Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2021 – 03:04 pm BST

PDB ID	:	6ZG4
Title	:	Structure of M1-StaR-T4L in complex with HTL0009936 at 2.35A
Authors	:	Rucktooa, P.; Cooke, R.M.
Deposited on	:	2020-06-18
Resolution	:	2.33 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 following versions of software and data (see references ⓘ) were used in the production of this report:

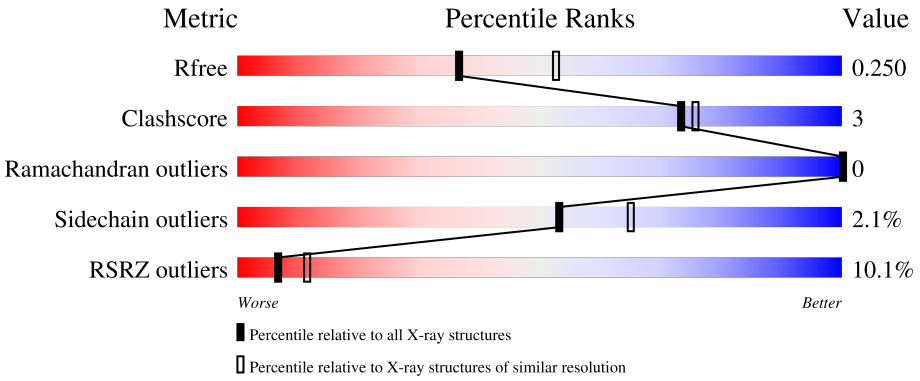
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	455	10% 91% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLA	A	1206	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLA	A	1212	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3899 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
			Total	C	N	O	S			
1	A	446	3556	2311	600	621	24	0	0	0

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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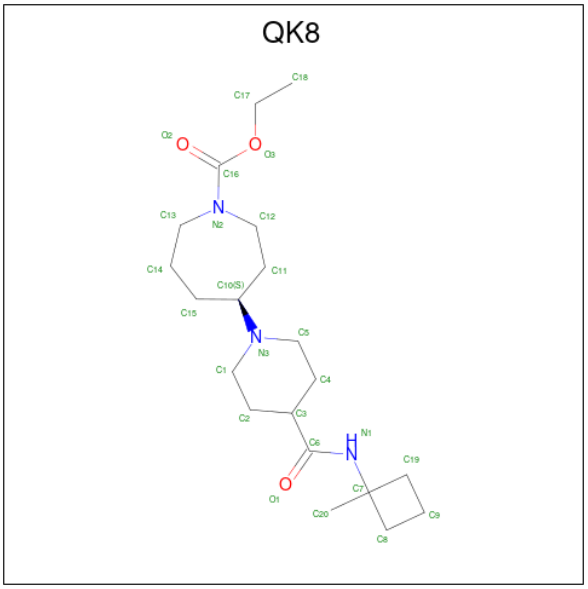
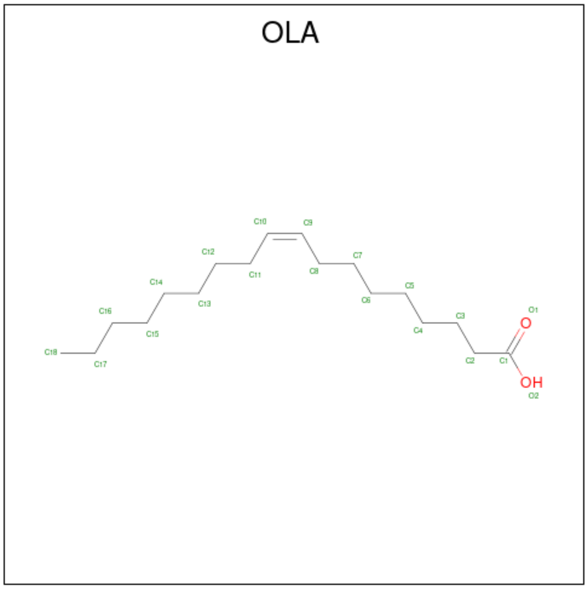
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	THR	engineered mutation	UNP P11229
A	101	ALA	TRP	engineered mutation	UNP P11229
A	112	ALA	SER	engineered mutation	UNP P11229
A	143	LEU	ALA	engineered mutation	UNP P11229
A	196	THR	ALA	engineered mutation	UNP P11229
A	1012	GLY	ARG	conflict	UNP P00720
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 ethyl (4 {S})-4-[4-[(1-methylcyclobutyl)carbamoyl]piperidin-1-yl]azepane-1-carboxylate (three-letter code: QK8) (formula: $C_{20}H_{35}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



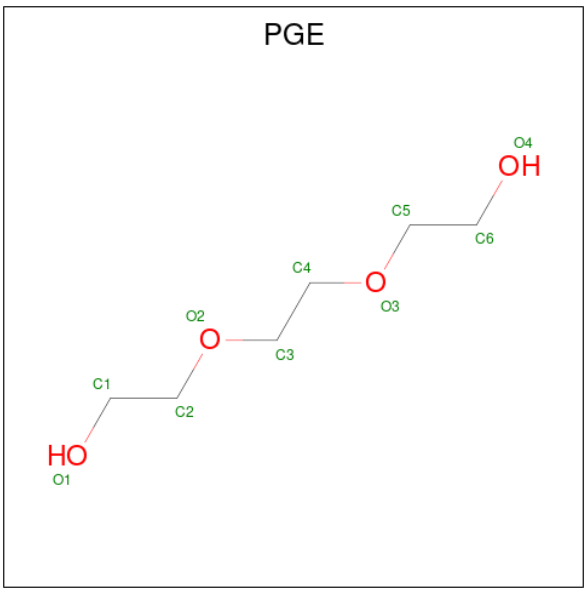
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 26	C 20	N 3	O 3	0	0

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



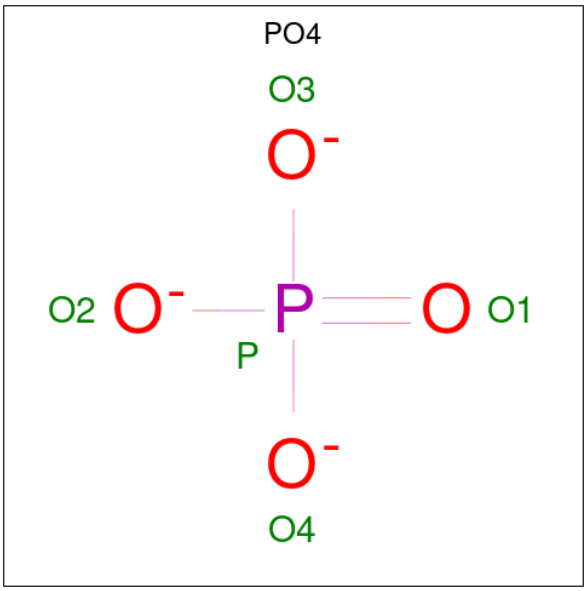
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1	Total 20	C 18	O 2	0	0
3	A	1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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

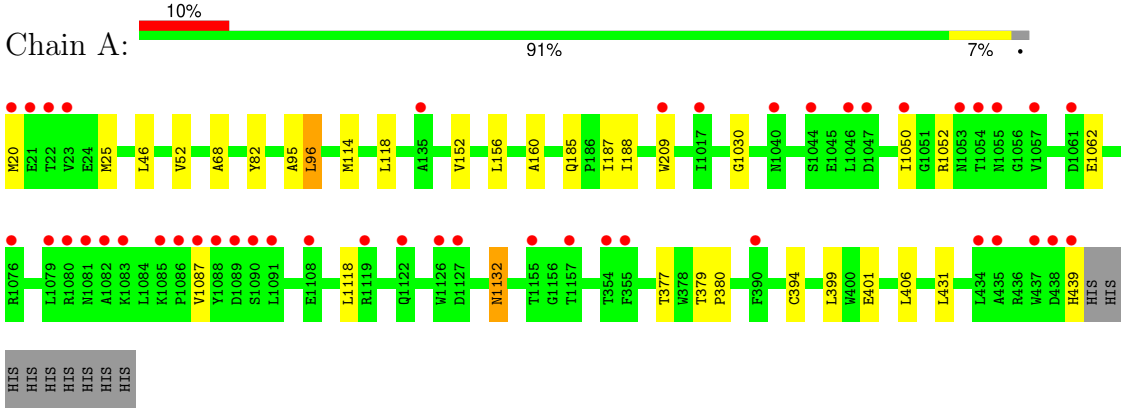
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	72	Total O 72 72	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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.47Å 65.45Å 154.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.33 49.98 – 2.33	Depositor EDS
% Data completeness (in resolution range)	74.0 (49.98-2.33) 74.0 (49.98-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.204 , 0.234 0.216 , 0.250	Depositor DCC
R_{free} test set	1000 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PO4, OLA, QK8

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	0.46	0/3634	0.62	0/4942

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3556	0	3636	26	0
2	A	26	0	0	0	0
3	A	220	0	363	14	0
4	A	10	0	14	0	0
5	A	15	0	0	0	0
6	A	72	0	0	0	0
All	All	3899	0	4013	26	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.

All (26) 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:96:LEU:HB2	3:A:1213:OLA:H62	1.74	0.68
1:A:95:ALA:CB	3:A:1213:OLA:H22	2.35	0.57
1:A:1087:VAL:HG11	1:A:1118:LEU:HD22	1.87	0.55
1:A:114:MET:HE1	3:A:1205:OLA:H10	1.87	0.55
1:A:96:LEU:HB2	3:A:1213:OLA:C6	2.38	0.54
1:A:96:LEU:H	3:A:1213:OLA:H62	1.73	0.53
1:A:95:ALA:H	3:A:1213:OLA:H42	1.74	0.52
1:A:377:THR:HB	1:A:406:LEU:O	2.11	0.51
1:A:160:ALA:HB2	3:A:1215:OLA:H9	1.93	0.50
1:A:1030:GLY:HA3	3:A:1207:OLA:H42	1.95	0.48
1:A:95:ALA:N	3:A:1213:OLA:H42	2.30	0.47
1:A:118:LEU:HD21	3:A:1205:OLA:H9	1.95	0.47
1:A:379:THR:HG21	3:A:1202:OLA:H162	1.95	0.47
1:A:187:ILE:HD12	1:A:188:ILE:HG13	1.97	0.47
1:A:156:LEU:HG	3:A:1215:OLA:H171	1.96	0.47
1:A:20:MET:HE3	1:A:25:MET:HG2	1.96	0.46
1:A:152:VAL:O	1:A:156:LEU:HB2	2.16	0.45
1:A:82:TYR:OH	1:A:401:GLU:HA	2.16	0.44
1:A:46:LEU:HD23	1:A:68:ALA:HB2	1.99	0.44
1:A:1050:ILE:HD12	1:A:1062:GLU:HB3	1.99	0.43
1:A:185:GLN:HB3	1:A:188:ILE:HD12	2.00	0.43
1:A:95:ALA:HB2	3:A:1213:OLA:H22	2.01	0.42
1:A:380:PRO:HG2	1:A:406:LEU:HD13	2.01	0.42
1:A:1132:ASN:HD22	1:A:1132:ASN:N	2.18	0.42
1:A:95:ALA:HB3	3:A:1213:OLA:H22	2.02	0.41
1:A:1050:ILE:HG22	1:A:1052:ARG:HG2	2.02	0.41

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	444/455 (98%)	436 (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	376/385 (98%)	368 (98%)	8 (2%)	53 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	96	LEU
1	A	209	TRP
1	A	1132	ASN
1	A	394	CYS
1	A	399	LEU
1	A	431	LEU
1	A	439	HIS

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

Mol	Chain	Res	Type
1	A	1069	GLN
1	A	1132	ASN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OLA	A	1203	-	16,19,19	0.23	0	15,19,19	0.14	0
2	QK8	A	1201	-	26,28,28	2.07	6 (23%)	25,39,39	1.78	5 (20%)
3	OLA	A	1215	-	16,19,19	0.21	0	15,19,19	0.15	0
3	OLA	A	1212	-	16,19,19	0.21	0	15,19,19	0.15	0
3	OLA	A	1206	-	16,19,19	0.21	0	15,19,19	0.17	0
4	PGE	A	1208	-	9,9,9	0.21	0	8,8,8	0.10	0
3	OLA	A	1214	-	16,19,19	0.20	0	15,19,19	0.18	0
3	OLA	A	1207	-	16,19,19	0.23	0	15,19,19	0.26	0
3	OLA	A	1213	-	16,19,19	0.20	0	15,19,19	0.17	0
5	PO4	A	1216	-	4,4,4	2.49	1 (25%)	6,6,6	0.51	0
5	PO4	A	1209	-	4,4,4	2.47	1 (25%)	6,6,6	0.47	0
3	OLA	A	1205	-	16,19,19	0.22	0	15,19,19	0.22	0
3	OLA	A	1202	-	16,19,19	0.23	0	15,19,19	0.21	0
3	OLA	A	1204	-	16,19,19	0.25	0	15,19,19	0.16	0
3	OLA	A	1211	-	16,19,19	0.22	0	15,19,19	0.15	0
5	PO4	A	1210	-	4,4,4	2.49	1 (25%)	6,6,6	0.39	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	1203	-	-	7/15/17/17	-
2	QK8	A	1201	-	-	4/19/49/49	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	A	1215	-	-	9/15/17/17	-
3	OLA	A	1212	-	-	8/15/17/17	-
3	OLA	A	1206	-	-	10/15/17/17	-
4	PGE	A	1208	-	-	6/7/7/7	-
3	OLA	A	1214	-	-	9/15/17/17	-
3	OLA	A	1207	-	-	9/15/17/17	-
3	OLA	A	1213	-	-	8/15/17/17	-
3	OLA	A	1205	-	-	9/15/17/17	-
3	OLA	A	1202	-	-	10/15/17/17	-
3	OLA	A	1204	-	-	8/15/17/17	-
3	OLA	A	1211	-	-	12/15/17/17	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	QK8	C5-N3	5.23	1.57	1.47
2	A	1201	QK8	C1-N3	4.98	1.56	1.47
2	A	1201	QK8	C16-N2	4.26	1.42	1.35
5	A	1210	PO4	P-O1	4.14	1.60	1.50
5	A	1216	PO4	P-O1	4.12	1.60	1.50
5	A	1209	PO4	P-O1	4.10	1.60	1.50
2	A	1201	QK8	C10-N3	2.93	1.56	1.48
2	A	1201	QK8	O2-C16	2.54	1.24	1.21
2	A	1201	QK8	C11-C12	2.27	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	QK8	C17-O3-C16	5.61	124.00	115.59
2	A	1201	QK8	O1-C6-C3	-2.94	118.29	122.12
2	A	1201	QK8	C5-N3-C1	2.60	113.83	109.08
2	A	1201	QK8	C14-C13-N2	2.48	120.48	113.93
2	A	1201	QK8	C4-C3-C2	2.19	114.60	109.97

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	QK8	C11-C10-N3-C1

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Mol	Chain	Res	Type	Atoms
3	A	1202	OLA	C1-C2-C3-C4
3	A	1203	OLA	C1-C2-C3-C4
3	A	1203	OLA	C11-C10-C9-C8
3	A	1205	OLA	C1-C2-C3-C4
3	A	1206	OLA	C1-C2-C3-C4
3	A	1206	OLA	C11-C10-C9-C8
3	A	1211	OLA	C1-C2-C3-C4
3	A	1212	OLA	C1-C2-C3-C4
3	A	1212	OLA	C11-C10-C9-C8
3	A	1213	OLA	C1-C2-C3-C4
3	A	1214	OLA	C11-C10-C9-C8
3	A	1202	OLA	C11-C10-C9-C8
3	A	1211	OLA	C11-C10-C9-C8
3	A	1213	OLA	C11-C10-C9-C8
4	A	1208	PGE	O3-C5-C6-O4
3	A	1207	OLA	C14-C15-C16-C17
3	A	1215	OLA	C4-C5-C6-C7
3	A	1204	OLA	C2-C3-C4-C5
3	A	1207	OLA	C11-C10-C9-C8
3	A	1212	OLA	C12-C13-C14-C15
3	A	1204	OLA	C5-C6-C7-C8
3	A	1207	OLA	C12-C13-C14-C15
3	A	1202	OLA	C2-C3-C4-C5
3	A	1214	OLA	C11-C12-C13-C14
3	A	1214	OLA	C4-C5-C6-C7
3	A	1206	OLA	C5-C6-C7-C8
3	A	1215	OLA	C12-C13-C14-C15
3	A	1211	OLA	C13-C14-C15-C16
3	A	1212	OLA	C14-C15-C16-C17
3	A	1214	OLA	C14-C15-C16-C17
3	A	1214	OLA	C6-C7-C8-C9
3	A	1207	OLA	C13-C14-C15-C16
3	A	1215	OLA	C14-C15-C16-C17
3	A	1211	OLA	C3-C4-C5-C6
3	A	1212	OLA	C13-C14-C15-C16
3	A	1202	OLA	C14-C15-C16-C17
3	A	1204	OLA	C13-C14-C15-C16
3	A	1206	OLA	C11-C12-C13-C14
3	A	1214	OLA	C12-C13-C14-C15
3	A	1211	OLA	C14-C15-C16-C17
3	A	1205	OLA	C11-C10-C9-C8
3	A	1204	OLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	A	1213	OLA	C13-C14-C15-C16
3	A	1202	OLA	C12-C13-C14-C15
3	A	1206	OLA	C2-C3-C4-C5
3	A	1207	OLA	C3-C4-C5-C6
3	A	1213	OLA	C4-C5-C6-C7
3	A	1203	OLA	C10-C11-C12-C13
3	A	1205	OLA	C4-C5-C6-C7
3	A	1215	OLA	C13-C14-C15-C16
3	A	1213	OLA	C5-C6-C7-C8
3	A	1202	OLA	C13-C14-C15-C16
3	A	1204	OLA	C4-C5-C6-C7
3	A	1202	OLA	C6-C7-C8-C9
3	A	1205	OLA	C6-C7-C8-C9
3	A	1206	OLA	C10-C11-C12-C13
3	A	1213	OLA	C10-C11-C12-C13
3	A	1202	OLA	C11-C12-C13-C14
3	A	1204	OLA	C11-C10-C9-C8
3	A	1212	OLA	C4-C5-C6-C7
3	A	1202	OLA	C10-C11-C12-C13
3	A	1203	OLA	C5-C6-C7-C8
3	A	1211	OLA	C4-C5-C6-C7
3	A	1205	OLA	C15-C16-C17-C18
3	A	1215	OLA	C15-C16-C17-C18
3	A	1207	OLA	C10-C11-C12-C13
3	A	1203	OLA	C15-C16-C17-C18
3	A	1215	OLA	C2-C3-C4-C5
3	A	1215	OLA	C10-C11-C12-C13
3	A	1211	OLA	C12-C13-C14-C15
3	A	1203	OLA	C3-C4-C5-C6
3	A	1211	OLA	C11-C12-C13-C14
3	A	1205	OLA	C2-C3-C4-C5
3	A	1204	OLA	C15-C16-C17-C18
3	A	1206	OLA	C13-C14-C15-C16
3	A	1204	OLA	C3-C4-C5-C6
3	A	1207	OLA	C5-C6-C7-C8
3	A	1205	OLA	C7-C8-C9-C10
3	A	1211	OLA	C15-C16-C17-C18
2	A	1201	QK8	C2-C3-C6-O1
3	A	1211	OLA	C6-C7-C8-C9
3	A	1212	OLA	C2-C3-C4-C5
4	A	1208	PGE	C1-C2-O2-C3
4	A	1208	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	1214	OLA	C10-C11-C12-C13
3	A	1205	OLA	C11-C12-C13-C14
3	A	1206	OLA	C4-C5-C6-C7
4	A	1208	PGE	C6-C5-O3-C4
3	A	1212	OLA	C15-C16-C17-C18
3	A	1214	OLA	C5-C6-C7-C8
4	A	1208	PGE	C3-C4-O3-C5
3	A	1207	OLA	C9-C10-C11-C12
2	A	1201	QK8	C2-C3-C6-N1
3	A	1202	OLA	C7-C8-C9-C10
3	A	1211	OLA	C10-C11-C12-C13
3	A	1207	OLA	C15-C16-C17-C18
3	A	1215	OLA	C6-C7-C8-C9
3	A	1214	OLA	C3-C4-C5-C6
3	A	1206	OLA	C6-C7-C8-C9
3	A	1213	OLA	C11-C12-C13-C14
3	A	1205	OLA	C10-C11-C12-C13
3	A	1203	OLA	C7-C8-C9-C10
3	A	1215	OLA	C7-C8-C9-C10
3	A	1206	OLA	C3-C4-C5-C6
3	A	1213	OLA	C9-C10-C11-C12
2	A	1201	QK8	C15-C10-N3-C1
3	A	1211	OLA	C9-C10-C11-C12
4	A	1208	PGE	O2-C3-C4-O3

There are no ring outliers.

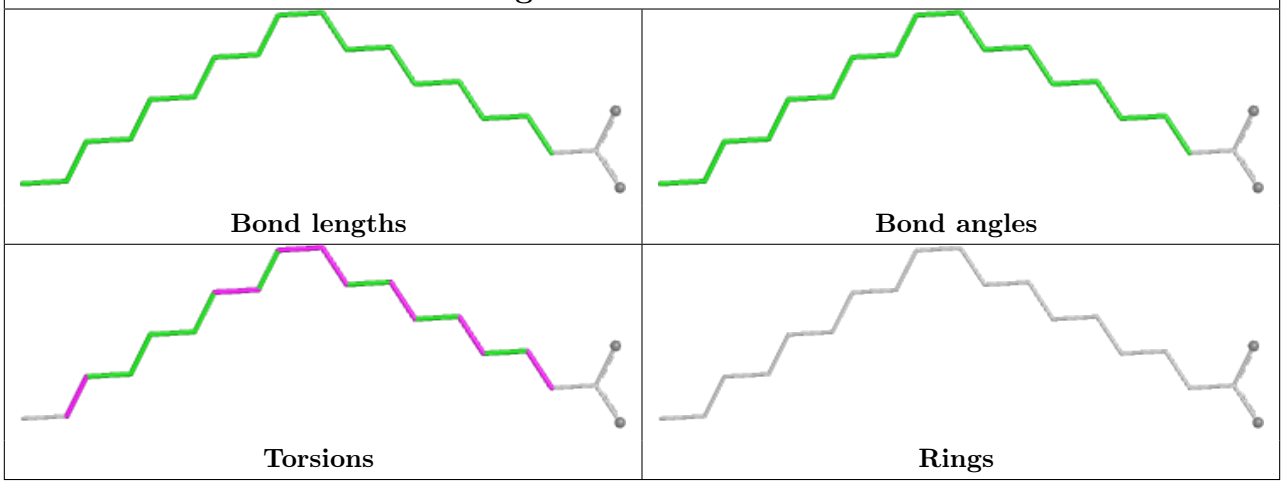
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1215	OLA	2	0
3	A	1207	OLA	1	0
3	A	1213	OLA	8	0
3	A	1205	OLA	2	0
3	A	1202	OLA	1	0

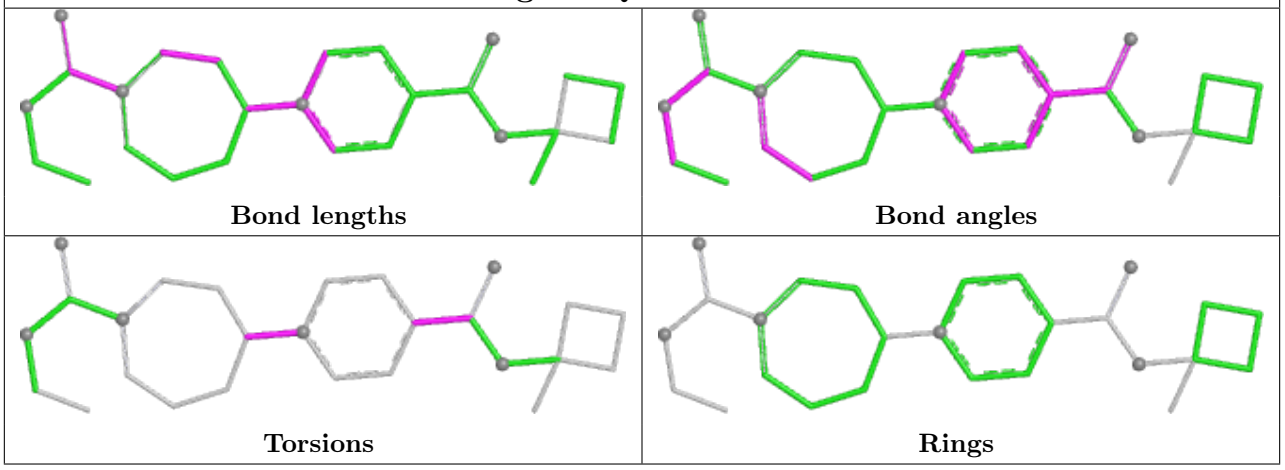
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

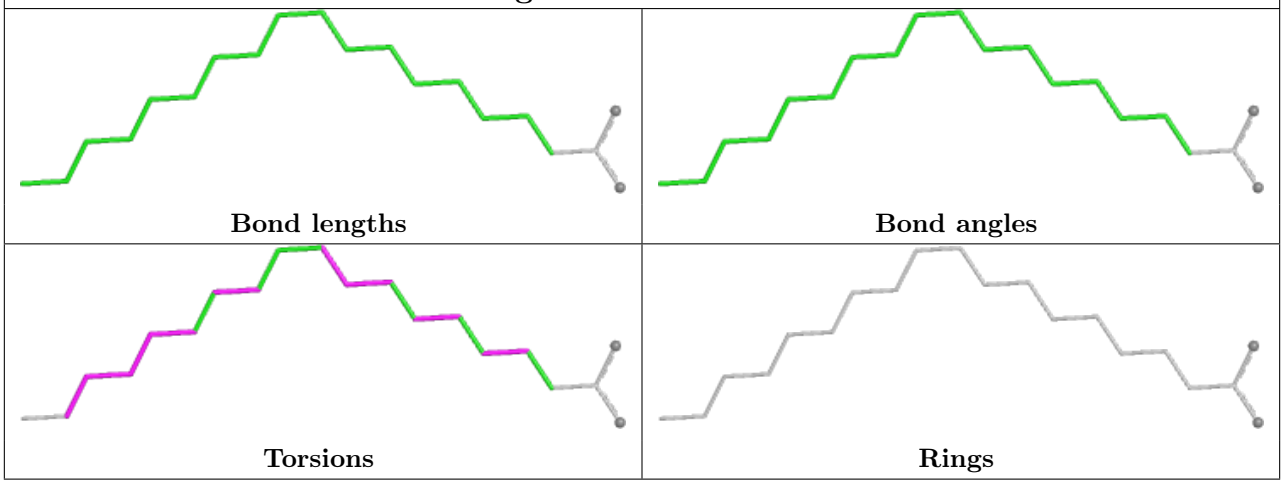
Ligand OLA A 1203



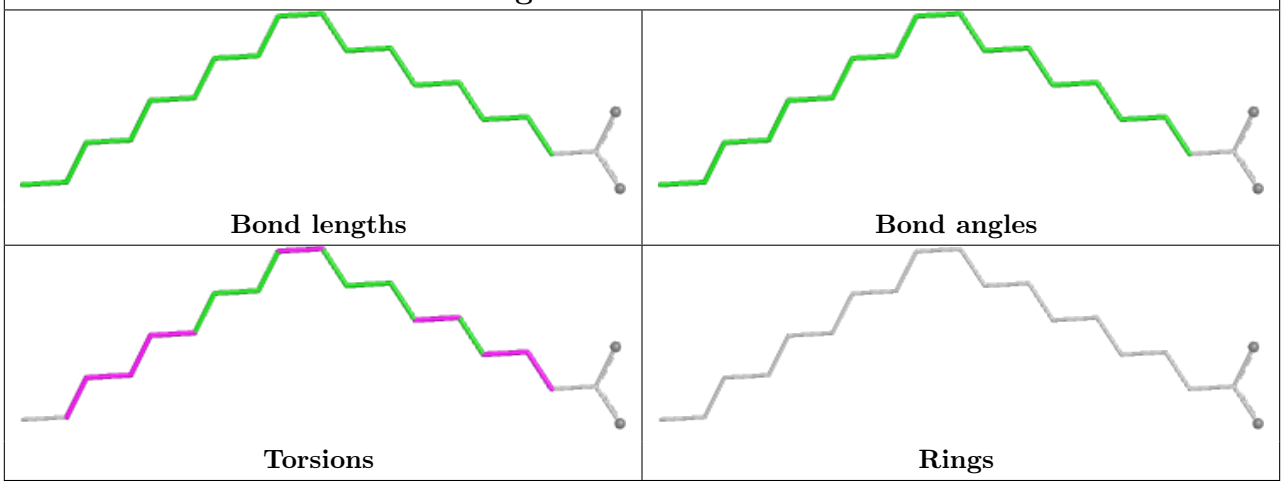
Ligand QK8 A 1201



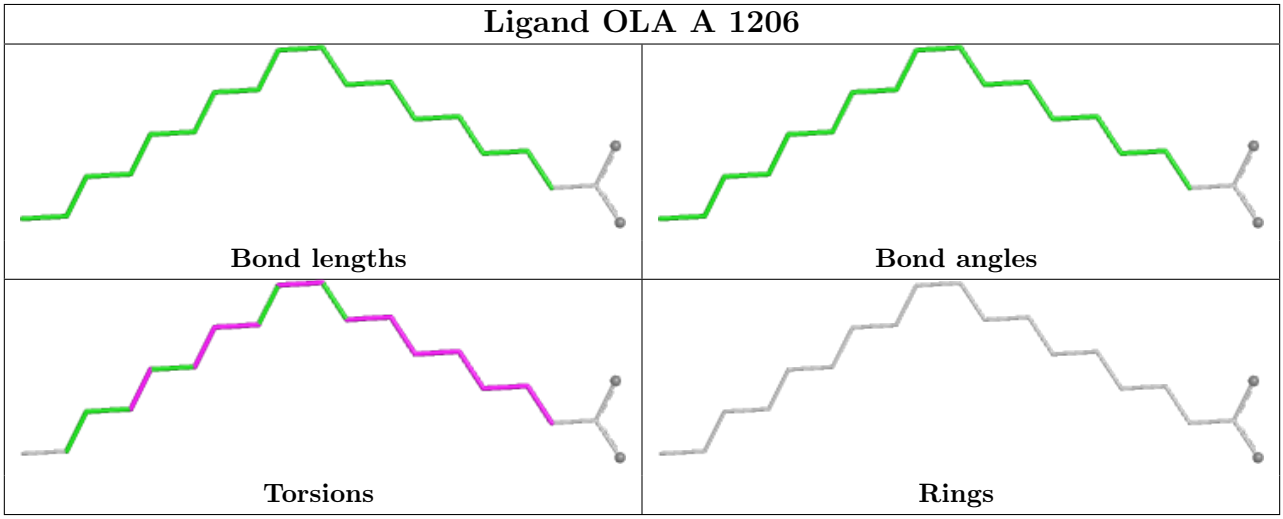
Ligand OLA A 1215



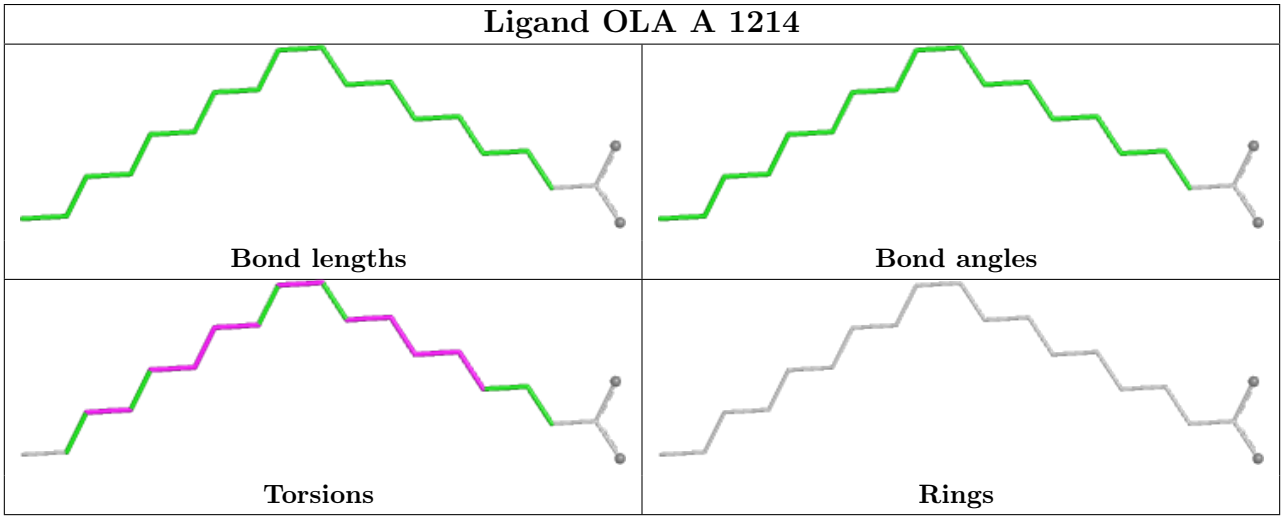
Ligand OLA A 1212



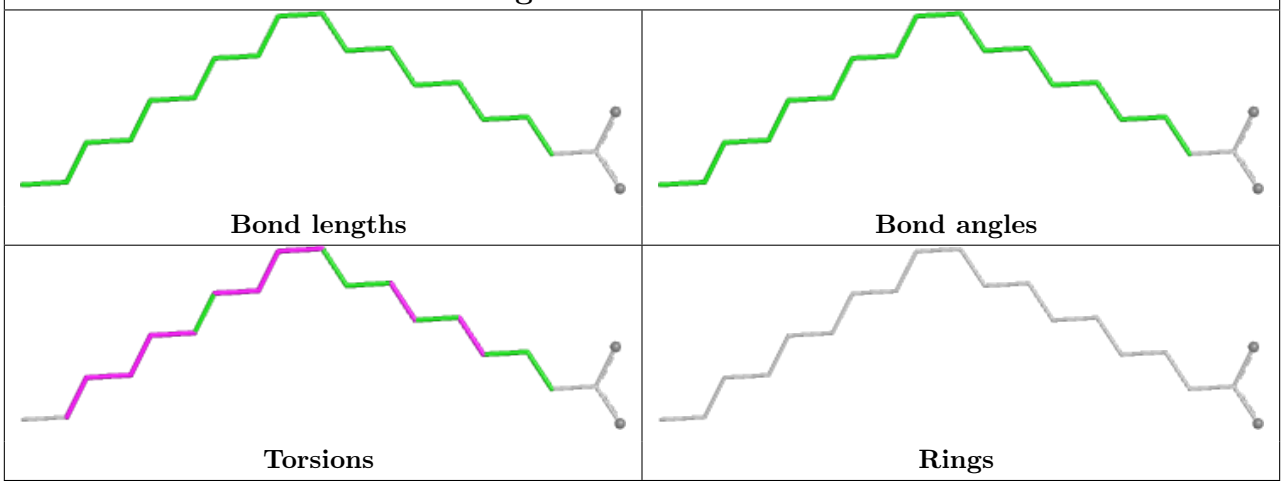
Ligand OLA A 1206



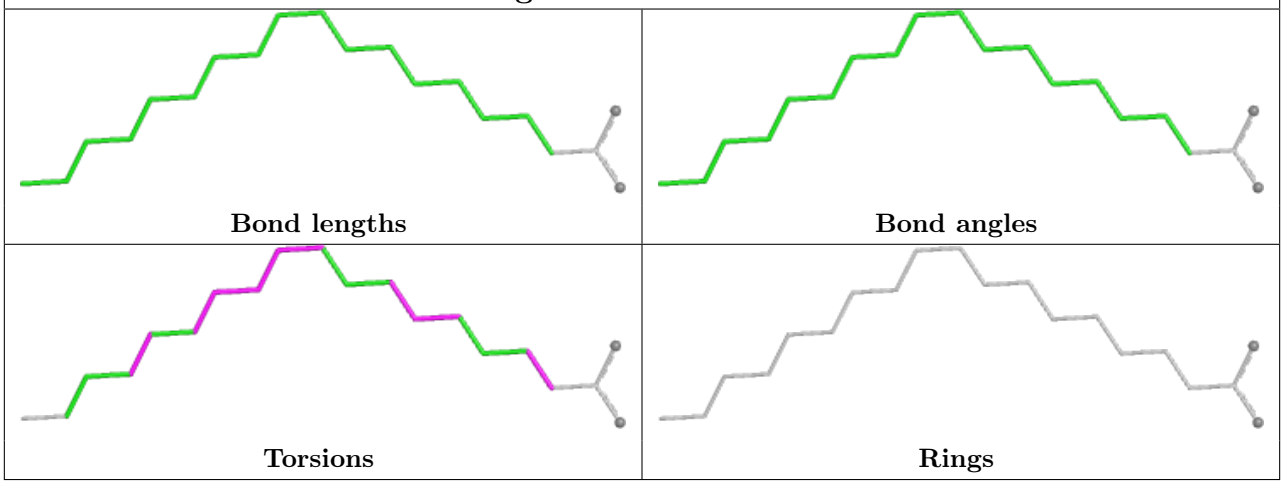
Ligand OLA A 1214



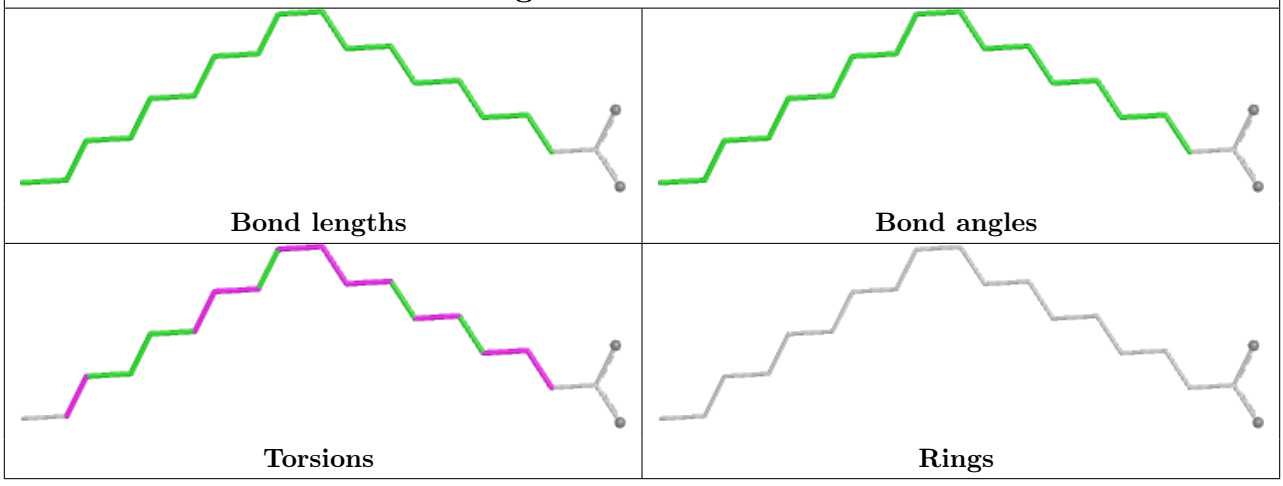
Ligand OLA A 1207

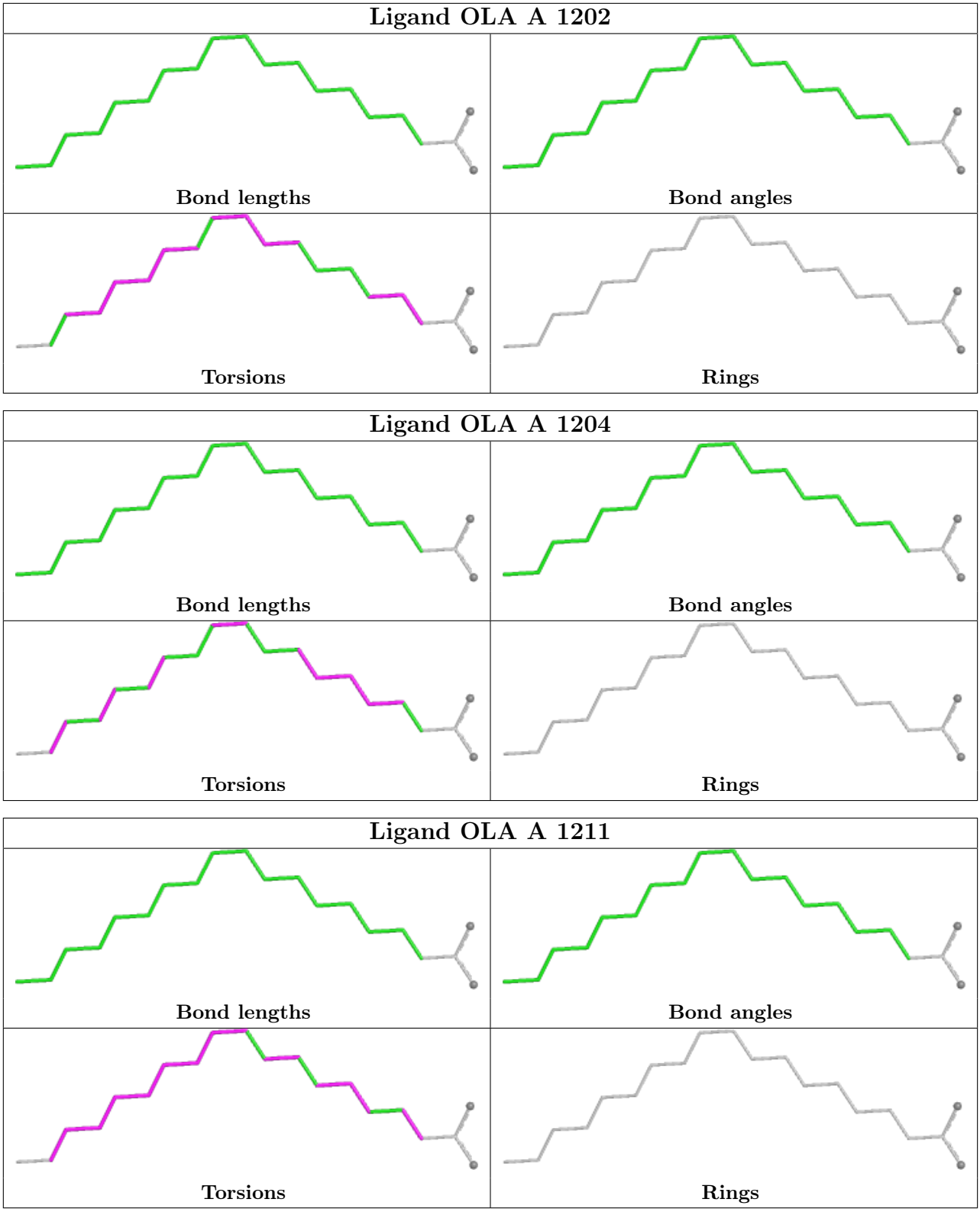


Ligand OLA A 1213



Ligand OLA A 1205





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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	446/455 (98%)	0.60	45 (10%)	7	11	12, 30, 60, 82	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	TRP	7.2
1	A	438	ASP	6.2
1	A	354	THR	6.2
1	A	1054	THR	5.6
1	A	1057	VAL	4.7
1	A	1047	ASP	4.6
1	A	1082	ALA	4.5
1	A	1080	ARG	4.1
1	A	1053	ASN	4.1
1	A	1079	LEU	4.1
1	A	1087	VAL	3.7
1	A	439	HIS	3.6
1	A	1017	ILE	3.5
1	A	23	VAL	3.5
1	A	1126	TRP	3.4
1	A	1090	SER	3.2
1	A	209	TRP	3.1
1	A	1085	LYS	3.1
1	A	1088	TYR	3.0
1	A	1046	LEU	3.0
1	A	1083	LYS	3.0
1	A	22	THR	2.9
1	A	20	MET	2.8
1	A	1122	GLN	2.8
1	A	1086	PRO	2.7
1	A	1081	ASN	2.7
1	A	434	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1076	ARG	2.6
1	A	1155	THR	2.6
1	A	355	PHE	2.6
1	A	135	ALA	2.6
1	A	1127	ASP	2.5
1	A	1055	ASN	2.5
1	A	1119	ARG	2.5
1	A	1108	GLU	2.4
1	A	390	PHE	2.4
1	A	435	ALA	2.4
1	A	1050	ILE	2.3
1	A	1089	ASP	2.3
1	A	21	GLU	2.2
1	A	1040	ASN	2.2
1	A	1091	LEU	2.2
1	A	1157	THR	2.1
1	A	1061	ASP	2.1
1	A	1044	SER	2.1

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	RSR	B-factors(Å^2)	Q<0.9
3	OLA	A	1212	20/20	0.57	0.51	67,75,82,82	0
3	OLA	A	1211	20/20	0.62	0.34	73,74,77,77	0
3	OLA	A	1207	20/20	0.63	0.38	68,70,73,73	0
5	PO4	A	1216	5/5	0.64	0.28	117,117,118,118	0
3	OLA	A	1206	20/20	0.65	0.44	54,58,63,63	0

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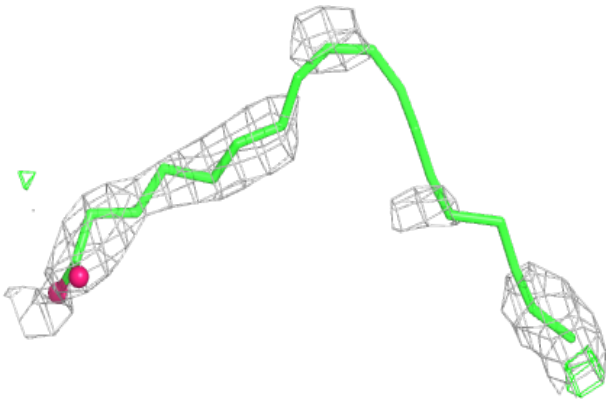
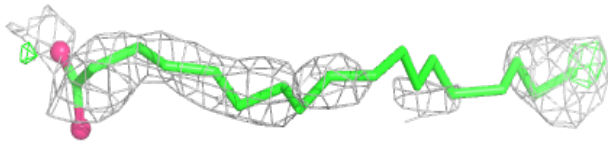
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	A	1215	20/20	0.72	0.29	42,51,59,59	0
4	PGE	A	1208	10/10	0.74	0.20	46,50,53,54	0
3	OLA	A	1213	20/20	0.75	0.30	51,57,59,59	0
3	OLA	A	1203	20/20	0.77	0.27	33,39,59,60	0
3	OLA	A	1205	20/20	0.79	0.28	44,50,60,60	0
3	OLA	A	1214	20/20	0.80	0.20	47,50,53,54	0
3	OLA	A	1204	20/20	0.82	0.19	33,40,57,60	0
3	OLA	A	1202	20/20	0.87	0.27	27,31,42,42	0
5	PO4	A	1210	5/5	0.92	0.26	79,80,82,82	0
5	PO4	A	1209	5/5	0.93	0.18	68,68,69,70	0
2	QK8	A	1201	26/26	0.96	0.15	13,15,29,30	0

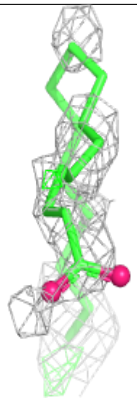
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1212:

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

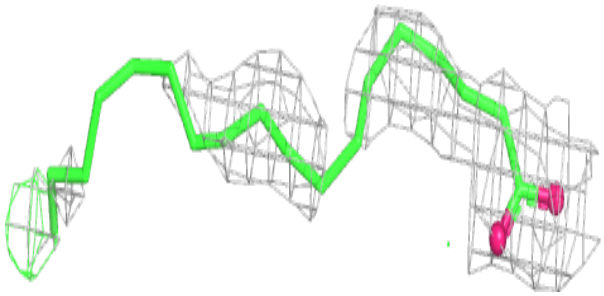


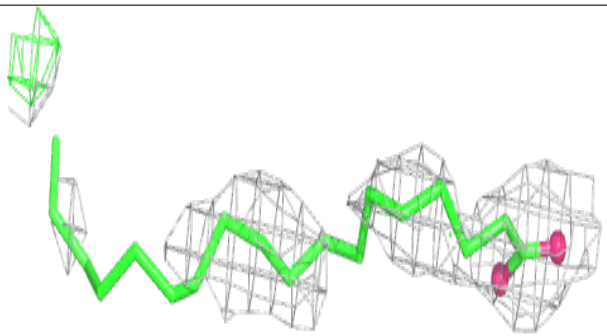


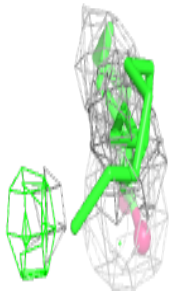


Electron density around OLA A 1211:

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

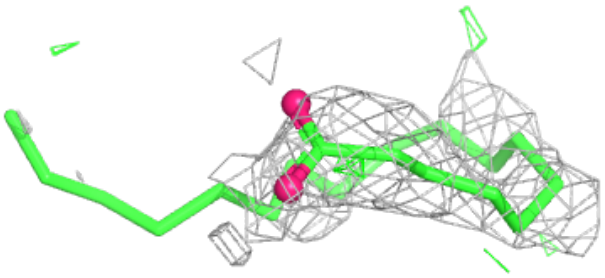


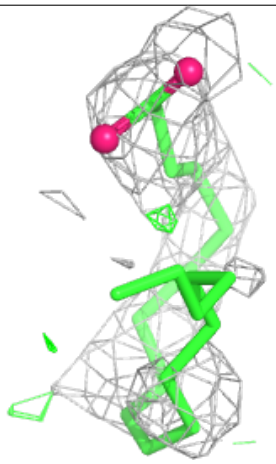




Electron density around OLA A 1207:

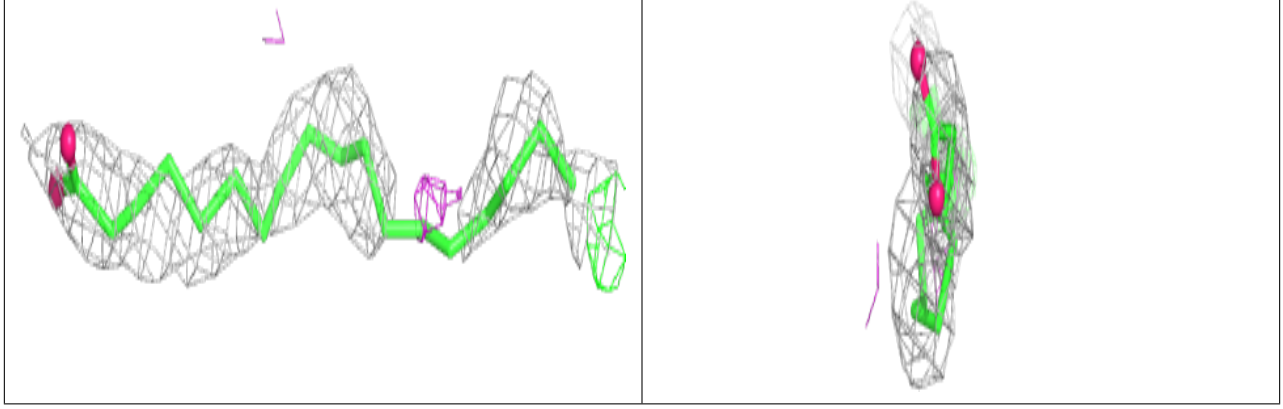
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





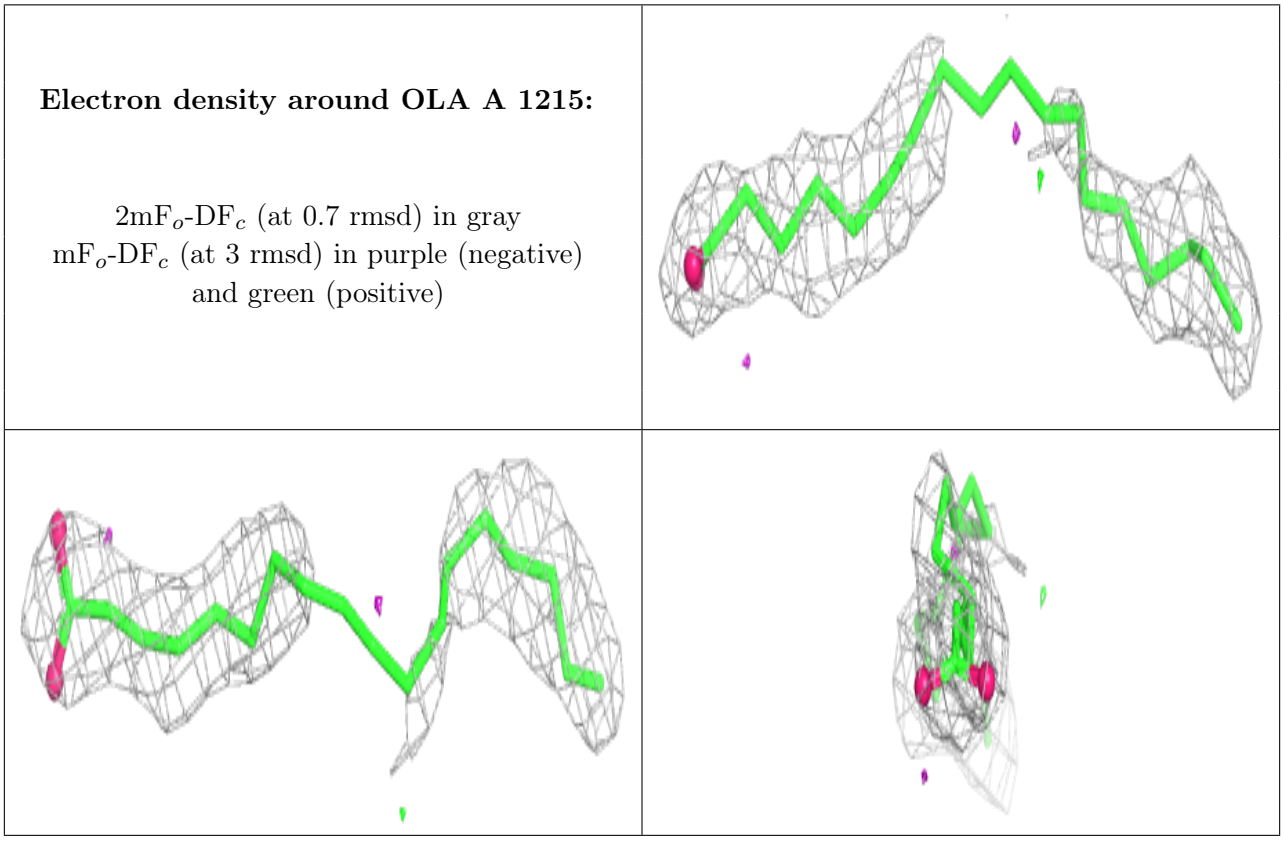
Electron density around OLA A 1206:

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



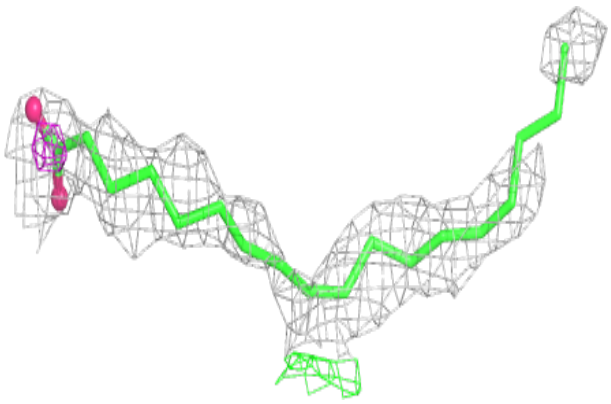
Electron density around OLA A 1215:

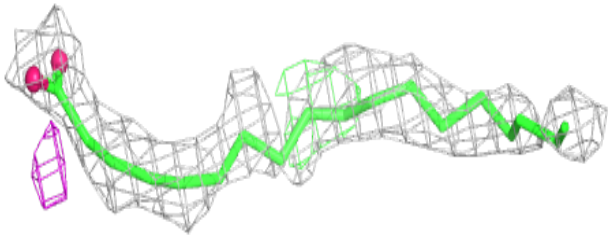
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

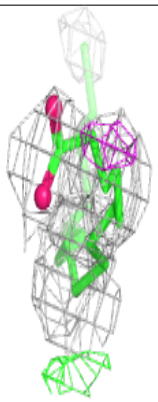


Electron density around OLA A 1213:

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

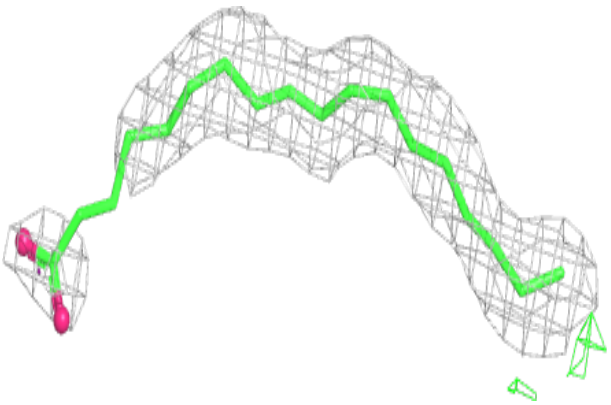


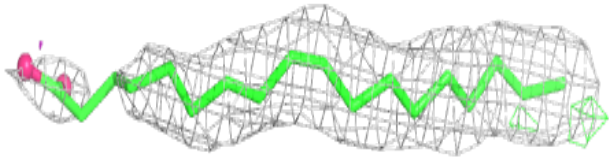


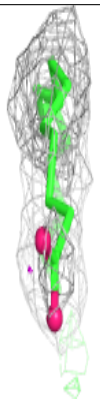


Electron density around OLA A 1203:

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

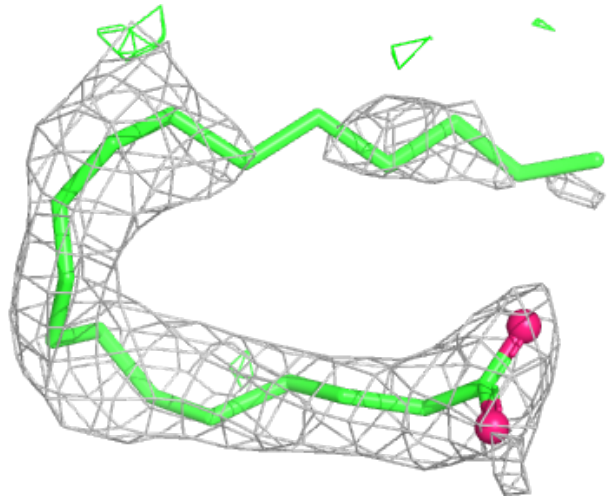


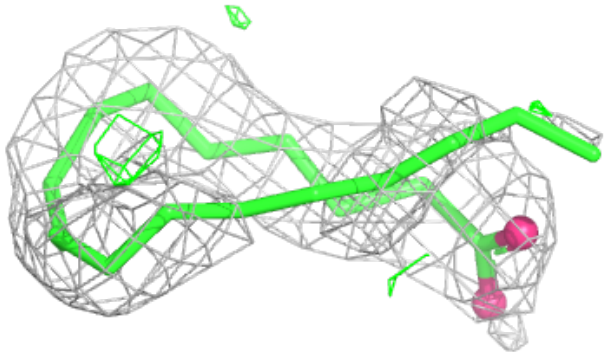


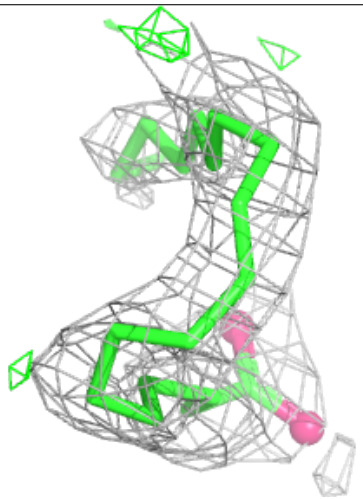


Electron density around OLA A 1205:

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

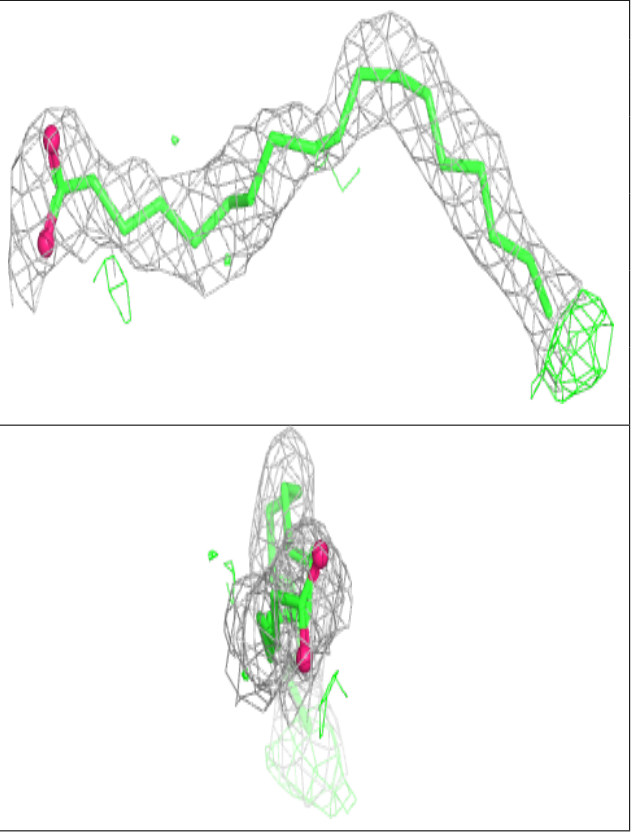


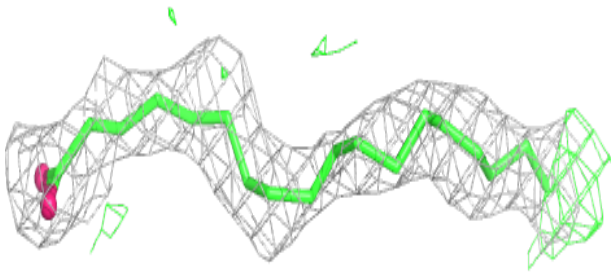




Electron density around OLA A 1214:

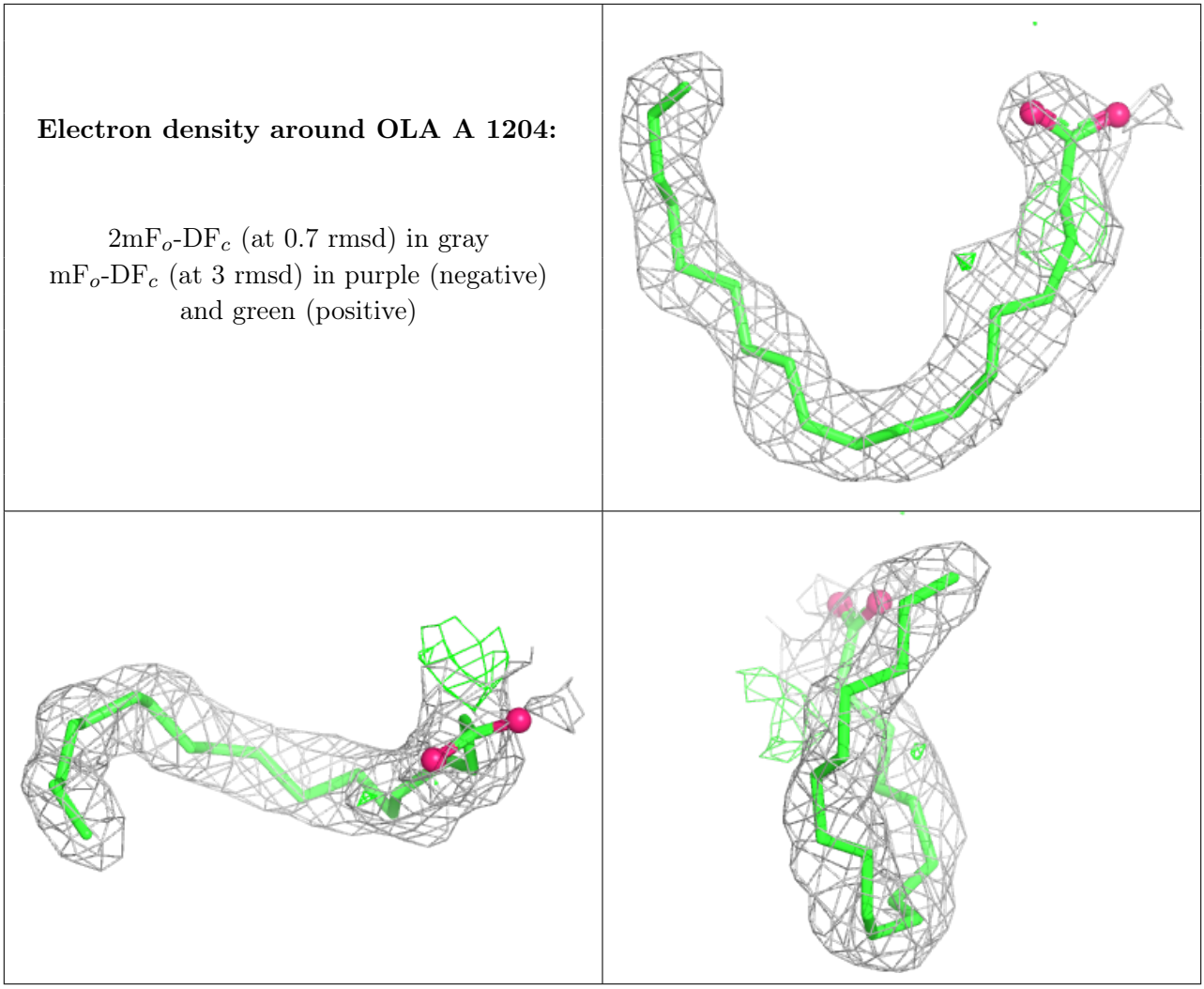
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





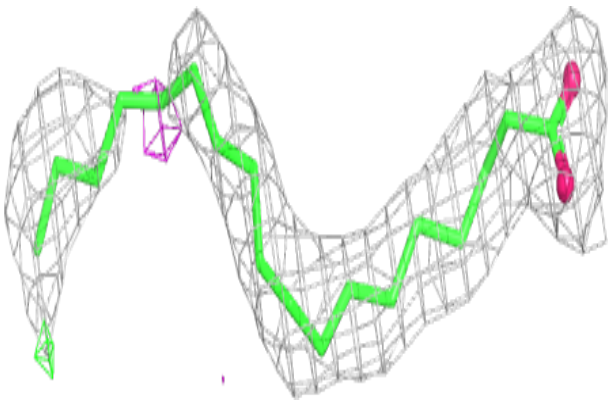
Electron density around OLA A 1204:

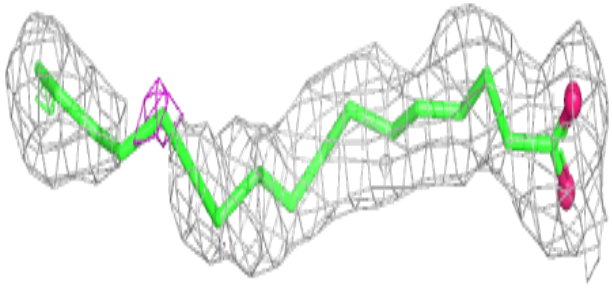
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

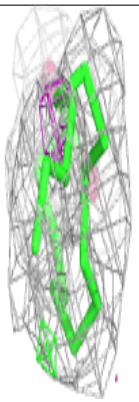


Electron density around OLA A 1202:

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

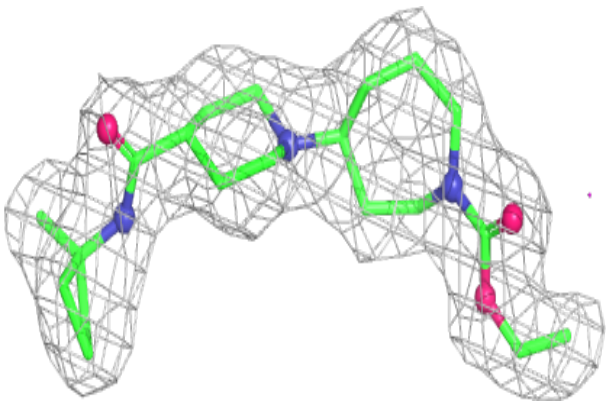


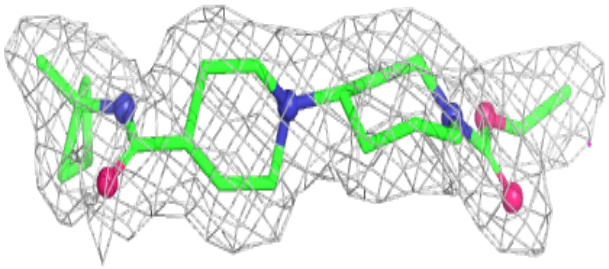


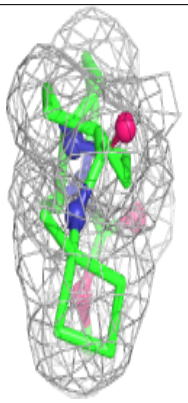


Electron density around QK8 A 1201:

$2mF_o$-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.