



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:02 AM UTC

PDB ID : 6ZFF / pdb_00006zff
Title : Structure of M1-StaR-T4L in complex with 77-LH-28-1 at 2.17Å
Authors : Rucktooa, P.; Cooke, R.M.
Deposited on : 2020-06-18
Resolution : 2.17 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

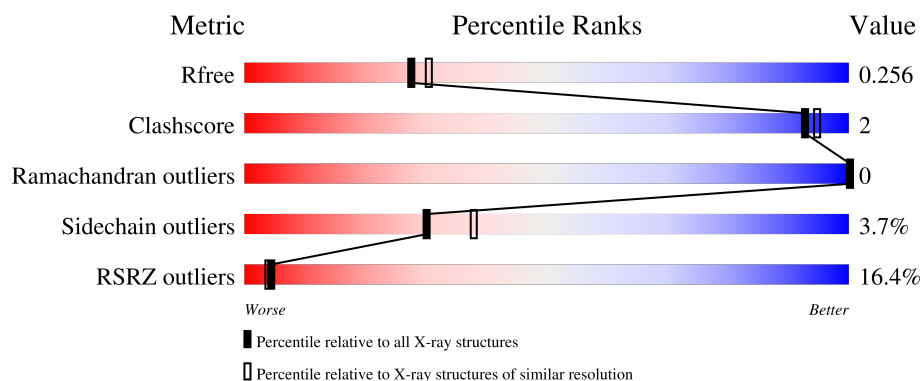
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	455	16% 91% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3855 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 Muscarinic acetylcholine receptor M1,Endolysin,Muscarinic acetylcholine receptor M1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	2	0
			3573	2325	601	623	24			

There are 49 discrepancies between the modelled and reference sequences:

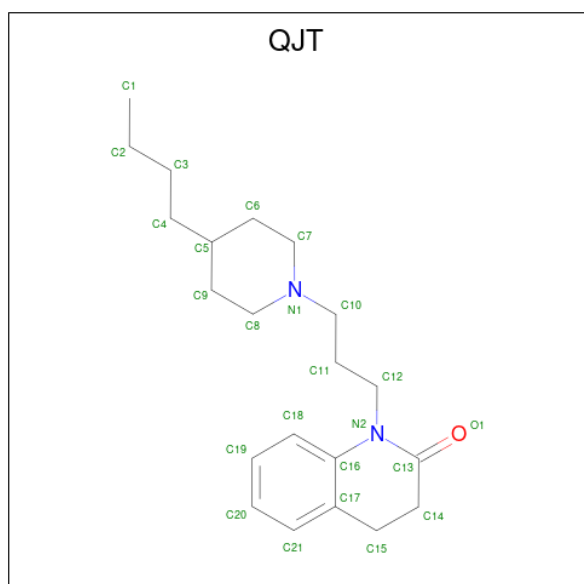
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP P11229
A	21	GLU	-	expression tag	UNP P11229
A	22	THR	-	expression tag	UNP P11229
A	23	VAL	-	expression tag	UNP P11229
A	24	GLU	-	expression tag	UNP P11229
A	25	MET	-	expression tag	UNP P11229
A	26	VAL	-	expression tag	UNP P11229
A	27	ALA	PHE	engineered mutation	UNP P11229
A	29	ALA	GLY	conflict	UNP P11229
A	30	THR	ILE	conflict	UNP P11229
A	31	VAL	THR	conflict	UNP P11229
A	32	ALA	THR	engineered mutation	UNP P11229
A	44	ILE	LEU	engineered mutation	UNP P11229
A	46	LEU	VAL	engineered mutation	UNP P11229
A	47	MET	LEU	conflict	UNP P11229
A	48	LEU	ILE	conflict	UNP P11229
A	50	ILE	PHE	conflict	UNP P11229
A	54	ARG	THR	conflict	UNP P11229
A	55	GLN	GLU	conflict	UNP P11229
A	57	GLN	LYS	conflict	UNP P11229
A	64	ALA	LEU	engineered mutation	UNP P11229
A	65	PHE	LEU	conflict	UNP P11229
A	76	ALA	THR	engineered mutation	UNP P11229
A	84	VAL	THR	engineered mutation	UNP P11229
A	86	ILE	LEU	conflict	UNP P11229
A	87	ILE	LEU	conflict	UNP P11229

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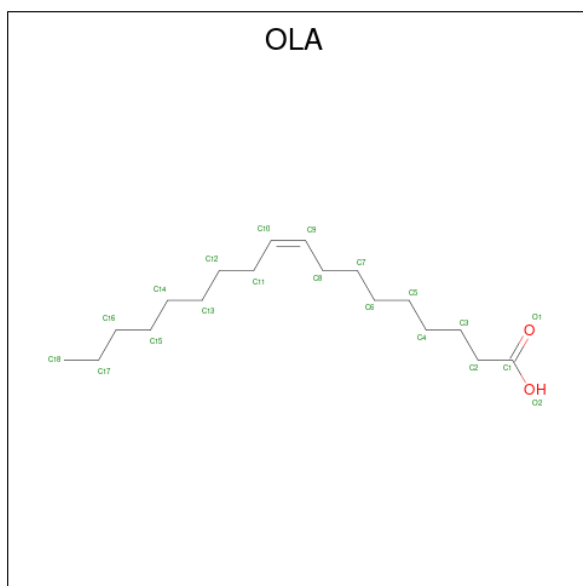
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	THR	engineered mutation	UNP P11229
A	101	ALA	TRP	engineered mutation	UNP P11229
A	112	ALA	SER	engineered mutation	UNP P11229
A	143	LEU	ALA	engineered mutation	UNP P11229
A	196	THR	ALA	engineered mutation	UNP P11229
A	1012	GLY	ARG	conflict	UNP P00720
A	1054	THR	CYS	conflict	UNP P00720
A	1097	ALA	CYS	conflict	UNP P00720
A	1137	ARG	ILE	conflict	UNP P00720
A	362	ALA	LYS	engineered mutation	UNP P11229
A	364	LEU	ALA	engineered mutation	UNP P11229
A	411	ALA	SER	engineered mutation	UNP P11229
A	435	ALA	CYS	conflict	UNP P11229
A	439	HIS	-	expression tag	UNP P11229
A	440	HIS	-	expression tag	UNP P11229
A	441	HIS	-	expression tag	UNP P11229
A	442	HIS	-	expression tag	UNP P11229
A	443	HIS	-	expression tag	UNP P11229
A	444	HIS	-	expression tag	UNP P11229
A	445	HIS	-	expression tag	UNP P11229
A	446	HIS	-	expression tag	UNP P11229
A	447	HIS	-	expression tag	UNP P11229
A	448	HIS	-	expression tag	UNP P11229

- Molecule 2 is 1-[3-(4-butylpiperidin-1-yl)propyl]-3,4-dihydroquinolin-2-one (CCD ID: QJT) (formula: C₂₁H₃₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	21	2	1		

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



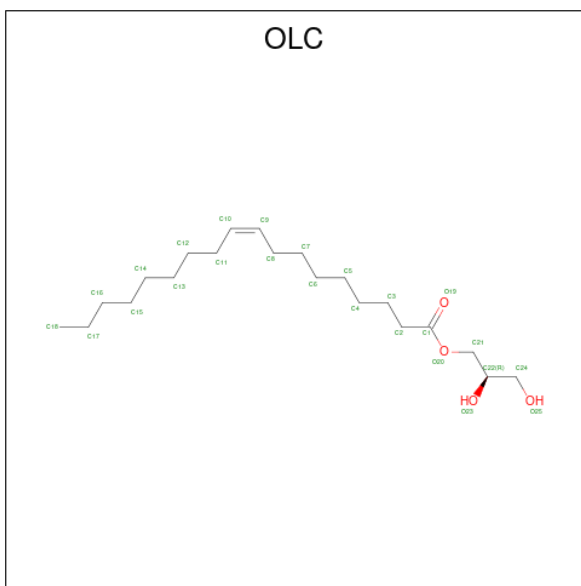
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



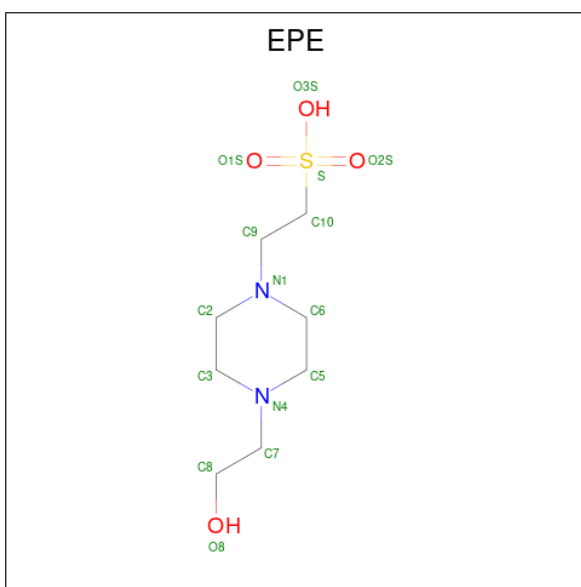
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



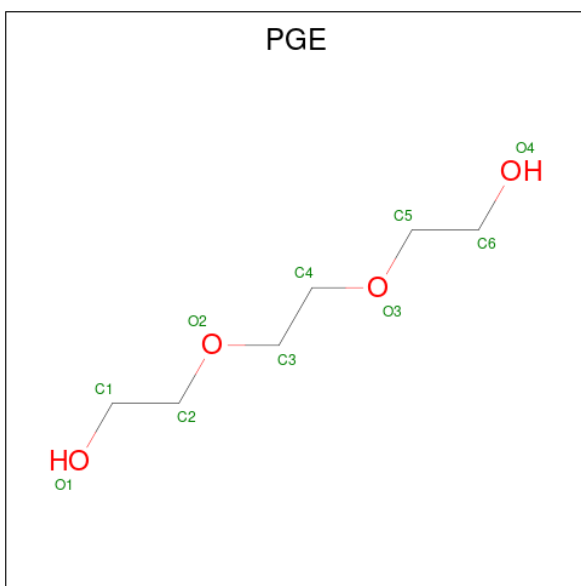
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		

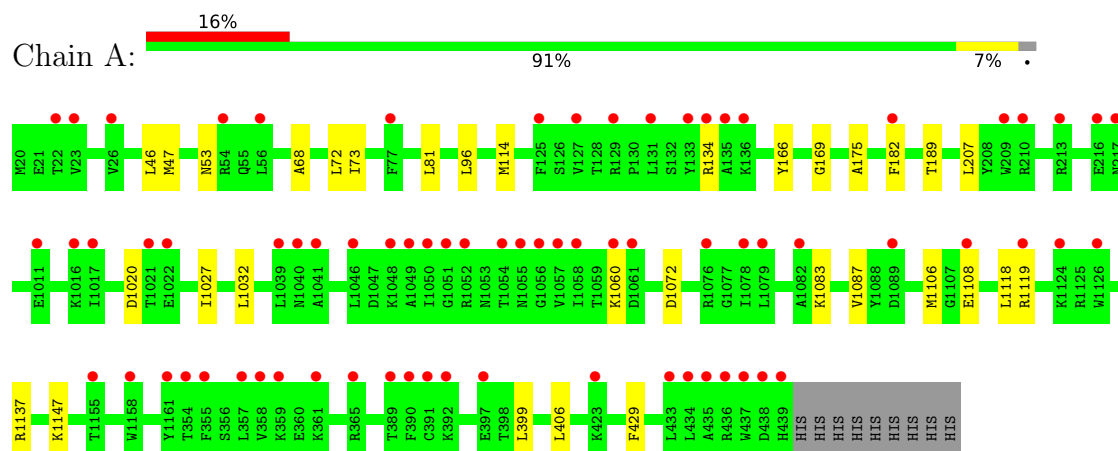
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total 33	O 33	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: Muscarinic acetylcholine receptor M1,Endolysin,Muscarinic acetylcholine receptor M1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.34Å 65.63Å 156.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.30 – 2.17 50.30 – 2.17	Depositor EDS
% Data completeness (in resolution range)	72.3 (50.30-2.17) 72.4 (50.30-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.214 , 0.242 0.226 , 0.256	Depositor DCC
R_{free} test set	1194 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3855	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: QJT, OLC, PO4, OLA, PGE, EPE

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	0.77	0/3659	1.36	6/4977 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	182	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	1020	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	53	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	1137	ARG	CA-C-N	5.02	127.31	120.54
1	A	1137	ARG	C-N-CA	5.02	127.31	120.54

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	3573	0	3652	12	0
2	A	24	0	0	0	0
3	A	160	0	264	2	0
4	A	5	0	0	0	0
5	A	25	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	15	0	18	4	0
7	A	20	0	28	2	0
8	A	33	0	0	0	0
All	All	3855	0	4002	12	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 2.

All (12) 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:166:TYR:HA	6:A:1212:EPE:H32	1.80	0.62
1:A:46:LEU:HD23	1:A:68:ALA:HB2	1.87	0.56
1:A:166:TYR:HD1	6:A:1212:EPE:H52	1.70	0.55
1:A:73:ILE:HD11	3:A:1202:OLA:H162	1.90	0.53
1:A:175:ALA:HA	7:A:1214:PGE:H5	1.91	0.52
1:A:189:THR:HG21	7:A:1213:PGE:H6	1.92	0.51
1:A:47:MET:HE1	1:A:72:LEU:HD22	1.92	0.51
1:A:166:TYR:CD1	6:A:1212:EPE:H52	2.48	0.48
1:A:81:LEU:HD11	3:A:1205:OLA:H81	2.00	0.42
1:A:1087:VAL:HG11	1:A:1118:LEU:HD22	2.01	0.42
1:A:169:GLY:C	6:A:1212:EPE:H31	2.46	0.41
1:A:114:MET:HE3	5:A:1211:OLC:H21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	446/455 (98%)	438 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	378/385 (98%)	364 (96%)	14 (4%)	30 38

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	134	ARG
1	A	207	LEU
1	A	1027	ILE
1	A	1032	LEU
1	A	1060	LYS
1	A	1072	ASP
1	A	1083	LYS
1	A	1106	MET
1	A	1108	GLU
1	A	1119	ARG
1	A	1147	LYS
1	A	399	LEU
1	A	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1002	ASN
1	A	1055	ASN
1	A	410	ASN
1	A	414	ASN
1	A	439	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	1210	-	19,19,19	0.53	0	19,19,19	0.48	0
6	EPE	A	1212	-	15,15,15	1.96	1 (6%)	19,20,20	1.53	4 (21%)
3	OLA	A	1205	-	19,19,19	0.53	0	19,19,19	0.48	0
4	PO4	A	1206	-	4,4,4	2.55	2 (50%)	6,6,6	0.50	0
3	OLA	A	1204	-	19,19,19	0.53	0	19,19,19	0.48	0
3	OLA	A	1208	-	19,19,19	0.52	0	19,19,19	0.48	0
7	PGE	A	1213	-	9,9,9	0.17	0	8,8,8	0.11	0
3	OLA	A	1207	-	19,19,19	0.54	0	19,19,19	0.48	0
2	QJT	A	1201	-	26,26,26	1.60	5 (19%)	33,34,34	1.29	4 (12%)
3	OLA	A	1202	-	19,19,19	0.54	0	19,19,19	0.47	0
5	OLC	A	1211	-	24,24,24	0.98	1 (4%)	25,25,25	0.86	1 (4%)
3	OLA	A	1203	-	19,19,19	0.56	0	19,19,19	0.46	0
3	OLA	A	1209	-	19,19,19	0.53	0	19,19,19	0.48	0
7	PGE	A	1214	-	9,9,9	0.16	0	8,8,8	0.09	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	1210	-	-	9/17/17/17	-
6	EPE	A	1212	-	-	5/9/19/19	0/1/1/1
3	OLA	A	1205	-	-	12/17/17/17	-
7	PGE	A	1213	-	-	5/7/7/7	-
3	OLA	A	1204	-	-	11/17/17/17	-
3	OLA	A	1208	-	-	14/17/17/17	-
3	OLA	A	1207	-	-	13/17/17/17	-
2	QJT	A	1201	-	-	2/10/33/33	0/3/3/3
3	OLA	A	1202	-	-	11/17/17/17	-
5	OLC	A	1211	-	-	17/24/24/24	-
3	OLA	A	1203	-	-	12/17/17/17	-
3	OLA	A	1209	-	-	9/17/17/17	-
7	PGE	A	1214	-	-	3/7/7/7	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1212	EPE	C10-S	-7.24	1.67	1.77
5	A	1211	OLC	O20-C1	4.53	1.46	1.33
4	A	1206	PO4	P-O1	4.22	1.60	1.50
2	A	1201	QJT	C8-N1	3.68	1.56	1.46
2	A	1201	QJT	C10-N1	3.35	1.55	1.47
2	A	1201	QJT	C7-N1	3.32	1.55	1.46
2	A	1201	QJT	C16-N2	2.33	1.45	1.41
2	A	1201	QJT	C14-C13	2.09	1.55	1.51
4	A	1206	PO4	P-O3	2.04	1.60	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	QJT	C12-N2-C13	-2.89	115.04	118.08
6	A	1212	EPE	O3S-S-C10	2.87	111.62	106.00
5	A	1211	OLC	O20-C1-C2	2.70	120.08	111.83
2	A	1201	QJT	O1-C13-N2	2.61	126.13	122.47
6	A	1212	EPE	C6-N1-C2	2.59	114.42	108.84
6	A	1212	EPE	O2S-S-C10	2.57	110.61	106.73
6	A	1212	EPE	C5-C6-N1	2.43	115.54	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	QJT	C16-N2-C13	2.25	126.00	121.44
2	A	1201	QJT	C6-C7-N1	-2.06	107.74	111.08

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1212	EPE	C10-C9-N1-C6
6	A	1212	EPE	S-C10-C9-N1
3	A	1203	OLA	C11-C10-C9-C8
3	A	1205	OLA	C11-C10-C9-C8
3	A	1202	OLA	C11-C10-C9-C8
3	A	1204	OLA	C11-C10-C9-C8
3	A	1208	OLA	C1-C2-C3-C4
3	A	1209	OLA	C11-C10-C9-C8
5	A	1211	OLC	O20-C21-C22-O23
7	A	1214	PGE	O2-C3-C4-O3
5	A	1211	OLC	C2-C1-O20-C21
5	A	1211	OLC	O20-C21-C22-C24
5	A	1211	OLC	O19-C1-O20-C21
7	A	1214	PGE	O3-C5-C6-O4
3	A	1203	OLA	C2-C3-C4-C5
5	A	1211	OLC	C5-C6-C7-C8
3	A	1203	OLA	C5-C6-C7-C8
3	A	1209	OLA	C3-C4-C5-C6
3	A	1210	OLA	C3-C4-C5-C6
3	A	1205	OLA	C12-C13-C14-C15
3	A	1207	OLA	C12-C13-C14-C15
3	A	1204	OLA	C3-C4-C5-C6
3	A	1204	OLA	C5-C6-C7-C8
5	A	1211	OLC	C6-C7-C8-C9
3	A	1207	OLA	C11-C12-C13-C14
3	A	1202	OLA	C3-C4-C5-C6
3	A	1207	OLA	C5-C6-C7-C8
3	A	1210	OLA	C2-C3-C4-C5
3	A	1208	OLA	C11-C12-C13-C14
3	A	1202	OLA	C12-C13-C14-C15
3	A	1207	OLA	C14-C15-C16-C17
3	A	1208	OLA	C13-C14-C15-C16
3	A	1208	OLA	C14-C15-C16-C17
5	A	1211	OLC	C13-C14-C15-C16
3	A	1202	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	1203	OLA	C1-C2-C3-C4
3	A	1202	OLA	C6-C7-C8-C9
3	A	1210	OLA	C6-C7-C8-C9
3	A	1205	OLA	C4-C5-C6-C7
3	A	1209	OLA	C14-C15-C16-C17
3	A	1205	OLA	C3-C4-C5-C6
3	A	1205	OLA	C5-C6-C7-C8
3	A	1207	OLA	C1-C2-C3-C4
3	A	1204	OLA	C6-C7-C8-C9
3	A	1207	OLA	C6-C7-C8-C9
5	A	1211	OLC	C10-C11-C12-C13
3	A	1204	OLA	C2-C3-C4-C5
3	A	1207	OLA	C4-C5-C6-C7
3	A	1210	OLA	C5-C6-C7-C8
3	A	1203	OLA	C6-C7-C8-C9
3	A	1203	OLA	C10-C11-C12-C13
3	A	1208	OLA	C5-C6-C7-C8
5	A	1211	OLC	C11-C12-C13-C14
7	A	1213	PGE	O3-C5-C6-O4
3	A	1204	OLA	C12-C13-C14-C15
3	A	1208	OLA	C12-C13-C14-C15
7	A	1213	PGE	O2-C3-C4-O3
3	A	1205	OLA	C6-C7-C8-C9
3	A	1205	OLA	C10-C11-C12-C13
3	A	1203	OLA	C4-C5-C6-C7
3	A	1210	OLA	C13-C14-C15-C16
3	A	1205	OLA	C1-C2-C3-C4
3	A	1203	OLA	C11-C12-C13-C14
3	A	1209	OLA	C5-C6-C7-C8
3	A	1207	OLA	C10-C11-C12-C13
3	A	1209	OLA	C6-C7-C8-C9
5	A	1211	OLC	C3-C4-C5-C6
5	A	1211	OLC	C4-C5-C6-C7
5	A	1211	OLC	C15-C16-C17-C18
3	A	1205	OLA	C15-C16-C17-C18
3	A	1202	OLA	C15-C16-C17-C18
3	A	1204	OLA	C10-C11-C12-C13
5	A	1211	OLC	C14-C15-C16-C17
3	A	1202	OLA	C2-C3-C4-C5
3	A	1208	OLA	C4-C5-C6-C7
3	A	1210	OLA	C15-C16-C17-C18
3	A	1203	OLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	A	1211	OLC	C2-C3-C4-C5
7	A	1213	PGE	C4-C3-O2-C2
3	A	1208	OLA	C2-C3-C4-C5
3	A	1209	OLA	C12-C13-C14-C15
7	A	1213	PGE	C6-C5-O3-C4
6	A	1212	EPE	C8-C7-N4-C5
7	A	1214	PGE	C4-C3-O2-C2
3	A	1203	OLA	C12-C13-C14-C15
2	A	1201	QJT	C1-C2-C3-C4
3	A	1209	OLA	C13-C14-C15-C16
3	A	1205	OLA	C14-C15-C16-C17
3	A	1202	OLA	C13-C14-C15-C16
6	A	1212	EPE	C10-C9-N1-C2
3	A	1208	OLA	C11-C10-C9-C8
5	A	1211	OLC	C7-C8-C9-C10
3	A	1202	OLA	C14-C15-C16-C17
3	A	1204	OLA	O2-C1-C2-C3
3	A	1208	OLA	O1-C1-C2-C3
3	A	1210	OLA	O1-C1-C2-C3
3	A	1205	OLA	O2-C1-C2-C3
3	A	1208	OLA	O2-C1-C2-C3
3	A	1208	OLA	C3-C4-C5-C6
3	A	1202	OLA	O1-C1-C2-C3
3	A	1210	OLA	O2-C1-C2-C3
3	A	1202	OLA	O2-C1-C2-C3
3	A	1209	OLA	O2-C1-C2-C3
3	A	1204	OLA	C14-C15-C16-C17
3	A	1209	OLA	O1-C1-C2-C3
3	A	1205	OLA	O1-C1-C2-C3
3	A	1207	OLA	C3-C4-C5-C6
3	A	1203	OLA	C14-C15-C16-C17
3	A	1210	OLA	C12-C13-C14-C15
3	A	1204	OLA	O1-C1-C2-C3
7	A	1213	PGE	O1-C1-C2-O2
6	A	1212	EPE	C8-C7-N4-C3
5	A	1211	OLC	C9-C10-C11-C12
3	A	1203	OLA	C9-C10-C11-C12
3	A	1208	OLA	C6-C7-C8-C9
3	A	1207	OLA	O2-C1-C2-C3
3	A	1207	OLA	C13-C14-C15-C16
3	A	1207	OLA	C15-C16-C17-C18
3	A	1207	OLA	O1-C1-C2-C3

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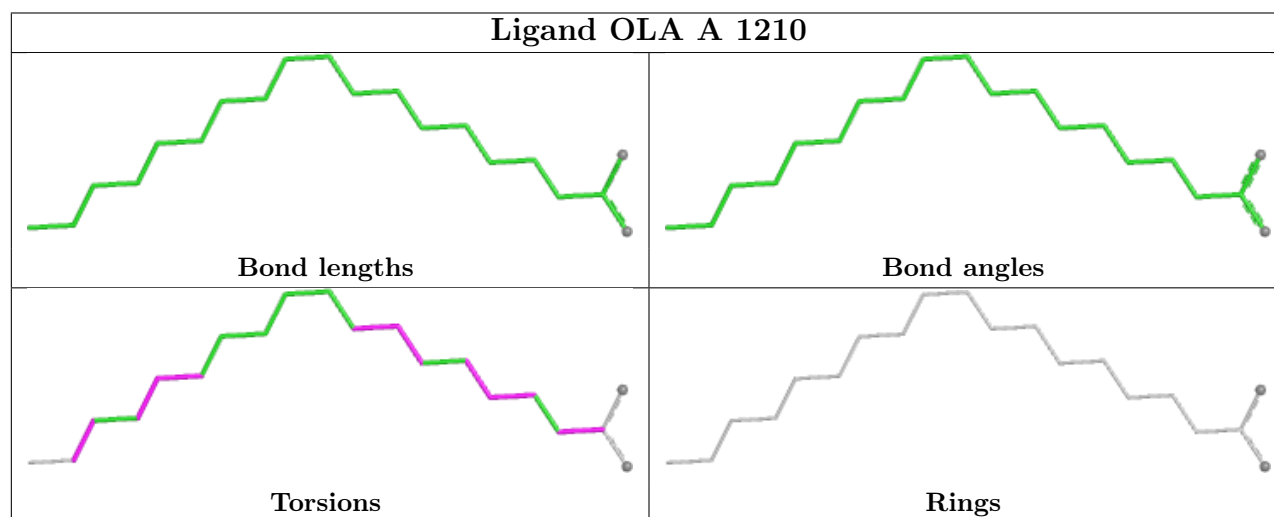
Mol	Chain	Res	Type	Atoms
2	A	1201	QJT	C3-C4-C5-C6
3	A	1208	OLA	C10-C11-C12-C13
5	A	1211	OLC	C1-C2-C3-C4
3	A	1204	OLA	C1-C2-C3-C4

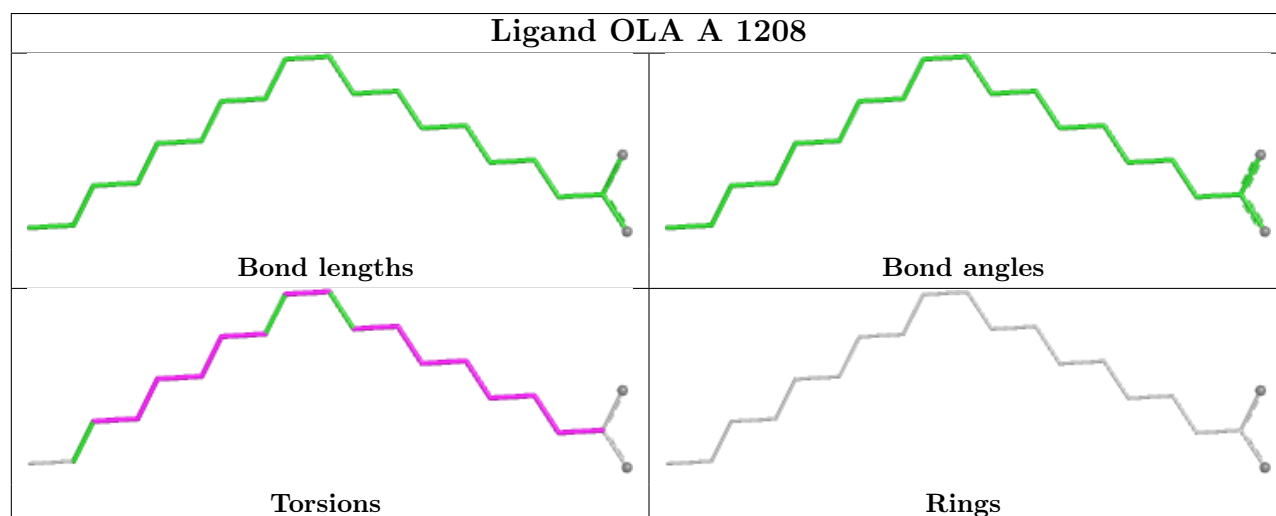
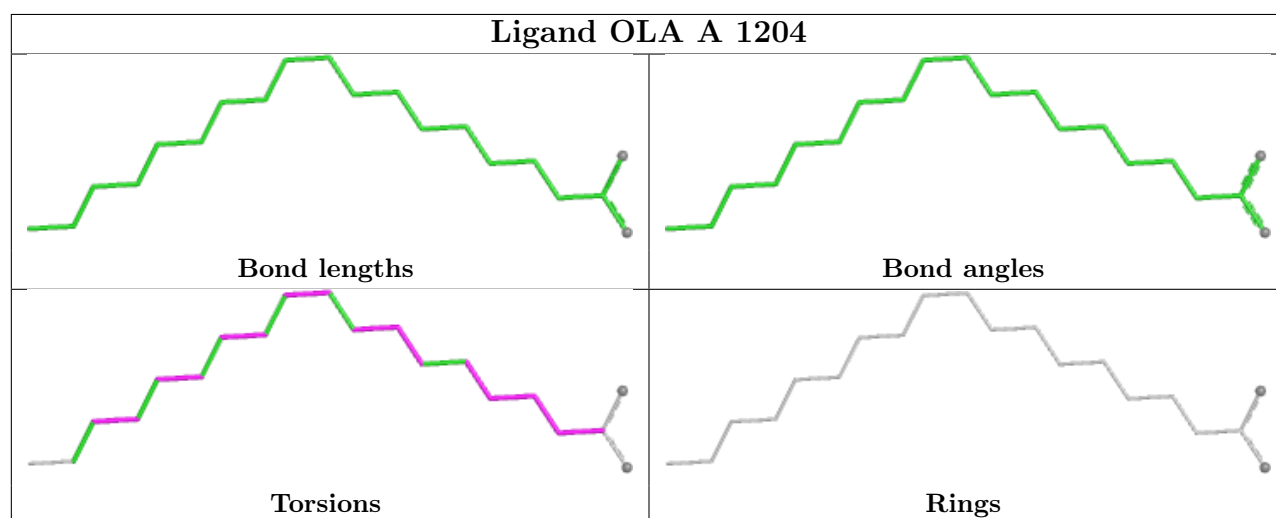
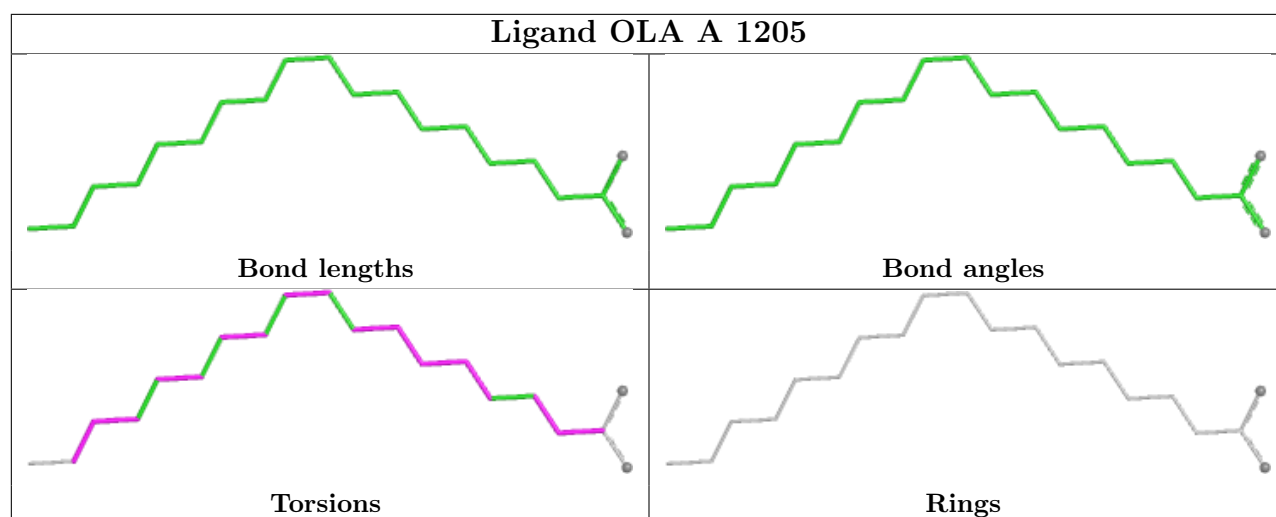
There are no ring outliers.

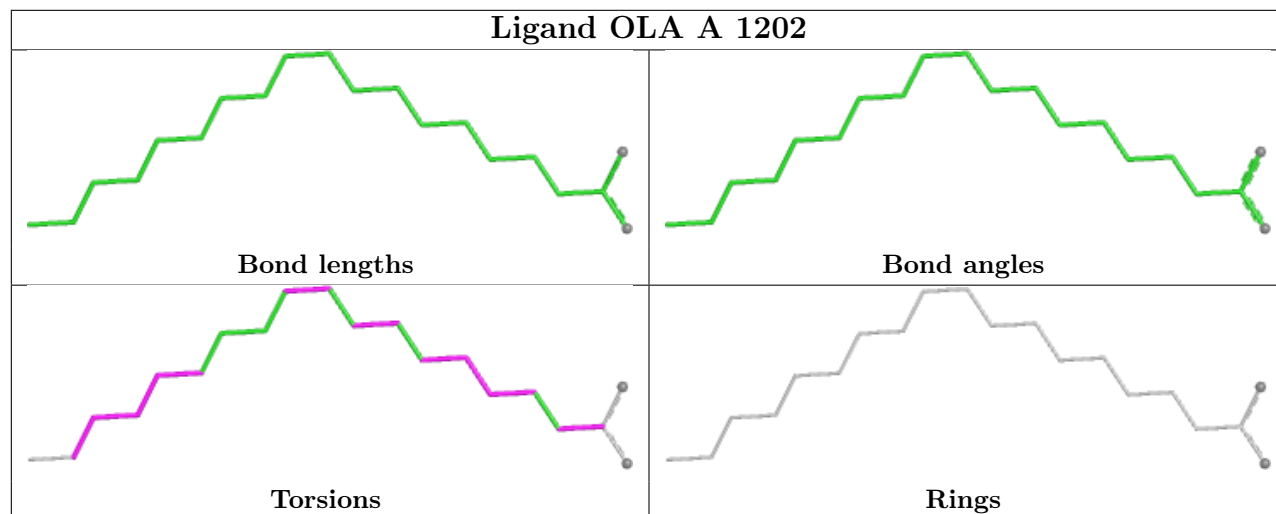
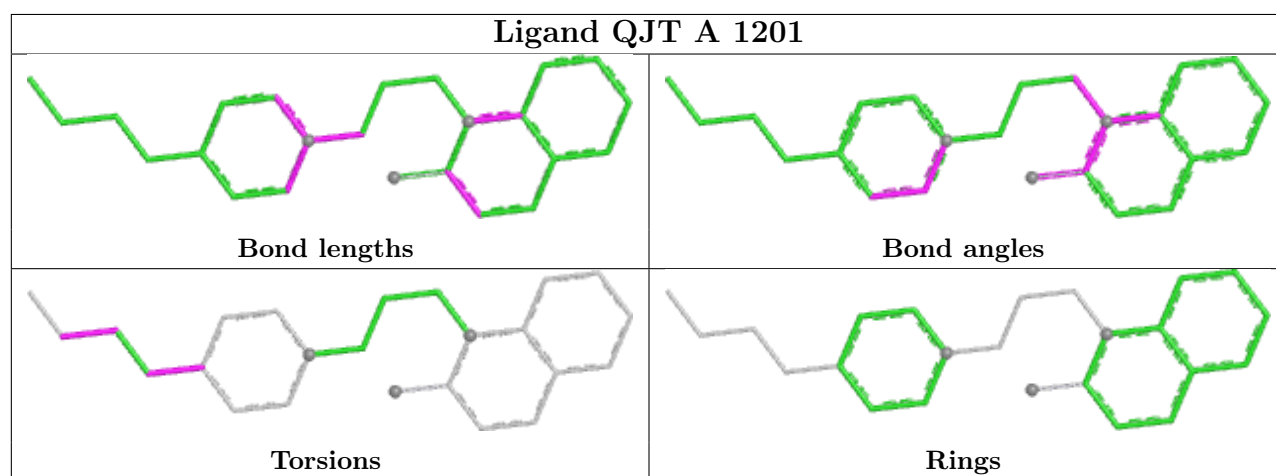
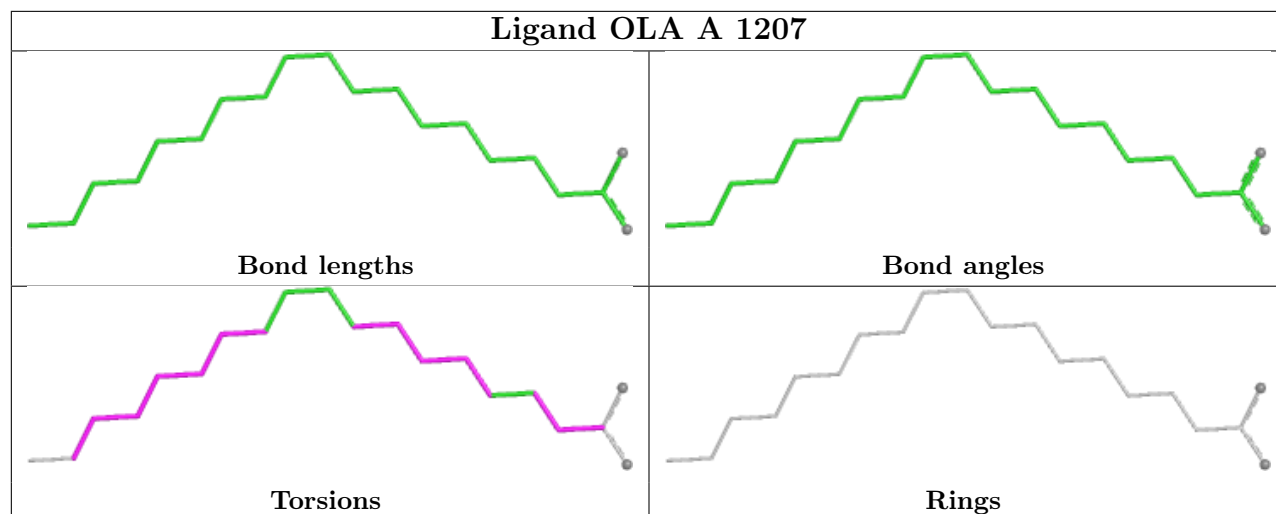
6 monomers are involved in 9 short contacts:

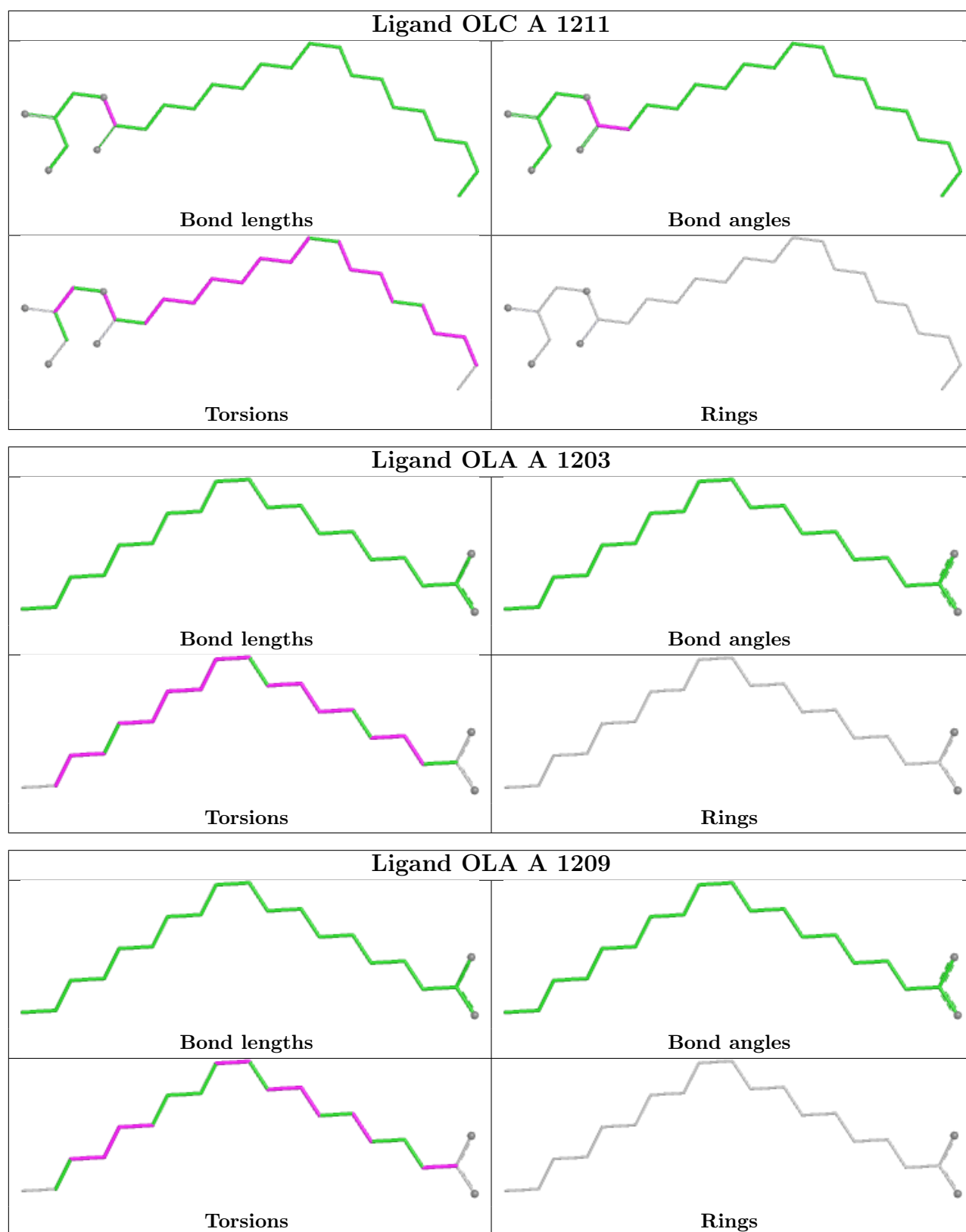
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1212	EPE	4	0
3	A	1205	OLA	1	0
7	A	1213	PGE	1	0
3	A	1202	OLA	1	0
5	A	1211	OLC	1	0
7	A	1214	PGE	1	0

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 than 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.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	446/455 (98%)	0.83	73 (16%) 4 4	20, 41, 76, 138	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	TRP	7.3
1	A	354	THR	5.2
1	A	209[A]	TRP	4.9
1	A	390	PHE	4.2
1	A	136	LYS	4.0
1	A	1126	TRP	4.0
1	A	439	HIS	4.0
1	A	392	LYS	3.9
1	A	1050	ILE	3.7
1	A	358	VAL	3.6
1	A	1051	GLY	3.6
1	A	391	CYS	3.4
1	A	355	PHE	3.4
1	A	357	LEU	3.3
1	A	22	THR	3.3
1	A	213	ARG	3.2
1	A	361	LYS	3.2
1	A	26	VAL	3.2
1	A	1158	TRP	3.1
1	A	1046	LEU	3.1
1	A	135	ALA	3.0
1	A	438	ASP	3.0
1	A	133	TYR	2.8
1	A	1078	ILE	2.8
1	A	54	ARG	2.8
1	A	134	ARG	2.8
1	A	1079	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	210	ARG	2.7
1	A	1017	ILE	2.7
1	A	389	THR	2.7
1	A	23	VAL	2.7
1	A	1052	ARG	2.6
1	A	216[A]	GLU	2.6
1	A	397	GLU	2.6
1	A	434	LEU	2.6
1	A	1161	TYR	2.6
1	A	1060	LYS	2.5
1	A	1108	GLU	2.5
1	A	436	ARG	2.5
1	A	125	PHE	2.4
1	A	1021	THR	2.4
1	A	1049	ALA	2.4
1	A	359	LYS	2.4
1	A	131	LEU	2.4
1	A	1055	ASN	2.4
1	A	1040	ASN	2.4
1	A	423	LYS	2.3
1	A	1056	GLY	2.3
1	A	1076	ARG	2.3
1	A	77	PHE	2.3
1	A	182	PHE	2.3
1	A	217	ASN	2.3
1	A	435	ALA	2.3
1	A	433	LEU	2.3
1	A	1119	ARG	2.2
1	A	127	VAL	2.2
1	A	1016	LYS	2.2
1	A	1061	ASP	2.2
1	A	1048	LYS	2.2
1	A	1155	THR	2.2
1	A	1022	GLU	2.2
1	A	1058	ILE	2.1
1	A	1057	VAL	2.1
1	A	1054	THR	2.1
1	A	1041	ALA	2.1
1	A	365	ARG	2.1
1	A	1011	GLU	2.0
1	A	1082	ALA	2.0
1	A	56	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1039	LEU	2.0
1	A	1089	ASP	2.0
1	A	129	ARG	2.0
1	A	1124	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

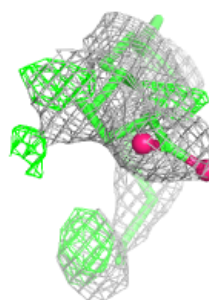
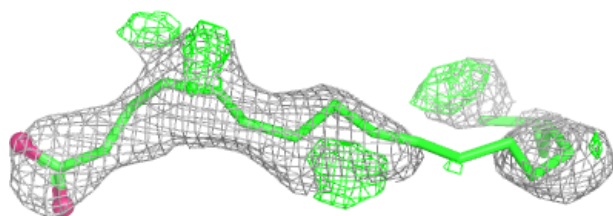
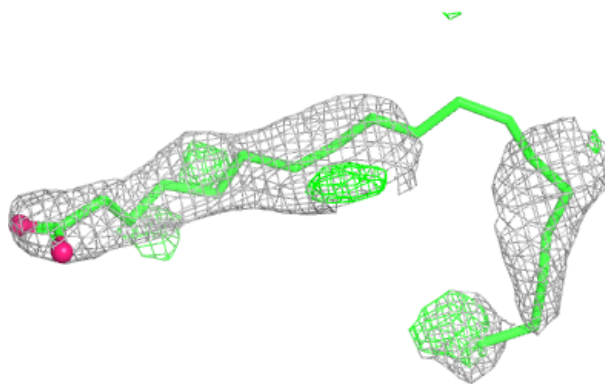
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EPE	A	1212	15/15	0.66	0.29	83,85,91,93	0
3	OLA	A	1210	20/20	0.69	0.34	83,84,85,85	0
4	PO4	A	1206	5/5	0.70	0.18	102,103,103,103	0
7	PGE	A	1214	10/10	0.71	0.27	61,70,78,78	0
3	OLA	A	1208	20/20	0.72	0.26	57,63,74,74	0
3	OLA	A	1202	20/20	0.76	0.25	54,58,69,70	0
3	OLA	A	1207	20/20	0.77	0.23	65,70,79,80	0
5	OLC	A	1211	25/25	0.77	0.26	68,76,82,82	0
3	OLA	A	1204	20/20	0.78	0.20	47,58,79,79	0
3	OLA	A	1205	20/20	0.79	0.28	65,73,85,85	0
3	OLA	A	1203	20/20	0.79	0.24	51,55,64,64	0
3	OLA	A	1209	20/20	0.80	0.25	50,65,67,67	0
7	PGE	A	1213	10/10	0.82	0.19	54,62,67,67	0
2	QJT	A	1201	24/24	0.93	0.09	27,31,37,39	0

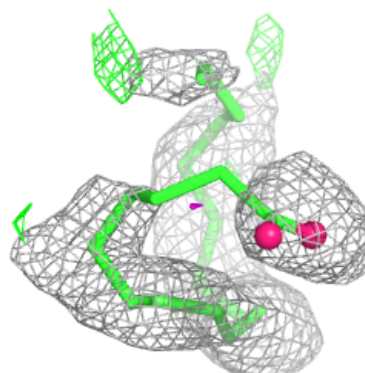
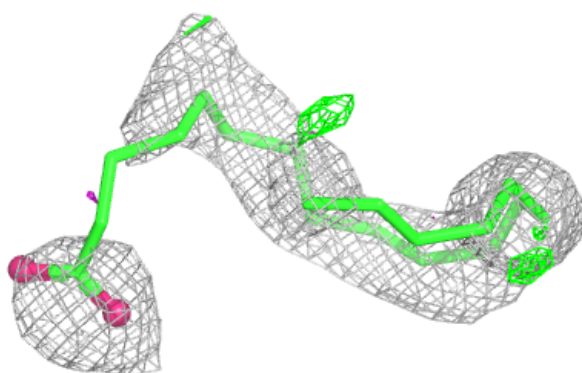
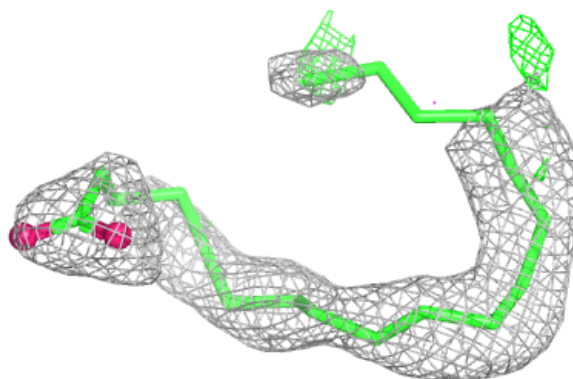
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1210:

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

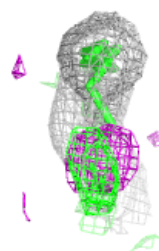
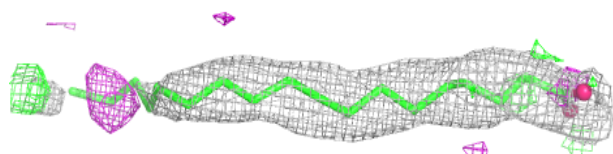
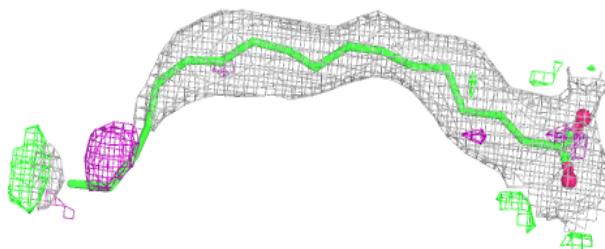
**Electron density around OLA A 1208:**

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

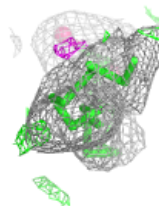
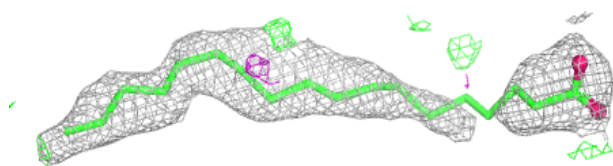
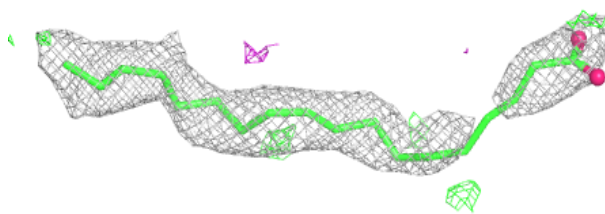


Electron density around OLA A 1202:

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

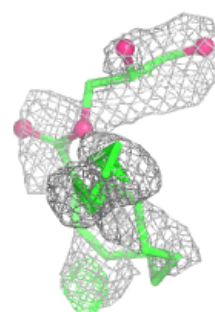
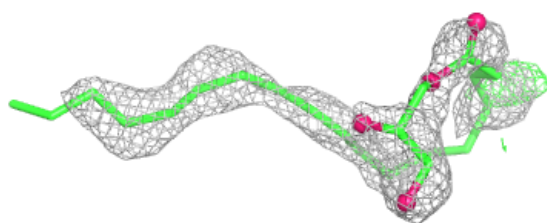
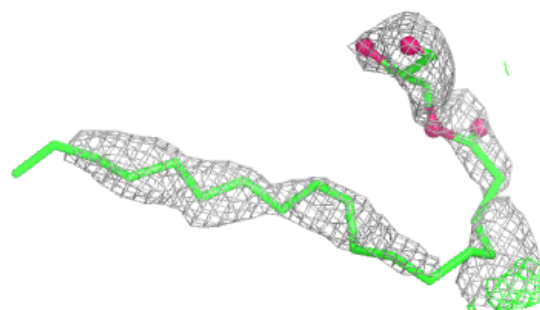
**Electron density around OLA A 1207:**

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



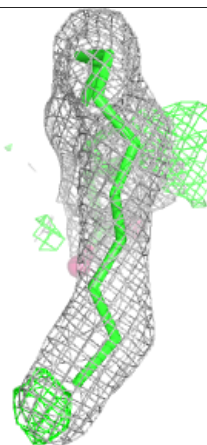
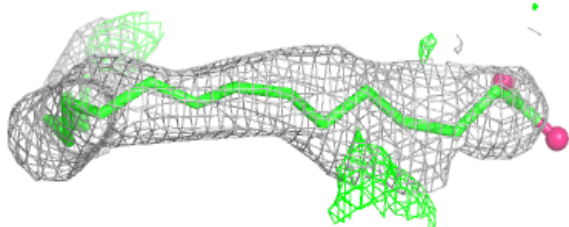
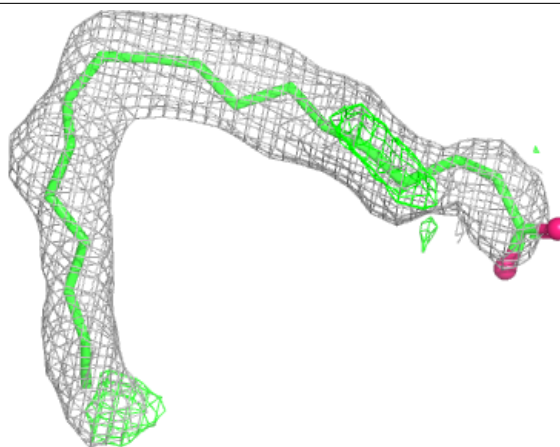
Electron density around OLC A 1211:

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

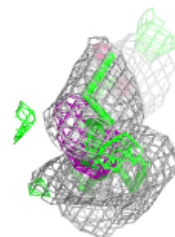
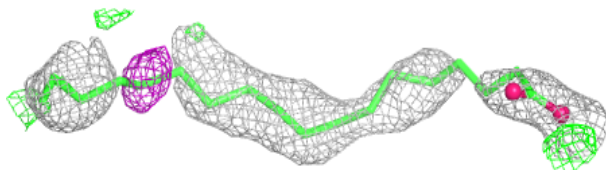
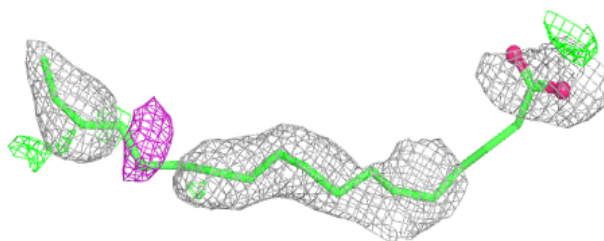


Electron density around OLA A 1204:

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

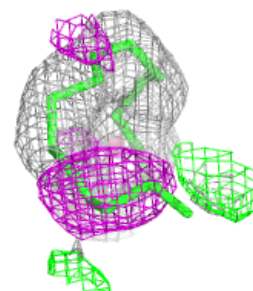
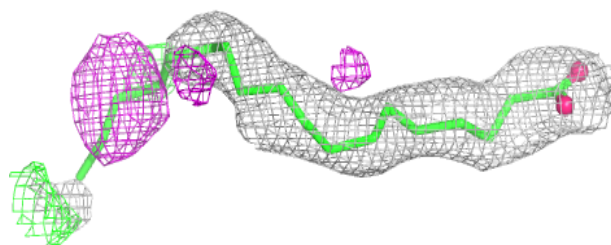
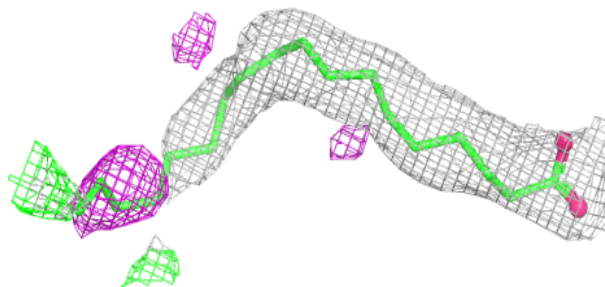
**Electron density around OLA A 1205:**

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

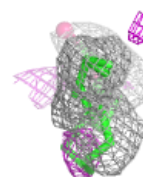
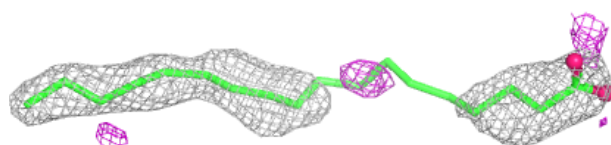
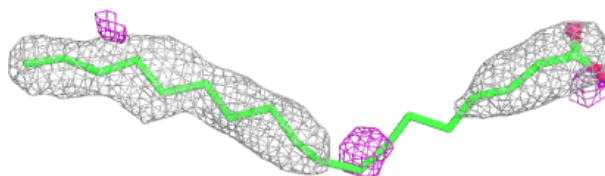


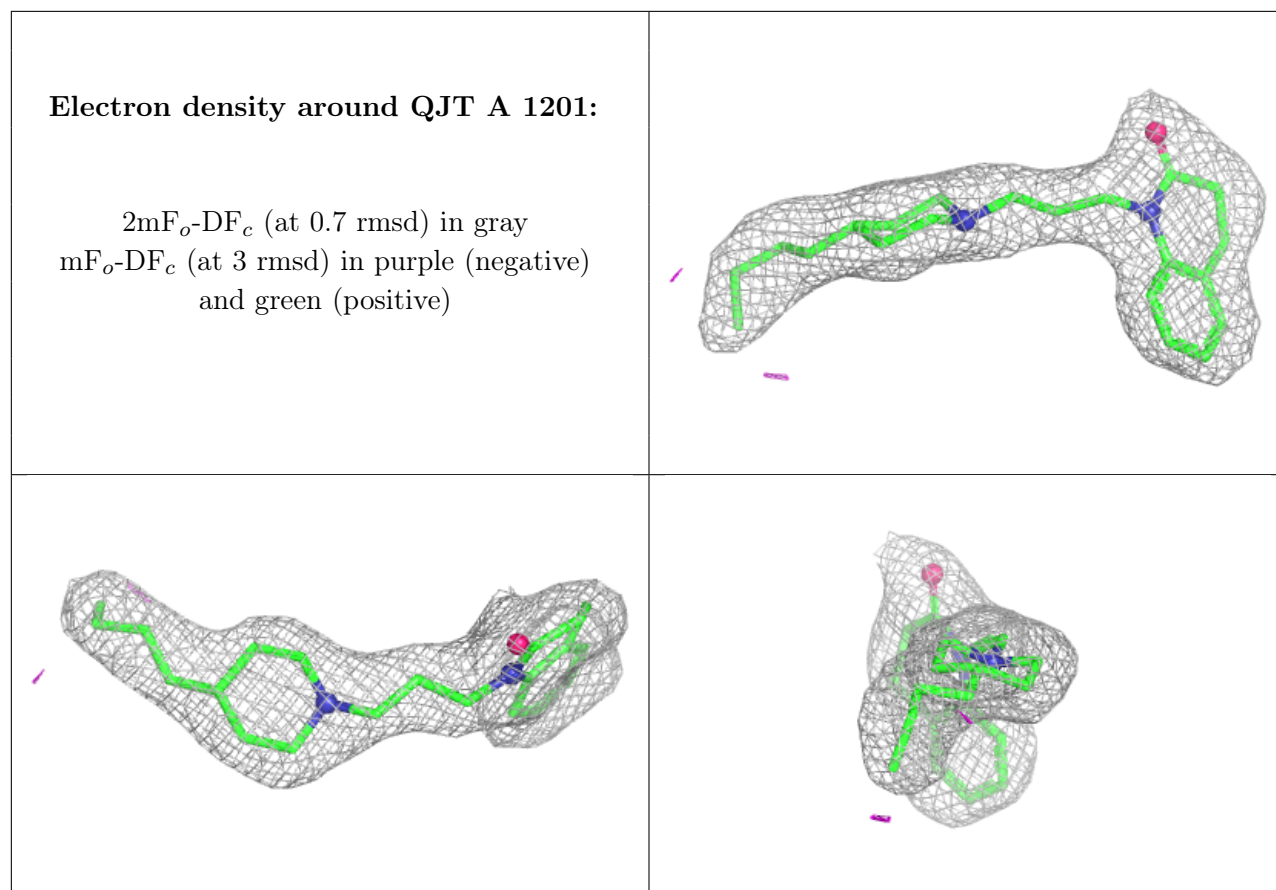
Electron density around OLA A 1203:

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

**Electron density around OLA A 1209:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.