Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 12:12 am GMT

PDB ID	:	5EE7
Title	:	Crystal structure of the human glucagon receptor (GCGR) in complex with the antagonist MK-0893
Authors	:	Jazayeri, A.; Dore, A.S.; Lamb, D.; Krishnamurthy, H.; Southall, S.M.; Baig, A.H.; Bortolato, A.; Koglin, M.; Robertson, N.J.; Errey, J.C.; Andrews, S.P.; Brown, A.J.H.; Cooke, R.M.; Weir, M.; Marshall, F.H.
Deposited on	:	2015-10-22
Resolution	:	2.50 Å(reported)

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

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

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

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

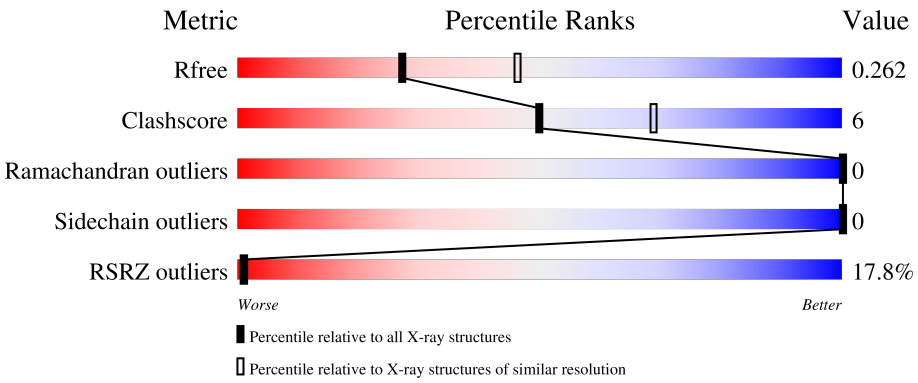
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	452	16% 79% 13% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3619 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 Glucagon receptor,Endolysin,Glucagon receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3331	2184	573	560	14	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	MET	engineered mutation	UNP P47871
A	154	ALA	GLY	engineered mutation	UNP P47871
A	173	ALA	ARG	engineered mutation	UNP P47871
A	182	LEU	ALA	engineered mutation	UNP P47871
A	190	ALA	SER	engineered mutation	UNP P47871
A	193	PHE	VAL	engineered mutation	UNP P47871
A	207	GLU	GLY	engineered mutation	UNP P47871
A	223	ALA	GLY	engineered mutation	UNP P47871
A	255	LEU	MET	linker	UNP P00720
A	1010	GLY	ARG	engineered mutation	UNP P00720
A	1052	THR	CYS	engineered mutation	UNP P00720
A	1095	ALA	CYS	engineered mutation	UNP P00720
A	1135	ARG	ILE	engineered mutation	UNP P00720
A	1159	TYR	-	linker	UNP P00720
A	276	ALA	MET	engineered mutation	UNP P47871
A	344	ALA	LYS	engineered mutation	UNP P47871
A	362	PHE	GLU	engineered mutation	UNP P47871
A	387	ALA	PHE	engineered mutation	UNP P47871
A	418	ALA	-	expression tag	UNP P47871
A	419	ALA	-	expression tag	UNP P47871
A	420	ALA	-	expression tag	UNP P47871
A	421	HIS	-	expression tag	UNP P47871
A	422	HIS	-	expression tag	UNP P47871
A	423	HIS	-	expression tag	UNP P47871
A	424	HIS	-	expression tag	UNP P47871
A	425	HIS	-	expression tag	UNP P47871
A	426	HIS	-	expression tag	UNP P47871

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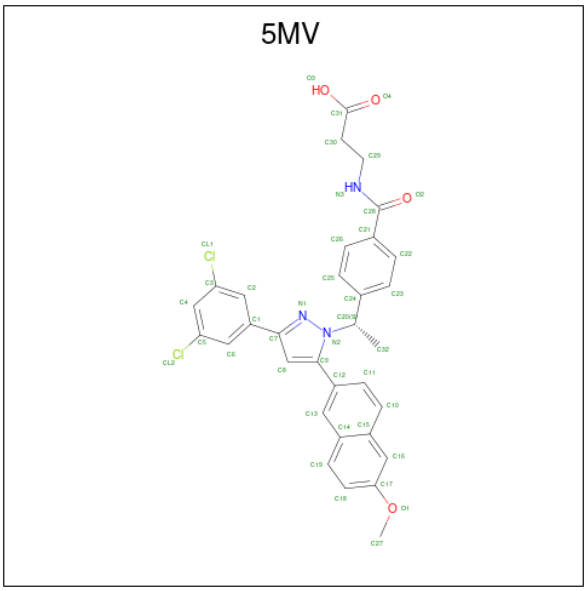
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP P47871
A	428	HIS	-	expression tag	UNP P47871
A	429	HIS	-	expression tag	UNP P47871
A	430	HIS	-	expression tag	UNP P47871

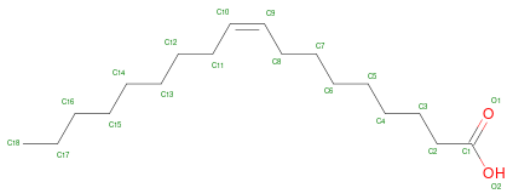
- Molecule 2 is 3-[[4-[(1 {S})-1-[3-[3,5-bis(chloranyl)phenyl]-5-(6-methoxynaphthalen-2-yl)pyrazol-1-yl]ethyl]phenyl]carbonylamino]propanoic acid (three-letter code: 5MV) (formula: $C_{32}H_{27}Cl_2N_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	41	32	2	3	4	0	0

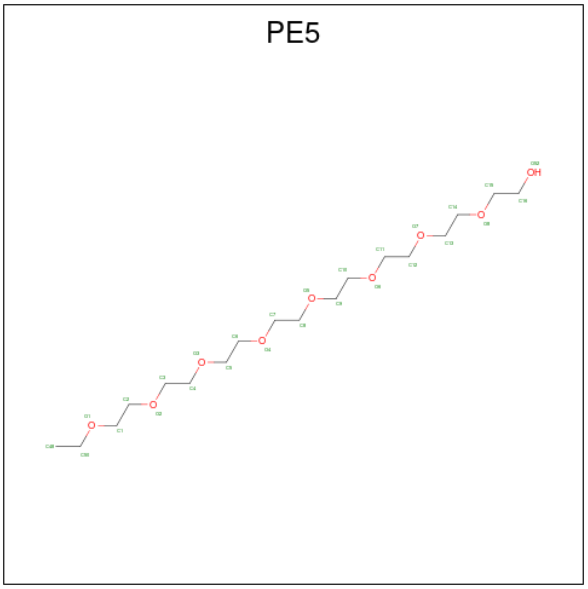
- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

OLA



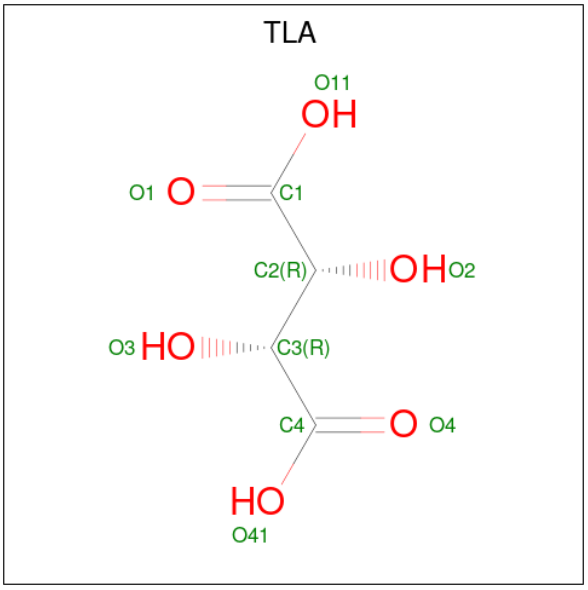
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 8 2	0	0
3	A	1	Total C O 15 13 2	0	0
3	A	1	Total C O 15 13 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 11 9 2	0	0

- Molecule 4 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: $C_{18}H_{38}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	24	16	8	0	0

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 6 is water.

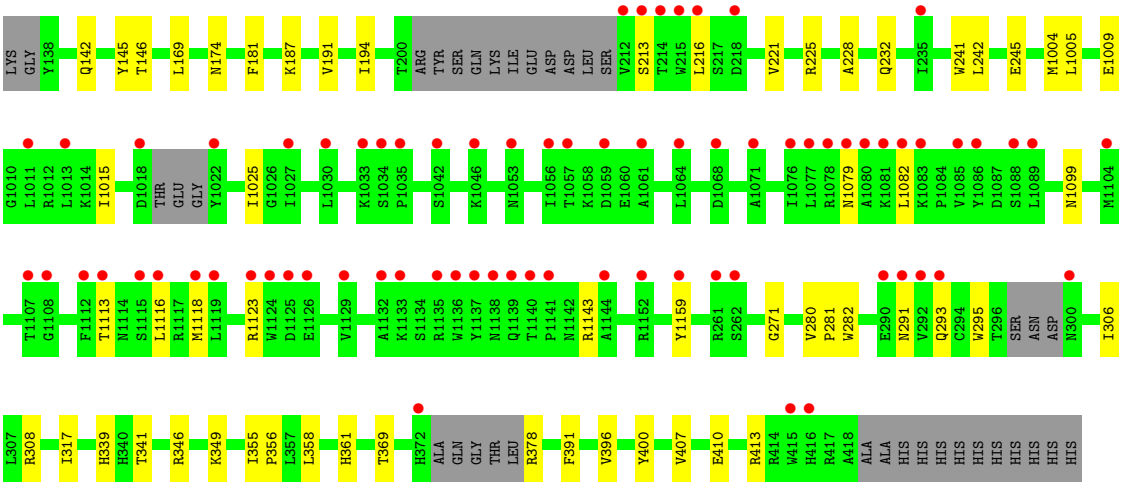
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	24	24	24	0	0

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: Glucagon receptor,Endolysin,Glucagon receptor

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.58Å 71.48Å 183.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 32.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (19.97-2.50) 89.7 (32.73-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.263 0.228 , 0.262	Depositor DCC
R_{free} test set	777 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3619	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PE5, OLA, 5MV, TLA

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	0.26	0/3408	0.43	0/4618

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3331	0	3403	38	0
2	A	41	0	0	2	0
3	A	189	0	271	6	0
4	A	24	0	33	7	0
5	A	10	0	4	1	0
6	A	24	0	0	0	0
All	All	3619	0	3711	42	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 6.

All (42) 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:306:ILE:H	1:A:306:ILE:HD12	1.42	0.84
1:A:391:PHE:HB3	3:A:1204:OLA:H9	1.69	0.74
1:A:1118:MET:HG2	1:A:1123:ARG:HH21	1.54	0.71
1:A:308:ARG:NH2	1:A:369:THR:OG1	2.25	0.68
1:A:242:LEU:HD21	1:A:355:ILE:HA	1.77	0.67
1:A:369:THR:O	1:A:378:ARG:NH1	2.28	0.66
1:A:225:ARG:NH1	1:A:293:GLN:O	2.26	0.66
1:A:356:PRO:HA	5:A:1217:TLA:H2	1.81	0.62
1:A:242:LEU:HD22	1:A:358:LEU:HD12	1.80	0.62
1:A:410:GLU:OE1	1:A:413:ARG:NH2	2.27	0.58
1:A:1113:THR:HA	1:A:1116:LEU:HD12	1.87	0.56
1:A:191:VAL:HG13	4:A:1216:PE5:H111	1.86	0.56
3:A:1212:OLA:H9	3:A:1213:OLA:H51	1.87	0.56
1:A:339:HIS:NE2	1:A:341:THR:OG1	2.40	0.55
1:A:194:ILE:HG21	4:A:1216:PE5:H132	1.89	0.55
1:A:1079:ASN:HB3	1:A:1082:LEU:HB2	1.90	0.54
1:A:1005:LEU:HD21	1:A:1099:ASN:HA	1.90	0.53
2:A:1201:5MV:CL1	3:A:1214:OLA:H71	2.46	0.53
1:A:245:GLU:HG2	1:A:400:TYR:OH	2.10	0.52
1:A:213:SER:HA	1:A:216:LEU:HD13	1.92	0.52
1:A:1004:MET:HG3	1:A:1159:TYR:CZ	2.44	0.52
1:A:142:GLN:HA	1:A:145:TYR:CE2	2.45	0.51
2:A:1201:5MV:CL1	3:A:1214:OLA:H52	2.49	0.50
1:A:181:PHE:HE1	1:A:396:VAL:HG12	1.76	0.50
1:A:169:LEU:O	1:A:174:ASN:ND2	2.31	0.49
1:A:241:TRP:CE2	1:A:271:GLY:HA3	2.48	0.48
1:A:1009:GLU:OE2	1:A:1143:ARG:NH1	2.35	0.48
1:A:346:ARG:HA	1:A:349:LYS:HD3	1.96	0.47
1:A:146:THR:HG21	3:A:1206:OLA:H42	1.96	0.47
4:A:1216:PE5:H101	4:A:1216:PE5:H81	1.70	0.46
1:A:361:HIS:CD2	4:A:1216:PE5:H21	2.50	0.46
1:A:216:LEU:HB3	1:A:221:VAL:HG13	1.96	0.46
1:A:145:TYR:CZ	4:A:1216:PE5:H102	2.50	0.45
1:A:187:LYS:HZ1	4:A:1216:PE5:H11	1.81	0.45
1:A:228:ALA:O	1:A:232:GLN:HG2	2.18	0.44
1:A:187:LYS:NZ	4:A:1216:PE5:H11	2.32	0.44
1:A:291:ASN:HA	1:A:295:TRP:HE1	1.83	0.43
1:A:169:LEU:HD13	1:A:407:VAL:HG22	2.02	0.42
1:A:317:ILE:HG12	3:A:1209:OLA:H132	2.01	0.41
1:A:280:VAL:HB	1:A:281:PRO:HD3	2.02	0.41
1:A:282:TRP:NE1	1:A:306:ILE:HD13	2.35	0.41
1:A:1015:ILE:HG23	1:A:1025:ILE:HD12	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	406/452 (90%)	397 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	348/378 (92%)	348 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	1139	GLN

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)

17 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	1211	-	6,6,19	0.13	0	5,5,19	0.26	0
3	OLA	A	1214	-	13,13,19	0.57	0	12,13,19	0.78	0
4	PE5	A	1216	-	23,23,26	0.63	0	22,22,25	0.42	0
3	OLA	A	1212	-	10,10,19	0.27	0	8,9,19	0.34	0
3	OLA	A	1205	-	10,10,19	0.61	0	10,10,19	0.84	0
3	OLA	A	1207	-	19,19,19	0.47	0	19,19,19	0.68	0
3	OLA	A	1208	-	19,19,19	0.48	0	19,19,19	0.68	0
3	OLA	A	1213	-	6,6,19	0.14	0	5,5,19	0.28	0
2	5MV	A	1201	-	45,45,45	1.25	3 (6%)	61,64,64	0.91	0
3	OLA	A	1202	-	9,9,19	0.64	0	9,9,19	0.92	0
3	OLA	A	1210	-	16,16,19	0.51	0	16,16,19	0.72	0
3	OLA	A	1215	-	10,10,19	0.61	0	10,10,19	0.85	0
3	OLA	A	1206	-	10,10,19	0.60	0	10,10,19	0.87	0
3	OLA	A	1209	-	19,19,19	0.47	0	19,19,19	0.69	0
3	OLA	A	1204	-	14,14,19	0.55	0	14,14,19	0.74	0
5	TLA	A	1217	-	9,9,9	1.01	0	12,12,12	1.35	2 (16%)
3	OLA	A	1203	-	14,14,19	0.56	0	14,14,19	0.75	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	1211	-	-	2/4/4/17	-
3	OLA	A	1214	-	-	3/11/11/17	-
4	PE5	A	1216	-	-	10/21/21/24	-
3	OLA	A	1212	-	-	4/8/8/17	-
3	OLA	A	1205	-	-	2/8/8/17	-
3	OLA	A	1207	-	-	9/17/17/17	-
3	OLA	A	1208	-	-	5/17/17/17	-
3	OLA	A	1213	-	-	0/4/4/17	-
2	5MV	A	1201	-	-	4/26/28/28	0/5/5/5
3	OLA	A	1202	-	-	6/7/7/17	-
3	OLA	A	1210	-	-	5/14/14/17	-
3	OLA	A	1215	-	-	6/8/8/17	-
3	OLA	A	1206	-	-	6/8/8/17	-
3	OLA	A	1209	-	-	7/17/17/17	-
3	OLA	A	1204	-	-	7/12/12/17	-
5	TLA	A	1217	-	-	8/12/12/12	-
3	OLA	A	1203	-	-	5/12/12/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	5MV	C16-C17	2.81	1.42	1.37
2	A	1201	5MV	C19-C18	2.24	1.41	1.36
2	A	1201	5MV	C25-C24	2.08	1.42	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1217	TLA	O41-C4-C3	2.61	120.33	113.27
5	A	1217	TLA	O11-C1-C2	2.48	119.97	113.27

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	OLA	C10-C11-C12-C13
3	A	1212	OLA	C9-C10-C11-C12
5	A	1217	TLA	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	1217	TLA	O3-C3-C4-O41
3	A	1215	OLA	C1-C2-C3-C4
3	A	1209	OLA	C1-C2-C3-C4
3	A	1210	OLA	C5-C6-C7-C8
3	A	1206	OLA	C3-C4-C5-C6
3	A	1206	OLA	C1-C2-C3-C4
3	A	1214	OLA	C5-C6-C7-C8
3	A	1203	OLA	C10-C11-C12-C13
5	A	1217	TLA	C2-C3-C4-O4
3	A	1204	OLA	C1-C2-C3-C4
5	A	1217	TLA	C2-C3-C4-O41
3	A	1215	OLA	C2-C3-C4-C5
3	A	1207	OLA	C6-C7-C8-C9
3	A	1207	OLA	C10-C11-C12-C13
3	A	1207	OLA	C11-C12-C13-C14
3	A	1215	OLA	C5-C6-C7-C8
3	A	1208	OLA	C11-C12-C13-C14
3	A	1212	OLA	C3-C4-C5-C6
3	A	1215	OLA	C6-C7-C8-C9
3	A	1204	OLA	C6-C7-C8-C9
5	A	1217	TLA	O11-C1-C2-C3
3	A	1211	OLA	C5-C6-C7-C8
3	A	1212	OLA	C2-C3-C4-C5
4	A	1216	PE5	C10-C9-O5-C8
3	A	1203	OLA	C6-C7-C8-C9
3	A	1207	OLA	C14-C15-C16-C17
3	A	1206	OLA	C5-C6-C7-C8
2	A	1201	5MV	C18-C17-O1-C27
3	A	1207	OLA	C15-C16-C17-C18
5	A	1217	TLA	O1-C1-C2-C3
3	A	1208	OLA	C14-C15-C16-C17
3	A	1211	OLA	C2-C3-C4-C5
2	A	1201	5MV	C16-C17-O1-C27
4	A	1216	PE5	O6-C11-C12-O7
3	A	1215	OLA	C4-C5-C6-C7
3	A	1202	OLA	C4-C5-C6-C7
3	A	1207	OLA	C5-C6-C7-C8
3	A	1214	OLA	C9-C10-C11-C12
3	A	1214	OLA	C2-C3-C4-C5
4	A	1216	PE5	C2-C1-O1-C50
3	A	1206	OLA	C6-C7-C8-C9
2	A	1201	5MV	C29-C30-C31-O3

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Mol	Chain	Res	Type	Atoms
2	A	1201	5MV	C29-C30-C31-O4
4	A	1216	PE5	O1-C1-C2-O2
4	A	1216	PE5	C8-C7-O4-C6
3	A	1202	OLA	C5-C6-C7-C8
4	A	1216	PE5	C1-C2-O2-C3
4	A	1216	PE5	O7-C13-C14-O8
3	A	1208	OLA	C13-C14-C15-C16
3	A	1202	OLA	C2-C3-C4-C5
3	A	1207	OLA	C9-C10-C11-C12
3	A	1209	OLA	C7-C8-C9-C10
3	A	1209	OLA	C4-C5-C6-C7
5	A	1217	TLA	O11-C1-C2-O2
4	A	1216	PE5	C7-C8-O5-C9
3	A	1206	OLA	O1-C1-C2-C3
3	A	1209	OLA	C12-C13-C14-C15
3	A	1205	OLA	O1-C1-C2-C3
3	A	1202	OLA	C1-C2-C3-C4
4	A	1216	PE5	C48-C50-O1-C1
3	A	1204	OLA	O1-C1-C2-C3
3	A	1206	OLA	O2-C1-C2-C3
5	A	1217	TLA	O1-C1-C2-O2
3	A	1204	OLA	O2-C1-C2-C3
3	A	1205	OLA	O2-C1-C2-C3
3	A	1203	OLA	C7-C8-C9-C10
3	A	1209	OLA	C9-C10-C11-C12
4	A	1216	PE5	C5-C6-O4-C7
3	A	1203	OLA	C9-C10-C11-C12
3	A	1209	OLA	O1-C1-C2-C3
3	A	1210	OLA	C4-C5-C6-C7
3	A	1208	OLA	C7-C8-C9-C10
3	A	1210	OLA	C9-C10-C11-C12
3	A	1207	OLA	C13-C14-C15-C16
3	A	1203	OLA	C4-C5-C6-C7
3	A	1207	OLA	C7-C8-C9-C10
3	A	1209	OLA	O2-C1-C2-C3
3	A	1204	OLA	C7-C8-C9-C10
3	A	1212	OLA	C7-C8-C9-C10
3	A	1208	OLA	C9-C10-C11-C12
3	A	1204	OLA	C2-C3-C4-C5
3	A	1210	OLA	C7-C8-C9-C10
3	A	1202	OLA	O2-C1-C2-C3
3	A	1210	OLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	1202	OLA	O1-C1-C2-C3
3	A	1215	OLA	O1-C1-C2-C3

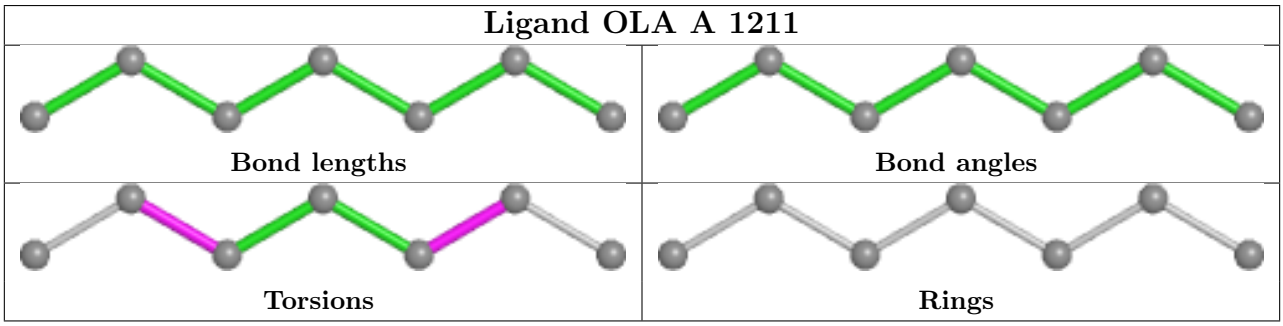
There are no ring outliers.

9 monomers are involved in 14 short contacts:

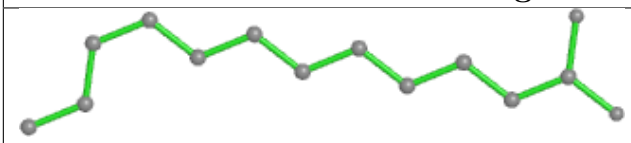
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1214	OLA	2	0
4	A	1216	PE5	7	0
3	A	1212	OLA	1	0
3	A	1213	OLA	1	0
2	A	1201	5MV	2	0
3	A	1206	OLA	1	0
3	A	1209	OLA	1	0
3	A	1204	OLA	1	0
5	A	1217	TLA	1	0

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.

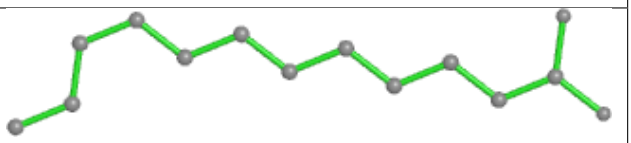
Ligand OLA A 1211



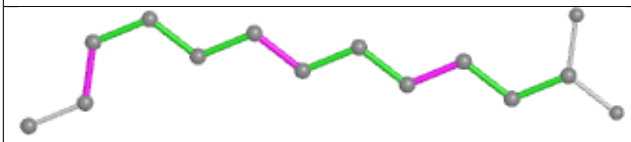
Ligand OLA A 1214



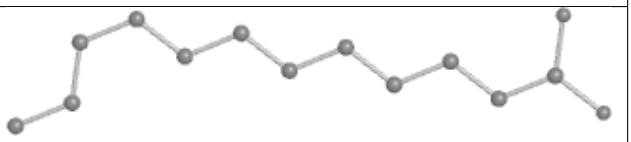
Bond lengths



Bond angles

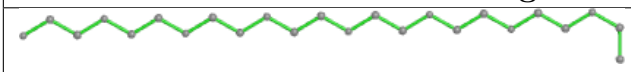


Torsions



Rings

Ligand PE5 A 1216



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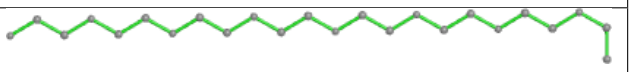
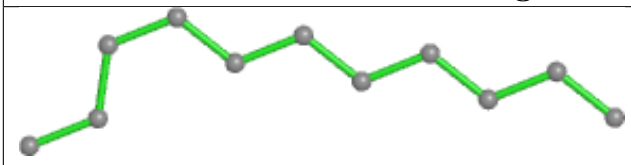


Bond angles

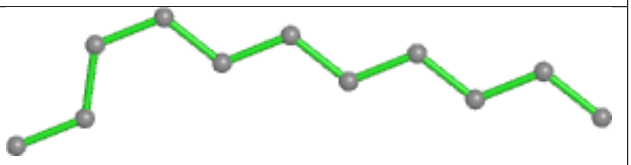
Torsions

Rings

Ligand OLA A 1212



Bond lengths



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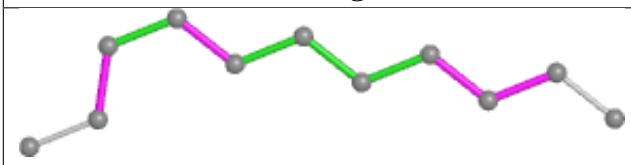
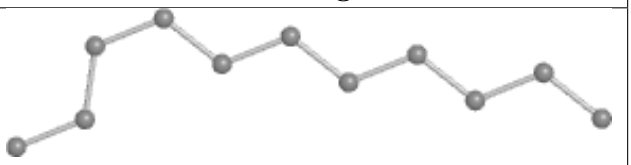
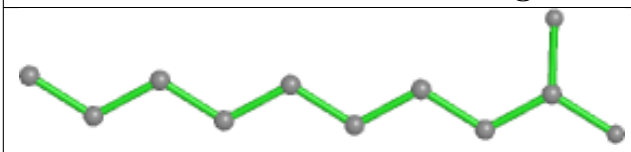


Torsions



Rings

Ligand OLA A 1205



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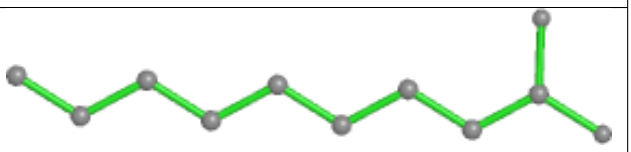
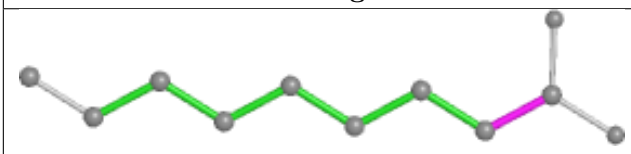
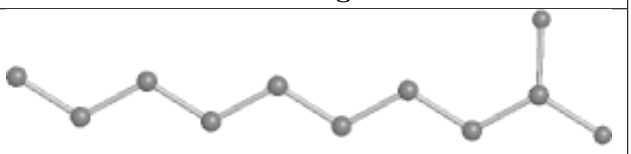


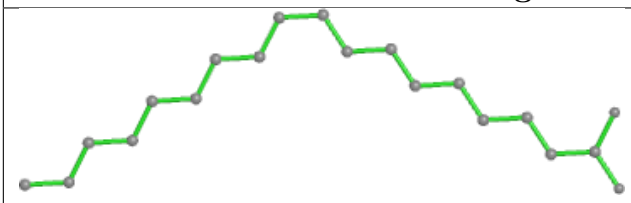
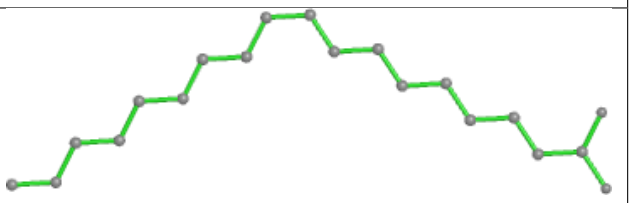
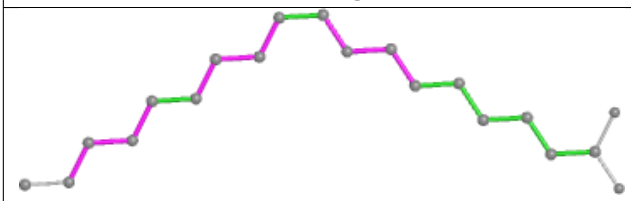
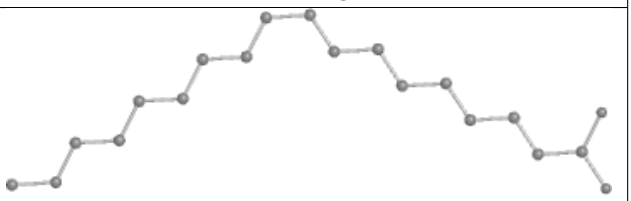
Bond angles



Torsions



Rings

Ligand OLA A 1207	
 Bond lengths	 Bond angles
 Torsions	 Rings

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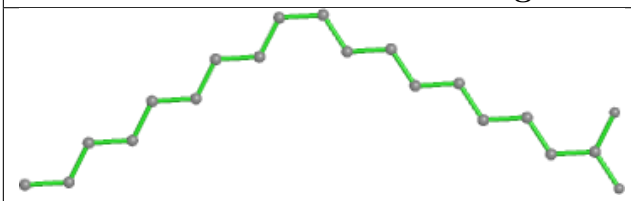
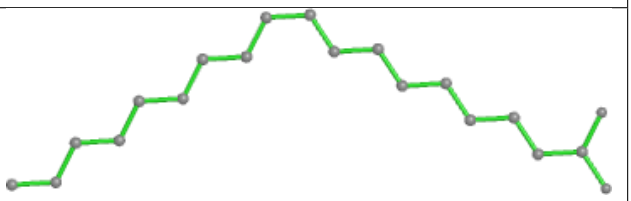
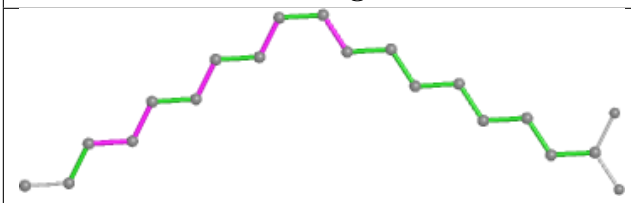
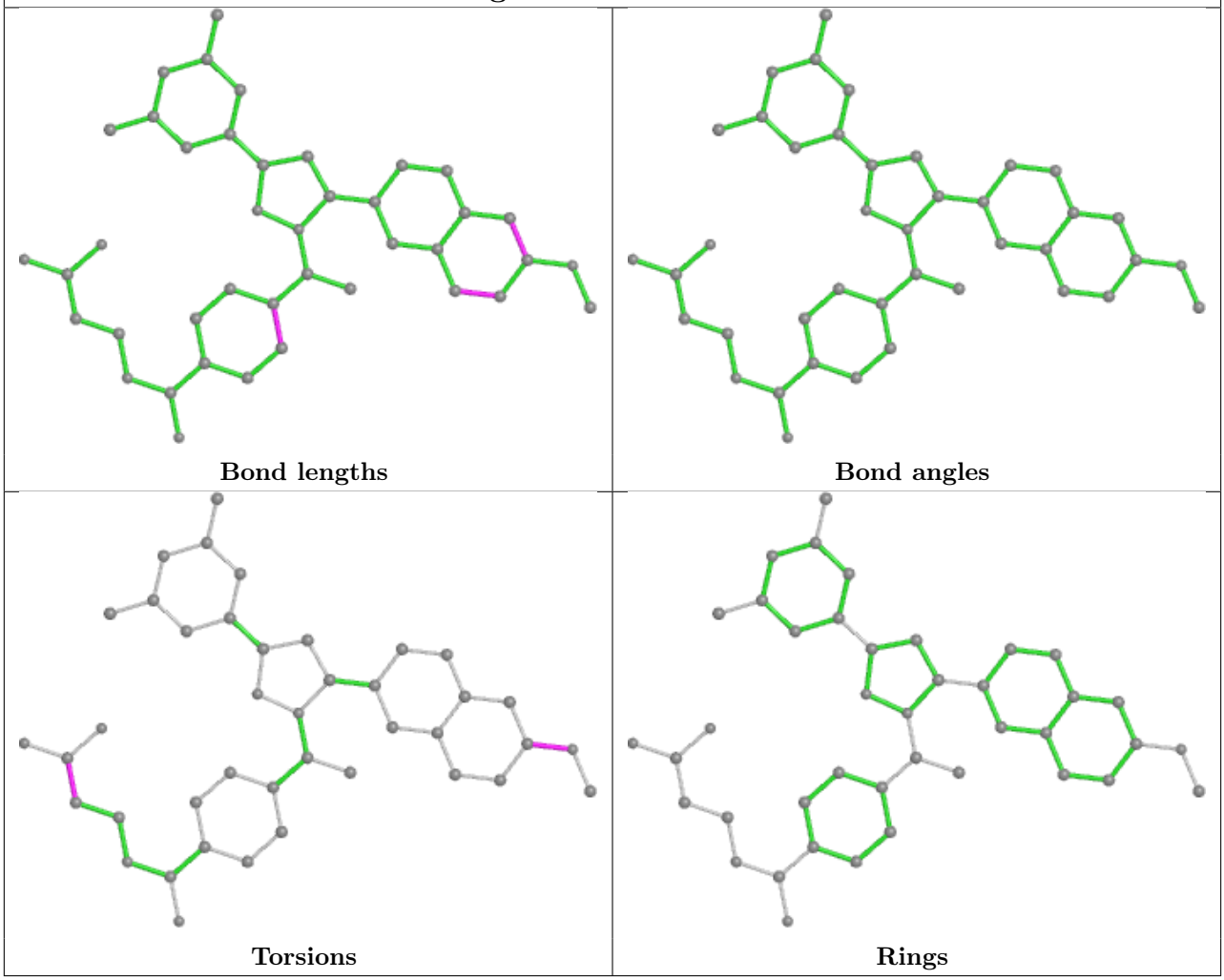
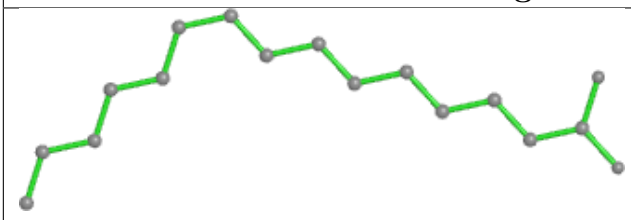
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand 5MV A 1201

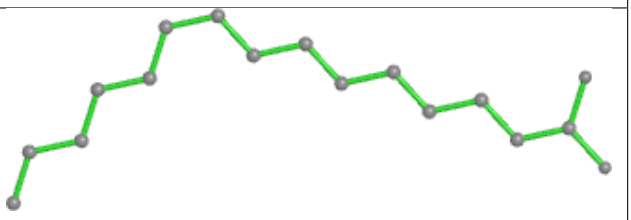


Ligand OLA A 1202

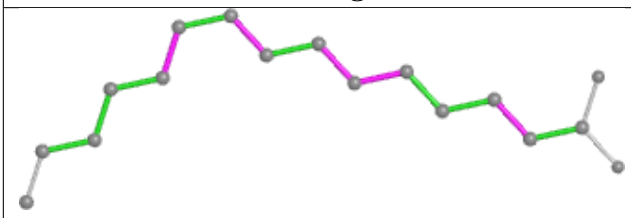
Ligand OLA A 1210



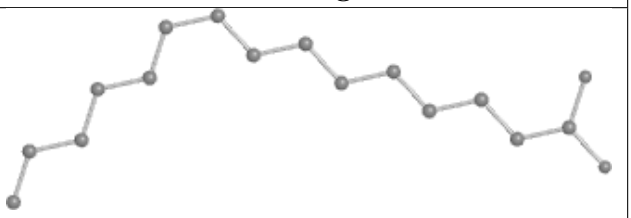
Bond lengths



Bond angles

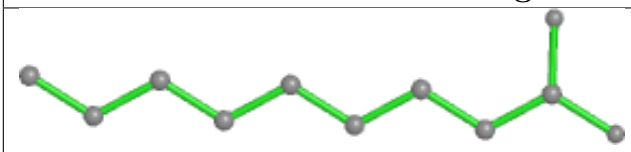


Torsions



Rings

Ligand OLA A 1215



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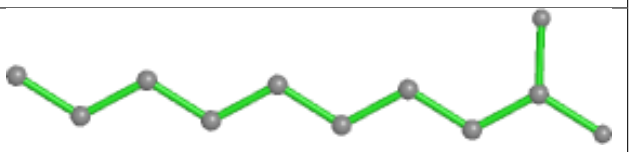
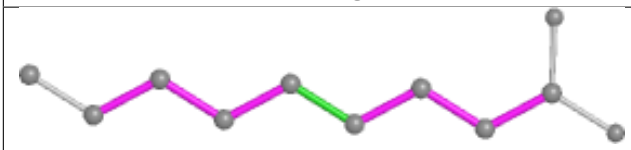


Bond angles



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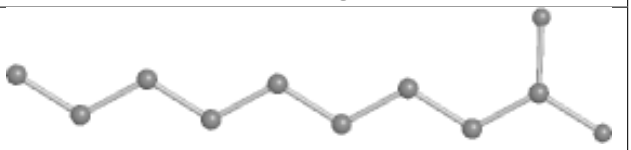
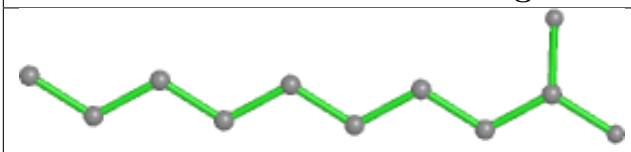


Rings

Ligand OLA A 1206



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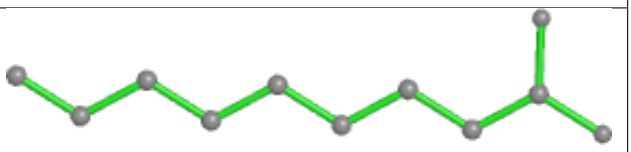
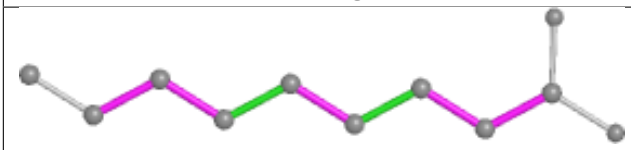


Bond angles



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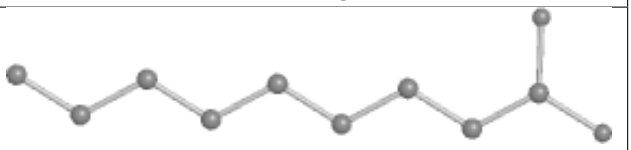

Rings

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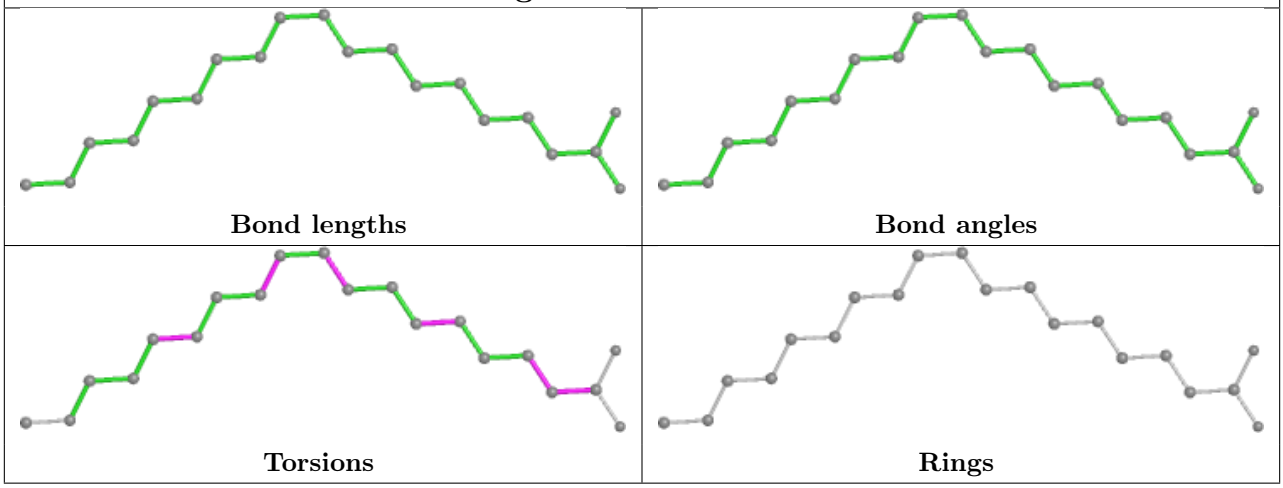

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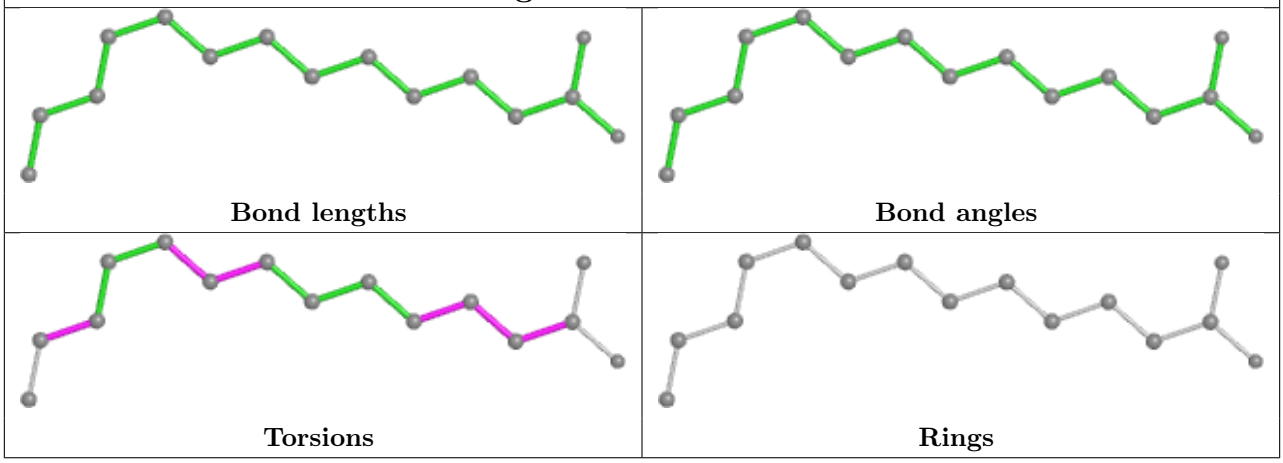
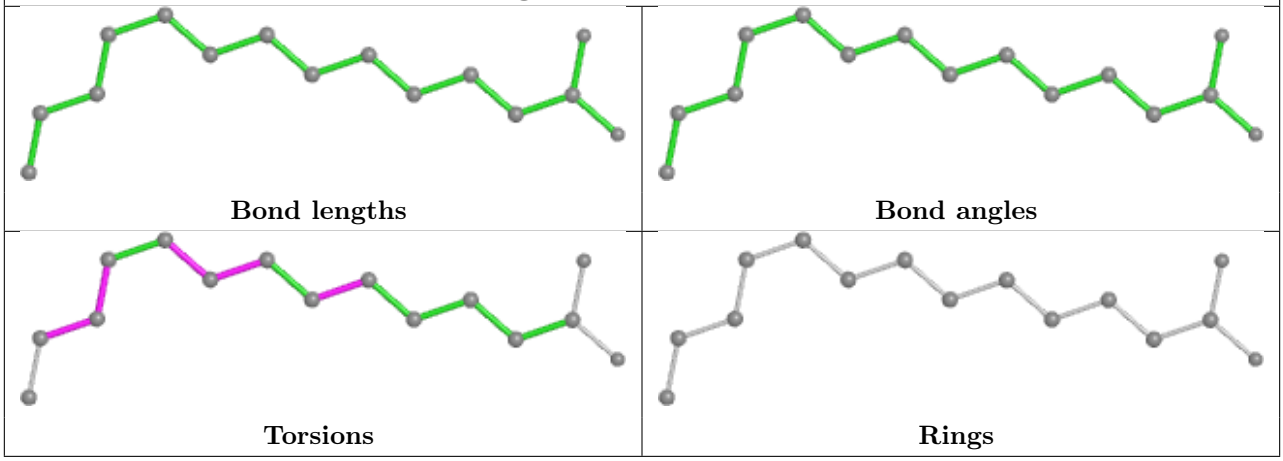


Ligand OLA A 1203



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	416/452 (92%)	0.88	74 (17%) 1 1	25, 60, 127, 144	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1081	LYS	7.9
1	A	1140	THR	6.8
1	A	1133	LYS	5.9
1	A	1107	THR	5.6
1	A	1138	ASN	5.4
1	A	1129	VAL	5.2
1	A	1077	LEU	4.9
1	A	1112	PHE	4.9
1	A	1136	TRP	4.9
1	A	1011	LEU	4.8
1	A	1082	LEU	4.8
1	A	1085	VAL	4.6
1	A	261	ARG	4.5
1	A	1135	ARG	4.5
1	A	1057	THR	4.4
1	A	262	SER	4.4
1	A	415	TRP	4.3
1	A	1137	TYR	4.3
1	A	293	GLN	4.1
1	A	1125	ASP	4.0
1	A	1035	PRO	3.9
1	A	1053	ASN	3.8
1	A	1113	THR	3.8
1	A	1123	ARG	3.8
1	A	1088	SER	3.7
1	A	1126	GLU	3.6
1	A	1078	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	213	SER	3.5
1	A	1139	GLN	3.5
1	A	291	ASN	3.4
1	A	1116	LEU	3.3
1	A	215	TRP	3.2
1	A	416	HIS	3.2
1	A	1119	LEU	3.2
1	A	1033	LYS	3.1
1	A	1152	ARG	3.1
1	A	1132	ALA	2.9
1	A	300	ASN	2.8
1	A	1056	ILE	2.8
1	A	1144	ALA	2.7
1	A	1027	ILE	2.7
1	A	212	VAL	2.6
1	A	1059	ASP	2.6
1	A	214	THR	2.6
1	A	218	ASP	2.6
1	A	1115	SER	2.6
1	A	290	GLU	2.6
1	A	1083	LYS	2.6
1	A	1159	TYR	2.6
1	A	1079	ASN	2.5
1	A	292	VAL	2.5
1	A	1034	SER	2.4
1	A	1042	SER	2.4
1	A	1022	TYR	2.4
1	A	1071	ALA	2.3
1	A	1080	ALA	2.3
1	A	1018	ASP	2.3
1	A	1061	ALA	2.3
1	A	1104	MET	2.3
1	A	1046	LYS	2.2
1	A	372	HIS	2.2
1	A	1089	LEU	2.2
1	A	1068	ASP	2.2
1	A	1076	ILE	2.2
1	A	1013	LEU	2.2
1	A	1141	PRO	2.2
1	A	1118	MET	2.1
1	A	1124	TRP	2.1
1	A	1064	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1086	TYR	2.1
1	A	1030	LEU	2.1
1	A	216	LEU	2.1
1	A	235	ILE	2.0
1	A	1108	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

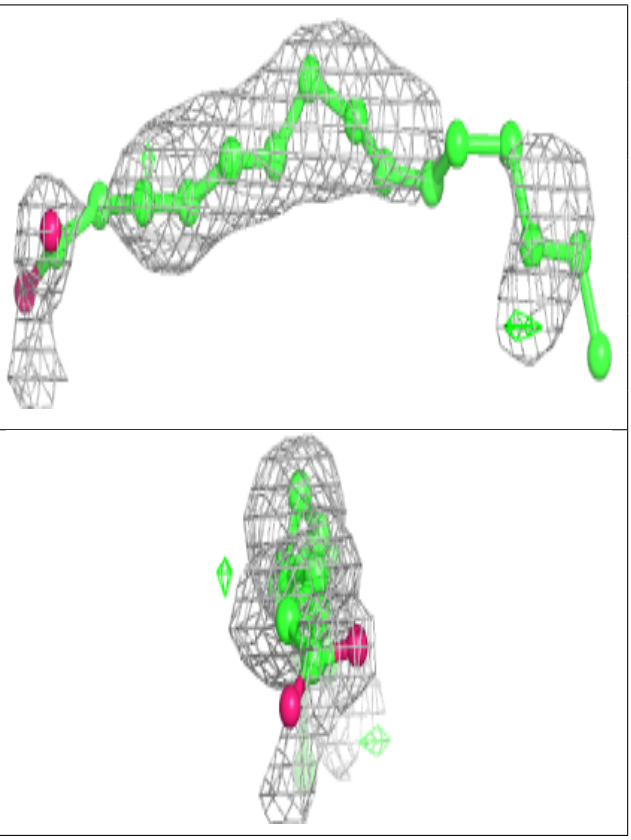
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

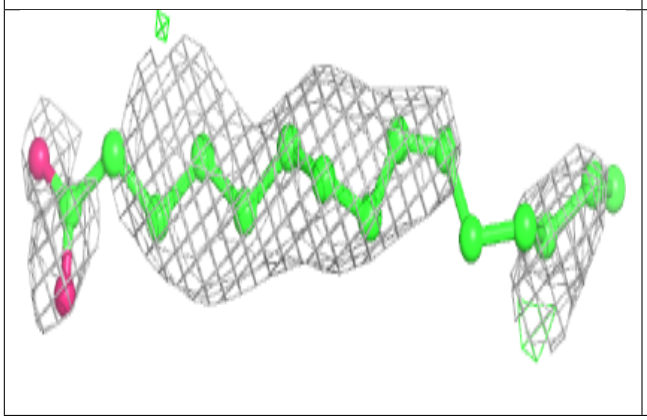
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	A	1210	17/20	0.63	0.33	54,66,91,93	0
3	OLA	A	1203	15/20	0.78	0.21	46,51,68,76	0
3	OLA	A	1215	11/20	0.78	0.16	59,63,68,68	0
3	OLA	A	1208	20/20	0.81	0.20	43,51,63,65	0
3	OLA	A	1204	15/20	0.83	0.22	40,42,62,64	0
3	OLA	A	1202	10/20	0.84	0.17	45,51,61,61	0
3	OLA	A	1205	11/20	0.84	0.19	33,39,45,57	0
3	OLA	A	1206	11/20	0.84	0.22	39,49,62,72	0
3	OLA	A	1214	14/20	0.85	0.19	46,52,57,63	0
3	OLA	A	1207	20/20	0.86	0.26	33,45,54,54	0
3	OLA	A	1212	11/20	0.86	0.23	50,52,55,55	0
4	PE5	A	1216	24/27	0.86	0.27	42,52,70,77	0
3	OLA	A	1209	20/20	0.87	0.17	40,49,66,73	0
3	OLA	A	1213	7/20	0.88	0.14	35,44,48,49	0
5	TLA	A	1217	10/10	0.89	0.17	43,52,58,61	0
3	OLA	A	1211	7/20	0.90	0.23	45,48,55,58	0
2	5MV	A	1201	41/41	0.94	0.15	24,37,49,63	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:

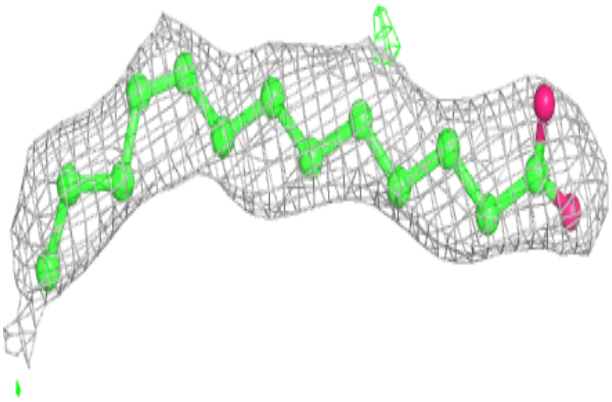
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

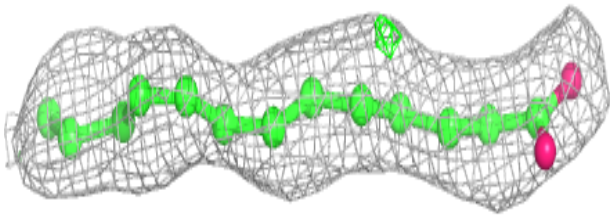


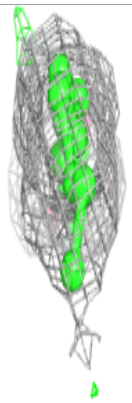


Electron density around OLA A 1203:

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

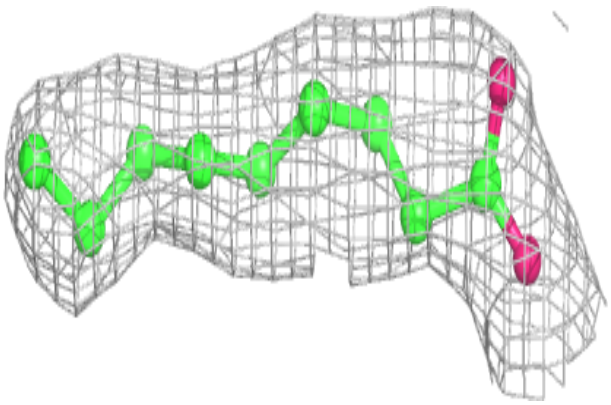


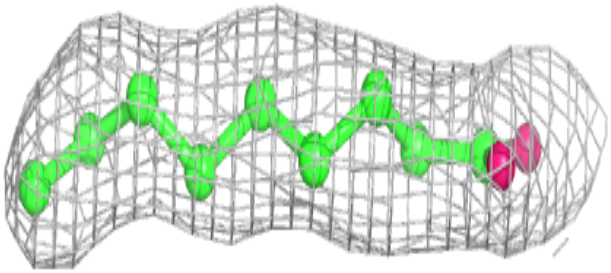


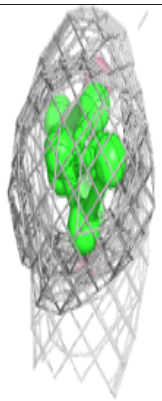


Electron density around OLA A 1215:

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

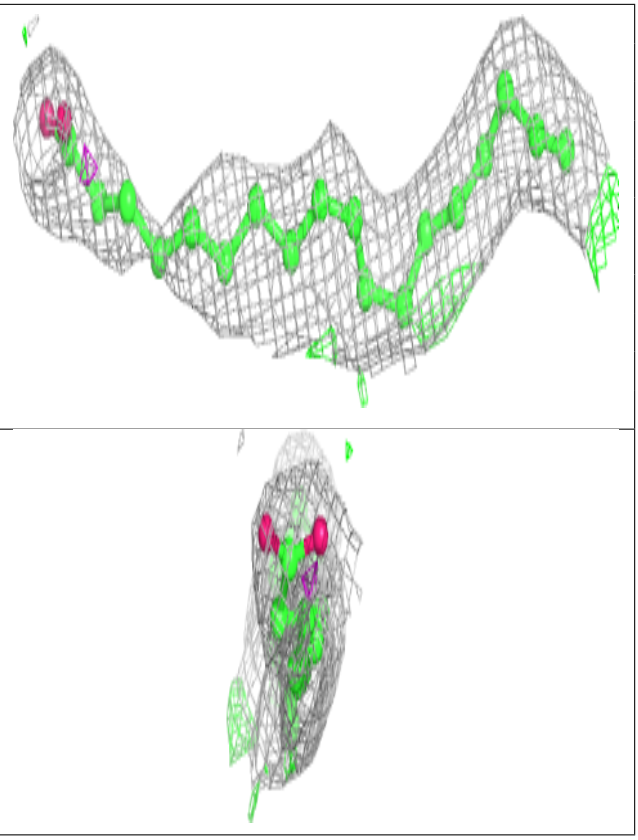






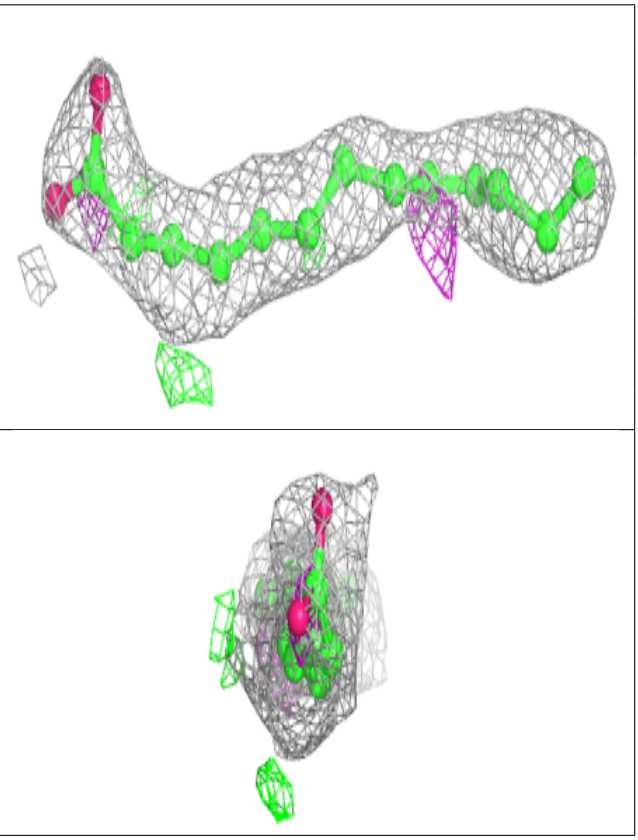
Electron density around OLA A 1208:

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



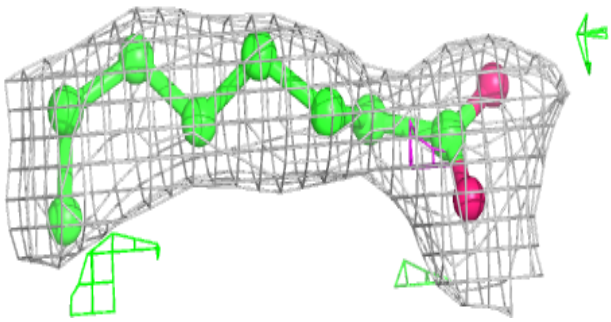
Electron density around OLA A 1204:

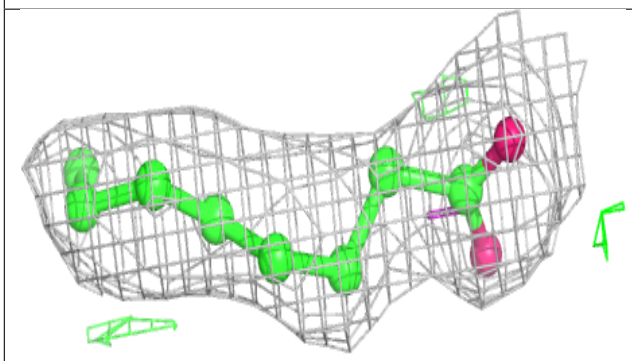
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

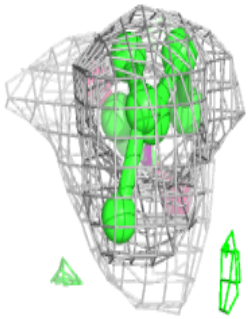


Electron density around OLA A 1202:

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

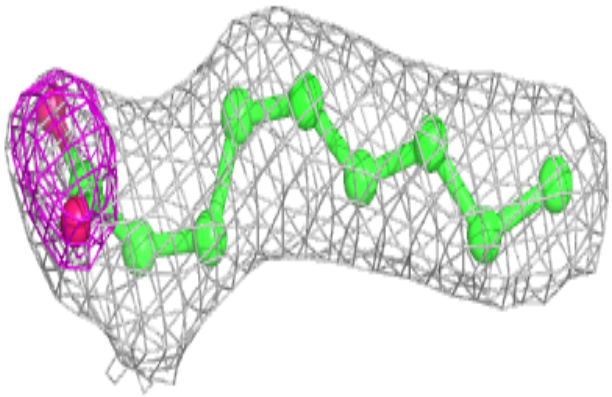


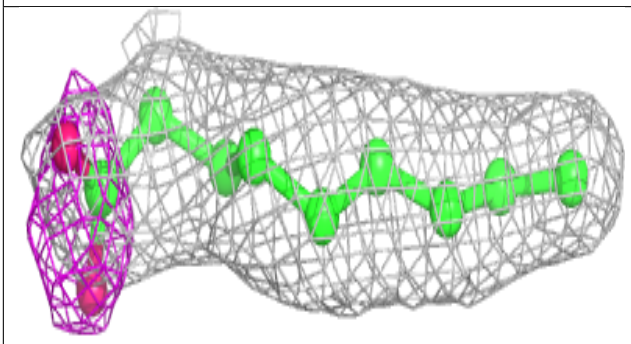


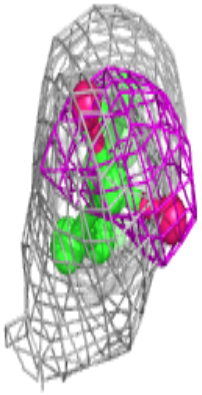


Electron density around OLA A 1205:

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

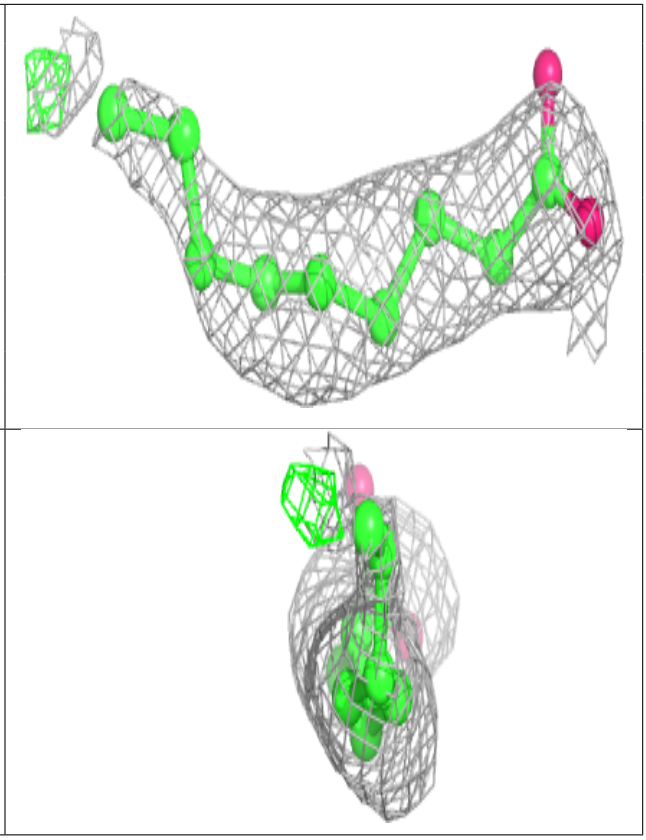






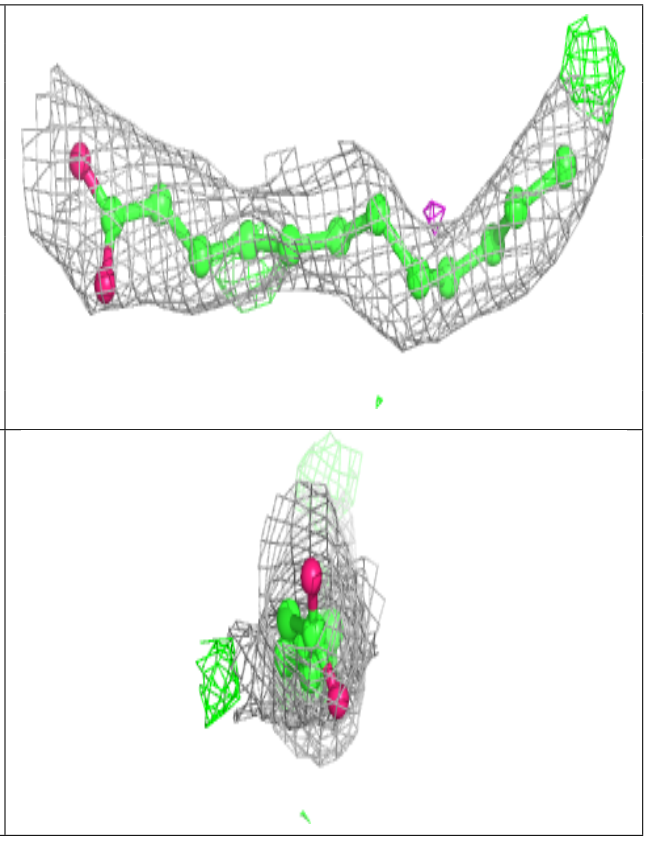
Electron density around OLA A 1206:

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



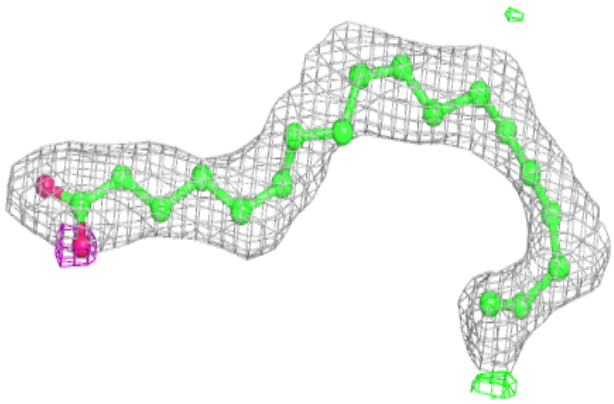
Electron density around OLA A 1214:

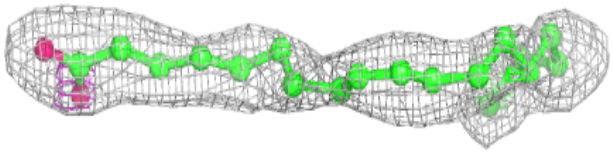
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

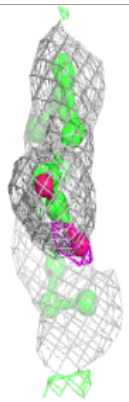


Electron density around OLA A 1207:

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

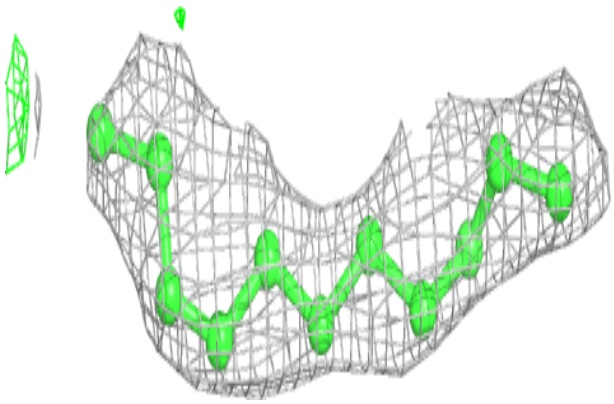


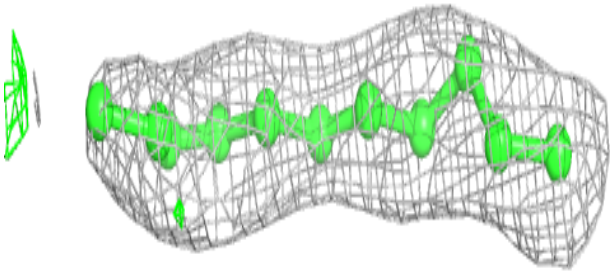


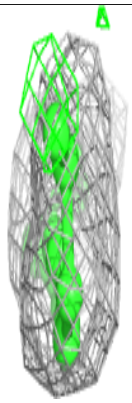


Electron density around OLA A 1212:

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







Electron density around PE5 A 1216:

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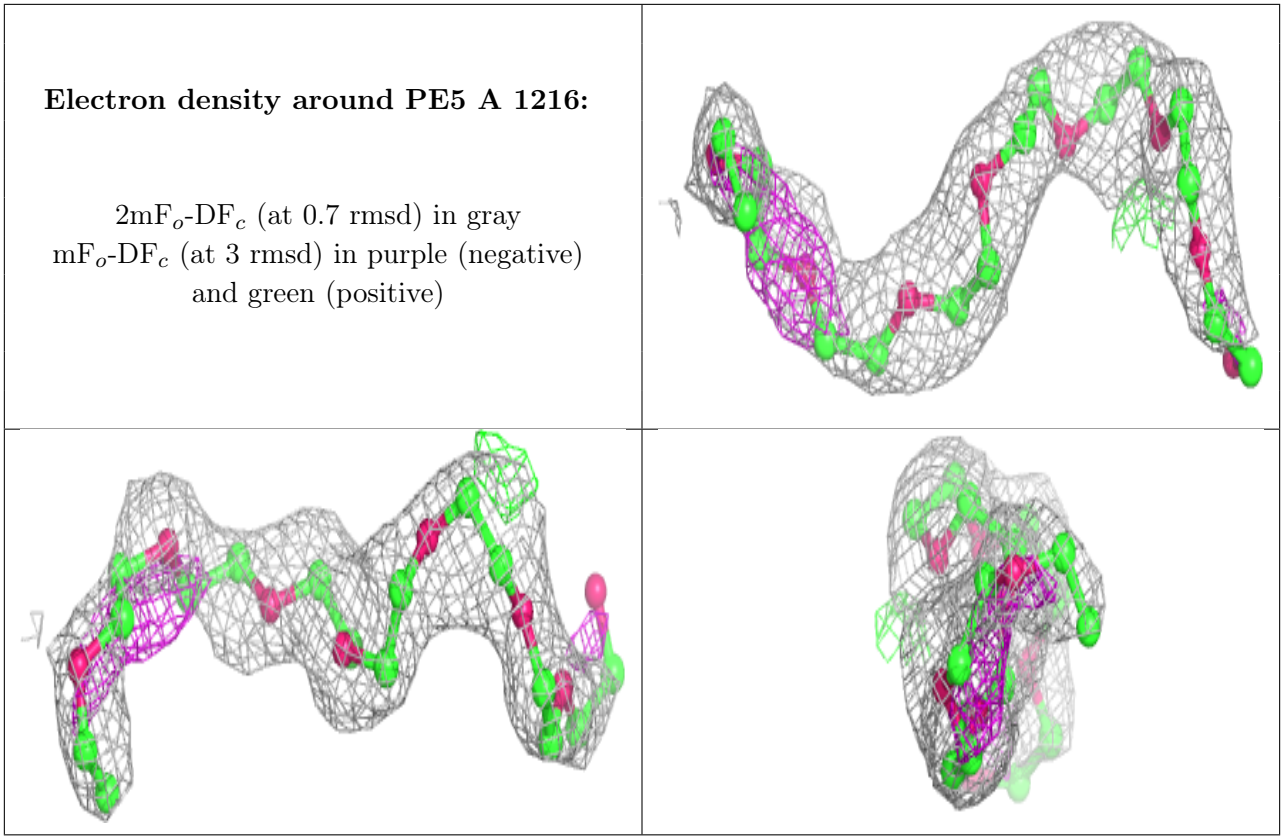
and green (positive)



Electron density around OLA A 1209:

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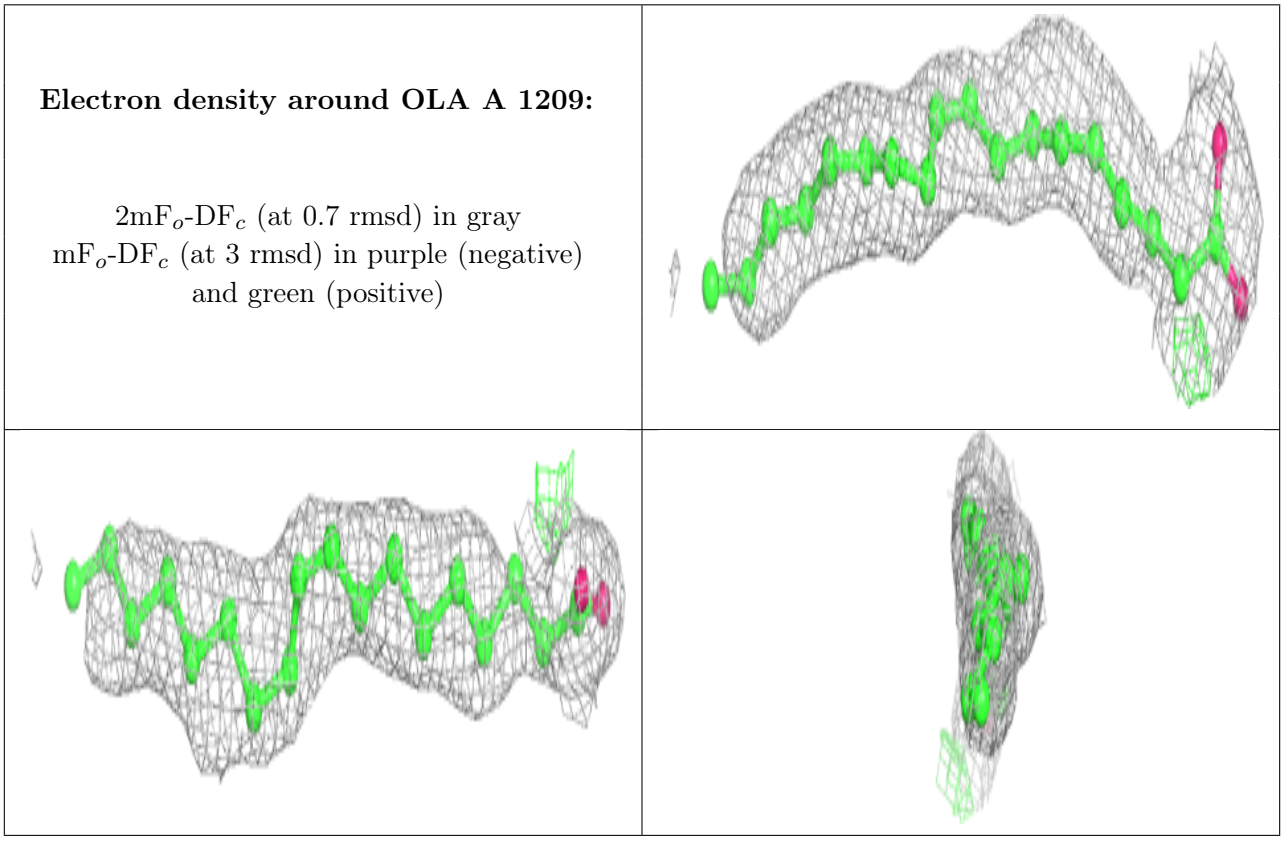
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA A 1211:

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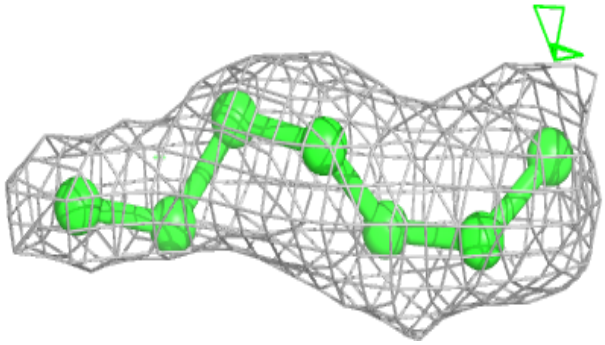
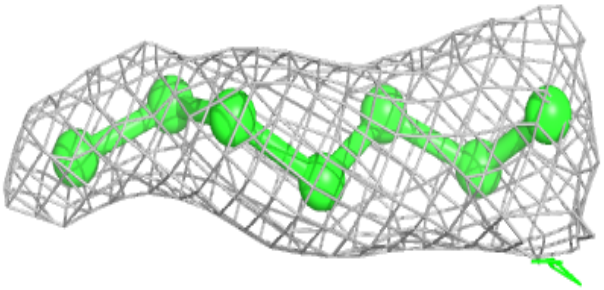
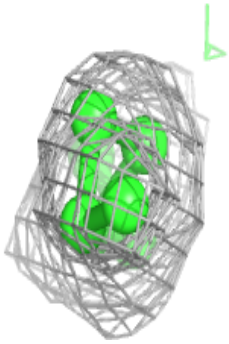
and green (positive)







Electron density around 5MV A 1201:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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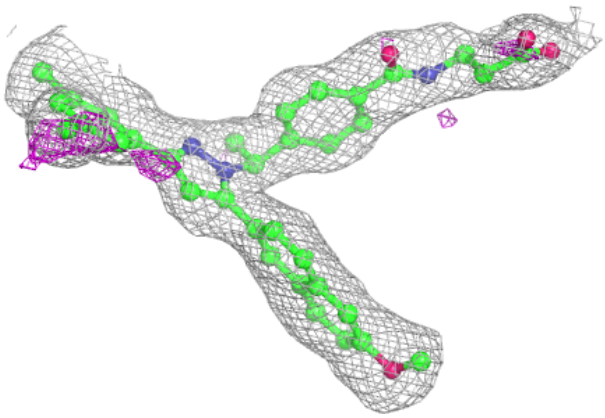

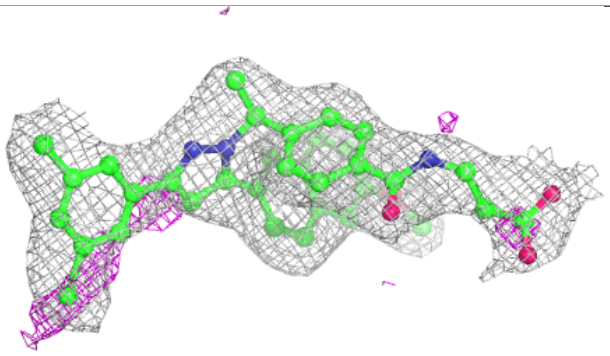

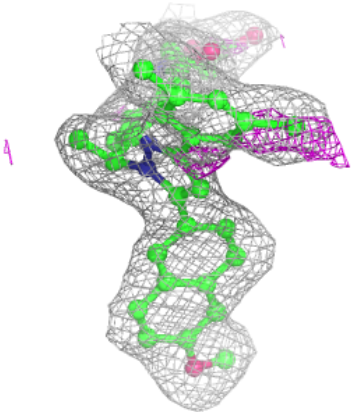

6.5 Other polymers (i)

There are no such residues in this entry.