Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 06:41 pm GMT

PDB ID	:	6RNK
Title	:	Crystal structure of a humanized (K18E, K269N) rat succinate receptor SUCNR1 (GPR91) in complex with a nanobody and antagonist NF-56-EJ40.
Authors	:	Haffke, M.; Jaakola, V.-P.
Deposited on	:	2019-05-08
Resolution	:	1.94 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 (i) 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 (i)) were used in the production of this report:

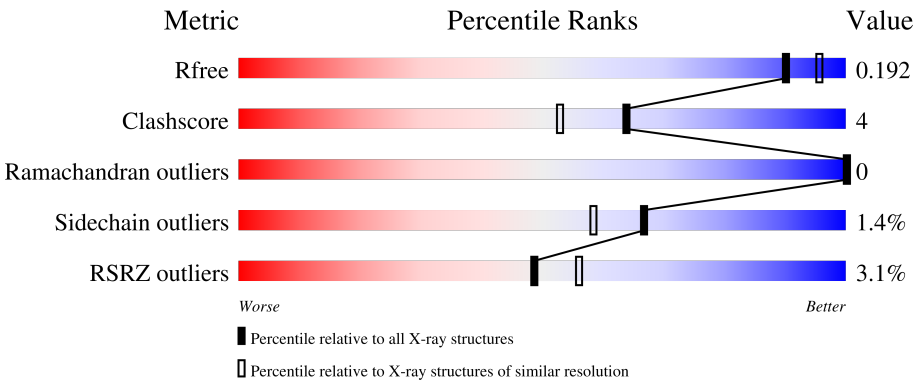
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	2% 76% 8% 17%
2	B	142	5% 82% 8% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	415	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3809 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 Succinate receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2319	1554	361	386	18	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP Q6IYF9
A	-5	TYR	-	expression tag	UNP Q6IYF9
A	-4	LYS	-	expression tag	UNP Q6IYF9
A	-3	ASP	-	expression tag	UNP Q6IYF9
A	-2	ASP	-	expression tag	UNP Q6IYF9
A	-1	ASP	-	expression tag	UNP Q6IYF9
A	0	ASP	-	expression tag	UNP Q6IYF9
A	1	LYS	-	expression tag	UNP Q6IYF9
A	18	GLU	LYS	engineered mutation	UNP Q6IYF9
A	269	ASN	LYS	engineered mutation	UNP Q6IYF9
A	318	LEU	-	expression tag	UNP Q6IYF9
A	319	GLU	-	expression tag	UNP Q6IYF9
A	320	VAL	-	expression tag	UNP Q6IYF9
A	321	LEU	-	expression tag	UNP Q6IYF9
A	322	PHE	-	expression tag	UNP Q6IYF9
A	323	GLN	-	expression tag	UNP Q6IYF9
A	324	GLY	-	expression tag	UNP Q6IYF9
A	325	PRO	-	expression tag	UNP Q6IYF9
A	326	HIS	-	expression tag	UNP Q6IYF9
A	327	HIS	-	expression tag	UNP Q6IYF9
A	328	HIS	-	expression tag	UNP Q6IYF9
A	329	HIS	-	expression tag	UNP Q6IYF9
A	330	HIS	-	expression tag	UNP Q6IYF9
A	331	HIS	-	expression tag	UNP Q6IYF9
A	332	HIS	-	expression tag	UNP Q6IYF9
A	333	HIS	-	expression tag	UNP Q6IYF9
A	334	HIS	-	expression tag	UNP Q6IYF9

Continued on next page...

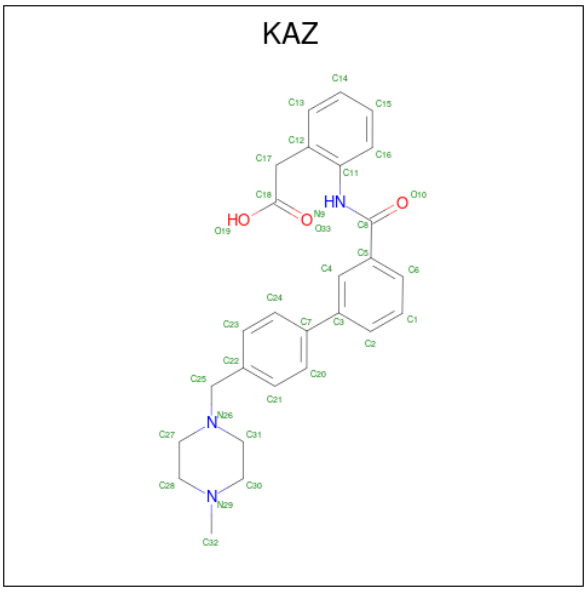
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP Q6IYF9

- Molecule 2 is a protein called Nanobody6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	129	962	599	164	194	5	0	0	0

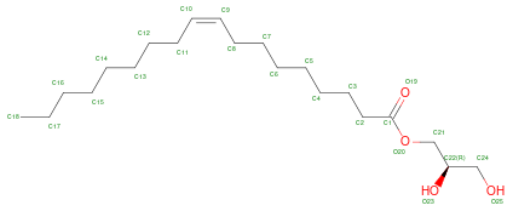
- Molecule 3 is 2-[2-[[3-[4-[(4-methylpiperazin-1-yl)methyl]phenyl]phenyl]carbonylamino]phenyl]ethanoic acid (three-letter code: KAZ) (formula: $C_{27}H_{29}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	27	3	3	0	0

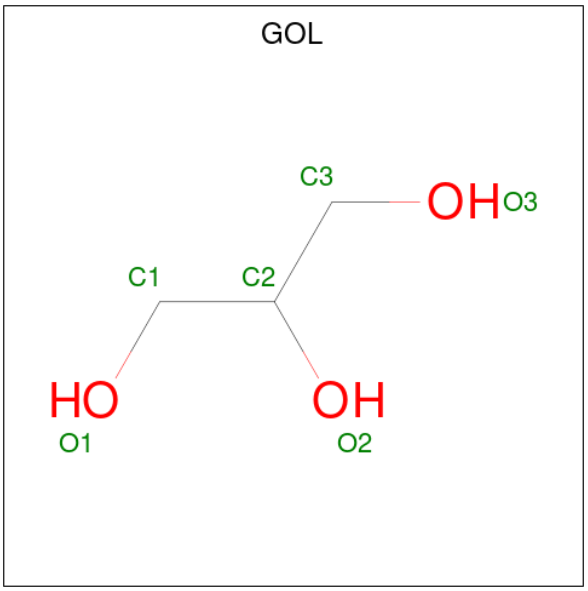
- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).

OLC



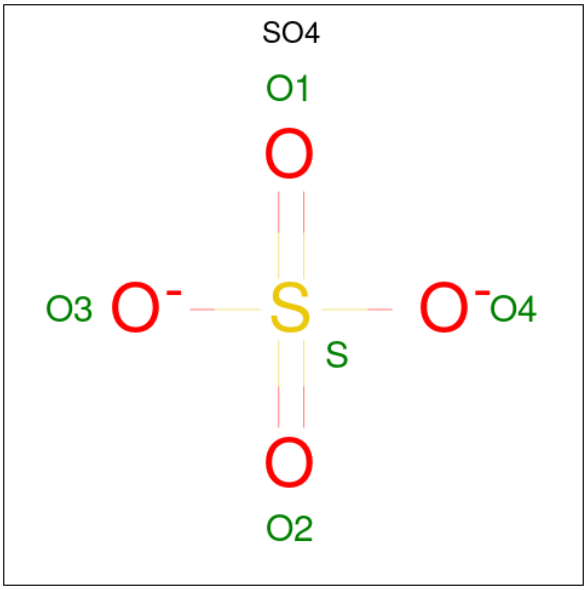
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	19	15	4	0	0
			Total	C	O		
4	A	1	19	15	4	0	0
			Total	C	O		
4	A	1	25	21	4	0	0
			Total	C	O		
4	A	1	19	15	4	0	0
			Total	C	O		
4	A	1	21	17	4	0	0
			Total	C	O		
4	A	1	14	10	4	0	0
			Total	C	O		
4	A	1	25	21	4	0	0
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	A	1	12	8	4	0	0
			Total	C	O		
4	A	1	11	7	4	0	0
			Total	C	O		
4	A	1	25	21	4	0	0
			Total	C	O		
4	A	1	17	13	4	0	0
			Total	C	O		
4	A	1	25	21	4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0

- Molecule 7 is water.

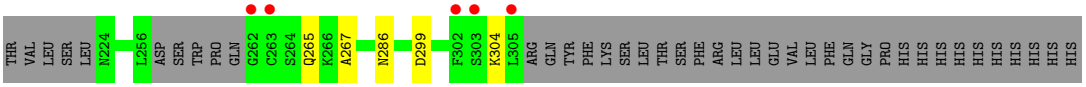
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	159	159	159	0	0
			Total	O		
7	B	83	83	83	0	0

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.

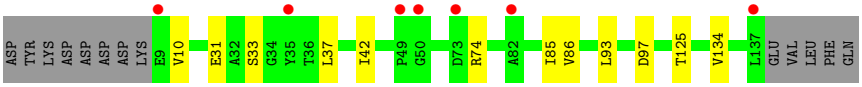
• Molecule 1: Succinate receptor 1

Chain A:



• Molecule 2: Nanobody6

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	76.83Å 150.93Å 68.23Å 90.00° 112.42° 90.00°	Depositor
Resolution (Å)	75.47 – 1.94 75.47 – 1.94	Depositor EDS
% Data completeness (in resolution range)	76.6 (75.47-1.94) 76.7 (75.47-1.94)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.94Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.177 , 0.199 0.180 , 0.192	Depositor DCC
R_{free} test set	1992 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3809	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KAZ, SO4, GOL, 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	0.53	0/2380	0.58	0/3230
2	B	0.47	0/980	0.66	0/1329
All	All	0.52	0/3360	0.61	0/4559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2319	0	2382	22	0
2	B	962	0	913	6	0
3	A	33	0	0	0	0
4	A	242	0	336	13	0
5	A	6	0	8	5	0
6	A	5	0	0	0	0
7	A	159	0	0	2	0
7	B	83	0	0	0	0
All	All	3809	0	3639	30	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 4.

All (30) 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:132:LYS:HB2	4:A:404:OLC:H21	1.61	0.81
2:B:31:GLU:HG2	2:B:85:ILE:HG12	1.69	0.73
1:A:131:LYS:HD2	4:A:404:OLC:H2A	1.73	0.70
1:A:267:ALA:HB1	4:A:413:OLC:H3	1.76	0.68
1:A:133:GLU:OE2	4:A:404:OLC:H3	1.97	0.65
1:A:170:ASP:HB2	5:A:415:GOL:C3	2.27	0.64
1:A:170:ASP:HB2	5:A:415:GOL:H31	1.84	0.59
2:B:37:LEU:HD11	2:B:42:ILE:HD11	1.85	0.59
4:A:404:OLC:H21A	7:A:521:HOH:O	2.03	0.58
1:A:99:HIS:HB3	1:A:150:VAL:HG22	1.87	0.57
1:A:131:LYS:HG3	4:A:404:OLC:H6	1.89	0.55
1:A:170:ASP:HB2	5:A:415:GOL:H32	1.91	0.53
1:A:95:ARG:HH12	5:A:415:GOL:H31	1.74	0.53
1:A:36:GLY:HA3	7:A:507:HOH:O	2.12	0.49
1:A:182:ILE:HG12	4:A:411:OLC:H24A	1.95	0.49
1:A:67:ALA:HA	4:A:407:OLC:H3	1.93	0.49
4:A:402:OLC:H2A	4:A:403:OLC:H4	1.95	0.48
1:A:95:ARG:HH22	5:A:415:GOL:H31	1.79	0.47
1:A:51:TRP:CZ3	4:A:406:OLC:H2	2.49	0.47
1:A:201:PHE:HB2	4:A:408:OLC:H3A	1.97	0.47
1:A:129:LEU:HD23	1:A:134:PHE:CE2	2.50	0.47
1:A:84:TRP:CZ2	1:A:86:TYR:HB2	2.50	0.47
1:A:65:ASP:OD2	1:A:286:ASN:OD1	2.33	0.46
2:B:10:VAL:HG23	2:B:125:THR:HG21	1.99	0.45
2:B:74:ARG:HH22	2:B:97:ASP:CG	2.20	0.45
1:A:71:THR:HG22	4:A:407:OLC:H24	1.98	0.44
1:A:51:TRP:CZ2	4:A:409:OLC:H24	2.53	0.43
2:B:93:LEU:HB3	2:B:134:VAL:HG21	2.03	0.41
2:B:42:ILE:HG13	2:B:86:VAL:HG21	2.03	0.41
1:A:47:CYS:SG	1:A:304:LYS:HG3	2.61	0.41

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	279/342 (82%)	275 (99%)	4 (1%)	0	100	100
2	B	127/142 (89%)	121 (95%)	6 (5%)	0	100	100
All	All	406/484 (84%)	396 (98%)	10 (2%)	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	260/315 (82%)	256 (98%)	4 (2%)	65	56
2	B	102/118 (86%)	101 (99%)	1 (1%)	76	71
All	All	362/433 (84%)	357 (99%)	5 (1%)	67	58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	77	ARG
1	A	265	GLN
1	A	299	ASP
2	B	33	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
6	SO4	A	416	-	4,4,4	0.22	0	6,6,6	0.14	0
4	OLC	A	403	-	18,18,24	0.73	0	18,19,25	0.52	0
4	OLC	A	413	-	16,16,24	0.76	0	17,17,25	0.48	0
3	KAZ	A	401	-	36,36,36	1.05	1 (2%)	49,49,49	1.01	3 (6%)
4	OLC	A	405	-	18,18,24	0.70	0	18,19,25	0.65	0
4	OLC	A	407	-	13,13,24	0.71	0	14,14,25	0.50	0
5	GOL	A	415	-	5,5,5	0.58	0	5,5,5	0.48	0
4	OLC	A	406	-	20,20,24	0.66	0	21,21,25	0.47	0
4	OLC	A	412	-	24,24,24	0.70	0	25,25,25	0.43	0
4	OLC	A	404	-	24,24,24	0.77	0	25,25,25	0.63	0
4	OLC	A	409	-	9,9,24	0.70	0	10,10,25	0.63	0
4	OLC	A	414	-	24,24,24	0.72	0	25,25,25	0.57	0
4	OLC	A	402	-	18,18,24	0.63	0	18,19,25	0.62	0
4	OLC	A	408	-	24,24,24	0.71	0	25,25,25	0.53	0
4	OLC	A	411	-	10,10,24	0.72	0	11,11,25	0.53	0
4	OLC	A	410	-	11,11,24	0.74	0	12,12,25	0.48	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	403	-	-	14/18/18/24	-
4	OLC	A	413	-	-	5/16/16/24	-
3	KAZ	A	401	-	-	0/20/30/30	0/4/4/4
4	OLC	A	405	-	-	7/18/18/24	-
4	OLC	A	407	-	-	8/13/13/24	-
5	GOL	A	415	-	-	4/4/4/4	-
4	OLC	A	406	-	-	9/20/20/24	-
4	OLC	A	412	-	-	14/24/24/24	-
4	OLC	A	404	-	-	14/24/24/24	-
4	OLC	A	409	-	-	2/9/9/24	-
4	OLC	A	414	-	-	13/24/24/24	-
4	OLC	A	402	-	-	8/18/18/24	-
4	OLC	A	408	-	-	10/24/24/24	-
4	OLC	A	411	-	-	5/10/10/24	-
4	OLC	A	410	-	-	4/11/11/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	KAZ	C17-C12	2.04	1.54	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	KAZ	O10-C8-C5	-3.24	115.16	120.94
3	A	401	KAZ	C30-N29-C28	2.84	113.50	109.52
3	A	401	KAZ	C5-C8-N9	2.50	121.42	115.92

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	OLC	C9-C10-C11-C12
4	A	404	OLC	O20-C21-C22-C24
4	A	407	OLC	O20-C21-C22-C24
4	A	408	OLC	C21-C22-C24-O25
4	A	411	OLC	C21-C22-C24-O25
4	A	411	OLC	O20-C21-C22-O23
4	A	414	OLC	O20-C21-C22-O23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	415	GOL	C1-C2-C3-O3
4	A	408	OLC	O19-C1-O20-C21
4	A	412	OLC	O19-C1-O20-C21
4	A	411	OLC	O19-C1-O20-C21
4	A	406	OLC	C2-C1-O20-C21
4	A	408	OLC	C2-C1-O20-C21
4	A	412	OLC	C2-C1-O20-C21
4	A	411	OLC	C2-C1-O20-C21
4	A	406	OLC	O19-C1-O20-C21
4	A	407	OLC	O20-C21-C22-O23
4	A	412	OLC	C2-C3-C4-C5
4	A	405	OLC	C2-C1-O20-C21
4	A	409	OLC	C2-C1-O20-C21
4	A	412	OLC	C1-C2-C3-C4
4	A	409	OLC	O19-C1-O20-C21
4	A	404	OLC	O20-C21-C22-O23
4	A	406	OLC	C1-C2-C3-C4
4	A	405	OLC	O19-C1-O20-C21
4	A	403	OLC	O20-C21-C22-O23
4	A	406	OLC	O20-C21-C22-O23
4	A	402	OLC	C2-C1-O20-C21
4	A	414	OLC	C5-C6-C7-C8
4	A	406	OLC	O20-C21-C22-C24
4	A	411	OLC	O20-C21-C22-C24
4	A	403	OLC	C2-C3-C4-C5
4	A	408	OLC	C13-C14-C15-C16
4	A	404	OLC	C11-C12-C13-C14
4	A	402	OLC	C21-C22-C24-O25
4	A	403	OLC	C21-C22-C24-O25
4	A	404	OLC	C21-C22-C24-O25
5	A	415	GOL	O1-C1-C2-C3
4	A	407	OLC	C1-C2-C3-C4
4	A	412	OLC	C11-C12-C13-C14
4	A	412	OLC	C12-C13-C14-C15
4	A	414	OLC	C11-C12-C13-C14
4	A	413	OLC	C2-C1-O20-C21
4	A	402	OLC	C5-C6-C7-C8
4	A	407	OLC	C3-C4-C5-C6
5	A	415	GOL	O2-C2-C3-O3
4	A	404	OLC	C14-C15-C16-C17
4	A	404	OLC	C5-C6-C7-C8
4	A	406	OLC	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	404	OLC	C10-C11-C12-C13
4	A	410	OLC	C1-C2-C3-C4
4	A	412	OLC	C14-C15-C16-C17
4	A	402	OLC	O19-C1-O20-C21
4	A	412	OLC	C4-C5-C6-C7
4	A	413	OLC	O19-C1-O20-C21
4	A	405	OLC	C3-C4-C5-C6
4	A	403	OLC	C5-C6-C7-C8
4	A	412	OLC	C10-C11-C12-C13
4	A	403	OLC	O20-C21-C22-C24
4	A	410	OLC	O20-C21-C22-C24
4	A	412	OLC	C13-C14-C15-C16
4	A	403	OLC	C4-C5-C6-C7
4	A	405	OLC	C1-C2-C3-C4
4	A	405	OLC	C6-C7-C8-C9
4	A	403	OLC	C6-C7-C8-C9
4	A	414	OLC	C12-C13-C14-C15
4	A	408	OLC	C15-C16-C17-C18
4	A	404	OLC	C6-C7-C8-C9
4	A	413	OLC	C6-C7-C8-C9
4	A	414	OLC	C6-C7-C8-C9
4	A	407	OLC	C2-C3-C4-C5
4	A	414	OLC	C9-C10-C11-C12
4	A	404	OLC	C1-C2-C3-C4
4	A	404	OLC	C15-C16-C17-C18
4	A	414	OLC	C3-C4-C5-C6
4	A	402	OLC	O23-C22-C24-O25
4	A	407	OLC	C4-C5-C6-C7
4	A	412	OLC	C15-C16-C17-C18
4	A	402	OLC	C6-C7-C8-C9
4	A	408	OLC	C9-C10-C11-C12
4	A	403	OLC	C3-C4-C5-C6
4	A	404	OLC	C2-C1-O20-C21
4	A	407	OLC	C2-C1-O20-C21
4	A	412	OLC	O20-C21-C22-C24
4	A	407	OLC	O19-C1-O20-C21
4	A	414	OLC	O19-C1-O20-C21
4	A	405	OLC	C2-C3-C4-C5
4	A	410	OLC	O20-C21-C22-O23
4	A	414	OLC	O20-C21-C22-C24
4	A	414	OLC	C2-C1-O20-C21
4	A	404	OLC	O19-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	415	GOL	O1-C1-C2-O2
4	A	404	OLC	C13-C14-C15-C16
4	A	410	OLC	C2-C3-C4-C5
4	A	414	OLC	C13-C14-C15-C16
4	A	402	OLC	C1-C2-C3-C4
4	A	403	OLC	O23-C22-C24-O25
4	A	408	OLC	O23-C22-C24-O25
4	A	413	OLC	C4-C5-C6-C7
4	A	414	OLC	C7-C8-C9-C10
4	A	405	OLC	O20-C1-C2-C3
4	A	403	OLC	C7-C8-C9-C10
4	A	413	OLC	C7-C8-C9-C10
4	A	406	OLC	C3-C4-C5-C6
4	A	406	OLC	C9-C10-C11-C12
4	A	403	OLC	C2-C1-O20-C21
4	A	403	OLC	O19-C1-O20-C21
4	A	414	OLC	C2-C3-C4-C5
4	A	406	OLC	C10-C11-C12-C13
4	A	404	OLC	C7-C8-C9-C10
4	A	408	OLC	C14-C15-C16-C17
4	A	403	OLC	O20-C1-C2-C3
4	A	408	OLC	O20-C21-C22-O23
4	A	412	OLC	C9-C10-C11-C12
4	A	412	OLC	C21-C22-C24-O25
4	A	408	OLC	C11-C12-C13-C14
4	A	403	OLC	O19-C1-C2-C3

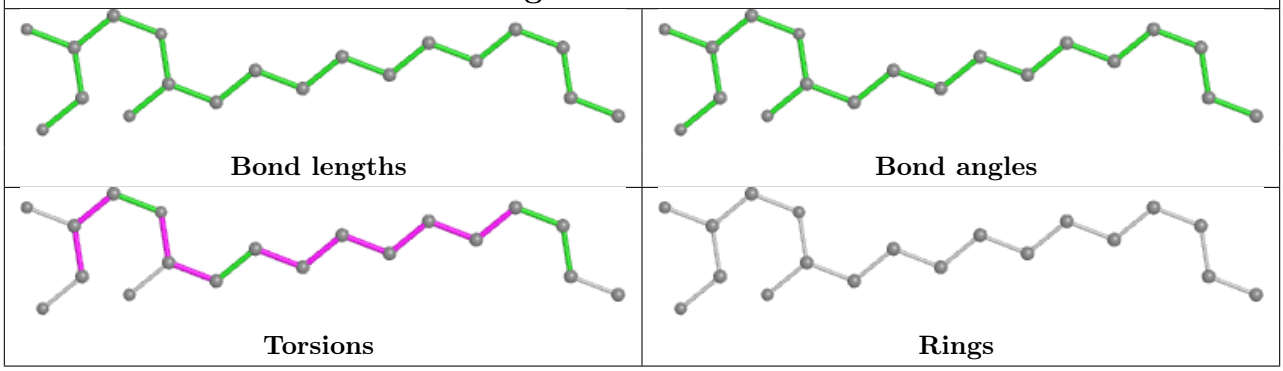
There are no ring outliers.

10 monomers are involved in 18 short contacts:

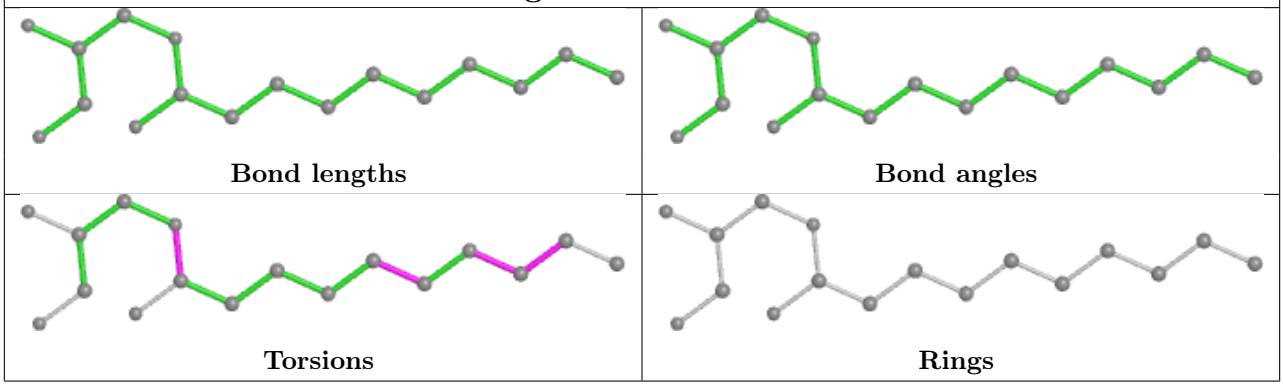
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	OLC	1	0
4	A	413	OLC	1	0
4	A	407	OLC	2	0
5	A	415	GOL	5	0
4	A	406	OLC	1	0
4	A	404	OLC	5	0
4	A	409	OLC	1	0
4	A	402	OLC	1	0
4	A	408	OLC	1	0
4	A	411	OLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

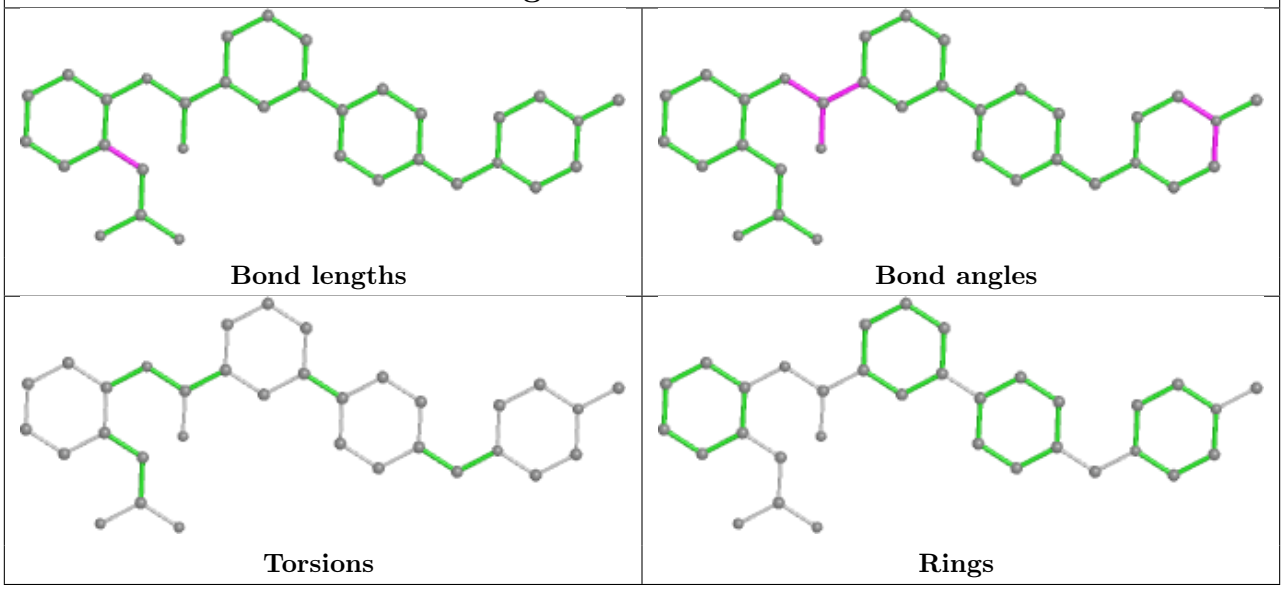
Ligand OLC A 403



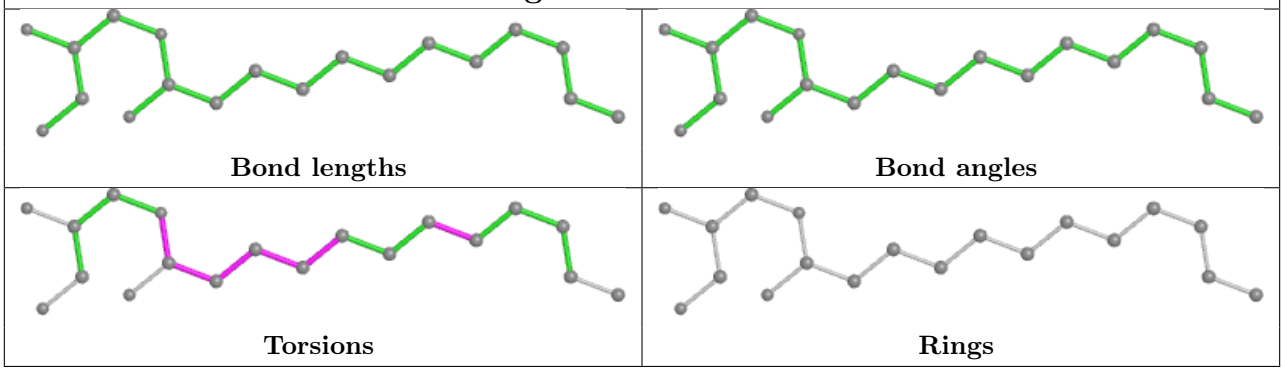
Ligand OLC A 413



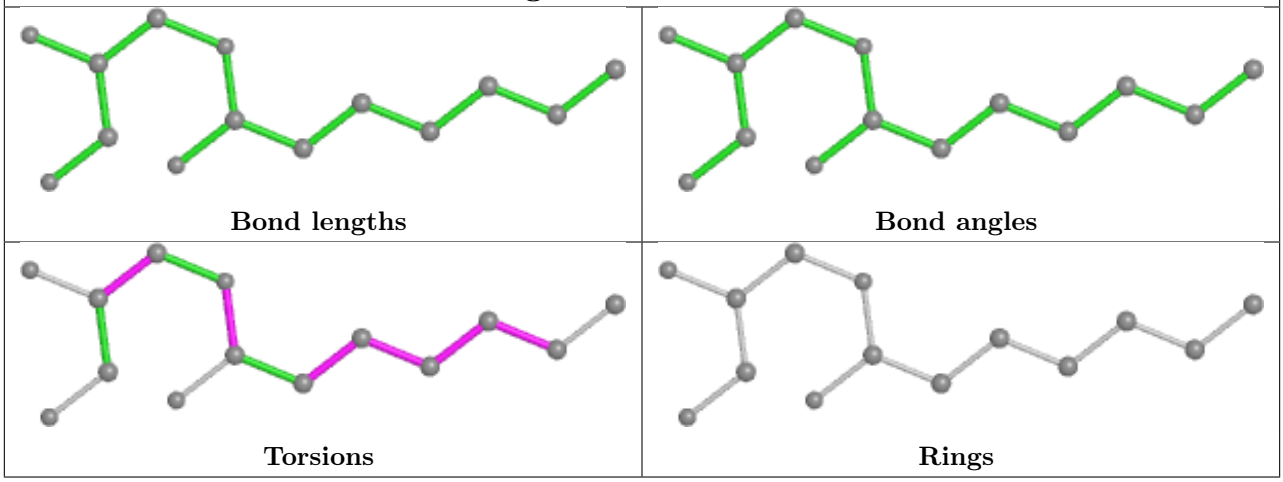
Ligand KAZ A 401



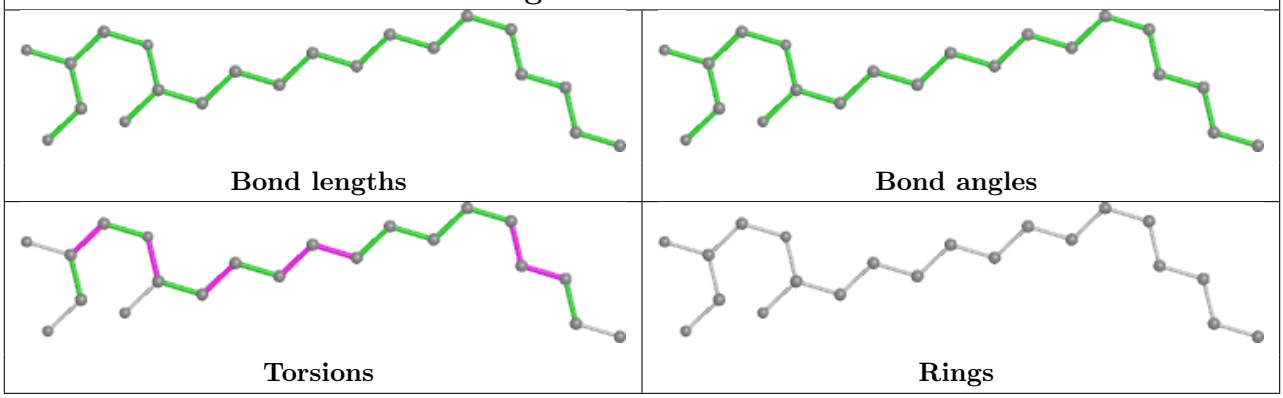
Ligand OLC A 405



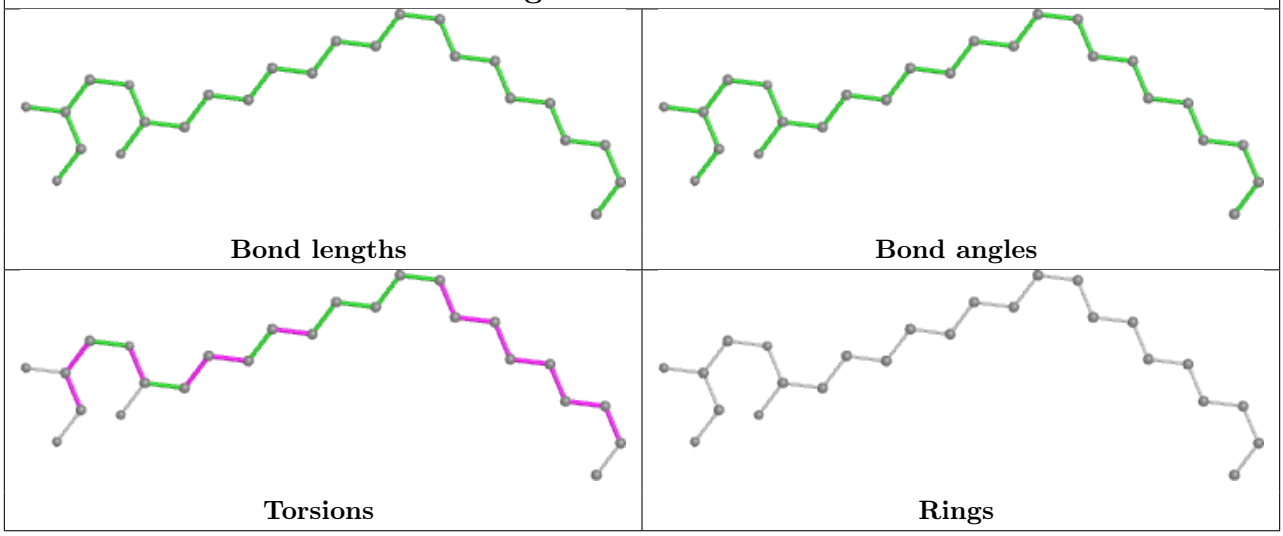
Ligand OLC A 407



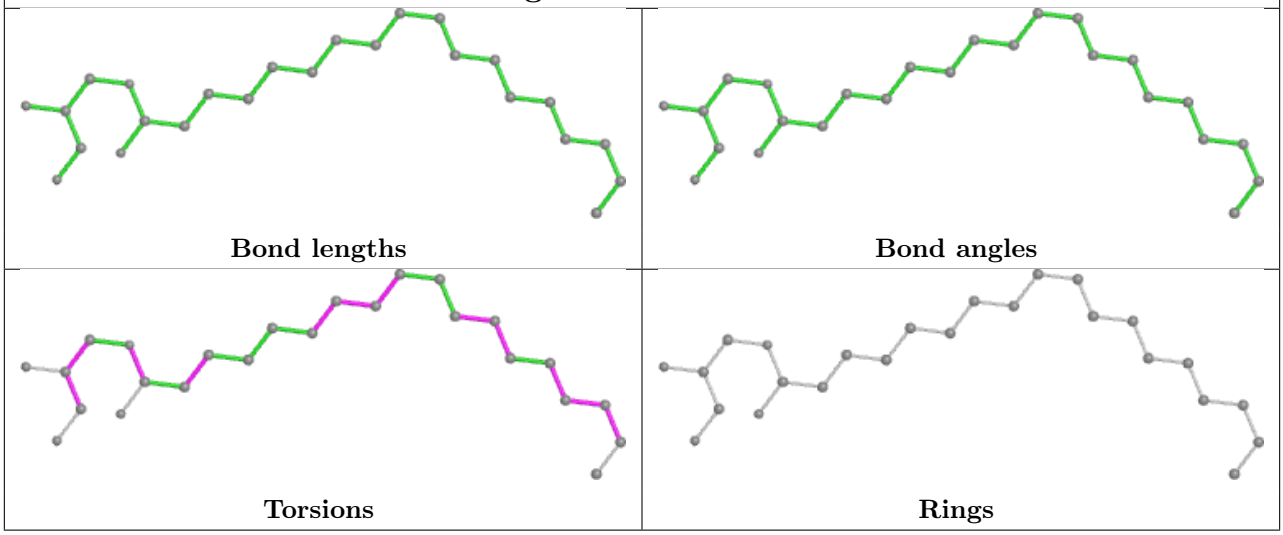
Ligand OLC A 406



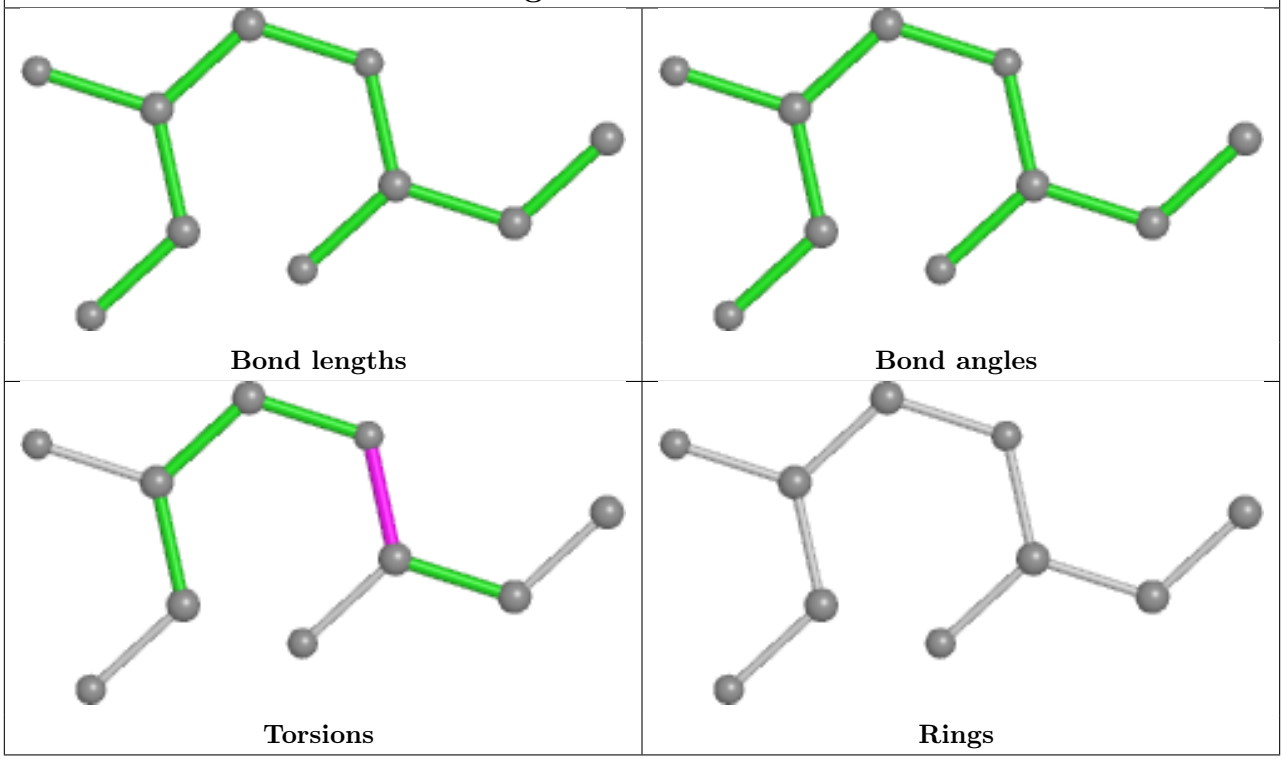
Ligand OLC A 412



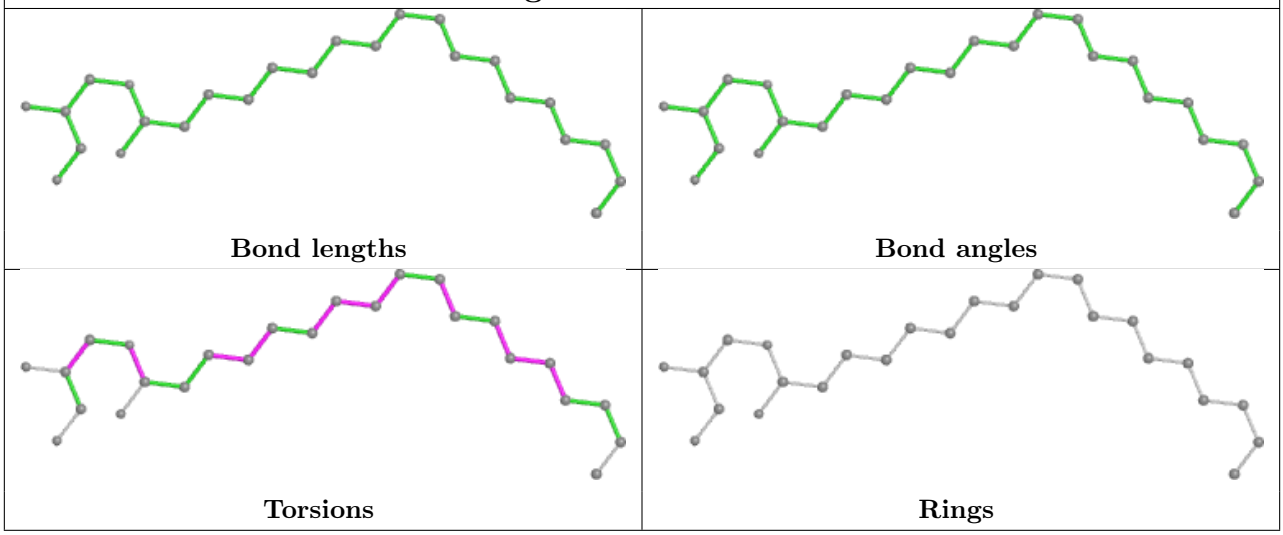
Ligand OLC A 404



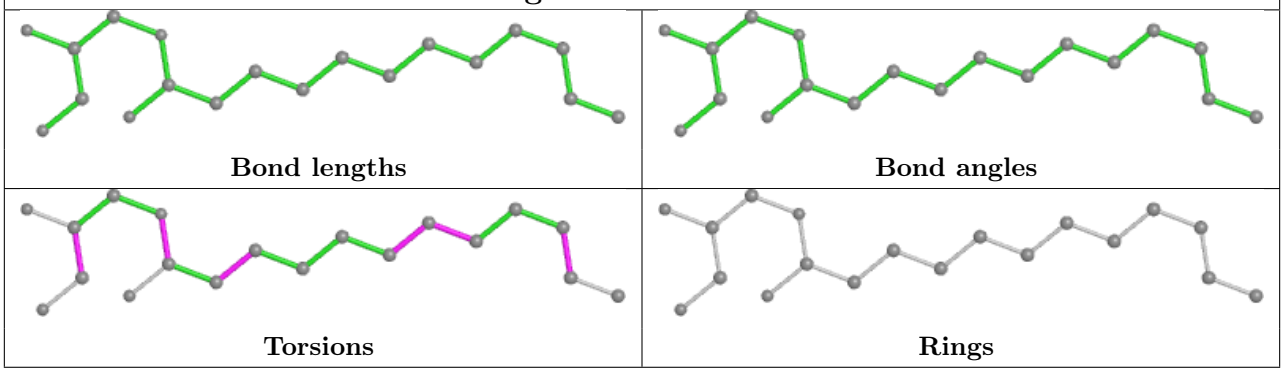
Ligand OLC A 409



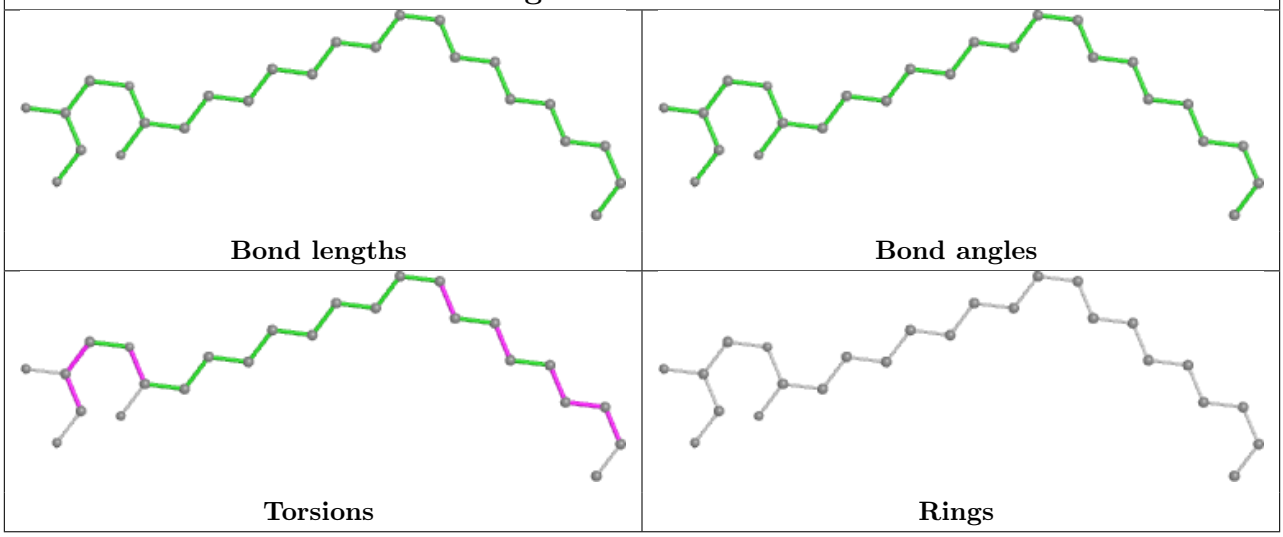
Ligand OLC A 414



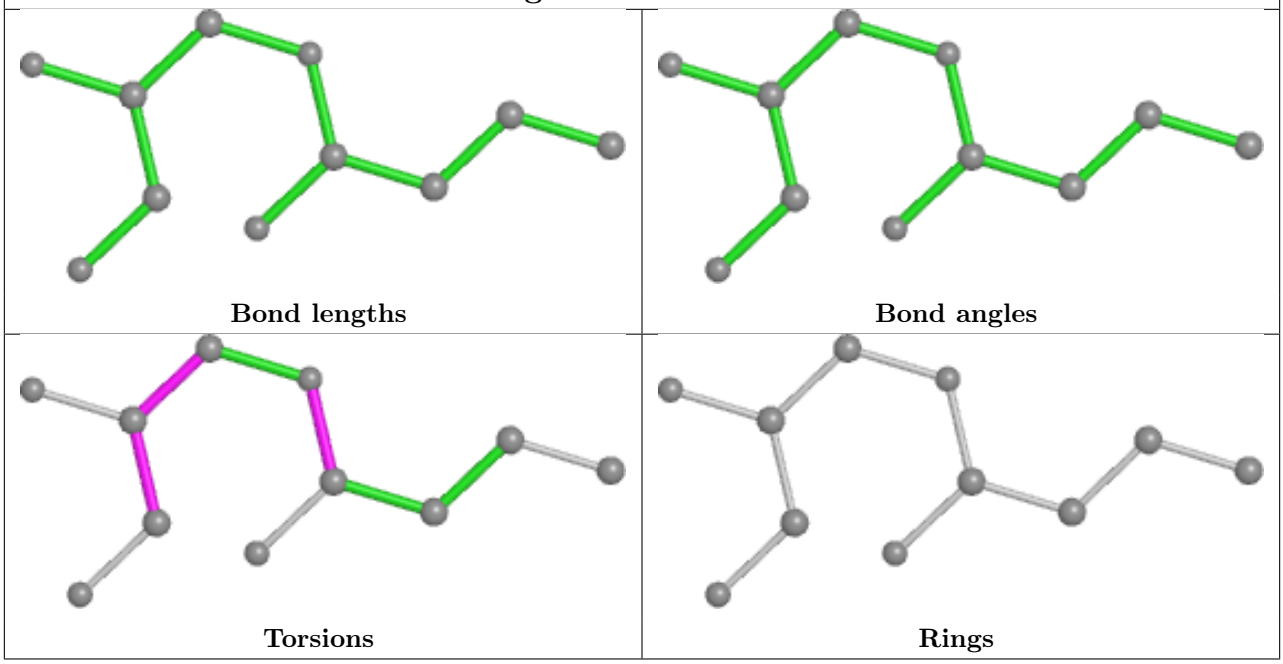
Ligand OLC A 402

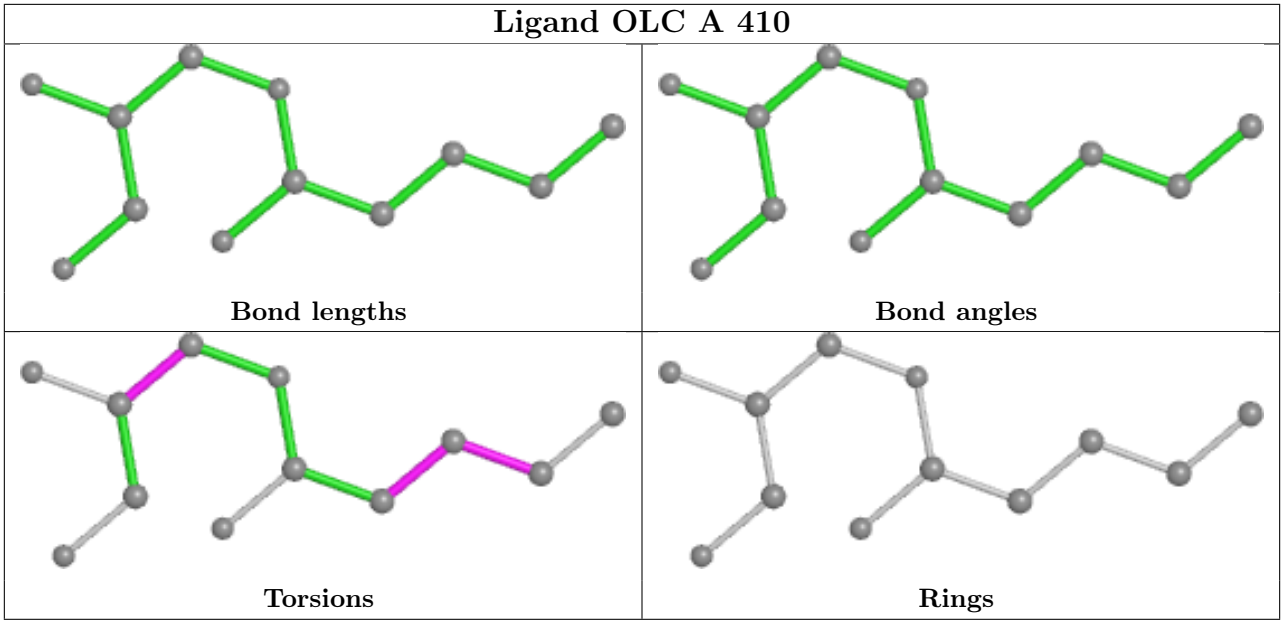


Ligand OLC A 408



Ligand OLC A 411





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	285/342 (83%)	-0.13	6 (2%)	63	70	27, 36, 72, 119	0
2	B	129/142 (90%)	0.00	7 (5%)	25	32	29, 41, 78, 100	0
All	All	414/484 (85%)	-0.09	13 (3%)	49	56	27, 38, 76, 119	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	35	TYR	6.2
1	A	262	GLY	5.2
1	A	305	LEU	4.5
2	B	137	LEU	4.3
1	A	302	PHE	4.1
1	A	303	SER	3.3
2	B	50	GLY	2.8
2	B	49	PRO	2.5
2	B	9	GLU	2.4
2	B	82	ALA	2.4
1	A	46	PHE	2.2
1	A	263	CYS	2.2
2	B	73	ASP	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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

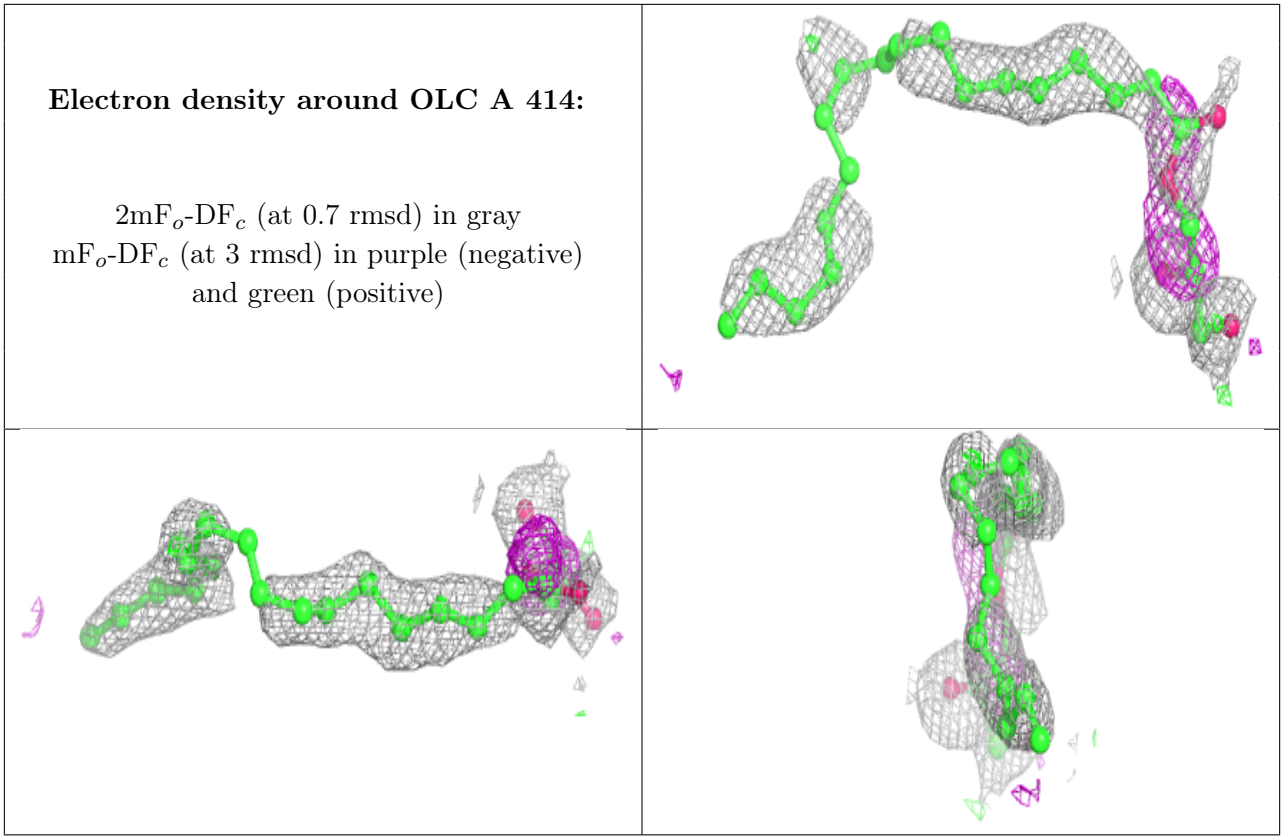
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	414	25/25	0.58	0.31	45,75,79,80	0
4	OLC	A	404	25/25	0.60	0.22	65,72,75,76	0
4	OLC	A	412	25/25	0.64	0.27	74,79,96,97	0
4	OLC	A	407	14/25	0.67	0.18	79,83,87,89	0
4	OLC	A	408	25/25	0.68	0.26	49,76,89,89	0
4	OLC	A	406	21/25	0.70	0.23	81,83,86,87	0
4	OLC	A	405	19/25	0.71	0.20	54,63,78,79	0
4	OLC	A	410	12/25	0.71	0.24	63,74,78,79	0
4	OLC	A	413	17/25	0.74	0.24	61,81,92,92	0
4	OLC	A	409	10/25	0.75	0.30	82,85,87,88	0
4	OLC	A	402	19/25	0.77	0.18	42,65,68,73	0
4	OLC	A	411	11/25	0.81	0.32	81,83,87,88	0
4	OLC	A	403	19/25	0.85	0.17	45,61,84,85	0
5	GOL	A	415	6/6	0.85	0.18	45,56,57,59	0
3	KAZ	A	401	33/33	0.98	0.09	25,28,40,40	0
6	SO4	A	416	5/5	1.00	0.08	28,29,30,30	5

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.

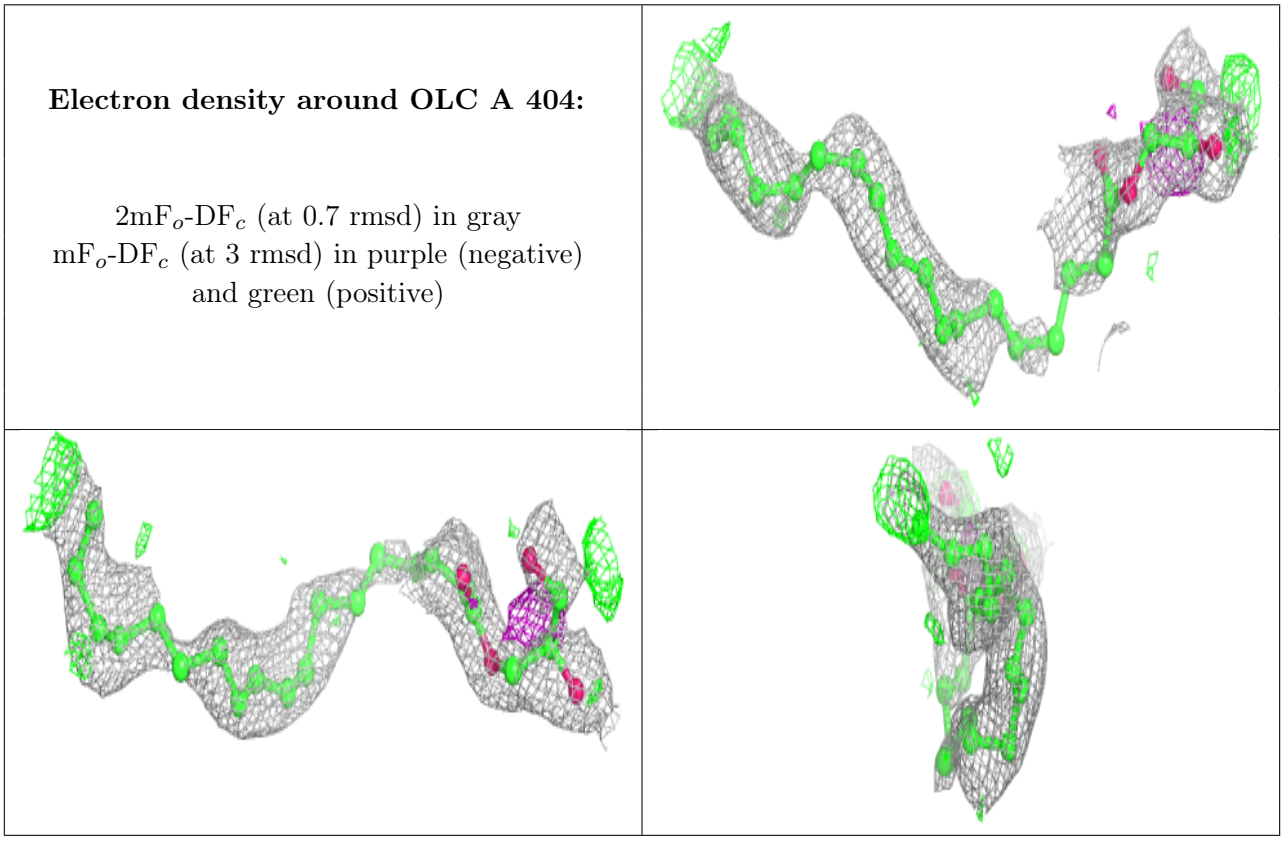
Electron density around OLC A 414:

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



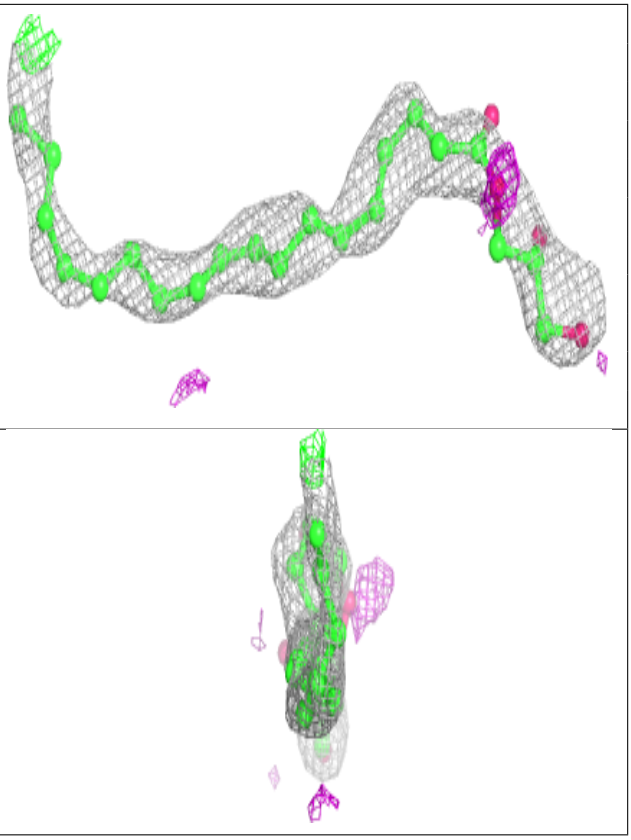
Electron density around OLC A 404:

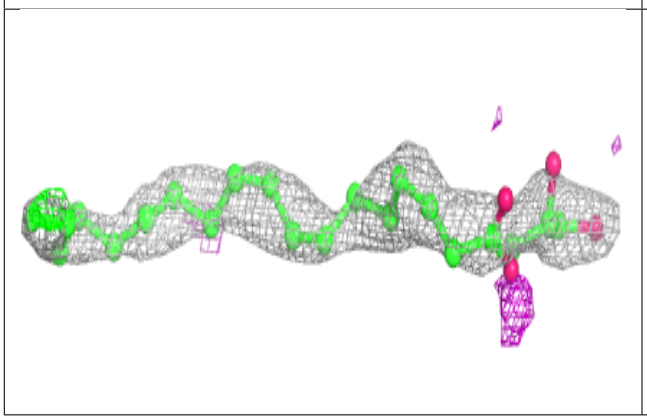
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC A 412:

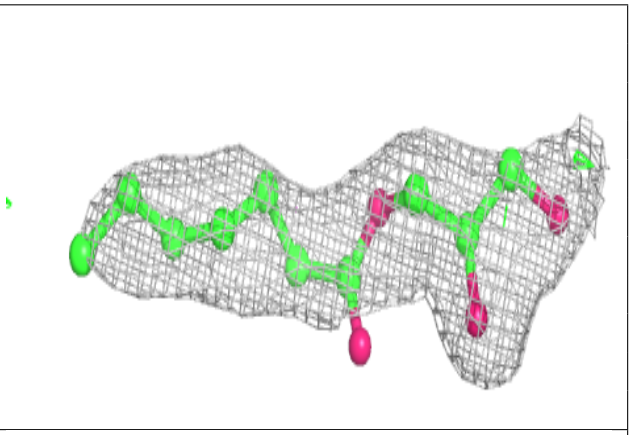
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

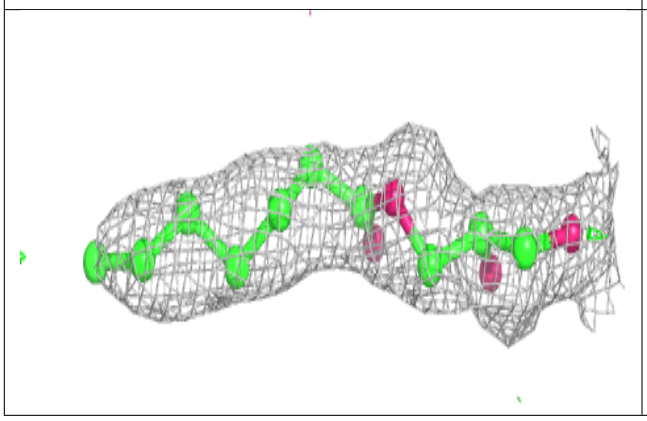




Electron density around OLC A 407:

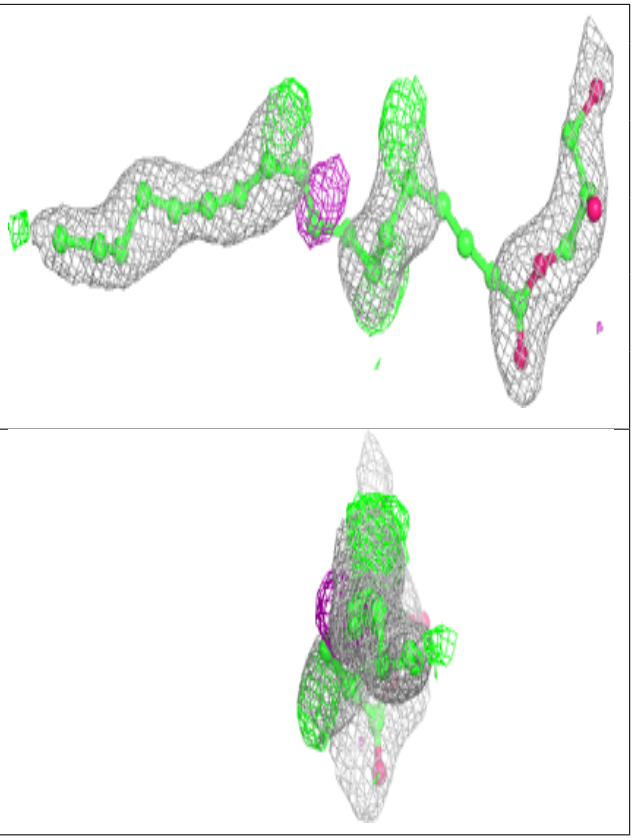
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





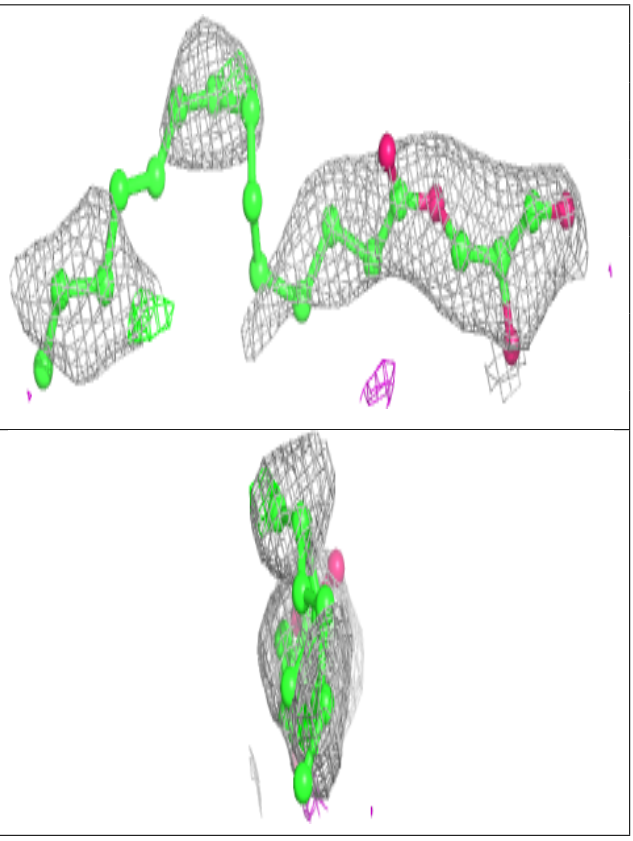
Electron density around OLC A 408:

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



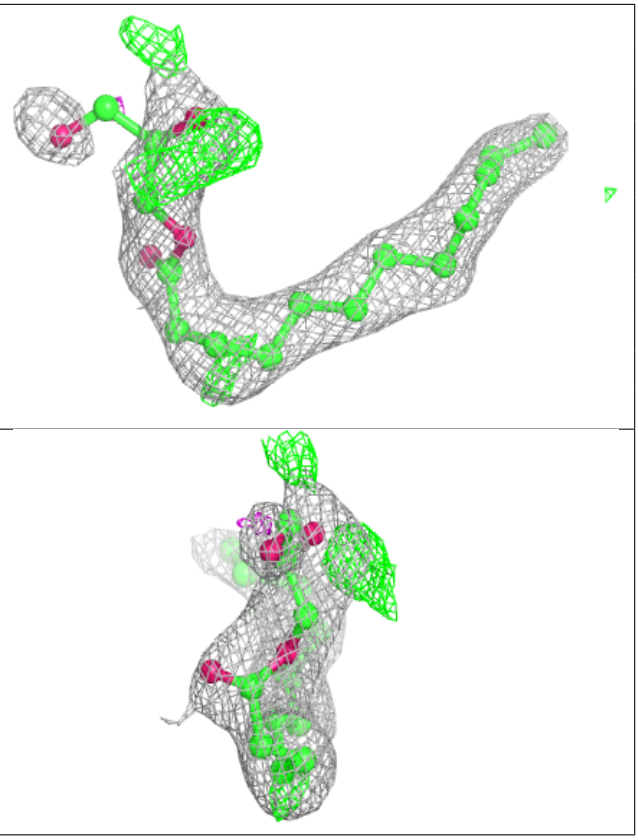
Electron density around OLC A 406:

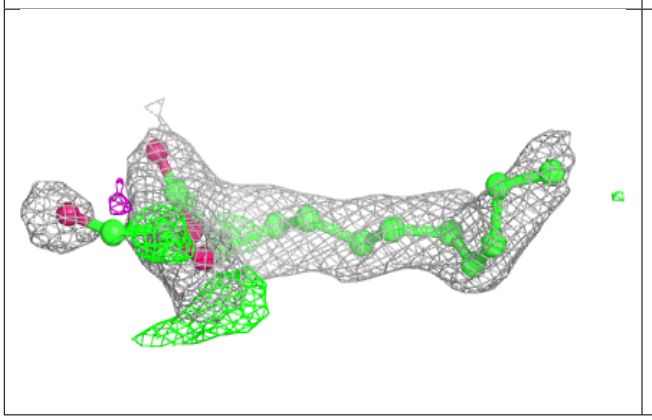
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC A 405:

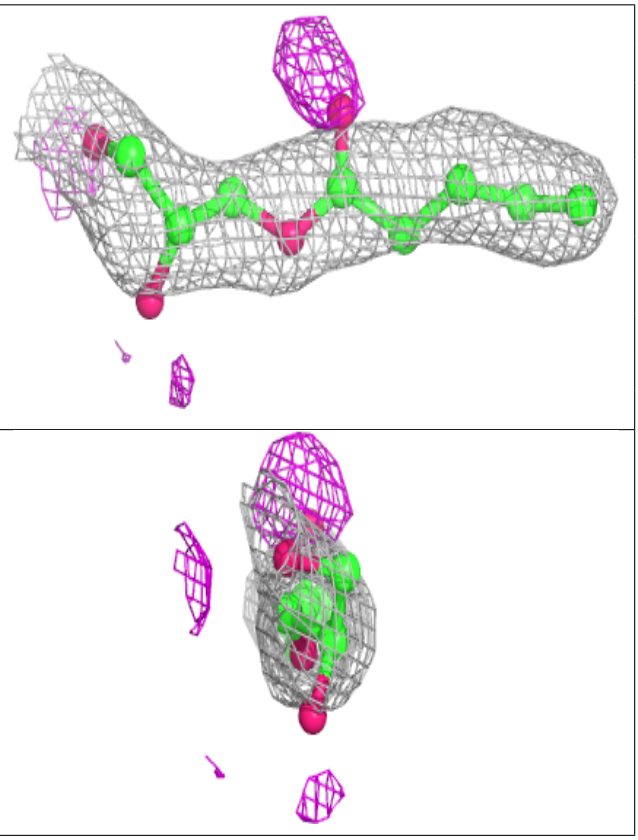
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

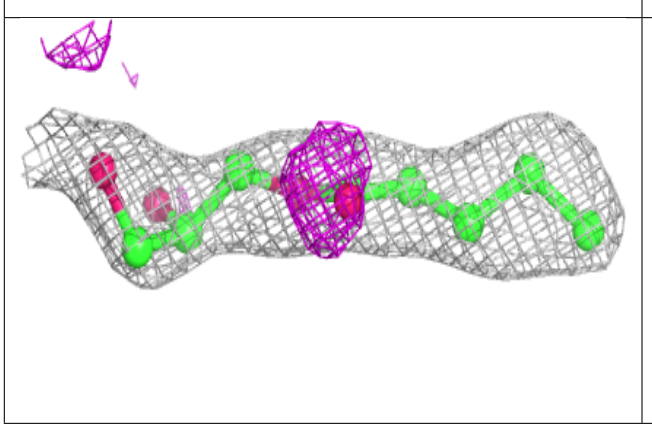




Electron density around OLC A 410:

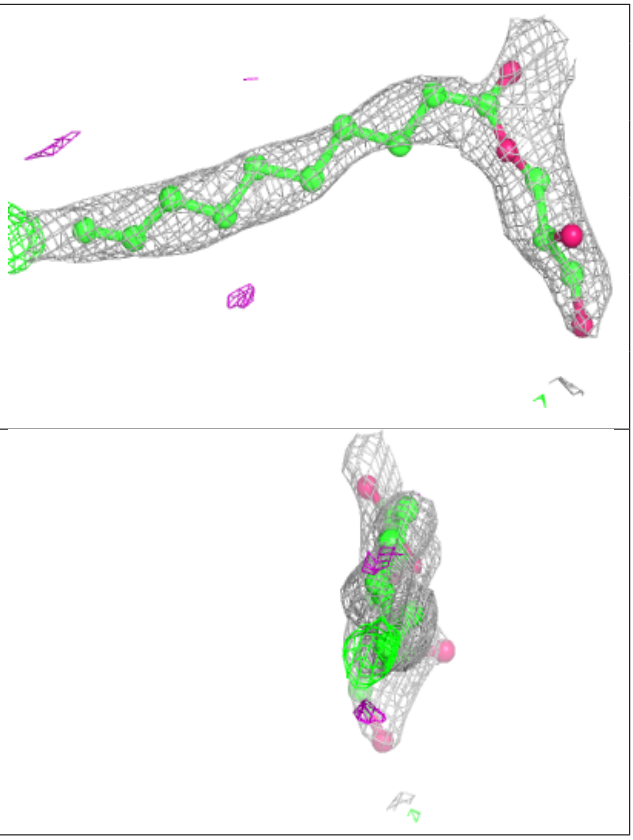
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





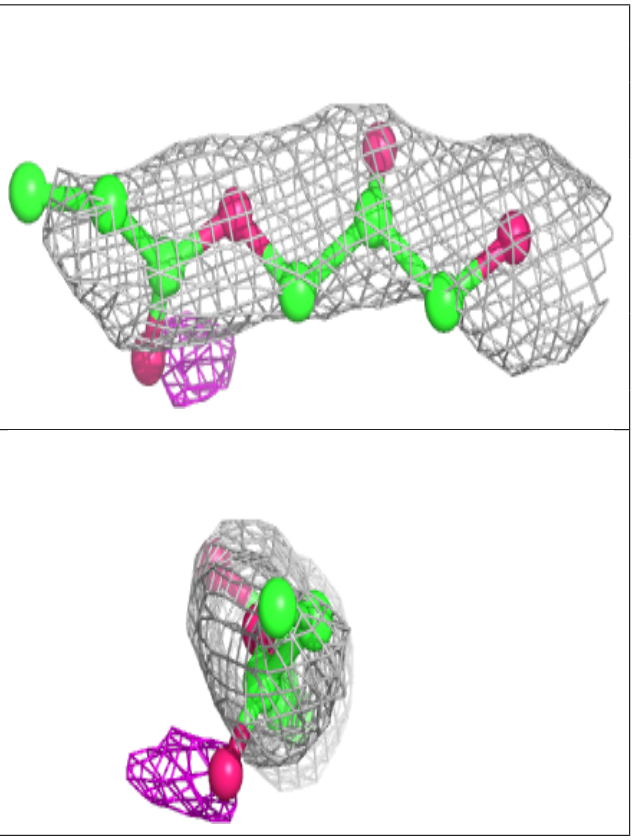
Electron density around OLC A 413:

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



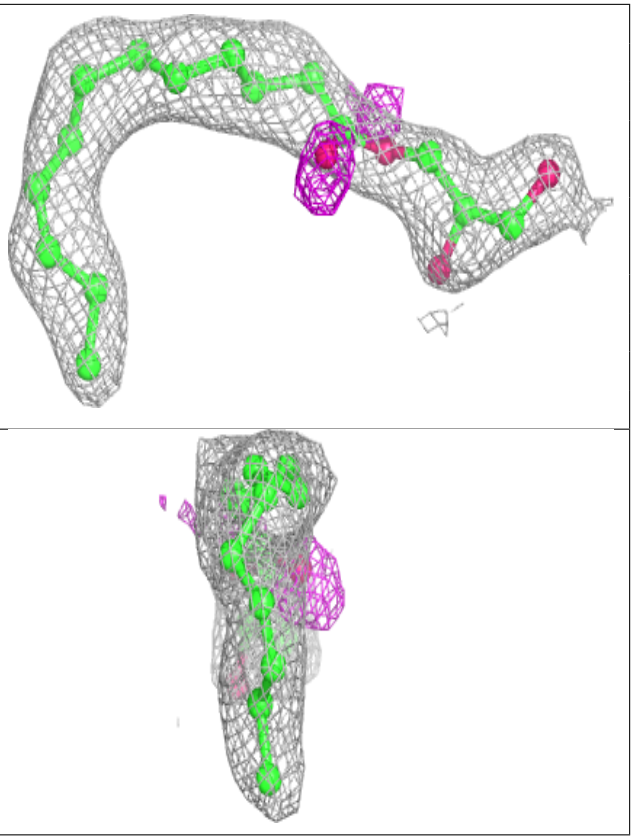
Electron density around OLC A 409:

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



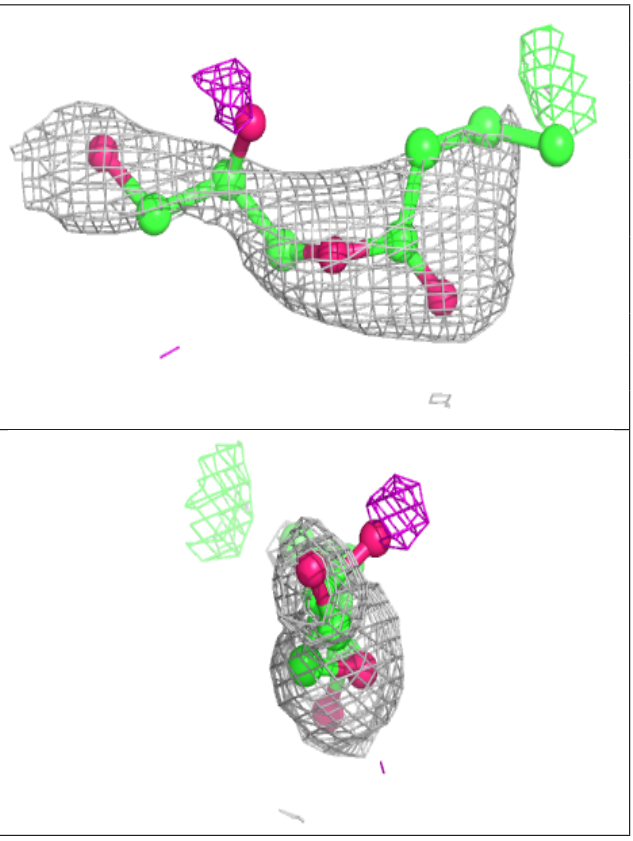
Electron density around OLC A 402:

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



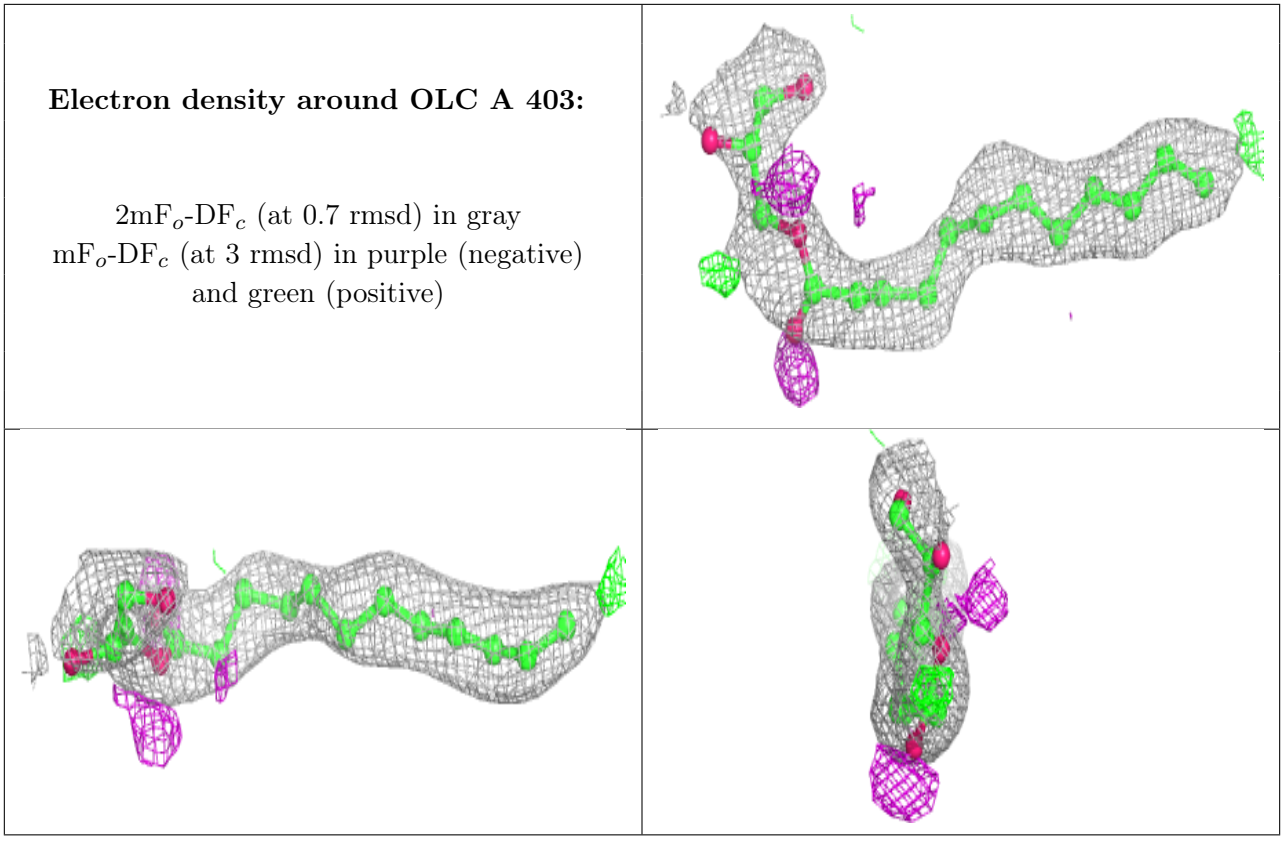
Electron density around OLC A 411:

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



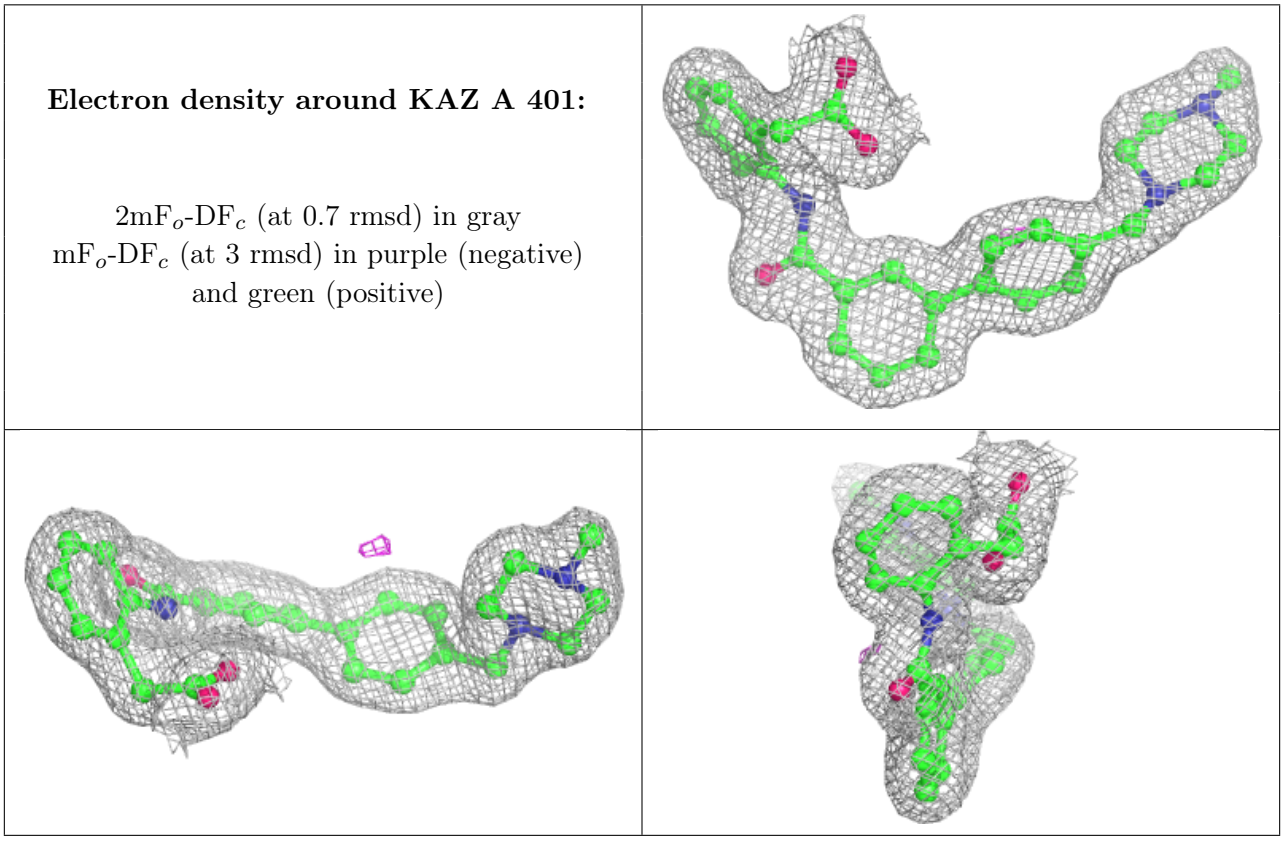
Electron density around OLC A 403:

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



Electron density around KAZ 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.