wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 04:11 pm BST

PDB ID	:	8PWN
Title	:	Structure of A2A adenosine receptor A2AR-StaR2-bRIL, solved at wavelength 2.75 A
Authors	:	El Omari, K.; Duman, R.; Mykhaylyk, V.; Orr, C.; Romano, M.; Moraes, I.; Wagner, A.
Deposited on	:	2023-07-20
Resolution	:	2.40 Å(reported)

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

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

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

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

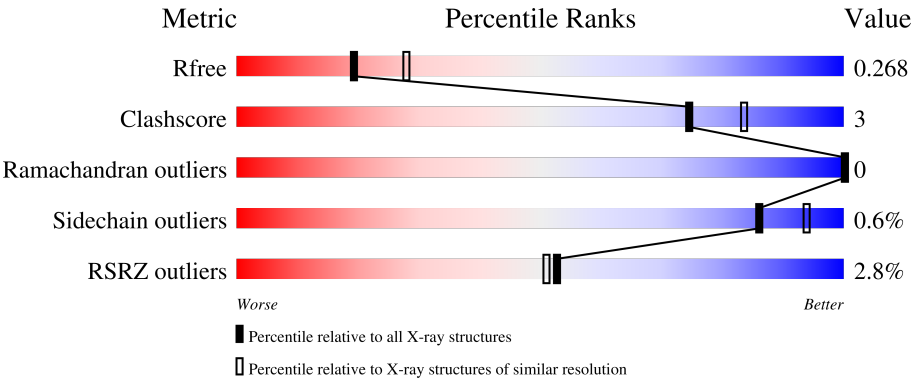
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	433	3% 83% 7% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3321 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 Adenosine receptor A2a,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	3007	1960	508	518	21	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ASP	-	expression tag	UNP P29274
A	18	TYR	-	expression tag	UNP P29274
A	19	LYS	-	expression tag	UNP P29274
A	20	ASP	-	expression tag	UNP P29274
A	21	ASP	-	expression tag	UNP P29274
A	22	ASP	-	expression tag	UNP P29274
A	23	ASP	-	expression tag	UNP P29274
A	24	GLY	-	expression tag	UNP P29274
A	25	ALA	-	expression tag	UNP P29274
A	26	PRO	-	expression tag	UNP P29274
A	79	LEU	ALA	conflict	UNP P29274
A	113	ALA	THR	conflict	UNP P29274
A	132	ALA	ARG	conflict	UNP P29274
A	147	ALA	LYS	conflict	UNP P29274
A	179	ALA	ASN	conflict	UNP P29274
A	227	ALA	LEU	conflict	UNP P29274
A	240	TRP	MET	conflict	UNP P0ABE7
A	335	ILE	-	linker	UNP P0ABE7
A	336	GLN	-	linker	UNP P0ABE7
A	337	LYS	-	linker	UNP P0ABE7
A	338	TYR	-	linker	UNP P0ABE7
A	339	LEU	-	linker	UNP P0ABE7
A	356	ALA	LEU	conflict	UNP P29274
A	360	ALA	VAL	conflict	UNP P29274
A	398	ALA	SER	conflict	UNP P29274
A	439	ALA	GLY	conflict	UNP P29274
A	440	HIS	-	expression tag	UNP P29274

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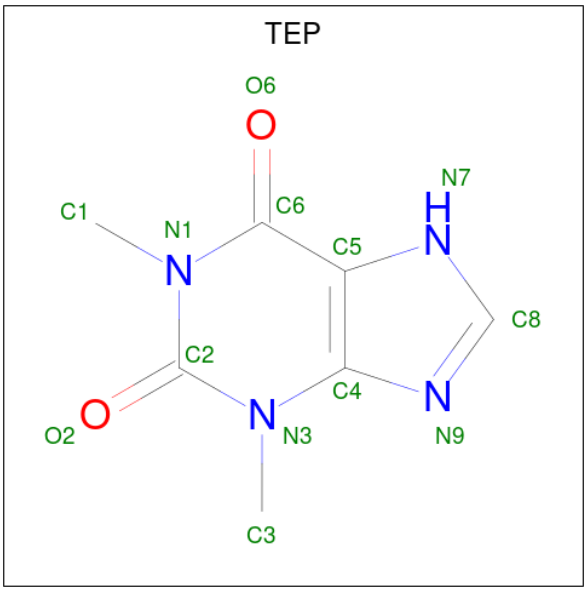
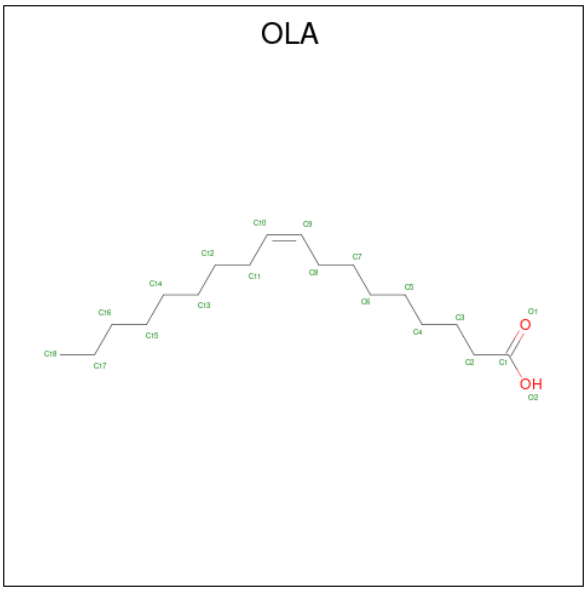
Chain	Residue	Modelled	Actual	Comment	Reference
A	441	HIS	-	expression tag	UNP P29274
A	442	HIS	-	expression tag	UNP P29274
A	443	HIS	-	expression tag	UNP P29274
A	444	HIS	-	expression tag	UNP P29274
A	445	HIS	-	expression tag	UNP P29274
A	446	HIS	-	expression tag	UNP P29274
A	447	HIS	-	expression tag	UNP P29274
A	448	HIS	-	expression tag	UNP P29274
A	449	HIS	-	expression tag	UNP P29274

- Molecule 2 is THEOPHYLLINE (three-letter code: TEP) (formula: $C_7H_8N_4O_2$).



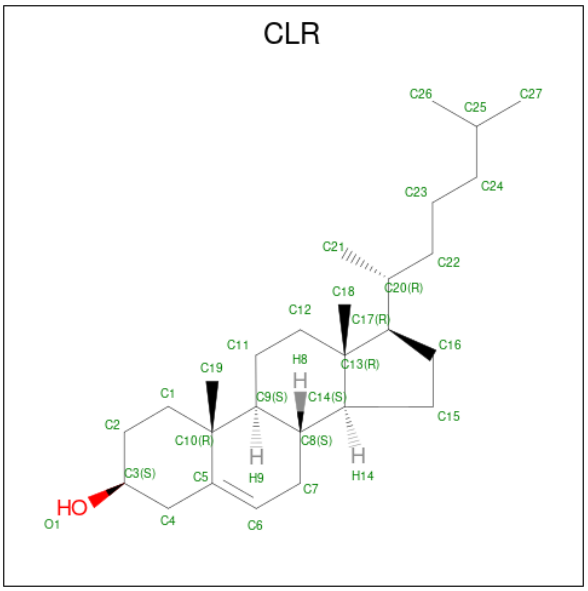
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	4	2		

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 9 7 2	0	0
3	A	1	Total C O 13 11 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 15 13 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 18 16 2	0	0
3	A	1	Total C O 20 18 2	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0

- Molecule 5 is water.

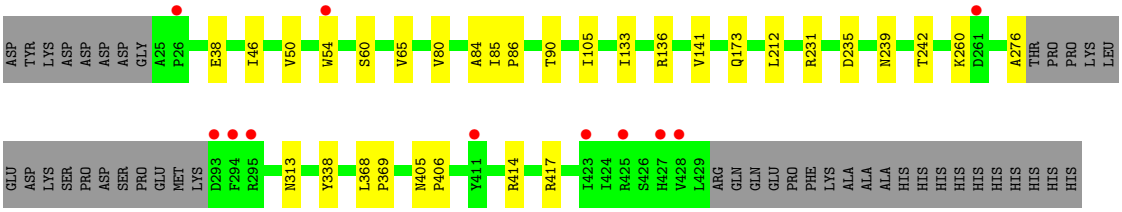
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0

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: Adenosine receptor A2a,Soluble cytochrome b562

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.31Å 179.64Å 139.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.82 – 2.40 89.82 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.82-2.40) 99.9 (89.82-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.222 , 0.261 0.228 , 0.268	Depositor DCC
R_{free} test set	1176 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.7	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	0.94	EDS
Total number of atoms	3321	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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: CLR, TEP, 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	0.58	0/3072	0.58	0/4181

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3007	0	3072	21	1
2	A	13	0	8	0	0
3	A	191	0	267	1	0
4	A	84	0	138	3	0
5	A	26	0	0	0	0
All	All	3321	0	3485	22	1

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 3.

The worst 5 of 22 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:38:GLU:HG3	1:A:85:ILE:HG23	1.64	0.78
1:A:231:ARG:NH1	1:A:235:ASP:OD1	2.22	0.73
1:A:86:PRO:O	1:A:90:THR:HG23	1.91	0.70
1:A:414:ARG:HG2	1:A:417:ARG:NH2	2.10	0.67
1:A:133:ILE:HG22	1:A:136:ARG:HB2	1.85	0.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:NE2	1:A:173:GLN:NE2[3_656]	1.94	0.26

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	385/433 (89%)	378 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	313/353 (89%)	311 (99%)	2 (1%)	86 94

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

Mol	Chain	Res	Type
1	A	54	TRP
1	A	60	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OLA	A	501	-	16,16,19	0.62	0	16,16,19	0.51	0
4	CLR	A	514	-	31,31,31	0.28	0	48,48,48	0.41	0
2	TEP	A	500	-	6,14,14	0.95	0	8,21,21	3.26	3 (37%)
3	OLA	A	502	-	13,13,19	0.64	0	12,13,19	0.58	0
3	OLA	A	507	-	14,14,19	0.63	0	14,14,19	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OLA	A	509	-	16,16,19	0.60	0	16,16,19	0.52	0
3	OLA	A	504	-	12,12,19	0.72	0	12,12,19	0.60	0
3	OLA	A	505	-	16,16,19	0.56	0	16,16,19	0.59	0
4	CLR	A	513	-	31,31,31	0.30	0	48,48,48	0.48	0
4	CLR	A	515	-	31,31,31	0.31	0	48,48,48	0.48	0
3	OLA	A	508	-	16,16,19	0.60	0	16,16,19	0.55	0
3	OLA	A	506	-	16,16,19	0.58	0	16,16,19	0.55	0
3	OLA	A	511	-	17,17,19	0.56	0	17,17,19	0.50	0
3	OLA	A	510	-	16,16,19	0.58	0	16,16,19	0.54	0
3	OLA	A	512	-	19,19,19	0.52	0	19,19,19	0.48	0
3	OLA	A	503	-	8,8,19	0.81	0	8,8,19	0.69	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
3	OLA	A	501	-	-	9/14/14/17	-
4	CLR	A	514	-	-	2/10/68/68	0/4/4/4
3	OLA	A	502	-	-	3/11/11/17	-
3	OLA	A	507	-	-	7/12/12/17	-
2	TEP	A	500	-	-	-	0/2/2/2
3	OLA	A	509	-	-	8/14/14/17	-
3	OLA	A	504	-	-	6/10/10/17	-
3	OLA	A	505	-	-	8/14/14/17	-
4	CLR	A	513	-	-	3/10/68/68	0/4/4/4
4	CLR	A	515	-	-	2/10/68/68	0/4/4/4
3	OLA	A	508	-	-	7/14/14/17	-
3	OLA	A	506	-	-	12/14/14/17	-
3	OLA	A	511	-	-	7/15/15/17	-
3	OLA	A	510	-	-	8/14/14/17	-
3	OLA	A	512	-	-	9/17/17/17	-
3	OLA	A	503	-	-	2/6/6/17	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	TEP	C5-C6-N1	-5.94	111.87	118.20
2	A	500	TEP	C4-C5-C6	5.15	123.27	119.96
2	A	500	TEP	C4-C5-N7	-4.09	105.14	109.40

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	OLA	C1-C2-C3-C4
3	A	506	OLA	C1-C2-C3-C4
4	A	515	CLR	C22-C23-C24-C25
3	A	510	OLA	C10-C11-C12-C13
3	A	506	OLA	C4-C5-C6-C7

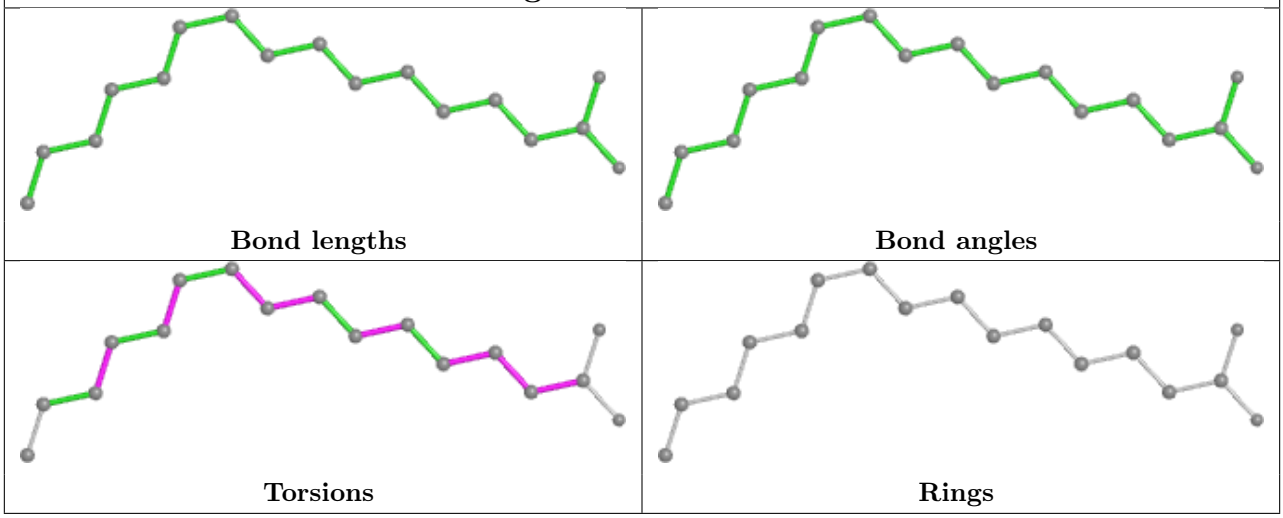
There are no ring outliers.

2 monomers are involved in 3 short contacts:

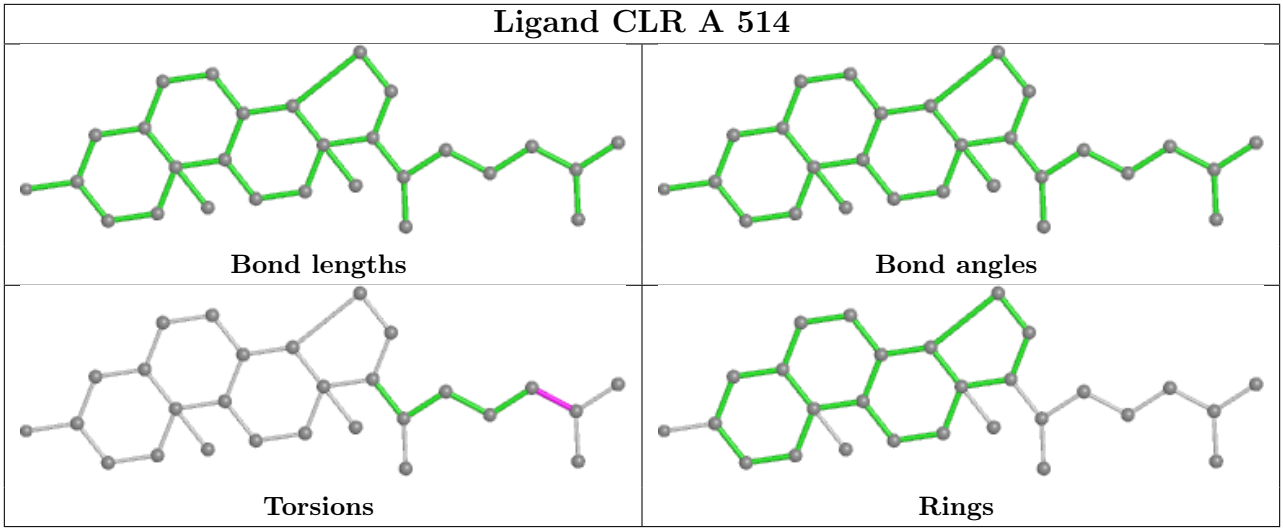
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	513	CLR	3	0
3	A	506	OLA	1	0

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.

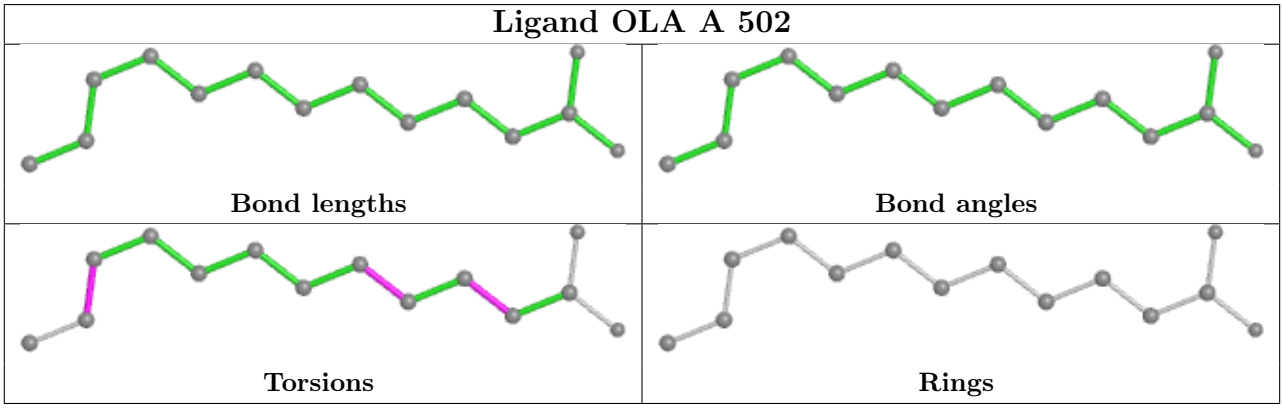
Ligand OLA A 501



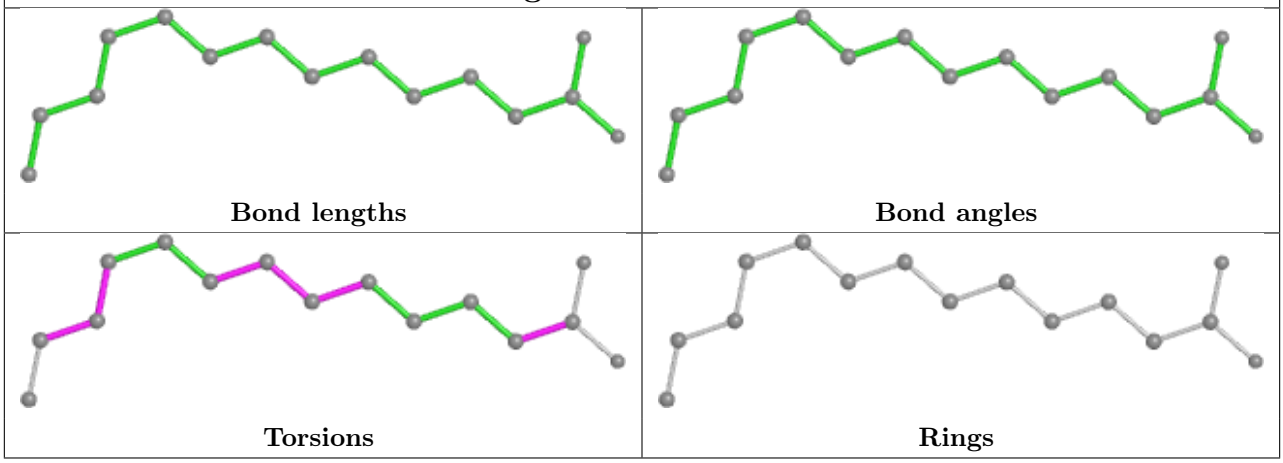
Ligand CLR A 514



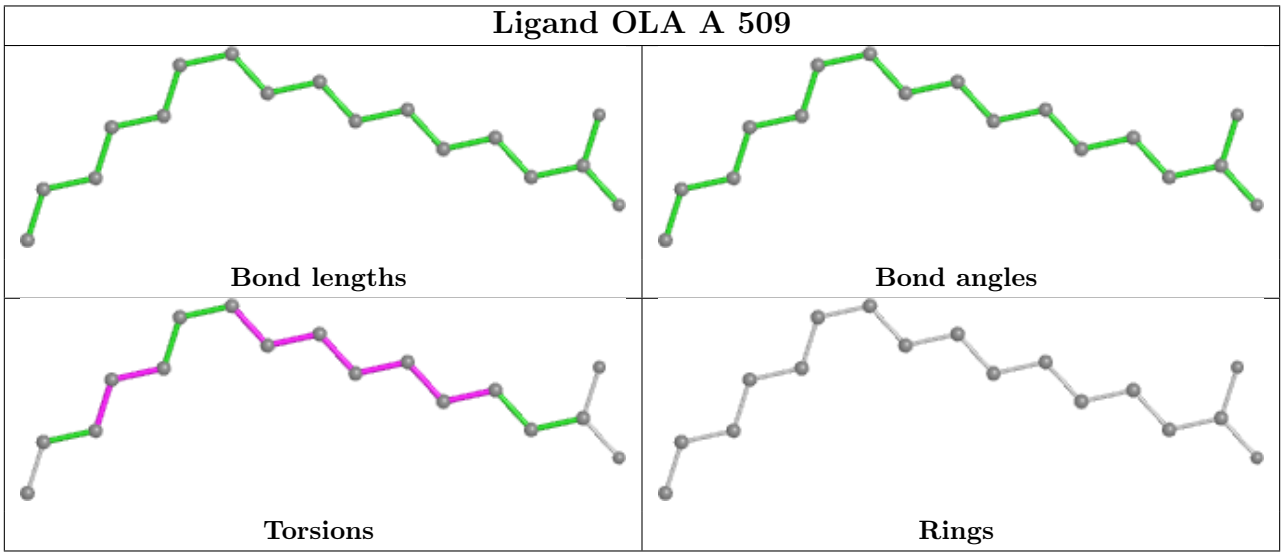
Ligand OLA A 502



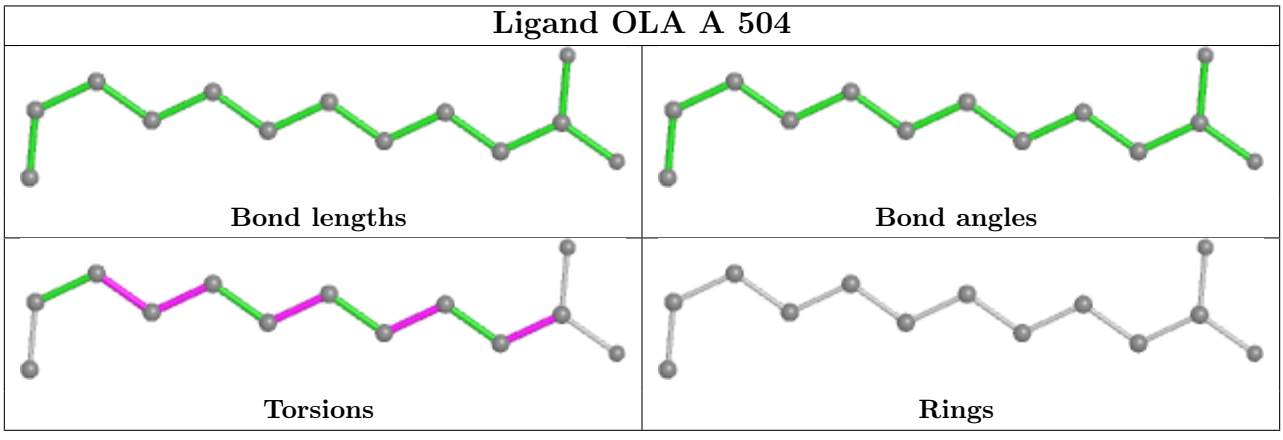
Ligand OLA A 507



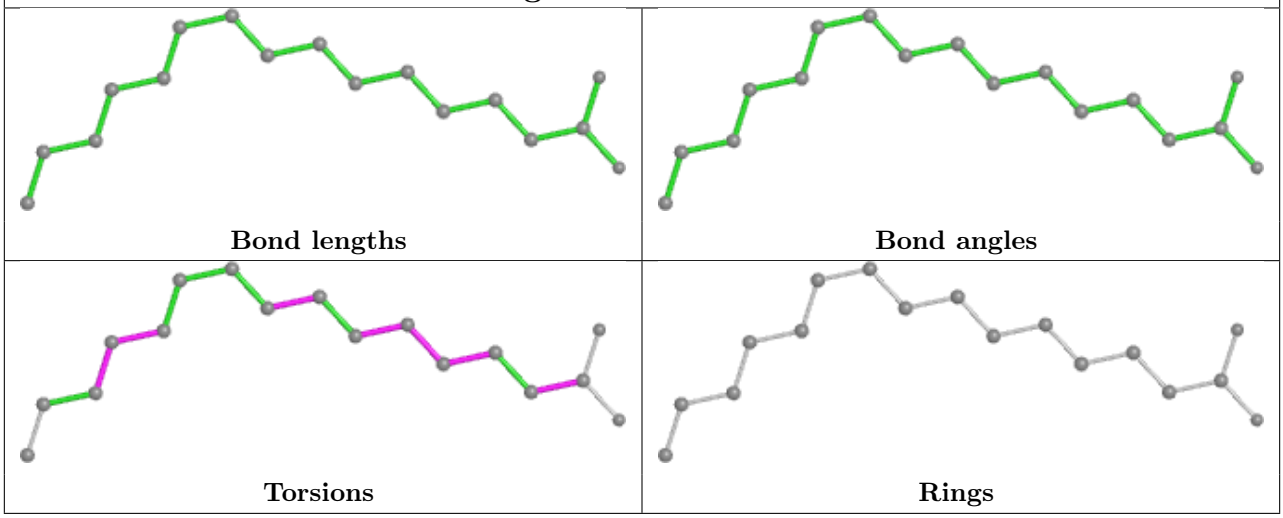
Ligand OLA A 509



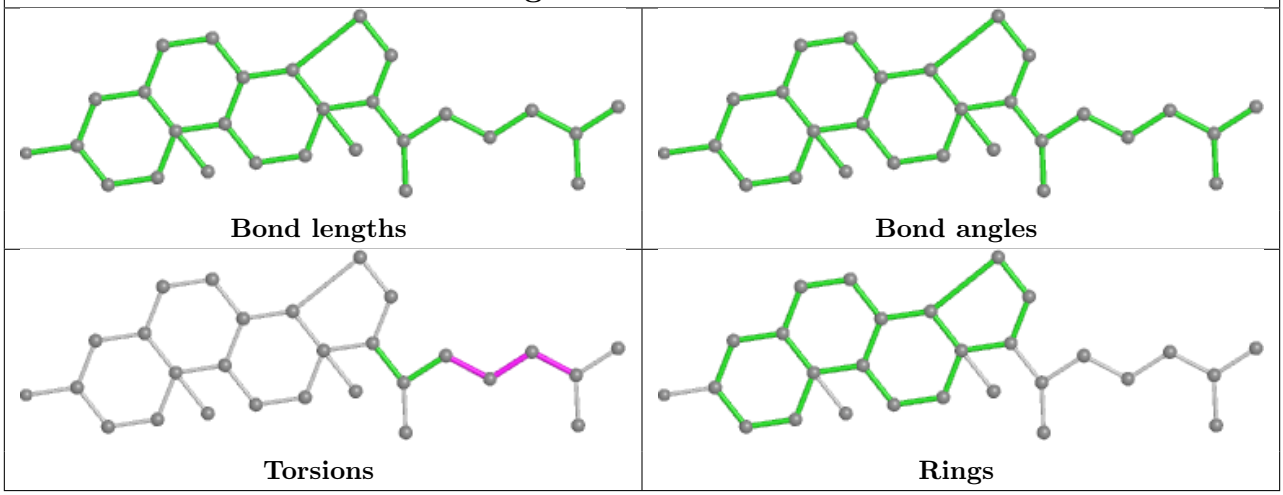
Ligand OLA A 504



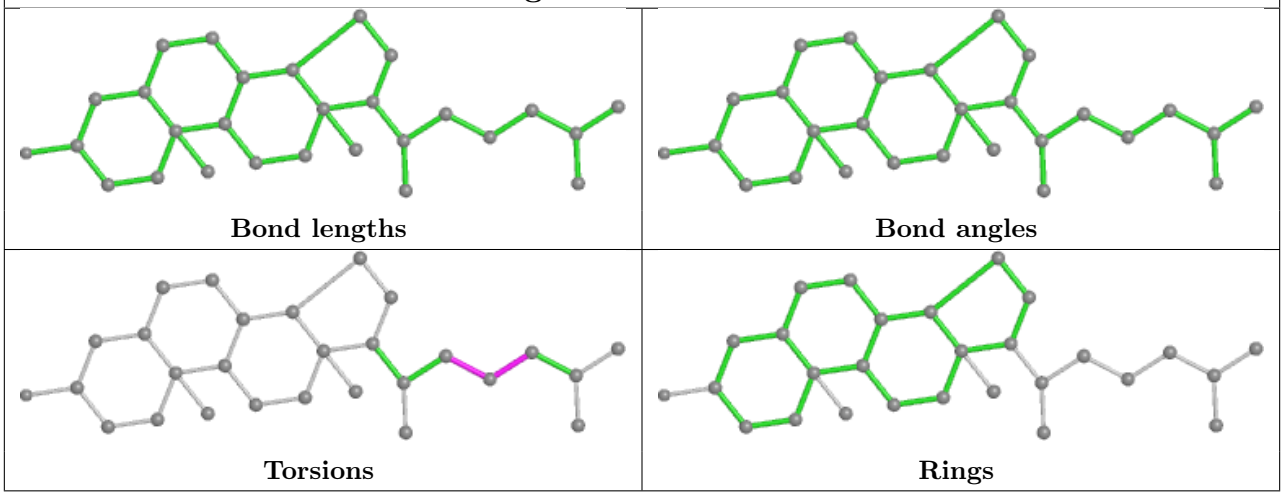
Ligand OLA A 505



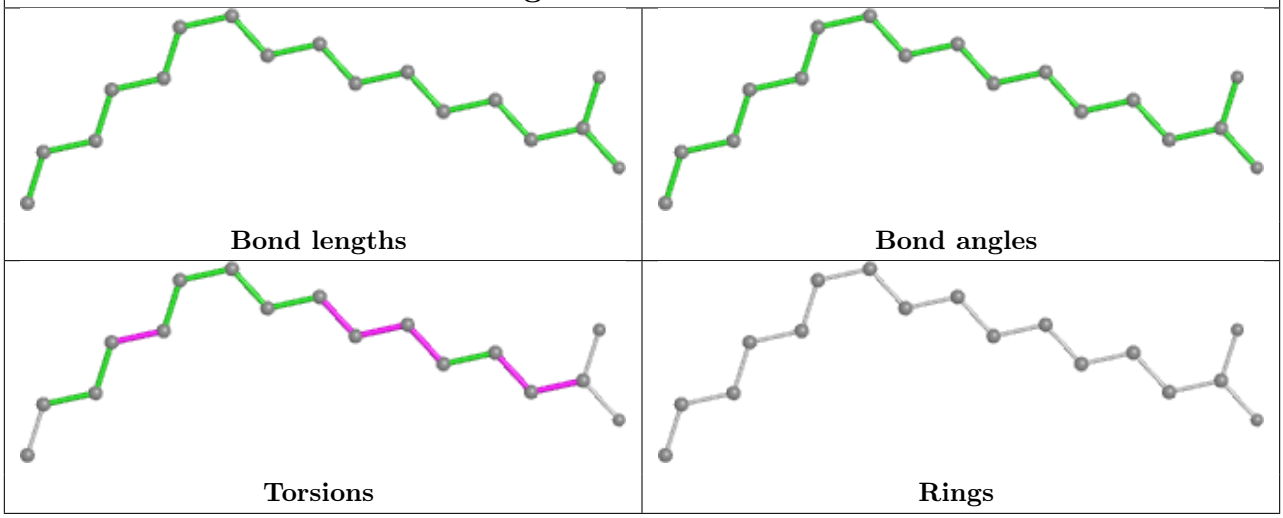
Ligand CLR A 513



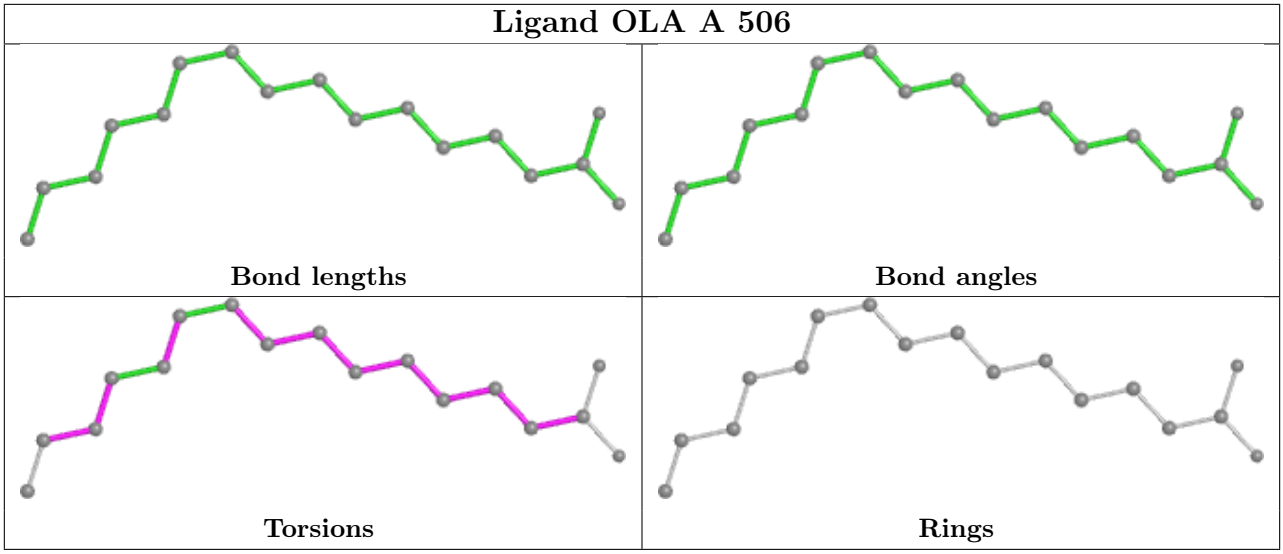
Ligand CLR A 515



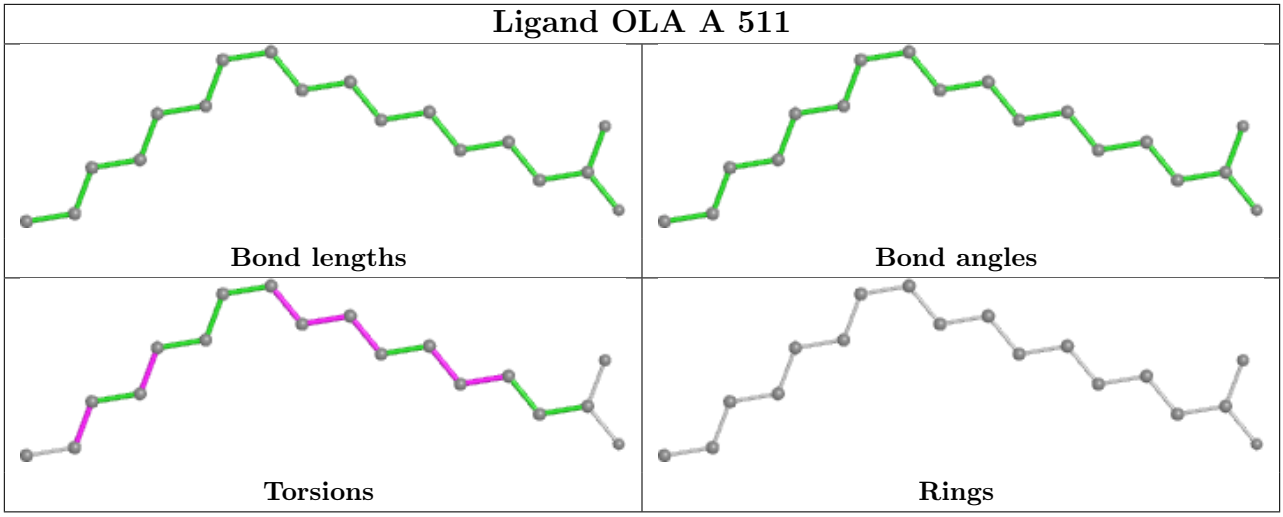
Ligand OLA A 508

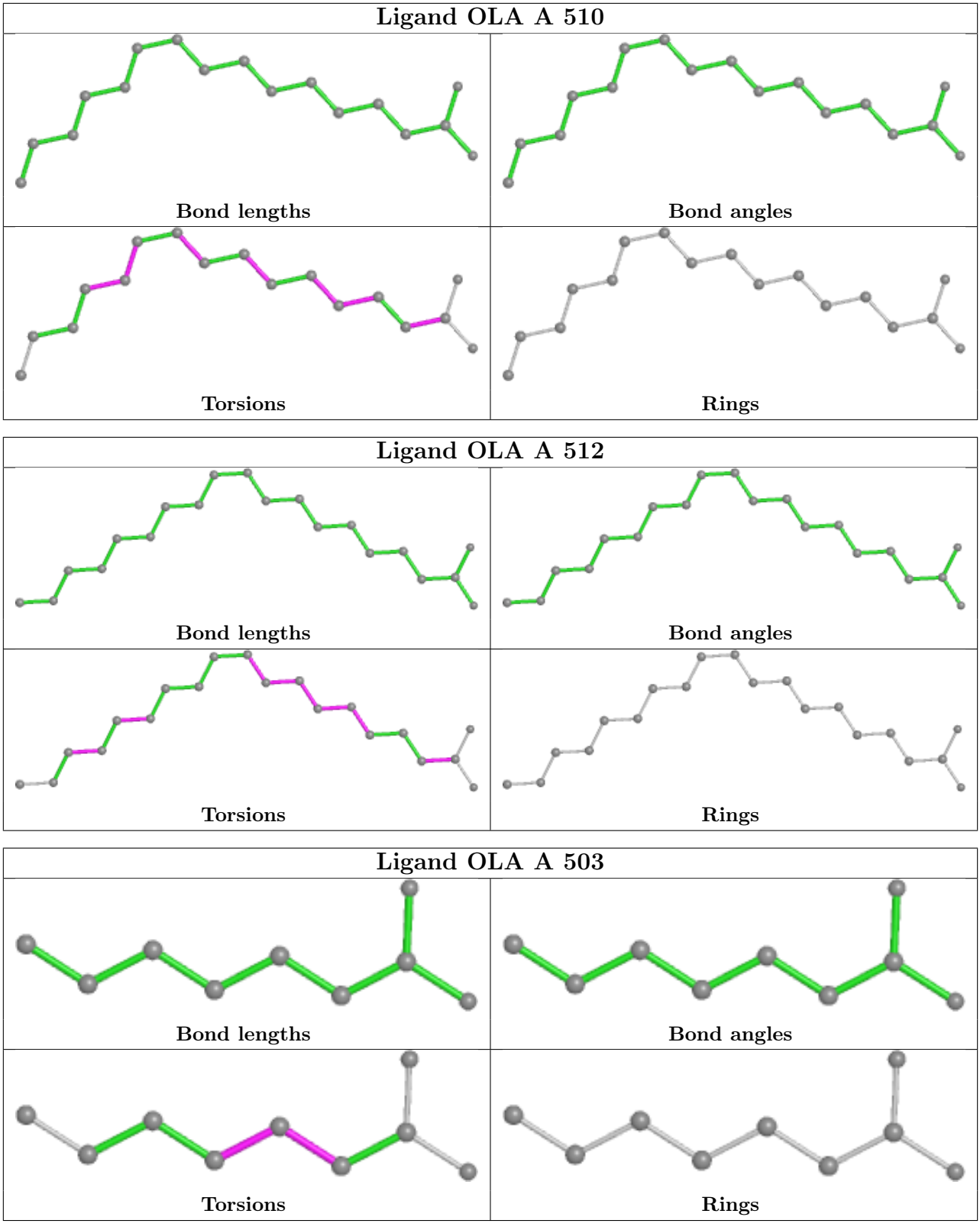


Ligand OLA A 506



Ligand OLA A 511





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	389/433 (89%)	0.05	11 (2%) 53 51	34, 55, 94, 134	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	VAL	4.9
1	A	427	HIS	4.3
1	A	294	PHE	4.3
1	A	425	ARG	3.5
1	A	261	ASP	3.0

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

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	OLA	A	509	17/20	0.58	0.35	75,85,93,102	0
3	OLA	A	510	17/20	0.58	0.35	70,83,105,107	0

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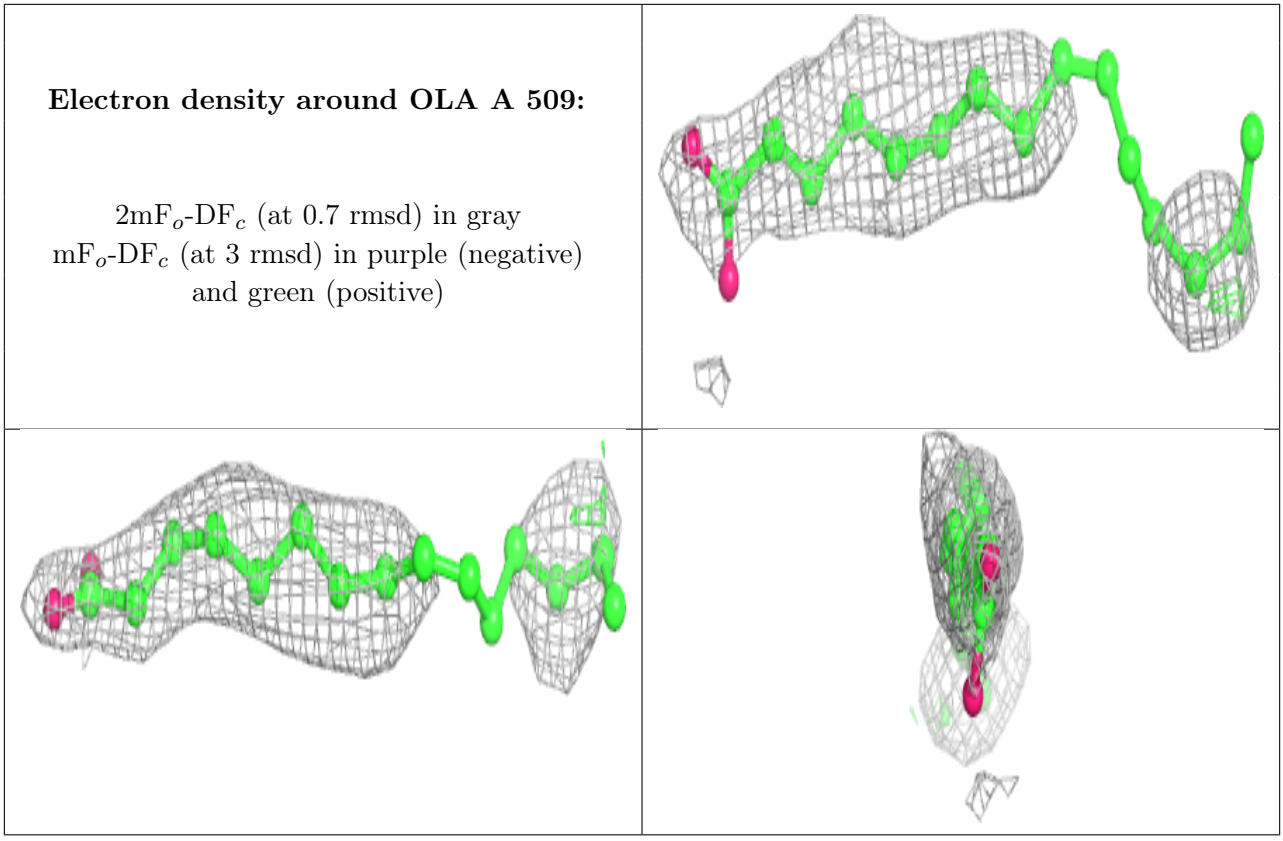
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	A	504	13/20	0.70	0.21	74,80,83,89	0
3	OLA	A	507	15/20	0.72	0.30	59,65,94,103	0
3	OLA	A	511	18/20	0.73	0.25	70,81,95,96	0
3	OLA	A	508	17/20	0.76	0.30	66,74,90,93	0
3	OLA	A	505	17/20	0.76	0.23	58,66,85,88	0
3	OLA	A	501	17/20	0.80	0.30	60,68,77,80	0
3	OLA	A	502	14/20	0.82	0.20	60,68,84,88	0
3	OLA	A	503	9/20	0.84	0.21	65,69,78,79	0
3	OLA	A	512	20/20	0.85	0.28	55,65,83,92	0
3	OLA	A	506	17/20	0.86	0.22	50,57,74,76	0
2	TEP	A	500	13/13	0.94	0.14	40,44,45,46	0
4	CLR	A	513	28/28	0.94	0.18	40,47,76,80	0
4	CLR	A	515	28/28	0.95	0.15	43,48,76,80	0
4	CLR	A	514	28/28	0.96	0.16	48,52,59,62	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.

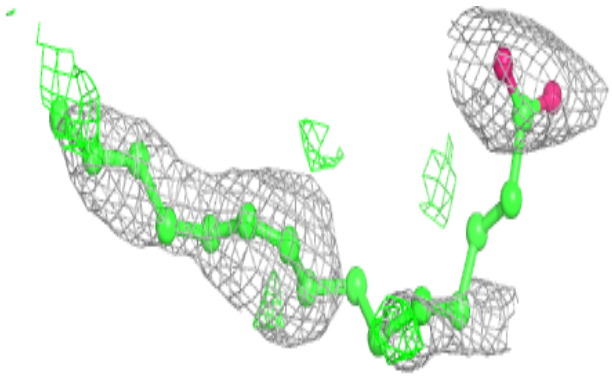
Electron density around OLA A 509:

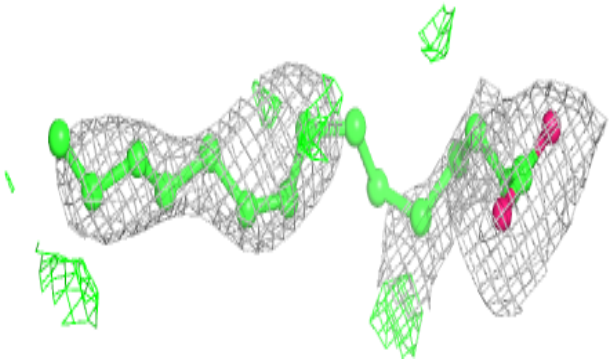
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

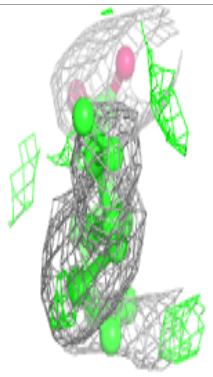


Electron density around OLA A 510:

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

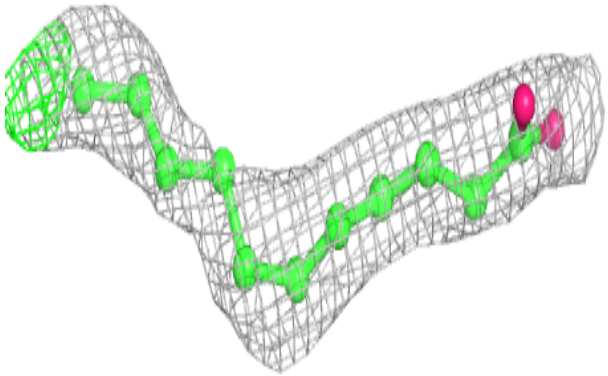


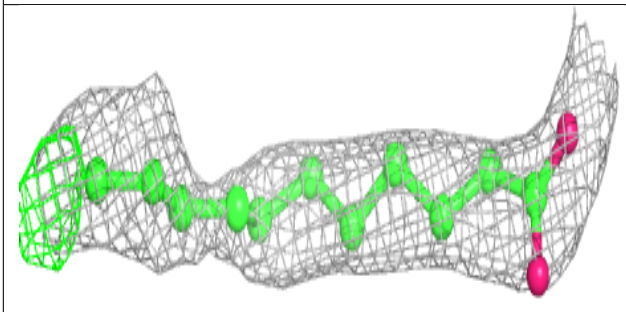


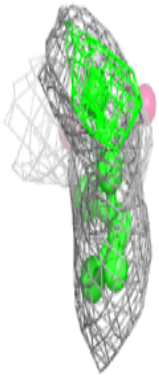


Electron density around OLA A 504:

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

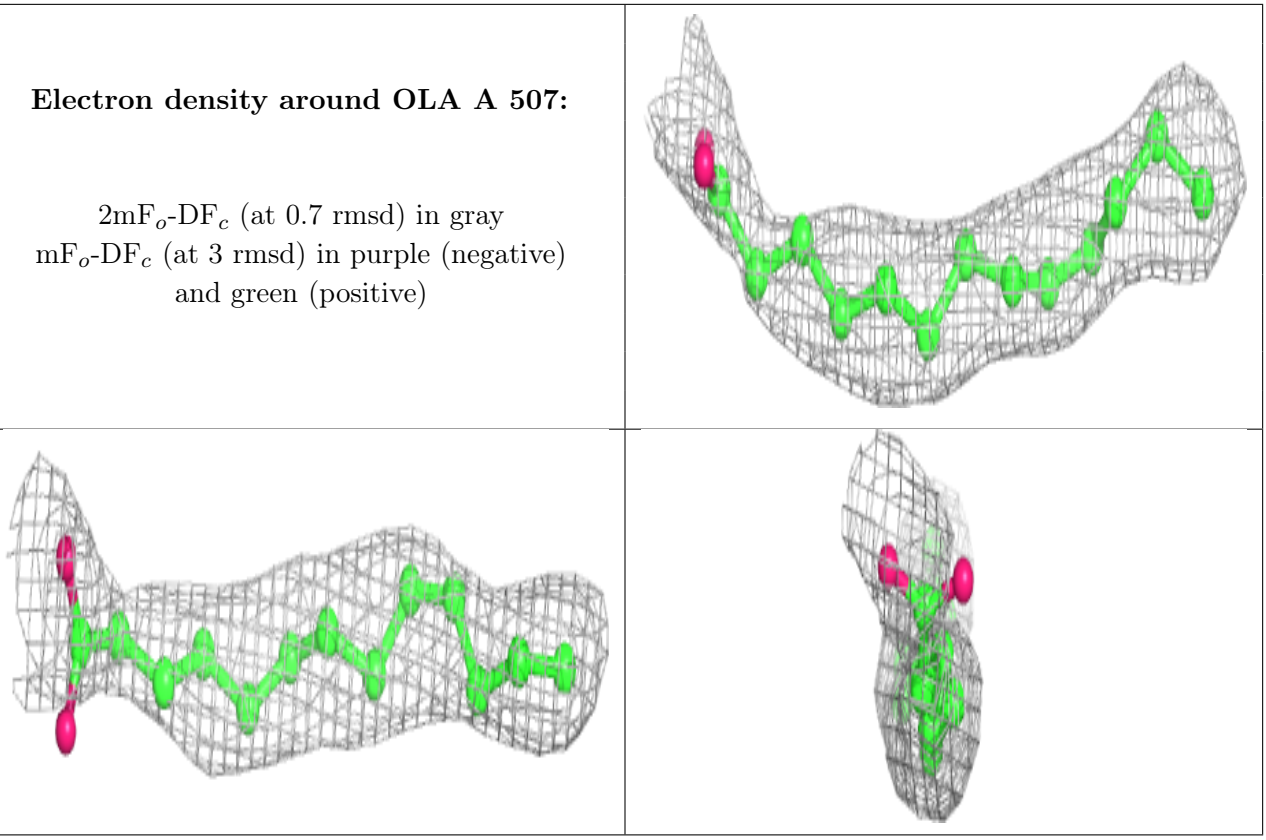






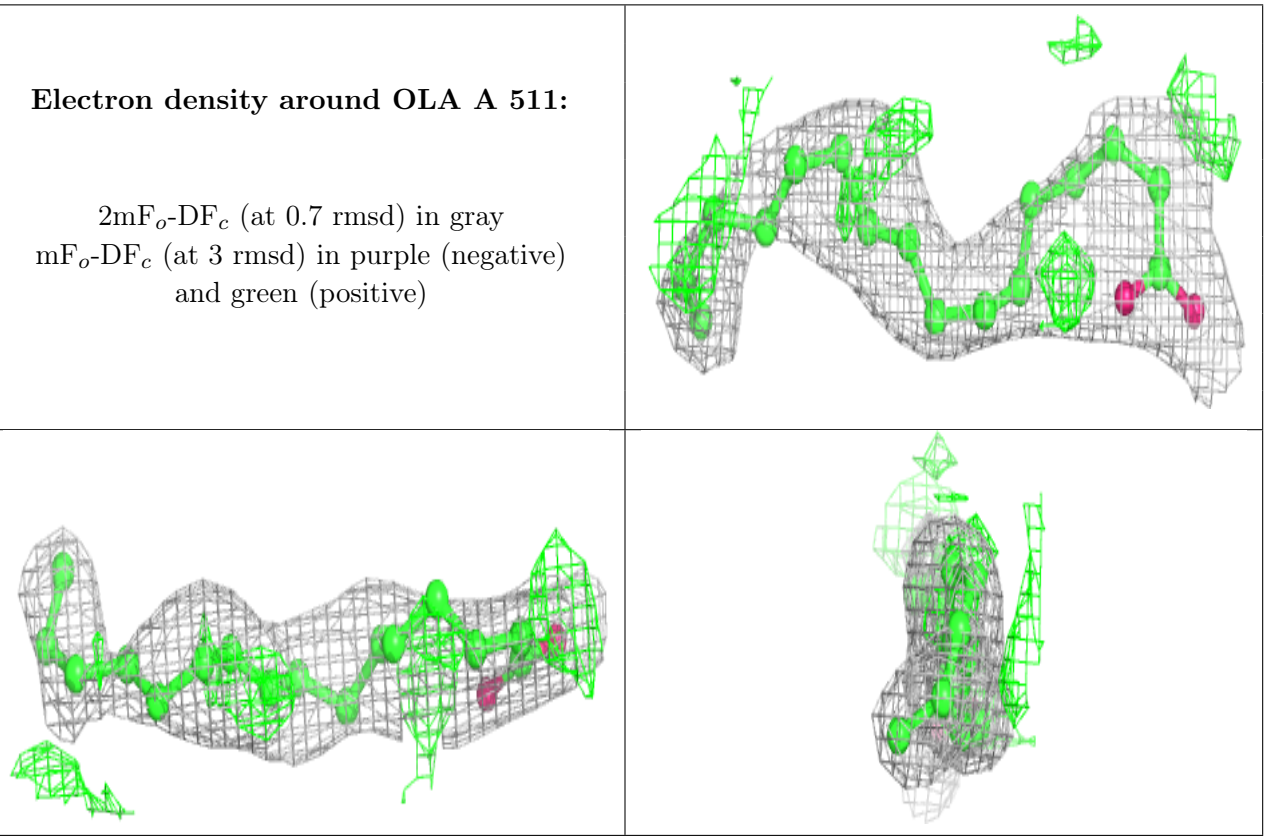
Electron density around OLA A 507:

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



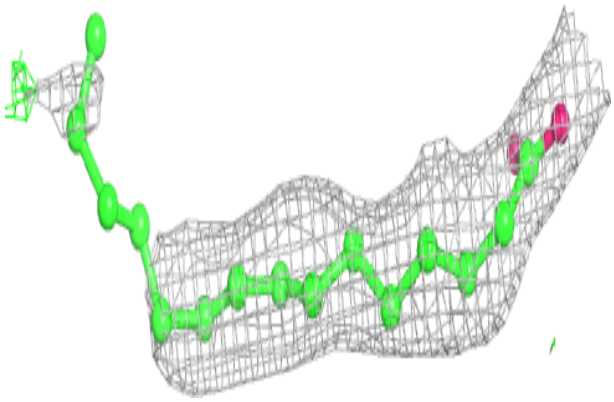
Electron density around OLA A 511:

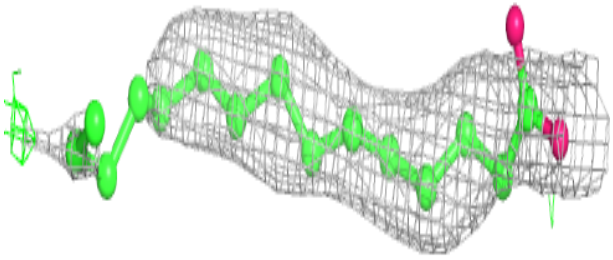
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

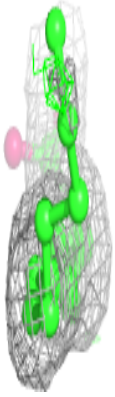


Electron density around OLA A 508:

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

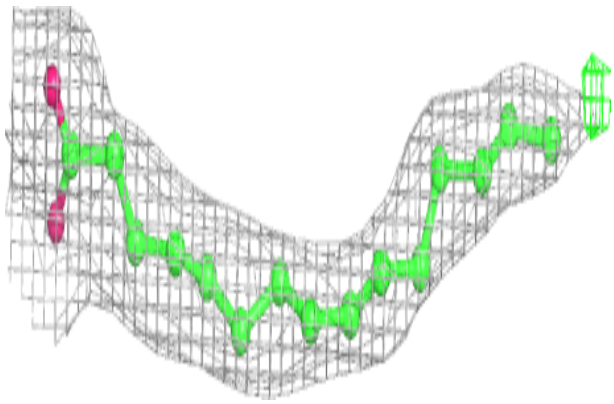


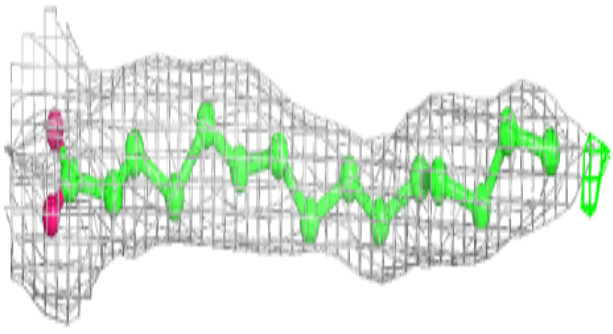


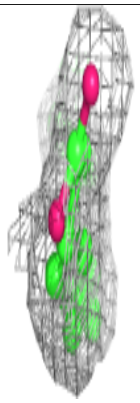


Electron density around OLA A 505:

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

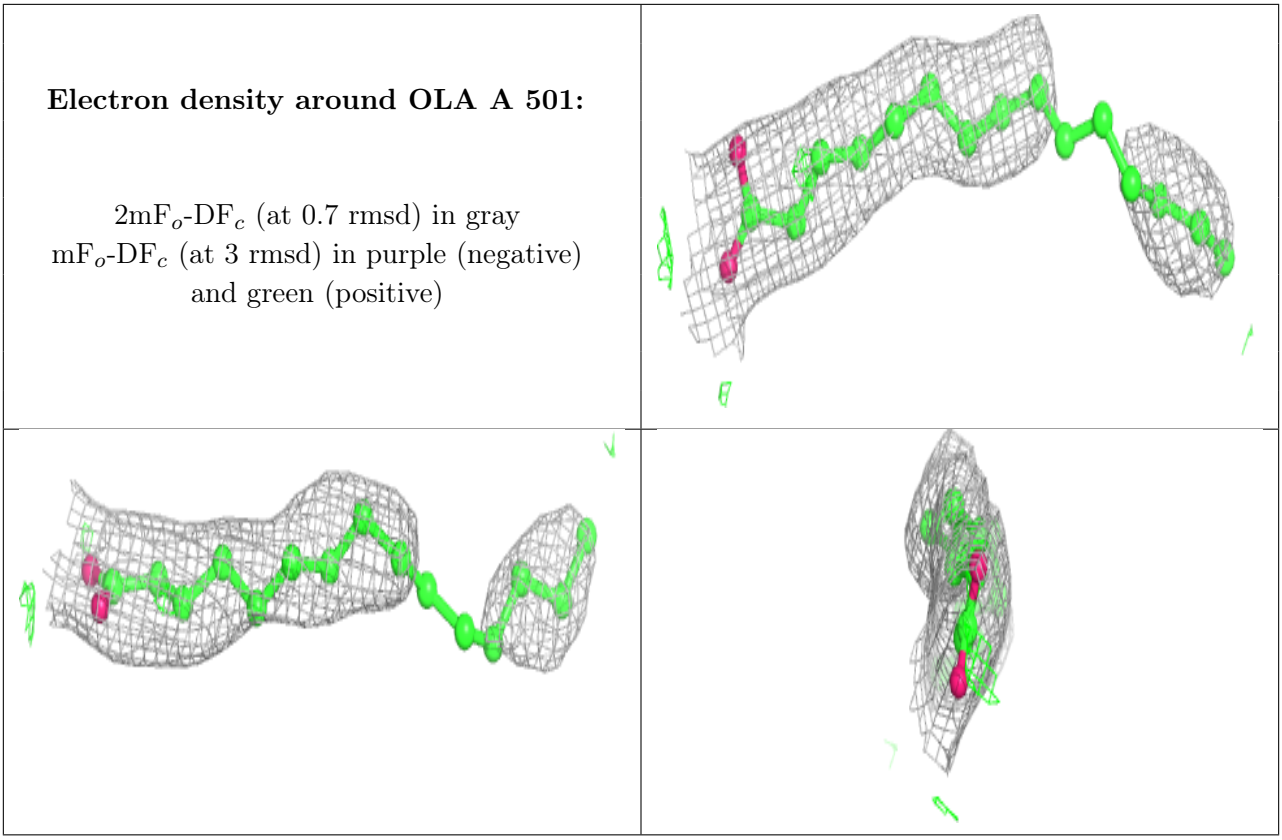






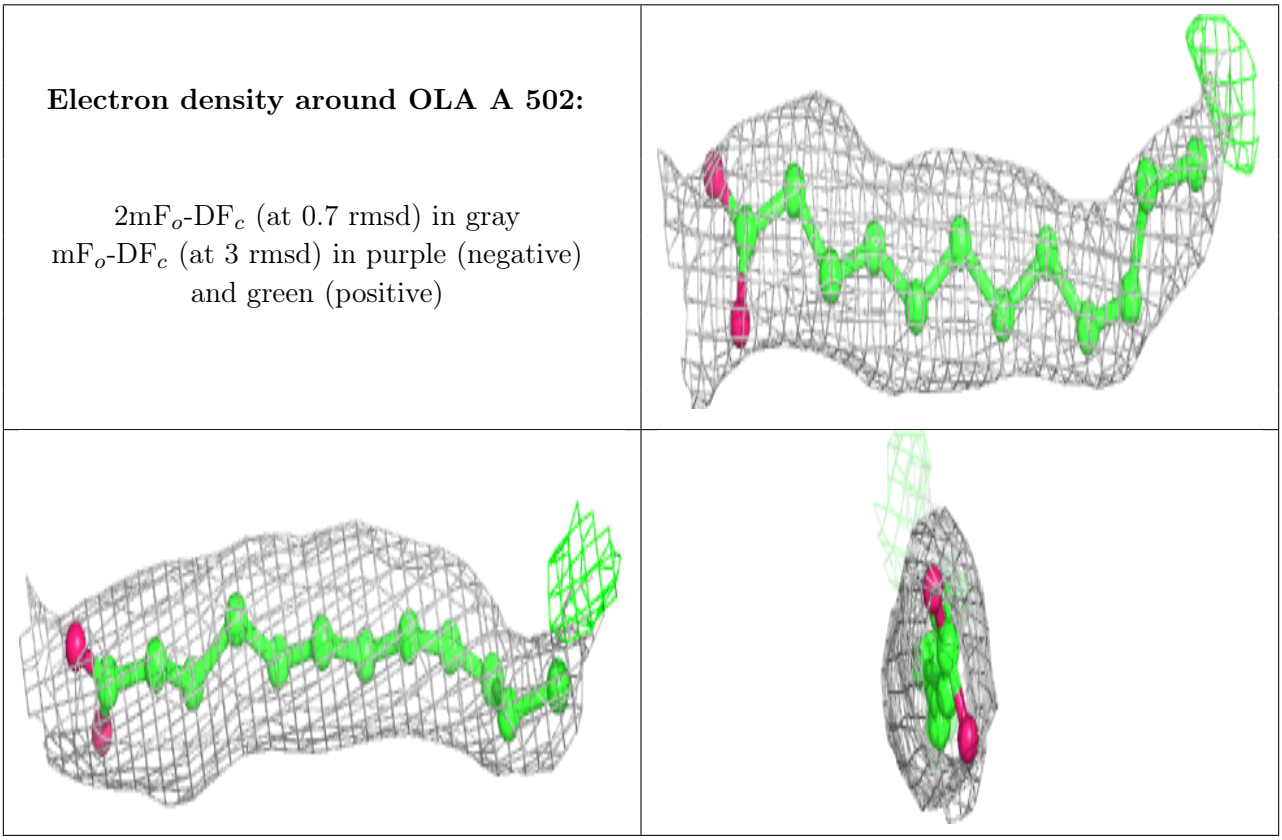
Electron density around OLA A 501:

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



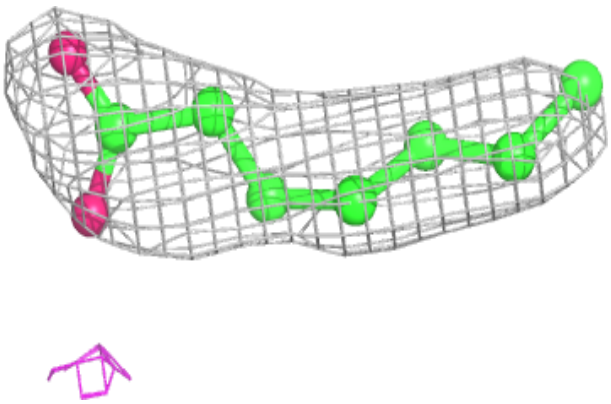
Electron density around OLA A 502:

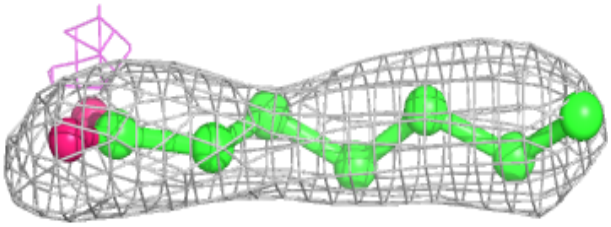
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

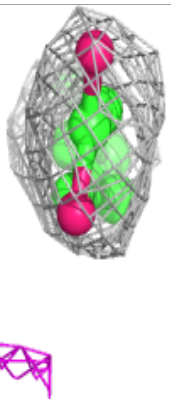


Electron density around OLA A 503:

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

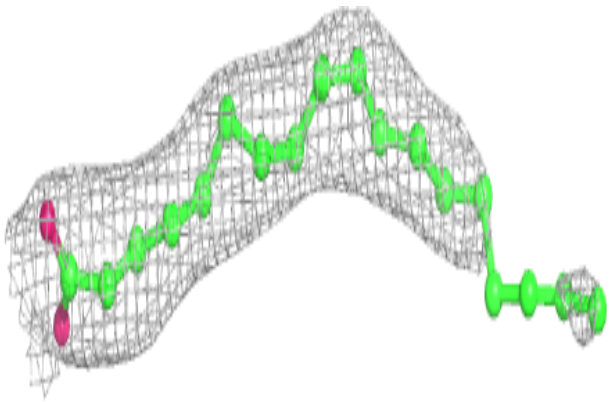


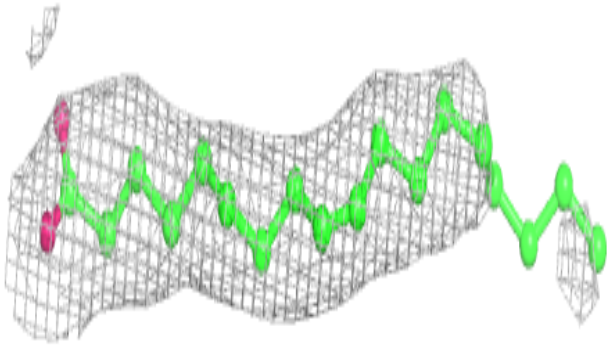


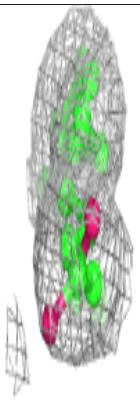


Electron density around OLA A 512:

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

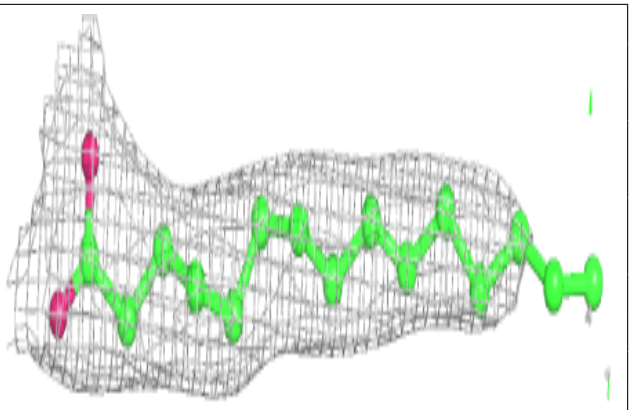


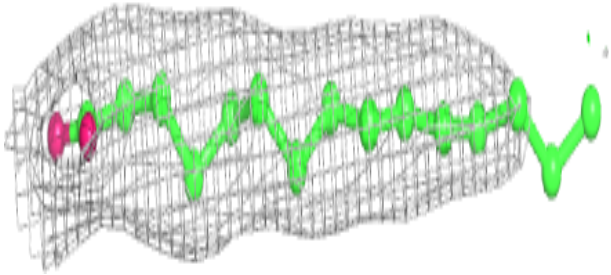


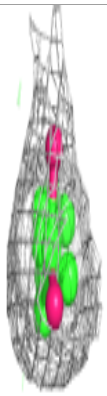


Electron density around OLA A 506:

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

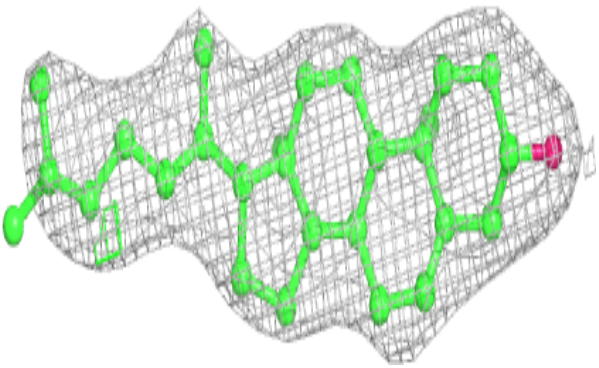


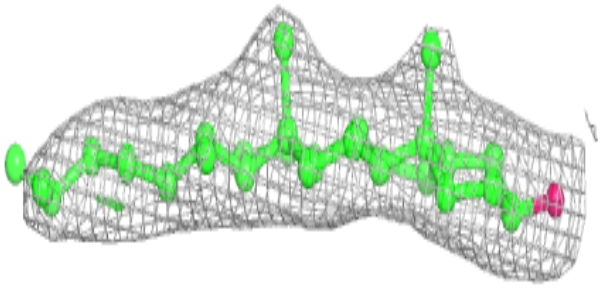


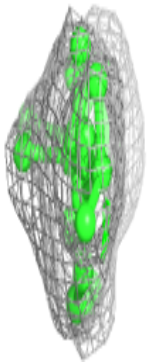


Electron density around CLR A 513:

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

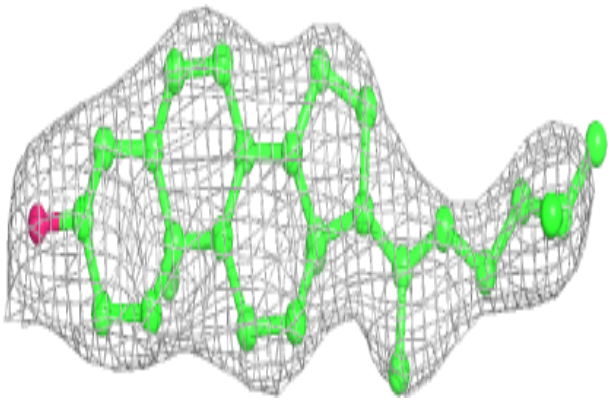


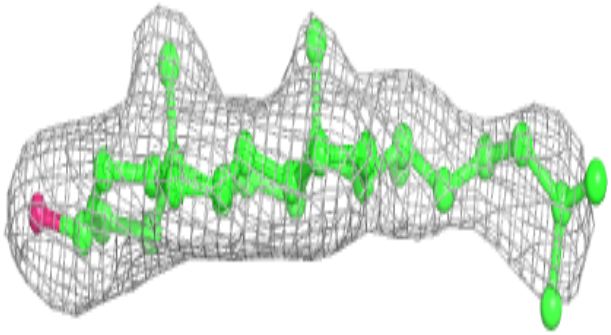


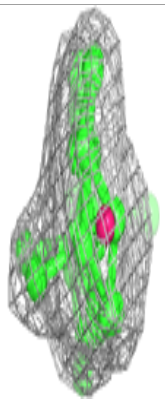


Electron density around CLR A 515:

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

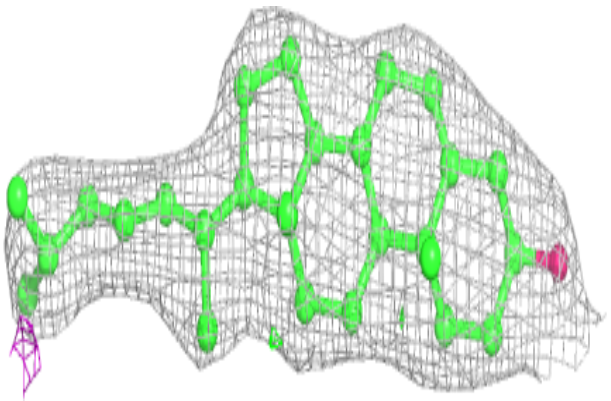


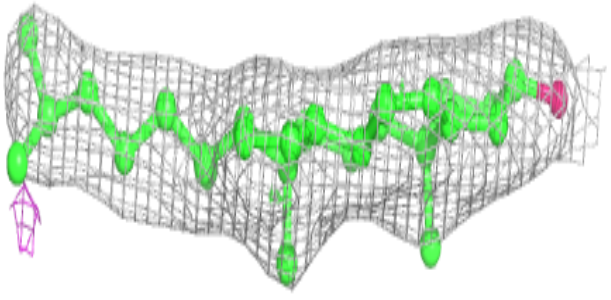


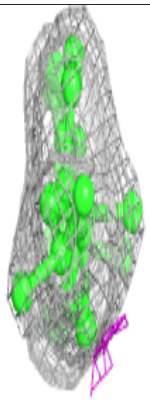


Electron density around CLR A 514:

$2mF_o$-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.