



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2021 – 05:26 PM JST

PDB ID : 7E6Y
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 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 : 2.18
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)

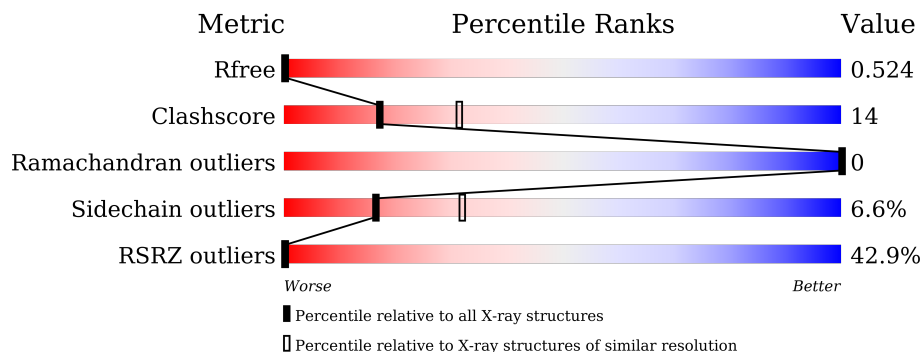
1 Overall quality at a glance

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}	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 $\leq 5\%$. 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	<div> <div>36%</div> <div>63%</div> <div>19%</div> <div>•</div> <div>17%</div> </div>
2	E	2	<div>100%</div>

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.18

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:

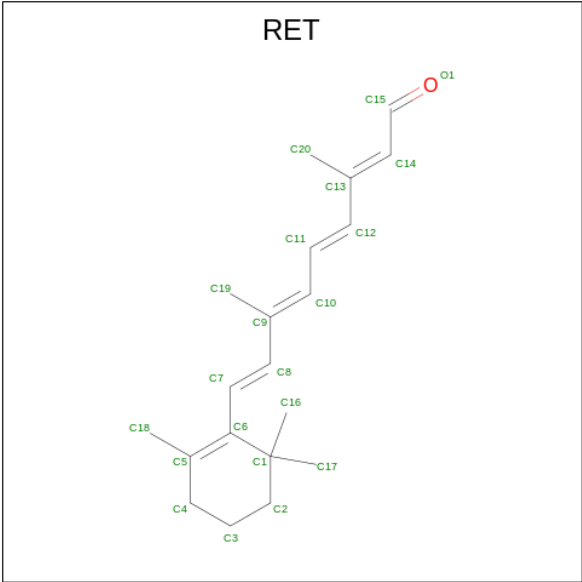
Chain	Residue	Modelled	Actual	Comment	Reference
A	349	SER	-	expression tag	UNP Q8RUT8
A	350	SER	-	expression tag	UNP Q8RUT8
A	351	GLU	-	expression tag	UNP Q8RUT8
A	352	ASP	-	expression tag	UNP Q8RUT8
A	353	LEU	-	expression tag	UNP Q8RUT8
A	354	TYR	-	expression tag	UNP Q8RUT8
A	355	PHE	-	expression tag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



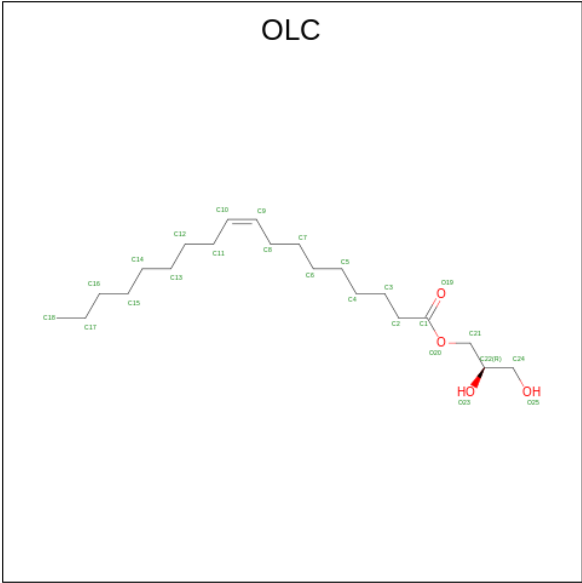
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is RETINAL (three-letter code: RET) (formula: 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 (three-letter code: 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

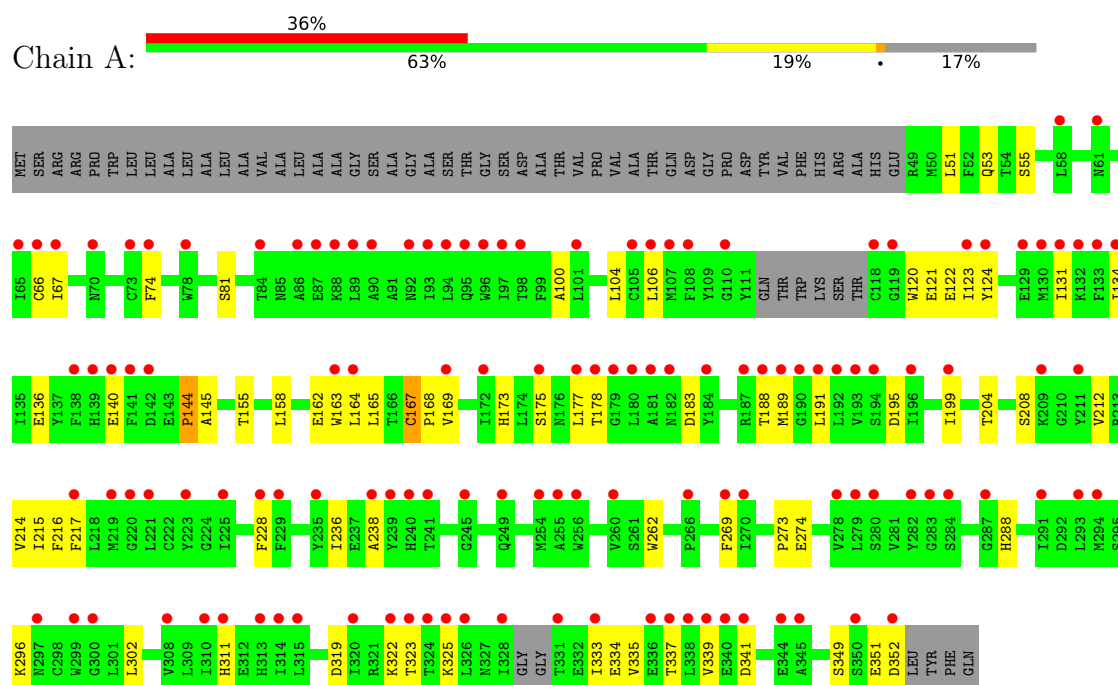
- Molecule 5 is water.

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

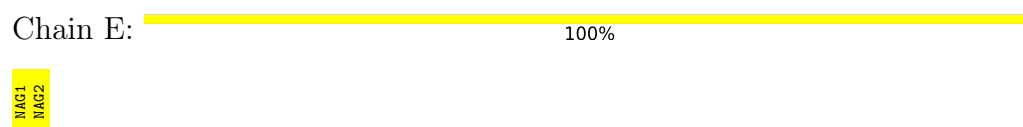
3 Residue-property plots [i](#)

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)	74.1 (14.96-2.50) 74.5 (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 (4.94%)	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)	0.26 , 74.2	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	0.78	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.82	0/2377	0.87	1/3237 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
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 [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	67	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	69	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 (69) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/356 (82%)	274 (94%)	16 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	122	GLU
1	A	144	PRO
1	A	167	CYS
1	A	183	ASP
1	A	189	MET
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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	70	ASN
1	A	72	GLN
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	1,2	14,14,15	0.70	0	17,19,21	1.14	2 (11%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	2.08	2 (11%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	5.84	120.11	112.19
2	E	2	NAG	O5-C1-C2	-4.99	103.40	111.29
2	E	1	NAG	C2-N2-C7	2.38	126.29	122.90
2	E	1	NAG	C4-C3-C2	2.14	114.15	111.02

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.

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	402	-	24,24,24	0.53	0	25,25,25	0.75	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	2.99	4 (20%)	27,27,28	1.89	7 (25%)
4	OLC	A	405	-	15,15,24	0.57	0	16,16,25	0.65	0
4	OLC	A	404	-	13,13,24	0.75	0	14,14,25	0.54	0
4	OLC	A	408	-	6,9,24	0.51	0	5,9,25	0.34	0
4	OLC	A	403	-	12,15,24	0.61	0	11,15,25	0.38	0
4	OLC	A	410	-	7,7,24	0.63	0	6,6,25	0.29	0
4	OLC	A	407	-	6,9,24	0.83	0	5,9,25	0.38	0
4	OLC	A	406	-	17,17,24	0.50	0	18,18,25	0.67	0
4	OLC	A	409	-	8,8,24	0.67	0	7,7,25	0.29	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	402	-	-	12/24/24/24	-
3	RET	A	401	1	-	0/13/30/31	0/1/1/1
4	OLC	A	405	-	-	10/15/15/24	-
4	OLC	A	404	-	-	7/13/13/24	-
4	OLC	A	408	-	-	4/5/7/24	-
4	OLC	A	403	-	-	7/11/13/24	-
4	OLC	A	410	-	-	5/5/5/24	-
4	OLC	A	407	-	-	2/5/7/24	-
4	OLC	A	406	-	-	10/17/17/24	-
4	OLC	A	409	-	-	4/6/6/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	RET	C14-C13	10.42	1.41	1.33
3	A	401	RET	C10-C9	5.88	1.43	1.35
3	A	401	RET	C15-C14	-3.26	1.37	1.49
3	A	401	RET	C8-C9	-2.65	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	RET	C8-C9-C10	4.05	125.16	118.94
3	A	401	RET	C19-C9-C10	-3.87	117.50	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	RET	C2-C1-C6	3.59	116.01	110.48
3	A	401	RET	C12-C13-C14	3.43	129.67	118.80
3	A	401	RET	C20-C13-C14	-3.40	113.67	123.71
3	A	401	RET	C10-C11-C12	2.76	131.82	123.22
3	A	401	RET	C1-C6-C7	2.62	123.19	115.78

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

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

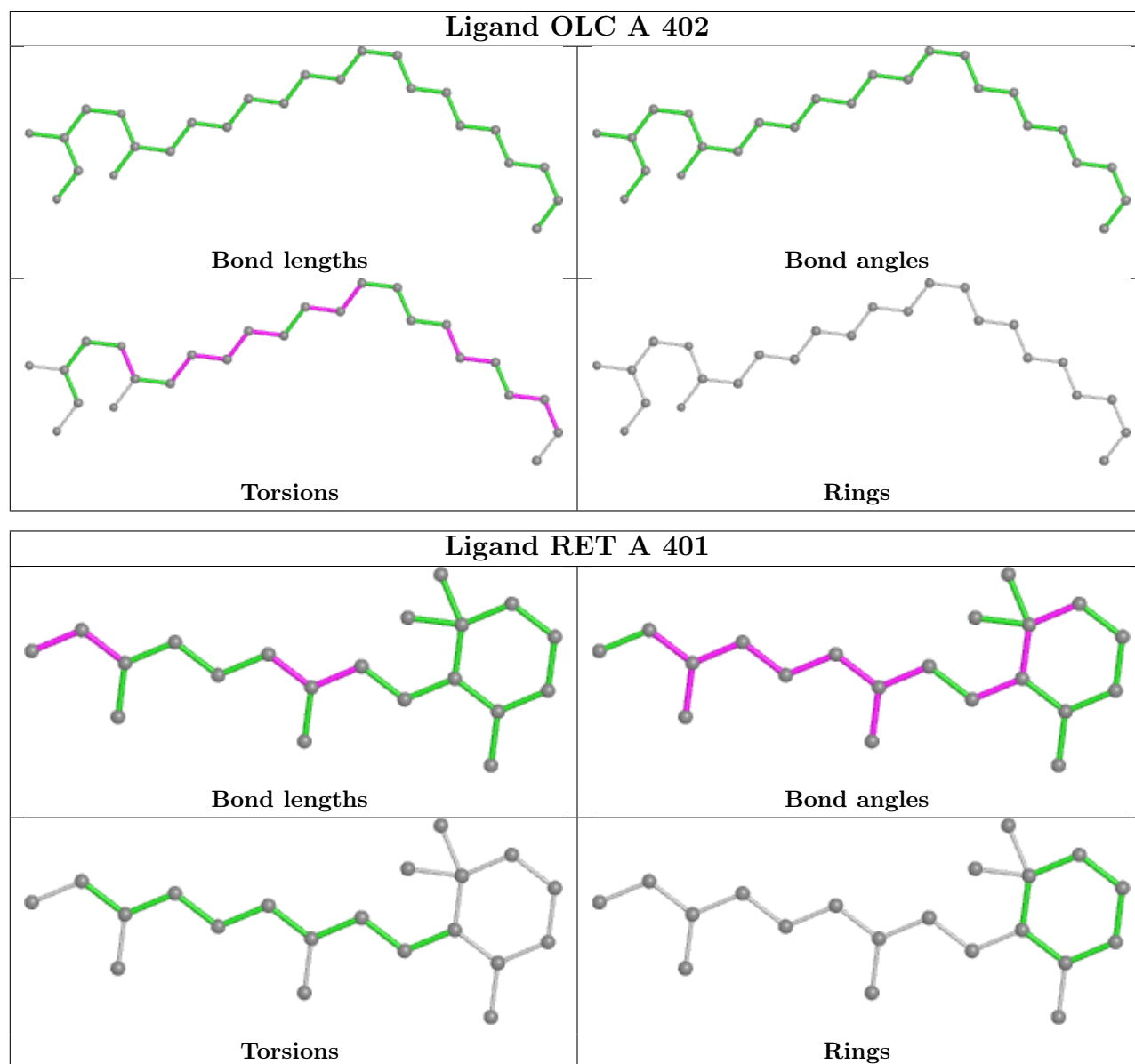
There are no ring outliers.

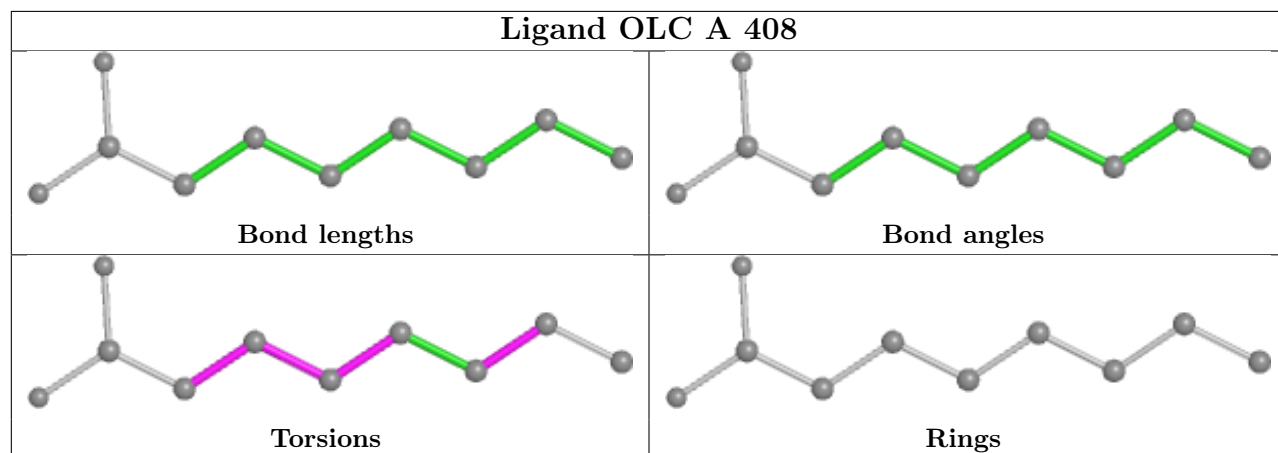
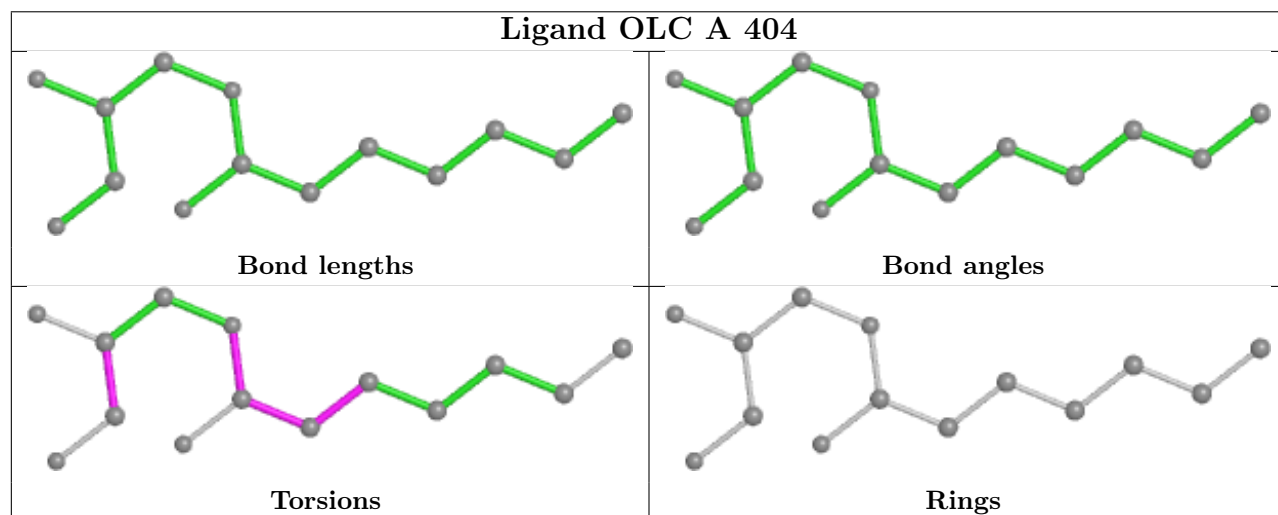
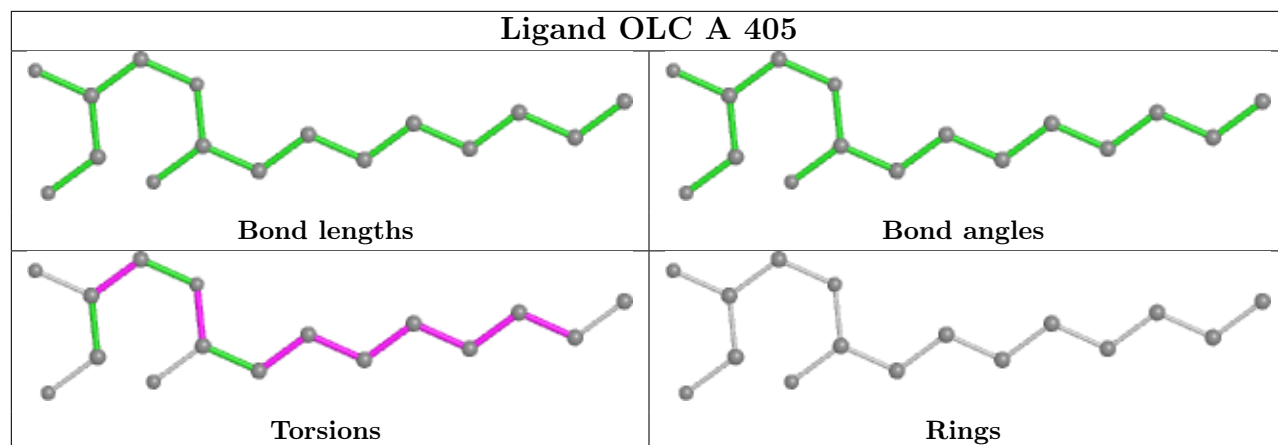
6 monomers are involved in 27 short contacts:

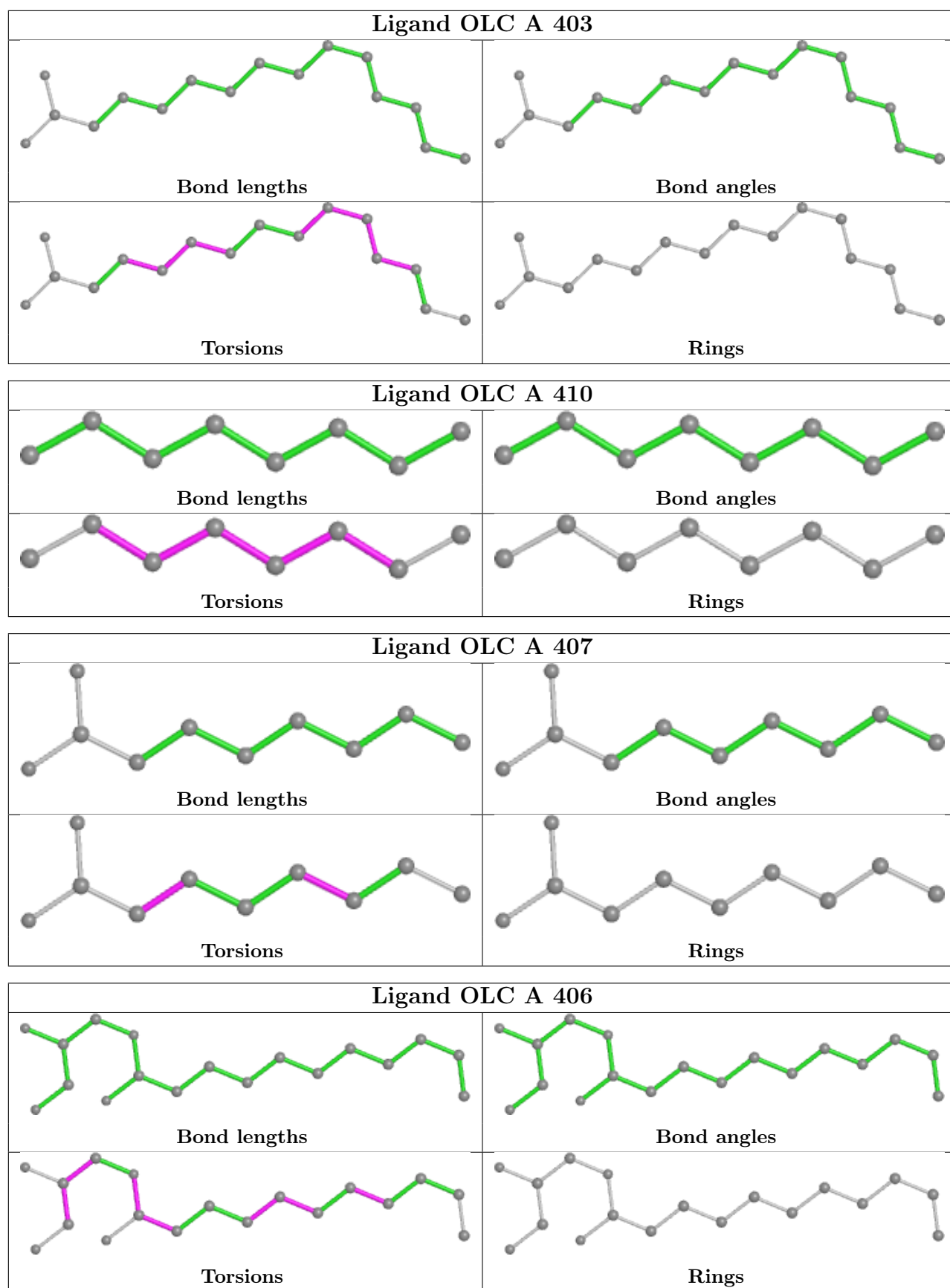
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	OLC	5	0
3	A	401	RET	3	0
4	A	403	OLC	11	0
4	A	407	OLC	1	0
4	A	406	OLC	5	0
4	A	409	OLC	2	0

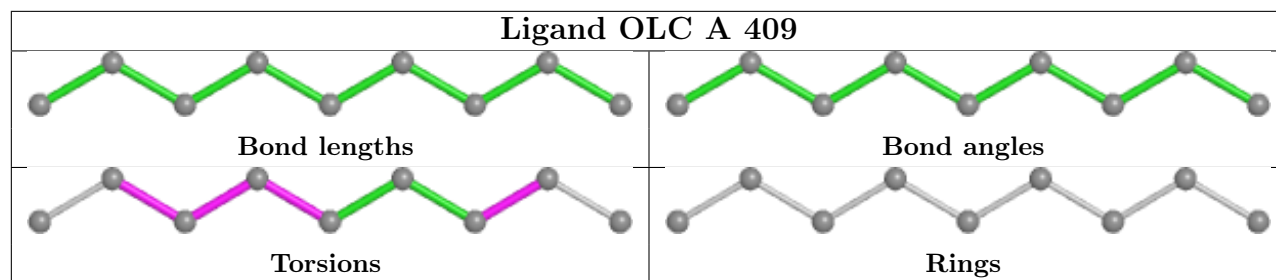
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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%)	2.19	127 (42%) 0 0	37, 72, 118, 173	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	ALA	14.0
1	A	229	PHE	11.7
1	A	84	THR	8.2
1	A	138	PHE	7.6
1	A	58	LEU	7.1
1	A	89	LEU	6.7
1	A	350	SER	6.5
1	A	191	LEU	6.4
1	A	337	THR	6.0
1	A	189	MET	5.9
1	A	86	ALA	5.6
1	A	182	ASN	5.5
1	A	211	TYR	5.4
1	A	93	ILE	5.3
1	A	338	LEU	5.2
1	A	325	LYS	5.0
1	A	256	TRP	5.0
1	A	96	TRP	4.9
1	A	139	HIS	4.9
1	A	322	LYS	4.9
1	A	61	ASN	4.8
1	A	352	ASP	4.7
1	A	192	LEU	4.7
1	A	282	TYR	4.7
1	A	340	GLU	4.6
1	A	341	ASP	4.6
1	A	313	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	92	ASN	4.6
1	A	190	GLY	4.5
1	A	172	ILE	4.4
1	A	221	LEU	4.4
1	A	326	LEU	4.3
1	A	131	ILE	4.3
1	A	179	GLY	4.3
1	A	278	VAL	4.3
1	A	140	GLU	4.2
1	A	310	ILE	4.2
1	A	141	PHE	4.1
1	A	219	MET	4.1
1	A	287	GLY	4.0
1	A	300	GLY	4.0
1	A	123	ILE	4.0
1	A	333	ILE	3.9
1	A	188	THR	3.9
1	A	291	ILE	3.9
1	A	311	HIS	3.9
1	A	220	GLY	3.8
1	A	169	VAL	3.7
1	A	217	PHE	3.7
1	A	245	GLY	3.6
1	A	260	VAL	3.6
1	A	178	THR	3.6
1	A	106	LEU	3.6
1	A	241	THR	3.5
1	A	228	PHE	3.5
1	A	133	PHE	3.4
1	A	328	ILE	3.4
1	A	108	PHE	3.4
1	A	142	ASP	3.4
1	A	66	CYS	3.4
1	A	225	ILE	3.4
1	A	297	ASN	3.4
1	A	345	ALA	3.3
1	A	180	LEU	3.3
1	A	199	ILE	3.3
1	A	269	PHE	3.3
1	A	119	GLY	3.2
1	A	320	ILE	3.2
1	A	283	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	118	CYS	3.2
1	A	293	LEU	3.2
1	A	65	ILE	3.1
1	A	315	LEU	3.1
1	A	249	GLN	3.1
1	A	299	TRP	3.1
1	A	101	LEU	3.0
1	A	110	GLY	3.0
1	A	97	ILE	3.0
1	A	70	ASN	3.0
1	A	130	MET	2.8
1	A	239	TYR	2.9
1	A	308	VAL	2.8
1	A	132	LYS	2.8
1	A	336	GLU	2.8
1	A	284	SER	2.8
1	A	209	LYS	2.8
1	A	314	ILE	2.7
1	A	105	CYS	2.6
1	A	194	SER	2.6
1	A	235	TYR	2.6
1	A	184	TYR	2.5
1	A	98	THR	2.5
1	A	255	ALA	2.5
1	A	324	THR	2.5
1	A	193	VAL	2.5
1	A	67	ILE	2.5
1	A	254	MET	2.5
1	A	223	TYR	2.4
1	A	279	LEU	2.4
1	A	323	THR	2.4
1	A	294	MET	2.4
1	A	187	ARG	2.4
1	A	78	TRP	2.4
1	A	238	ALA	2.4
1	A	163	TRP	2.3
1	A	94	LEU	2.3
1	A	87	GLU	2.3
1	A	88	LYS	2.3
1	A	90	ALA	2.3
1	A	177	LEU	2.3
1	A	339	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	164	LEU	2.2
1	A	129	GLU	2.2
1	A	196	ILE	2.2
1	A	175	SER	2.2
1	A	280	SER	2.2
1	A	240	HIS	2.1
1	A	331	THR	2.1
1	A	344	GLU	2.1
1	A	107	MET	2.1
1	A	134	ILE	2.1
1	A	124	TYR	2.0
1	A	95	GLN	2.0
1	A	270	ILE	2.0
1	A	73	CYS	2.0
1	A	74	PHE	2.0
1	A	266	PRO	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.

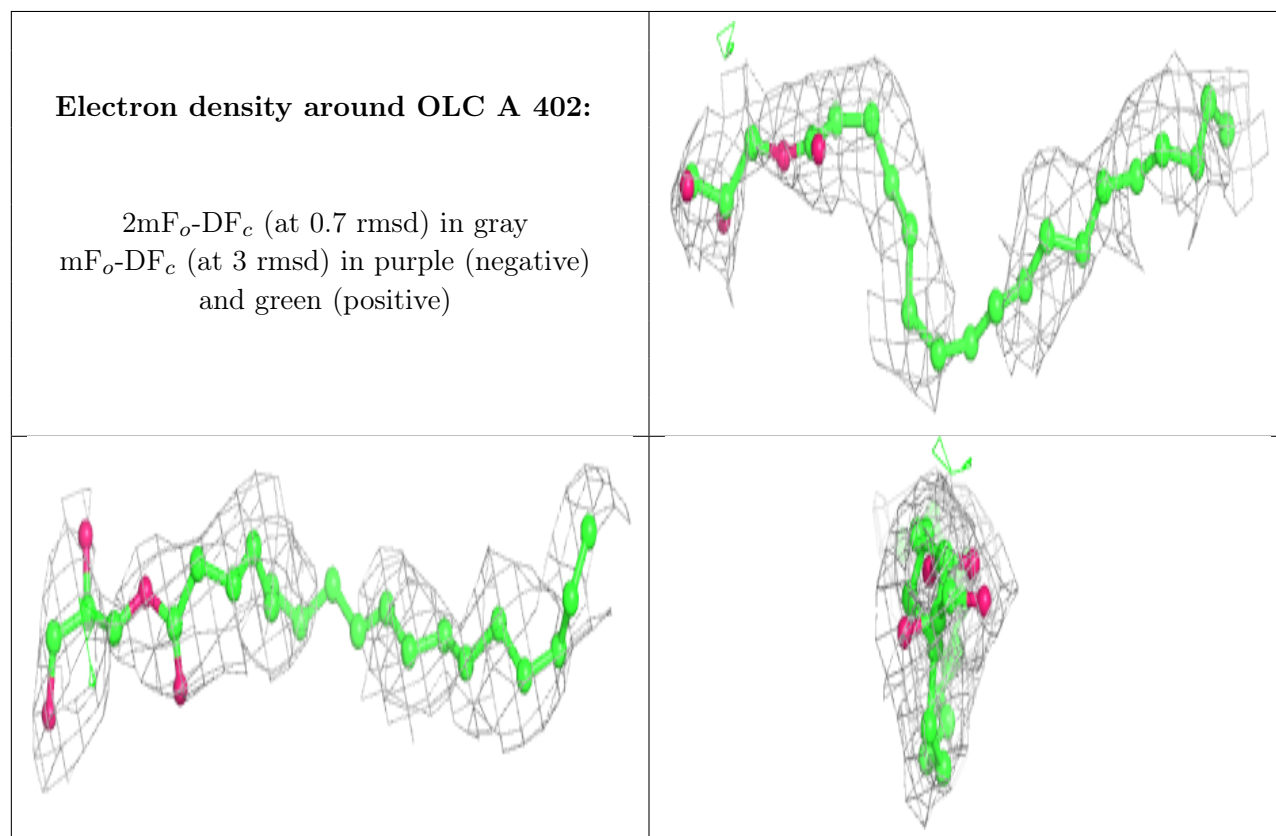
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	1	14/15	0.44	0.39	48,95,125,135	0
2	NAG	E	2	14/15	0.64	0.37	54,77,90,121	0

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.

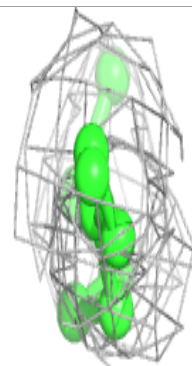
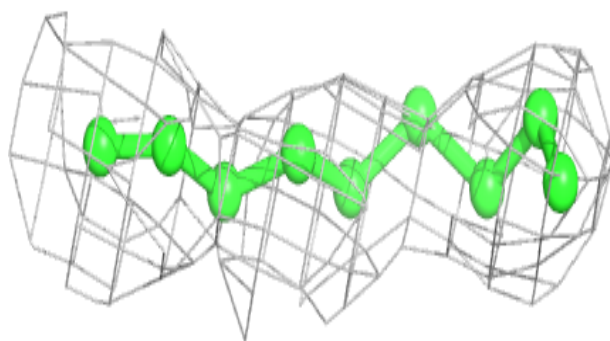
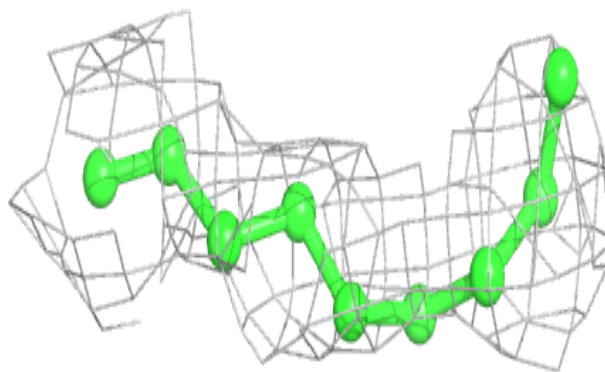
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OLC	A	402	25/25	0.30	0.39	58,79,100,104	0
4	OLC	A	409	9/25	0.46	0.27	58,65,76,83	0
4	OLC	A	403	16/25	0.48	0.26	53,63,85,89	0
4	OLC	A	410	8/25	0.56	0.39	67,84,98,105	0
4	OLC	A	406	18/25	0.61	0.33	48,59,77,78	0
4	OLC	A	404	14/25	0.71	0.36	46,76,101,107	0
3	RET	A	401	20/21	0.77	0.35	45,68,93,97	0
4	OLC	A	408	10/25	0.78	0.15	54,73,78,79	0
4	OLC	A	407	10/25	0.79	0.21	54,66,72,74	0
4	OLC	A	405	16/25	0.82	0.20	42,53,82,97	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.

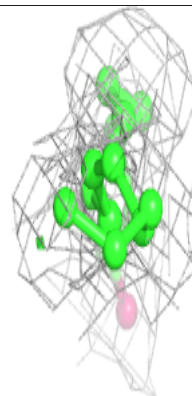
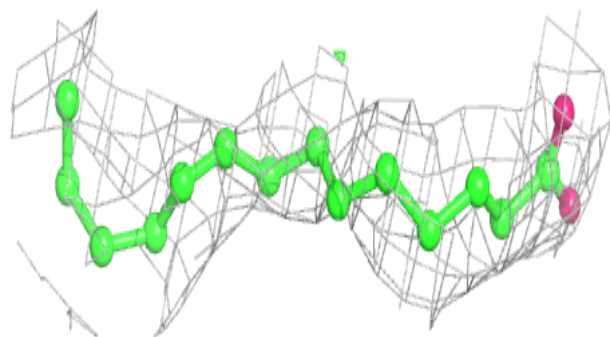
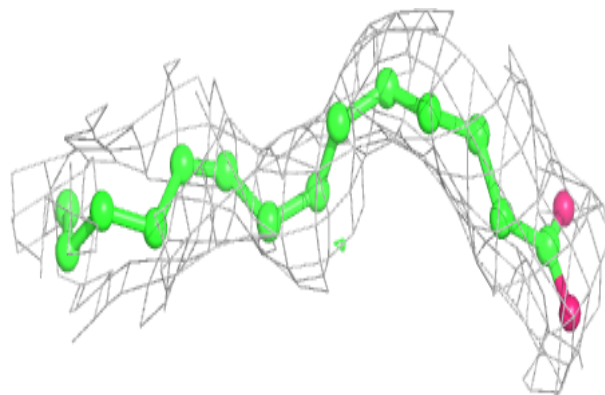


Electron density around OLC A 409:

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

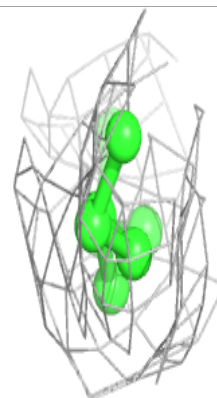
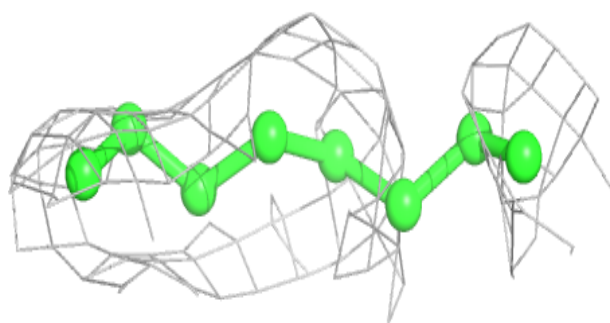
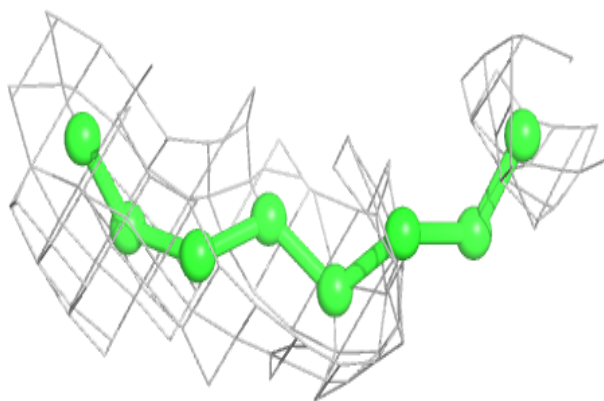
**Electron density around OLC A 403:**

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

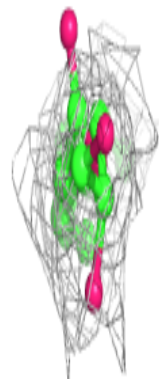
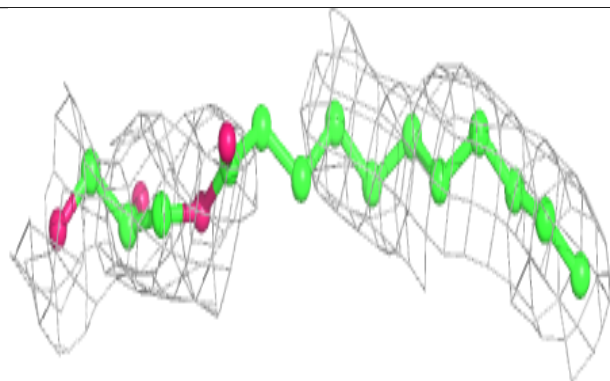
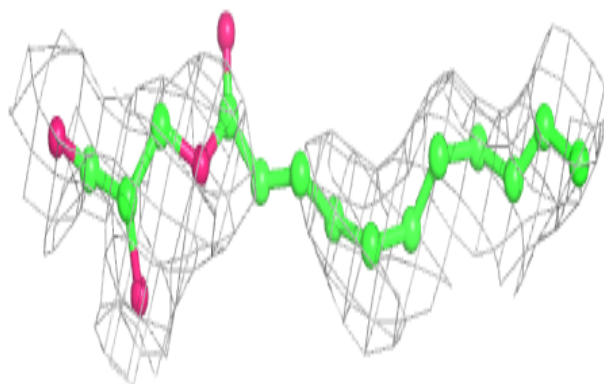


Electron density around OLC A 410:

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

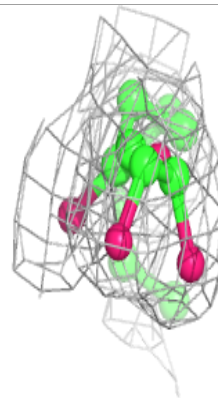
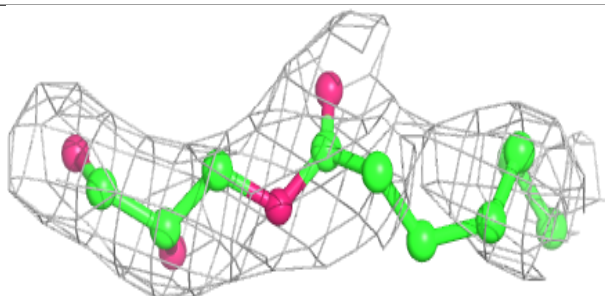
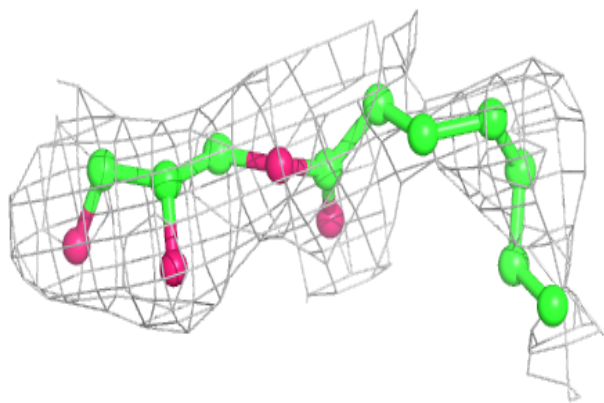
**Electron density around OLC A 406:**

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

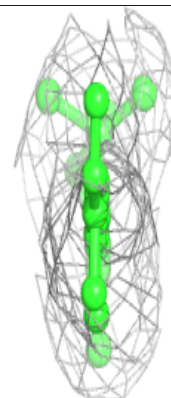
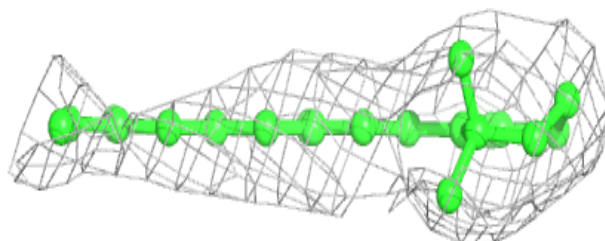
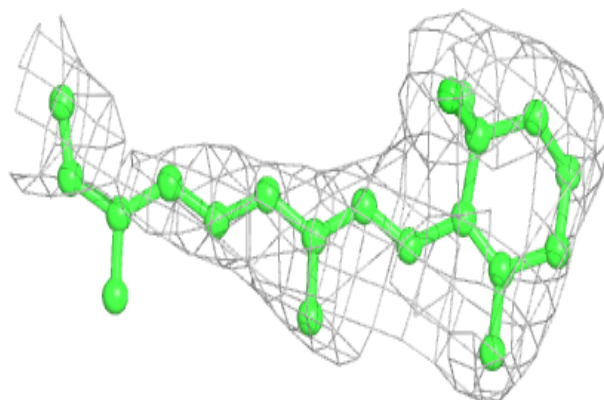


Electron density around OLC A 404:

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

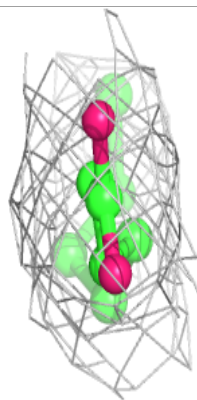
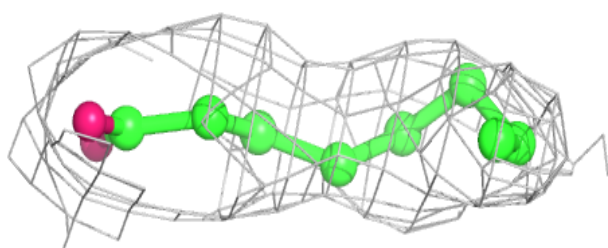
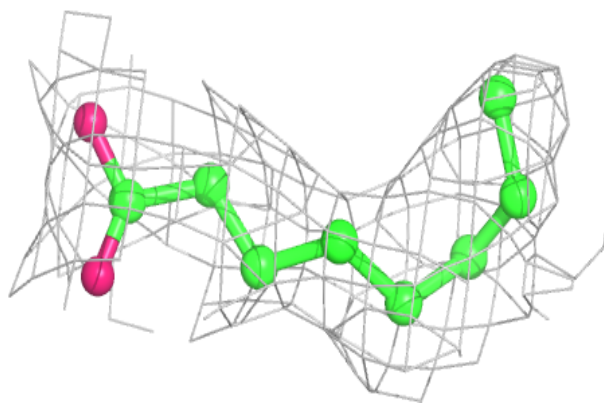
**Electron density around RET A 401:**

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

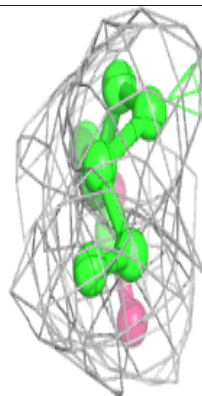
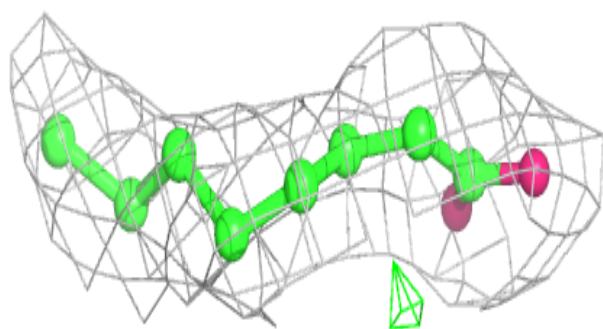
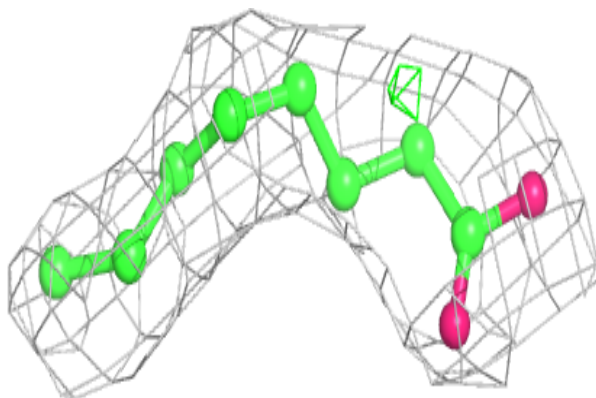


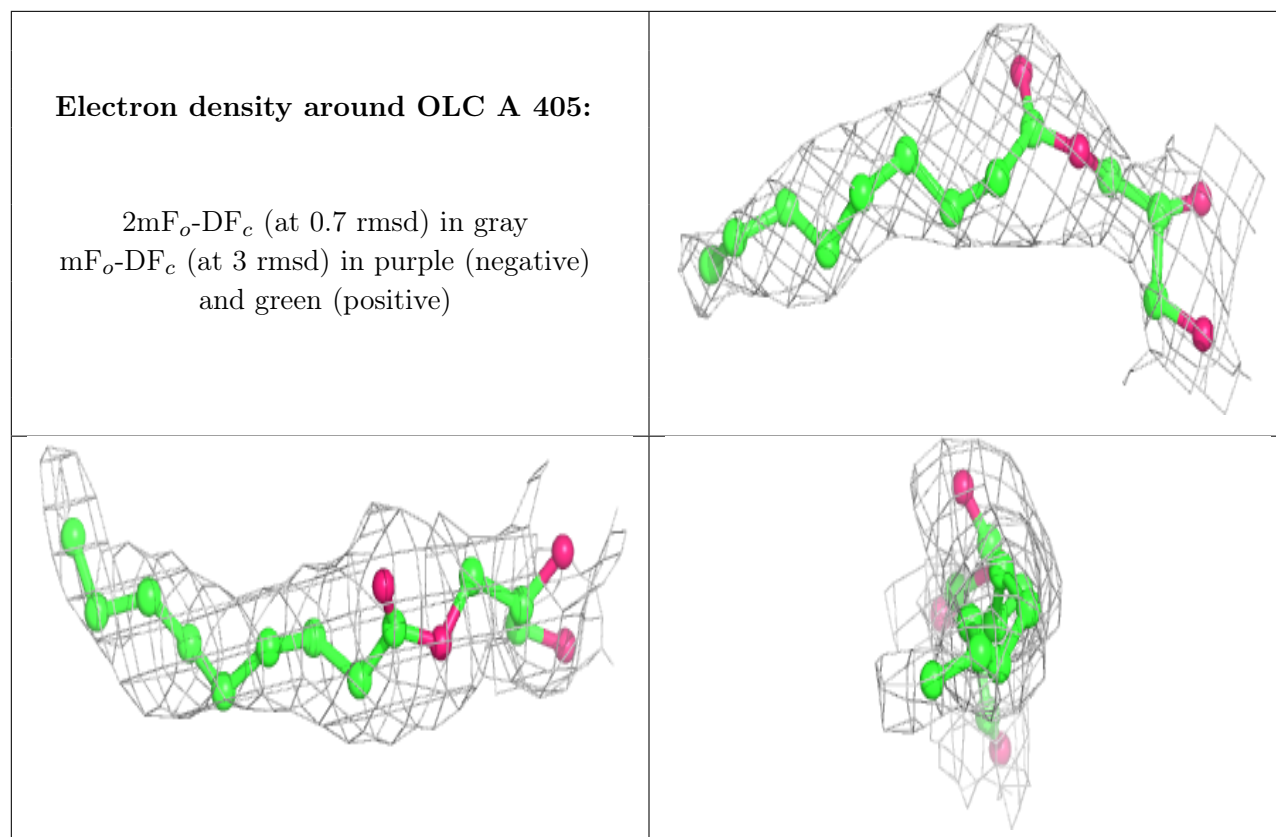
Electron density around OLC A 408:

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

**Electron density around OLC A 407:**

$2mF_o-DF_c$ (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.