



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 05:29 PM EST

PDB ID : 6PT2
Title : Crystal structure of the active delta opioid receptor in complex with the peptide agonist KGCHM07
Authors : Claff, T.; Yu, J.; Blais, V.; Patel, N.; Martin, C.; Wu, L.; Han, G.W.; Holleran, B.J.; Van der Poorten, O.; Hanson, M.A.; Sarret, P.; Gendron, L.; Cherezov, V.; Katritch, V.; Ballet, S.; Liu, Z.; Muller, C.E.; Stevens, R.C.
Deposited on : 2019-07-14
Resolution : 2.80 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

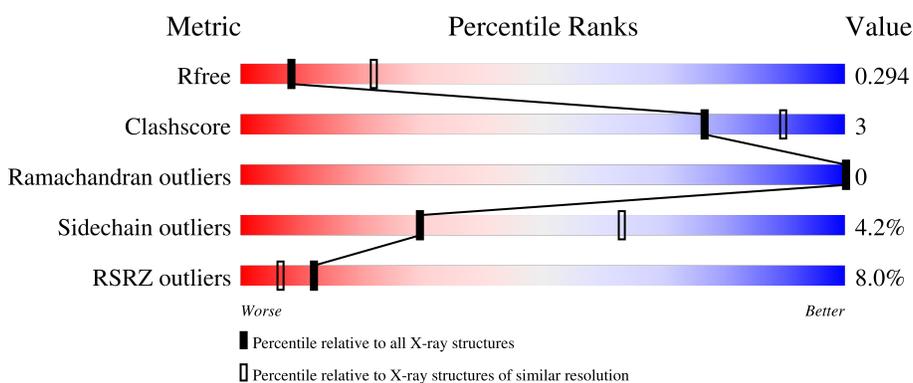
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	454	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 77% 10% 13%</p>
1	B	454	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 73% 7% 20%</p>
2	C	5	<div style="display: flex; align-items: center;"> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">40% 60%</p>
2	D	5	<div style="display: flex; align-items: center;"> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">60% 40%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLA	A	1202	-	-	-	X
4	OLA	A	1203	-	-	-	X
4	OLA	B	1201	-	-	-	X
4	OLA	B	1204	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5972 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.

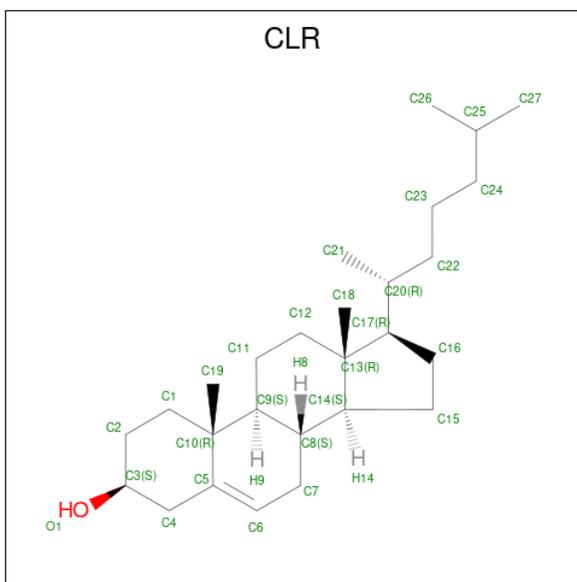
- Molecule 1 is a protein called Delta opioid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	Total	C	N	O	S	0	0	0
			3055	1994	502	534	25			
1	B	361	Total	C	N	O	S	0	0	0
			2662	1744	430	464	24			

- Molecule 2 is a protein called Peptide agonist KGCHM07.

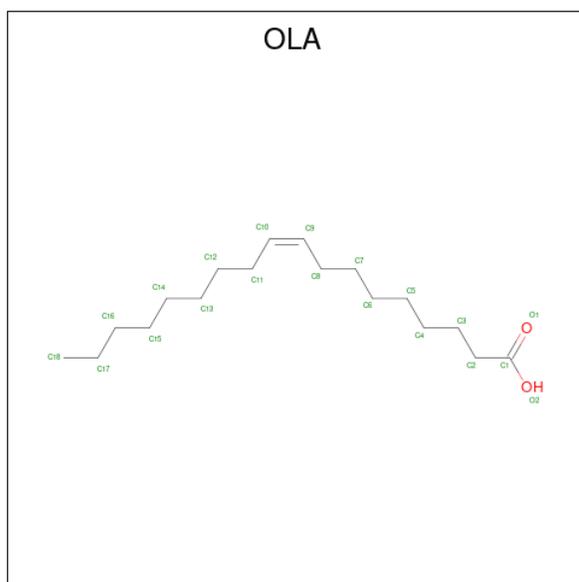
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
2	C	5	Total	C	F	N	O	0	0	0
			58	39	6	8	5			
2	D	5	Total	C	F	N	O	0	0	0
			58	39	6	8	5			

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



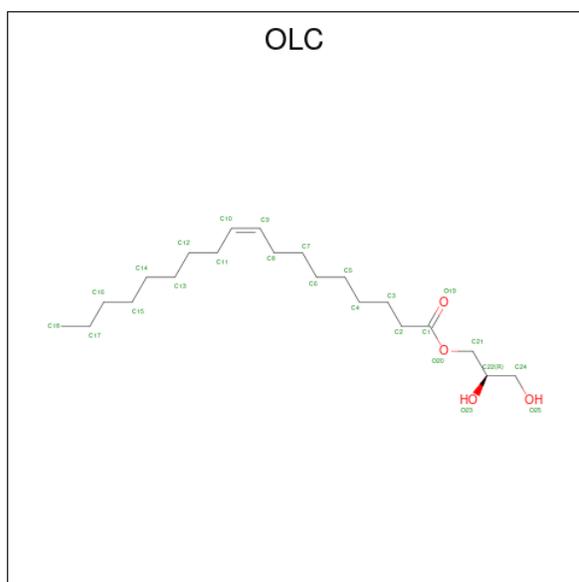
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C		0	0
			13	13			
4	B	1	Total	C		0	0
			9	9			
4	B	1	Total	C		0	0
			9	9			
4	B	1	Total	C		0	0
			9	9			
4	B	1	Total	C	O	0	0
			9	7	2		
			9	7	2		

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	C O	0	0
			19	15 4		

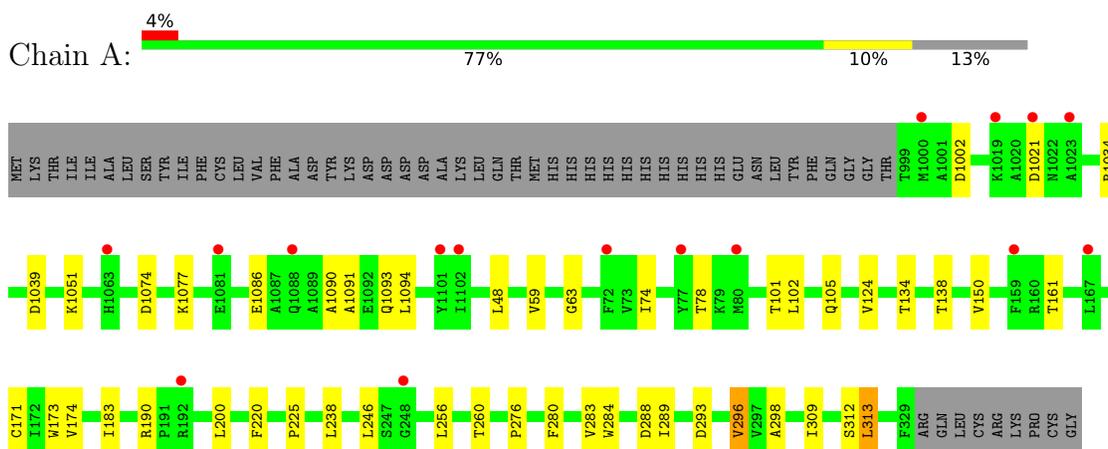
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		

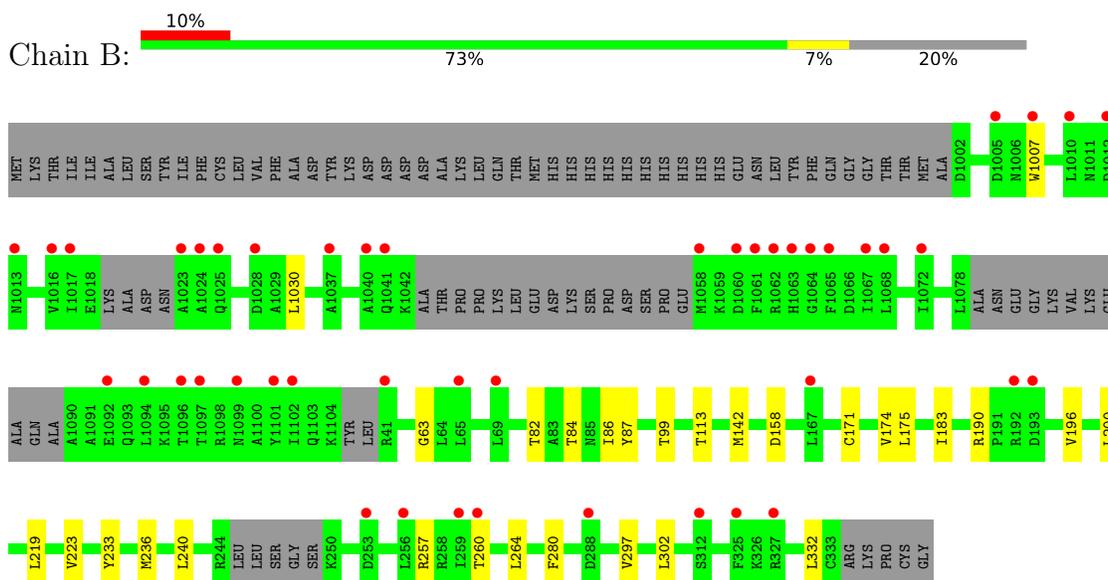
3 Residue-property plots [i](#)

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: Delta opioid receptor



- Molecule 1: Delta opioid receptor



- Molecule 2: Peptide agonist KGCHM07





- Molecule 2: Peptide agonist KGCHM07

Chain D:
60% 40%

A horizontal bar representing the overall quality of Chain D. The bar is divided into two segments: a green segment on the left representing 60% and a yellow segment on the right representing 40%.



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.96Å 140.88Å 158.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.80 45.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.51-2.80) 93.3 (45.03-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.81Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.246 , 0.282 0.251 , 0.294	Depositor DCC
R_{free} test set	1269 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	94.7	Xtrriage
Anisotropy	0.537	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5972	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.74% 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: OLC, DAR, DI7, OLA, SAR, OXJ, CLR

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	0.50	0/3119	0.62	0/4253
1	B	0.51	0/2714	0.63	0/3716
2	C	0.90	0/11	1.05	0/13
2	D	1.02	0/11	1.24	0/13
All	All	0.50	0/5855	0.63	0/7995

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	3055	0	3144	21	0
1	B	2662	0	2611	13	0
2	C	58	0	40	1	0
2	D	58	0	40	0	0
3	A	28	0	46	2	0
4	A	40	0	66	1	0
4	B	49	0	84	1	0
5	B	19	0	25	0	0
6	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
All	All	5972	0	6056	36	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 (36) 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:B:87:TYR:HB3	1:B:142:MET:HG2	1.75	0.69
1:A:276:PRO:HG3	3:A:1201:CLR:H242	1.76	0.67
1:B:113:THR:HG23	1:B:196:VAL:H	1.58	0.67
1:A:101:THR:HG23	1:A:124:VAL:HG13	1.78	0.66
1:A:309:ILE:O	1:A:313:LEU:HB2	2.01	0.60
1:A:173:TRP:CG	4:A:1203:OLA:H10	2.38	0.58
1:A:284:TRP:HA	1:A:289:ILE:HD12	1.87	0.56
1:B:87:TYR:HB3	1:B:142:MET:CG	2.36	0.55
1:A:1074:ASP:HA	1:A:1077:LYS:HE3	1.89	0.54
1:A:293:ASP:HB3	1:A:296:VAL:HG13	1.91	0.53
1:B:63:GLY:HA3	1:B:99:THR:HG21	1.89	0.53
1:A:183:ILE:HG23	1:A:200:LEU:HD21	1.90	0.53
1:A:101:THR:CG2	1:A:105:GLN:HE21	2.23	0.52
1:B:219:LEU:HA	1:B:223:VAL:HG22	1.93	0.51
1:B:219:LEU:HD12	1:B:223:VAL:CG2	2.43	0.48
1:A:48:LEU:HD11	1:A:298:ALA:HB2	1.94	0.48
1:B:86:ILE:HG23	4:B:1203:OLA:H122	1.96	0.47
1:A:59:VAL:HG23	1:A:102:LEU:HD13	1.97	0.47
1:A:220:PHE:O	1:A:225:PRO:HD3	2.15	0.47
1:A:1091:ALA:HA	1:A:1094:LEU:HD12	1.96	0.46
1:B:233:TYR:CE1	1:B:264:LEU:HB2	2.50	0.46
1:A:150:VAL:HG22	1:A:256:LEU:HD22	1.96	0.46
1:A:283:VAL:HG12	1:A:289:ILE:HD11	1.98	0.45
1:B:240:LEU:HD21	1:B:257:ARG:HA	1.98	0.44
1:A:63:GLY:HA2	1:A:312:SER:HB2	2.00	0.44
3:A:1201:CLR:H222	3:A:1201:CLR:H162	1.64	0.43
1:A:1090:ALA:O	1:A:1093:GLN:HG2	2.19	0.43
1:A:171:CYS:HA	1:A:174:VAL:HG12	2.01	0.42
1:B:236:MET:HB3	1:B:260:THR:HG22	2.01	0.42
1:A:74:ILE:HA	1:A:78:THR:HG23	2.02	0.41
1:B:183:ILE:HG23	1:B:200:LEU:HD21	2.02	0.41
2:C:3:PHE:HA	2:C:4:SAR:HA3	1.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:HG22	1:A:105:GLN:HE21	1.83	0.41
1:A:134:THR:O	1:A:138:THR:HG22	2.21	0.41
1:B:171:CYS:HA	1:B:174:VAL:HG12	2.03	0.41
1:B:171:CYS:O	1:B:175:LEU:HB2	2.21	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	395/454 (87%)	386 (98%)	9 (2%)	0	100	100
1	B	349/454 (77%)	339 (97%)	10 (3%)	0	100	100
2	C	1/5 (20%)	1 (100%)	0	0	100	100
2	D	1/5 (20%)	1 (100%)	0	0	100	100
All	All	746/918 (81%)	727 (98%)	19 (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	328/390 (84%)	313 (95%)	15 (5%)	27	60
1	B	268/390 (69%)	258 (96%)	10 (4%)	34	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	598/782 (76%)	573 (96%)	25 (4%)	30	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	ASP
1	A	1021	ASP
1	A	1034	ARG
1	A	1039	ASP
1	A	1051	LYS
1	A	1086	GLU
1	A	161	THR
1	A	190	ARG
1	A	238	LEU
1	A	246	LEU
1	A	260	THR
1	A	280	PHE
1	A	288	ASP
1	A	296	VAL
1	A	313	LEU
1	B	1007	TRP
1	B	1030	LEU
1	B	82	THR
1	B	84	THR
1	B	158	ASP
1	B	190	ARG
1	B	280	PHE
1	B	297	VAL
1	B	302	LEU
1	B	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	324	ASN
1	B	67	ASN
1	B	105	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](#)

6 non-standard protein/DNA/RNA residues 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
2	DI7	C	1	2	13,14,15	1.00	1 (7%)	15,19,21	1.11	1 (6%)
2	SAR	C	4	2	4,4,5	1.23	0	1,3,5	1.97	0
2	DI7	D	1	2	13,14,15	0.88	0	15,19,21	1.11	1 (6%)
2	SAR	D	4	2	4,4,5	0.93	0	1,3,5	2.69	1 (100%)

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
2	DI7	C	1	2	-	0/5/6/8	0/1/1/1
2	SAR	C	4	2	-	1/1/2/3	-
2	DI7	D	1	2	-	0/5/6/8	0/1/1/1
2	SAR	D	4	2	-	1/1/2/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DI7	CD1-CD	2.43	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	SAR	O-C-CA	-2.69	117.64	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	DI7	CE3-CD1-CE1	-2.37	115.11	119.49
2	D	1	DI7	CE3-CD1-CE1	-2.30	115.24	119.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	SAR	C-CA-N-CN
2	D	4	SAR	C-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	SAR	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
4	OLA	B	1204	-	8,8,19	0.29	0	7,7,19	0.48	0
5	OLC	B	1206	-	18,18,24	0.51	0	18,19,25	0.90	1 (5%)
4	OLA	B	1201	-	12,12,19	0.34	0	11,11,19	0.40	0
4	OLA	B	1203	-	8,8,19	0.26	0	7,7,19	0.51	0
3	CLR	A	1201	-	31,31,31	0.35	0	48,48,48	0.55	0
4	OLA	A	1203	-	19,19,19	0.50	0	19,19,19	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLA	B	1205	-	8,8,19	0.75	0	8,8,19	1.18	1 (12%)
4	OLA	A	1202	-	19,19,19	0.56	0	19,19,19	0.92	2 (10%)
4	OLA	B	1202	-	8,8,19	0.25	0	7,7,19	0.53	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
4	OLA	B	1204	-	-	3/6/6/17	-
5	OLC	B	1206	-	-	9/18/18/24	-
4	OLA	B	1201	-	-	5/10/10/17	-
4	OLA	B	1203	-	-	5/6/6/17	-
3	CLR	A	1201	-	-	8/10/68/68	0/4/4/4
4	OLA	A	1203	-	-	9/17/17/17	-
4	OLA	B	1205	-	-	6/6/6/17	-
4	OLA	A	1202	-	-	11/17/17/17	-
4	OLA	B	1202	-	-	3/6/6/17	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1202	OLA	O2-C1-C2	2.62	122.44	114.03
5	B	1206	OLC	O20-C1-C2	2.32	119.18	111.91
4	A	1202	OLA	O2-C1-O1	-2.24	117.71	123.30
4	B	1205	OLA	O2-C1-C2	2.05	120.61	114.03

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	CLR	C16-C17-C20-C21
3	A	1201	CLR	C13-C17-C20-C21
3	A	1201	CLR	C13-C17-C20-C22
5	B	1206	OLC	C2-C1-O20-C21
3	A	1201	CLR	C16-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1206	OLC	O19-C1-O20-C21
3	A	1201	CLR	C20-C22-C23-C24
4	B	1203	OLA	C13-C14-C15-C16
3	A	1201	CLR	C23-C24-C25-C27
4	B	1203	OLA	C11-C12-C13-C14
4	B	1202	OLA	C12-C13-C14-C15
4	B	1204	OLA	C14-C15-C16-C17
4	A	1202	OLA	C11-C12-C13-C14
5	B	1206	OLC	C1-C2-C3-C4
4	B	1201	OLA	C13-C14-C15-C16
3	A	1201	CLR	C23-C24-C25-C26
4	B	1202	OLA	C14-C15-C16-C17
5	B	1206	OLC	C2-C3-C4-C5
4	A	1202	OLA	C1-C2-C3-C4
4	A	1203	OLA	C1-C2-C3-C4
4	B	1205	OLA	C2-C3-C4-C5
4	A	1203	OLA	C4-C5-C6-C7
4	B	1204	OLA	C13-C14-C15-C16
5	B	1206	OLC	C6-C7-C8-C9
4	A	1203	OLA	C3-C4-C5-C6
4	A	1202	OLA	C2-C3-C4-C5
4	B	1205	OLA	C1-C2-C3-C4
4	A	1202	OLA	C4-C5-C6-C7
5	B	1206	OLC	C5-C6-C7-C8
4	A	1203	OLA	C5-C6-C7-C8
5	B	1206	OLC	C3-C4-C5-C6
3	A	1201	CLR	C22-C23-C24-C25
4	A	1202	OLA	C5-C6-C7-C8
4	B	1203	OLA	C10-C11-C12-C13
4	A	1202	OLA	C14-C15-C16-C17
4	A	1202	OLA	C12-C13-C14-C15
4	B	1201	OLA	C15-C16-C17-C18
4	B	1201	OLA	C6-C7-C8-C9
4	A	1202	OLA	C15-C16-C17-C18
4	A	1202	OLA	C10-C11-C12-C13
4	B	1203	OLA	C15-C16-C17-C18
4	B	1202	OLA	C15-C16-C17-C18
4	B	1205	OLA	O1-C1-C2-C3
4	B	1204	OLA	C12-C13-C14-C15
4	B	1203	OLA	C14-C15-C16-C17
4	A	1203	OLA	C10-C11-C12-C13
4	A	1203	OLA	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

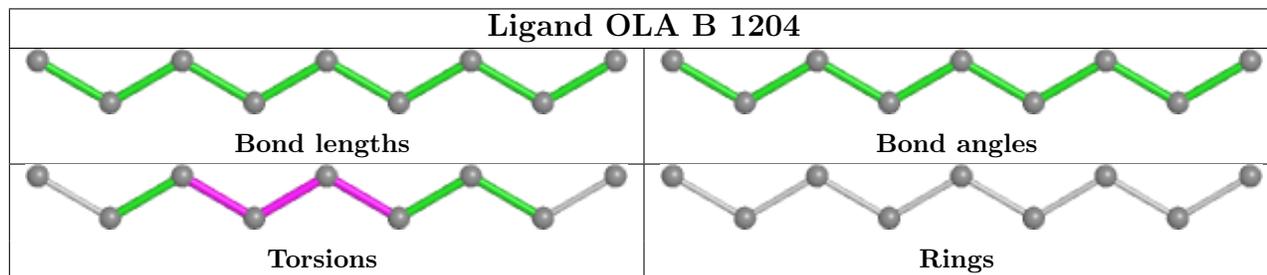
Mol	Chain	Res	Type	Atoms
4	B	1205	OLA	O2-C1-C2-C3
4	A	1203	OLA	O2-C1-C2-C3
4	B	1201	OLA	C11-C12-C13-C14
4	B	1205	OLA	C3-C4-C5-C6
4	A	1203	OLA	O1-C1-C2-C3
5	B	1206	OLC	O20-C1-C2-C3
4	A	1202	OLA	C9-C10-C11-C12
4	B	1205	OLA	C4-C5-C6-C7
4	A	1202	OLA	C7-C8-C9-C10
4	B	1201	OLA	C7-C8-C9-C10
4	A	1203	OLA	C2-C3-C4-C5
5	B	1206	OLC	O19-C1-C2-C3

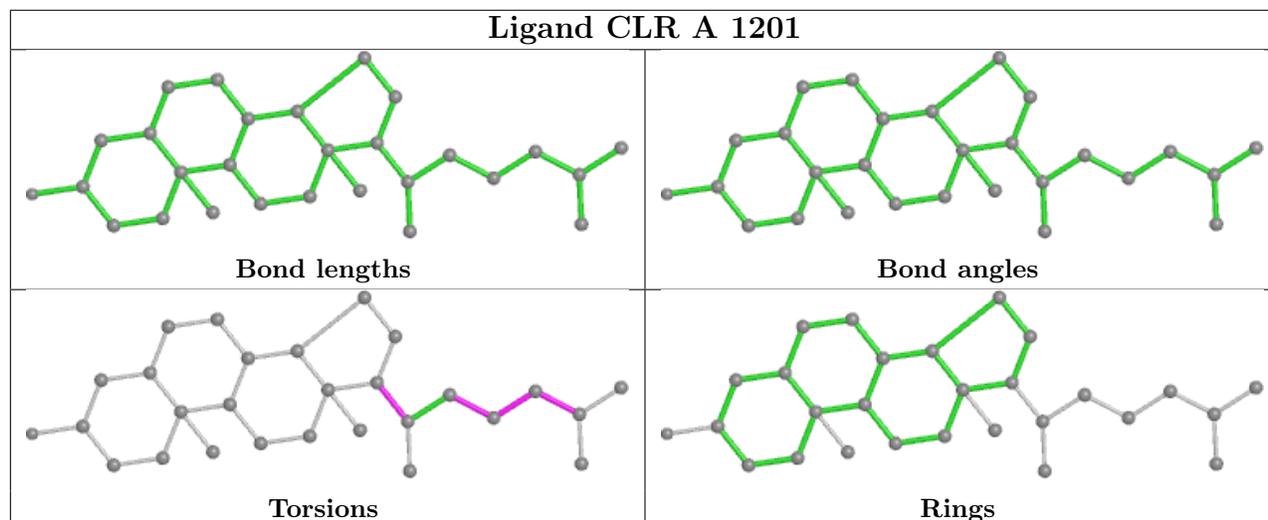
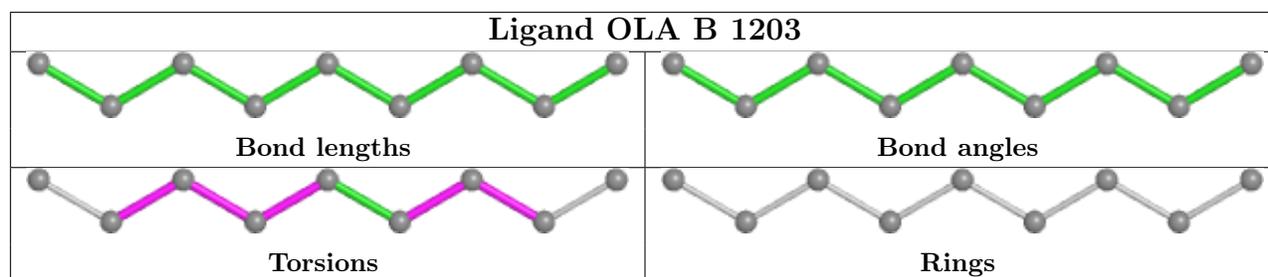
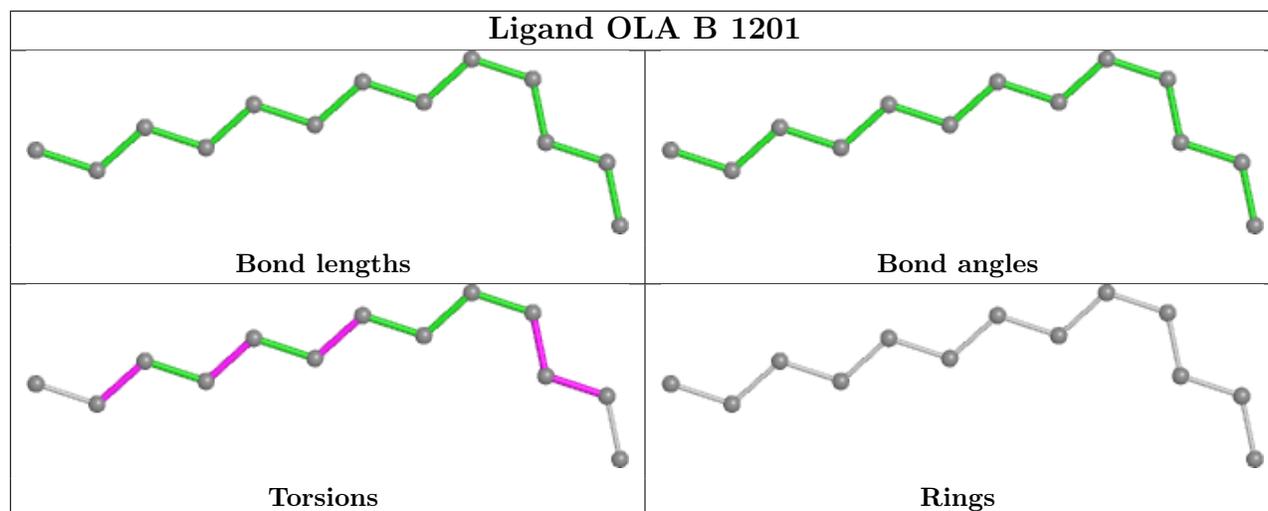
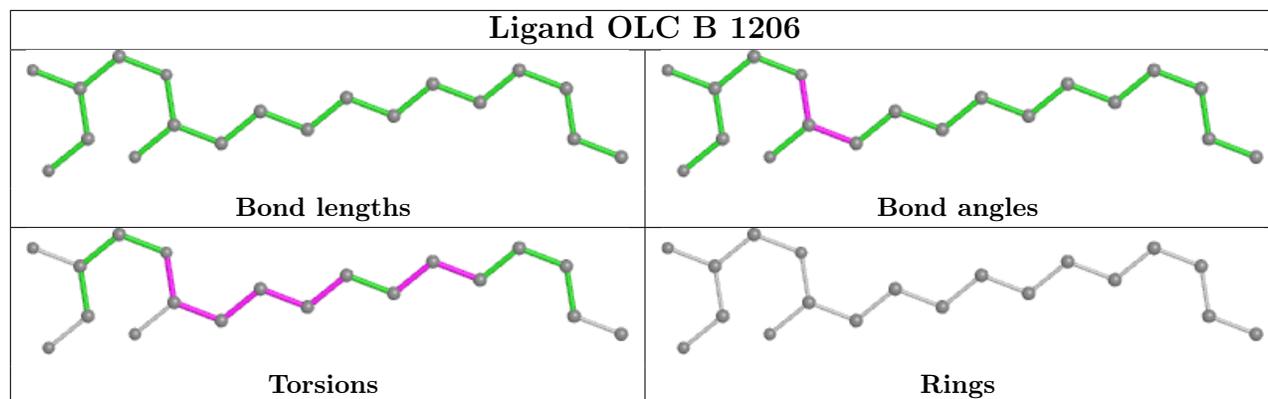
There are no ring outliers.

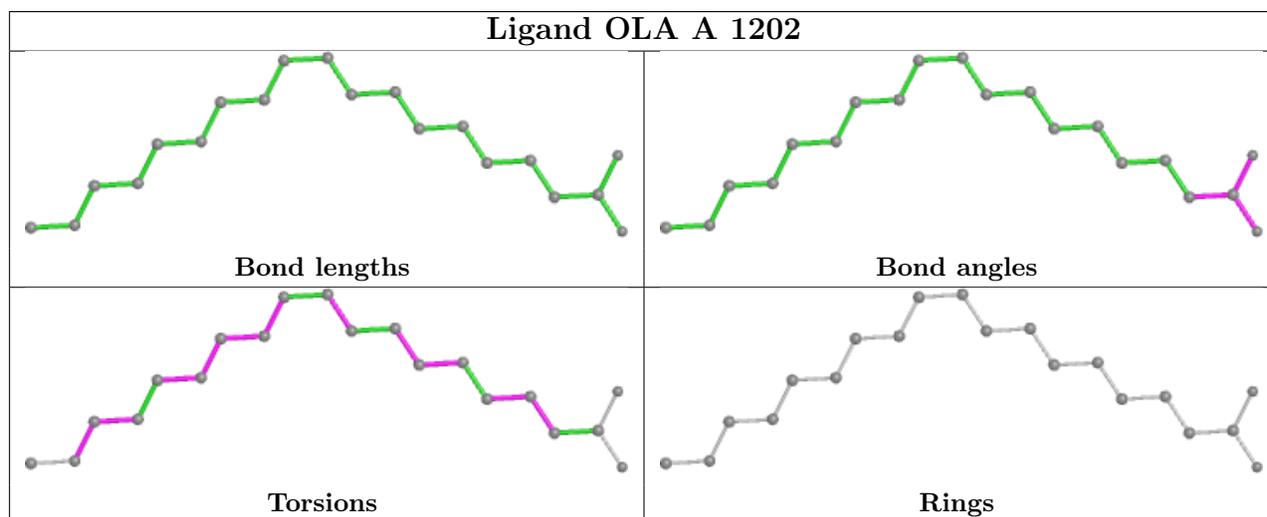
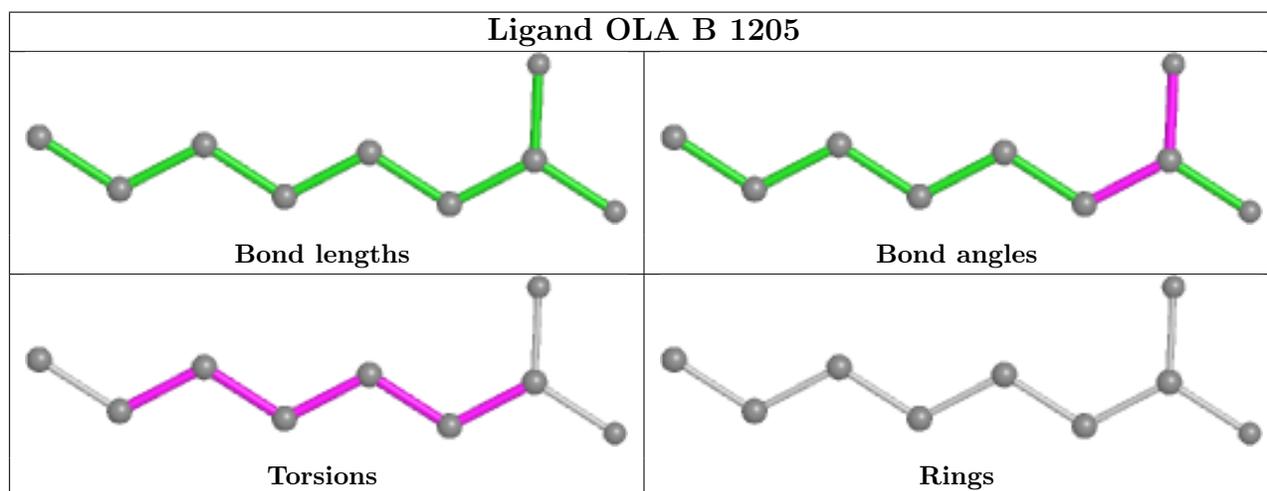
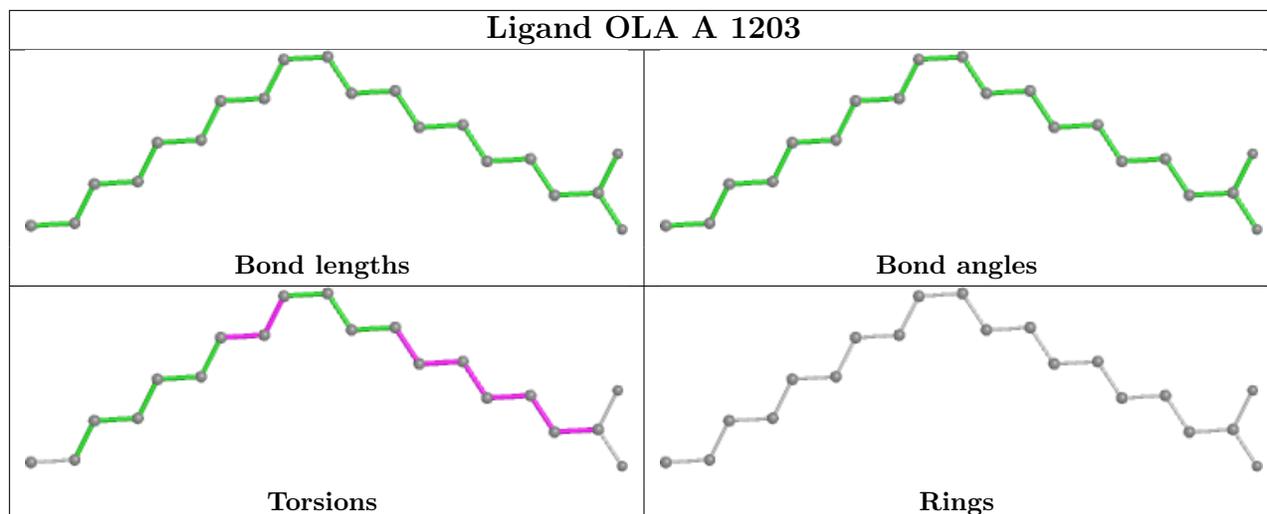
3 monomers are involved in 4 short contacts:

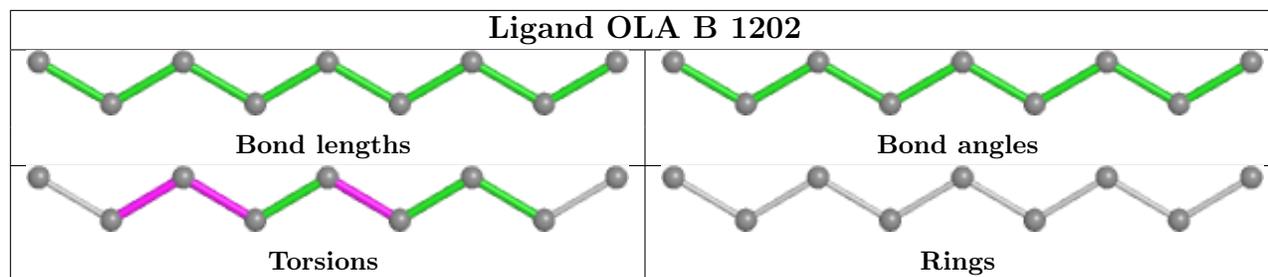
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1203	OLA	1	0
3	A	1201	CLR	2	0
4	A	1203	OLA	1	0

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 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 [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, 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	397/454 (87%)	0.32	16 (4%) 38 28	79, 104, 170, 207	0
1	B	361/454 (79%)	0.62	45 (12%) 3 2	84, 110, 177, 207	0
2	C	1/5 (20%)	0.77	0 100 100	80, 80, 80, 80	0
2	D	1/5 (20%)	0.31	0 100 100	82, 82, 82, 82	0
All	All	760/918 (82%)	0.47	61 (8%) 12 6	79, 106, 174, 207	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	LEU	6.8
1	B	1063	HIS	6.4
1	B	1068	LEU	6.3
1	B	193	ASP	6.3
1	B	1040	ALA	5.9
1	B	1101	TYR	5.3
1	A	1101	TYR	5.2
1	B	1058	MET	5.2
1	B	1013	ASN	5.1
1	B	1064	GLY	4.8
1	B	1102	ILE	4.4
1	B	1007	TRP	4.3
1	B	327	ARG	4.2
1	B	167	LEU	3.9
1	B	41	ARG	3.8
1	A	1021	ASP	3.8
1	A	77	TYR	3.5
1	B	1024	ALA	3.5
1	B	1096	THR	3.4
1	B	325	PHE	3.4
1	B	1025	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1028	ASP	3.3
1	A	1081	GLU	3.2
1	B	1061	PHE	3.2
1	B	1037	ALA	3.1
1	B	65	LEU	3.1
1	A	1019	LYS	3.1
1	B	1060	ASP	3.1
1	A	248	GLY	3.1
1	B	192	ARG	3.1
1	B	259	ILE	3.0
1	A	192	ARG	3.0
1	B	288	ASP	2.9
1	A	1063	HIS	2.9
1	A	72	PHE	2.8
1	B	1041	GLN	2.8
1	B	1065	PHE	2.7
1	B	1067	ILE	2.7
1	B	1016	VAL	2.7
1	B	1005	ASP	2.7
1	A	1088	GLN	2.7
1	A	167	LEU	2.7
1	B	260	THR	2.7
1	A	80	MET	2.6
1	B	1023	ALA	2.5
1	B	253	ASP	2.5
1	B	1017	ILE	2.5
1	A	1102	ILE	2.5
1	B	1010	LEU	2.5
1	A	159	PHE	2.4
1	A	1000	MET	2.4
1	B	1012	ASP	2.4
1	A	1023	ALA	2.3
1	B	69	LEU	2.3
1	B	1099	ASN	2.2
1	B	1072	ILE	2.2
1	B	312	SER	2.2
1	B	1062	ARG	2.1
1	B	1092	GLU	2.1
1	B	1097	THR	2.0
1	B	1094	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DAR	C	2	11/12	0.93	0.23	80,88,99,99	0
2	DAR	D	2	11/12	0.93	0.33	78,90,97,99	0
2	DI7	C	1	14/15	0.95	0.18	71,73,82,85	0
2	DI7	D	1	14/15	0.95	0.28	76,79,84,84	0
2	SAR	D	4	5/6	0.96	0.23	81,83,86,91	0
2	SAR	C	4	5/6	0.97	0.16	78,81,82,85	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

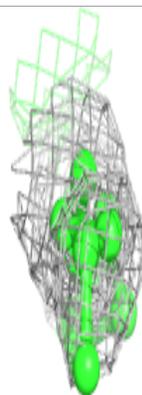
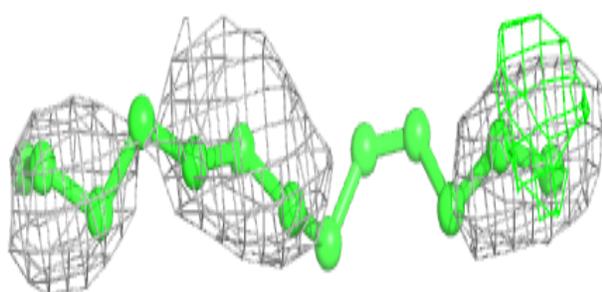
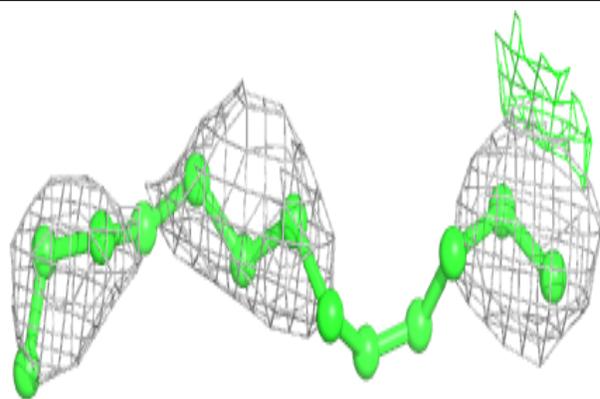
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLA	B	1201	13/20	0.45	0.46	110,115,122,123	0
4	OLA	B	1204	9/20	0.54	0.42	97,99,103,104	0
4	OLA	A	1202	20/20	0.62	0.72	92,107,121,121	0
4	OLA	A	1203	20/20	0.67	0.43	112,119,139,139	0
4	OLA	B	1202	9/20	0.69	0.39	108,109,112,112	0
4	OLA	B	1203	9/20	0.81	0.35	104,105,106,107	0
5	OLC	B	1206	19/25	0.81	0.25	119,124,127,128	0
3	CLR	A	1201	28/28	0.85	0.35	121,133,138,139	0
4	OLA	B	1205	9/20	0.87	0.25	122,123,129,130	0

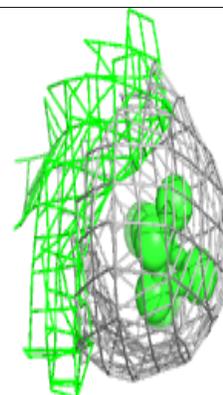
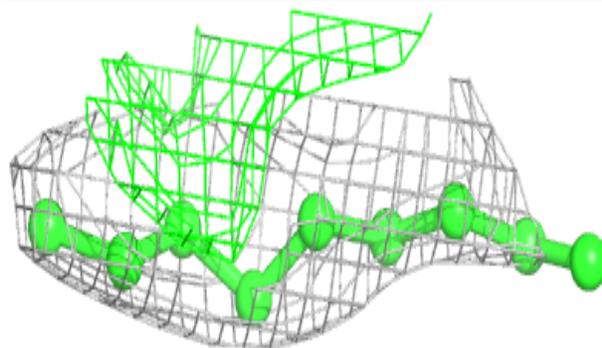
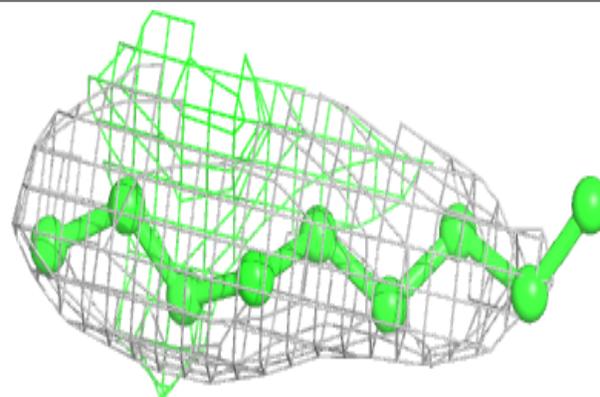
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA B 1201:

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

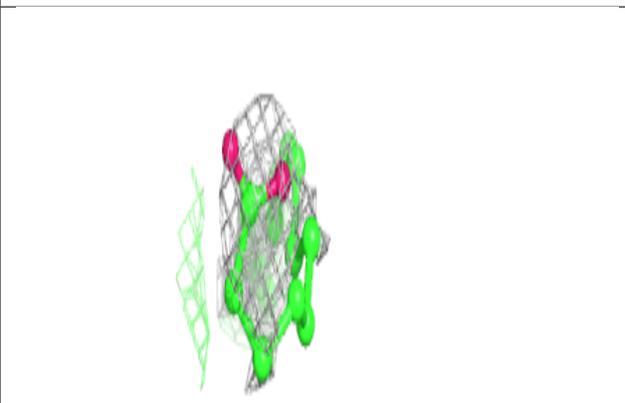
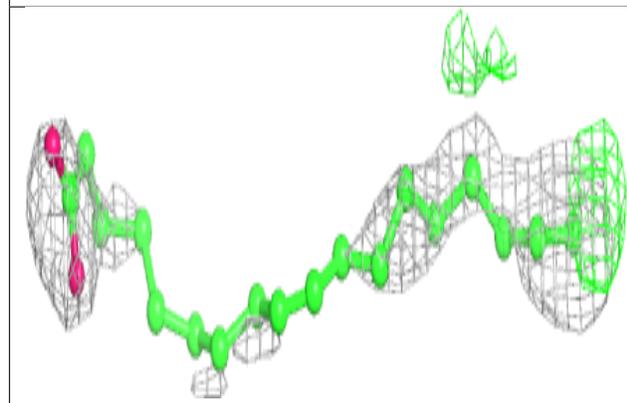
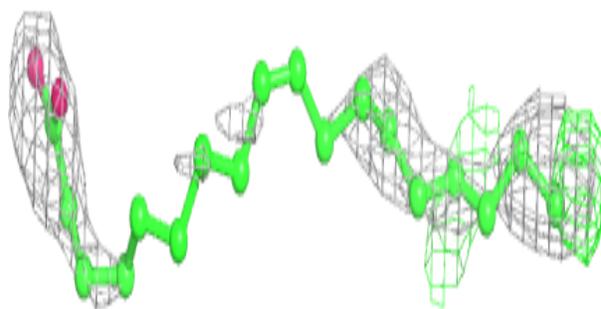
**Electron density around OLA B 1204:**

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

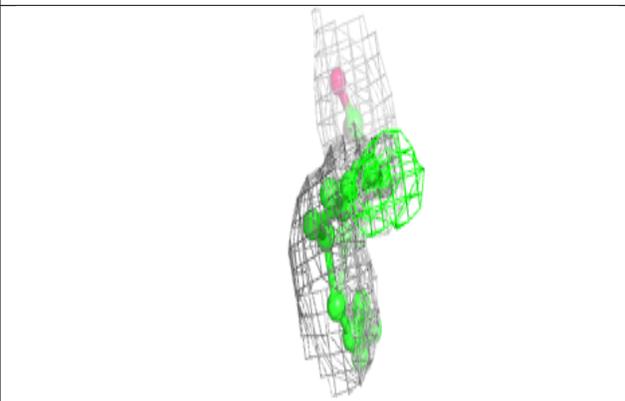
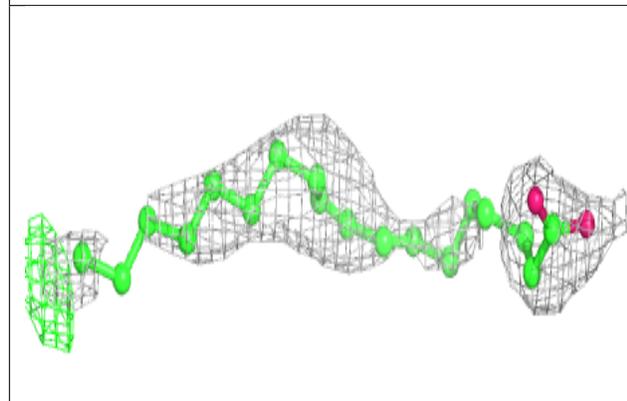
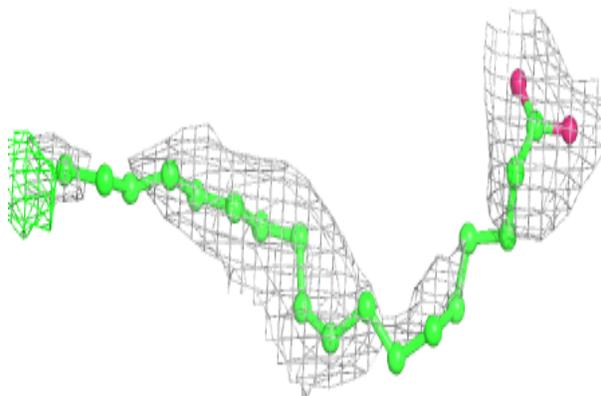


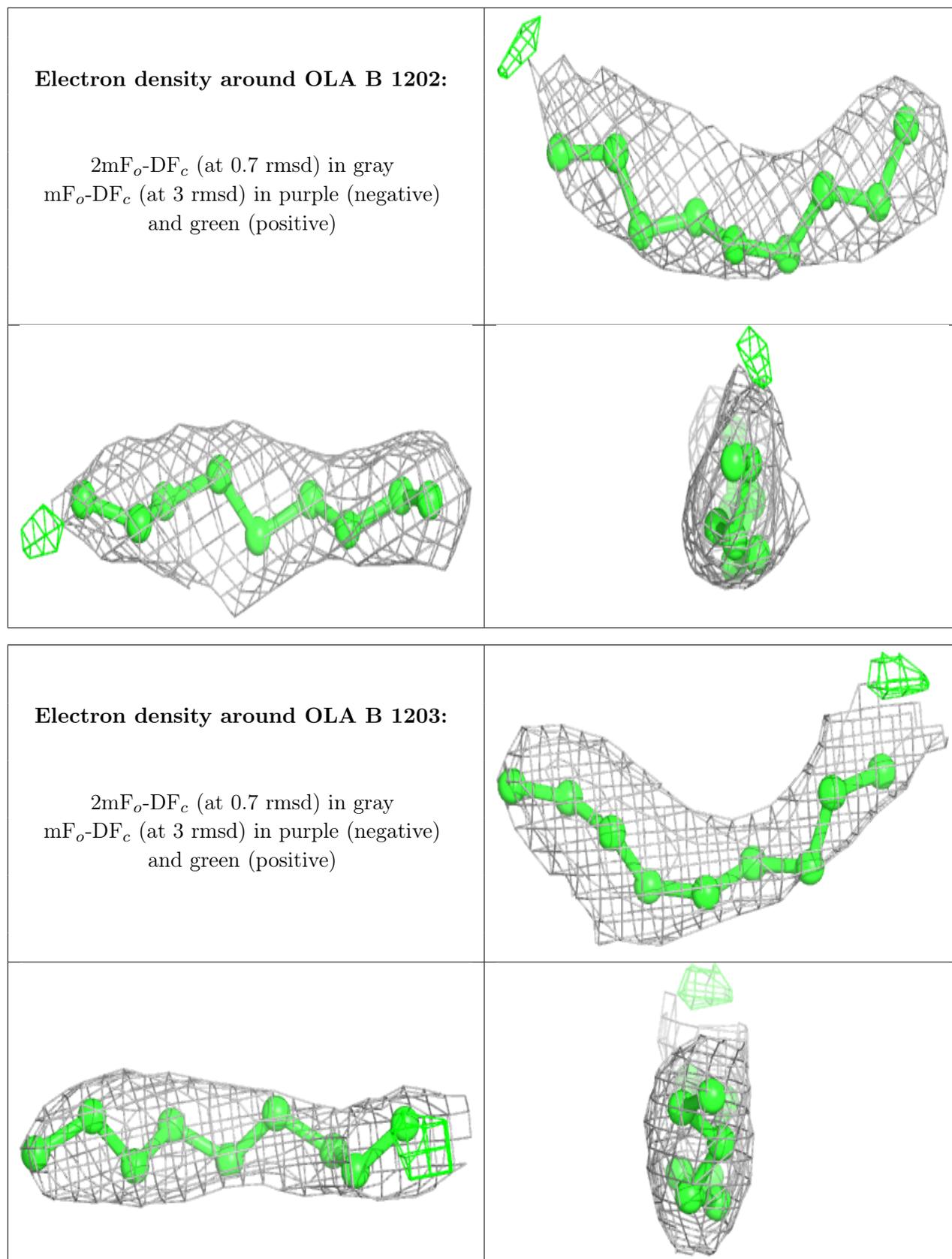
Electron density around OLA A 1202:

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

**Electron density around OLA A 1203:**

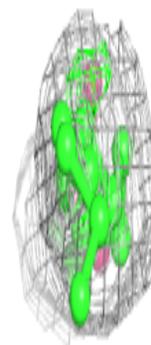
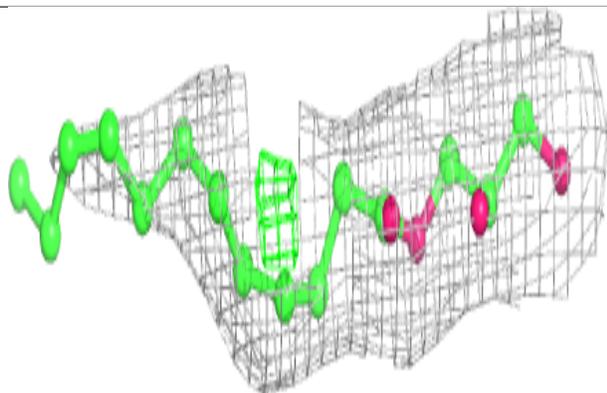
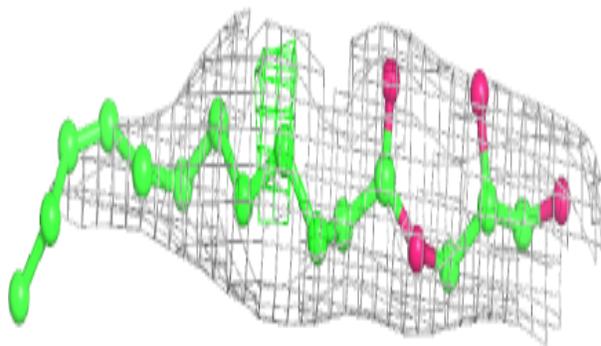
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



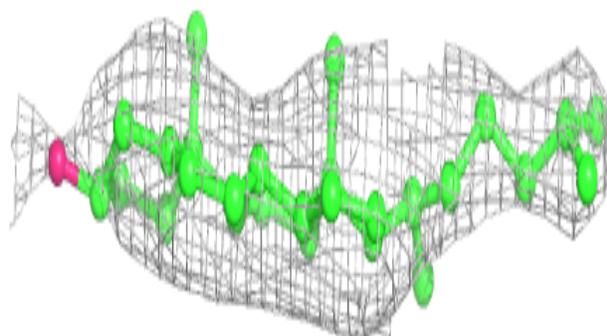
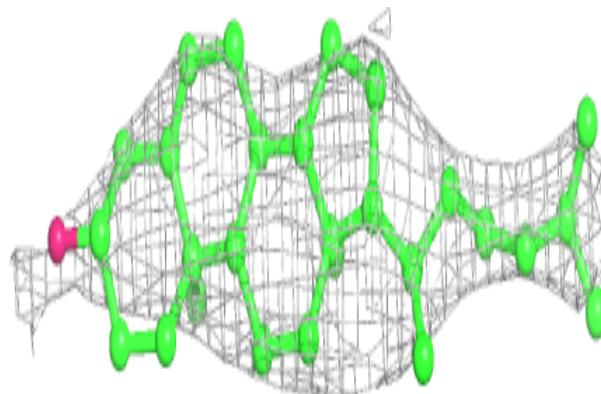


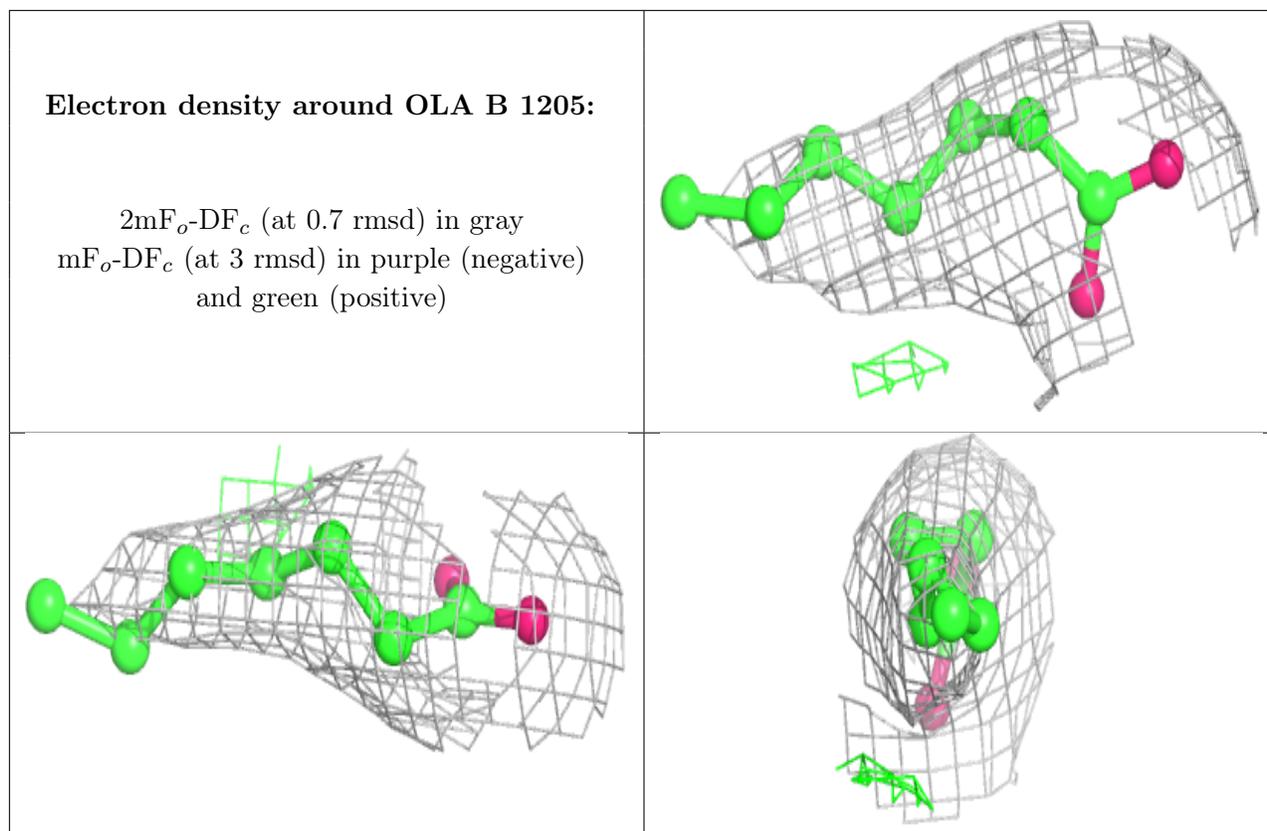
Electron density around OLC B 1206:

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

**Electron density around CLR 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.