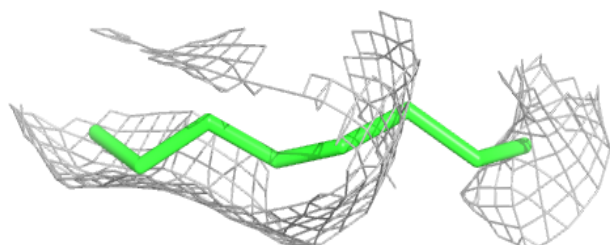
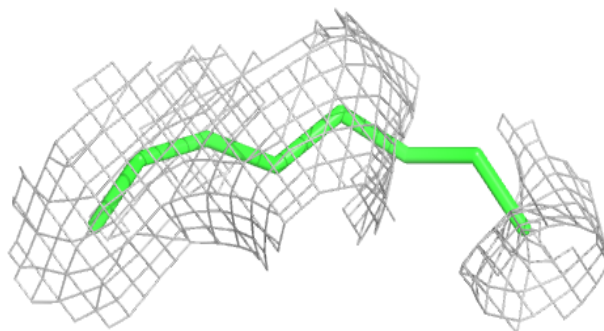


Electron density around OLC A 403:

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

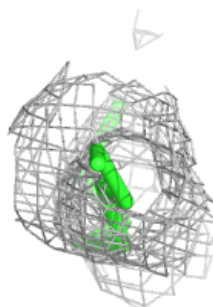
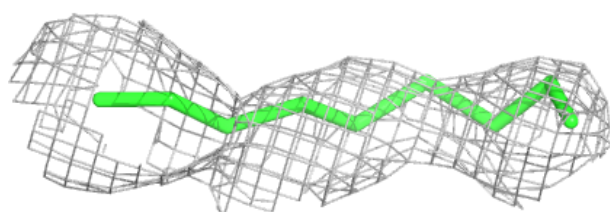
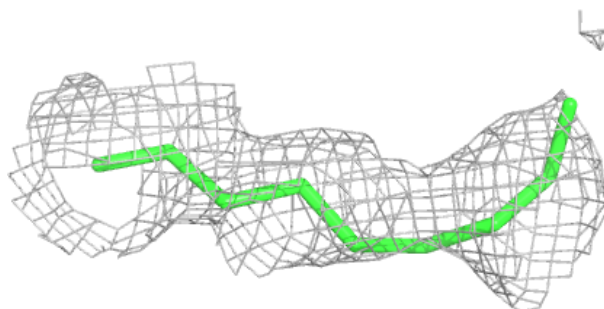
**Electron density around OLC A 410:**

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

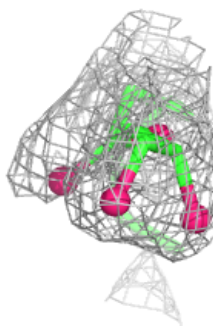
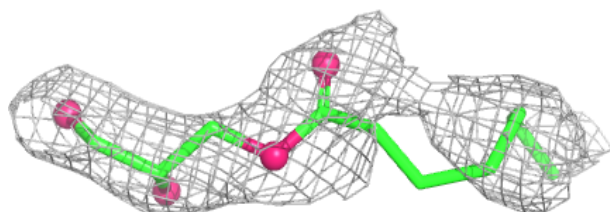
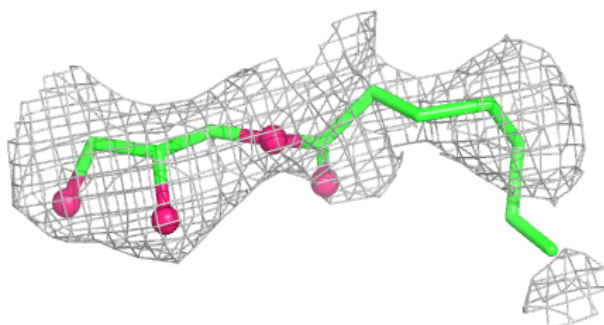


Electron density around OLC A 409:

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

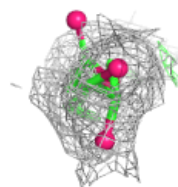
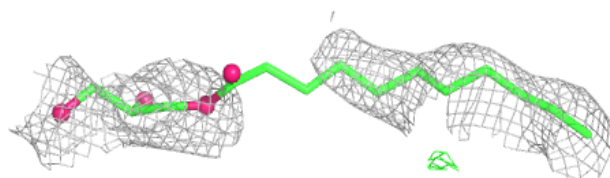
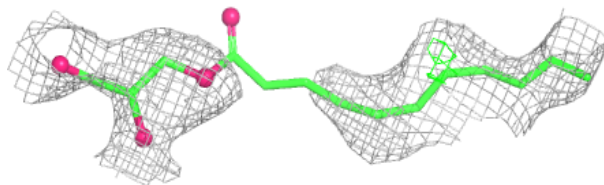
**Electron density around OLC A 404:**

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

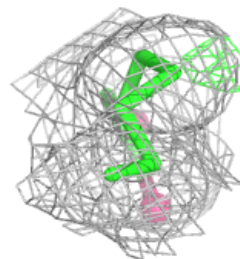
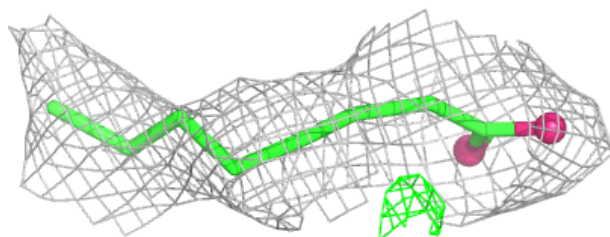
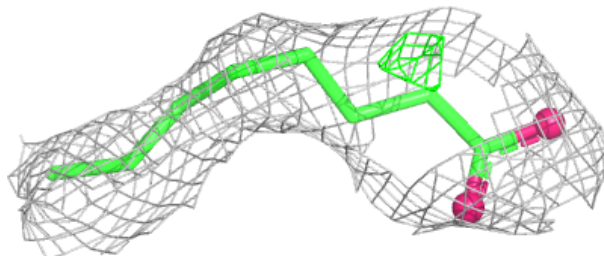


Electron density around OLC A 406:

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

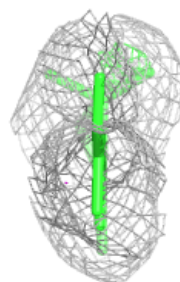
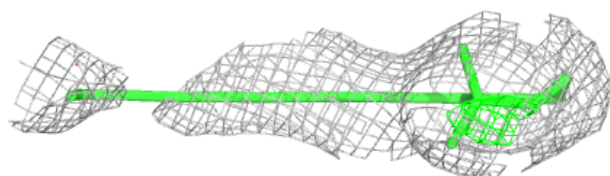
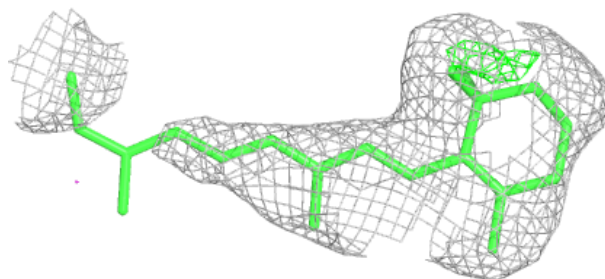
**Electron density around OLC A 407:**

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

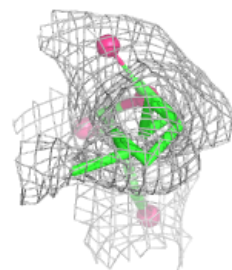
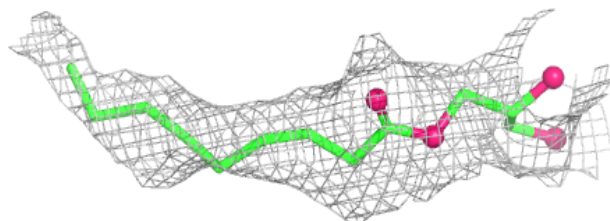


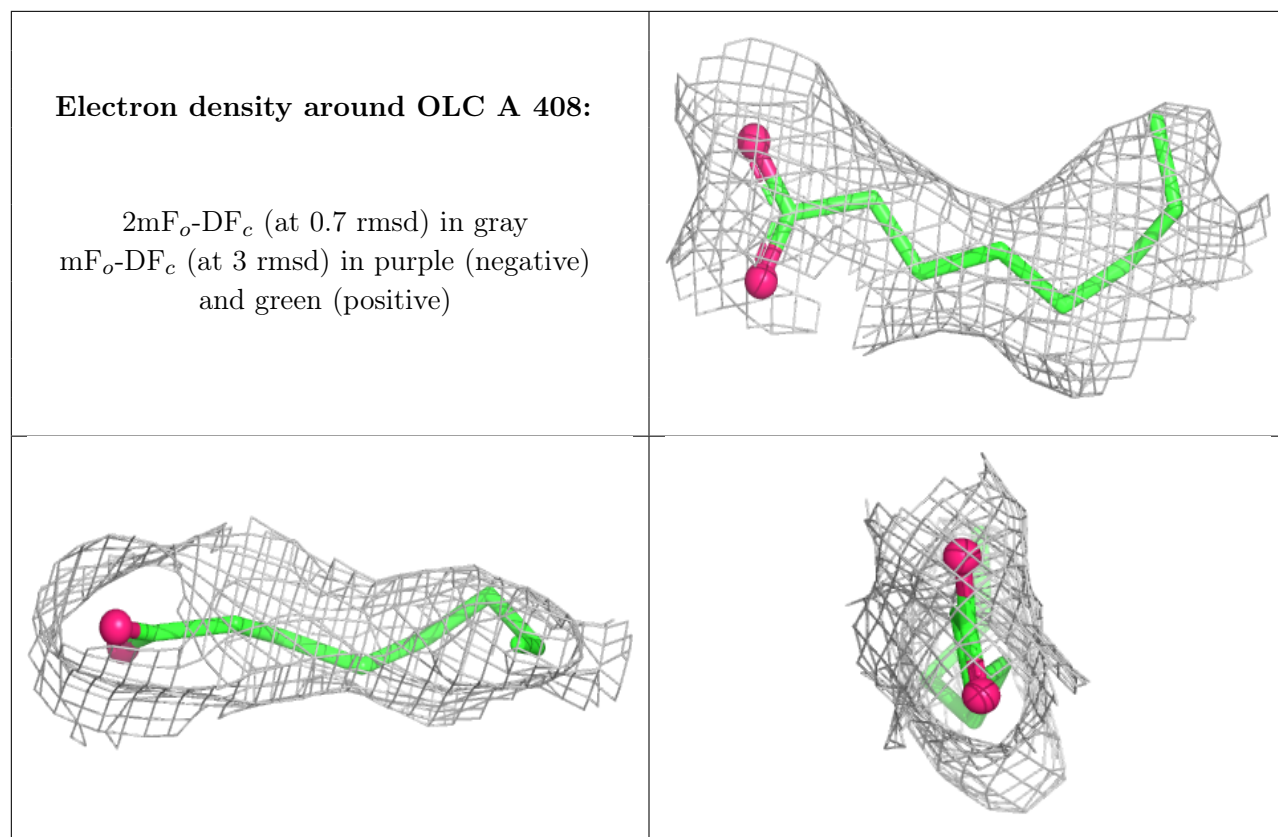
Electron density around RET A 401:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.