Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:06 am BST

PDB ID	:	5N6H
Title	:	Structure of the membrane integral lipoprotein N-acyltransferase Lnt from E. coli
Authors	:	Huang, C.-Y.; Boland, C.; Howe, N.; Wiktor, M.; Vogeley, L.; Weichert, D.; Bailey, J.; Olieric, V.; Wang, M.; Caffrey, M.
Deposited on	:	2017-02-15
Resolution	:	2.90 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:

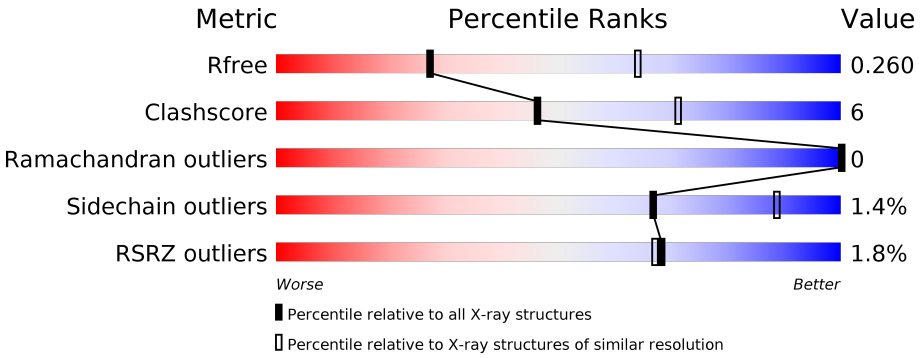
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

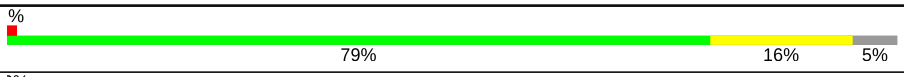
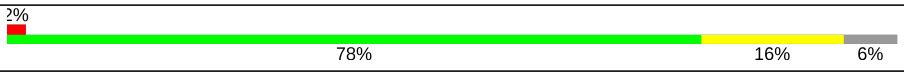
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	532	
1	B	532	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLC	A	605	-	-	-	X
2	OLC	A	607	-	-	-	X
2	OLC	B	604	-	-	-	X
3	GOL	A	619	-	-	-	X
3	GOL	B	607	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8282 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 Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3957	2604	656	683	14			
1	B	498	Total	C	N	O	S	0	0	0
			3905	2566	648	677	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23930
A	-18	GLY	-	expression tag	UNP P23930
A	-17	SER	-	expression tag	UNP P23930
A	-16	SER	-	expression tag	UNP P23930
A	-15	HIS	-	expression tag	UNP P23930
A	-14	HIS	-	expression tag	UNP P23930
A	-13	HIS	-	expression tag	UNP P23930
A	-12	HIS	-	expression tag	UNP P23930
A	-11	HIS	-	expression tag	UNP P23930
A	-10	HIS	-	expression tag	UNP P23930
A	-9	SER	-	expression tag	UNP P23930
A	-8	SER	-	expression tag	UNP P23930
A	-7	GLY	-	expression tag	UNP P23930
A	-6	LEU	-	expression tag	UNP P23930
A	-5	VAL	-	expression tag	UNP P23930
A	-4	PRO	-	expression tag	UNP P23930
A	-3	ARG	-	expression tag	UNP P23930
A	-2	GLY	-	expression tag	UNP P23930
A	-1	SER	-	expression tag	UNP P23930
A	0	HIS	-	expression tag	UNP P23930
B	-19	MET	-	initiating methionine	UNP P23930
B	-18	GLY	-	expression tag	UNP P23930
B	-17	SER	-	expression tag	UNP P23930
B	-16	SER	-	expression tag	UNP P23930
B	-15	HIS	-	expression tag	UNP P23930

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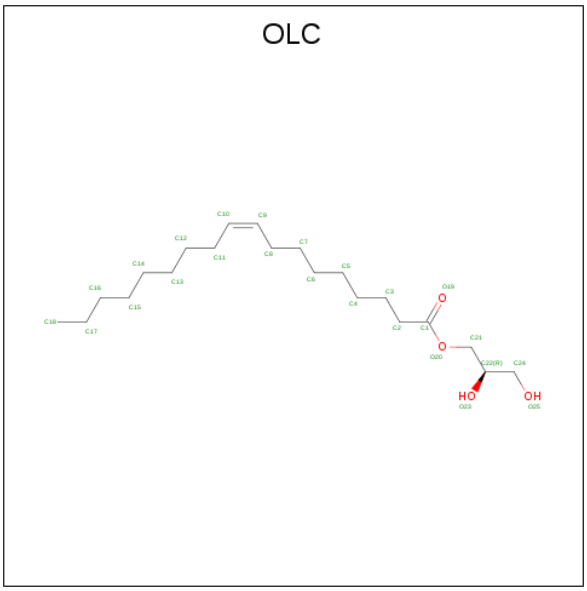
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P23930
B	-13	HIS	-	expression tag	UNP P23930
B	-12	HIS	-	expression tag	UNP P23930
B	-11	HIS	-	expression tag	UNP P23930
B	-10	HIS	-	expression tag	UNP P23930
B	-9	SER	-	expression tag	UNP P23930
B	-8	SER	-	expression tag	UNP P23930
B	-7	GLY	-	expression tag	UNP P23930
B	-6	LEU	-	expression tag	UNP P23930
B	-5	VAL	-	expression tag	UNP P23930
B	-4	PRO	-	expression tag	UNP P23930
B	-3	ARG	-	expression tag	UNP P23930
B	-2	GLY	-	expression tag	UNP P23930
B	-1	SER	-	expression tag	UNP P23930
B	0	HIS	-	expression tag	UNP P23930

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 9 4	0	0
2	A	1	Total C O 11 7 4	0	0
2	A	1	Total C O 25 21 4	0	0

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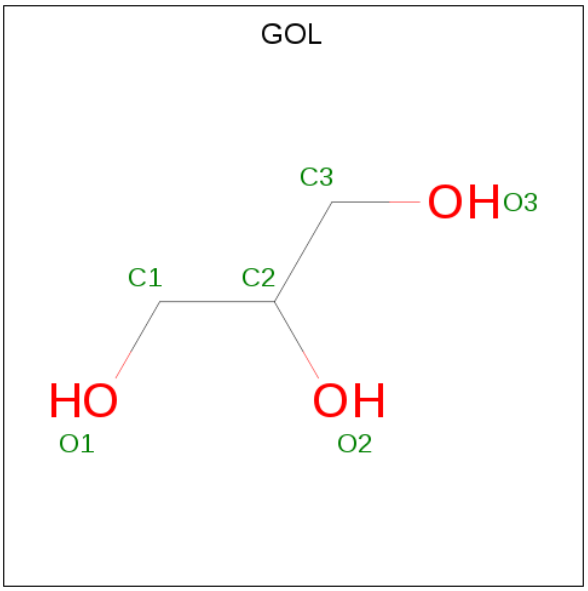
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 14 10 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 16 12 4	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	A	1	Total C O 16 12 4	0	0
2	A	1	Total C O 16 12 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	B	1	Total C O 13 9 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 17 13 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 15 11 4	0	0
2	B	1	Total C O 11 7 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

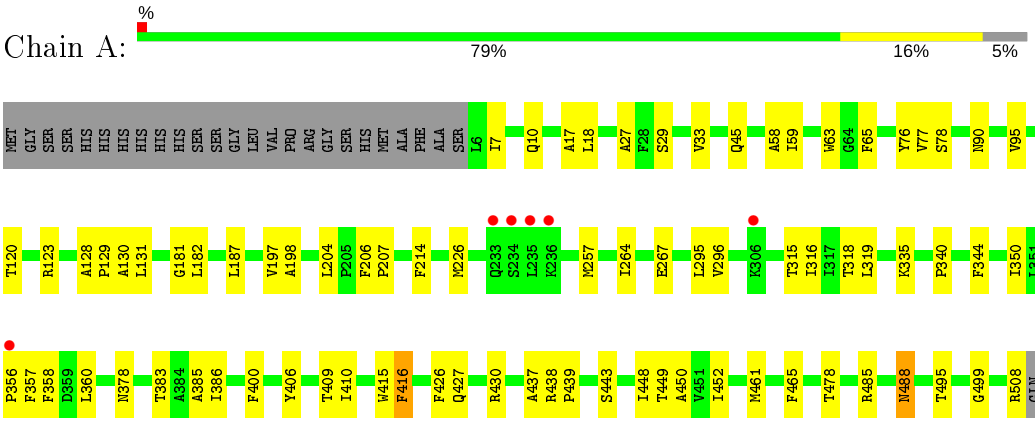
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

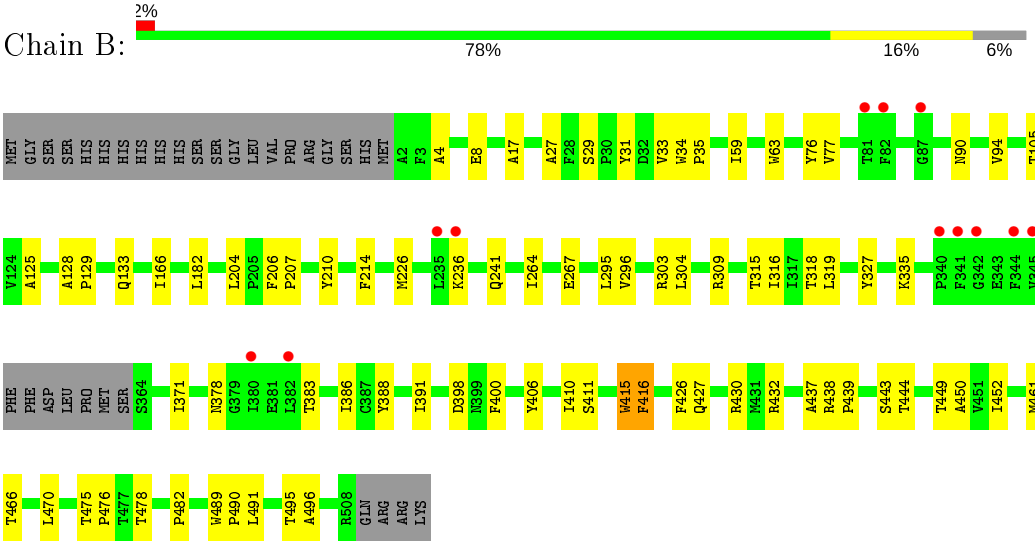
- Molecule 1: Apolipoprotein N-acyltransferase

Chain A:



- Molecule 1: Apolipoprotein N-acyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.20Å 142.30Å 199.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.90 49.10 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.10-2.90) 100.0 (49.10-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.91Å)	Xtriage
Refinement program	BUSTER, PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.219 , 0.249 0.226 , 0.260	Depositor DCC
R_{free} test set	1764 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8282	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/4071	0.49	0/5564
1	B	0.26	0/4015	0.48	0/5485
All	All	0.26	0/8086	0.48	0/11049

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	PHE	Peptide

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	3957	0	4022	54	0
1	B	3905	0	3960	49	0
2	A	211	0	290	11	0
2	B	106	0	146	3	0
3	A	42	0	54	1	0
3	B	36	0	47	0	0
4	A	18	0	0	0	0
4	B	7	0	0	0	0
All	All	8282	0	8519	105	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 6.

All (105) 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:485:ARG:NH1	2:A:609:OLC:O25	2.12	0.82
1:A:499:GLY:HA3	2:A:605:OLC:H10	1.61	0.81
1:A:45:GLN:HG2	1:A:181:GLY:HA2	1.63	0.79
1:B:133:GLN:HG2	1:B:495:THR:HG21	1.66	0.75
1:B:443:SER:HA	1:B:449:THR:HG23	1.72	0.72
1:A:197:VAL:HG11	2:A:603:OLC:H5	1.73	0.70
1:A:354:LEU:HD13	1:A:360:LEU:HB2	1.74	0.69
1:A:443:SER:HA	1:A:449:THR:HG23	1.78	0.66
1:A:438:ARG:NH2	1:A:478:THR:O	2.29	0.66
1:B:296:VAL:HG22	1:B:318:THR:HG22	1.79	0.65
1:A:352:ARG:HB2	1:A:353:PRO:HD3	1.79	0.65
1:A:355:ALA:HB3	1:A:356:PRO:HD3	1.81	0.62
1:B:236:LYS:O	1:B:241:GLN:NE2	2.33	0.62
1:A:77:VAL:HG21	1:A:416:PHE:HA	1.81	0.61
1:A:267:GLU:HA	1:A:410:ILE:HD12	1.84	0.60
1:A:488:ASN:HD22	1:A:488:ASN:H	1.47	0.60
1:B:267:GLU:HA	1:B:410:ILE:HD12	1.84	0.60
1:B:438:ARG:NH2	1:B:478:THR:O	2.33	0.59
1:A:430:ARG:HG2	1:A:452:ILE:HG12	1.83	0.59
1:B:430:ARG:HG2	1:B:452:ILE:HG12	1.85	0.58
1:A:295:LEU:HD23	1:A:319:LEU:HD13	1.86	0.58
1:A:10:GLN:HB3	3:A:617:GOL:H2	1.85	0.57
1:A:296:VAL:HG22	1:A:318:THR:HG22	1.86	0.57
1:A:450:ALA:HB2	1:A:461:MET:HG3	1.86	0.57
1:B:29:SER:HB2	1:B:427:GLN:HB2	1.86	0.57
1:B:63:TRP:HE3	1:B:105:THR:HG21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:SER:HB2	1:A:416:PHE:HE1	1.70	0.56
1:B:295:LEU:HD23	1:B:319:LEU:HD13	1.87	0.56
1:A:27:ALA:HA	1:A:33:VAL:O	2.05	0.56
1:A:340:PRO:HA	1:A:344:PHE:CE1	2.40	0.56
1:A:63:TRP:HE3	1:A:105:THR:HG21	1.70	0.56
1:A:350:ILE:O	1:A:353:PRO:HD2	2.06	0.55
1:B:335:LYS:HG3	1:B:386:ILE:HB	1.90	0.54
1:B:63:TRP:CE3	1:B:105:THR:HG21	2.43	0.54
1:A:29:SER:HB2	1:A:427:GLN:HB2	1.88	0.53
1:B:27:ALA:HA	1:B:33:VAL:O	2.08	0.53
1:A:63:TRP:CE3	1:A:105:THR:HG21	2.43	0.53
1:A:214:PHE:HB3	1:A:437:ALA:HB1	1.91	0.53
1:B:450:ALA:HB2	1:B:461:MET:HG3	1.90	0.52
1:A:335:LYS:HG3	1:A:386:ILE:HB	1.90	0.52
1:A:426:PHE:CG	1:A:448:ILE:HG21	2.45	0.52
1:B:77:VAL:HB	1:B:416:PHE:HA	1.90	0.52
1:B:214:PHE:HB3	1:B:437:ALA:HB1	1.91	0.52
1:A:187:LEU:HB2	2:A:612:OLC:H5	1.91	0.51
2:A:604:OLC:H24	2:A:606:OLC:H24A	1.92	0.51
1:A:18:LEU:HG	2:A:611:OLC:H8A	1.94	0.50
1:A:58:ALA:HB1	2:A:604:OLC:H2	1.94	0.49
1:B:120:THR:HG23	1:B:123:ARG:H	1.77	0.49
1:B:426:PHE:CE1	1:B:452:ILE:HD11	2.48	0.49
1:A:315:THR:HG22	1:A:316:ILE:N	2.29	0.48
1:A:17:ALA:HB2	1:A:59:ILE:HG23	1.96	0.48
1:A:206:PHE:HB3	1:A:207:PRO:HD3	1.95	0.48
1:A:316:ILE:HG12	1:A:410:ILE:HD11	1.95	0.47
1:A:226:MET:HG2	1:A:264:ILE:HB	1.96	0.47
1:B:316:ILE:HG12	1:B:410:ILE:HD11	1.96	0.47
1:A:204:LEU:O	1:A:207:PRO:HD2	2.16	0.46
1:A:120:THR:HG23	1:A:123:ARG:H	1.80	0.46
1:A:488:ASN:N	1:A:488:ASN:HD22	2.13	0.46
1:B:206:PHE:HB3	1:B:207:PRO:HD3	1.98	0.46
1:B:315:THR:HG22	1:B:316:ILE:N	2.31	0.46
1:A:426:PHE:CE1	1:A:452:ILE:HD11	2.51	0.45
1:B:411:SER:HB3	1:B:444:THR:HG22	1.99	0.45
1:B:210:TYR:O	2:B:605:OLC:H22	2.17	0.45
1:A:7:ILE:HD13	1:B:31:TYR:HA	2.00	0.44
1:A:131:LEU:HD13	2:A:605:OLC:H13	2.00	0.44
1:B:415:TRP:HB2	1:B:416:PHE:CE1	2.53	0.44
1:B:76:TYR:HB2	1:B:94:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HA	1:A:495:THR:HG23	2.00	0.43
1:A:95:VAL:HG22	2:A:611:OLC:H2	2.00	0.43
1:A:410:ILE:O	1:A:410:ILE:HG13	2.17	0.43
1:B:204:LEU:O	1:B:207:PRO:HD2	2.18	0.43
1:B:303:ARG:NH2	1:B:327:TYR:O	2.51	0.43
1:A:406:TYR:HD1	1:A:439:PRO:HB2	1.83	0.43
1:B:410:ILE:HG13	1:B:410:ILE:O	2.18	0.43
1:B:489:TRP:CG	1:B:490:PRO:HD3	2.54	0.43
1:B:371:ILE:HD11	1:B:398:ASP:HB3	1.99	0.43
1:A:65:PHE:HZ	1:A:95:VAL:HG13	1.84	0.43
2:B:604:OLC:H11	2:B:604:OLC:H8A	1.85	0.43
1:B:76:TYR:CE1	1:B:90:ASN:HB2	2.53	0.43
1:B:128:ALA:HB3	1:B:129:PRO:HD3	2.01	0.43
1:A:257:MET:HB3	1:A:257:MET:HE2	1.74	0.43
1:B:34:TRP:CG	1:B:35:PRO:HD3	2.55	0.42
1:B:462:ILE:HG23	1:B:470:LEU:HD13	2.02	0.42
1:B:304:LEU:HA	1:B:309:ARG:O	2.20	0.42
1:A:128:ALA:HB3	1:A:129:PRO:HD3	2.02	0.42
1:B:464:GLN:O	1:B:466:THR:HG23	2.20	0.41
1:B:125:ALA:HB2	1:B:182:LEU:HD21	2.02	0.41
1:B:475:THR:HA	1:B:476:PRO:HD3	1.95	0.41
1:B:432:ARG:HD3	1:B:432:ARG:HA	1.93	0.41
1:A:354:LEU:HA	1:A:360:LEU:HD12	2.02	0.41
1:A:385:ALA:O	1:A:409:THR:HA	2.21	0.41
1:B:166:ILE:HA	1:B:482:PRO:HB2	2.02	0.41
1:B:383:THR:HG21	1:B:400:PHE:HA	2.02	0.41
1:B:406:TYR:HD1	1:B:439:PRO:HB2	1.86	0.41
1:B:226:MET:HG2	1:B:264:ILE:HB	2.02	0.41
1:B:388:TYR:O	1:B:391:ILE:HG12	2.21	0.41
1:B:491:LEU:O	1:B:495:THR:HG23	2.21	0.41
1:B:496:ALA:HB2	2:B:604:OLC:H8A	2.03	0.41
1:A:76:TYR:CE1	1:A:90:ASN:HB2	2.56	0.40
1:B:4:ALA:O	1:B:8:GLU:HG3	2.20	0.40
1:A:383:THR:HG21	1:A:400:PHE:HA	2.02	0.40
1:B:17:ALA:HB2	1:B:59:ILE:HG23	2.04	0.40
2:A:603:OLC:H11	2:A:603:OLC:H8A	1.76	0.40
1:A:182:LEU:HB2	1:A:198:ALA:HB2	2.04	0.40
1:A:10:GLN:HE21	2:A:604:OLC:H21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/532 (94%)	484 (97%)	17 (3%)	0	100	100
1	B	494/532 (93%)	476 (96%)	18 (4%)	0	100	100
All	All	995/1064 (94%)	960 (96%)	35 (4%)	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	418/444 (94%)	410 (98%)	8 (2%)	57	84
1	B	411/444 (93%)	407 (99%)	4 (1%)	76	92
All	All	829/888 (93%)	817 (99%)	12 (1%)	67	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	A	358	PHE
1	A	378	ASN
1	A	415	TRP
1	A	416	PHE
1	A	465	PHE
1	A	488	ASN
1	A	508	ARG

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Mol	Chain	Res	Type
1	B	378	ASN
1	B	415	TRP
1	B	416	PHE
1	B	465	PHE

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

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

31 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	$\#\|Z\| > 2$
2	OLC	A	612	-	14,14,24	0.86	1 (7%)	15,15,25	1.11	1 (6%)
2	OLC	A	605	-	24,24,24	0.68	1 (4%)	25,25,25	0.93	1 (4%)
3	GOL	B	607	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	A	616	-	5,5,5	0.33	0	5,5,5	0.29	0
2	OLC	B	606	-	10,10,24	1.01	1 (10%)	11,11,25	1.10	1 (9%)
3	GOL	A	619	-	5,5,5	0.32	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	610	-	5,5,5	0.35	0	5,5,5	0.40	0
2	OLC	A	607	-	14,14,24	0.85	1 (7%)	14,14,25	1.14	1 (7%)
2	OLC	A	609	-	14,14,24	0.86	1 (7%)	15,15,25	1.05	1 (6%)
3	GOL	B	612	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GOL	A	615	-	5,5,5	0.33	0	5,5,5	0.29	0
2	OLC	A	604	-	13,13,24	0.91	1 (7%)	14,14,25	1.09	1 (7%)
3	GOL	A	617	-	5,5,5	0.33	0	5,5,5	0.28	0
3	GOL	B	609	-	5,5,5	0.33	0	5,5,5	0.29	0
2	OLC	B	604	-	24,24,24	0.68	1 (4%)	25,25,25	0.95	1 (4%)
2	OLC	A	601	-	12,12,24	0.93	1 (8%)	13,13,25	1.06	1 (7%)
2	OLC	B	601	-	12,12,24	0.93	1 (8%)	13,13,25	1.12	1 (7%)
3	GOL	B	611	-	5,5,5	0.34	0	5,5,5	0.34	0
2	OLC	A	608	-	19,19,24	0.77	1 (5%)	20,20,25	0.93	1 (5%)
2	OLC	A	603	-	24,24,24	0.67	1 (4%)	25,25,25	0.96	1 (4%)
2	OLC	A	611	-	15,15,24	0.84	1 (6%)	16,16,25	1.12	1 (6%)
2	OLC	B	603	-	16,16,24	0.85	1 (6%)	17,17,25	1.06	1 (5%)
2	OLC	A	602	-	10,10,24	1.02	1 (10%)	11,11,25	1.08	1 (9%)
2	OLC	A	606	-	24,24,24	0.68	1 (4%)	25,25,25	0.97	1 (4%)
3	GOL	A	618	-	5,5,5	0.34	0	5,5,5	0.39	0
2	OLC	B	605	-	14,14,24	0.89	1 (7%)	15,15,25	1.14	1 (6%)
2	OLC	B	602	-	24,24,24	0.68	1 (4%)	25,25,25	0.99	1 (4%)
2	OLC	A	610	-	15,15,24	0.83	1 (6%)	16,16,25	1.09	1 (6%)
3	GOL	B	608	-	5,5,5	0.34	0	5,5,5	0.34	0
3	GOL	A	614	-	5,5,5	0.32	0	5,5,5	0.37	0
3	GOL	A	613	-	5,5,5	0.32	0	5,5,5	0.22	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
2	OLC	A	612	-	-	4/14/14/24	-
2	OLC	A	605	-	-	13/24/24/24	-
3	GOL	B	607	-	-	2/4/4/4	-
3	GOL	A	616	-	-	2/4/4/4	-
2	OLC	B	606	-	-	0/10/10/24	-
3	GOL	A	619	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	610	-	-	2/4/4/4	-
2	OLC	A	607	-	-	5/12/12/24	-
2	OLC	A	609	-	-	8/14/14/24	-
3	GOL	B	612	-	-	2/4/4/4	-
3	GOL	A	615	-	-	2/4/4/4	-
2	OLC	A	604	-	-	9/13/13/24	-
3	GOL	A	617	-	-	2/4/4/4	-
3	GOL	B	609	-	-	4/4/4/4	-
2	OLC	B	604	-	-	10/24/24/24	-
2	OLC	A	601	-	-	4/12/12/24	-
2	OLC	B	601	-	-	7/12/12/24	-
3	GOL	B	611	-	-	2/4/4/4	-
2	OLC	A	608	-	-	14/19/19/24	-
2	OLC	A	603	-	-	16/24/24/24	-
2	OLC	A	611	-	-	10/15/15/24	-
2	OLC	B	603	-	-	6/16/16/24	-
2	OLC	A	602	-	-	6/10/10/24	-
2	OLC	A	606	-	-	14/24/24/24	-
3	GOL	A	618	-	-	2/4/4/4	-
2	OLC	B	605	-	-	5/14/14/24	-
2	OLC	B	602	-	-	18/24/24/24	-
2	OLC	A	610	-	-	9/15/15/24	-
3	GOL	B	608	-	-	4/4/4/4	-
3	GOL	A	614	-	-	2/4/4/4	-
3	GOL	A	613	-	-	0/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	OLC	O20-C1	2.69	1.41	1.33
2	A	608	OLC	O20-C1	2.69	1.41	1.33
2	B	605	OLC	O20-C1	2.69	1.41	1.33
2	A	611	OLC	O20-C1	2.66	1.41	1.33
2	A	606	OLC	O20-C1	2.66	1.41	1.33
2	A	604	OLC	O20-C1	2.64	1.41	1.33
2	A	602	OLC	O20-C1	2.64	1.41	1.33
2	B	604	OLC	O20-C1	2.63	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	OLC	O20-C1	2.63	1.41	1.33
2	B	603	OLC	O20-C1	2.62	1.41	1.33
2	A	601	OLC	O20-C1	2.62	1.41	1.33
2	A	612	OLC	O20-C1	2.61	1.41	1.33
2	B	602	OLC	O20-C1	2.60	1.40	1.33
2	B	606	OLC	O20-C1	2.60	1.40	1.33
2	A	607	OLC	O20-C1	2.59	1.40	1.33
2	A	603	OLC	O20-C1	2.59	1.40	1.33
2	A	610	OLC	O20-C1	2.56	1.40	1.33
2	A	609	OLC	O20-C1	2.56	1.40	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	607	OLC	O20-C1-C2	3.38	120.25	111.38
2	B	605	OLC	O20-C1-C2	2.96	121.20	111.91
2	B	604	OLC	O20-C1-C2	2.86	120.90	111.91
2	A	611	OLC	O20-C1-C2	2.85	120.85	111.91
2	B	601	OLC	O20-C1-C2	2.78	120.63	111.91
2	A	612	OLC	O20-C1-C2	2.77	120.60	111.91
2	A	604	OLC	O20-C1-C2	2.77	120.59	111.91
2	B	602	OLC	O20-C1-C2	2.75	120.53	111.91
2	A	603	OLC	O20-C1-C2	2.73	120.48	111.91
2	A	606	OLC	O20-C1-C2	2.72	120.45	111.91
2	A	605	OLC	O20-C1-C2	2.70	120.37	111.91
2	A	610	OLC	O20-C1-C2	2.69	120.36	111.91
2	A	608	OLC	O20-C1-C2	2.68	120.31	111.91
2	A	609	OLC	O20-C1-C2	2.61	120.10	111.91
2	B	603	OLC	O20-C1-C2	2.61	120.09	111.91
2	A	602	OLC	O20-C1-C2	2.60	120.08	111.91
2	A	601	OLC	O20-C1-C2	2.58	120.00	111.91
2	B	606	OLC	O20-C1-C2	2.57	119.96	111.91

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	612	OLC	O20-C21-C22-O23
2	A	605	OLC	O20-C21-C22-C24
2	A	605	OLC	O20-C21-C22-O23
3	B	607	GOL	C1-C2-C3-O3
3	B	610	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	609	OLC	C21-C22-C24-O25
2	A	609	OLC	O20-C21-C22-C24
2	A	604	OLC	C21-C22-C24-O25
2	A	604	OLC	O20-C21-C22-O23
3	B	609	GOL	O1-C1-C2-C3
3	B	609	GOL	C1-C2-C3-O3
2	B	601	OLC	O20-C21-C22-O23
2	A	608	OLC	C10-C11-C12-C13
2	A	608	OLC	O20-C21-C22-C24
2	A	603	OLC	C21-C22-C24-O25
2	A	611	OLC	C21-C22-C24-O25
2	A	611	OLC	O20-C21-C22-O23
2	A	606	OLC	O20-C21-C22-C24
3	A	618	GOL	C1-C2-C3-O3
2	B	602	OLC	C21-C22-C24-O25
2	B	602	OLC	O23-C22-C24-O25
2	A	610	OLC	C21-C22-C24-O25
3	B	608	GOL	O1-C1-C2-C3
3	B	608	GOL	C1-C2-C3-O3
3	A	614	GOL	O1-C1-C2-C3
2	A	608	OLC	C2-C1-O20-C21
2	A	608	OLC	O19-C1-O20-C21
2	B	604	OLC	C2-C1-O20-C21
2	B	601	OLC	C2-C1-O20-C21
2	B	605	OLC	C2-C1-O20-C21
2	A	605	OLC	O19-C1-O20-C21
2	A	605	OLC	C2-C1-O20-C21
2	B	603	OLC	C2-C1-O20-C21
2	B	604	OLC	O19-C1-O20-C21
2	B	601	OLC	O19-C1-O20-C21
2	B	605	OLC	O19-C1-O20-C21
2	A	609	OLC	C2-C1-O20-C21
2	B	602	OLC	C2-C1-O20-C21
2	A	608	OLC	O20-C21-C22-O23
2	A	609	OLC	O19-C1-O20-C21
2	B	603	OLC	O19-C1-O20-C21
2	B	602	OLC	O19-C1-O20-C21
2	A	607	OLC	C2-C1-O20-C21
2	A	604	OLC	C2-C1-O20-C21
2	A	601	OLC	C2-C1-O20-C21
2	A	610	OLC	C2-C1-O20-C21
2	A	604	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	B	601	OLC	O20-C21-C22-C24
2	A	603	OLC	O20-C21-C22-C24
2	A	606	OLC	C1-C2-C3-C4
2	A	609	OLC	O20-C21-C22-O23
2	A	606	OLC	O20-C21-C22-O23
2	A	604	OLC	O19-C1-O20-C21
2	A	610	OLC	O19-C1-O20-C21
3	A	616	GOL	O1-C1-C2-O2
2	A	604	OLC	O23-C22-C24-O25
3	B	611	GOL	O1-C1-C2-O2
2	A	607	OLC	O19-C1-O20-C21
2	A	611	OLC	C1-C2-C3-C4
2	B	601	OLC	C1-C2-C3-C4
2	A	601	OLC	O19-C1-O20-C21
2	A	603	OLC	O20-C21-C22-O23
2	A	602	OLC	C2-C1-O20-C21
2	A	603	OLC	C2-C1-O20-C21
2	A	603	OLC	C2-C3-C4-C5
2	B	601	OLC	C2-C3-C4-C5
2	A	606	OLC	C2-C3-C4-C5
2	B	602	OLC	C2-C3-C4-C5
2	A	610	OLC	C4-C5-C6-C7
2	B	603	OLC	C2-C3-C4-C5
2	A	606	OLC	C5-C6-C7-C8
2	B	602	OLC	C5-C6-C7-C8
2	B	604	OLC	C13-C14-C15-C16
2	B	604	OLC	C4-C5-C6-C7
2	A	608	OLC	C4-C5-C6-C7
2	A	608	OLC	C5-C6-C7-C8
2	A	603	OLC	C14-C15-C16-C17
2	B	605	OLC	C2-C3-C4-C5
3	A	616	GOL	O1-C1-C2-C3
3	A	619	GOL	O1-C1-C2-C3
3	B	612	GOL	C1-C2-C3-O3
3	A	615	GOL	O1-C1-C2-C3
3	A	617	GOL	C1-C2-C3-O3
3	B	611	GOL	O1-C1-C2-C3
2	A	608	OLC	C21-C22-C24-O25
2	B	602	OLC	O20-C21-C22-O23
2	A	610	OLC	O20-C21-C22-O23
2	B	603	OLC	C4-C5-C6-C7
2	B	604	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	A	603	OLC	C1-C2-C3-C4
2	A	606	OLC	C4-C5-C6-C7
2	A	602	OLC	O19-C1-O20-C21
2	A	611	OLC	C2-C1-O20-C21
2	B	604	OLC	C14-C15-C16-C17
2	B	605	OLC	C3-C4-C5-C6
2	A	604	OLC	C3-C4-C5-C6
2	A	603	OLC	O19-C1-O20-C21
3	A	617	GOL	O2-C2-C3-O3
3	B	609	GOL	O1-C1-C2-O2
3	B	609	GOL	O2-C2-C3-O3
2	A	603	OLC	O23-C22-C24-O25
3	A	618	GOL	O2-C2-C3-O3
2	A	610	OLC	O23-C22-C24-O25
3	B	608	GOL	O1-C1-C2-O2
3	B	608	GOL	O2-C2-C3-O3
2	A	603	OLC	C6-C7-C8-C9
2	A	610	OLC	C3-C4-C5-C6
2	A	608	OLC	C3-C4-C5-C6
2	A	606	OLC	C2-C1-O20-C21
2	A	611	OLC	O19-C1-O20-C21
2	A	610	OLC	O20-C21-C22-C24
2	A	604	OLC	C2-C3-C4-C5
2	B	604	OLC	C5-C6-C7-C8
2	A	604	OLC	C1-C2-C3-C4
2	B	604	OLC	C6-C7-C8-C9
2	A	605	OLC	C2-C3-C4-C5
2	A	611	OLC	C2-C3-C4-C5
2	A	606	OLC	O19-C1-O20-C21
2	A	608	OLC	C2-C3-C4-C5
2	A	603	OLC	C11-C12-C13-C14
2	A	605	OLC	C4-C5-C6-C7
2	A	610	OLC	C2-C3-C4-C5
2	A	609	OLC	C5-C6-C7-C8
2	A	603	OLC	C15-C16-C17-C18
3	B	607	GOL	O2-C2-C3-O3
3	A	615	GOL	O1-C1-C2-O2
2	B	602	OLC	C15-C16-C17-C18
2	B	602	OLC	O20-C21-C22-C24
2	B	601	OLC	C3-C4-C5-C6
2	A	609	OLC	C3-C4-C5-C6
2	A	608	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	605	OLC	C13-C14-C15-C16
2	A	611	OLC	C5-C6-C7-C8
2	B	602	OLC	C11-C12-C13-C14
2	A	603	OLC	C5-C6-C7-C8
2	A	612	OLC	C2-C1-O20-C21
2	A	611	OLC	O20-C21-C22-C24
3	A	619	GOL	O1-C1-C2-O2
3	B	610	GOL	O2-C2-C3-O3
2	A	611	OLC	O23-C22-C24-O25
3	A	614	GOL	O1-C1-C2-O2
2	A	602	OLC	C1-C2-C3-C4
2	A	605	OLC	C12-C13-C14-C15
2	B	603	OLC	C3-C4-C5-C6
2	B	602	OLC	C12-C13-C14-C15
2	A	611	OLC	C3-C4-C5-C6
2	B	602	OLC	C10-C11-C12-C13
2	A	603	OLC	C12-C13-C14-C15
2	A	605	OLC	C5-C6-C7-C8
2	A	606	OLC	C13-C14-C15-C16
2	A	601	OLC	C1-C2-C3-C4
2	A	612	OLC	O20-C21-C22-C24
2	A	603	OLC	C3-C4-C5-C6
2	B	602	OLC	C13-C14-C15-C16
2	A	612	OLC	O19-C1-O20-C21
2	A	609	OLC	O23-C22-C24-O25
2	A	602	OLC	O23-C22-C24-O25
2	A	605	OLC	C6-C7-C8-C9
2	B	604	OLC	C2-C3-C4-C5
2	A	602	OLC	C21-C22-C24-O25
2	A	603	OLC	C10-C11-C12-C13
2	A	605	OLC	C3-C4-C5-C6
2	A	606	OLC	C15-C16-C17-C18
2	A	606	OLC	C9-C10-C11-C12
2	B	602	OLC	C9-C10-C11-C12
2	A	608	OLC	O23-C22-C24-O25
2	A	606	OLC	C3-C4-C5-C6
2	A	606	OLC	C14-C15-C16-C17
2	A	602	OLC	O20-C21-C22-C24
2	A	605	OLC	C9-C10-C11-C12
2	A	608	OLC	C9-C10-C11-C12
3	B	612	GOL	O2-C2-C3-O3
2	A	607	OLC	O20-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	603	OLC	C7-C8-C9-C10
2	B	602	OLC	O20-C1-C2-C3
2	A	607	OLC	O19-C1-C2-C3
2	A	606	OLC	C10-C11-C12-C13
2	A	608	OLC	C7-C8-C9-C10
2	B	602	OLC	C6-C7-C8-C9
2	B	605	OLC	C1-C2-C3-C4
2	A	607	OLC	C21-C22-C24-O25
2	B	602	OLC	O19-C1-C2-C3
2	B	602	OLC	C3-C4-C5-C6
2	A	605	OLC	C7-C8-C9-C10
2	B	604	OLC	C15-C16-C17-C18
2	A	601	OLC	O20-C1-C2-C3

There are no ring outliers.

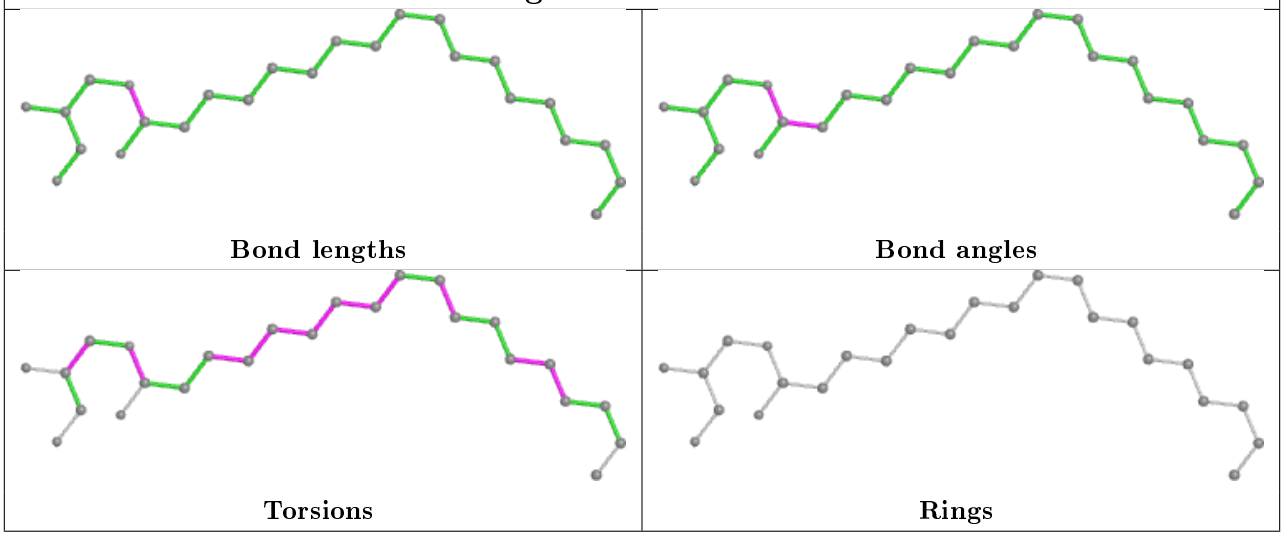
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	612	OLC	1	0
2	A	605	OLC	2	0
2	A	609	OLC	1	0
2	A	604	OLC	3	0
3	A	617	GOL	1	0
2	B	604	OLC	2	0
2	A	603	OLC	2	0
2	A	611	OLC	2	0
2	A	606	OLC	1	0
2	B	605	OLC	1	0

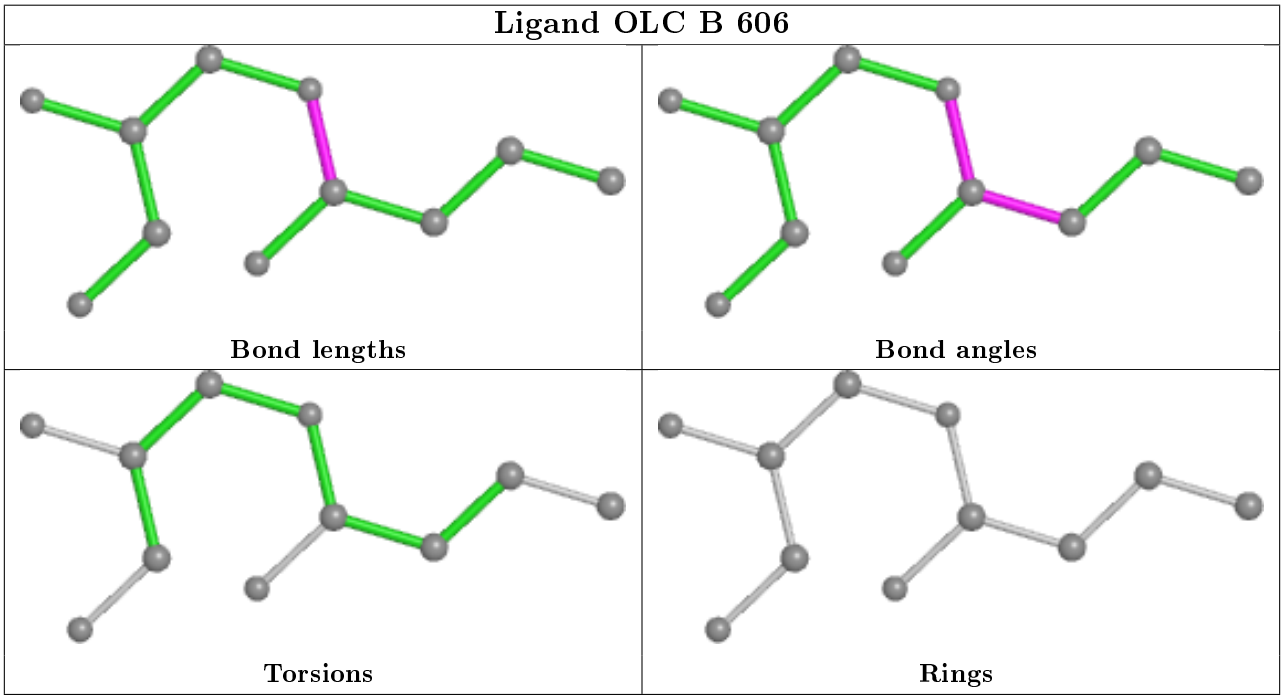
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 612

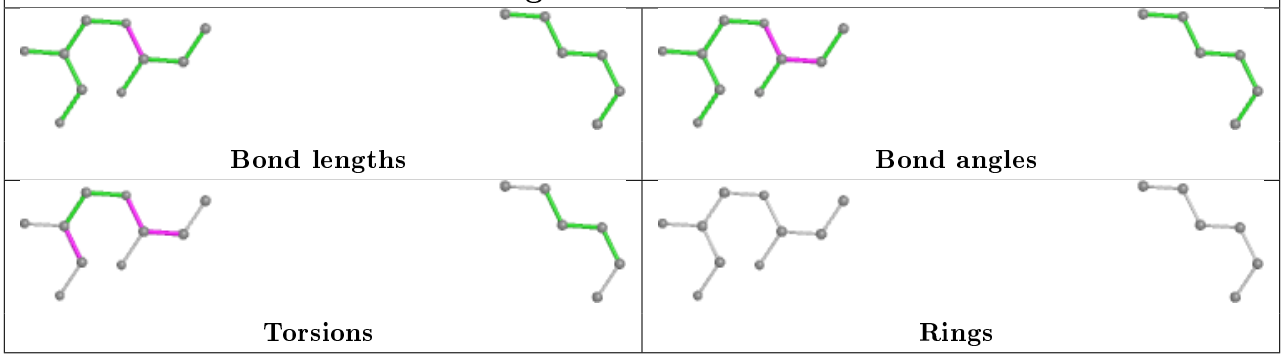
Ligand OLC A 605



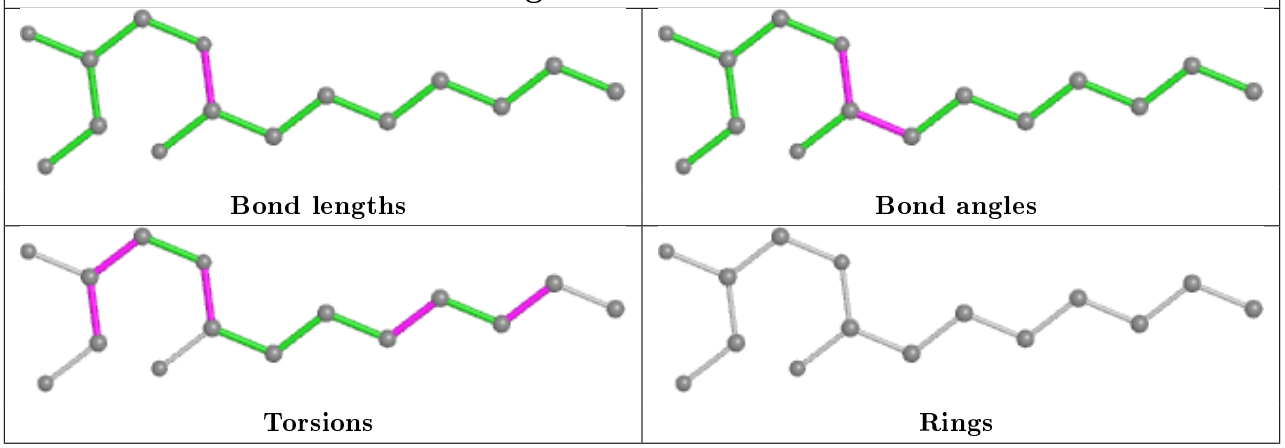
Ligand OLC B 606



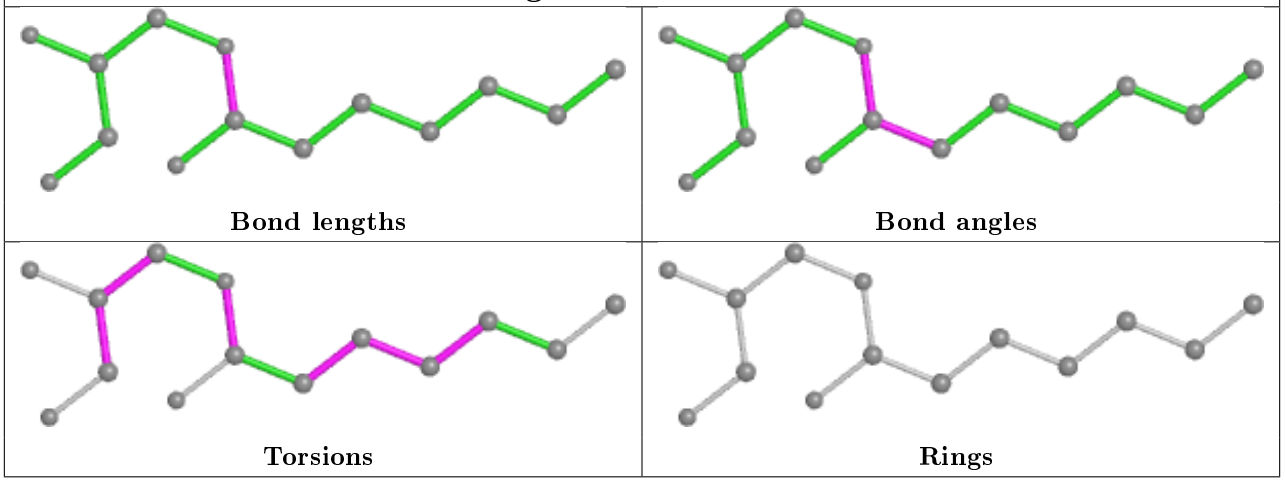
Ligand OLC A 607



Ligand OLC A 609



Ligand OLC A 604



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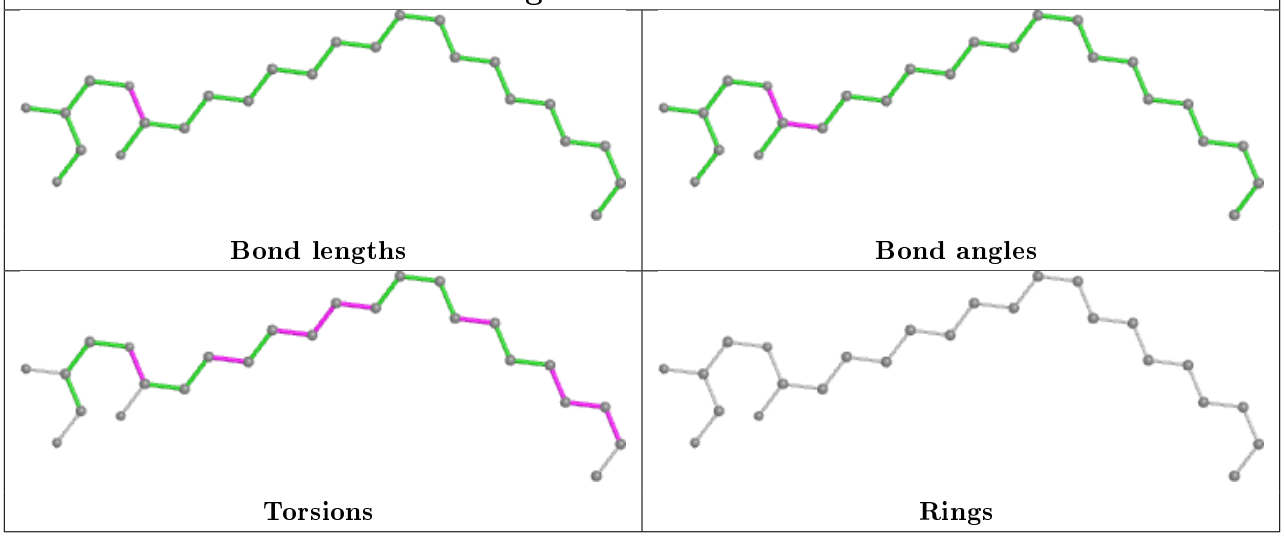
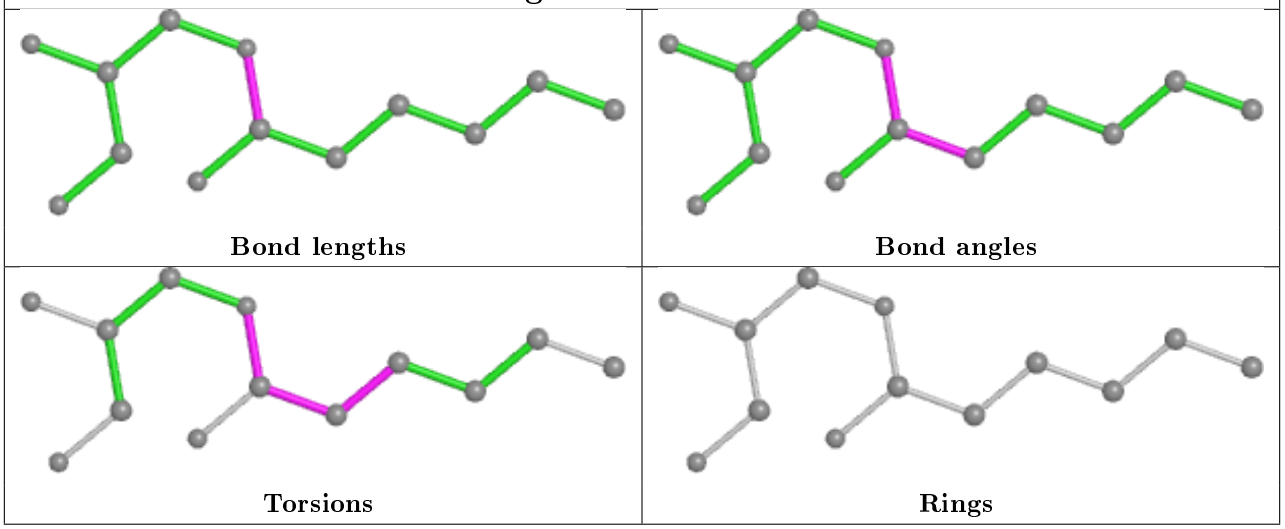


Ligand OLC A 601



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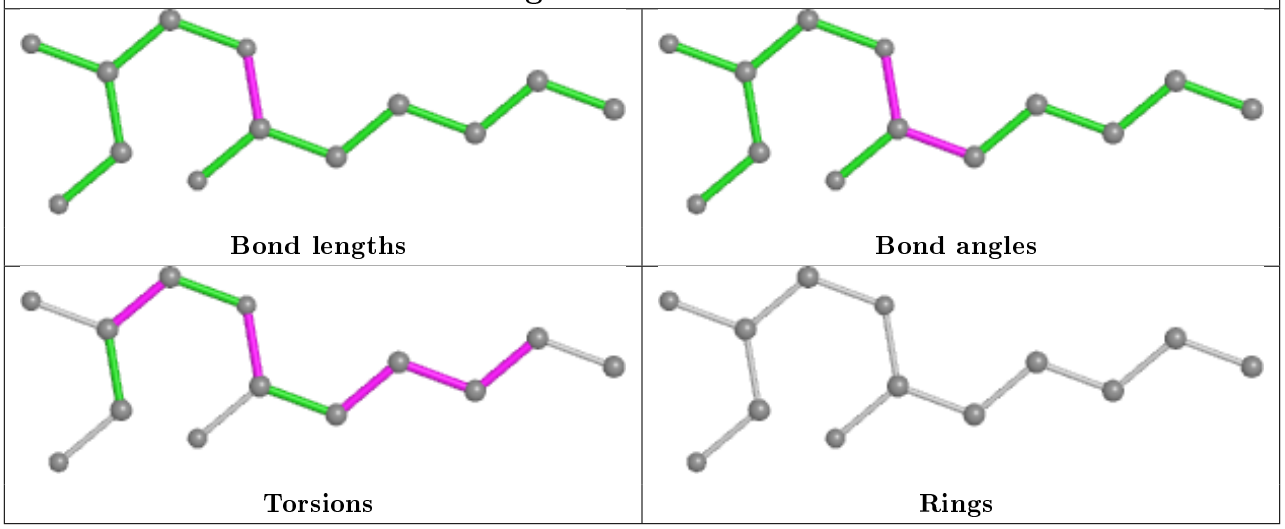
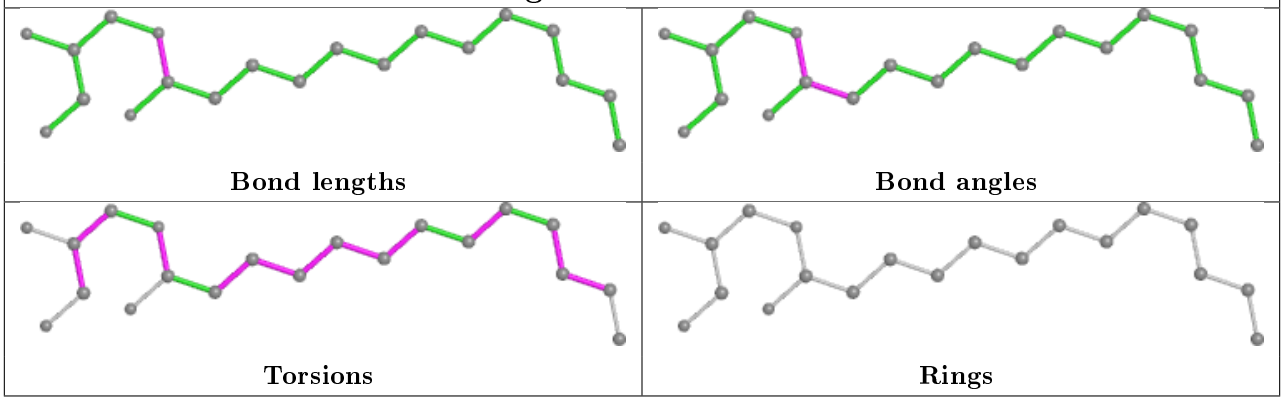
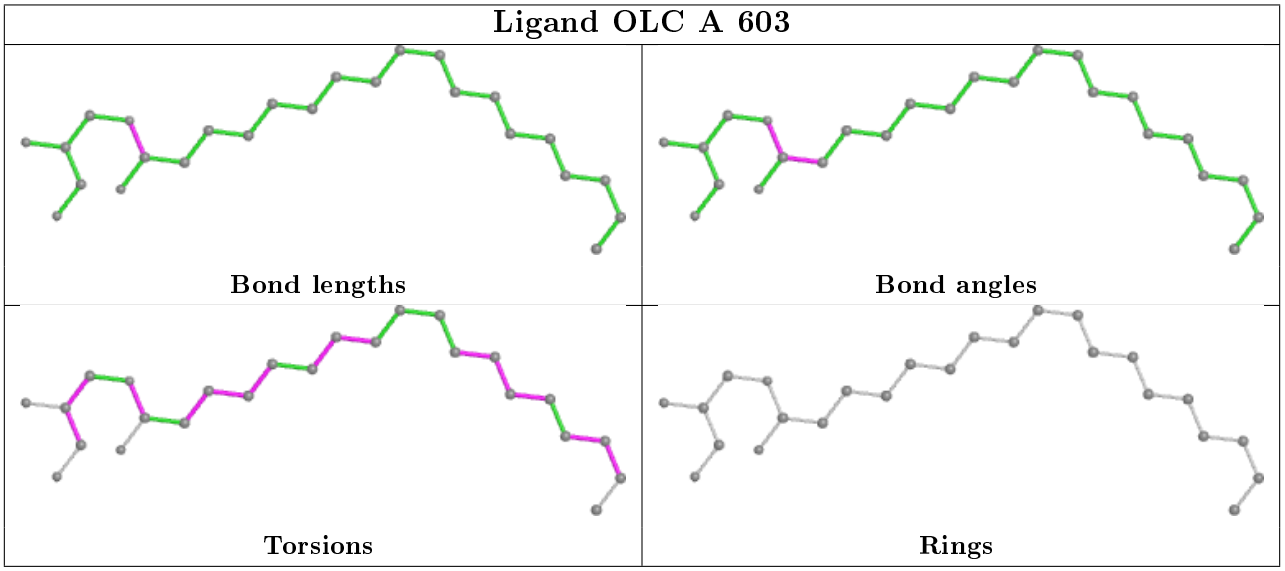


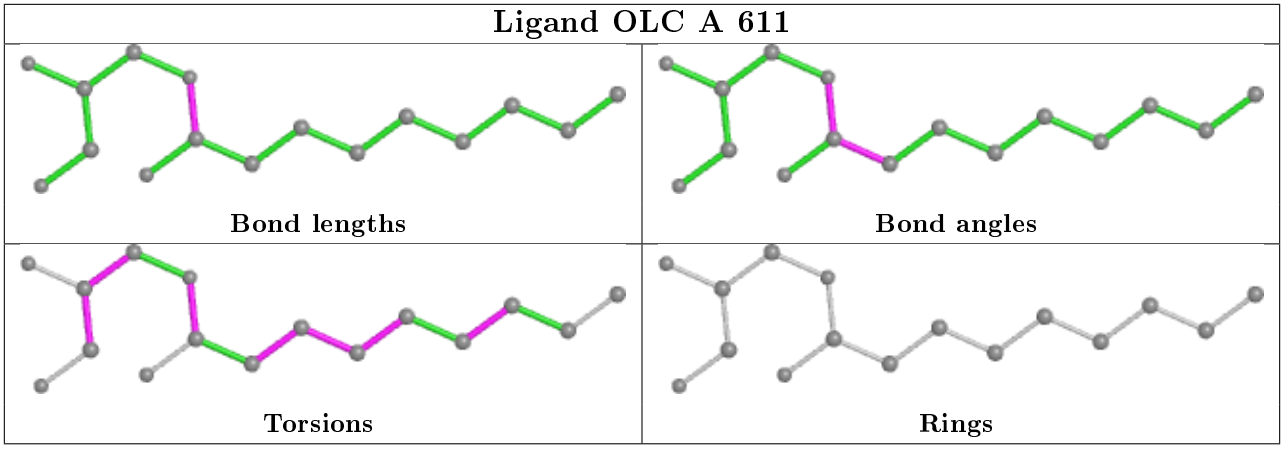
Ligand OLC A 608



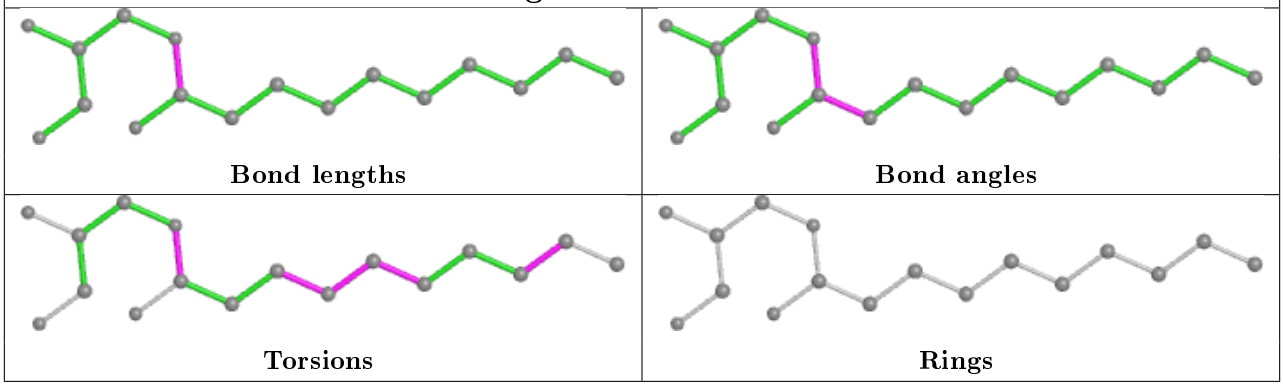
Ligand OLC A 603



Ligand OLC A 611



Ligand OLC B 603



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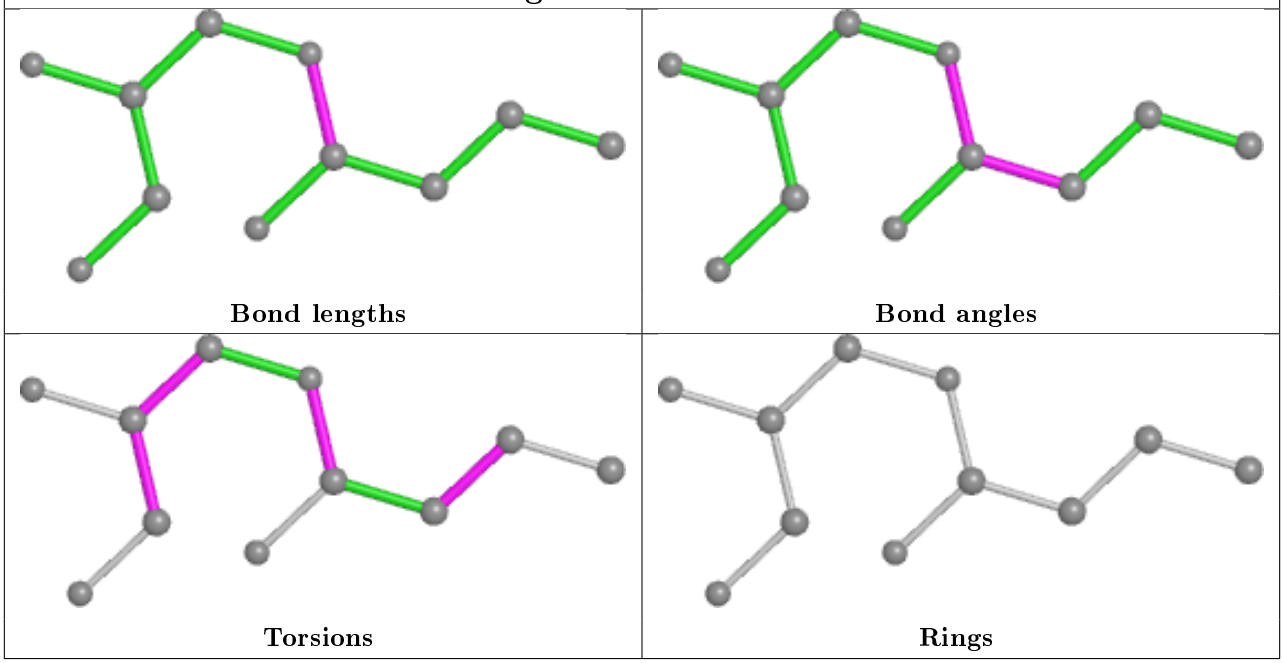
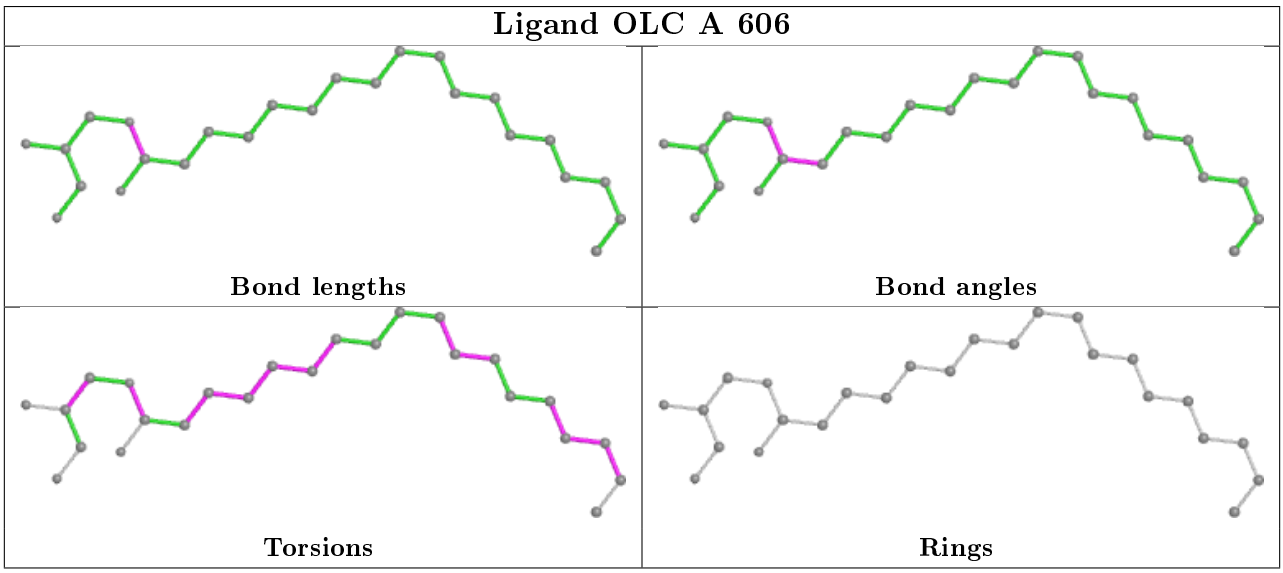
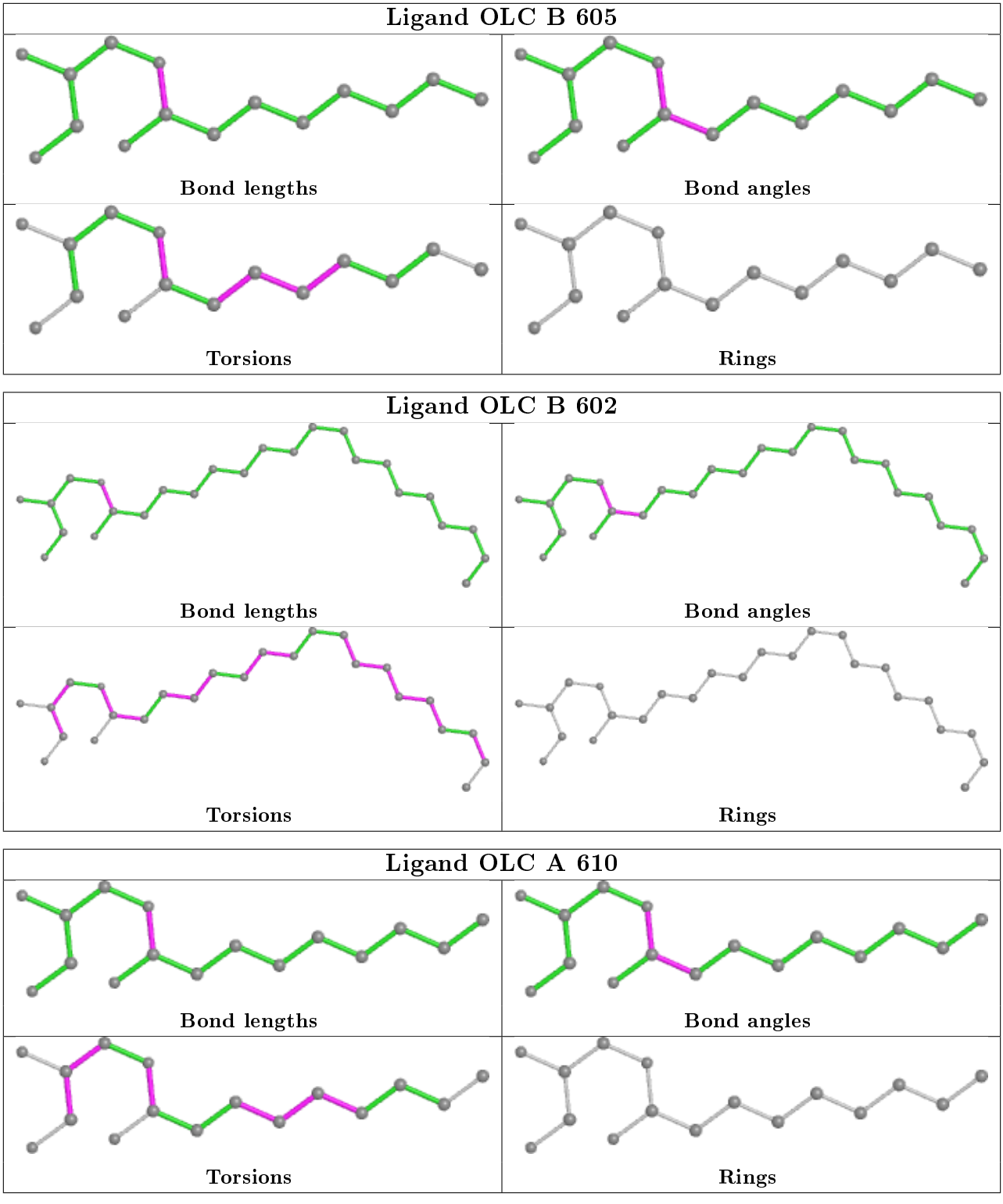


Ligand OLC A 606





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	503/532 (94%)	-0.30	6 (1%)	79	79	48, 67, 109, 142	0
1	B	498/532 (93%)	-0.16	12 (2%)	59	56	61, 83, 129, 170	0
All	All	1001/1064 (94%)	-0.23	18 (1%)	68	67	48, 77, 122, 170	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	7.7
1	A	234	SER	4.6
1	A	236	LYS	3.9
1	B	81	THR	3.8
1	B	382	LEU	3.5
1	A	233	GLN	3.5
1	B	82	PHE	3.1
1	B	236	LYS	3.0
1	B	235	LEU	2.9
1	B	345	VAL	2.6
1	B	344	PHE	2.6
1	B	380	ILE	2.4
1	B	340	PRO	2.4
1	A	306	LYS	2.3
1	B	341	PHE	2.3
1	B	87	GLY	2.2
1	B	342	GLY	2.0
1	A	356	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

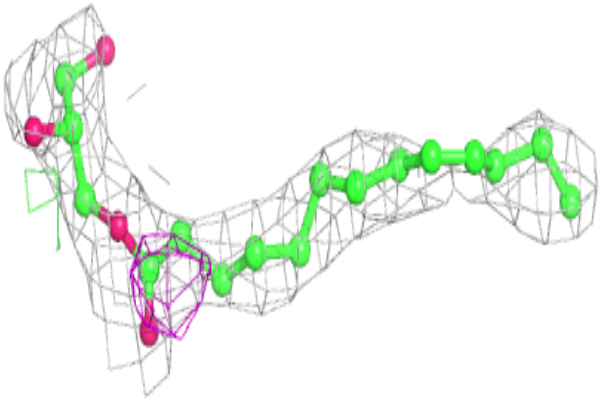
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

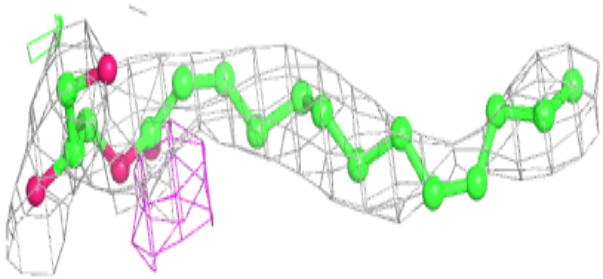
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	619	6/6	0.56	0.47	86,95,101,105	0
3	GOL	A	618	6/6	0.69	0.36	103,106,109,112	0
3	GOL	B	610	6/6	0.70	0.18	97,102,105,108	0
3	GOL	A	614	6/6	0.72	0.33	90,91,102,115	0
3	GOL	B	607	6/6	0.73	0.44	80,85,91,92	0
2	OLC	A	608	20/25	0.73	0.35	62,83,105,120	0
3	GOL	B	612	6/6	0.74	0.18	101,104,106,111	0
2	OLC	A	607	16/25	0.75	0.43	60,92,106,107	0
3	GOL	B	611	6/6	0.77	0.12	100,108,111,115	0
2	OLC	B	604	25/25	0.77	0.49	74,89,105,110	0
3	GOL	A	616	6/6	0.78	0.20	97,104,108,109	0
2	OLC	A	605	25/25	0.79	0.43	49,72,91,95	0
2	OLC	B	605	15/25	0.80	0.34	71,85,103,109	0
2	OLC	A	611	16/25	0.82	0.60	59,77,90,90	0
2	OLC	A	606	25/25	0.84	0.26	61,76,94,105	0
2	OLC	A	604	14/25	0.84	0.19	64,92,99,109	0
3	GOL	A	617	6/6	0.84	0.17	90,96,101,104	0
2	OLC	B	603	17/25	0.84	0.27	74,98,105,107	0
2	OLC	A	602	11/25	0.85	0.27	68,79,87,91	0
3	GOL	B	609	6/6	0.86	0.31	99,101,106,111	0
2	OLC	B	601	13/25	0.87	0.39	72,82,99,102	0
2	OLC	B	606	11/25	0.87	0.28	69,89,103,105	0
2	OLC	A	610	16/25	0.88	0.29	80,89,101,106	0
2	OLC	A	603	25/25	0.89	0.38	53,65,91,92	0
2	OLC	A	609	15/25	0.90	0.29	62,73,108,111	0
3	GOL	A	615	6/6	0.90	0.23	64,69,72,77	0
3	GOL	A	613	6/6	0.90	0.27	75,80,83,83	0
3	GOL	B	608	6/6	0.91	0.16	82,84,92,92	0
2	OLC	B	602	25/25	0.91	0.33	70,80,96,103	0
2	OLC	A	612	15/25	0.91	0.20	63,73,113,124	0
2	OLC	A	601	13/25	0.94	0.20	59,68,78,78	0

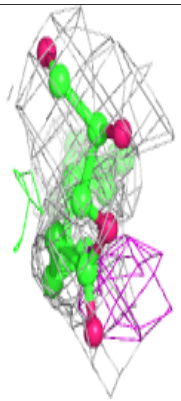
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 608:

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

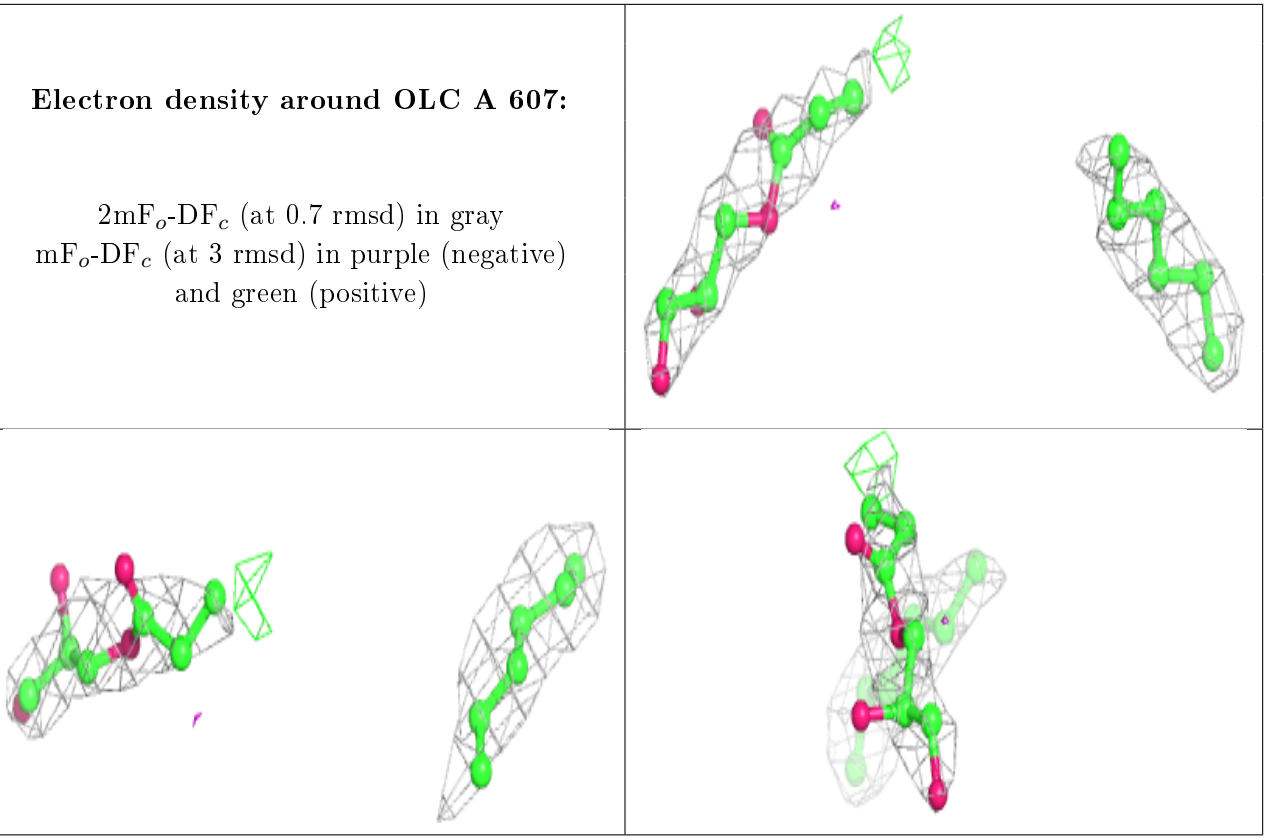






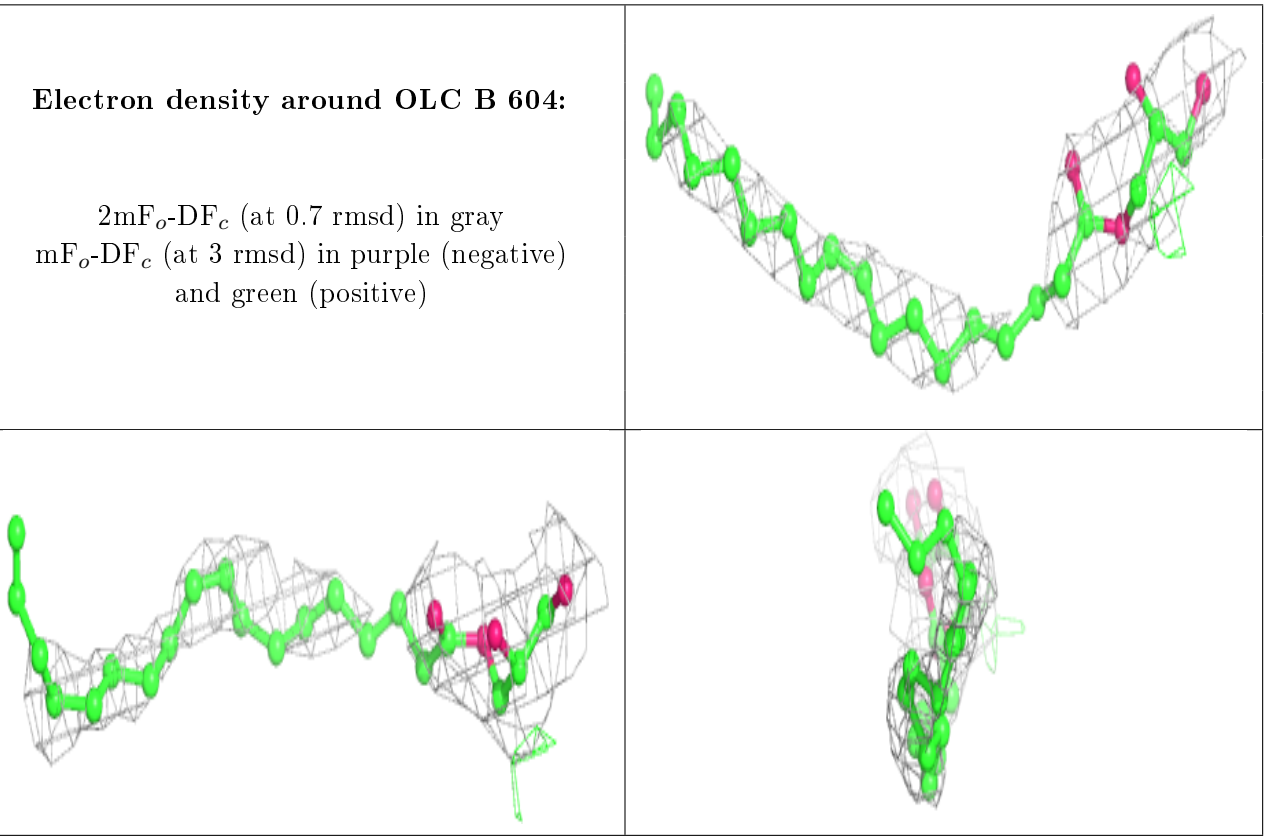
Electron density around OLC A 607:

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



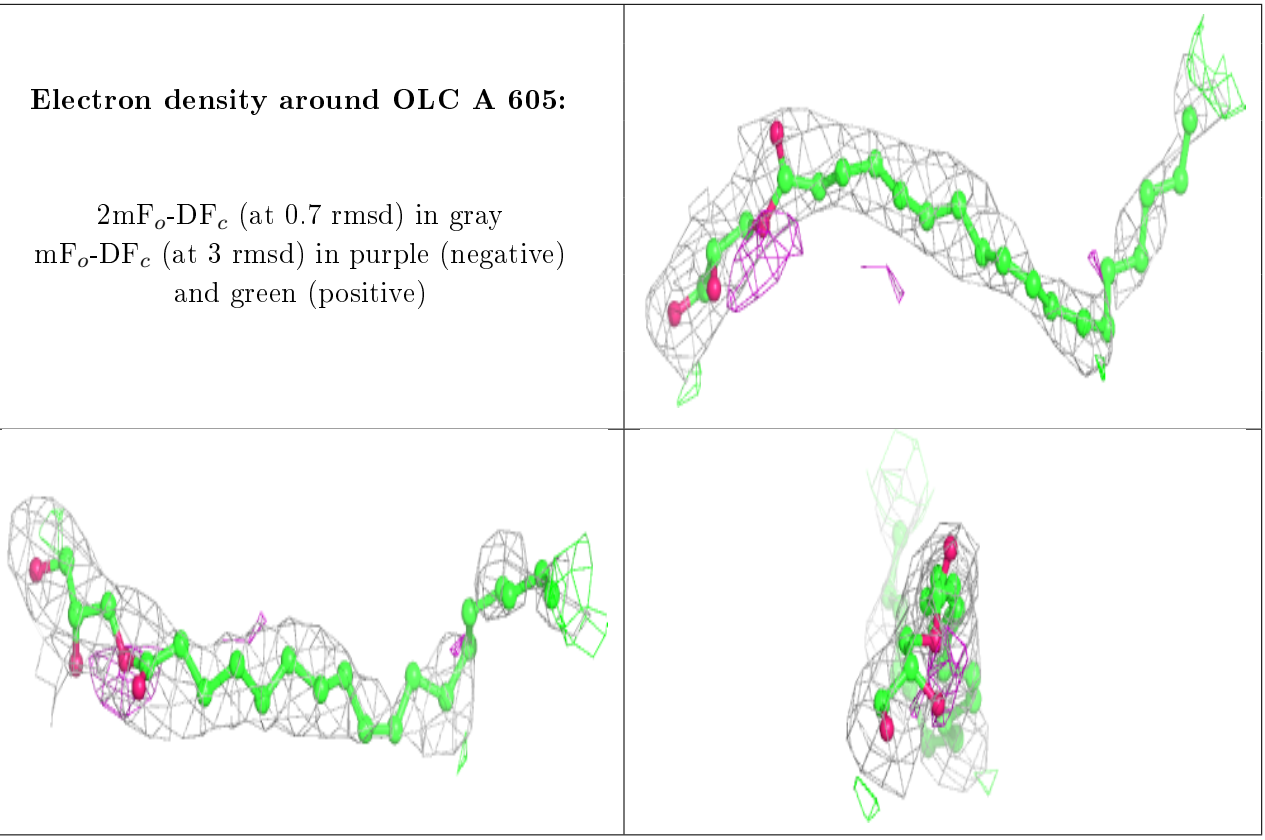
Electron density around OLC B 604:

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



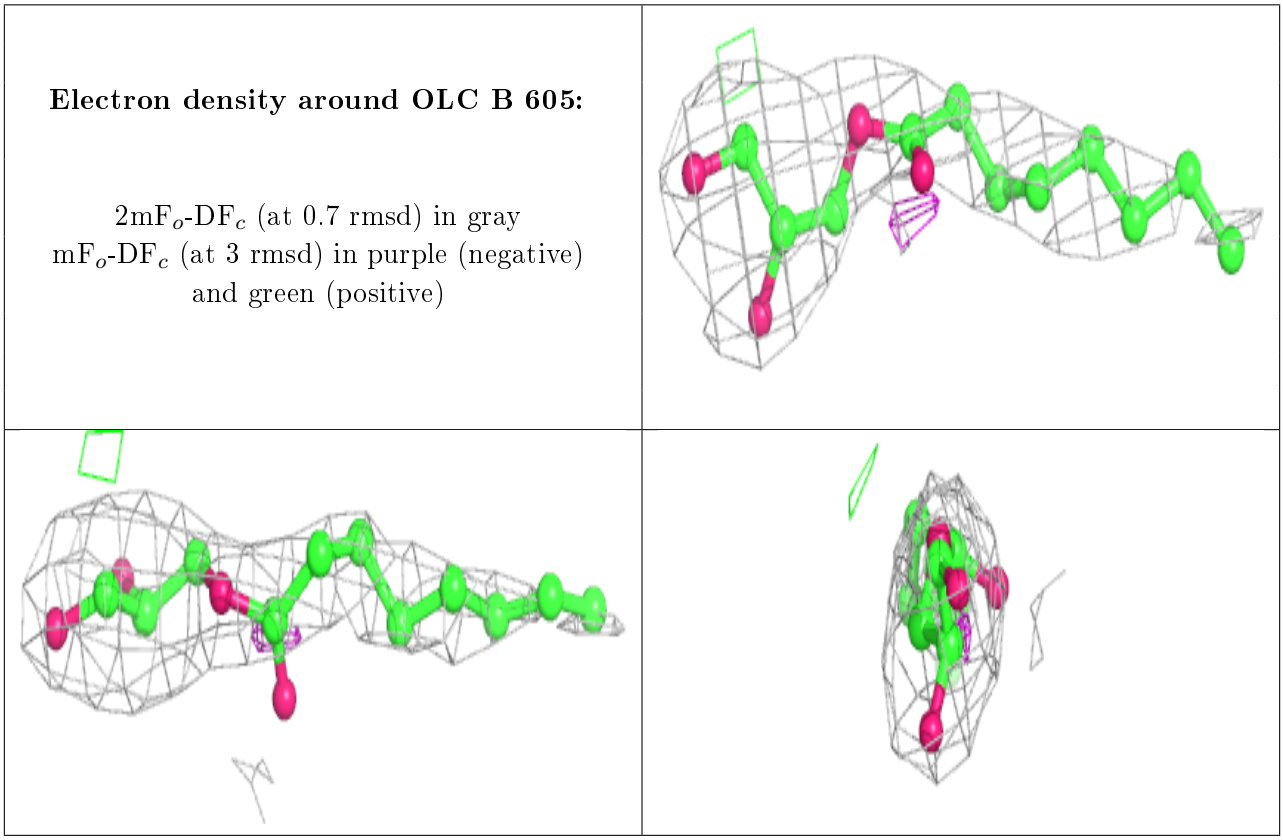
Electron density around OLC A 605:

$2mF_o$-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 B 605:

$2mF_o$-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 611:

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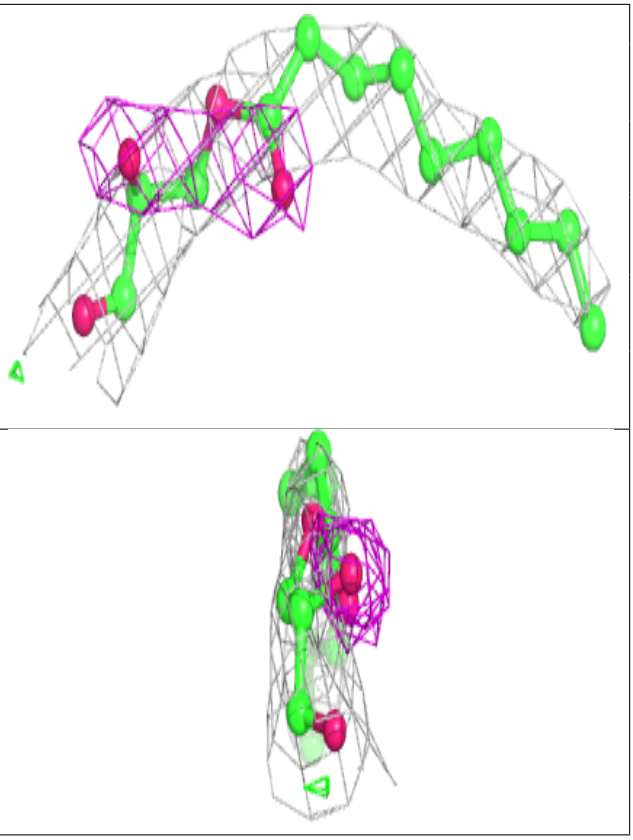
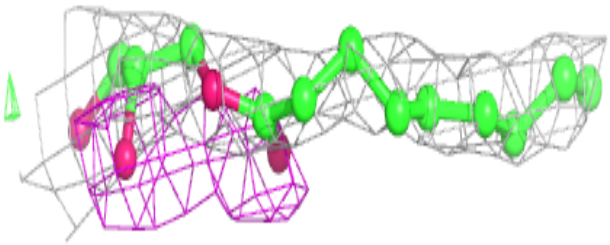
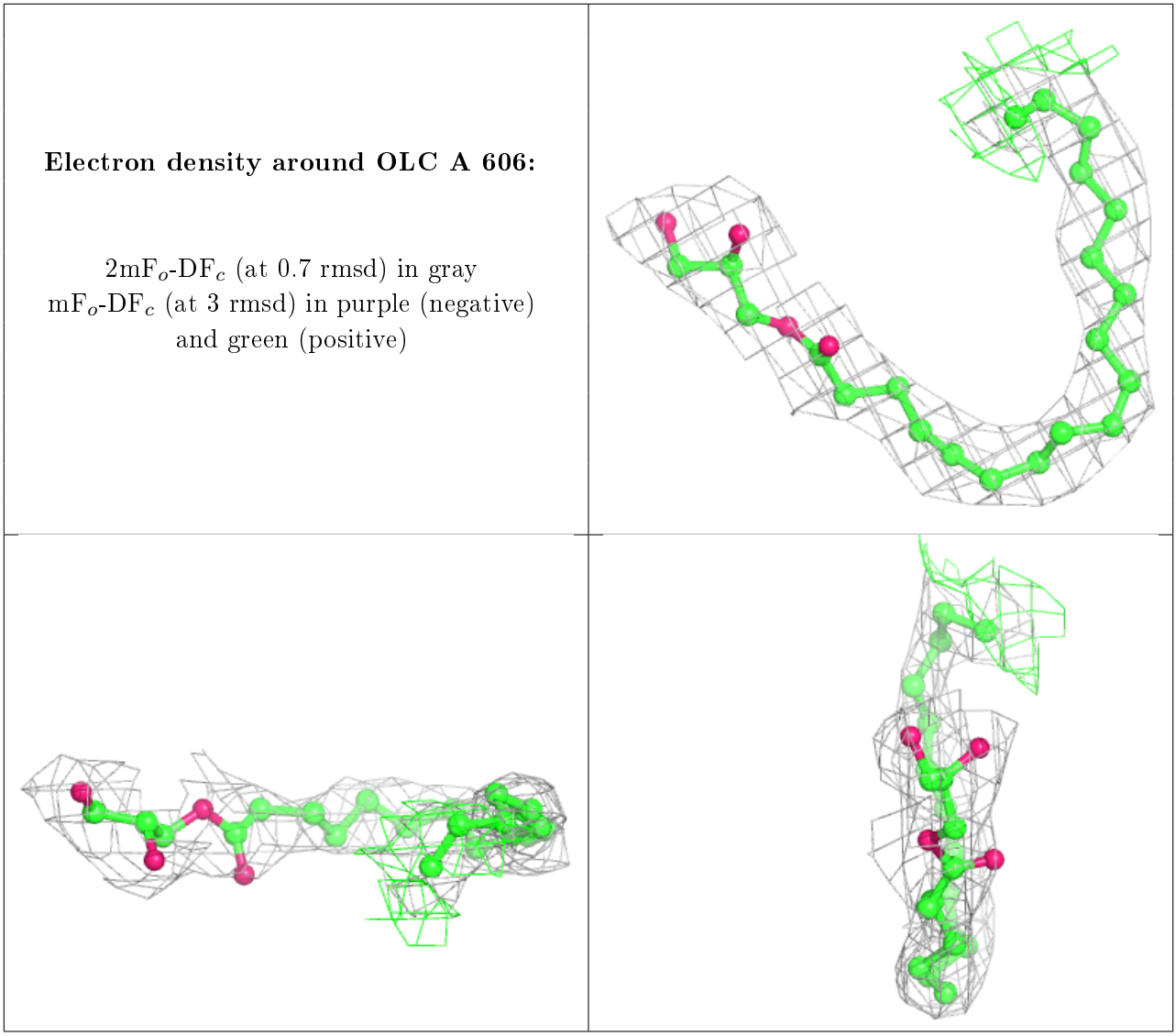
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around OLC A 606:

$2mF_o$-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 604:

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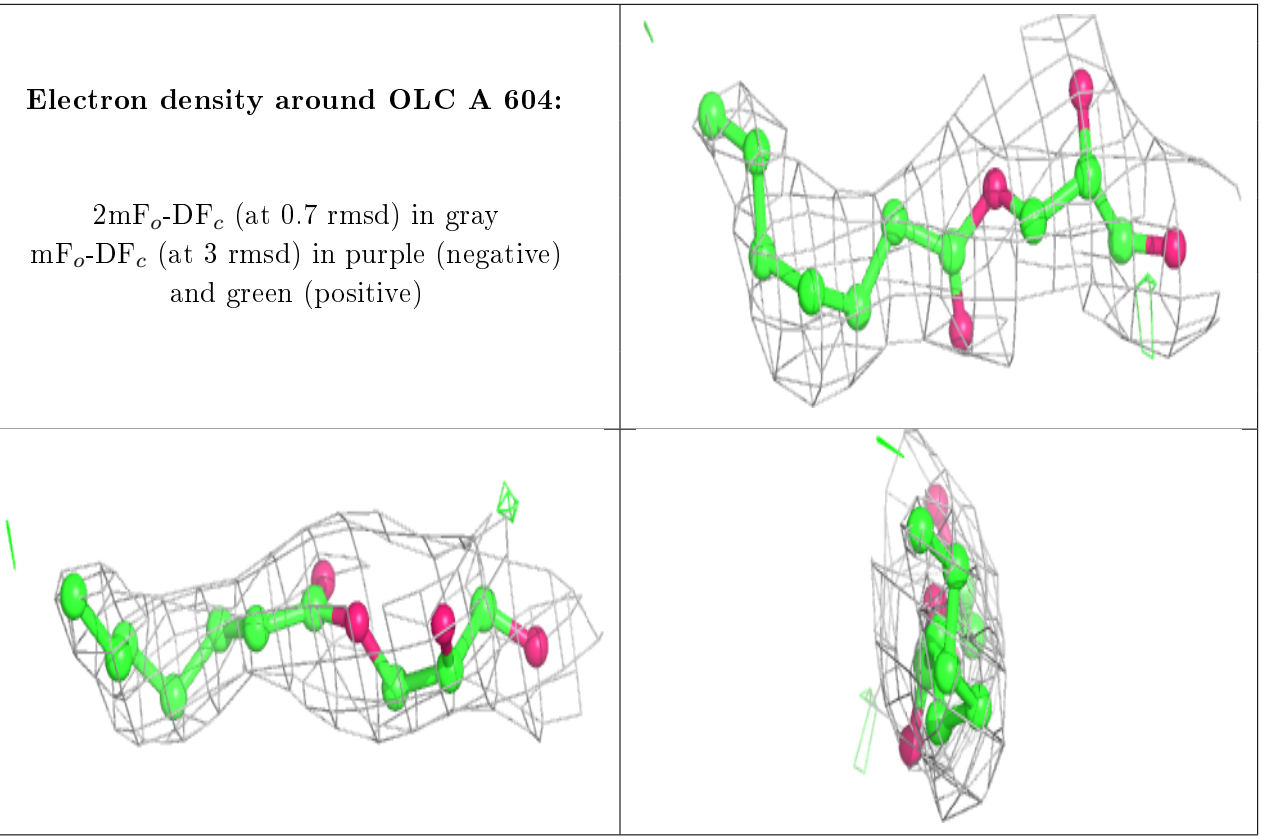
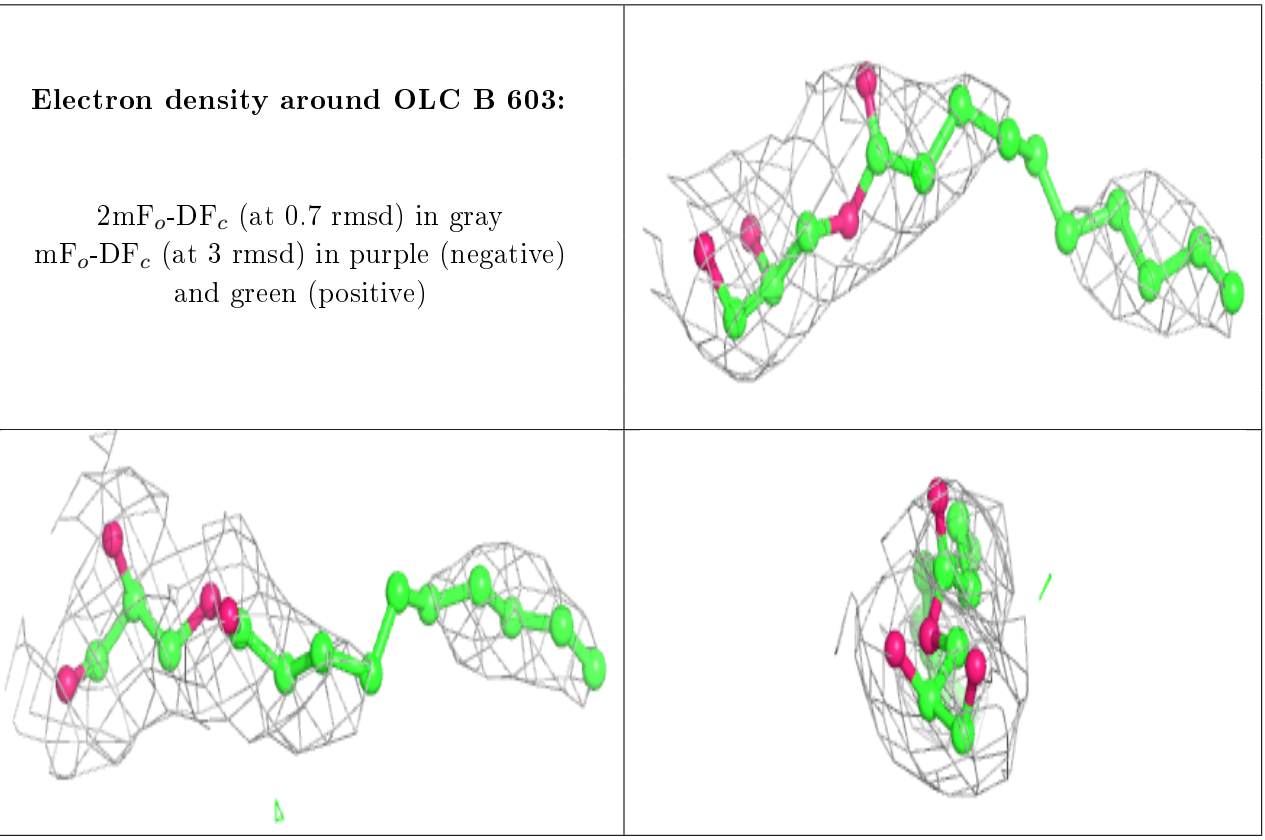
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



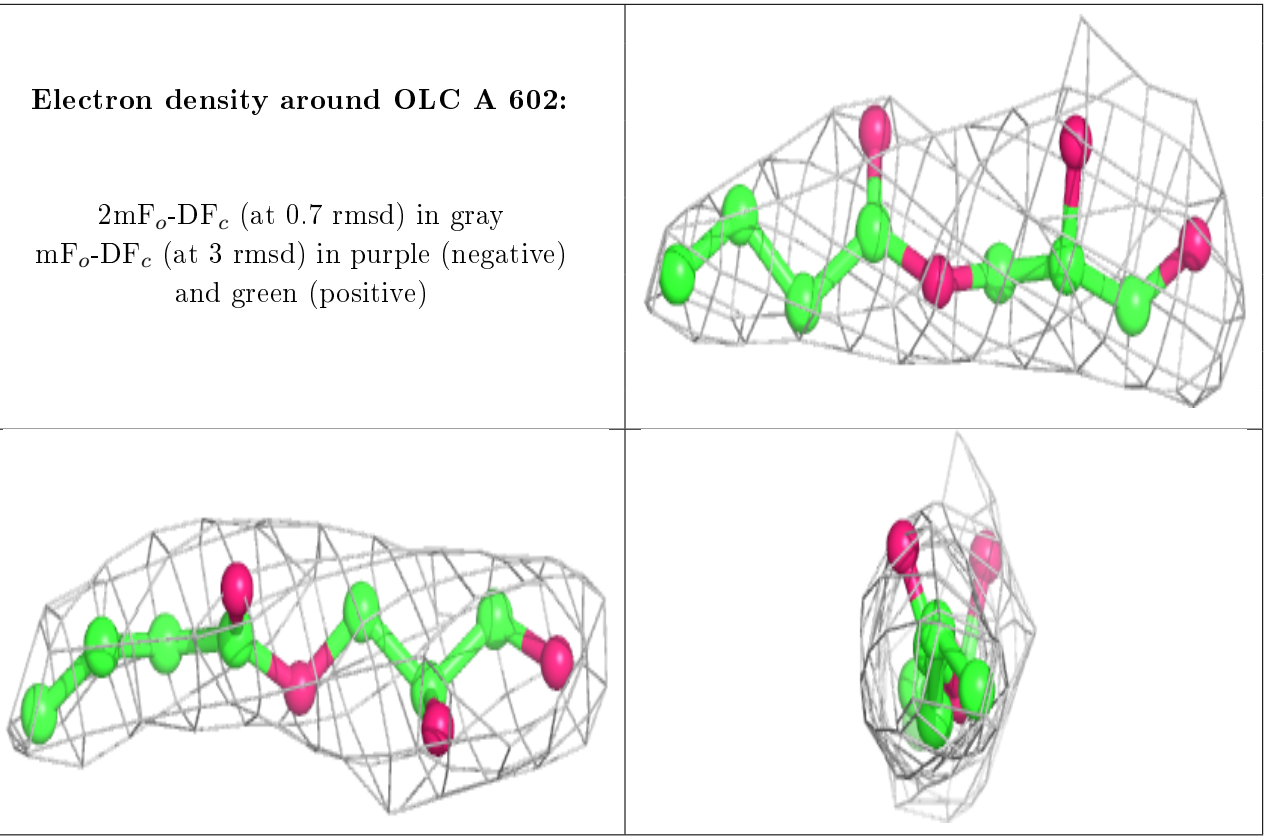
Electron density around OLC B 603:

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



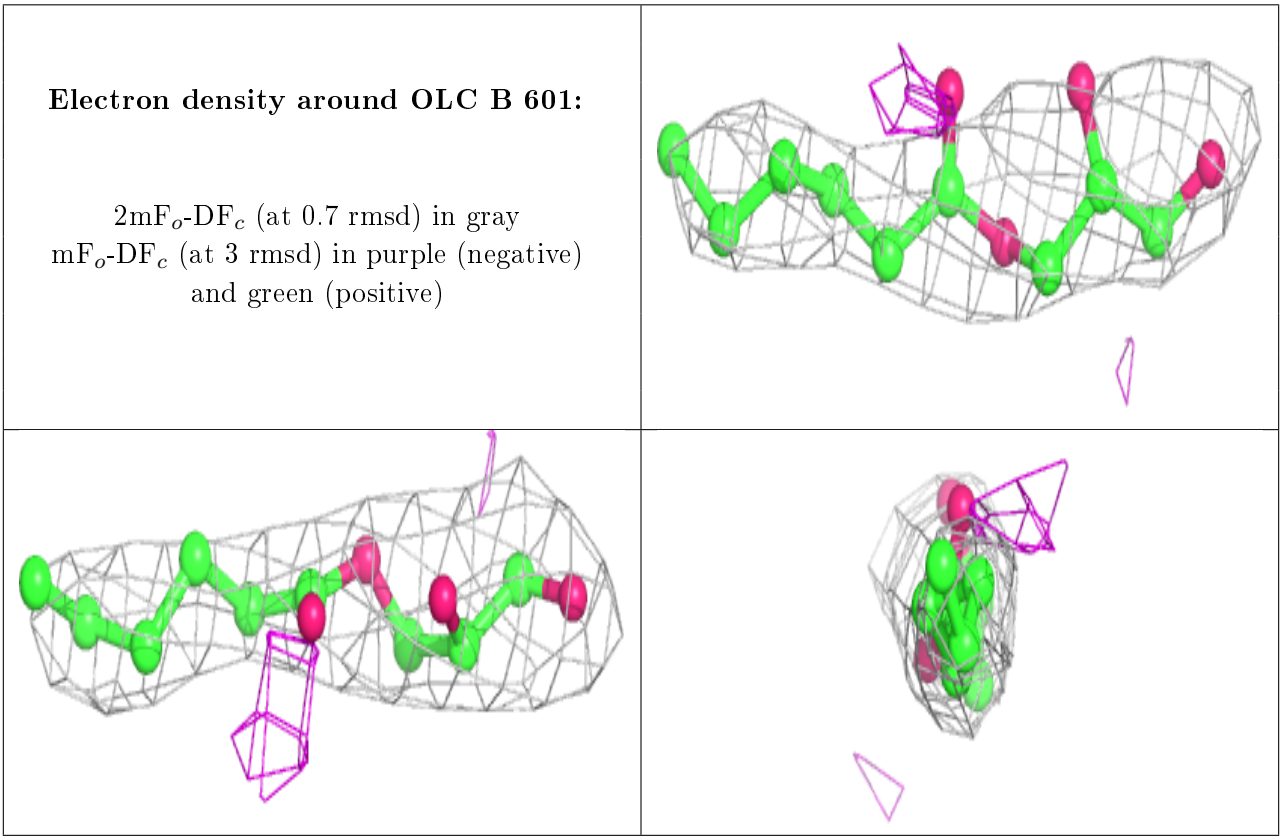
Electron density around OLC A 602:

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



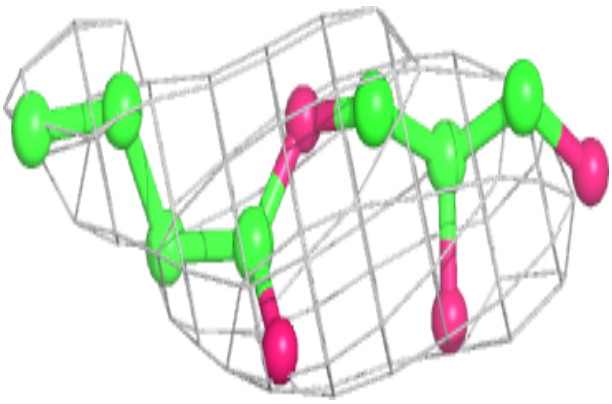
Electron density around OLC B 601:

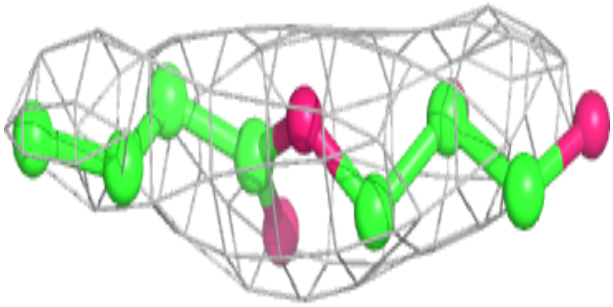
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

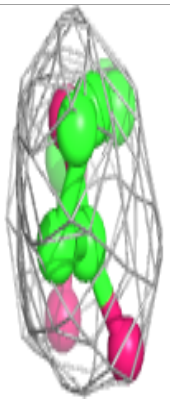


Electron density around OLC B 606:

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

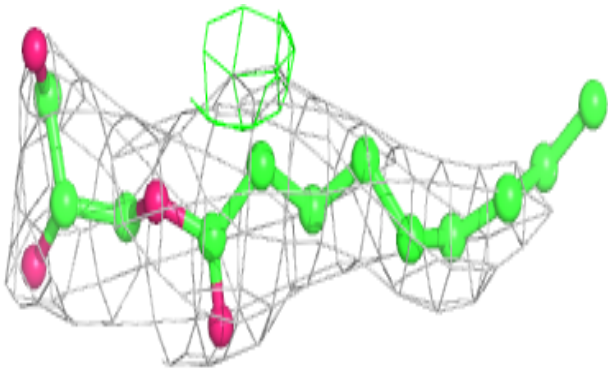


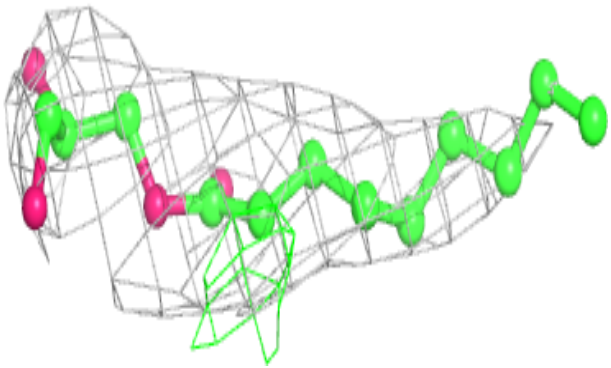




Electron density around OLC A 610:

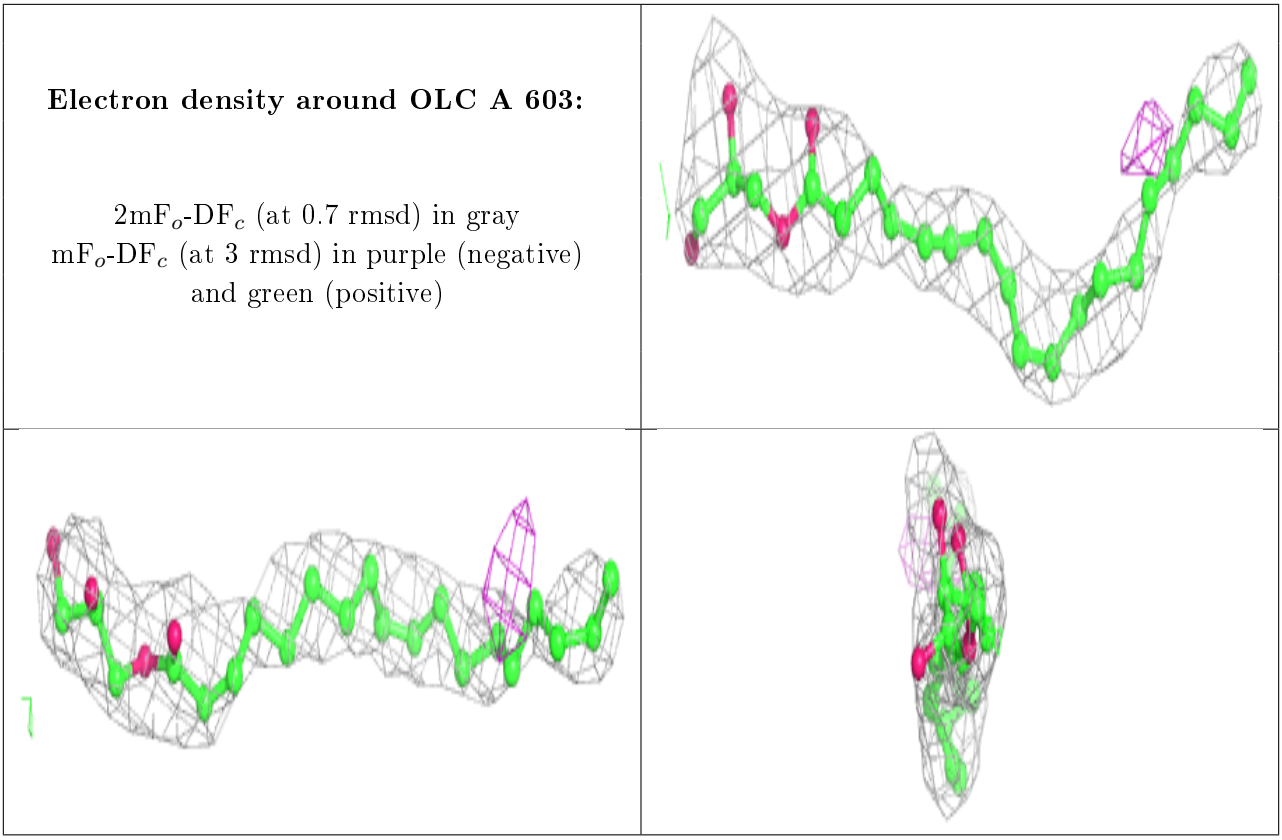
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





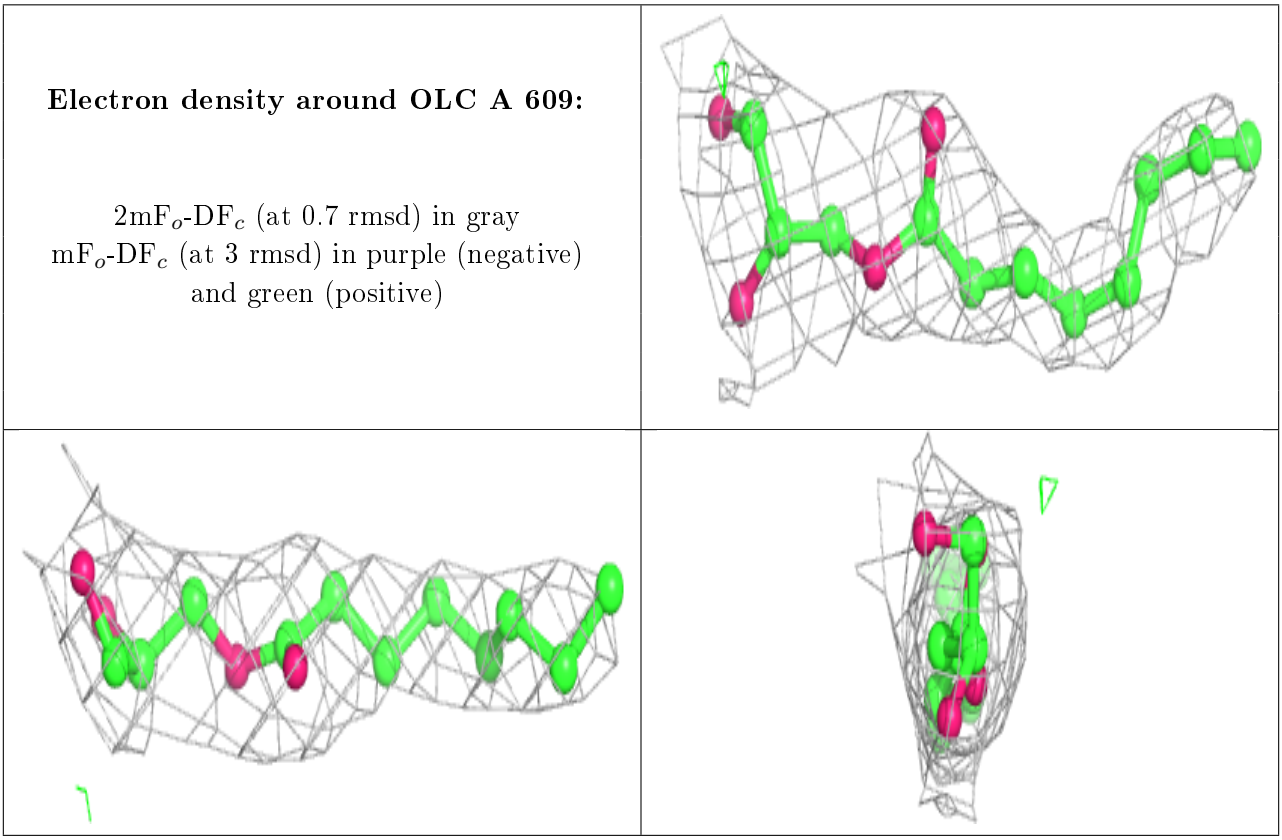
Electron density around OLC A 603:

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



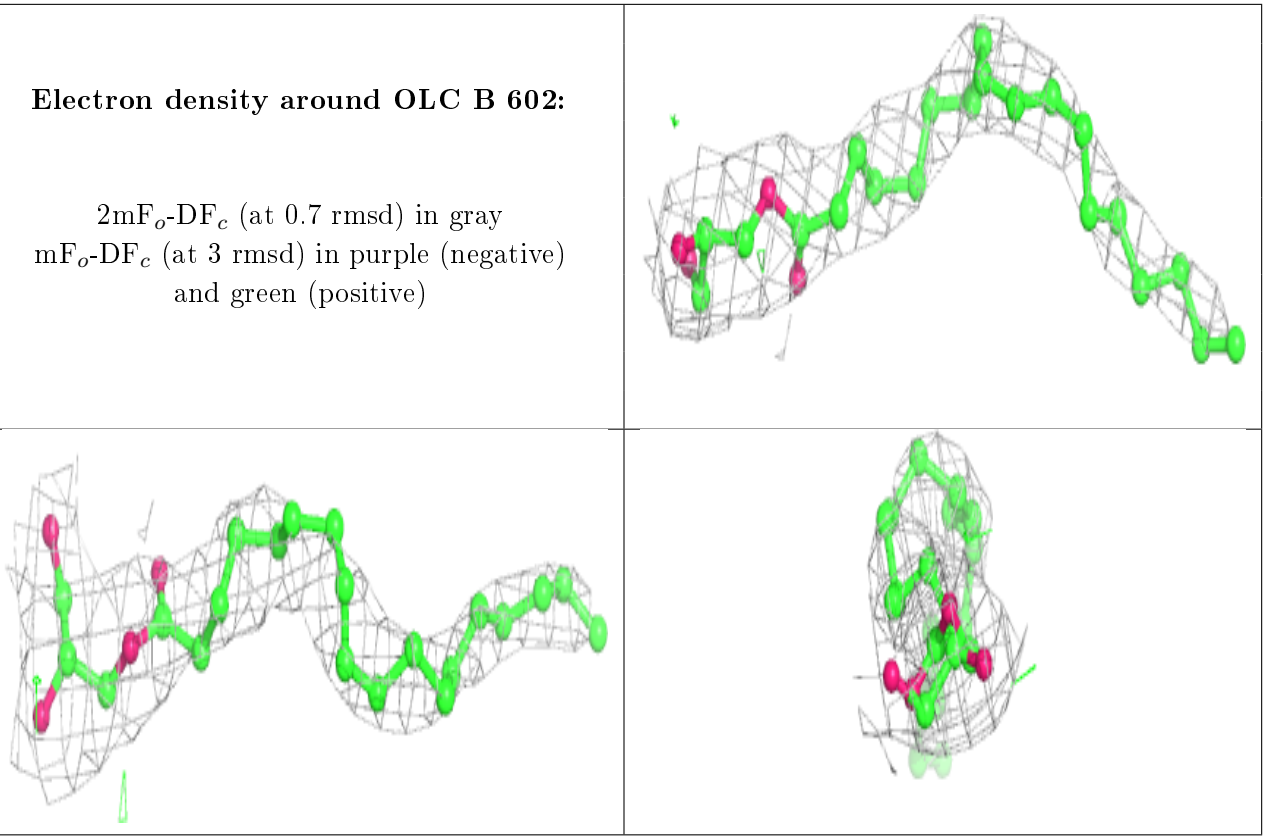
Electron density around OLC A 609:

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



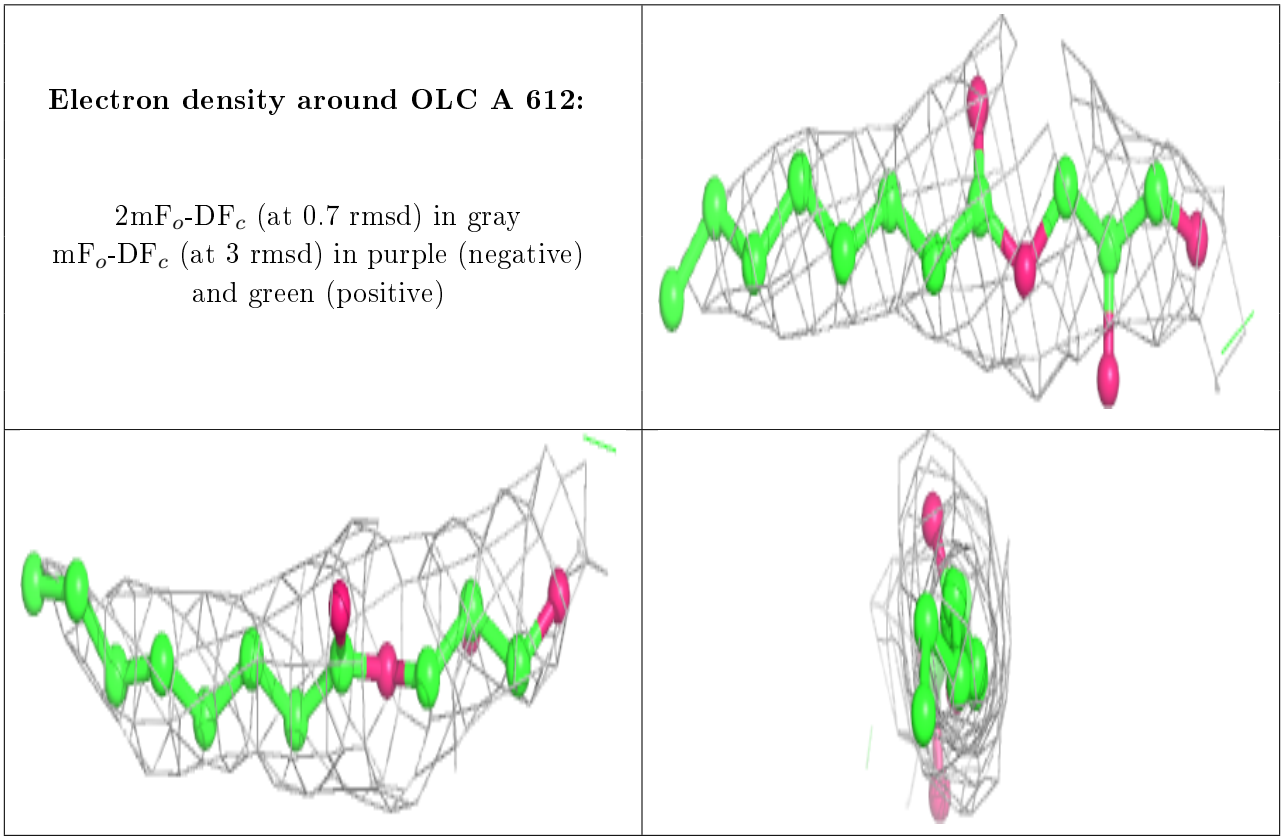
Electron density around OLC B 602:

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



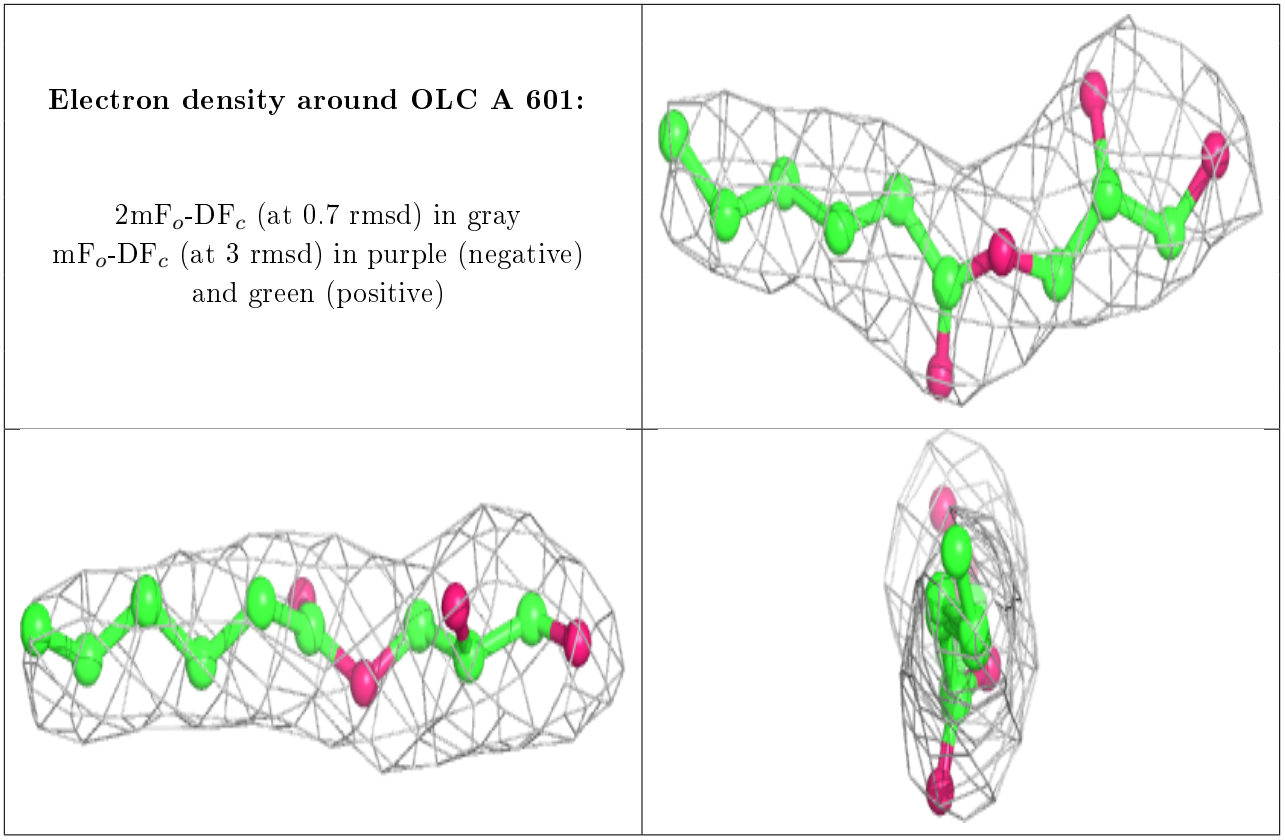
Electron density around OLC A 612:

$2mF_o$-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 601:

$2mF_o$-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.