Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:55 PM EDT

PDB ID	:	6GPX
Title	:	CRYSTAL STRUCTURE OF CCR2A IN COMPLEX WITH MK-0812
Authors	:	Pautsch, A.; Schnapp, G.; Cheng, R.; Apel, A.
Deposited on	:	2018-06-07
Resolution	:	2.70 Å(reported)

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

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

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

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

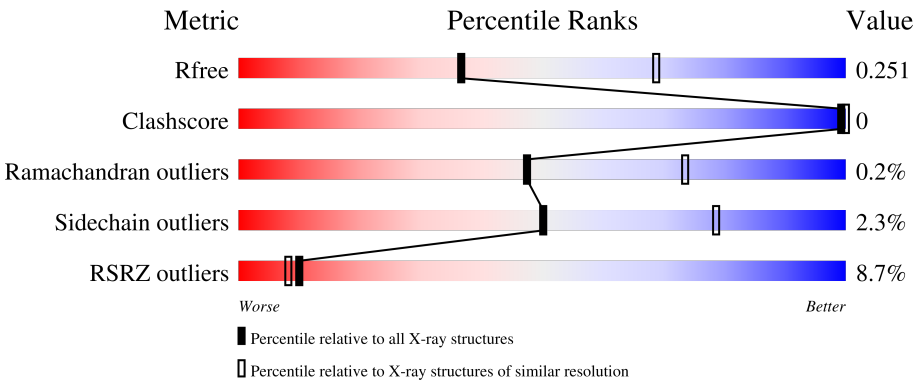
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	349	7%, 90%, 7%
1	B	349	8%, 73%, 25%

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
3	OLA	B	403	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10209 atoms, of which 5174 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 C-C chemokine receptor type 2,Rubredoxin,C-C chemokine receptor type 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	324	5200	1722	2611	400	448	19	2611	0	0
1	B	263	4282	1422	2176	322	348	14	2176	0	0

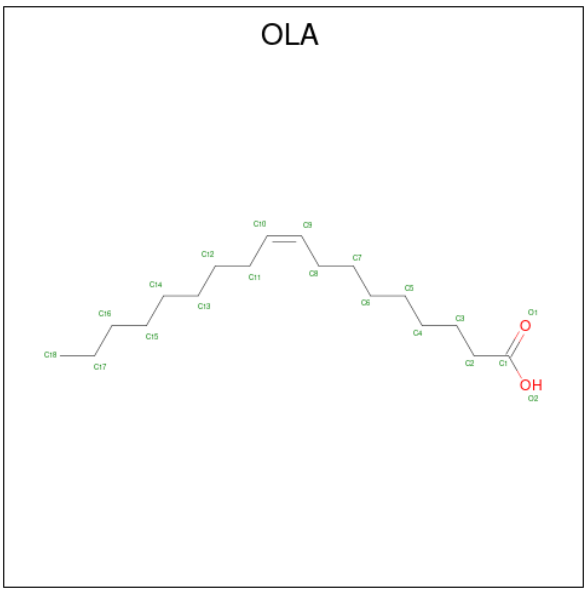
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	TYR	CYS	conflict	UNP P41597
A	175	ASN	GLY	conflict	UNP P41597
A	292	ASP	ALA	conflict	UNP P41597
A	373	GLU	-	expression tag	UNP P41597
A	374	VAL	-	expression tag	UNP P41597
A	375	LEU	-	expression tag	UNP P41597
A	376	PHE	-	expression tag	UNP P41597
A	377	GLN	-	expression tag	UNP P41597
B	70	TYR	CYS	conflict	UNP P41597
B	175	ASN	GLY	conflict	UNP P41597
B	241	ASP	ALA	conflict	UNP P41597
B	322	GLU	-	expression tag	UNP P41597
B	323	VAL	-	expression tag	UNP P41597
B	324	LEU	-	expression tag	UNP P41597
B	325	PHE	-	expression tag	UNP P41597
B	326	GLN	-	expression tag	UNP P41597

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- 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 H O 36 13 21 2	21	0
3	A	1	Total C H O 28 10 16 2	16	0
3	A	1	Total C H O 30 11 17 2	17	0
3	A	1	Total C H O 54 18 34 2	34	0
3	A	1	Total C H O 36 13 21 2	21	0
3	A	1	Total C H O 54 18 34 2	34	0
3	A	1	Total C H O 20 7 11 2	11	0
3	A	1	Total C H O 26 9 15 2	15	0
3	A	1	Total C H 42 15 27	27	0
3	A	1	Total C H O 30 11 17 2	17	0
3	A	1	Total C H O 54 18 34 2	34	0
3	B	1	Total C H O 26 9 15 2	15	0
3	B	1	Total C H O 36 13 21 2	21	0

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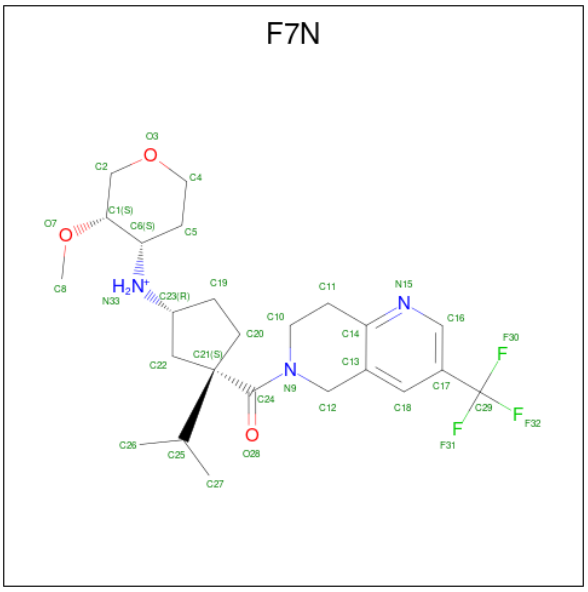
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	54	18	34	2	34	0

- Molecule 4 is [(3 {S},4 {S})-3-methoxyoxan-4-yl]-[(1 {R},3 {S})-3-propan-2-yl-3-[[3-(trifluoromethyl)-7,8-dihydro-5 {H}-1,6-naphthyridin-6-yl]carbonyl]cyclopentyl]azanium (three-letter code: F7N) (formula: $C_{24}H_{35}F_3N_3O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	H	N	O		
4	A	1	68	24	3	35	3	3	35	0
			Total	C	F	H	N	O		
4	B	1	68	24	3	35	3	3	35	0

- Molecule 5 is water.

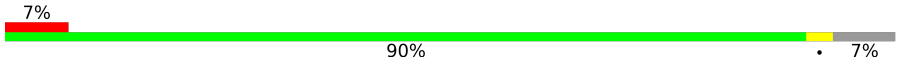
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	36	36	36	0	0
			Total	O		
5	B	28	28	28	0	0

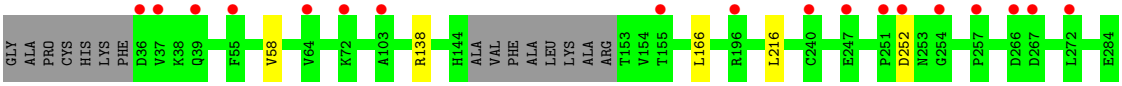
3 Residue-property plots (i)

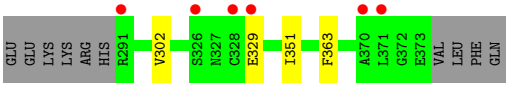
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: C-C chemokine receptor type 2,Rubredoxin,C-C chemokine receptor type 2

Chain A:

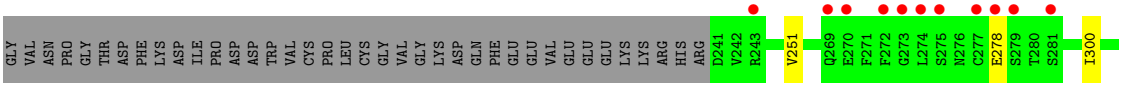


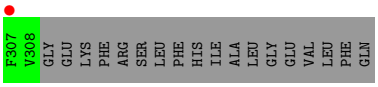




• Molecule 1: C-C chemokine receptor type 2,Rubredoxin,C-C chemokine receptor type 2

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.57Å 64.55Å 131.20Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	39.90 – 2.70 39.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.90-2.70) 100.0 (39.90-2.70)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.230 , 0.243 0.239 , 0.251	Depositor DCC
R_{free} test set	1266 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10209	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: F7N, OLA, ZN

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	0/2658	0.52	0/3622
1	B	0.39	0/2163	0.52	0/2952
All	All	0.38	0/4821	0.52	0/6574

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2589	2611	2611	1	0
1	B	2106	2176	2176	1	0
2	A	1	0	0	0	0
3	A	163	247	237	0	0
3	B	46	70	67	0	0
4	A	33	35	0	0	0
4	B	33	35	0	0	0
5	A	36	0	0	0	0
5	B	28	0	0	0	0
All	All	5035	5174	5091	2	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 0.

All (2) 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:302:VAL:HG11	1:A:351:ILE:HG21	1.97	0.46
1:B:251:VAL:HG11	1:B:300:ILE:HG21	1.98	0.45

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	318/349 (91%)	312 (98%)	6 (2%)	0	100	100
1	B	259/349 (74%)	253 (98%)	5 (2%)	1 (0%)	34	60
All	All	577/698 (83%)	565 (98%)	11 (2%)	1 (0%)	47	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	ASP

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	289/309 (94%)	282 (98%)	7 (2%)	49	77
1	B	234/309 (76%)	229 (98%)	5 (2%)	53	80
All	All	523/618 (85%)	511 (98%)	12 (2%)	50	78

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

Mol	Chain	Res	Type
1	A	58	VAL
1	A	138	ARG
1	A	166	LEU
1	A	216	LEU
1	A	252	ASP
1	A	329	GLU
1	A	363	PHE
1	B	39	GLN
1	B	58	VAL
1	B	166	LEU
1	B	216	LEU
1	B	278	GLU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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	404	-	12,12,19	0.25	0	12,12,19	0.18	0
3	OLA	A	412	-	19,19,19	0.16	0	19,19,19	0.19	0
4	F7N	A	413	-	35,36,36	0.61	1 (2%)	41,54,54	0.82	0
3	OLA	B	403	-	19,19,19	0.22	0	19,19,19	0.18	0
3	OLA	A	403	-	11,11,19	0.21	0	11,11,19	0.17	0
3	OLA	A	408	-	8,8,19	0.24	0	8,8,19	0.22	0
3	OLA	B	402	-	14,14,19	0.18	0	14,14,19	0.16	0
3	OLA	A	402	-	14,14,19	0.22	0	14,14,19	0.17	0
3	OLA	A	406	-	14,14,19	0.20	0	14,14,19	0.21	0
3	OLA	A	411	-	12,12,19	0.25	0	12,12,19	0.21	0
3	OLA	A	410	-	14,14,19	0.15	0	13,13,19	0.22	0
4	F7N	B	404	-	35,36,36	0.62	0	41,54,54	0.83	0
3	OLA	A	405	-	19,19,19	0.25	0	19,19,19	0.24	0
3	OLA	A	409	-	10,10,19	0.22	0	10,10,19	0.35	0
3	OLA	B	401	-	10,10,19	0.15	0	10,10,19	0.13	0
3	OLA	A	407	-	19,19,19	0.21	0	19,19,19	0.23	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	404	-	-	4/10/10/17	-
3	OLA	A	412	-	-	9/17/17/17	-
4	F7N	A	413	-	-	0/28/59/59	0/4/4/4
3	OLA	B	403	-	-	4/17/17/17	-
3	OLA	A	403	-	-	7/9/9/17	-
3	OLA	A	408	-	-	0/6/6/17	-
3	OLA	B	402	-	-	0/12/12/17	-
3	OLA	A	402	-	-	2/12/12/17	-
3	OLA	A	406	-	-	4/12/12/17	-
3	OLA	A	411	-	-	0/10/10/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	A	410	-	-	5/12/12/17	-
4	F7N	B	404	-	-	3/28/59/59	0/4/4/4
3	OLA	A	405	-	-	8/17/17/17	-
3	OLA	A	409	-	-	5/8/8/17	-
3	OLA	B	401	-	-	0/8/8/17	-
3	OLA	A	407	-	-	4/17/17/17	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	413	F7N	C21-C25	2.08	1.61	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	OLA	C11-C12-C13-C14
3	A	410	OLA	C5-C6-C7-C8
3	A	406	OLA	C3-C4-C5-C6
3	A	407	OLA	C12-C13-C14-C15
3	B	403	OLA	C14-C15-C16-C17
3	A	406	OLA	C5-C6-C7-C8
3	A	409	OLA	C4-C5-C6-C7
3	A	412	OLA	C14-C15-C16-C17
3	A	412	OLA	C11-C12-C13-C14
3	A	405	OLA	C4-C5-C6-C7
3	A	405	OLA	C1-C2-C3-C4
3	A	404	OLA	C4-C5-C6-C7
3	B	403	OLA	C3-C4-C5-C6
3	A	409	OLA	C3-C4-C5-C6
3	A	405	OLA	C6-C7-C8-C9
3	A	407	OLA	C1-C2-C3-C4
3	A	409	OLA	C5-C6-C7-C8
3	A	412	OLA	C1-C2-C3-C4
3	A	412	OLA	C3-C4-C5-C6
3	A	412	OLA	C4-C5-C6-C7
3	A	403	OLA	C4-C5-C6-C7
3	A	405	OLA	C5-C6-C7-C8
3	A	412	OLA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	403	OLA	C3-C4-C5-C6
4	B	404	F7N	C16-C17-C29-F30
3	A	405	OLA	C3-C4-C5-C6
3	A	403	OLA	C1-C2-C3-C4
3	B	403	OLA	O2-C1-C2-C3
3	A	406	OLA	O2-C1-C2-C3
3	B	403	OLA	O1-C1-C2-C3
3	A	403	OLA	O2-C1-C2-C3
3	A	407	OLA	C10-C11-C12-C13
3	A	403	OLA	O1-C1-C2-C3
3	A	406	OLA	O1-C1-C2-C3
3	A	405	OLA	O1-C1-C2-C3
3	A	405	OLA	O2-C1-C2-C3
3	A	404	OLA	O2-C1-C2-C3
3	A	412	OLA	O2-C1-C2-C3
3	A	412	OLA	O1-C1-C2-C3
3	A	404	OLA	O1-C1-C2-C3
3	A	410	OLA	C13-C14-C15-C16
4	B	404	F7N	C16-C17-C29-F31
3	A	412	OLA	C7-C8-C9-C10
4	B	404	F7N	C16-C17-C29-F32
3	A	404	OLA	C7-C8-C9-C10
3	A	402	OLA	O2-C1-C2-C3
3	A	405	OLA	C7-C8-C9-C10
3	A	410	OLA	C7-C8-C9-C10
3	A	407	OLA	C9-C10-C11-C12
3	A	402	OLA	O1-C1-C2-C3
3	A	410	OLA	C15-C16-C17-C18
3	A	409	OLA	O2-C1-C2-C3
3	A	409	OLA	O1-C1-C2-C3
3	A	403	OLA	C2-C3-C4-C5
3	A	403	OLA	C5-C6-C7-C8

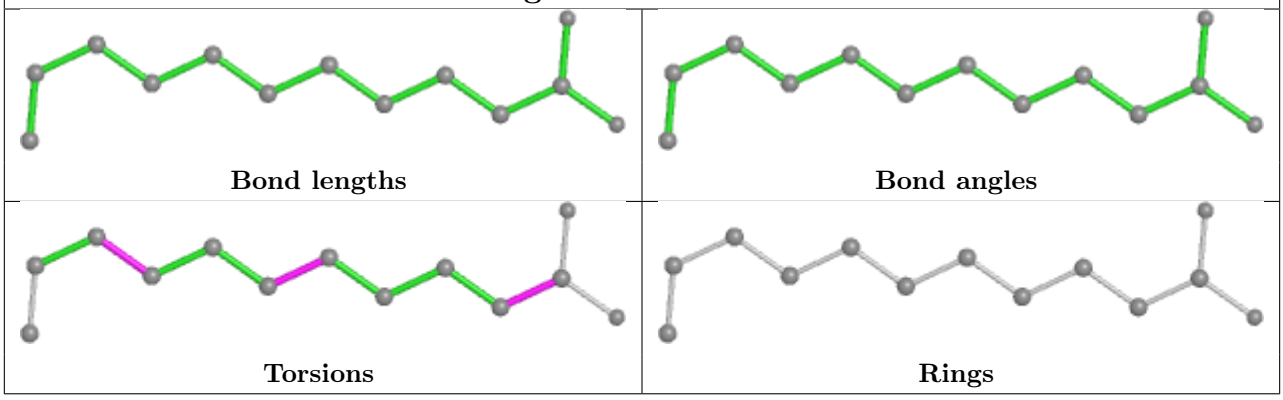
There are no ring outliers.

No monomer is involved in short contacts.

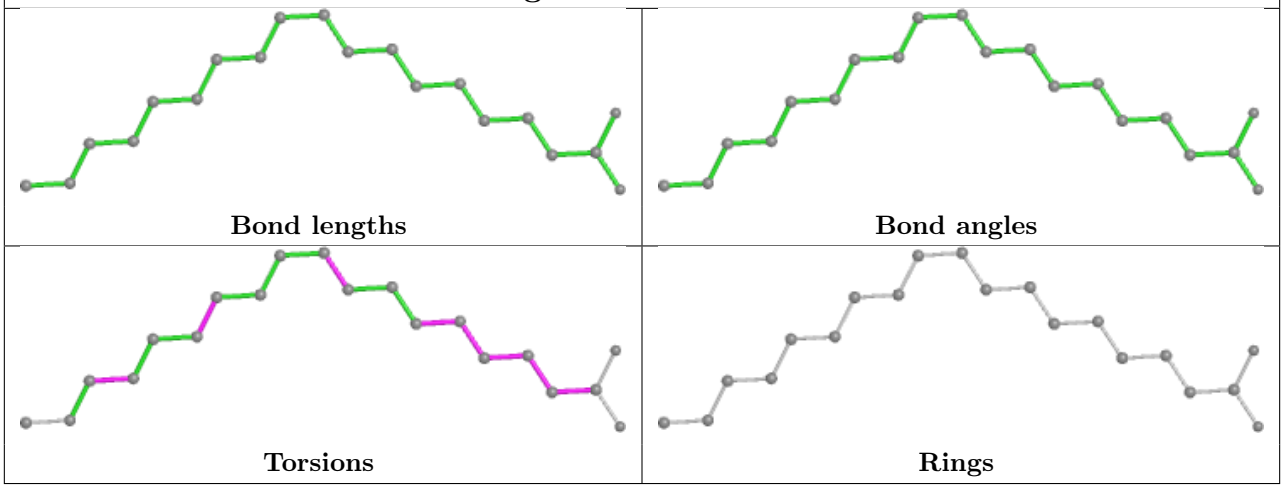
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

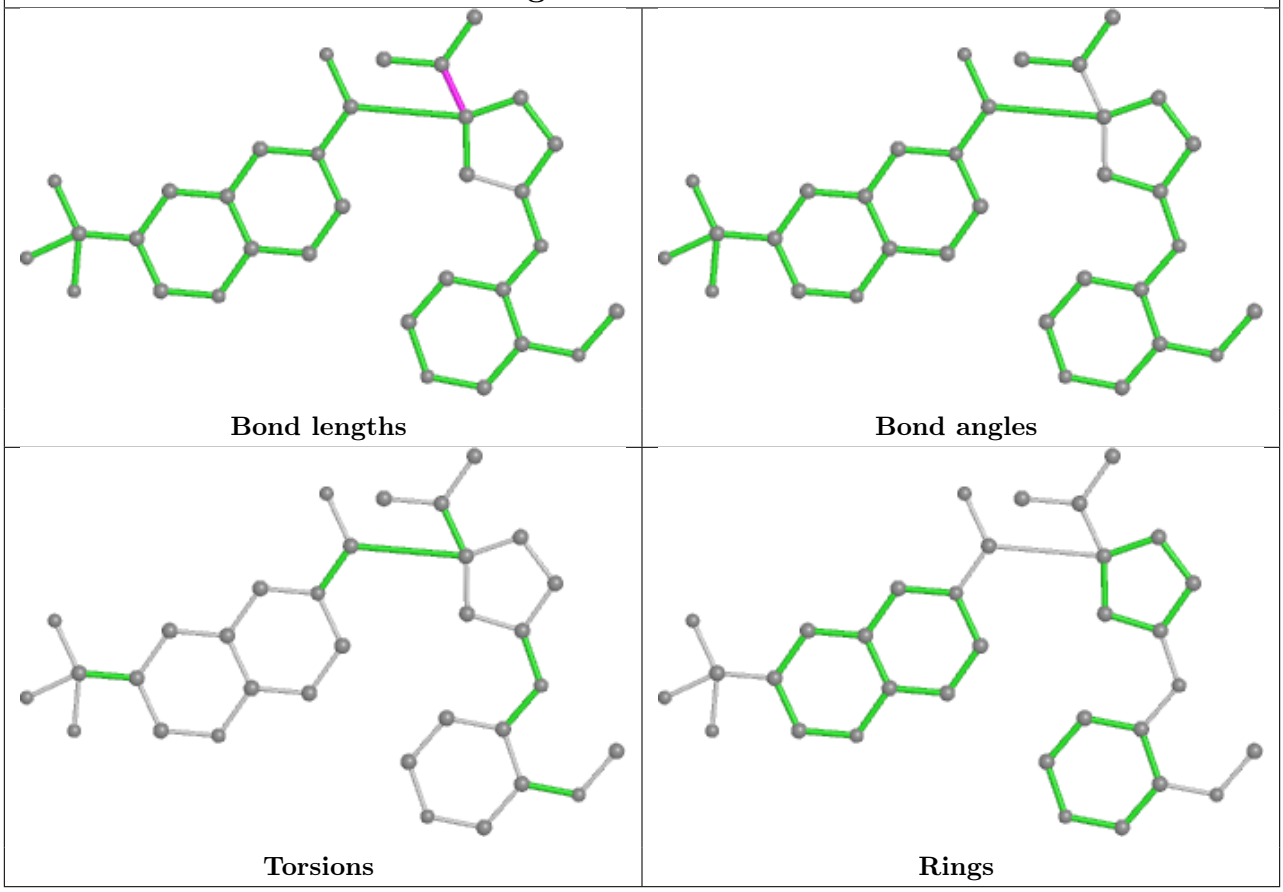
Ligand OLA A 404



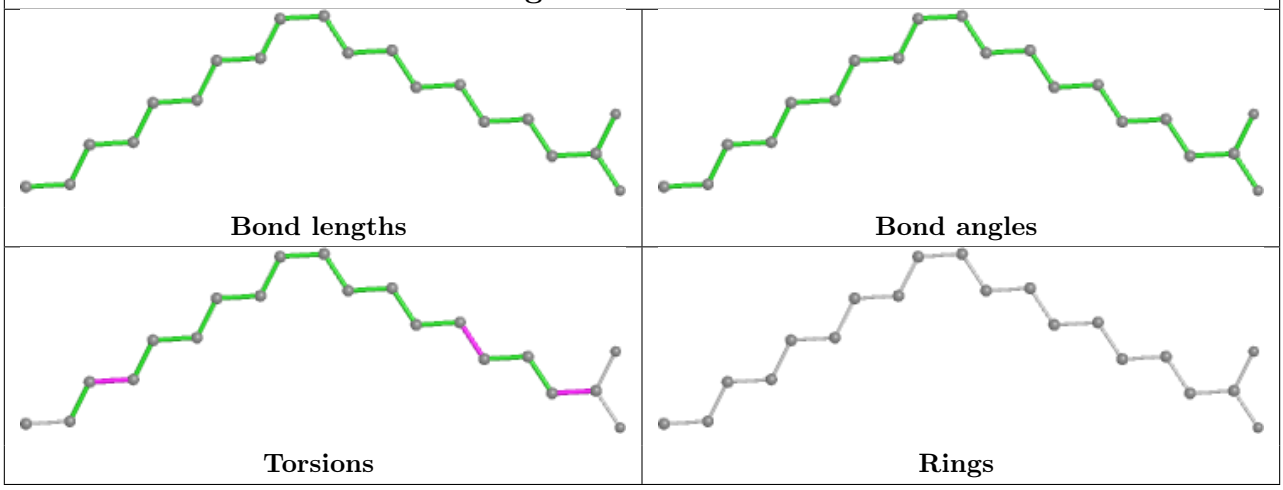
Ligand OLA A 412



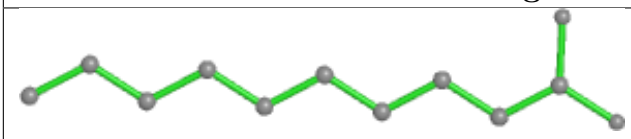
Ligand F7N A 413



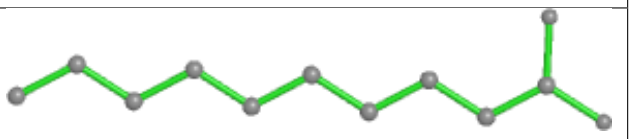
Ligand OLA B 403



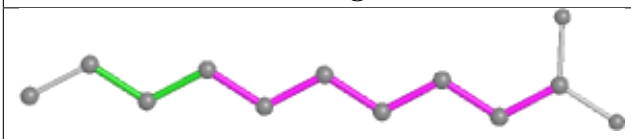
Ligand OLA A 403



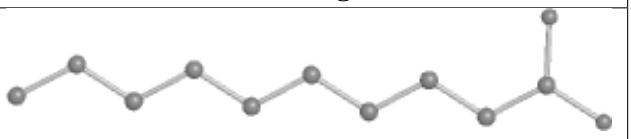
Bond lengths



Bond angles

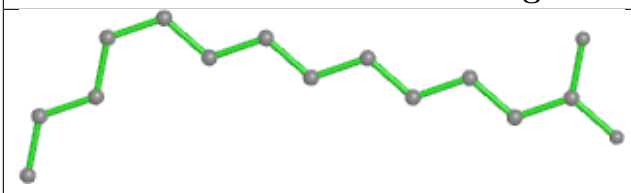


Torsions

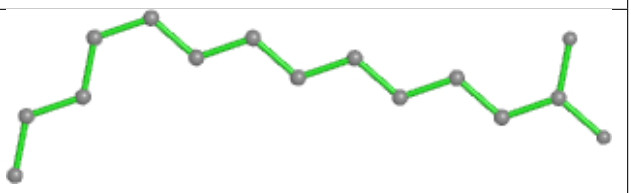


Rings

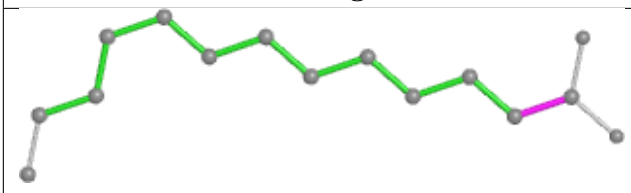
Ligand OLA A 402



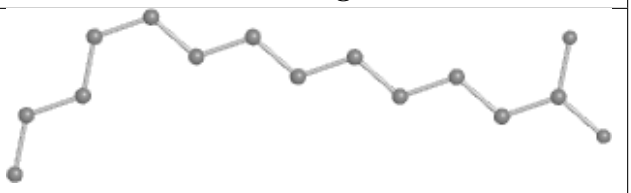
Bond lengths



Bond angles

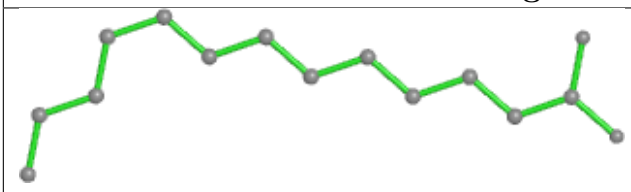


Torsions

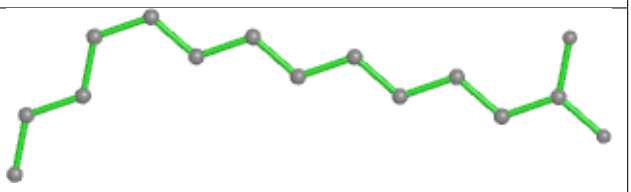


Rings

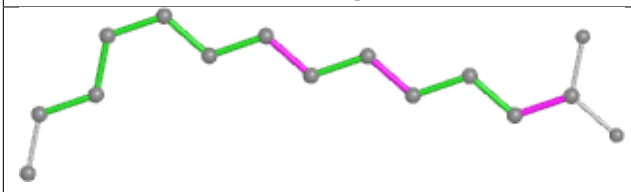
Ligand OLA A 406



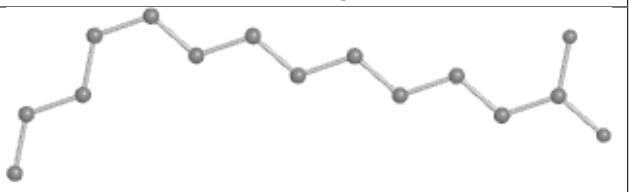
Bond lengths



Bond angles

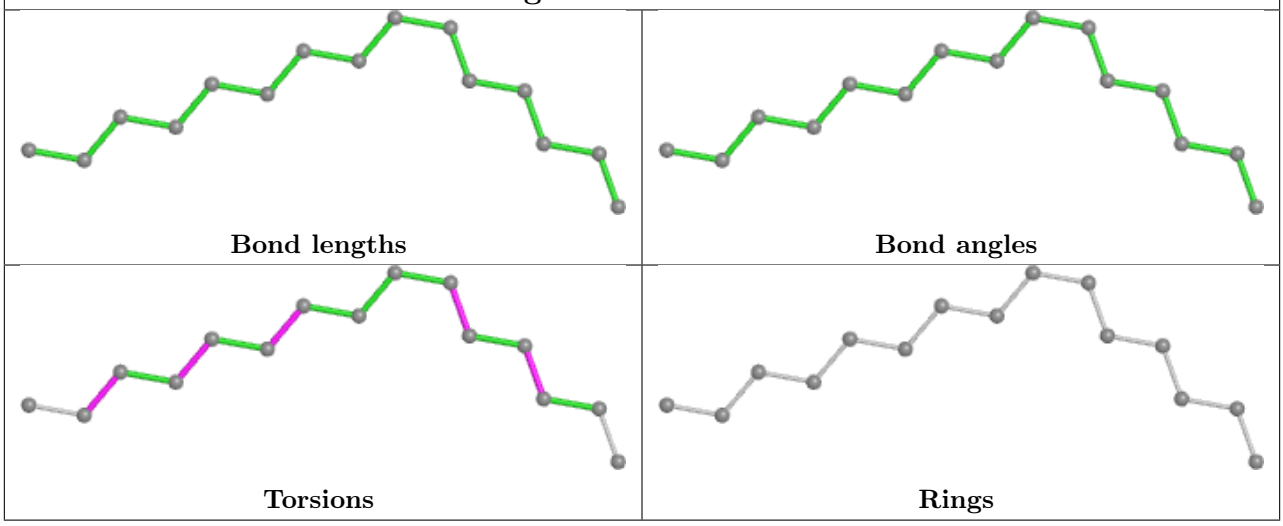


Torsions

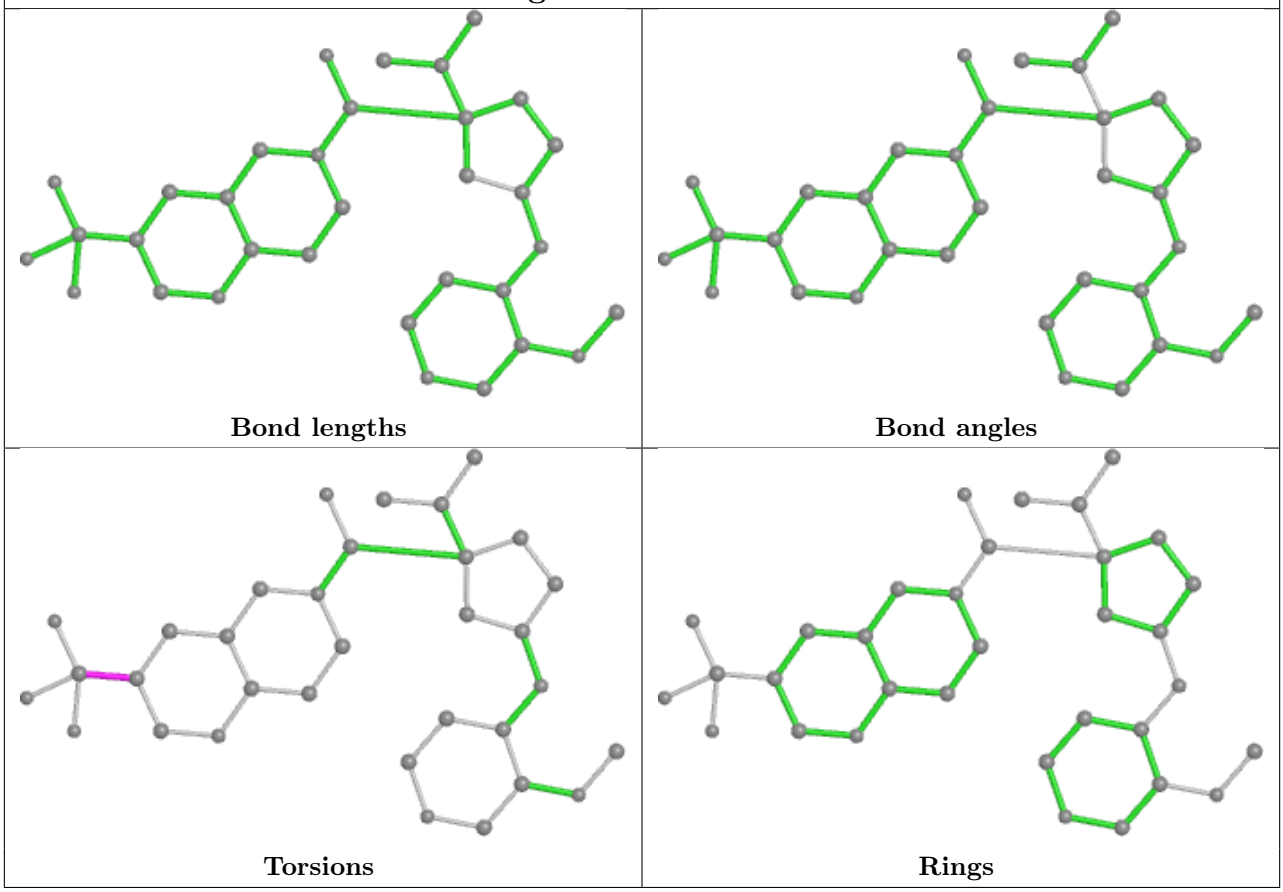


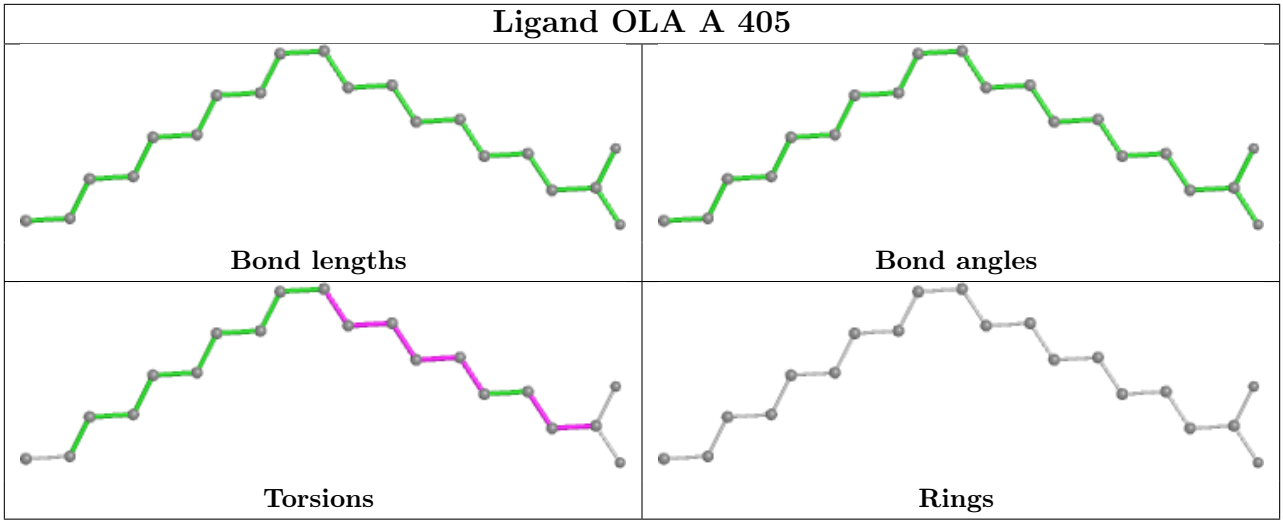
Rings

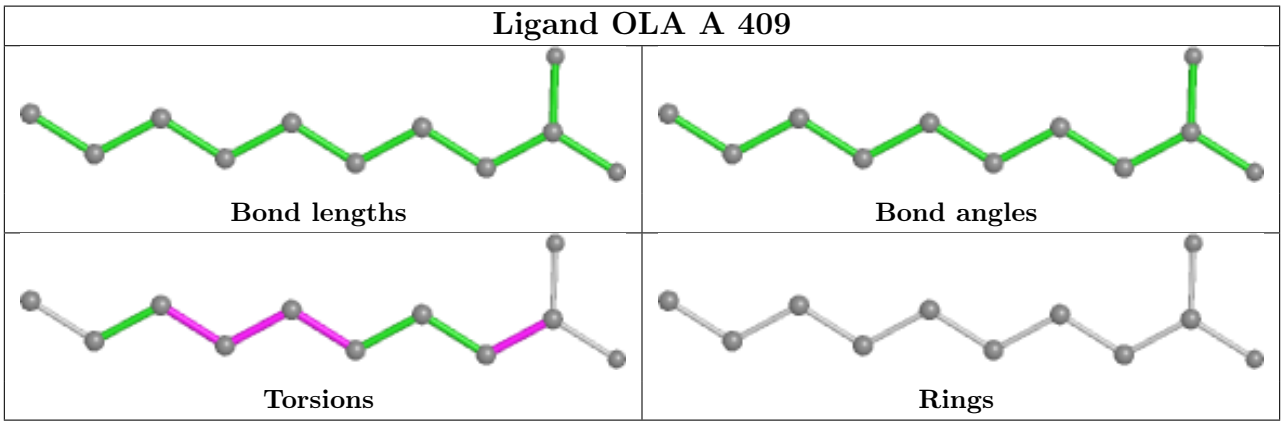
Ligand OLA A 410

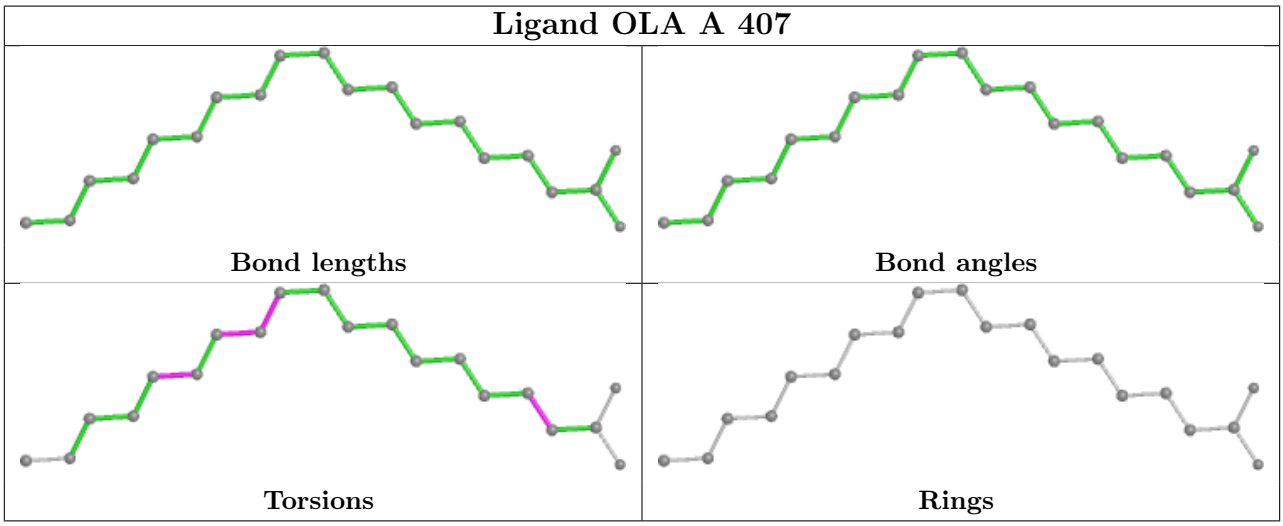


Ligand F7N B 404









5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/349 (92%)	0.41	24 (7%)	14	12	36, 58, 100, 152	0
1	B	263/349 (75%)	0.40	27 (10%)	6	5	36, 57, 102, 143	0
All	All	587/698 (84%)	0.41	51 (8%)	10	8	36, 58, 102, 152	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	PHE	9.6
1	A	36	ASP	5.2
1	A	329	GLU	5.0
1	B	36	ASP	4.7
1	A	196	ARG	4.7
1	B	281	SER	4.7
1	B	278	GLU	4.6
1	B	186	SER	4.6
1	B	227	LYS	4.5
1	A	252	ASP	4.1
1	A	328	CYS	4.0
1	B	187	VAL	3.8
1	B	228	THR	3.8
1	B	274	LEU	3.7
1	B	226	LEU	3.7
1	A	251	PRO	3.7
1	B	185	ASP	3.7
1	B	270	GLU	3.5
1	A	272	LEU	3.4
1	B	70	TYR	3.1
1	A	266	ASP	3.0
1	A	39	GLN	3.0
1	B	275	SER	2.8
1	A	37	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	155	THR	2.7
1	B	279	SER	2.7
1	A	247	GLU	2.7
1	A	326	SER	2.6
1	A	291	ARG	2.6
1	A	371	LEU	2.5
1	B	277	CYS	2.5
1	B	272	PHE	2.4
1	A	72	LYS	2.4
1	B	220	ILE	2.4
1	A	267	ASP	2.3
1	A	370	ALA	2.3
1	A	254	GLY	2.3
1	B	269	GLN	2.3
1	B	44	LEU	2.3
1	B	55	PHE	2.3
1	A	257	PRO	2.3
1	B	307	PHE	2.2
1	B	216	LEU	2.2
1	B	188	TYR	2.2
1	B	243	ARG	2.2
1	A	55	PHE	2.1
1	A	240	CYS	2.1
1	A	103	ALA	2.1
1	B	183	LYS	2.1
1	B	273	GLY	2.0
1	A	64	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

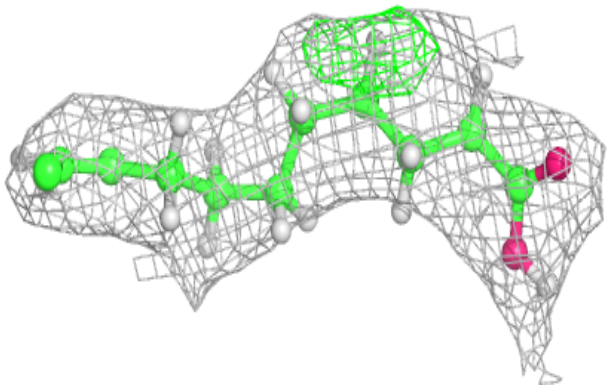
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

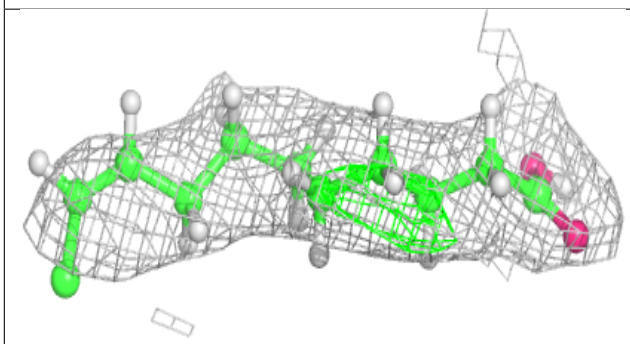
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	A	408	9/20	0.68	0.25	84,88,93,93	11
3	OLA	B	401	11/20	0.71	0.19	92,96,100,100	15
3	OLA	A	404	13/20	0.76	0.23	79,84,90,91	17
3	OLA	A	411	13/20	0.76	0.36	92,97,105,105	17
3	OLA	A	405	20/20	0.76	0.29	86,89,96,97	34
3	OLA	B	402	15/20	0.76	0.24	110,113,117,117	21
3	OLA	B	403	20/20	0.78	0.42	85,88,94,94	34
3	OLA	A	409	11/20	0.80	0.28	80,80,83,83	15
3	OLA	A	407	20/20	0.82	0.37	88,89,100,101	34
3	OLA	A	402	15/20	0.83	0.26	71,72,77,78	21
3	OLA	A	410	15/20	0.83	0.30	62,67,73,73	27
3	OLA	A	412	20/20	0.84	0.35	76,81,86,86	34
3	OLA	A	406	15/20	0.84	0.30	98,100,100,100	21
4	F7N	B	404	33/33	0.88	0.18	39,49,54,57	35
4	F7N	A	413	33/33	0.89	0.20	41,44,50,51	35
3	OLA	A	403	12/20	0.89	0.21	70,76,85,85	16
2	ZN	A	401	1/1	0.99	0.04	67,67,67,67	0

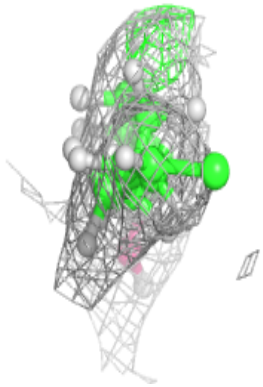
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 404:

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

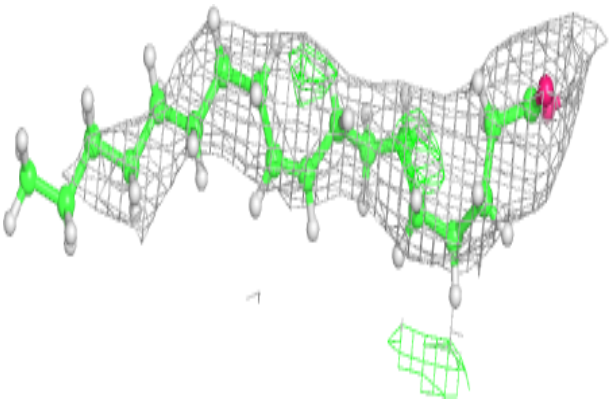


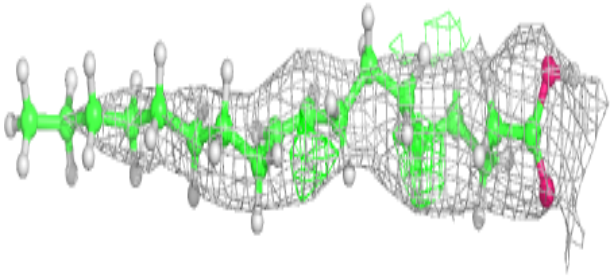


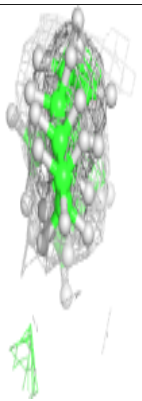


Electron density around OLA A 405:

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

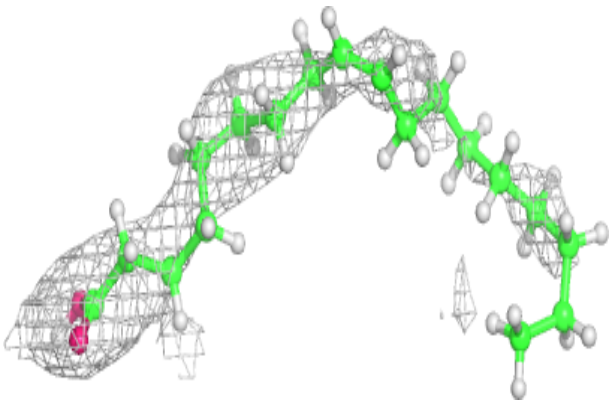


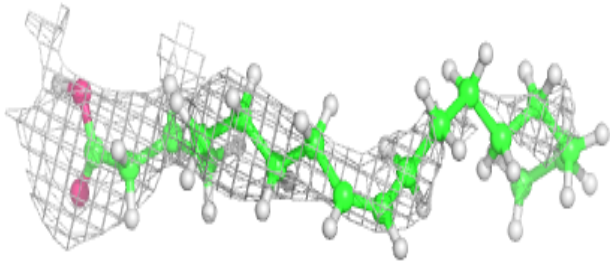


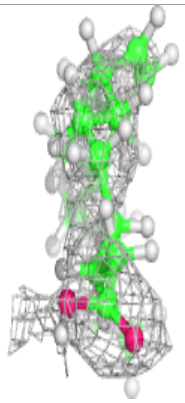


Electron density around OLA B 403:

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

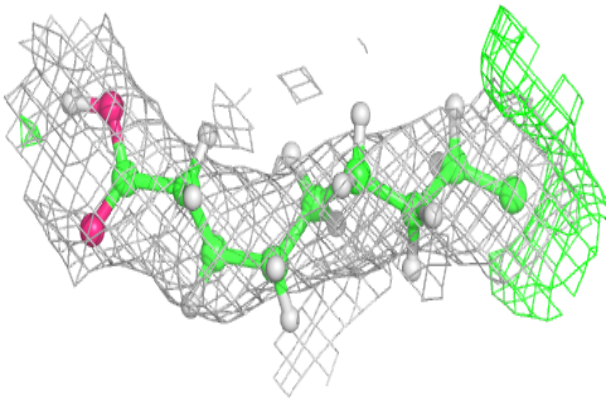


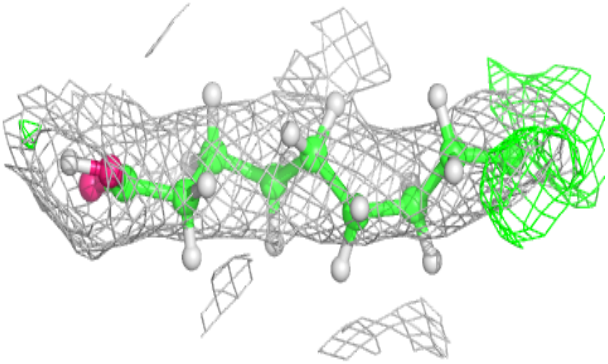


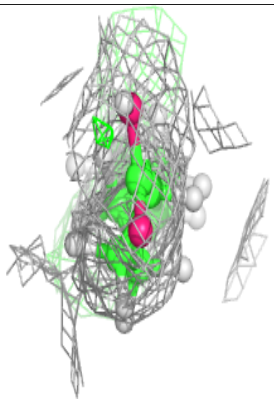


Electron density around OLA A 409:

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

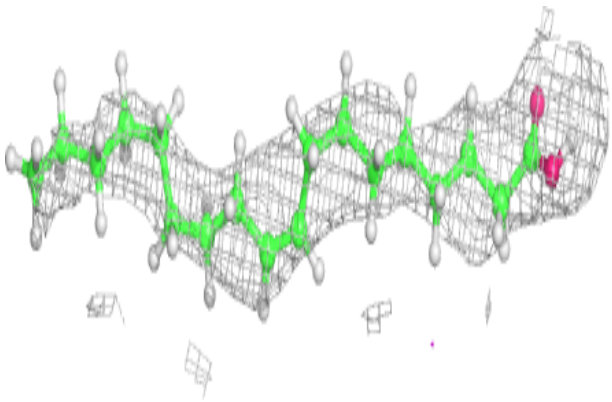


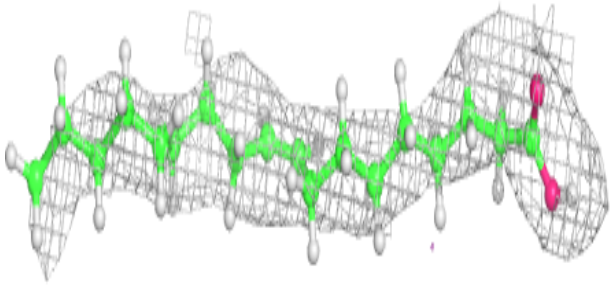


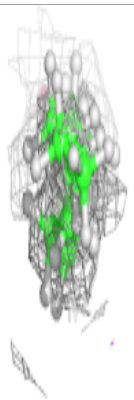


Electron density around OLA A 407:

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

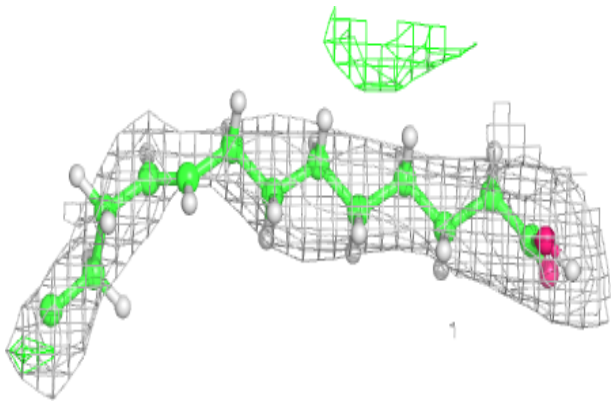


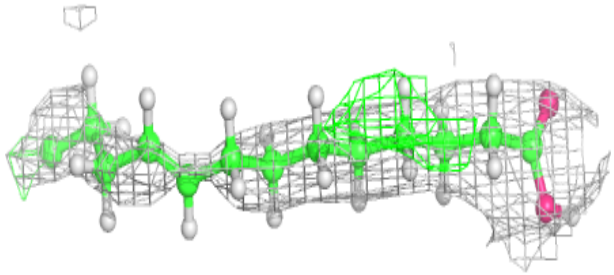


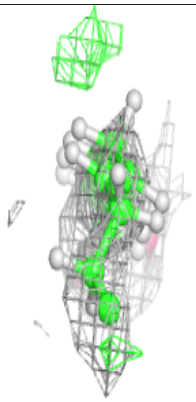


Electron density around OLA A 402:

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

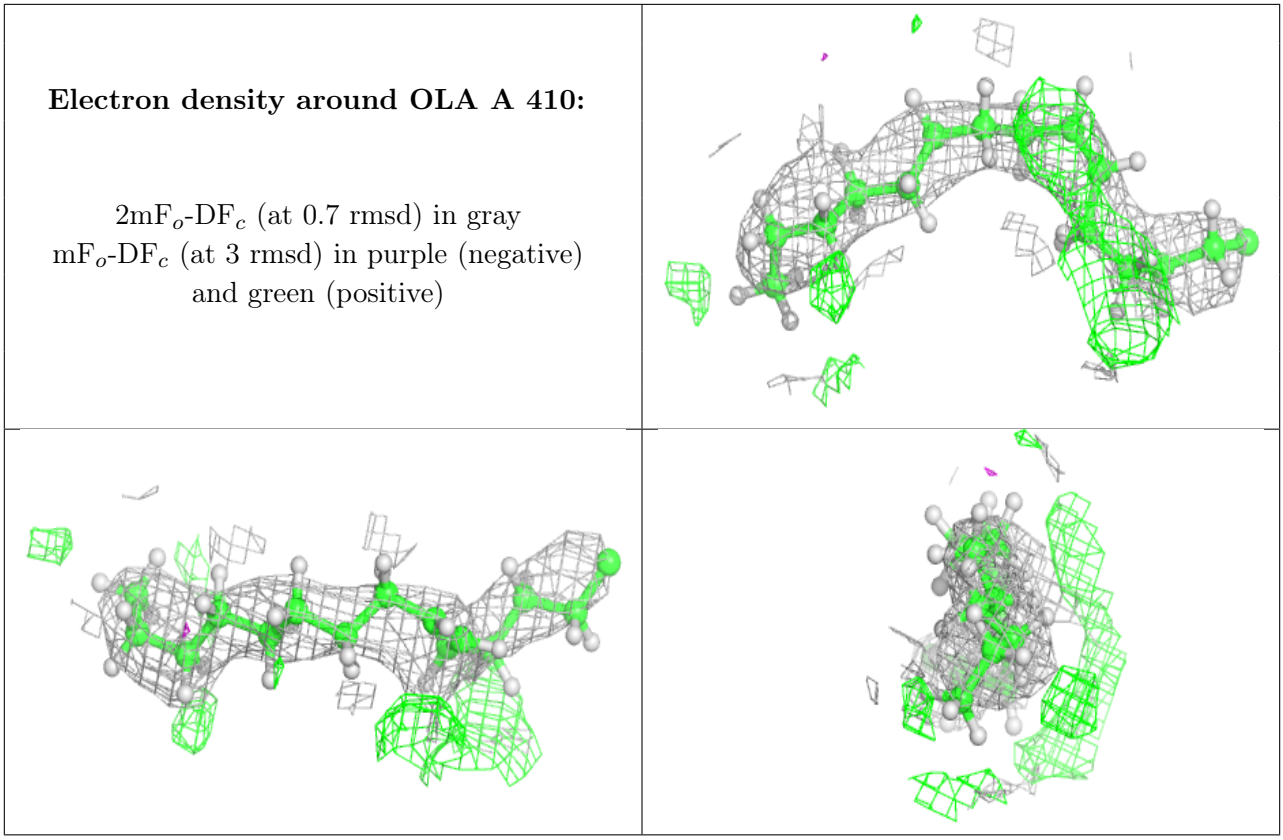






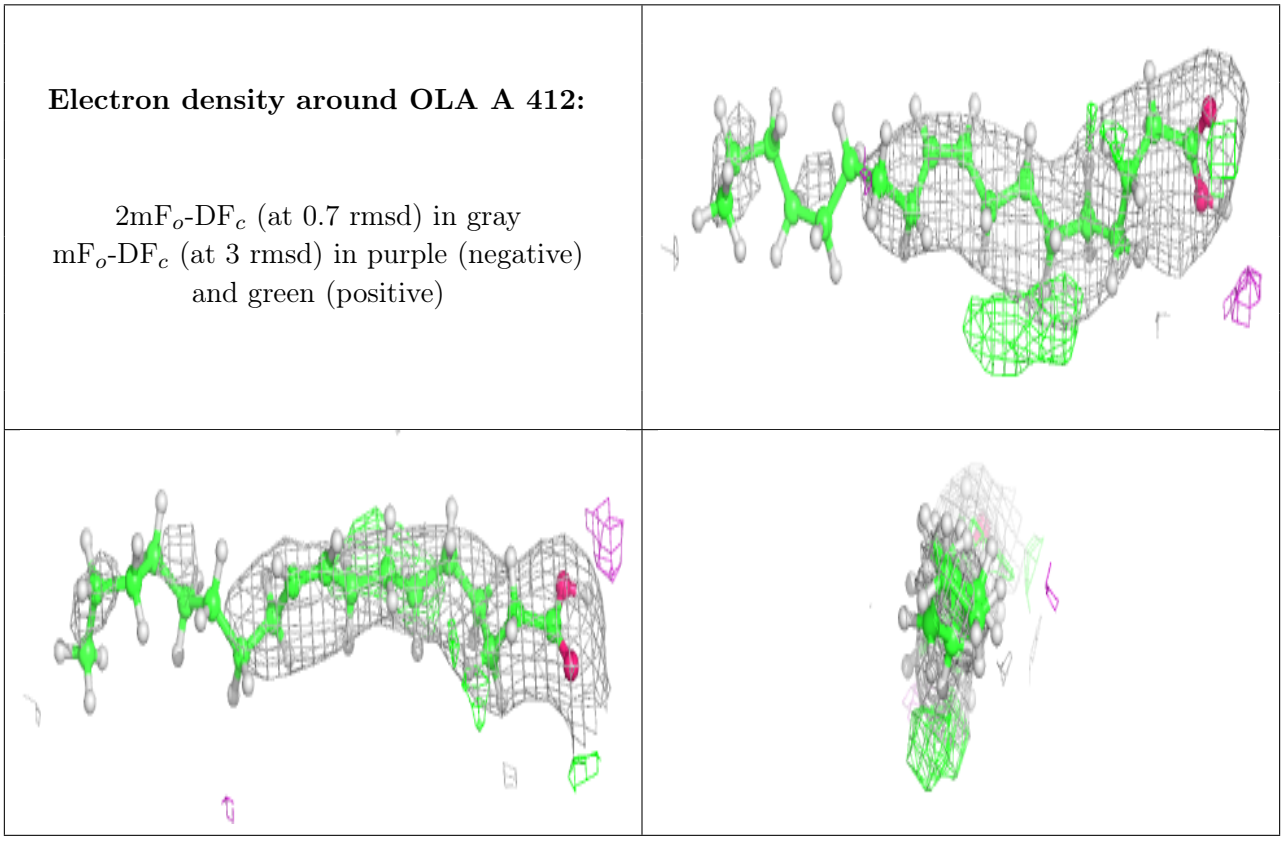
Electron density around OLA A 410:

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



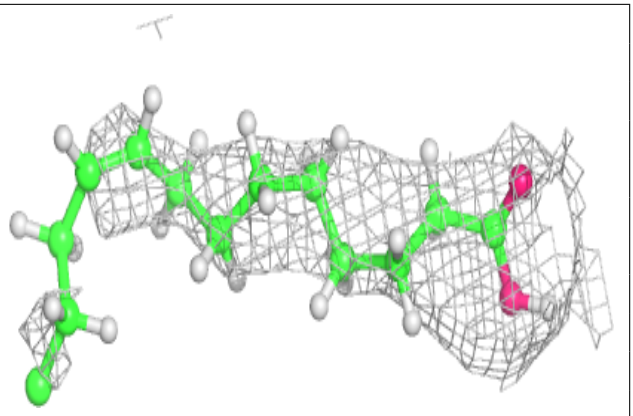
Electron density around OLA A 412:

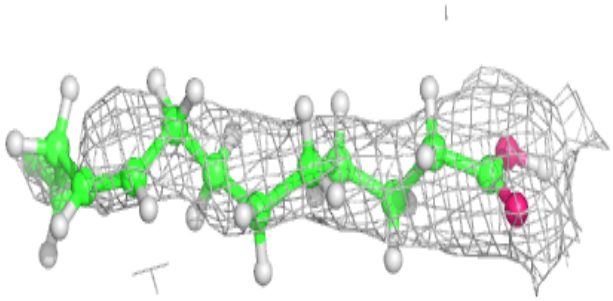
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

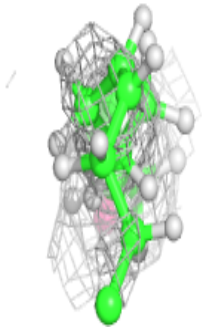


Electron density around OLA A 406:

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

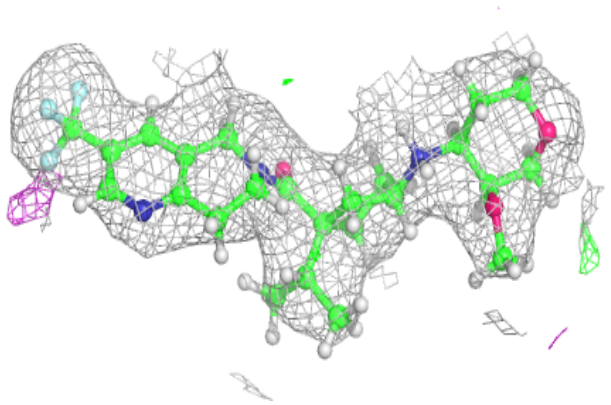


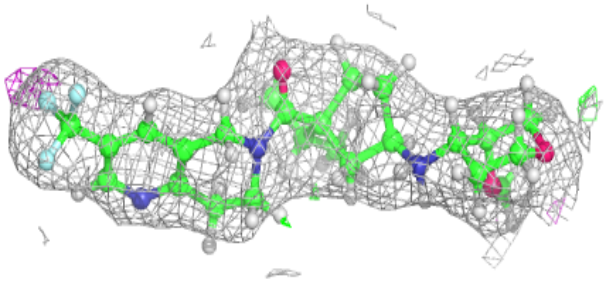


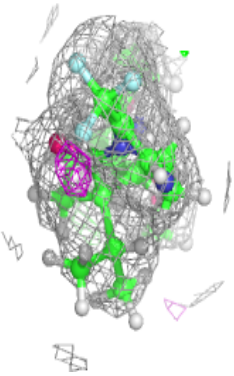


Electron density around F7N B 404:

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

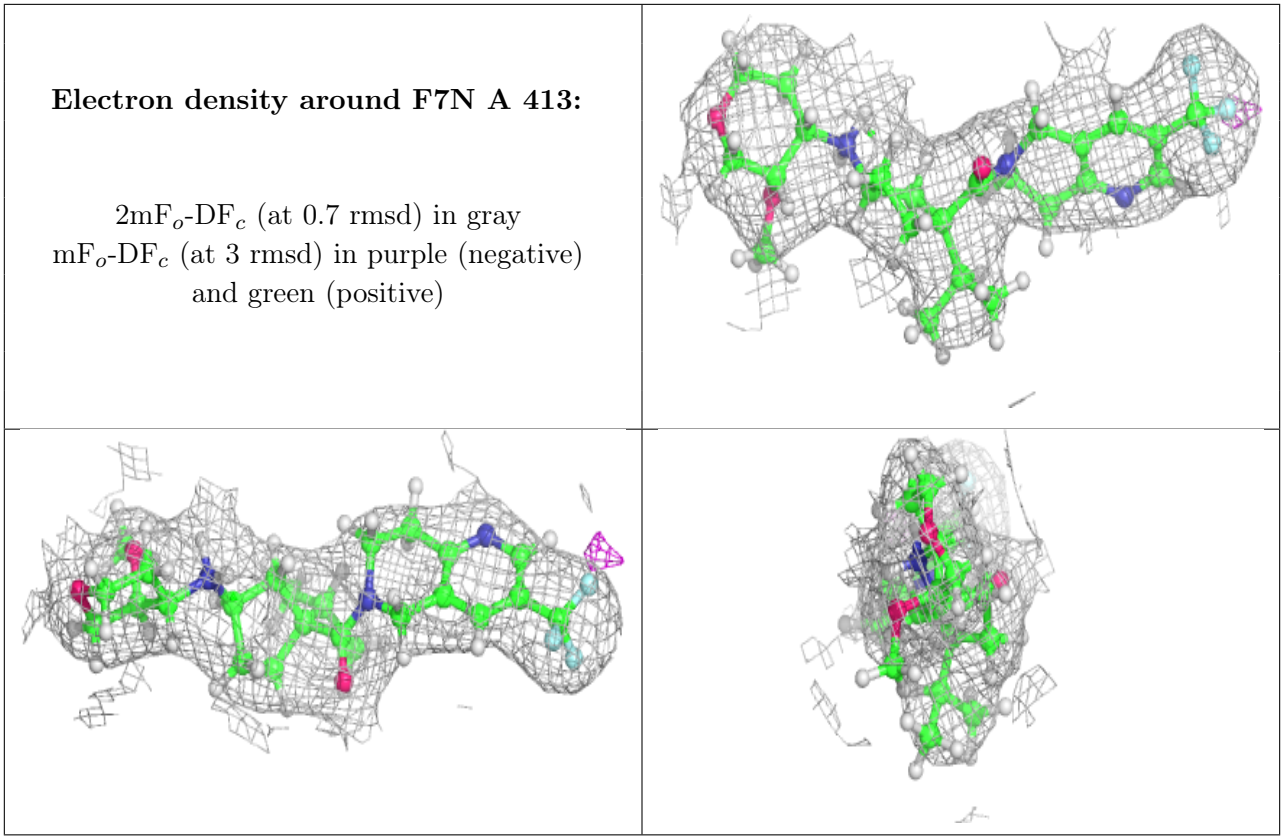






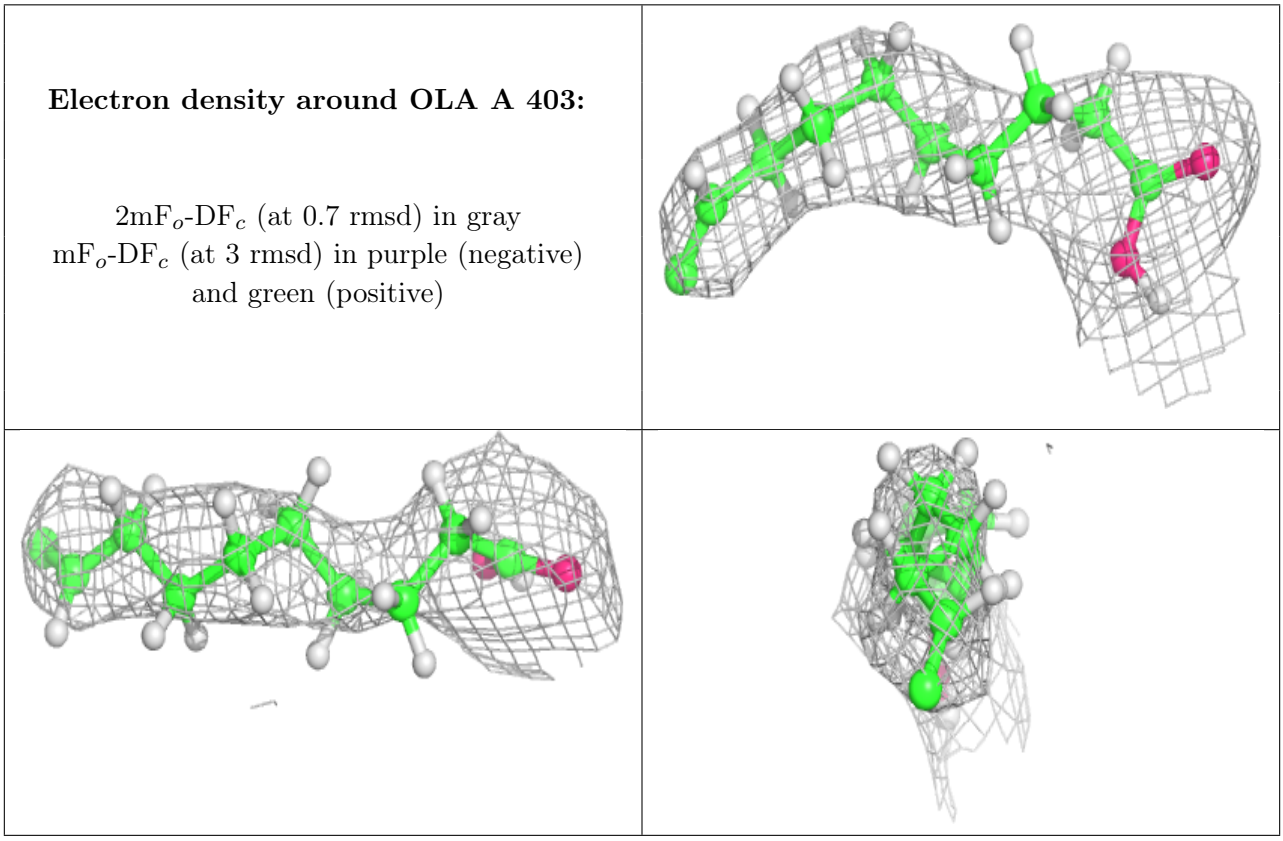
Electron density around F7N A 413:

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



Electron density around OLA A 403:

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



6.5 Other polymers (i)

There are no such residues in this entry.