Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 01:48 am GMT

PDB ID	:	6HLP
Title	:	Crystal structure of the Neurokinin 1 receptor in complex with the small molecule antagonist Netupitant
Authors	:	Schoppe, J.; Ehrenmann, J.; Klenk, C.; Rucktooa, P.; Schutz, M.; Dore, A.S.; Pluckthun, A.
Deposited on	:	2018-09-11
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

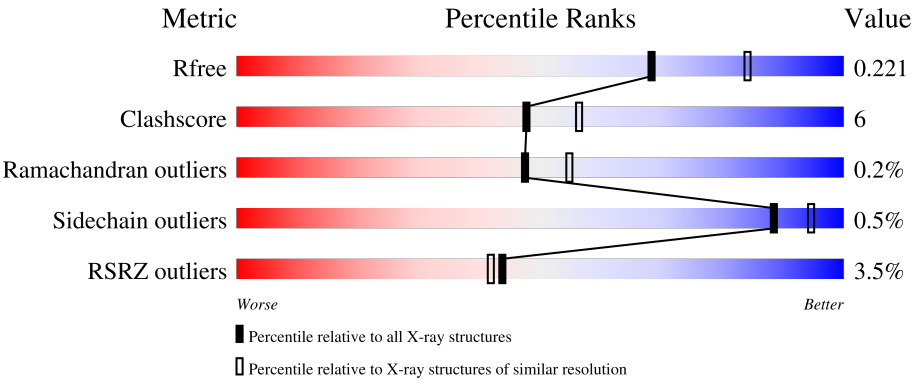
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	520	3%, 81%, 12%, 7%

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
4	OLA	A	1511	-	-	-	X
6	PEG	A	1517	-	-	-	X
6	PEG	A	1542	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4396 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.

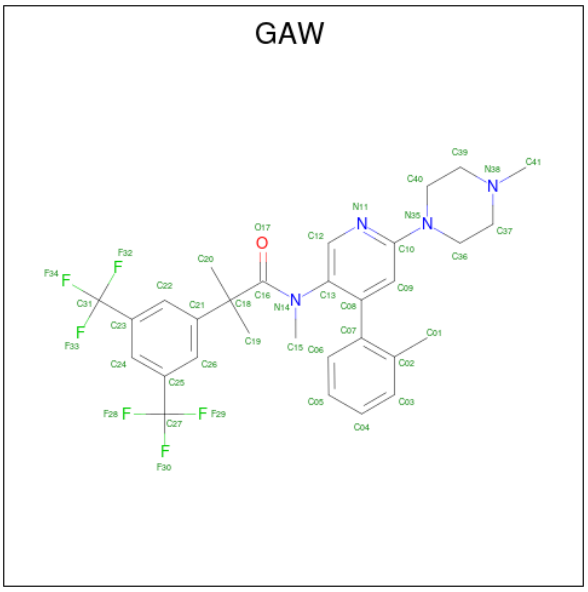
- Molecule 1 is a protein called Substance-P receptor,Substance-P receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3882	2560	630	662	30			

There are 8 discrepancies between the modelled and reference sequences:

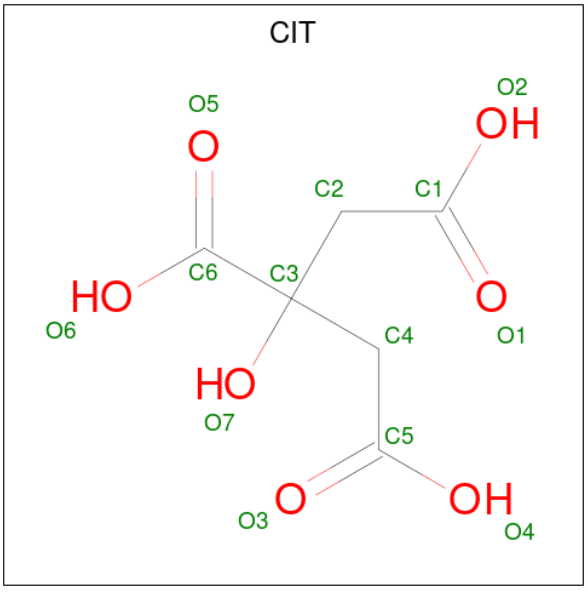
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	LEU	engineered mutation	UNP P25103
A	116	ILE	VAL	engineered mutation	UNP P25103
A	144	LEU	ALA	engineered mutation	UNP P25103
A	181	LYS	MET	engineered mutation	UNP P25103
A	215	LEU	ALA	engineered mutation	UNP P25103
A	224	ARG	TRP	engineered mutation	UNP P25103
A	1218	GLY	GLU	conflict	UNP P25103
A	243	ALA	LYS	engineered mutation	UNP P25103

- Molecule 2 is 2-[3,5-bis(trifluoromethyl)phenyl]- {N},2-dimethyl- {N}-[4-(2-methylphenyl)-6-(4-methylpiperazin-1-yl)pyridin-3-yl]propanamide (three-letter code: GAW) (formula: $C_{30}H_{32}F_6N_4O$).



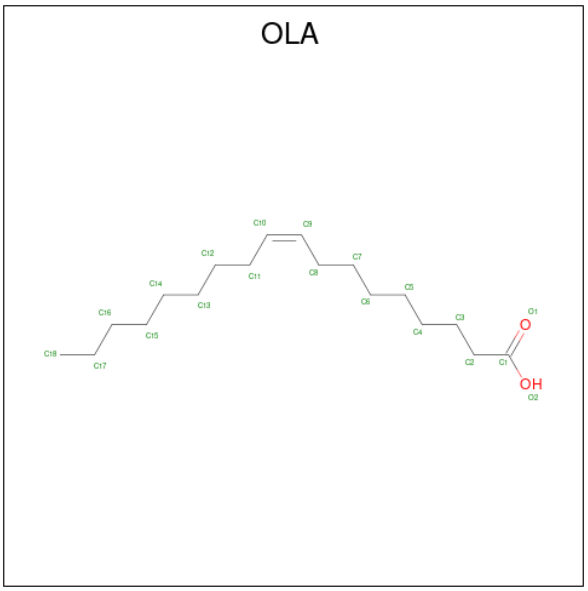
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			41	30	6	4	1		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



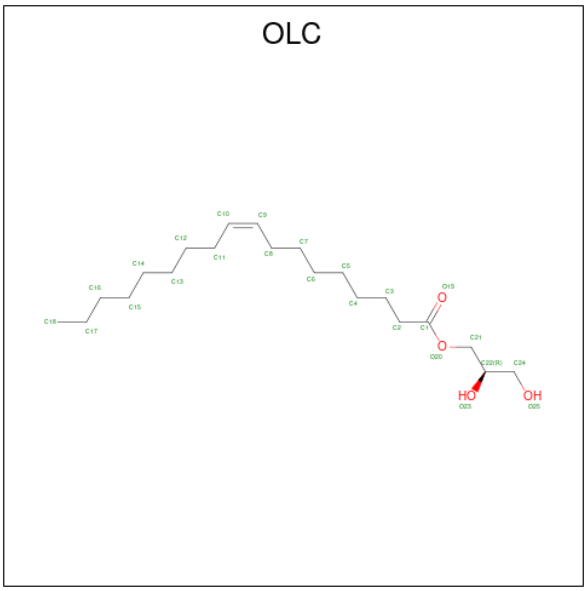
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			13	6	7			

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



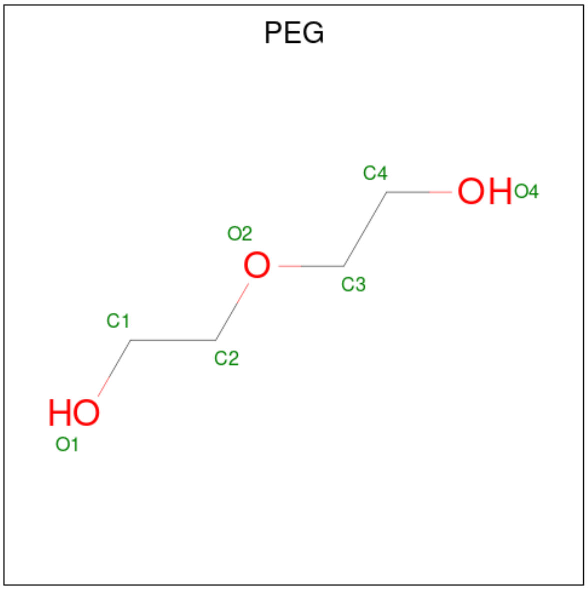
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 9 2	0	0
4	A	1	Total C O 14 12 2	0	0
4	A	1	Total C O 17 15 2	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C 10 10	0	0

- Molecule 5 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
5	A	1	Total C O 20 16 4	0	0
5	A	1	Total C O 23 19 4	0	0
5	A	1	Total C O 17 13 4	0	0
5	A	1	Total C O 17 13 4	0	0
5	A	1	Total C O 15 11 4	0	0
5	A	1	Total C O 17 13 4	0	0
5	A	1	Total C O 10 6 4	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0

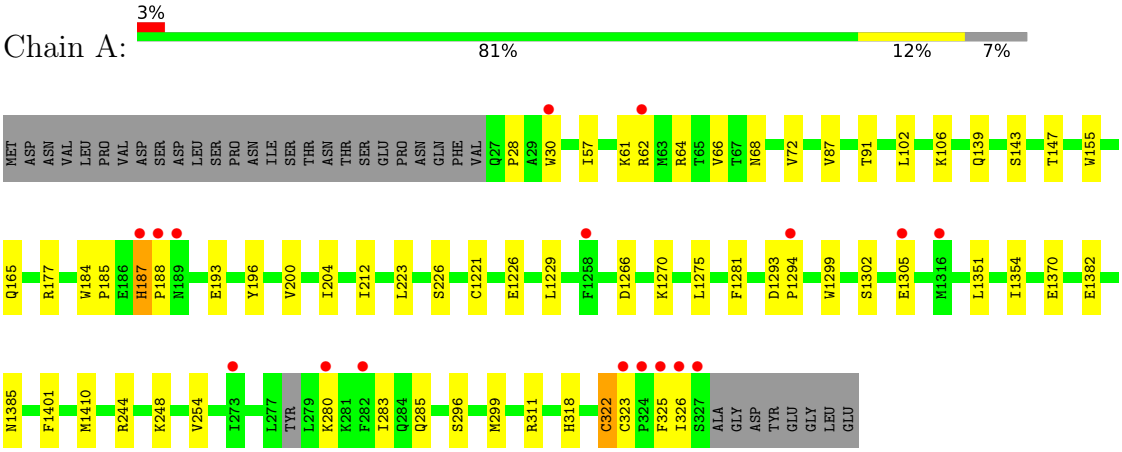
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	74	Total O 74 74	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: Substance-P receptor,Substance-P receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.66Å 76.57Å 166.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 2.20 49.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.24-2.20) 100.0 (49.50-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.203 , 0.225 0.206 , 0.221	Depositor DCC
R_{free} test set	1979 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4396	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% 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: OLC, CIT, YCM, GAW, PEG, OLA

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	0.38	1/3962 (0.0%)	0.53	1/5374 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1354	ILE	C-N	7.66	1.48	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	SER	O-C-N	-6.61	111.97	123.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3882	0	3941	50	0
2	A	41	0	0	0	0
3	A	13	0	5	3	0
4	A	99	0	147	1	0
5	A	119	0	154	6	0
6	A	168	0	240	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	74	0	0	3	0
All	All	4396	0	4487	54	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 (54) 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:187:HIS:HB3	1:A:188:PRO:CD	1.68	1.20
1:A:187:HIS:HB3	1:A:188:PRO:HD2	1.36	1.02
1:A:185:PRO:HB2	1:A:187:HIS:NE2	1.76	1.01
1:A:187:HIS:CB	1:A:188:PRO:HD2	1.94	0.97
1:A:187:HIS:CB	1:A:188:PRO:CD	2.42	0.94
1:A:187:HIS:HB3	1:A:188:PRO:HD3	1.48	0.93
1:A:102:LEU:H	3:A:1502:CIT:H42	1.54	0.73
4:A:1508:OLA:H42	5:A:1513:OLC:H5	1.72	0.71
1:A:139:GLN:HE22	5:A:1513:OLC:H21A	1.60	0.66
1:A:1370:GLU:OE2	7:A:1601:HOH:O	2.14	0.65
3:A:1502:CIT:O6	7:A:1602:HOH:O	2.14	0.64
1:A:185:PRO:HB2	1:A:187:HIS:CD2	2.33	0.63
1:A:187:HIS:HB2	1:A:188:PRO:HD2	1.84	0.57
1:A:280:LYS:O	1:A:283:ILE:HB	2.04	0.57
1:A:106:LYS:HD2	6:A:1518:PEG:H41	1.88	0.56
1:A:68:ASN:O	1:A:72:VAL:HG23	2.05	0.56
1:A:1229:LEU:HD11	1:A:1351:LEU:HD12	1.89	0.55
1:A:1266:ASP:OD2	7:A:1603:HOH:O	2.18	0.55
1:A:185:PRO:O	1:A:187:HIS:CD2	2.61	0.54
1:A:212:ILE:HG21	1:A:254:VAL:HG21	1.90	0.54
1:A:1226:GLU:HG3	1:A:1229:LEU:HD12	1.90	0.54
1:A:1385:ASN:HD22	6:A:1522:PEG:H42	1.75	0.52
1:A:66:VAL:HG22	1:A:147:THR:HG21	1.93	0.52
1:A:223:LEU:HB3	1:A:244:ARG:HG2	1.92	0.51
1:A:1382:GLU:HG3	6:A:1522:PEG:H32	1.93	0.51
1:A:155:TRP:CD1	5:A:1516:OLC:H5	2.47	0.50
1:A:165:GLN:HG3	1:A:196:TYR:CE1	2.47	0.49
1:A:177:ARG:HB2	6:A:1517:PEG:H41	1.95	0.49
1:A:28:PRO:HB2	1:A:30:TRP:CD1	2.48	0.49
1:A:143:SER:O	1:A:147:THR:HG23	2.12	0.49
1:A:1266:ASP:OD1	1:A:1266:ASP:N	2.47	0.48
1:A:87:VAL:O	1:A:91:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:HD2	5:A:1512:OLC:O23	2.16	0.46
1:A:1221:YCM:HA	1:A:1221:YCM:HD3	1.62	0.45
1:A:185:PRO:CB	1:A:187:HIS:NE2	2.65	0.45
1:A:1302:SER:HA	1:A:1305:GLU:HG2	1.98	0.45
1:A:248:LYS:HB2	5:A:1512:OLC:H21	1.97	0.45
1:A:285:GLN:OE1	1:A:285:GLN:N	2.42	0.45
1:A:200:VAL:O	1:A:204:ILE:HG12	2.17	0.45
1:A:62:ARG:HB3	1:A:311:ARG:HH12	1.82	0.45
1:A:1221:YCM:OZ1	1:A:1410:MET:HG2	2.17	0.44
1:A:296:SER:O	1:A:299:MET:HG2	2.18	0.44
5:A:1514:OLC:H6A	5:A:1514:OLC:H3	1.68	0.44
3:A:1502:CIT:O2	3:A:1502:CIT:O7	2.23	0.43
1:A:1293:ASP:HA	1:A:1294:PRO:HD3	1.89	0.43
1:A:66:VAL:HG13	1:A:147:THR:HG21	2.00	0.43
1:A:61:LYS:HG2	1:A:64:ARG:HH12	1.84	0.42
1:A:57:ILE:HG21	1:A:72:VAL:CG2	2.50	0.42
1:A:326:ILE:H	1:A:326:ILE:HD12	1.85	0.41
1:A:1270:LYS:HG3	1:A:1299:TRP:HH2	1.86	0.41
1:A:184:TRP:CD1	1:A:193:GLU:HB3	2.56	0.41
1:A:1275:LEU:O	1:A:1281:PHE:HB2	2.21	0.41
1:A:322:YCM:SG	1:A:323:CYS:N	2.94	0.41
1:A:323:CYS:HB3	1:A:325:PHE:CE2	2.56	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	479/520 (92%)	468 (98%)	10 (2%)	1 (0%)	47 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	HIS

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	415/450 (92%)	413 (100%)	2 (0%)	88 94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1401	PHE
1	A	318	HIS

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

Mol	Chain	Res	Type
1	A	139	GLN
1	A	1385	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	YCM	A	1221	1	7,9,10	0.95	0	4,10,12	0.85	0
1	YCM	A	322	1	7,9,10	1.01	1 (14%)	4,10,12	1.13	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
1	YCM	A	1221	1	-	0/6/8/10	-
1	YCM	A	322	1	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	YCM	CD-SG	-2.04	1.76	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	322	YCM	CA-CB-SG-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1221	YCM	2	0
1	A	322	YCM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

42 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	$\#\|Z\| > 2$
3	CIT	A	1502	-	12,12,12	1.15	0	17,17,17	1.50	3 (17%)
5	OLC	A	1513	-	22,22,24	0.97	1 (4%)	23,23,25	0.91	1 (4%)
6	PEG	A	1541	-	6,6,6	0.43	0	5,5,5	0.39	0
6	PEG	A	1535	-	6,6,6	0.43	0	5,5,5	0.29	0
5	OLC	A	1540	-	9,9,24	1.48	1 (11%)	10,10,25	1.31	1 (10%)
6	PEG	A	1529	-	6,6,6	0.44	0	5,5,5	0.26	0
6	PEG	A	1536	-	6,6,6	0.42	0	5,5,5	0.45	0
5	OLC	A	1516	-	14,14,24	1.19	1 (7%)	15,15,25	1.06	2 (13%)
6	PEG	A	1519	-	6,6,6	0.45	0	5,5,5	0.30	0
6	PEG	A	1526	-	6,6,6	0.43	0	5,5,5	0.30	0
6	PEG	A	1531	-	6,6,6	0.43	0	5,5,5	0.44	0
5	OLC	A	1514	-	16,16,24	1.16	1 (6%)	17,17,25	0.98	1 (5%)
6	PEG	A	1520	-	6,6,6	0.44	0	5,5,5	0.26	0
6	PEG	A	1542	-	6,6,6	0.42	0	5,5,5	0.34	0
4	OLA	A	1508	-	9,9,19	0.31	0	8,8,19	0.75	0
4	OLA	A	1503	-	10,10,19	0.57	0	10,10,19	1.17	2 (20%)
6	PEG	A	1528	-	6,6,6	0.46	0	5,5,5	0.28	0
4	OLA	A	1511	-	9,9,19	0.32	0	7,8,19	0.48	0
6	PEG	A	1521	-	6,6,6	0.43	0	5,5,5	0.30	0
6	PEG	A	1527	-	6,6,6	0.41	0	5,5,5	0.40	0
6	PEG	A	1533	-	6,6,6	0.44	0	5,5,5	0.33	0
6	PEG	A	1524	-	6,6,6	0.44	0	5,5,5	0.30	0
4	OLA	A	1504	-	13,13,19	0.59	0	12,13,19	0.98	1 (8%)
4	OLA	A	1505	-	16,16,19	0.54	0	16,16,19	0.85	1 (6%)
4	OLA	A	1507	-	10,10,19	0.29	0	9,9,19	0.68	0
6	PEG	A	1530	-	6,6,6	0.43	0	5,5,5	0.26	0
6	PEG	A	1517	-	6,6,6	0.42	0	5,5,5	0.48	0
6	PEG	A	1523	-	6,6,6	0.40	0	5,5,5	0.42	0
5	OLC	A	1512	-	19,19,24	1.02	1 (5%)	20,20,25	0.96	1 (5%)
6	PEG	A	1537	-	6,6,6	0.48	0	5,5,5	0.19	0
4	OLA	A	1510	-	12,12,19	0.25	0	11,11,19	0.46	0
6	PEG	A	1518	-	6,6,6	0.43	0	5,5,5	0.29	0
6	PEG	A	1534	-	6,6,6	0.44	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLA	A	1506	-	6,6,19	0.25	0	5,5,19	0.53	0
2	GAW	A	1501	-	43,44,44	3.18	13 (30%)	63,68,68	2.08	17 (26%)
5	OLC	A	1539	-	16,16,24	1.15	1 (6%)	17,17,25	1.13	1 (5%)
6	PEG	A	1525	-	6,6,6	0.42	0	5,5,5	0.36	0
6	PEG	A	1522	-	6,6,6	0.44	0	5,5,5	0.34	0
6	PEG	A	1538	-	6,6,6	0.38	0	5,5,5	0.38	0
4	OLA	A	1509	-	5,5,19	0.24	0	4,4,19	0.40	0
6	PEG	A	1532	-	6,6,6	0.44	0	5,5,5	0.26	0
5	OLC	A	1515	-	16,16,24	1.14	1 (6%)	17,17,25	1.03	1 (5%)

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
3	CIT	A	1502	-	-	10/16/16/16	-
5	OLC	A	1513	-	-	4/22/22/24	-
6	PEG	A	1541	-	-	0/4/4/4	-
6	PEG	A	1535	-	-	0/4/4/4	-
5	OLC	A	1540	-	-	4/9/9/24	-
6	PEG	A	1529	-	-	0/4/4/4	-
6	PEG	A	1536	-	-	1/4/4/4	-
5	OLC	A	1516	-	-	5/14/14/24	-
6	PEG	A	1519	-	-	1/4/4/4	-
6	PEG	A	1526	-	-	0/4/4/4	-
6	PEG	A	1531	-	-	2/4/4/4	-
5	OLC	A	1514	-	-	3/16/16/24	-
6	PEG	A	1520	-	-	1/4/4/4	-
6	PEG	A	1542	-	-	1/4/4/4	-
4	OLA	A	1508	-	-	1/7/7/17	-
4	OLA	A	1503	-	-	2/8/8/17	-
6	PEG	A	1528	-	-	2/4/4/4	-
4	OLA	A	1511	-	-	3/7/7/17	-
6	PEG	A	1521	-	-	0/4/4/4	-
6	PEG	A	1527	-	-	0/4/4/4	-
6	PEG	A	1533	-	-	0/4/4/4	-
6	PEG	A	1524	-	-	0/4/4/4	-
4	OLA	A	1504	-	-	2/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1505	-	-	5/14/14/17	-
4	OLA	A	1507	-	-	3/8/8/17	-
6	PEG	A	1530	-	-	2/4/4/4	-
6	PEG	A	1517	-	-	1/4/4/4	-
6	PEG	A	1523	-	-	0/4/4/4	-
5	OLC	A	1512	-	-	5/19/19/24	-
6	PEG	A	1537	-	-	1/4/4/4	-
4	OLA	A	1510	-	-	2/10/10/17	-
6	PEG	A	1518	-	-	2/4/4/4	-
6	PEG	A	1534	-	-	1/4/4/4	-
4	OLA	A	1506	-	-	0/4/4/17	-
2	GAW	A	1501	-	-	0/40/50/50	0/4/4/4
5	OLC	A	1539	-	-	5/16/16/24	-
6	PEG	A	1525	-	-	0/4/4/4	-
6	PEG	A	1522	-	-	1/4/4/4	-
6	PEG	A	1538	-	-	1/4/4/4	-
4	OLA	A	1509	-	-	0/3/3/17	-
6	PEG	A	1532	-	-	0/4/4/4	-
5	OLC	A	1515	-	-	1/16/16/24	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	GAW	C16-N14	15.05	1.47	1.36
2	A	1501	GAW	C10-N35	6.49	1.50	1.37
2	A	1501	GAW	C13-N14	4.69	1.49	1.44
5	A	1514	OLC	O20-C1	4.38	1.46	1.33
5	A	1539	OLC	O20-C1	4.36	1.46	1.33
5	A	1513	OLC	O20-C1	4.31	1.45	1.33
5	A	1515	OLC	O20-C1	4.30	1.45	1.33
5	A	1516	OLC	O20-C1	4.29	1.45	1.33
5	A	1540	OLC	O20-C1	4.28	1.45	1.33
2	A	1501	GAW	C27-C25	4.27	1.59	1.49
5	A	1512	OLC	O20-C1	4.19	1.45	1.33
2	A	1501	GAW	C31-C23	4.05	1.58	1.49
2	A	1501	GAW	C18-C21	4.05	1.58	1.53
2	A	1501	GAW	C09-C10	3.96	1.45	1.39
2	A	1501	GAW	C40-N35	3.94	1.52	1.46
2	A	1501	GAW	C12-C13	3.32	1.43	1.39
2	A	1501	GAW	C08-C13	2.86	1.44	1.41
2	A	1501	GAW	C36-N35	2.79	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	GAW	C09-C08	2.69	1.44	1.39
2	A	1501	GAW	C39-N38	2.24	1.51	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1501	GAW	C08-C09-C10	7.33	125.29	119.21
2	A	1501	GAW	C08-C13-N14	5.22	127.42	121.23
2	A	1501	GAW	C13-C12-N11	5.09	127.61	121.22
2	A	1501	GAW	C09-C10-N11	-4.69	114.60	122.73
2	A	1501	GAW	C39-C40-N35	3.75	117.98	110.70
5	A	1540	OLC	O20-C1-C2	3.37	120.22	111.38
3	A	1502	CIT	O6-C6-C3	3.23	118.66	113.05
2	A	1501	GAW	C41-N38-C37	-3.18	105.90	110.66
2	A	1501	GAW	O17-C16-N14	-3.16	116.52	120.00
2	A	1501	GAW	C41-N38-C39	-3.16	105.94	110.66
5	A	1539	OLC	O20-C1-C2	3.13	121.72	111.91
2	A	1501	GAW	C06-C07-C02	-3.06	115.53	119.35
5	A	1516	OLC	O20-C1-C2	2.92	121.07	111.91
2	A	1501	GAW	C40-N35-C36	-2.90	105.12	111.52
5	A	1513	OLC	O20-C1-C2	2.89	120.96	111.91
2	A	1501	GAW	N11-C10-N35	2.79	120.97	116.79
5	A	1515	OLC	O20-C1-C2	2.78	120.63	111.91
2	A	1501	GAW	C39-N38-C37	2.75	113.37	109.52
3	A	1502	CIT	O5-C6-C3	-2.75	118.36	122.25
5	A	1512	OLC	O20-C1-C2	2.54	119.88	111.91
5	A	1514	OLC	O20-C1-C2	2.41	119.47	111.91
2	A	1501	GAW	C19-C18-C20	2.32	111.17	107.89
2	A	1501	GAW	C12-N11-C10	2.29	121.47	117.30
3	A	1502	CIT	C3-C2-C1	-2.26	108.33	113.81
2	A	1501	GAW	C05-C06-C07	2.26	124.14	120.33
4	A	1505	OLA	C3-C2-C1	-2.20	108.92	114.47
4	A	1503	OLA	C3-C2-C1	-2.13	109.10	114.47
2	A	1501	GAW	C37-C36-N35	2.11	114.80	110.70
5	A	1516	OLC	O20-C1-O19	-2.08	118.35	123.59
4	A	1503	OLA	O1-C1-C2	-2.07	116.44	123.08
2	A	1501	GAW	C23-C22-C21	2.06	123.49	119.23
4	A	1504	OLA	C3-C2-C1	-2.02	109.39	114.47

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1502	CIT	O7-C3-C6-O5
3	A	1502	CIT	O7-C3-C6-O6
5	A	1516	OLC	C21-C22-C24-O25
5	A	1539	OLC	C21-C22-C24-O25
5	A	1512	OLC	C2-C1-O20-C21
5	A	1512	OLC	O19-C1-O20-C21
5	A	1516	OLC	C2-C1-O20-C21
5	A	1516	OLC	O19-C1-O20-C21
5	A	1540	OLC	O20-C21-C22-C24
6	A	1531	PEG	O1-C1-C2-O2
5	A	1516	OLC	C2-C3-C4-C5
6	A	1528	PEG	O2-C3-C4-O4
6	A	1530	PEG	O2-C3-C4-O4
5	A	1513	OLC	C3-C4-C5-C6
4	A	1511	OLA	C5-C6-C7-C8
5	A	1540	OLC	O20-C21-C22-O23
6	A	1518	PEG	O1-C1-C2-O2
5	A	1539	OLC	C2-C1-O20-C21
3	A	1502	CIT	C2-C3-C6-O5
3	A	1502	CIT	C2-C3-C6-O6
5	A	1514	OLC	C5-C6-C7-C8
5	A	1539	OLC	O23-C22-C24-O25
4	A	1507	OLA	C12-C13-C14-C15
4	A	1505	OLA	C10-C11-C12-C13
4	A	1505	OLA	C1-C2-C3-C4
5	A	1539	OLC	O19-C1-O20-C21
6	A	1534	PEG	O1-C1-C2-O2
6	A	1537	PEG	O2-C3-C4-O4
6	A	1517	PEG	O2-C3-C4-O4
6	A	1518	PEG	O2-C3-C4-O4
6	A	1519	PEG	O1-C1-C2-O2
4	A	1504	OLA	C5-C6-C7-C8
5	A	1516	OLC	O23-C22-C24-O25
5	A	1512	OLC	C2-C3-C4-C5
4	A	1504	OLA	C4-C5-C6-C7
4	A	1503	OLA	C1-C2-C3-C4
4	A	1505	OLA	C4-C5-C6-C7
5	A	1514	OLC	O20-C21-C22-O23
4	A	1503	OLA	C4-C5-C6-C7
5	A	1513	OLC	C2-C3-C4-C5
4	A	1511	OLA	C9-C10-C11-C12
4	A	1507	OLA	C11-C12-C13-C14
6	A	1542	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1505	OLA	C11-C12-C13-C14
6	A	1528	PEG	C1-C2-O2-C3
5	A	1539	OLC	C4-C5-C6-C7
5	A	1513	OLC	O20-C21-C22-O23
6	A	1538	PEG	O2-C3-C4-O4
6	A	1531	PEG	C1-C2-O2-C3
6	A	1536	PEG	C4-C3-O2-C2
6	A	1530	PEG	O1-C1-C2-O2
3	A	1502	CIT	C4-C3-C6-O6
5	A	1514	OLC	C4-C5-C6-C7
6	A	1520	PEG	O1-C1-C2-O2
4	A	1510	OLA	C6-C7-C8-C9
3	A	1502	CIT	O2-C1-C2-C3
5	A	1513	OLC	C4-C5-C6-C7
4	A	1511	OLA	C4-C5-C6-C7
4	A	1508	OLA	C5-C6-C7-C8
3	A	1502	CIT	C4-C3-C6-O5
3	A	1502	CIT	O1-C1-C2-C3
3	A	1502	CIT	C1-C2-C3-C4
5	A	1512	OLC	C5-C6-C7-C8
5	A	1540	OLC	C2-C1-O20-C21
4	A	1510	OLA	C7-C8-C9-C10
6	A	1522	PEG	C1-C2-O2-C3
3	A	1502	CIT	C1-C2-C3-C6
5	A	1512	OLC	C7-C8-C9-C10
5	A	1515	OLC	C1-C2-C3-C4
5	A	1540	OLC	O19-C1-O20-C21
4	A	1507	OLA	C9-C10-C11-C12
4	A	1505	OLA	O2-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	CIT	3	0
5	A	1513	OLC	2	0
5	A	1516	OLC	1	0
5	A	1514	OLC	1	0
4	A	1508	OLA	1	0
6	A	1517	PEG	1	0
5	A	1512	OLC	2	0
6	A	1518	PEG	1	0

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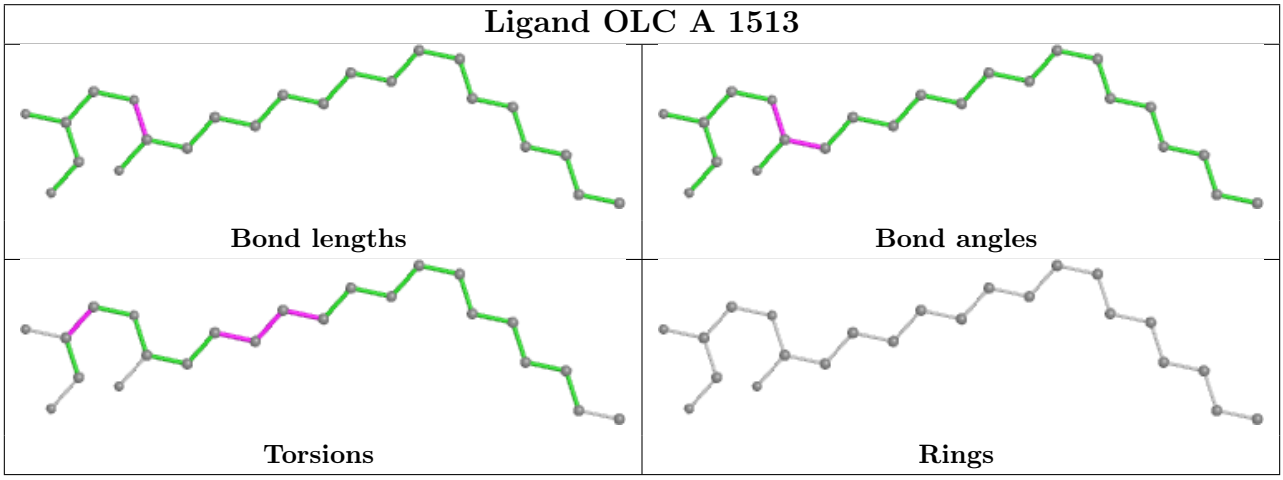
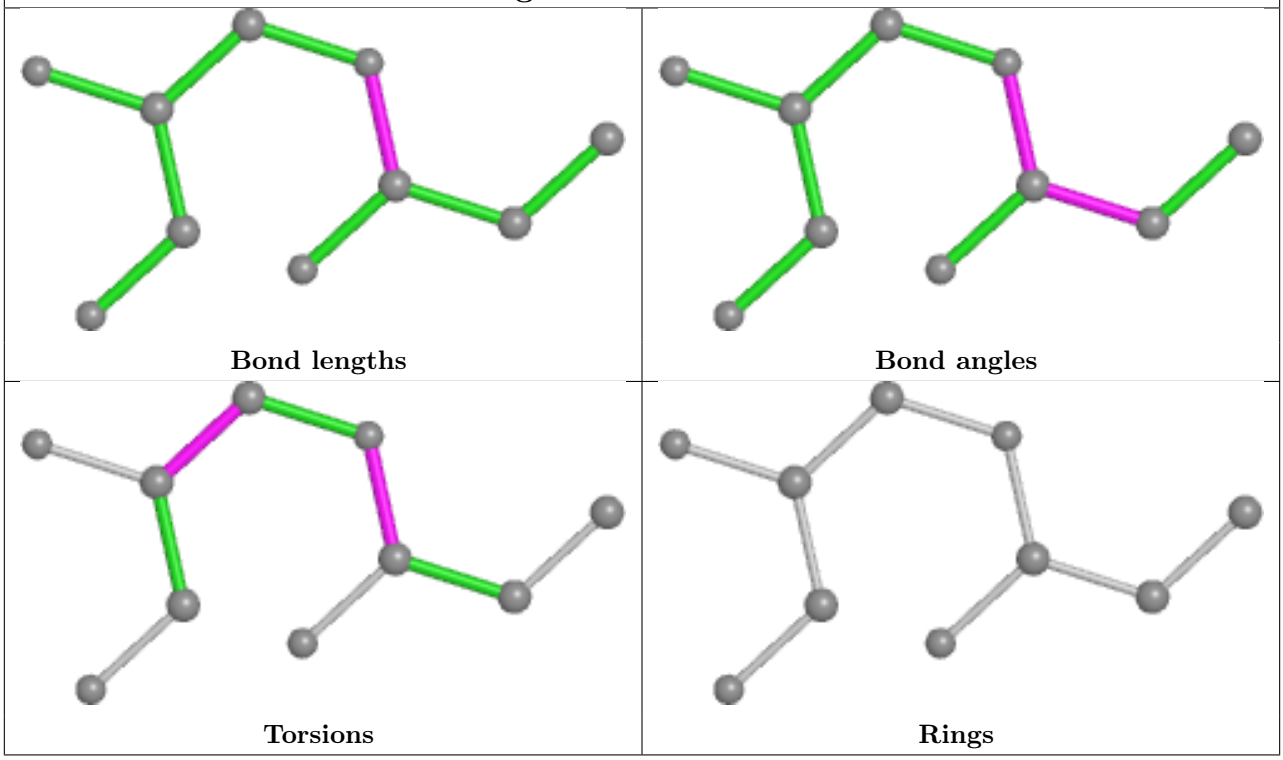
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1522	PEG	2	0

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 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 1540



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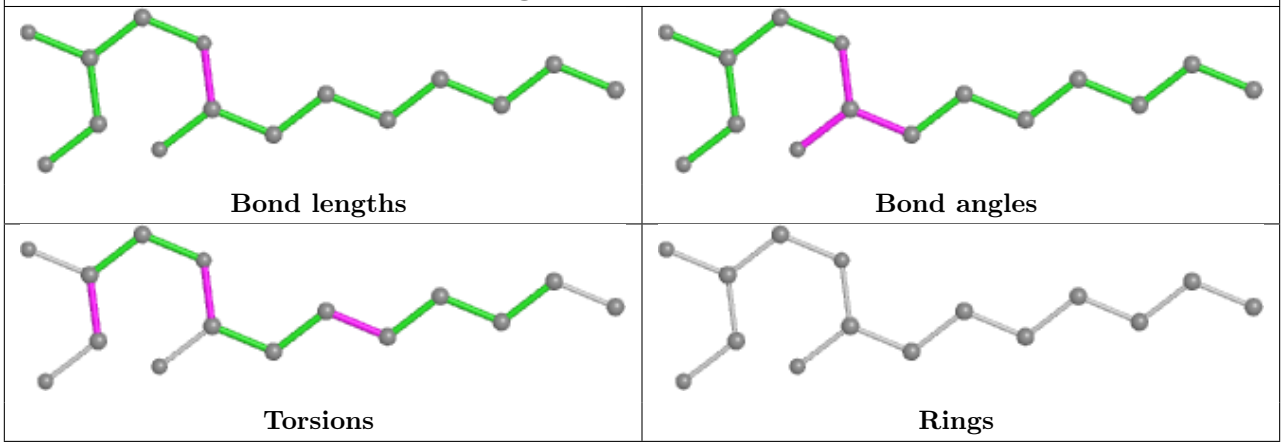

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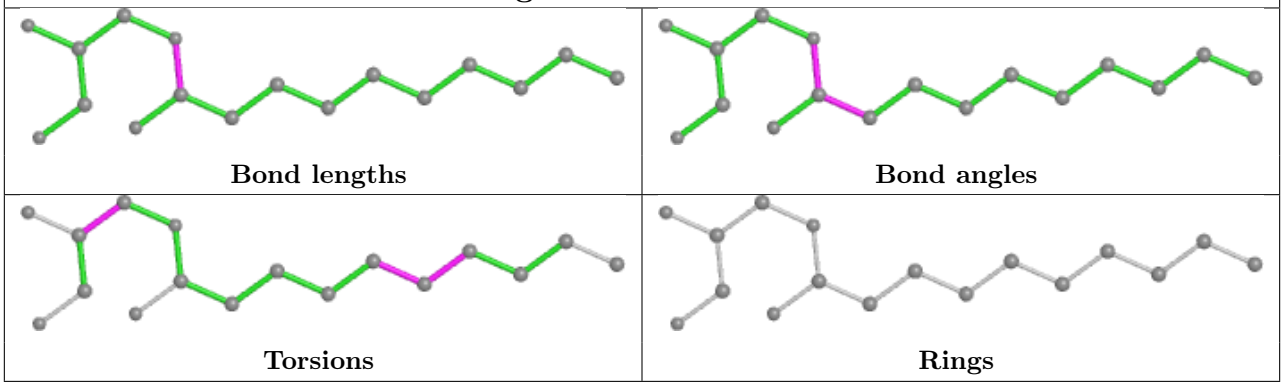

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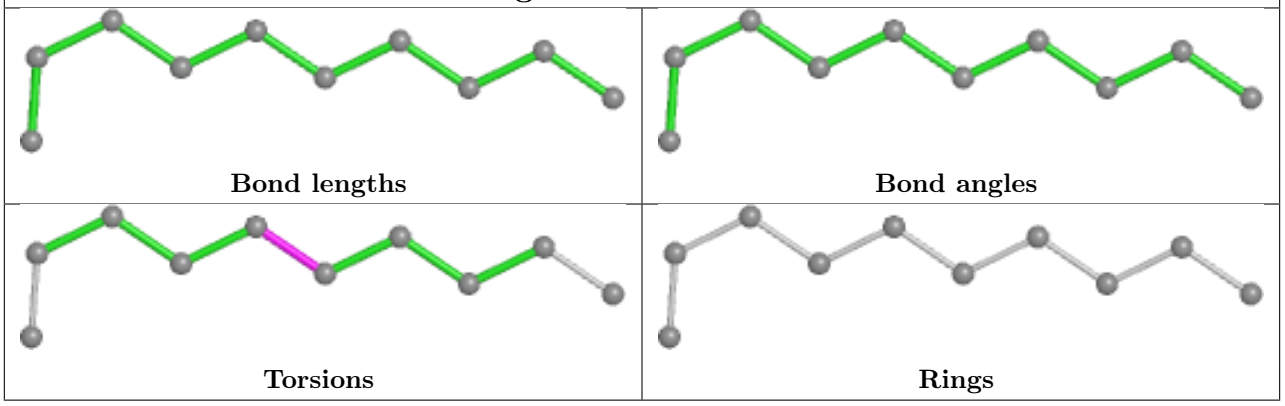

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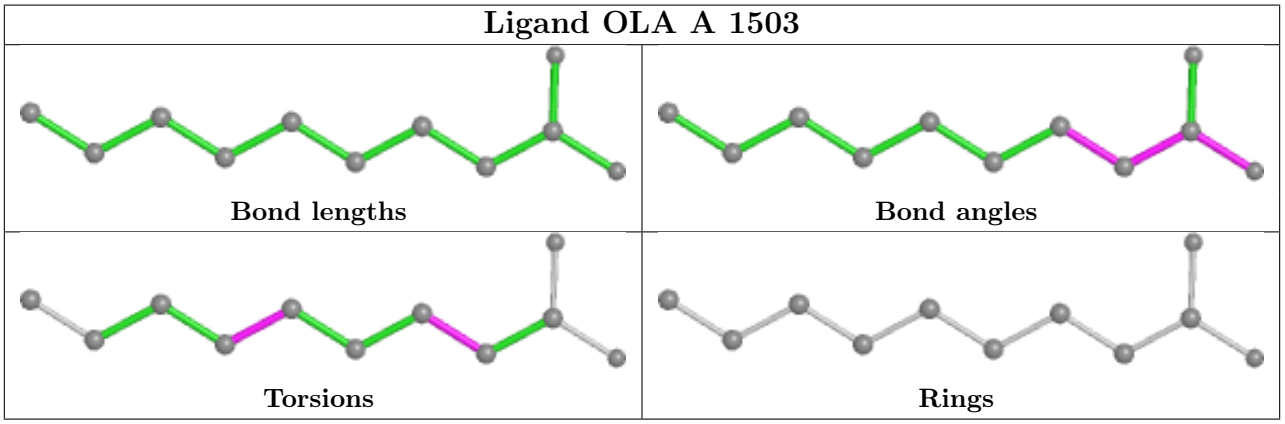

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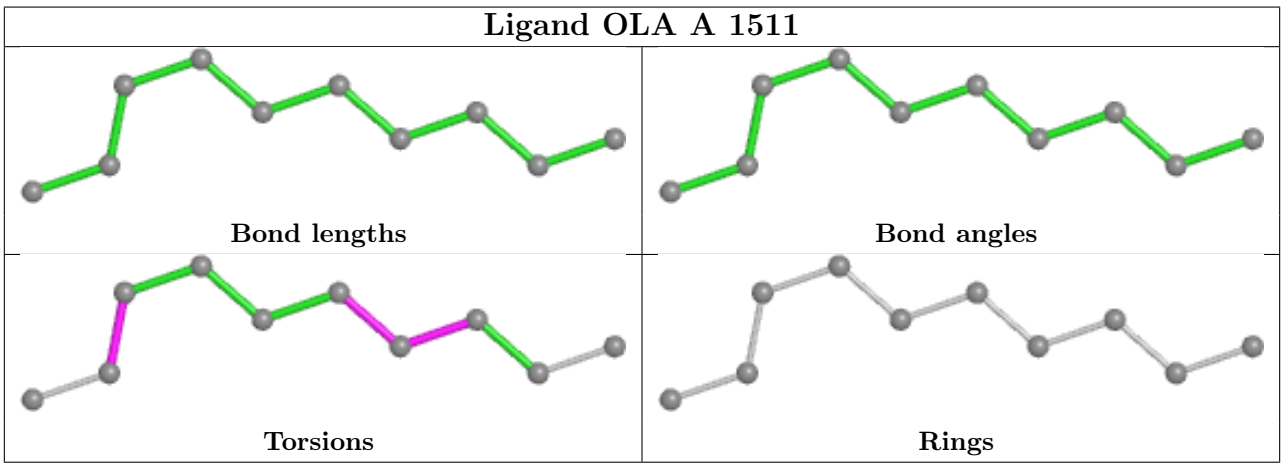

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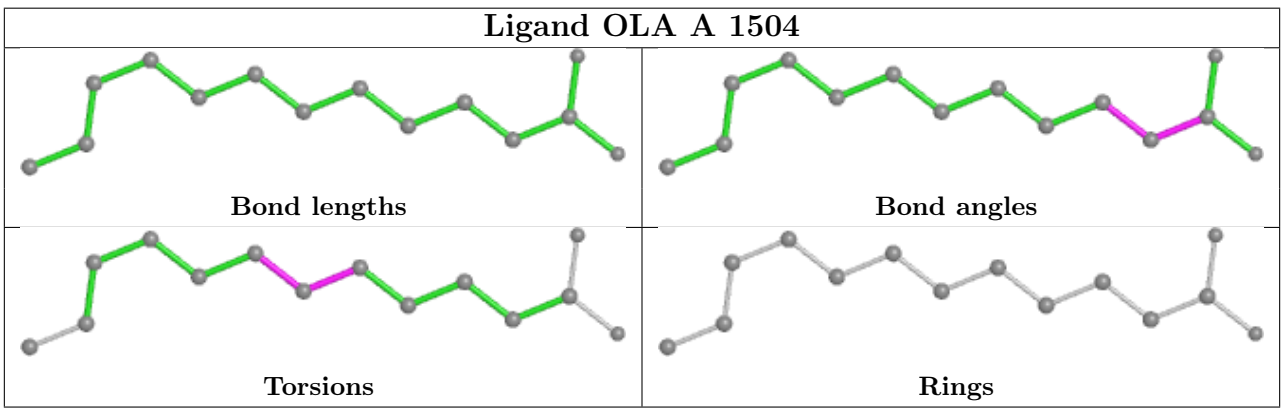

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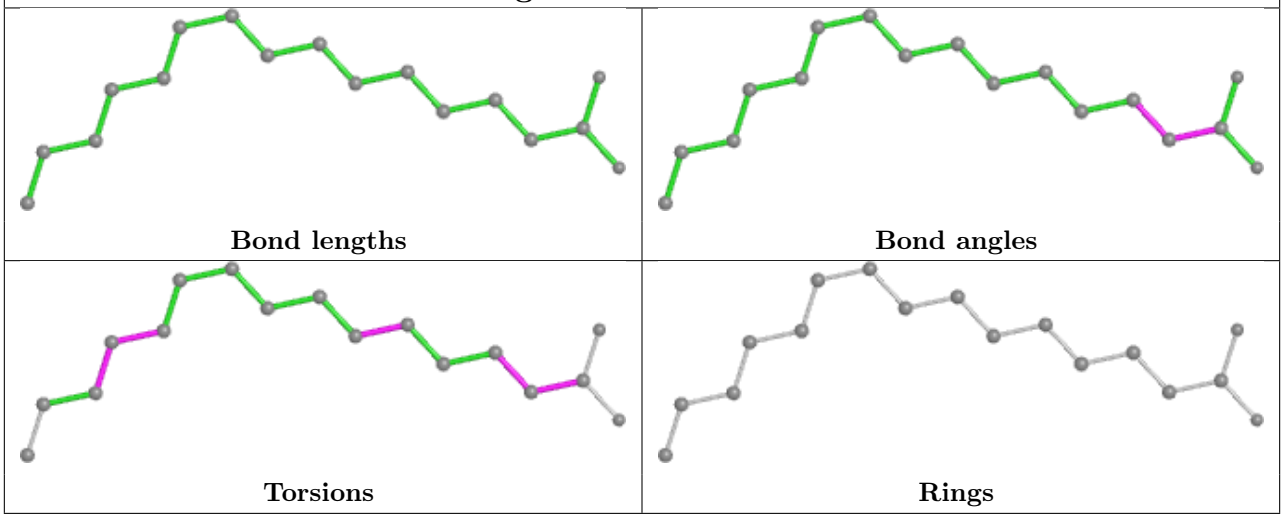

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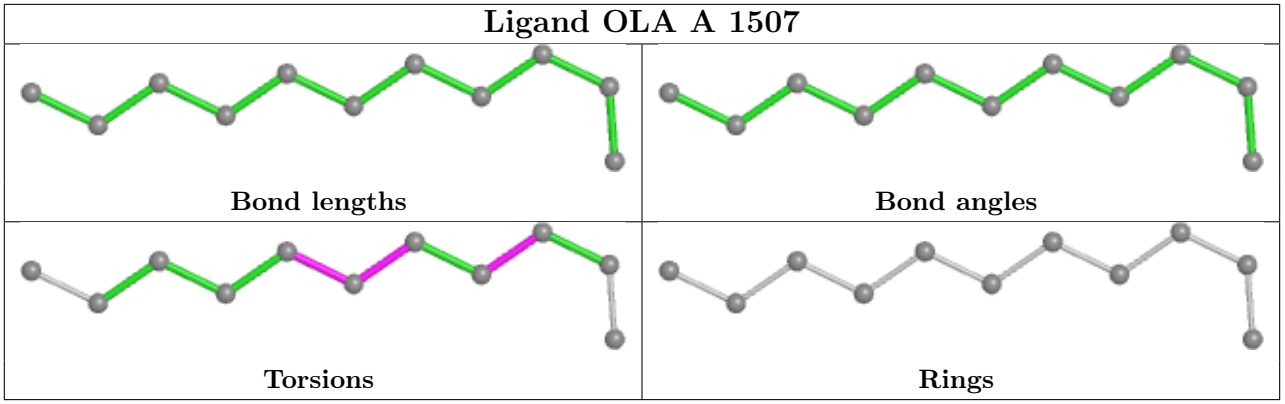
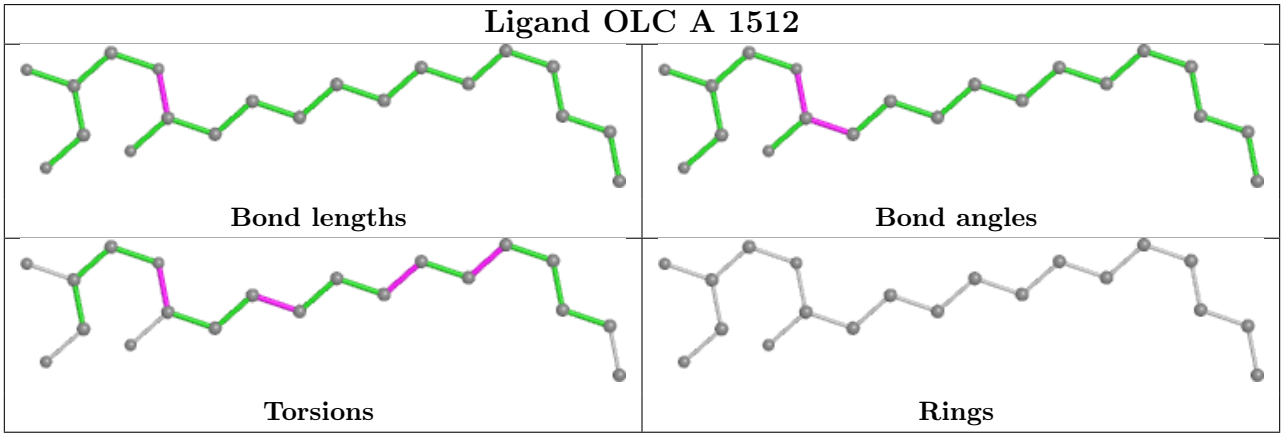
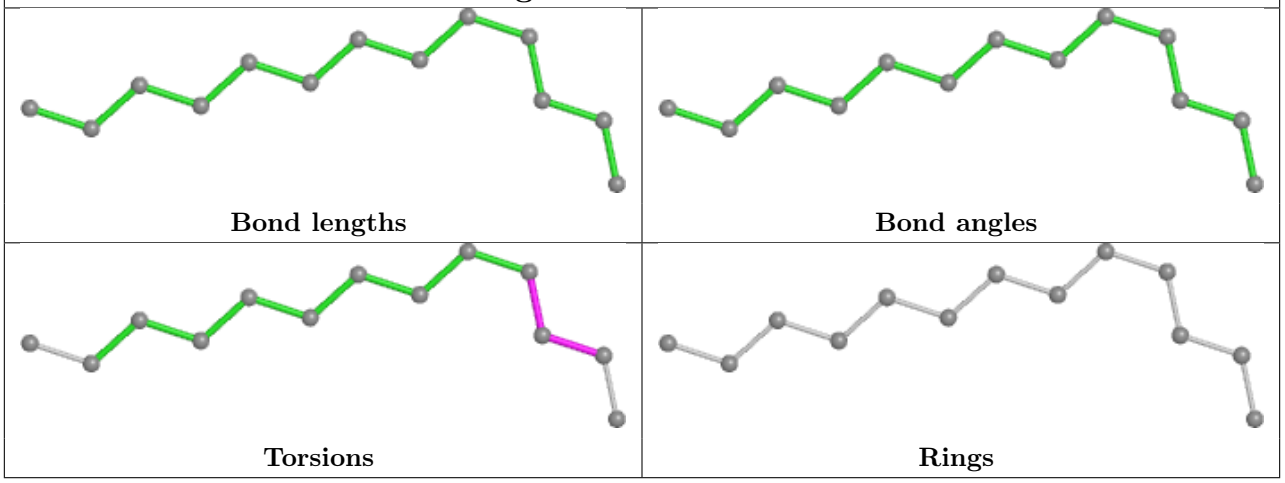


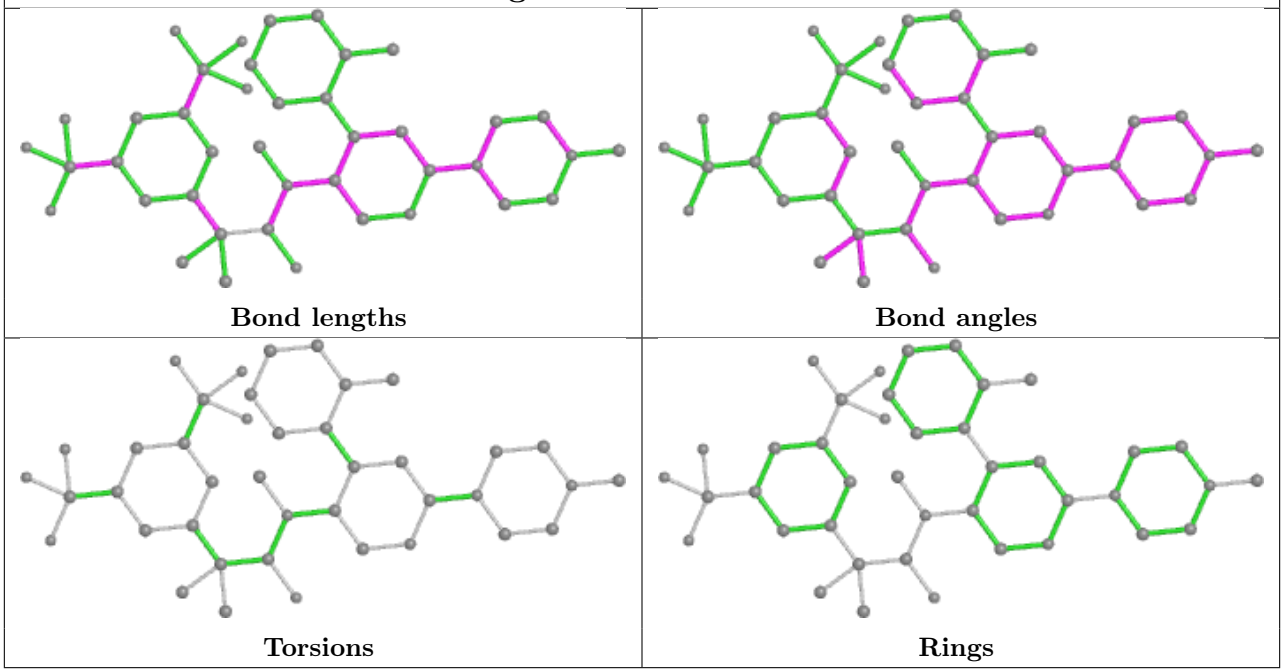
Ligand OLC A 1512



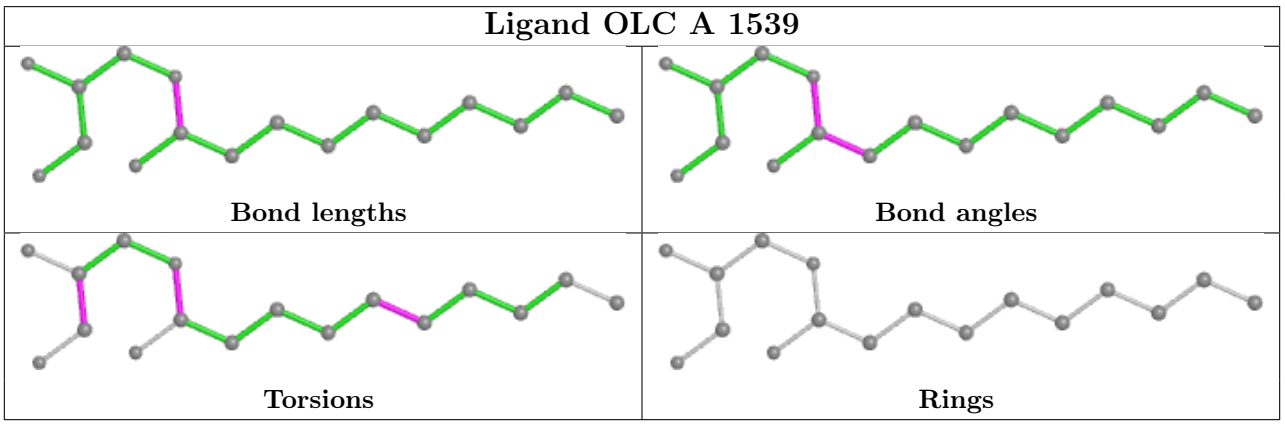
Ligand OLA A 1510

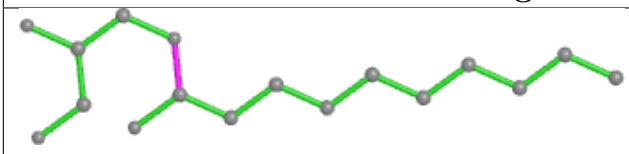
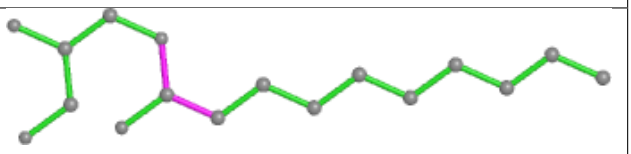
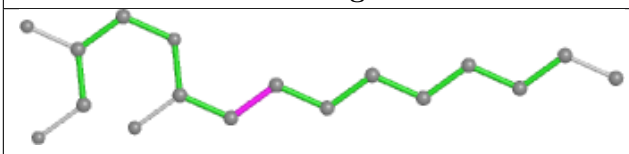
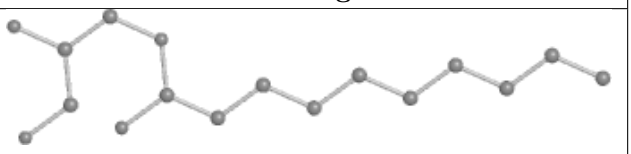


Ligand GAW A 1501



Ligand OLC A 1539



Ligand OLC A 1515	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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	483/520 (92%)	0.05	17 (3%) 44 42	37, 49, 89, 147	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	ASN	5.8
1	A	325	PHE	5.0
1	A	323	CYS	4.5
1	A	326	ILE	4.4
1	A	187	HIS	4.2
1	A	280	LYS	4.2
1	A	188	PRO	3.6
1	A	30	TRP	3.2
1	A	273	ILE	3.0
1	A	327	SER	3.0
1	A	324	PRO	2.8
1	A	282	PHE	2.8
1	A	62	ARG	2.5
1	A	1294	PRO	2.3
1	A	1316	MET	2.0
1	A	1258	PHE	2.0
1	A	1305	GLU	2.0

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

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
1	YCM	A	322	10/11	0.75	0.36	121,138,140,141	0
1	YCM	A	1221	10/11	0.92	0.14	53,60,65,69	0

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, 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
6	PEG	A	1538	7/7	0.41	0.29	105,112,119,121	0
6	PEG	A	1533	7/7	0.55	0.34	92,94,96,98	0
5	OLC	A	1514	17/25	0.56	0.31	68,88,97,98	0
4	OLA	A	1511	10/20	0.59	0.45	79,84,87,87	0
6	PEG	A	1530	7/7	0.64	0.27	80,81,83,83	0
6	PEG	A	1531	7/7	0.64	0.34	91,91,92,93	0
6	PEG	A	1537	7/7	0.65	0.24	80,81,82,82	0
5	OLC	A	1516	15/25	0.65	0.31	75,90,106,107	0
6	PEG	A	1517	7/7	0.66	0.44	67,72,82,82	0
4	OLA	A	1508	10/20	0.67	0.20	71,80,82,83	0
6	PEG	A	1542	7/7	0.67	0.43	106,107,108,108	0
6	PEG	A	1522	7/7	0.69	0.30	79,88,96,96	0
6	PEG	A	1526	7/7	0.70	0.27	95,97,100,101	0
6	PEG	A	1519	7/7	0.70	0.36	83,84,87,88	0
6	PEG	A	1535	7/7	0.70	0.23	96,97,98,101	0
6	PEG	A	1534	7/7	0.72	0.39	93,94,98,99	0
5	OLC	A	1515	17/25	0.73	0.21	75,83,106,108	0
5	OLC	A	1513	23/25	0.73	0.21	80,85,115,117	0
4	OLA	A	1510	13/20	0.74	0.27	71,74,81,81	0
6	PEG	A	1532	7/7	0.74	0.22	99,99,100,100	0
6	PEG	A	1528	7/7	0.75	0.26	79,80,90,91	0
6	PEG	A	1541	7/7	0.77	0.30	84,87,91,93	0
6	PEG	A	1525	7/7	0.78	0.26	92,97,98,98	0
6	PEG	A	1524	7/7	0.79	0.24	88,90,92,93	0
5	OLC	A	1539	17/25	0.81	0.21	74,85,98,100	0
6	PEG	A	1520	7/7	0.82	0.27	93,95,96,96	0
6	PEG	A	1536	7/7	0.82	0.25	122,123,123,124	0

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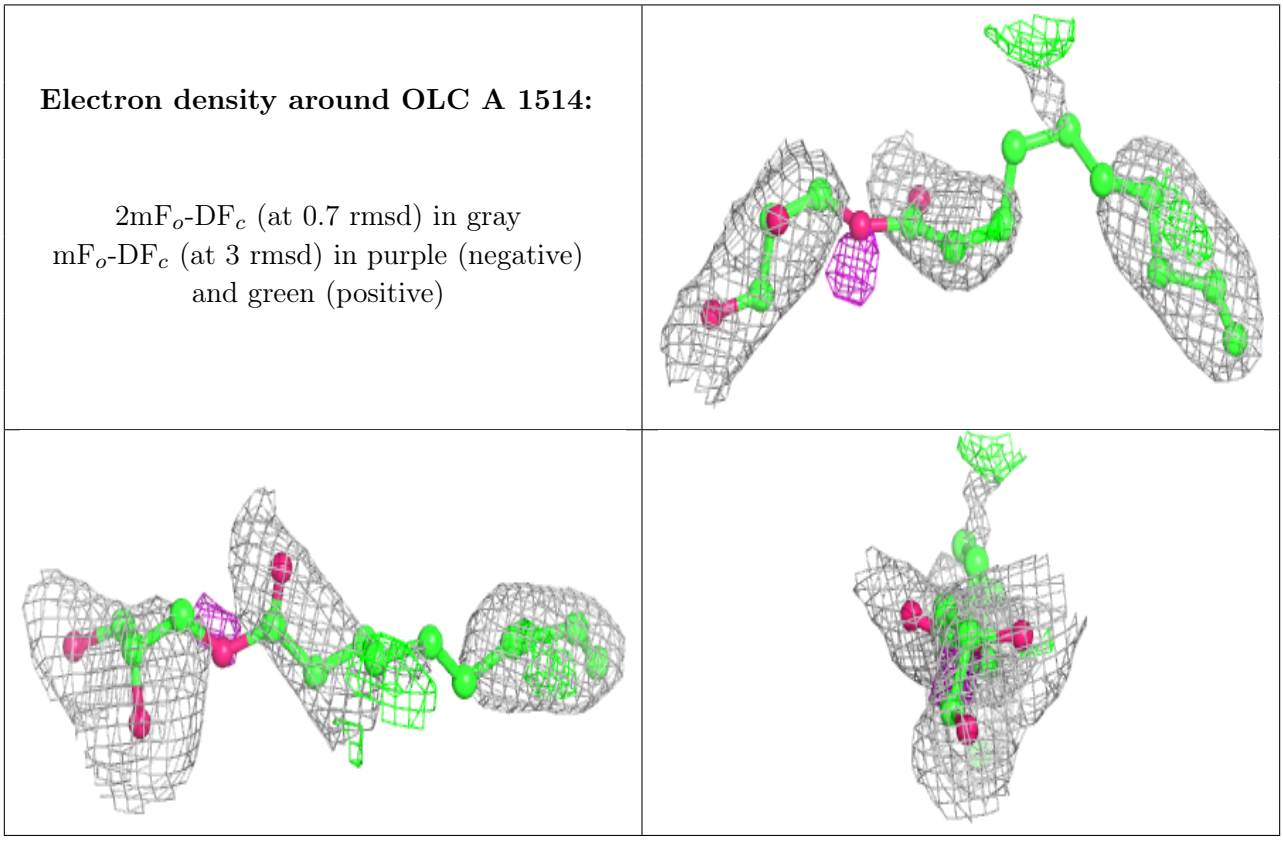
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	A	1529	7/7	0.83	0.12	75,75,80,82	0
6	PEG	A	1523	7/7	0.83	0.32	78,79,84,87	0
3	CIT	A	1502	13/13	0.85	0.22	49,64,67,68	0
6	PEG	A	1518	7/7	0.86	0.17	88,89,90,92	0
4	OLA	A	1504	14/20	0.86	0.27	69,71,74,77	0
6	PEG	A	1527	7/7	0.86	0.47	96,99,101,101	0
5	OLC	A	1512	20/25	0.86	0.28	64,76,87,89	0
5	OLC	A	1540	10/25	0.87	0.17	84,92,100,101	0
4	OLA	A	1505	17/20	0.87	0.22	80,86,95,97	0
4	OLA	A	1503	11/20	0.88	0.21	45,64,74,74	0
6	PEG	A	1521	7/7	0.89	0.18	81,81,83,85	0
4	OLA	A	1507	11/20	0.89	0.19	76,79,83,84	0
4	OLA	A	1506	7/20	0.91	0.15	63,68,76,78	0
4	OLA	A	1509	6/20	0.92	0.24	65,71,74,76	0
2	GAW	A	1501	41/41	0.94	0.12	38,50,65,68	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.

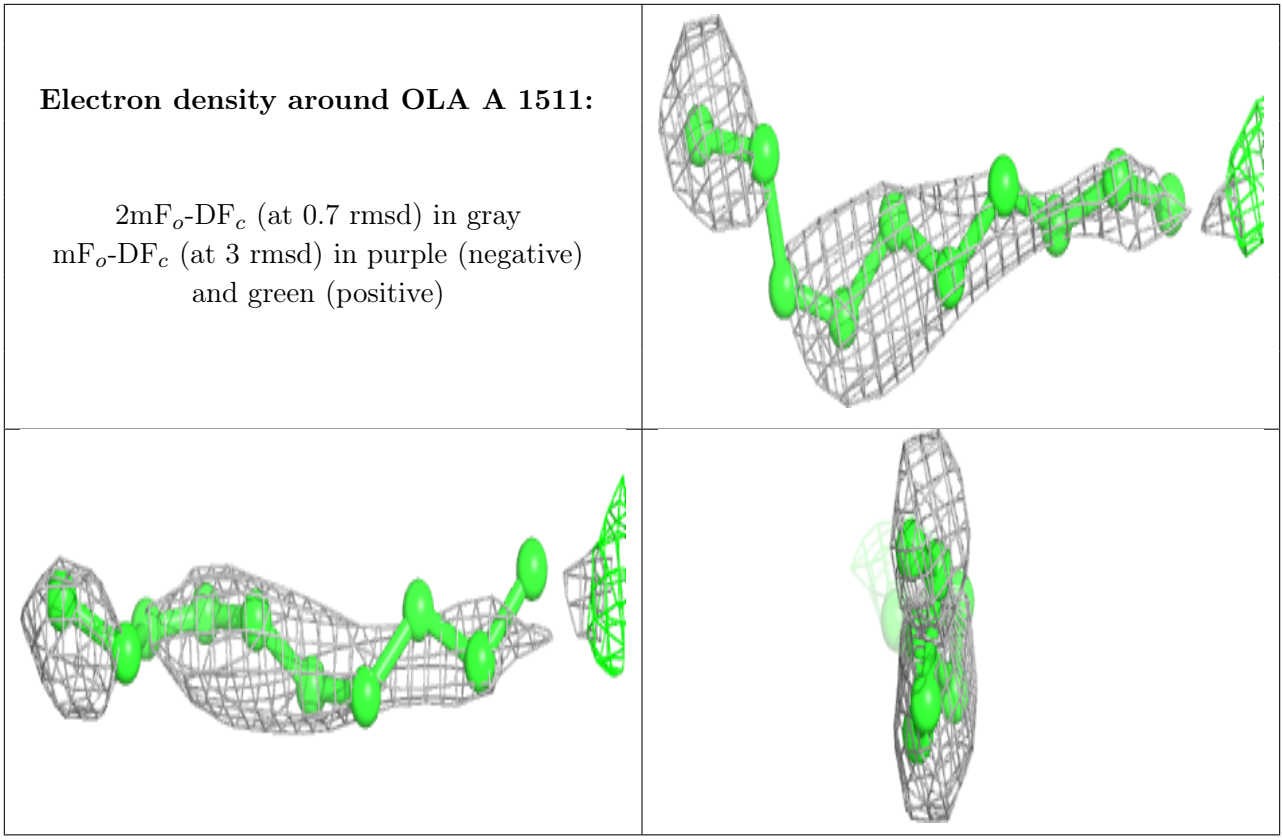
Electron density around OLC A 1514:

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



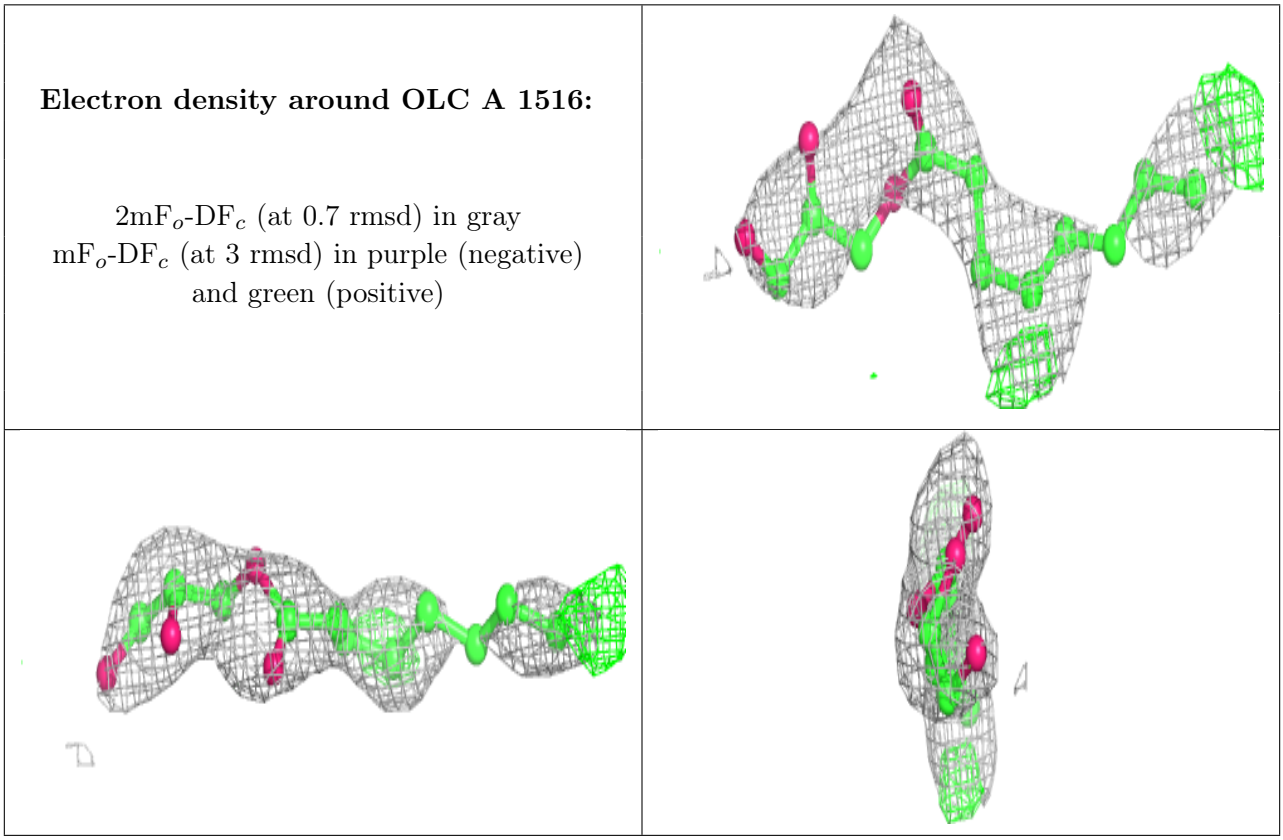
Electron density around OLA A 1511:

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



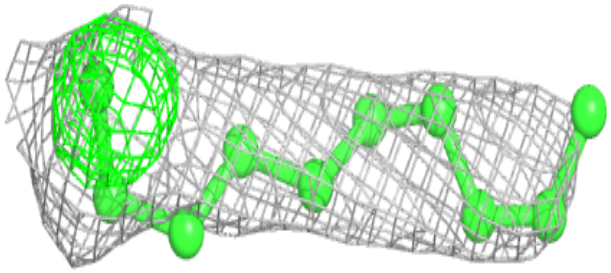
Electron density around OLC A 1516:

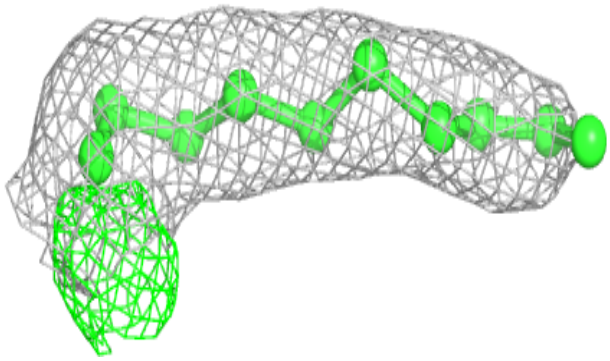
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

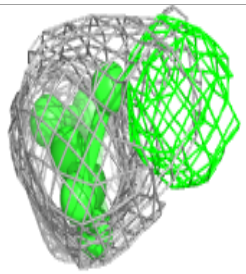


Electron density around OLA A 1508:

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

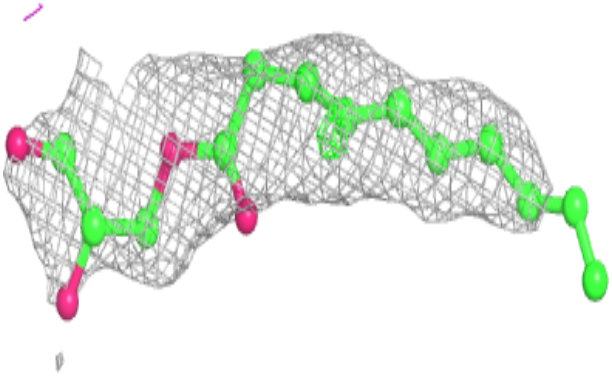


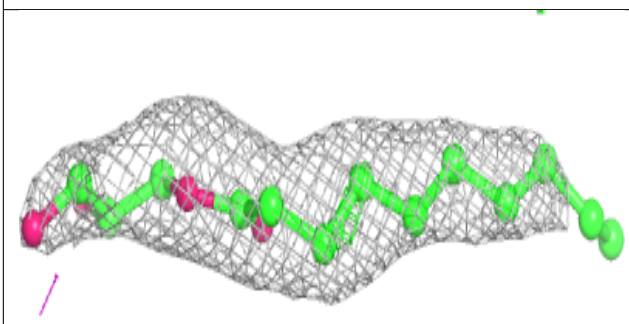


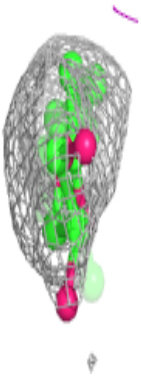


Electron density around OLC A 1515:

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

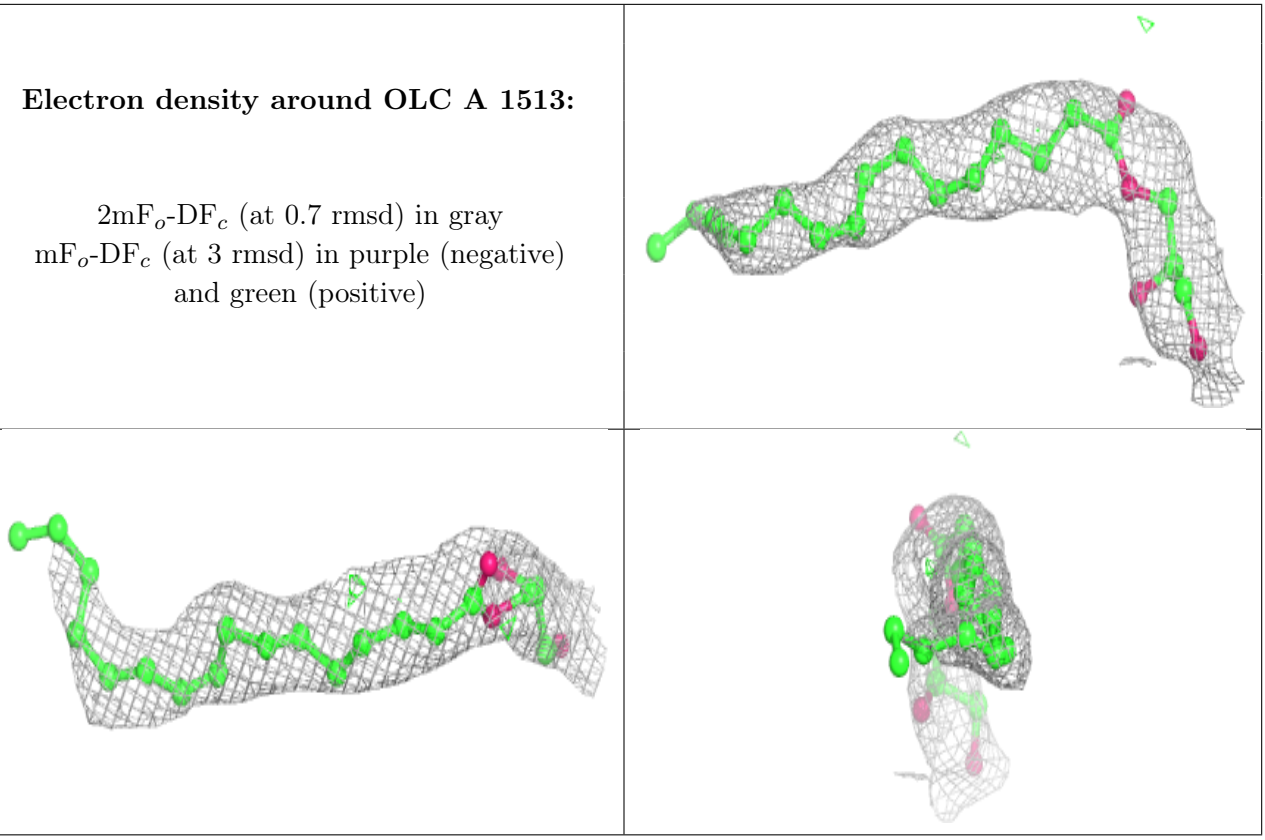






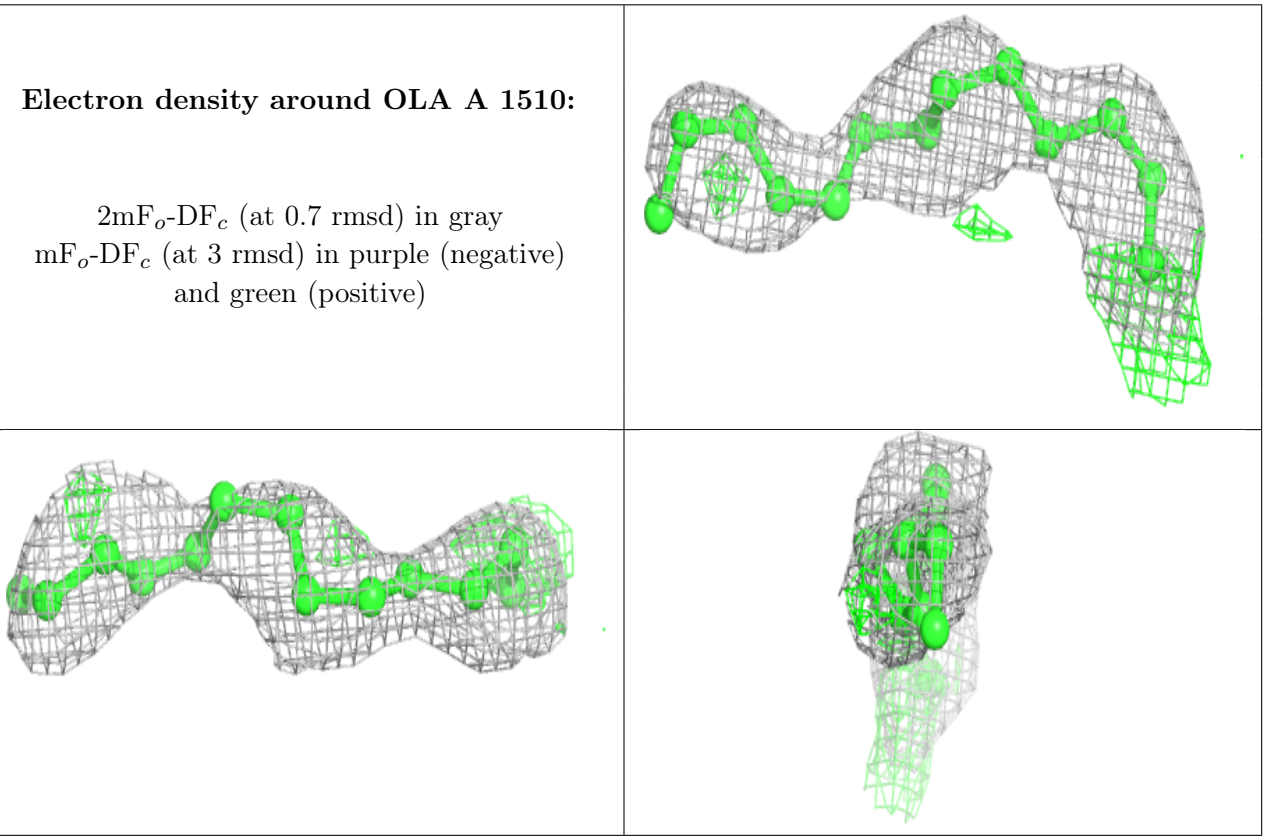
Electron density around OLC A 1513:

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



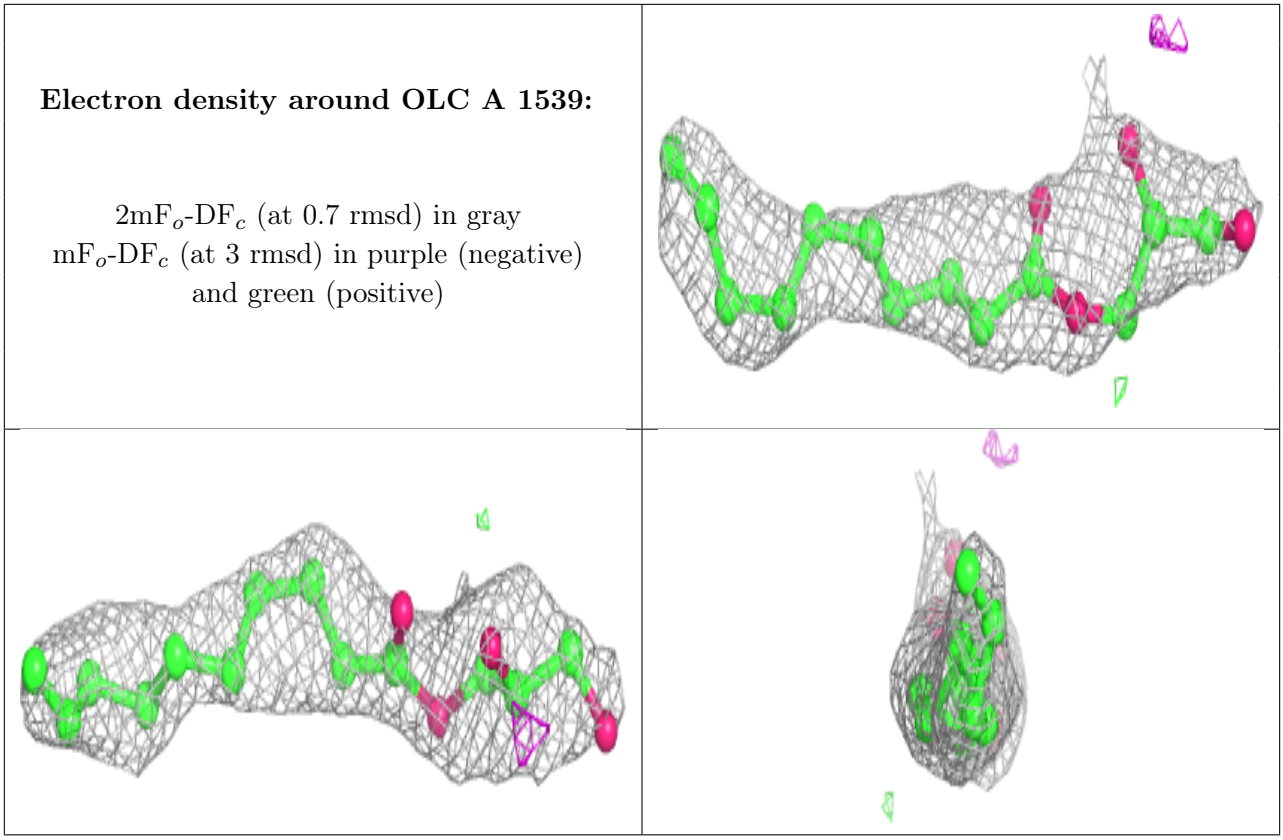
Electron density around OLA A 1510:

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



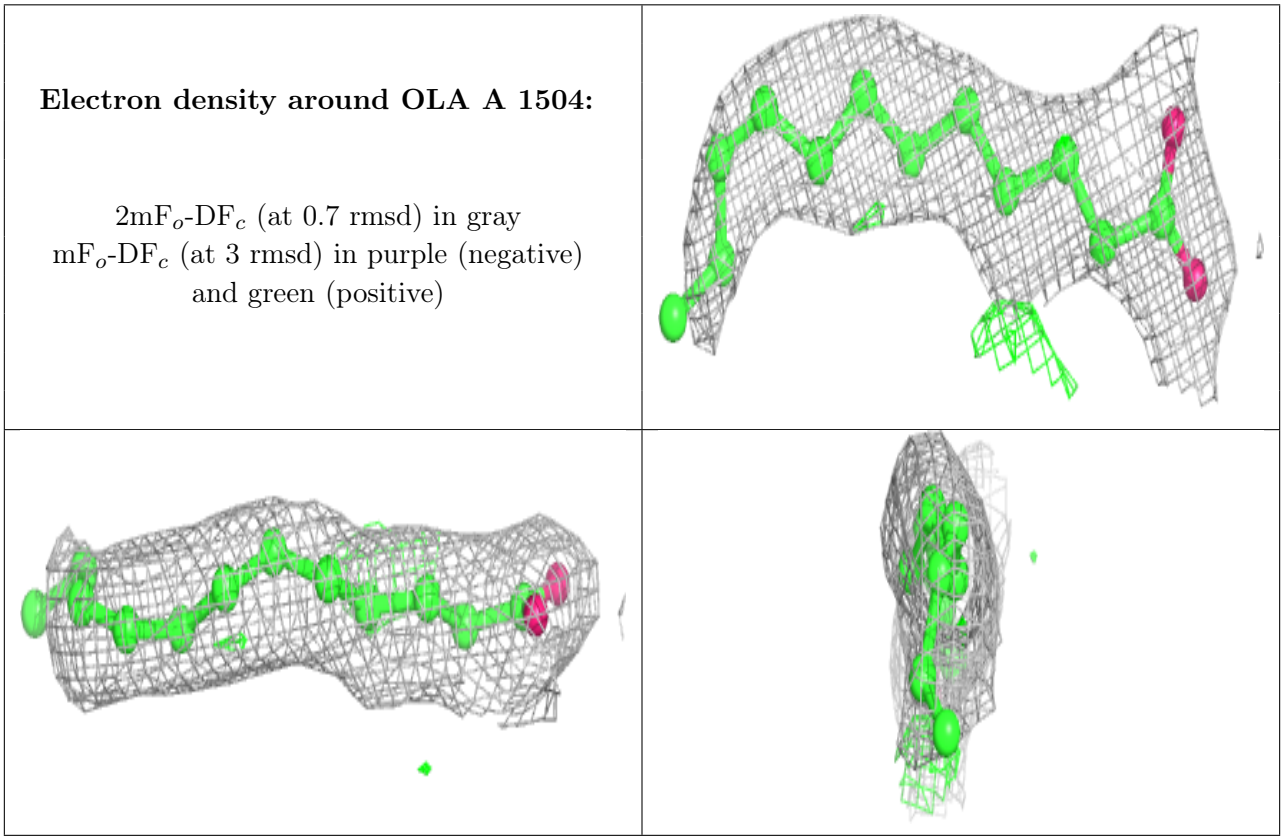
Electron density around OLC A 1539:

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



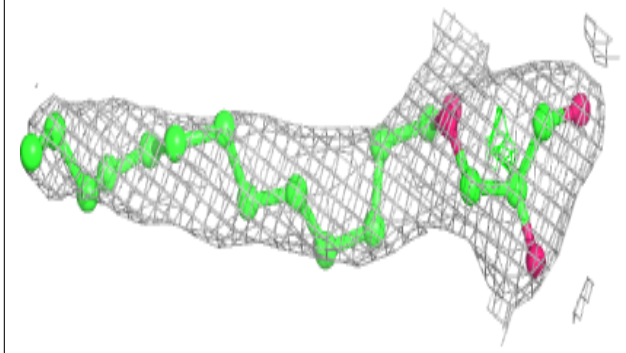
Electron density around OLA A 1504:

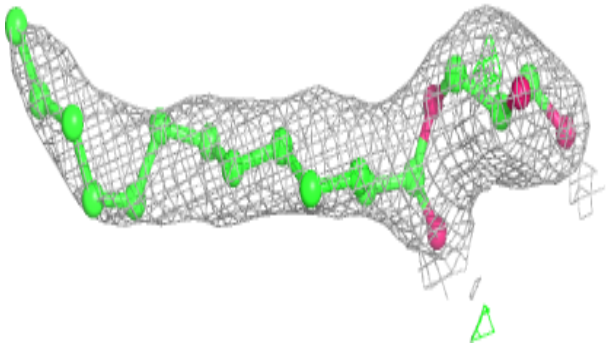
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

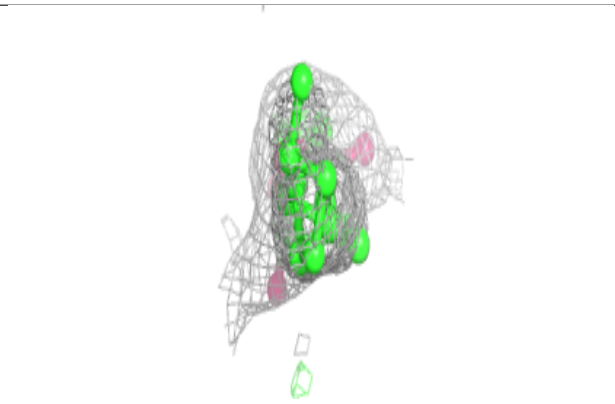


Electron density around OLC A 1512:

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

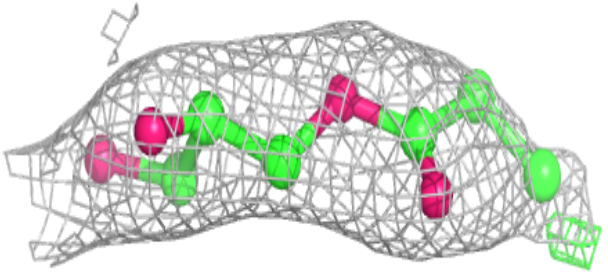


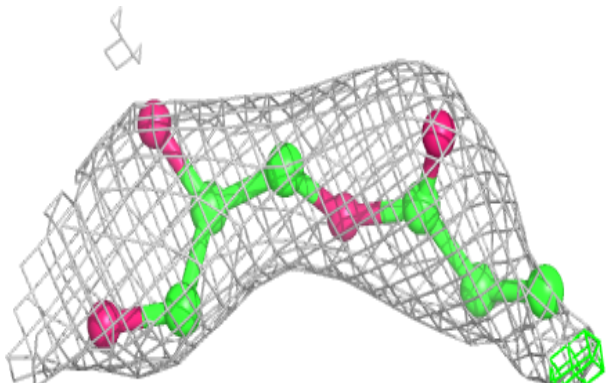


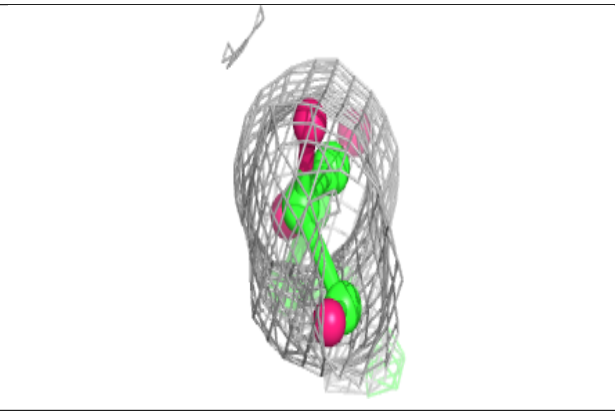


Electron density around OLC A 1540:

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

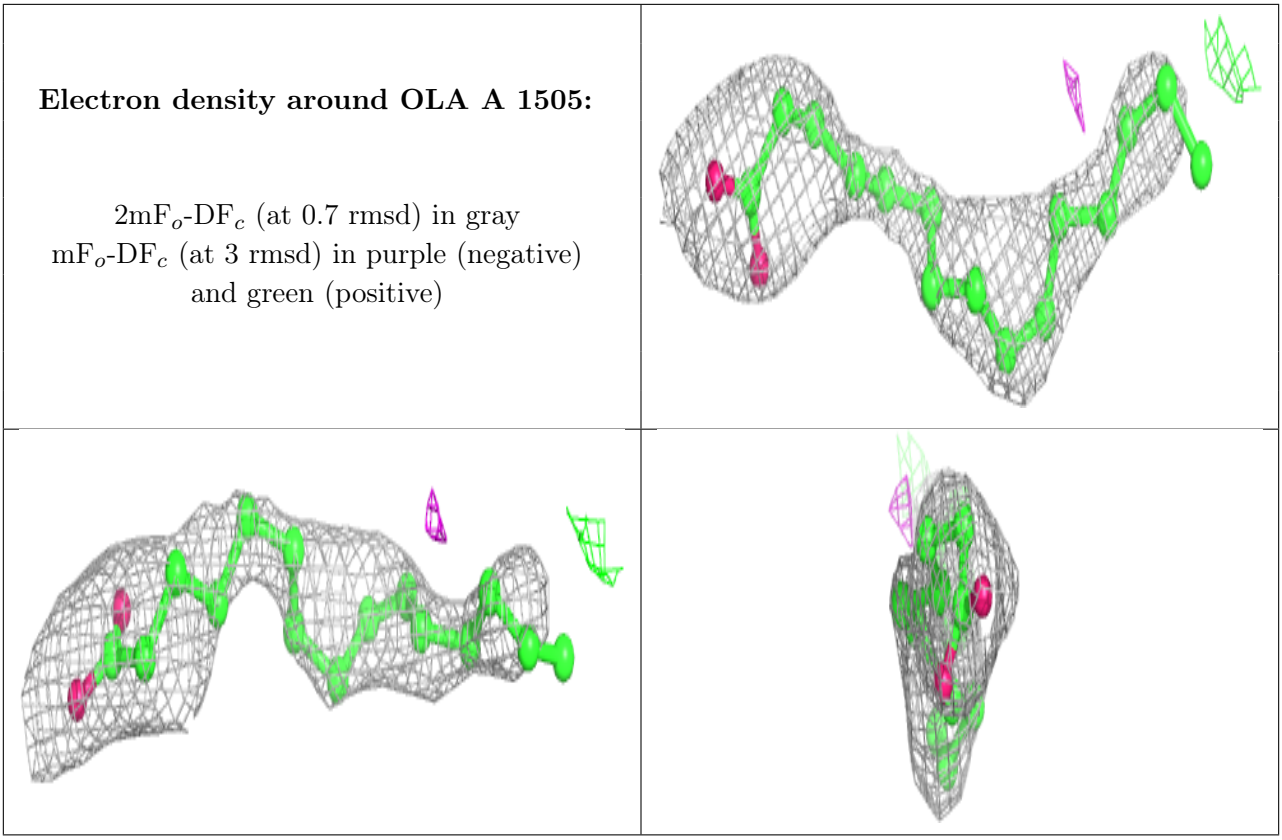






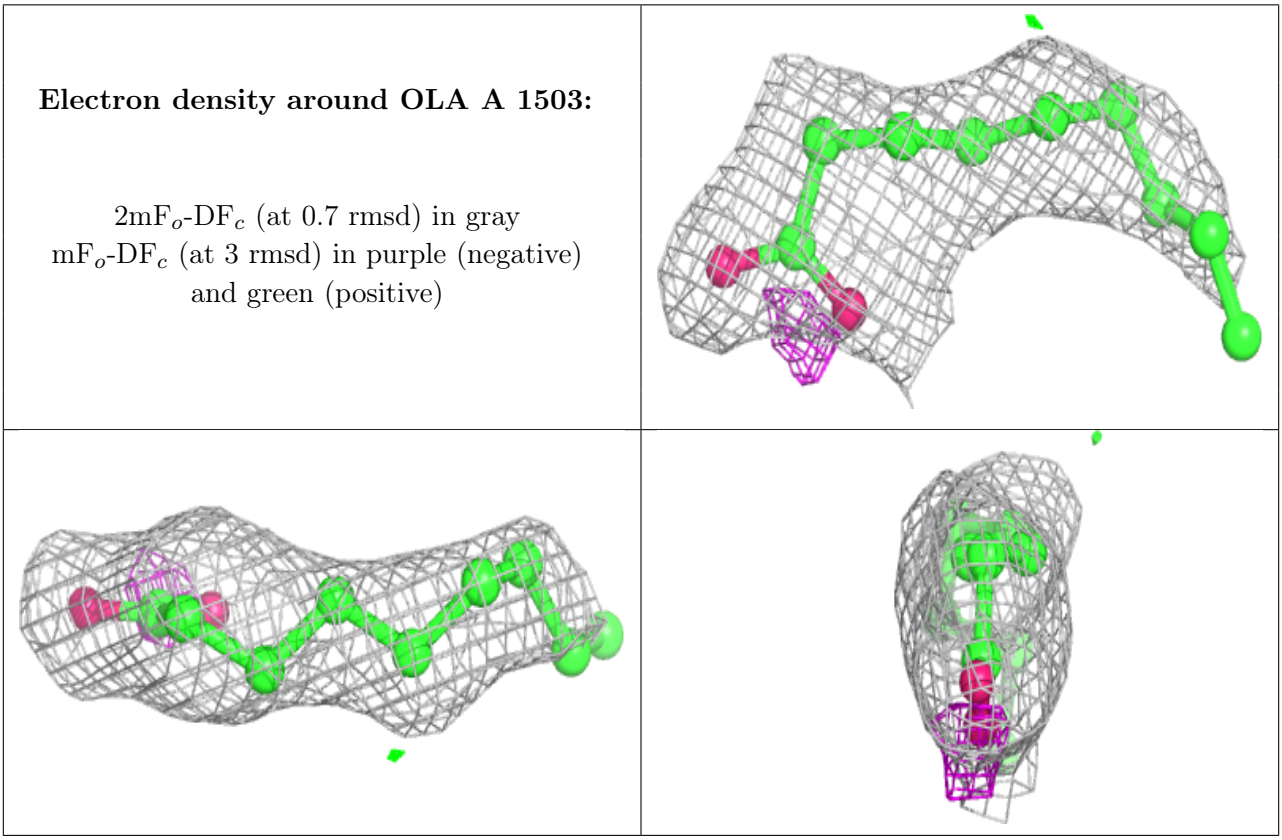
Electron density around OLA A 1505:

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



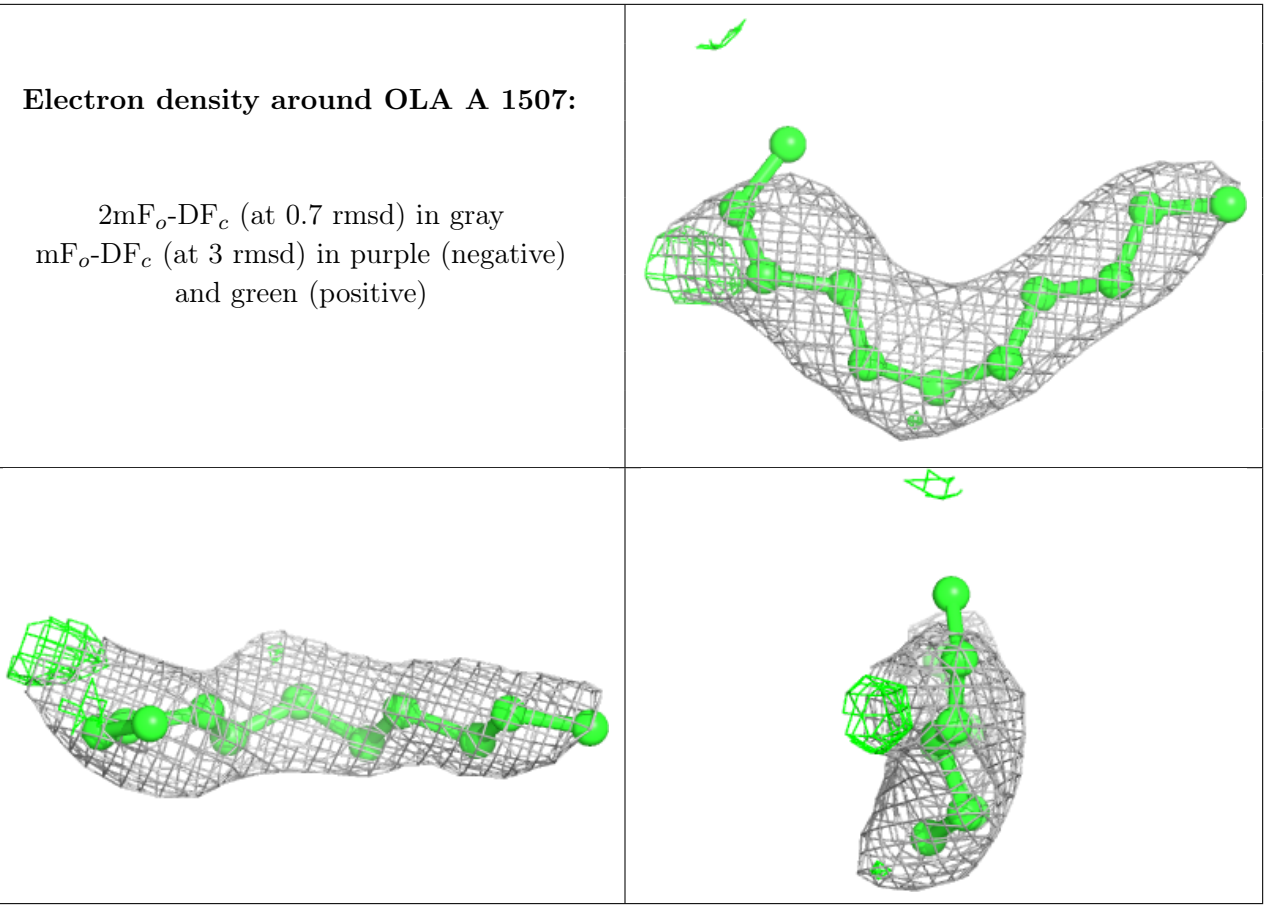
Electron density around OLA A 1503:

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



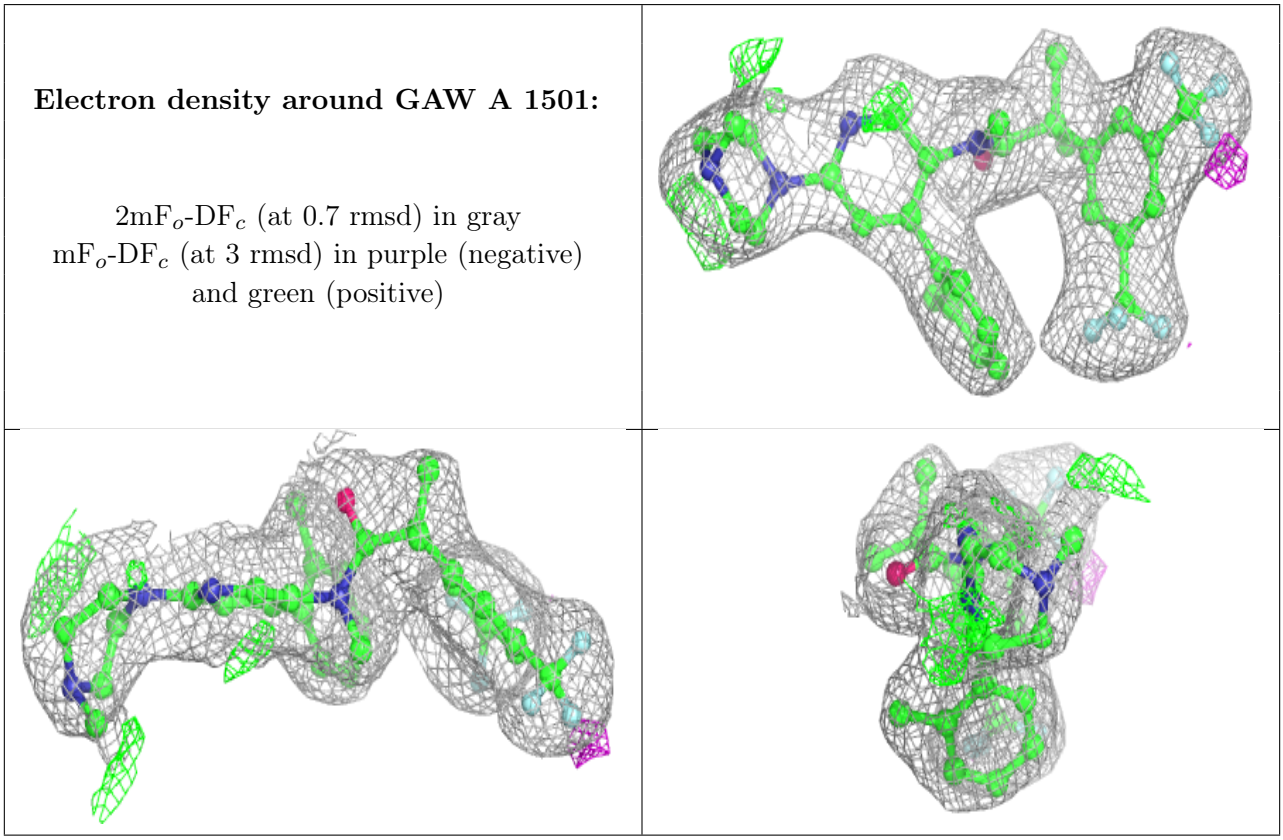
Electron density around OLA A 1507:

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



Electron density around GAW A 1501:

$2mF_o$-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.