

wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2023 - 10:47 am BST

PDB ID	:	8CIC
Title	:	Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in
		complex with clinical candidate Etrumadenant
Authors	:	Cheng, R.K.Y.; Markovic-Mueller, S.; Hennig, M.
Deposited on		
Resolution	:	2.10 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 (1)) were used in the production of this report:

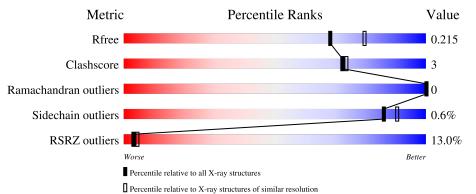
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.10 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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		
			12%		
1	А	433	83%	6%	11%

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	CLR	А	1203	-	_	-	X



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3689 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	
1	А	386	Total 3054	C 1991	N 515	O 525	S 23	0	25	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-8	ASP	_	expression tag	UNP P29274
А	-7	TYR	_	expression tag	UNP P29274
А	-6	LYS	-	expression tag	UNP P29274
А	-5	ASP	_	expression tag	UNP P29274
А	-4	ASP	-	expression tag	UNP P29274
А	-3	ASP	-	expression tag	UNP P29274
А	-2	ASP	-	expression tag	UNP P29274
А	-1	GLY	-	expression tag	UNP P29274
А	0	ALA	-	expression tag	UNP P29274
А	1	PRO	-	expression tag	UNP P29274
А	54	LEU	ALA	engineered mutation	UNP P29274
А	88	ALA	THR	engineered mutation	UNP P29274
А	107	ALA	ARG	engineered mutation	UNP P29274
А	122	ALA	LYS	engineered mutation	UNP P29274
А	154	ALA	ASN	engineered mutation	UNP P29274
А	202	ALA	LEU	engineered mutation	UNP P29274
А	1007	TRP	MET	engineered mutation	UNP P0ABE7
А	1102	ILE	HIS	engineered mutation	UNP P0ABE7
А	1106	LEU	ARG	engineered mutation	UNP P0ABE7
А	235	ALA	LEU	engineered mutation	UNP P29274
А	239	ALA	VAL	engineered mutation	UNP P29274
А	318	ALA	-	expression tag	UNP P29274
А	319	HIS	-	expression tag	UNP P29274
А	320	HIS	-	expression tag	UNP P29274
А	321	HIS	-	expression tag	UNP P29274
А	322	HIS	-	expression tag	UNP P29274
А	323	HIS	-	expression tag	UNP P29274

There are 32 discrepancies between the modelled and reference sequences:

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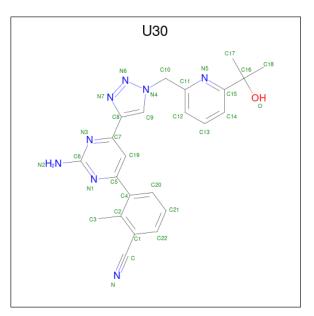
Chain	Residue	Modelled	Actual	Comment	Reference
А	324	HIS	-	expression tag	UNP P29274
А	325	HIS	-	expression tag	UNP P29274
А	326	HIS	-	expression tag	UNP P29274
А	327	HIS	-	expression tag	UNP P29274
А	328	HIS	-	expression tag	UNP P29274

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• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Na 1 1	0	0

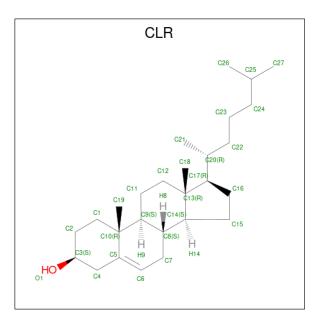
• Molecule 3 is 3-[2-azanyl-6-[1-[[6-(2-oxidanylpropan-2-yl)pyridin-2-yl]methyl]-1,2,3-tri azol-4-yl]pyrimidin-4-yl]-2-methyl-benzenecarbonitrile (three-letter code: U30) (formula: C₂₃H₂₂N₈O) (labeled as "Ligand of Interest" by depositor).



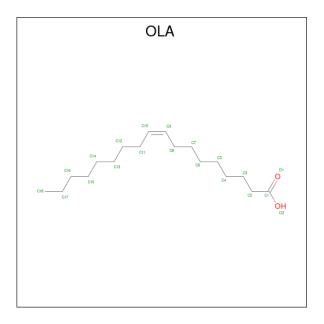
Mo	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Δ	1	Total	С	Ν	0	0	0
5	Π	L	32	23	8	1	0	0

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





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

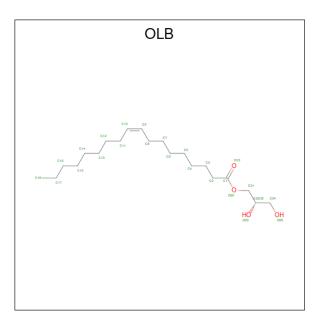




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C O 20 18 2	0	0
5	А	1	Total C O 15 13 2	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 7 & 2 \end{array}$	0	0
5	А	1	Total C O 19 17 2	0	0
5	А	1	Total C 10 10	0	0
5	А	1	Total C O 17 15 2	0	0
5	А	1	Total C 8 8	0	0
5	А	1	Total C 7 7	0	0
5	А	1	Total C O 16 14 2	0	0
5	А	1	Total C 11 11	0	0
5	А	1	Total C 12 12	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
5	А	1	Total C O 12 10 2	0	0
5	А	1	Total C O 20 18 2	0	0
5	А	1	Total C O 14 12 2	0	0

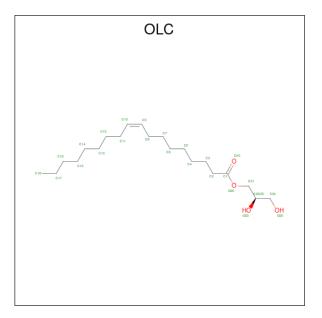
• Molecule 6 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: $C_{21}H_{40}O_4$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total C O 22 18 4	0	0
6	А	1	Total C O 19 15 4	0	0
6	А	1	Total C O 18 14 4	0	0

• Molecule 7 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
7	А	1	Total C O 25 21 4	0	0
7	А	1	Total C O 19 15 4	0	0
7	А	1	Total C O 21 17 4	0	0
7	А	1	Total C O 17 13 4	0	0
7	А	1	Total C O 25 21 4	0	0

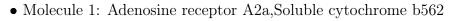
• Molecule 8 is water.

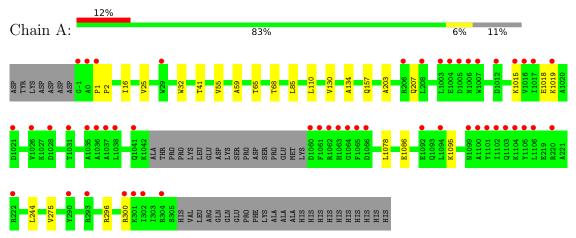
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	126	Total O 126 126	0	0



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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	39.36Å 179.09Å 140.57Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 - 2.10	Depositor
Resolution (A)	44.77 - 2.10	EDS
% Data completeness	99.9 (44.77-2.10)	Depositor
(in resolution range)	99.9 (44.77 - 2.10)	EDS
R _{merge}	0.17	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.00 (at 2.10 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14	Depositor
D D.	0.190 , 0.214	Depositor
R, R_{free}	0.191 , 0.215	DCC
R_{free} test set	1507 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 69.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3689	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: NA, OLB, OLC, CLR, OLA, U30

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/3120	0.39	0/4244	

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	А	3054	0	3105	20	0
2	А	1	0	0	0	0
3	А	32	0	0	2	0
4	А	112	0	184	2	0
5	А	198	0	284	8	0
6	А	59	0	79	2	0
7	А	107	0	151	3	0
8	А	126	0	0	1	0
All	All	3689	0	3803	25	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 3.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244[B]:LEU:HD11	5:A:1214:OLA:H41	1.69	0.75
5:A:1220:OLA:H10	5:A:1221:OLA:C12	2.26	0.66
5:A:1217:OLA:H62	7:A:1226:OLC:H6A	1.78	0.64
1:A:157[A]:GLN:NE2	8:A:1303:HOH:O	2.37	0.56
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.90	0.54

clash magnitude.

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	А	390/433~(90%)	388~(100%)	2~(0%)	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	А	319/354~(90%)	317~(99%)	2(1%)	86 90		

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



Mol	Chain	Res	Type
1	А	41	THR
1	А	110	LEU

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 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	Bo	ond leng	ths	Bond angles				
WIOI	Type	Ullalli	nes	nes	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLA	А	1215	-	$15,\!15,\!19$	0.53	0	$15,\!15,\!19$	0.98	2 (13%)		
5	OLA	А	1217	-	11,11,19	0.50	0	10,10,19	0.40	0		
4	CLR	А	1204	-	31,31,31	0.65	0	48,48,48	1.09	3 (6%)		
5	OLA	А	1212	-	16,16,19	0.53	0	16,16,19	0.92	2 (12%)		
5	OLA	А	1220	-	19,19,19	0.66	0	19,19,19	0.76	1 (5%)		
5	OLA	А	1209	-	8,8,19	0.86	0	8,8,19	1.14	1 (12%)		
5	OLA	А	1218	-	7,7,19	0.63	0	7,7,19	1.35	2 (28%)		
5	OLA	А	1207	-	19,19,19	0.67	0	19,19,19	0.77	1 (5%)		



Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	E	ond ang	gles
IVIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	OLA	А	1211	-	$9,\!9,\!19$	0.59	0	8,8,19	0.25	0
7	OLC	А	1227	-	20,20,24	1.47	4 (20%)	21,21,25	1.21	2 (9%)
6	OLB	А	1224	-	17,17,24	1.20	1 (5%)	18,18,25	0.91	1 (5%)
5	OLA	А	1216	-	$10,\!10,\!19$	0.39	0	9,9,19	0.25	0
5	OLA	А	1221	-	$13,\!13,\!19$	0.57	0	12,13,19	1.06	2 (16%)
6	OLB	А	1222	-	21,21,24	1.20	1 (4%)	22,22,25	0.94	1 (4%)
5	OLA	А	1210	-	18,18,19	0.67	0	18,18,19	0.78	1 (5%)
5	OLA	А	1219	-	11,11,19	0.62	0	11,11,19	1.14	2 (18%)
7	OLC	А	1229	-	24,24,24	1.42	4 (16%)	25,25,25	1.11	2 (8%)
4	CLR	А	1205	-	31,31,31	0.71	0	48,48,48	0.94	1 (2%)
7	OLC	А	1225	-	24,24,24	1.37	4 (16%)	25,25,25	1.11	2 (8%)
5	OLA	А	1214	-	6,6,19	0.26	0	$5,\!5,\!19$	0.16	0
7	OLC	А	1226	-	18,18,24	1.55	4 (22%)	18,19,25	1.30	2 (11%)
5	OLA	А	1208	-	14,14,19	0.71	0	14,14,19	0.89	1 (7%)
3	U30	А	1202	-	33,35,35	1.99	8 (24%)	40,51,51	2.12	11 (27%)
5	OLA	А	1213	-	7,7,19	0.61	0	6,6,19	0.28	0
4	CLR	А	1203	-	31,31,31	0.66	0	48,48,48	1.29	<u>6 (12%)</u>
4	CLR	А	1206	-	31,31,31	0.72	0	48,48,48	0.87	1 (2%)
7	OLC	А	1228	-	16,16,24	1.64	4 (25%)	17,17,25	1.34	2 (11%)
6	OLB	А	1223	-	18,18,24	1.23	1 (5%)	18,19,25	0.97	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
5	OLA	А	1215	-	-	5/13/13/17	-
5	OLA	А	1217	-	-	7/9/9/17	-
4	CLR	А	1204	-	-	0/10/68/68	0/4/4/4
5	OLA	А	1212	-	-	9/14/14/17	-
5	OLA	А	1220	-	-	6/17/17/17	-
5	OLA	А	1209	-	-	1/6/6/17	-
5	OLA	А	1218	-	-	1/5/5/17	-
5	OLA	А	1207	-	-	8/17/17/17	-
5	OLA	А	1211	-	-	5/7/7/17	_
7	OLC	А	1227	_	_	9/20/20/24	_

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLB	А	1224	-	-	7/17/17/24	-
5	OLA	А	1216	-	-	2/8/8/17	-
5	OLA	А	1221	-	-	5/11/11/17	-
6	OLB	А	1222	-	-	10/21/21/24	-
5	OLA	А	1210	-	-	5/16/16/17	-
5	OLA	А	1219	-	-	6/9/9/17	-
7	OLC	А	1229	-	-	12/24/24/24	-
4	CLR	А	1205	-	-	1/10/68/68	0/4/4/4
7	OLC	А	1225	-	-	14/24/24/24	-
5	OLA	А	1214	-	-	3/4/4/17	-
7	OLC	А	1226	-	-	10/18/18/24	-
5	OLA	А	1208	-	-	6/12/12/17	-
3	U30	А	1202	-	-	4/18/20/20	0/4/4/4
5	OLA	А	1213	-	-	1/5/5/17	-
4	CLR	А	1203	-	-	8/10/68/68	0/4/4/4
4	CLR	А	1206	-	-	2/10/68/68	0/4/4/4
7	OLC	А	1228	-	-	8/16/16/24	-
6	OLB	А	1223	-	-	10/18/18/24	-

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The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	1202	U30	C9-N4	6.74	1.42	1.35
3	А	1202	U30	N7-N6	-3.70	1.27	1.34
7	А	1229	OLC	O20-C1	3.68	1.44	1.33
7	А	1228	OLC	O20-C1	3.67	1.44	1.33
7	А	1226	OLC	O20-C1	3.65	1.44	1.33

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	1202	U30	C10-N4-C9	-5.19	122.58	129.19
3	А	1202	U30	C10-C11-N5	4.88	124.18	116.05
3	А	1202	U30	C10-C11-C12	-4.67	112.24	120.93
3	А	1202	U30	C2-C1-C	-4.22	116.31	120.01
7	А	1228	OLC	O20-C1-O19	-4.02	113.44	123.59

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	А	1202	U30	N3-C7-C8-C9
3	А	1202	U30	C19-C7-C8-C9
5	А	1216	OLA	C10-C11-C12-C13
6	А	1222	OLB	O20-C21-C22-O23
6	А	1222	OLB	O20-C21-C22-C24

5 of 165 torsion outliers are listed below:

There are no ring outliers.

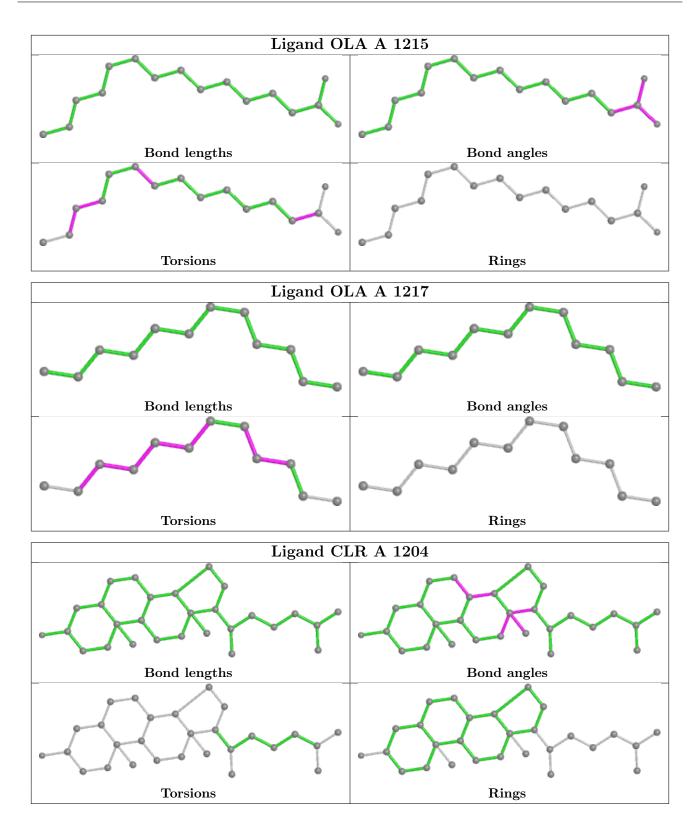
14 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	1217	OLA	1	0
5	А	1212	OLA	1	0
5	А	1220	OLA	1	0
6	А	1224	OLB	1	0
5	А	1221	OLA	2	0
6	А	1222	OLB	1	0
5	А	1210	OLA	2	0
7	А	1229	OLC	1	0
7	А	1225	OLC	1	0
5	А	1214	OLA	2	0
7	А	1226	OLC	1	0
3	А	1202	U30	2	0
4	А	1203	CLR	1	0
4	А	1206	CLR	1	0

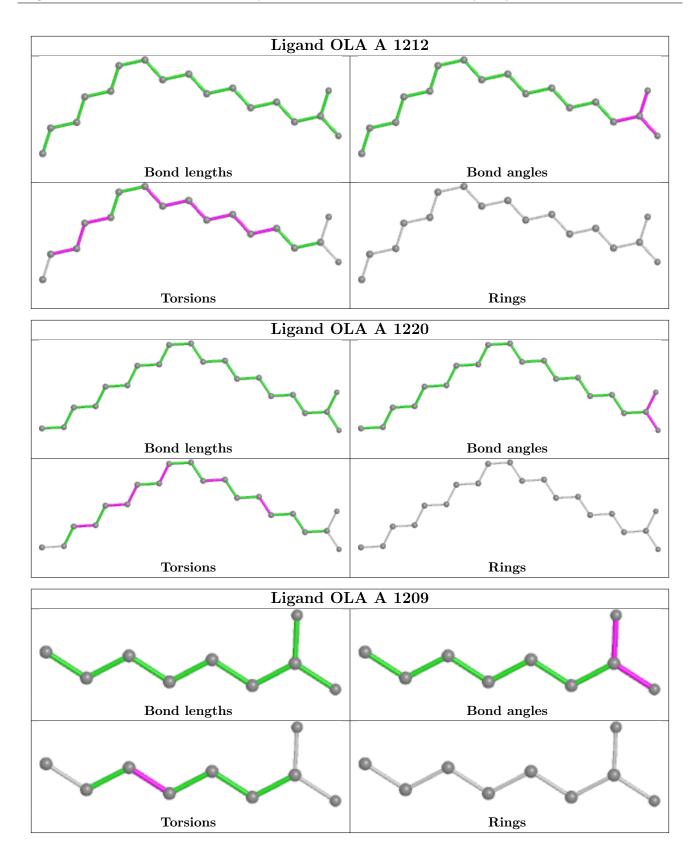
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





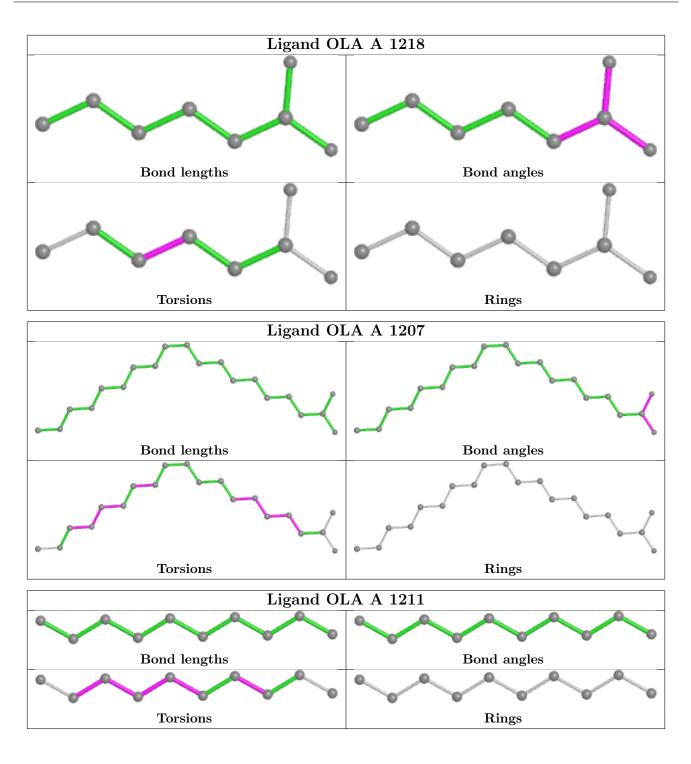






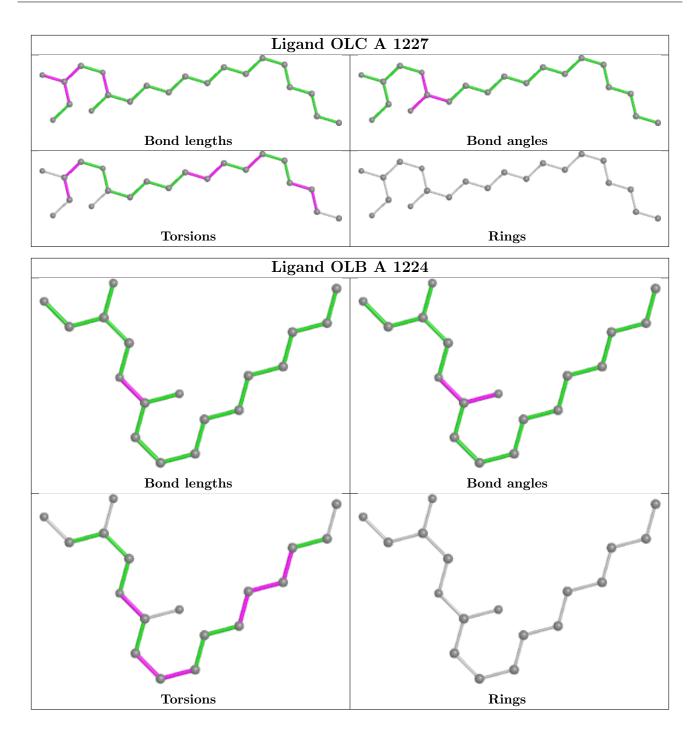




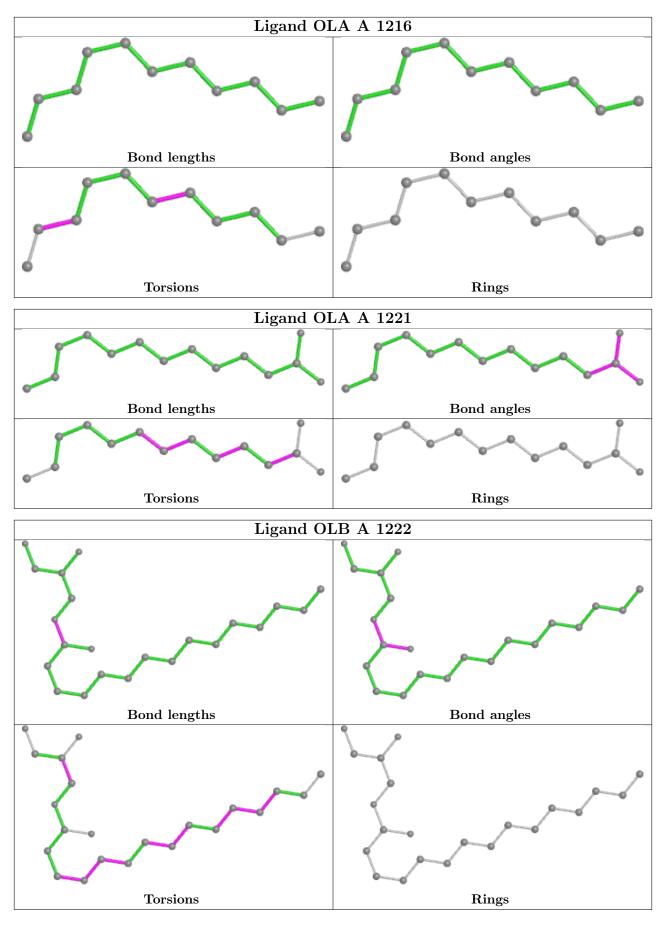




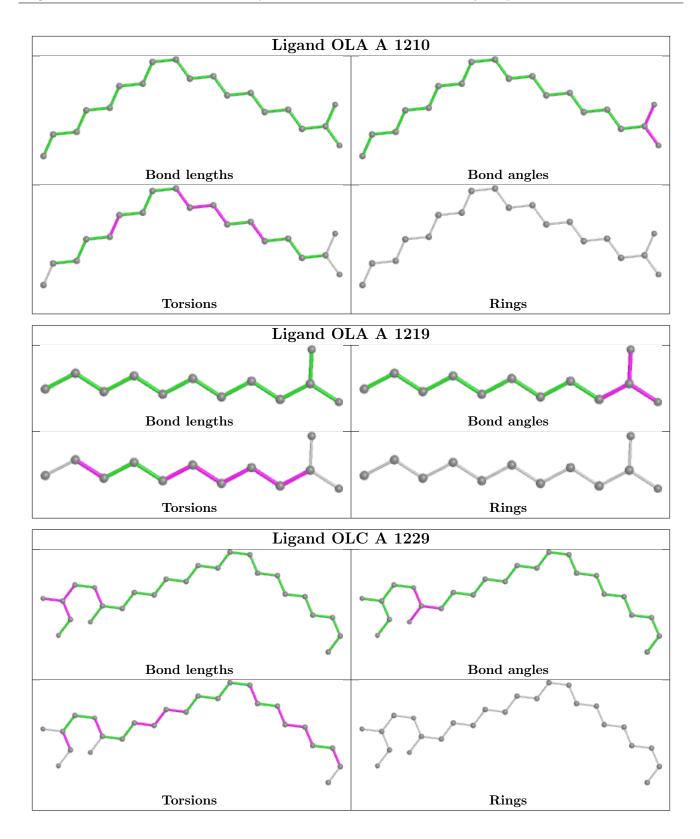






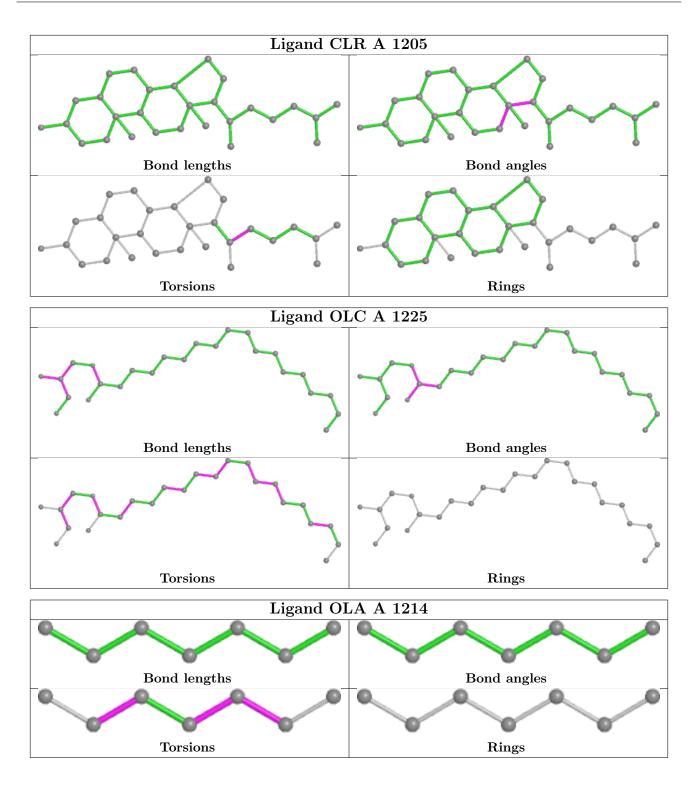




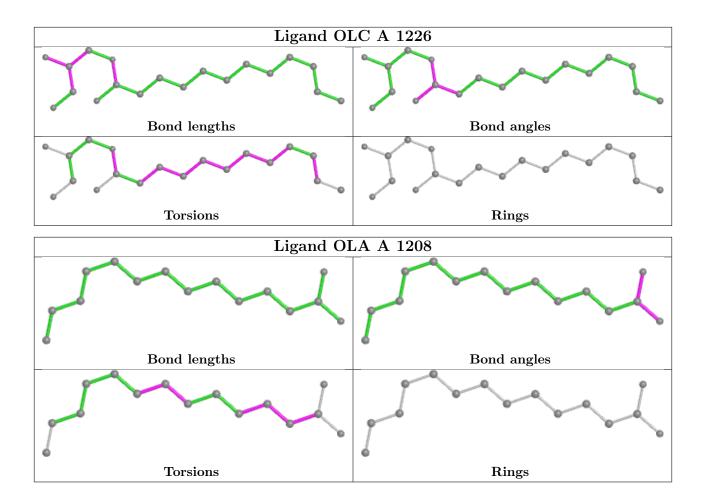






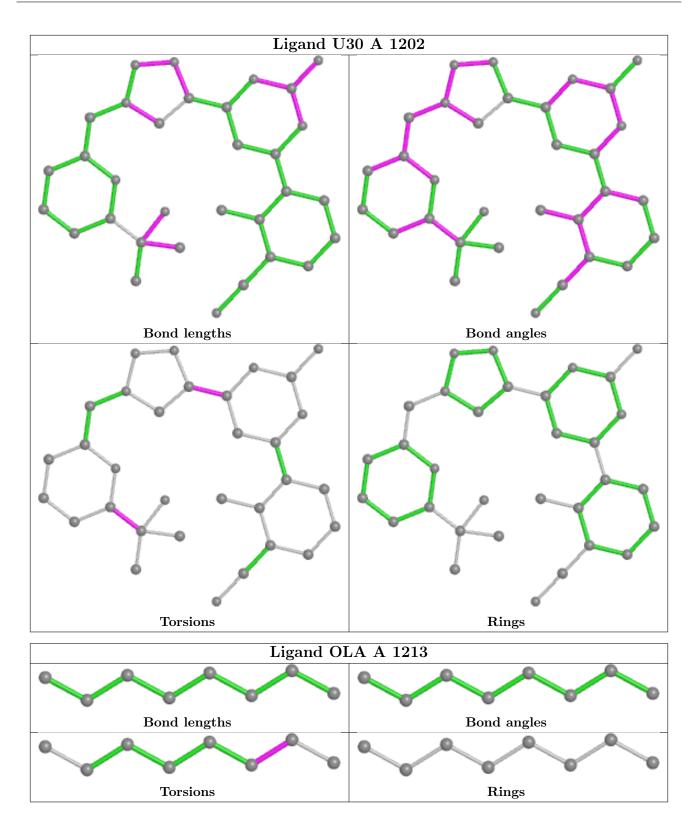






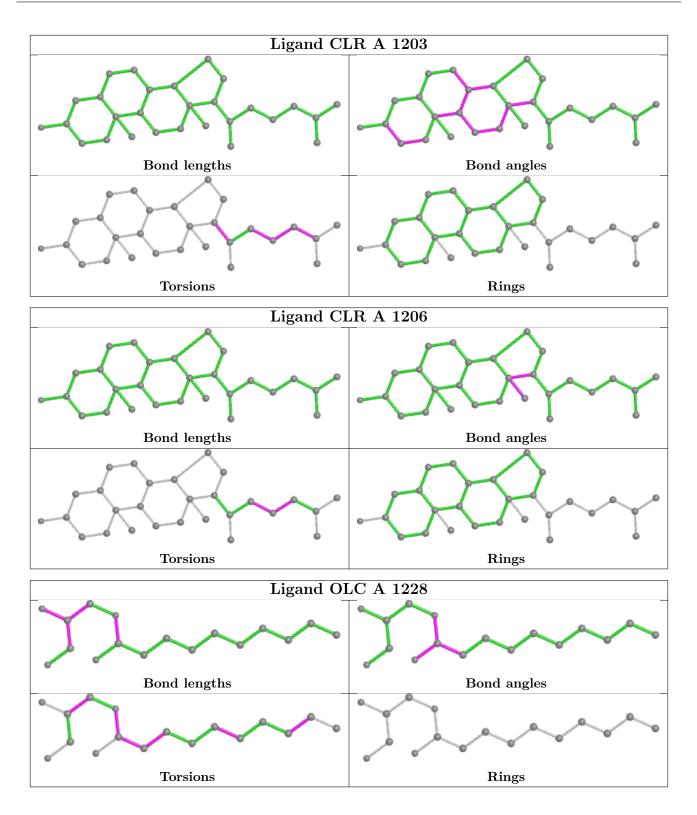






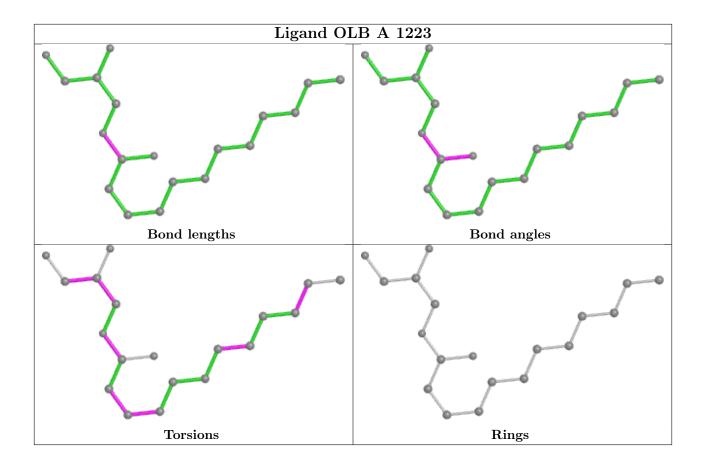












5.7 Other polymers (i)

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, 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	А	386/433~(89%)	0.63	50 (12%) 3 4	24, 42, 90, 128	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1061	PHE	8.3
1	А	1062	ARG	5.0
1	А	1101	TYR	5.0
1	А	1063	HIS	4.9
1	А	1105	TYR	4.9

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, 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	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
5	OLA	А	1218	8/20	0.42	0.28	$62,\!72,\!76,\!77$	0
4	CLR	А	1203	28/28	0.59	0.47	$102,\!118,\!125,\!125$	0

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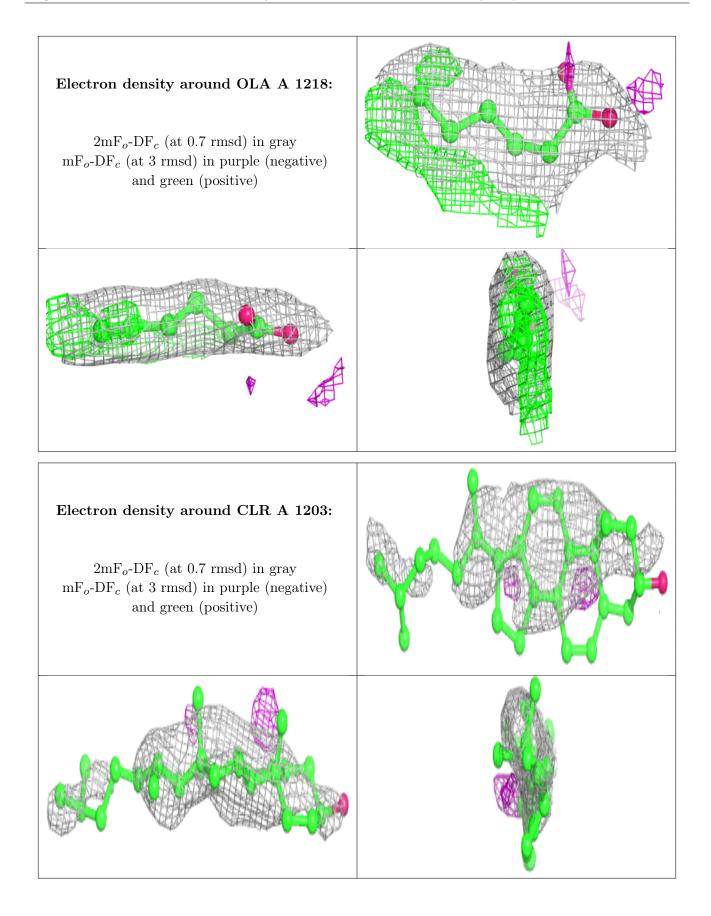
QCI	$\mathbf{\Omega}$
001	U

Mol	Type	m previoi Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OLA	A	1220	$\frac{20}{20}$	0.59	0.32	60,75,86,86	$\frac{Q < 0.3}{0}$
$\frac{5}{7}$	OLA	A		$\frac{20/20}{25/25}$				0
	OLC		1229	/	0.59	0.24	62,82,94,96	
5		A	1212	17/20	0.63	0.25	62,71,87,88	0
7	OLC	A	1226	19/25	0.67	0.26	47,53,85,88	0
5	OLA	A	1221	14/20	0.68	0.27	69,79,83,83	0
5	OLA	A	1210	19/20	0.68	0.23	67,72,75,76	0
5	OLA	A	1208	15/20	0.68	0.26	62,69,86,87	0
7	OLC	А	1228	17/25	0.70	0.30	70,74,87,87	0
5	OLA	A	1217	12/20	0.70	0.29	$57,\!63,\!65,\!66$	0
6	OLB	А	1224	18/25	0.72	0.26	$58,\!64,\!90,\!90$	0
5	OLA	А	1216	11/20	0.73	0.19	$64,\!67,\!72,\!72$	0
6	OLB	А	1223	19/25	0.74	0.31	$38,\!59,\!79,\!80$	0
7	OLC	А	1227	21/25	0.77	0.24	61,65,83,84	0
5	OLA	А	1215	16/20	0.78	0.28	54,65,96,96	0
5	OLA	А	1219	12/20	0.78	0.34	56,68,82,83	0
6	OLB	А	1222	22/25	0.78	0.32	56,68,83,89	0
5	OLA	А	1211	10/20	0.79	0.27	50,53,62,63	0
5	OLA	А	1214	7/20	0.80	0.25	64,65,66,66	0
7	OLC	А	1225	25/25	0.80	0.25	47,61,81,82	0
5	OLA	А	1207	20/20	0.81	0.22	49,68,85,86	0
5	OLA	А	1209	9/20	0.86	0.24	49,53,72,74	0
5	OLA	А	1213	8/20	0.89	0.20	47,52,55,56	0
2	NA	А	1201	1/1	0.92	0.13	51,51,51,51	0
4	CLR	А	1206	28/28	0.94	0.13	27,34,62,62	0
4	CLR	А	1204	28/28	0.94	0.14	34,37,64,70	0
4	CLR	А	1205	28/28	0.95	0.12	37,43,55,62	0
3	U30	А	1202	32/32	0.96	0.14	24,31,41,47	0

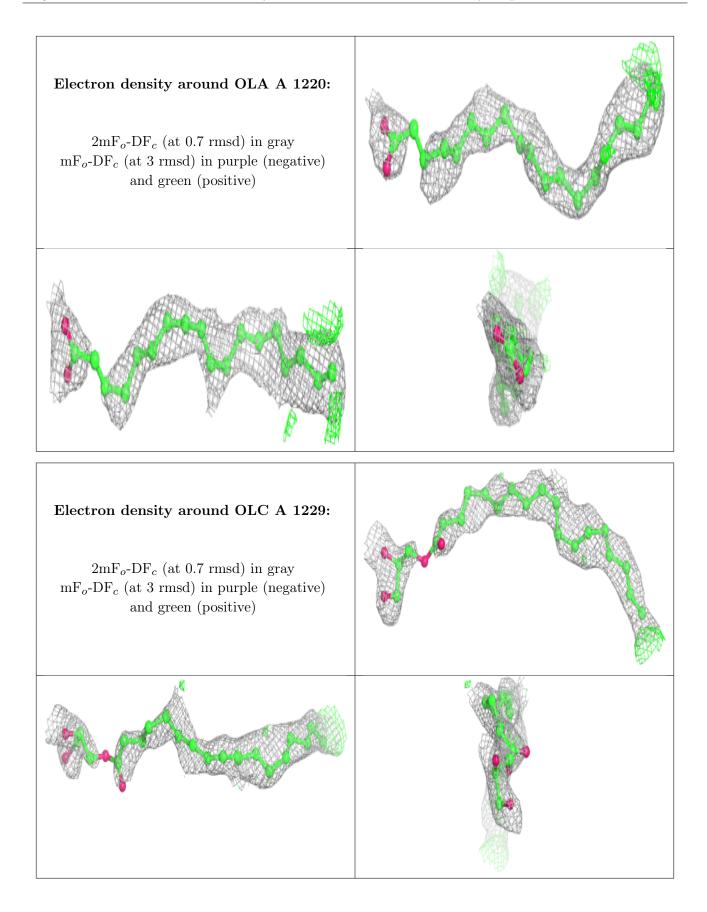
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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also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

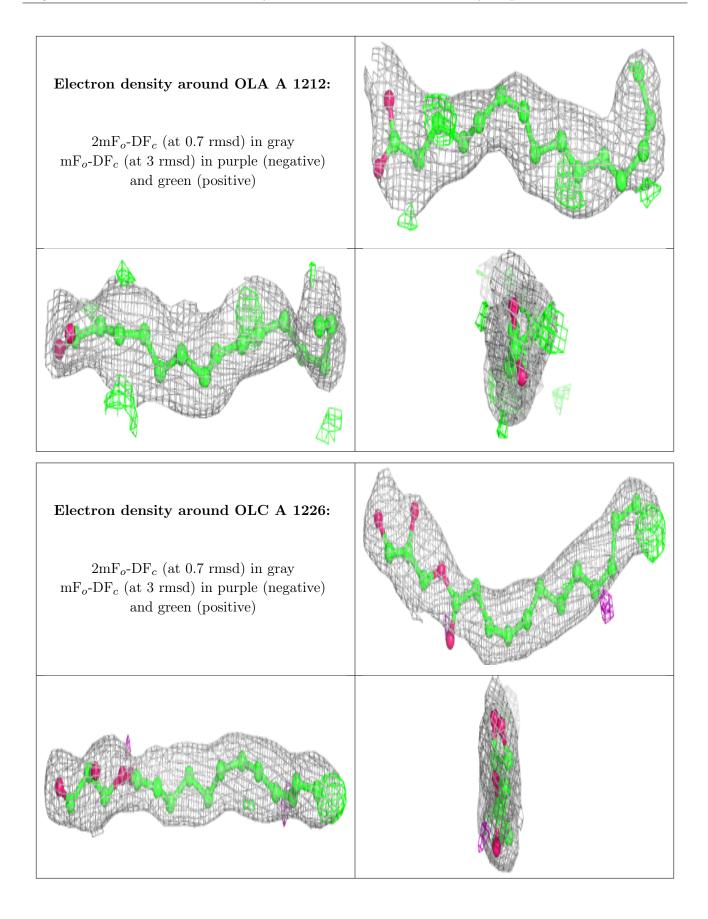




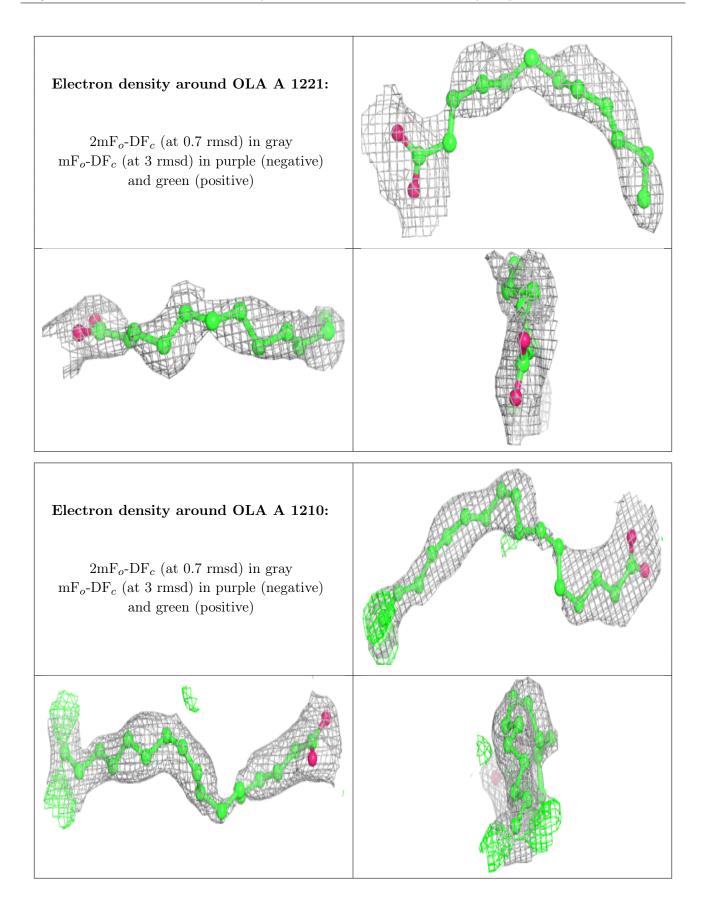




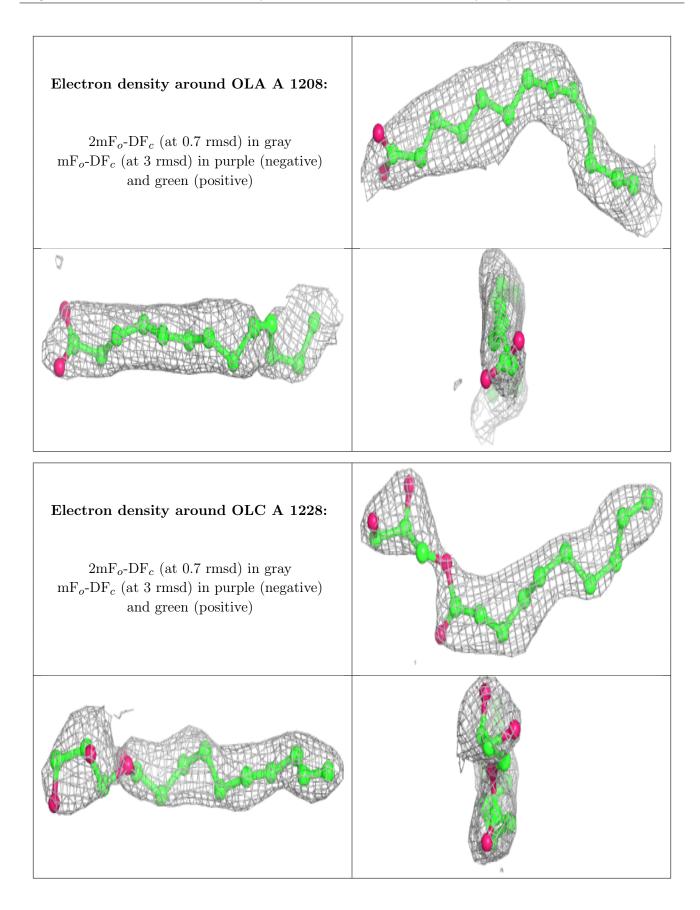




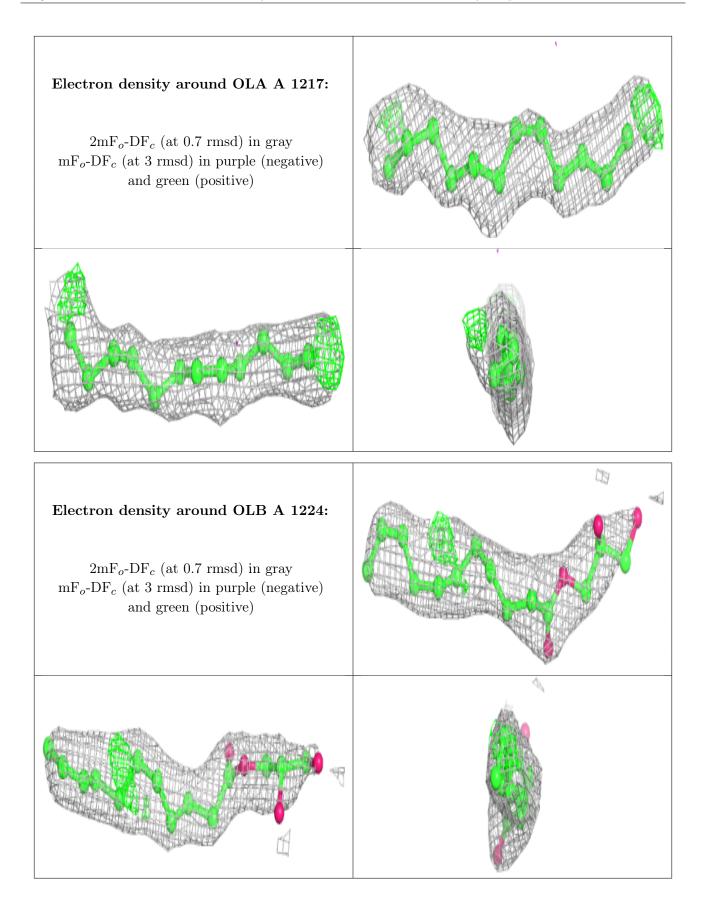




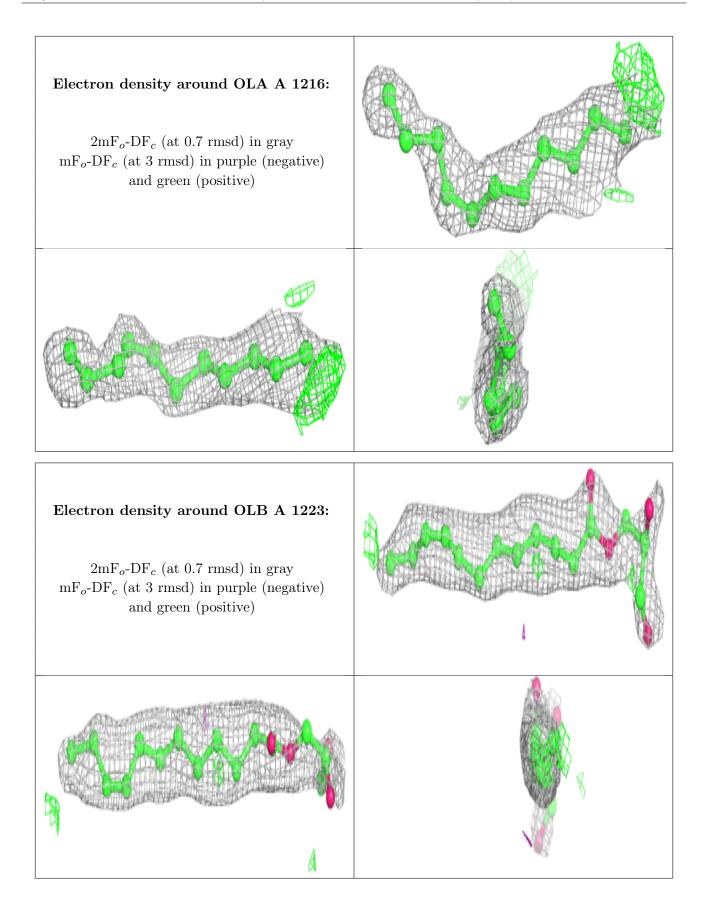




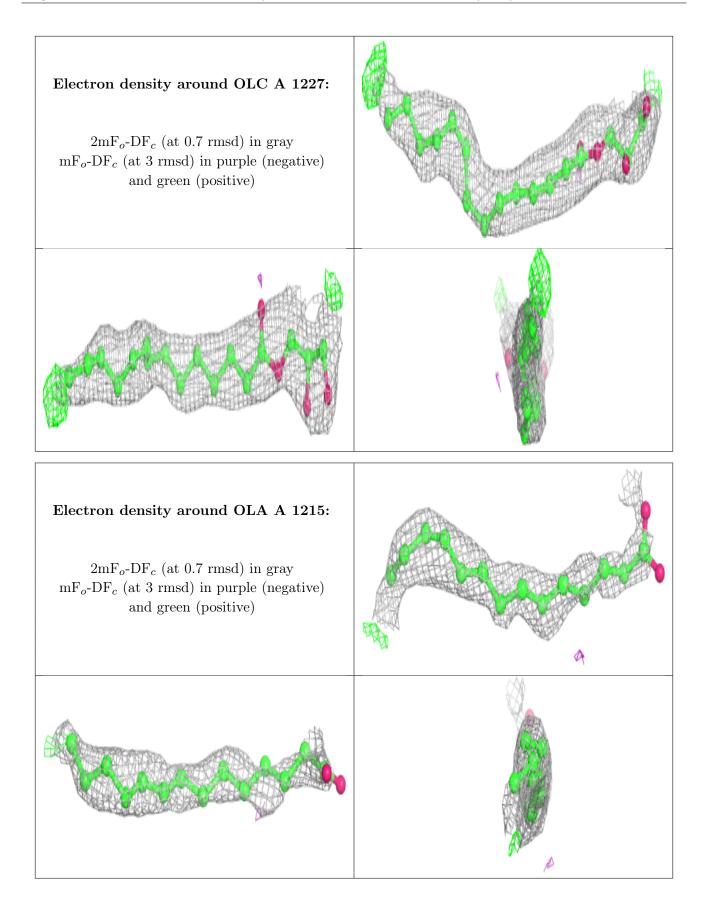




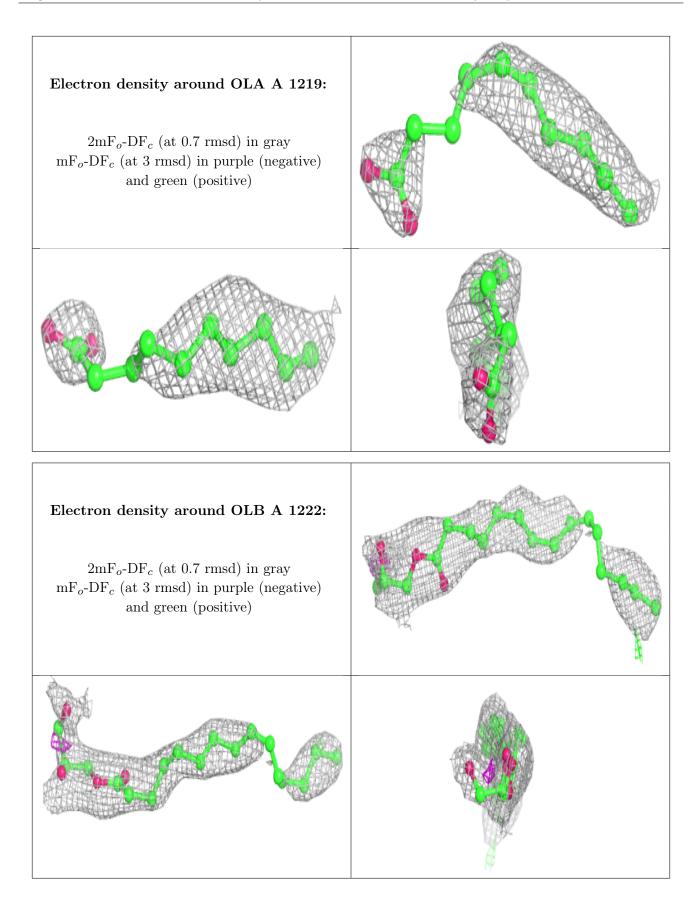




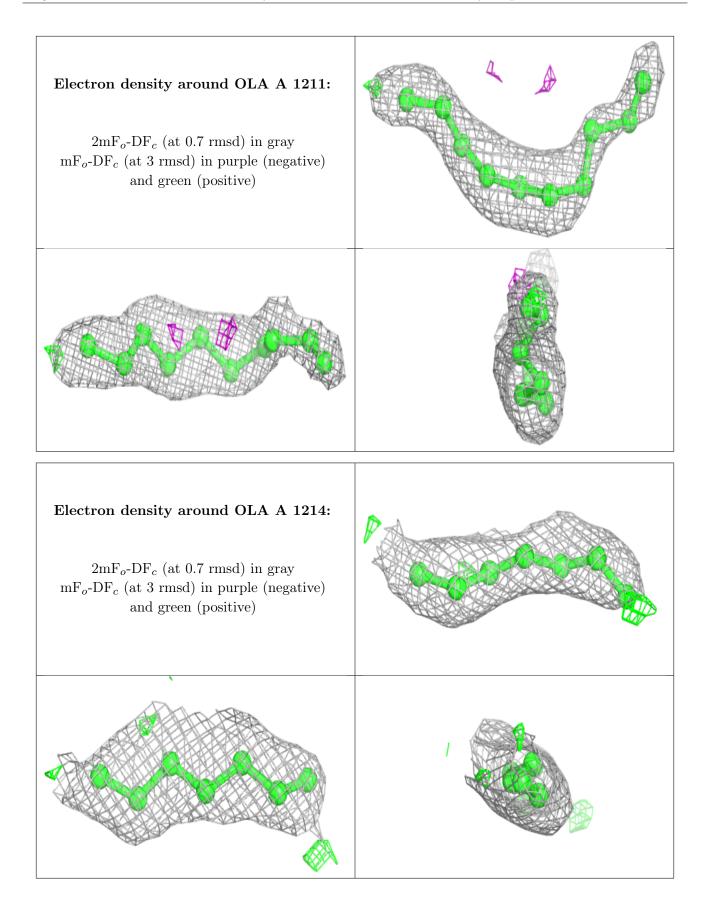




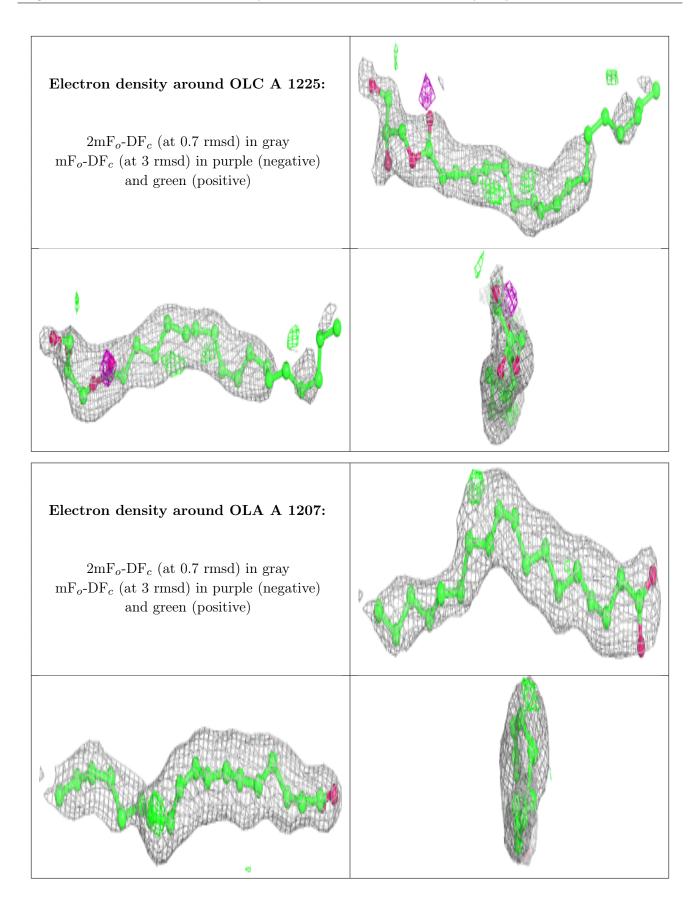




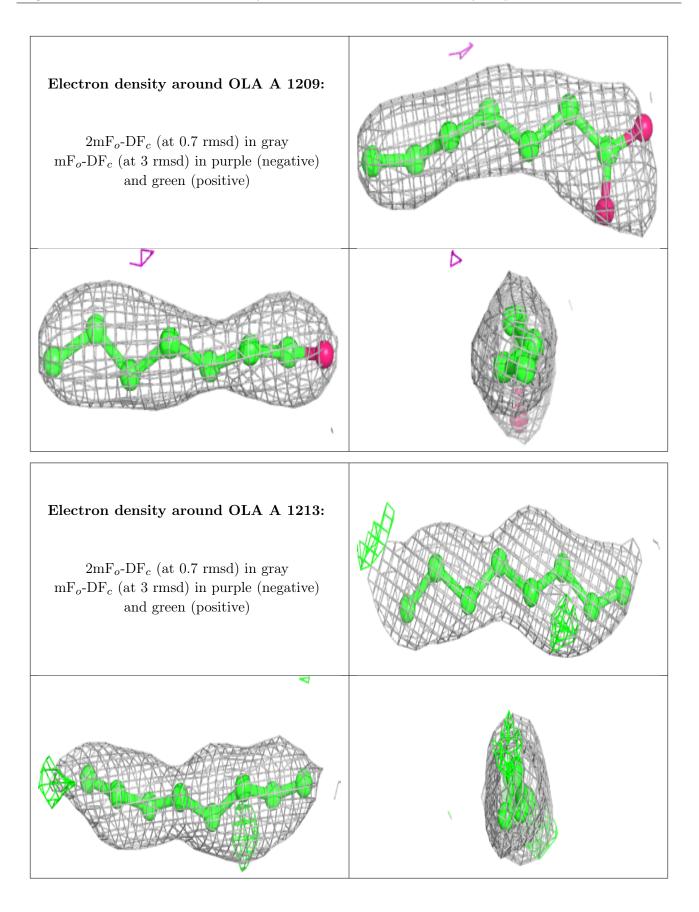




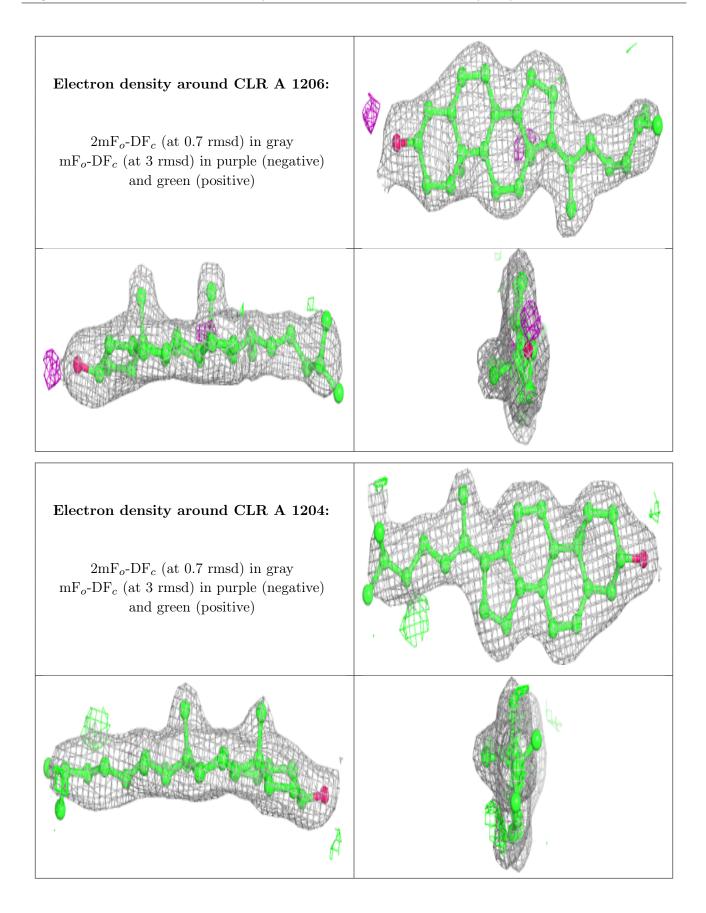




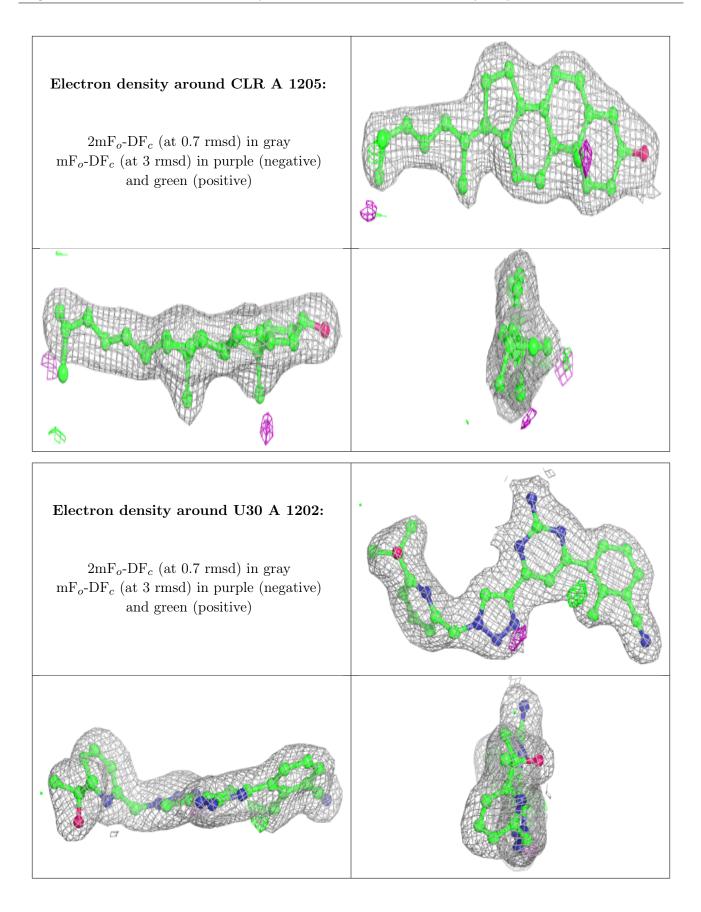














6.5 Other polymers (i)

There are no such residues in this entry.

