Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:49 pm BST

PDB ID	:	6K1Q
Title	:	Human endothelin receptor type-B in complex with inverse agonist IRL2500
Authors	:	Nagiri, C.; Shihoya, W.; Nureki, O.
Deposited on	:	2019-05-11
Resolution	:	2.70 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:

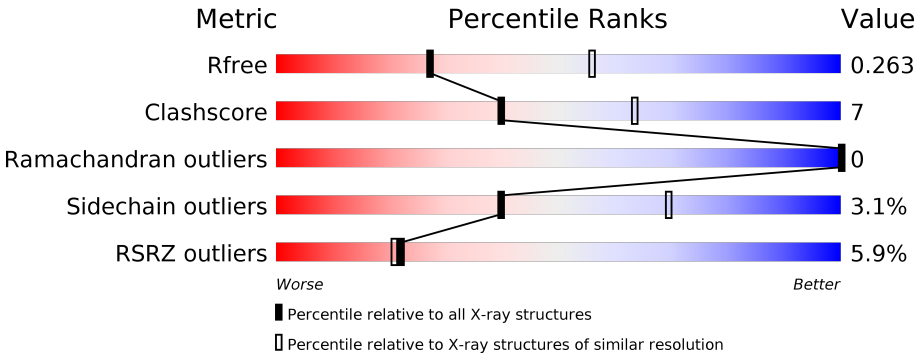
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	464	5% 72% 15% • 12%

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	PO4	A	1202	-	-	-	X
3	PO4	A	1203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	1207	-	-	-	X
4	OLC	A	1211	-	-	-	X
4	OLC	A	1212	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3541 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 Endothelin B receptor,Endolysin,Endothelin B receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3258	2136	539	559	24	0	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P24530
A	64	GLY	-	expression tag	UNP P24530
A	65	GLY	-	expression tag	UNP P24530
A	124	TYR	ARG	engineered mutation	UNP P24530
A	270	ALA	LYS	engineered mutation	UNP P24530
A	1002	ASN	-	linker	UNP P24530
A	1003	ILE	-	linker	UNP P24530
A	1004	PHE	-	linker	UNP P24530
A	1005	GLU	-	linker	UNP P24530
A	1006	MET	-	linker	UNP P24530
A	1007	LEU	-	linker	UNP P24530
A	1008	ARG	-	linker	UNP P24530
A	1009	ILE	-	linker	UNP P24530
A	1010	ASP	-	linker	UNP P24530
A	1011	GLU	-	linker	UNP P24530
A	1012	GLY	-	linker	UNP P24530
A	1012A	GLY	-	linker	UNP P24530
A	1012B	GLY	-	linker	UNP P24530
A	1012C	SER	-	linker	UNP P24530
A	1012D	GLY	-	linker	UNP P24530
A	1012E	GLY	-	linker	UNP P24530
A	1047	ALA	CYS	engineered mutation	UNP P00720
A	1087	ARG	ILE	engineered mutation	UNP P00720
A	342	ALA	SER	engineered mutation	UNP P24530
A	381	ALA	ILE	engineered mutation	UNP P24530
A	396	ALA	CYS	engineered mutation	UNP P24530
A	400	ALA	CYS	engineered mutation	UNP P24530

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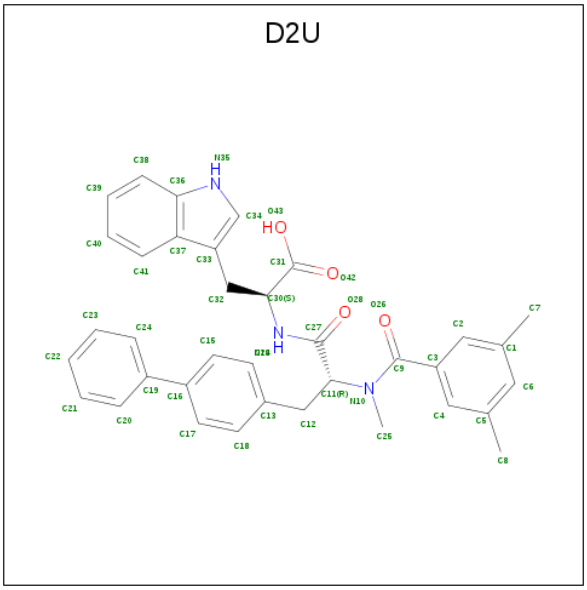
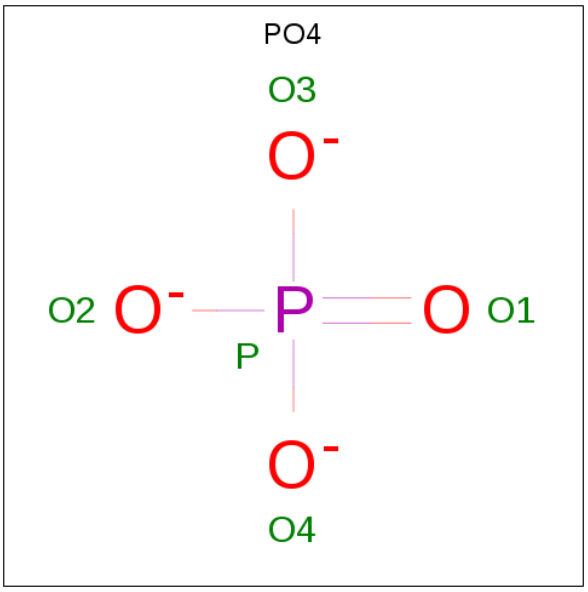
Chain	Residue	Modelled	Actual	Comment	Reference
A	405	ALA	CYS	engineered mutation	UNP P24530
A	408	PRO	-	expression tag	UNP P24530
A	409	SER	-	expression tag	UNP P24530
A	410	SER	-	expression tag	UNP P24530
A	411	GLU	-	expression tag	UNP P24530
A	412	ASN	-	expression tag	UNP P24530
A	413	LEU	-	expression tag	UNP P24530
A	414	TYR	-	expression tag	UNP P24530
A	415	PHE	-	expression tag	UNP P24530
A	416	GLN	-	expression tag	UNP P24530

- Molecule 2 is (2 {S})-2-[[(2 {R})-2-[(3,5-dimethylphenyl)carbonyl-methyl-amino]-3-(4-phenylphenyl)propanoyl]amino]-3-(1 {H}-indol-3-yl)propanoic acid (three-letter code: D2U) (formula: $C_{36}H_{35}N_3O_4$) (labeled as "Ligand of Interest" by author).



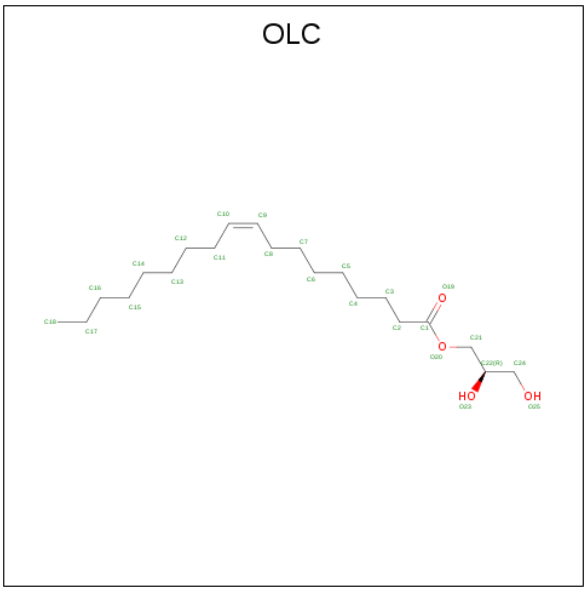
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	36	3	4		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 17 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0

- Molecule 5 is water.

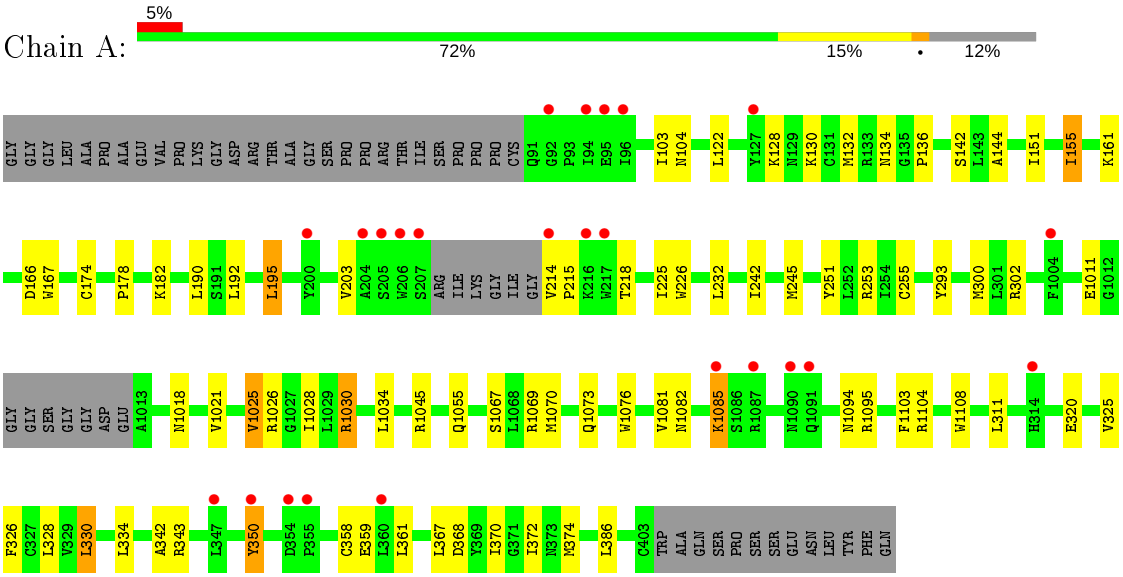
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Endothelin B receptor,Endolysin,Endothelin B receptor

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.91Å 109.91Å 291.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.70 48.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.47-2.70) 100.0 (48.47-2.70)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.222 , 0.265 0.221 , 0.263	Depositor DCC
R_{free} test set	1253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3541	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% 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: PO4, OLC, D2U

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	0.28	0/3331	0.42	0/4528

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	3258	0	3332	45	0
2	A	43	0	0	2	0
3	A	20	0	0	0	0
4	A	186	0	295	11	0
5	A	34	0	0	1	0
All	All	3541	0	3627	52	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 7.

All (52) 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:302:ARG:HH21	1:A:1018:ASN:HD21	1.38	0.71
4:A:1210:OLC:H8A	4:A:1211:OLC:H14A	1.81	0.63
1:A:182:LYS:NZ	5:A:1302:HOH:O	2.33	0.61
1:A:142:SER:HB2	1:A:226:TRP:HE1	1.65	0.61
1:A:128:LYS:O	1:A:130:LYS:NZ	2.37	0.57
1:A:330:LEU:HD13	4:A:1211:OLC:H13	1.88	0.56
1:A:151:ILE:HA	1:A:155:ILE:HG13	1.87	0.56
1:A:370:ILE:O	1:A:374:MET:HG2	2.09	0.53
1:A:178:PRO:HG3	2:A:1201:D2U:C40	2.39	0.53
1:A:203:VAL:HG11	1:A:300:MET:HG2	1.89	0.53
1:A:1076:TRP:HB3	1:A:1104:ARG:HA	1.91	0.52
1:A:342:ALA:HB2	1:A:367:LEU:HG	1.92	0.52
1:A:161:LYS:HD2	1:A:167:TRP:HZ3	1.72	0.52
1:A:242:ILE:HD13	1:A:255:CYS:HB2	1.92	0.51
4:A:1207:OLC:H14A	4:A:1208:OLC:H12A	1.92	0.51
1:A:134:ASN:HD22	1:A:136:PRO:HD2	1.76	0.51
1:A:190:LEU:HB2	1:A:225:ILE:HG23	1.94	0.50
1:A:328:LEU:HD11	1:A:386:LEU:HD21	1.94	0.50
1:A:1026:ARG:O	1:A:1030:ARG:HD3	2.12	0.50
1:A:232:LEU:HD23	4:A:1206:OLC:H8	1.92	0.49
1:A:1067:SER:OG	1:A:1082:ASN:ND2	2.42	0.48
1:A:166:ASP:OD2	1:A:253:ARG:NH1	2.30	0.47
4:A:1210:OLC:H7	4:A:1211:OLC:H12	1.96	0.47
1:A:1069:ARG:O	1:A:1073:GLN:HG2	2.15	0.47
1:A:293:TYR:HB2	1:A:326:PHE:CE1	2.49	0.47
1:A:1021:VAL:O	1:A:1025:VAL:HG13	2.16	0.46
1:A:104:ASN:ND2	1:A:372:ILE:HD11	2.30	0.46
1:A:1045:ARG:NE	1:A:1103:PHE:O	2.41	0.46
1:A:195:LEU:HB3	1:A:325:VAL:HG13	1.98	0.46
1:A:1081:VAL:O	1:A:1085:LYS:HG2	2.17	0.45
1:A:1028:ILE:HG23	1:A:1034:LEU:HB3	1.99	0.45
1:A:343:ARG:HH12	2:A:1201:D2U:C31	2.30	0.45
1:A:174:CYS:O	1:A:174:CYS:SG	2.75	0.44
1:A:132:MET:HA	1:A:132:MET:HE2	2.00	0.44
1:A:358:CYS:SG	1:A:359:GLU:N	2.90	0.44
4:A:1212:OLC:H15	4:A:1212:OLC:H12A	1.87	0.44
1:A:167:TRP:CZ2	1:A:174:CYS:HB2	2.52	0.44
1:A:1070:MET:HB2	1:A:1070:MET:HE3	1.72	0.43
4:A:1206:OLC:H8A	4:A:1206:OLC:H5	1.84	0.43
1:A:1055:GLN:HB2	1:A:1095:ARG:CZ	2.49	0.42
1:A:1108:TRP:O	1:A:311:LEU:HB2	2.20	0.42
1:A:334:LEU:HD12	4:A:1211:OLC:H15A	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HD13	4:A:1212:OLC:H8A	2.01	0.42
1:A:1011:GLU:OE1	1:A:1095:ARG:NH1	2.53	0.41
4:A:1210:OLC:H6	4:A:1210:OLC:H9	1.74	0.41
1:A:245:MET:O	1:A:251:TYR:HA	2.19	0.41
1:A:350:TYR:HD1	1:A:350:TYR:HA	1.67	0.41
1:A:368:ASP:O	1:A:372:ILE:HG23	2.20	0.41
4:A:1208:OLC:O19	4:A:1208:OLC:H24A	2.21	0.41
1:A:122:LEU:HD23	1:A:144:ALA:HB2	2.03	0.41
1:A:215:PRO:O	1:A:218:THR:HG22	2.21	0.41
1:A:214:VAL:N	1:A:215:PRO:HD2	2.36	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	404/464 (87%)	401 (99%)	3 (1%)	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	350/396 (88%)	339 (97%)	11 (3%)	40 69

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	A	192	LEU
1	A	195	LEU
1	A	1025	VAL
1	A	1030	ARG
1	A	1085	LYS
1	A	1094	ASN
1	A	320	GLU
1	A	330	LEU
1	A	350	TYR
1	A	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	1018	ASN
1	A	1066	ASN
1	A	1082	ASN
1	A	1094	ASN
1	A	317	GLN
1	A	382	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

13 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	OLC	A	1212	-	16,19,24	0.25	0	15,19,25	0.59	0
4	OLC	A	1206	-	20,20,24	1.00	1 (5%)	21,21,25	1.09	2 (9%)
3	PO4	A	1205	-	4,4,4	0.93	0	6,6,6	0.45	0
4	OLC	A	1208	-	24,24,24	0.92	1 (4%)	25,25,25	1.05	1 (4%)
3	PO4	A	1202	-	4,4,4	0.95	0	6,6,6	0.42	0
4	OLC	A	1213	-	16,19,24	0.23	0	15,19,25	0.65	0
4	OLC	A	1210	-	24,24,24	0.95	1 (4%)	25,25,25	0.92	1 (4%)
3	PO4	A	1204	-	4,4,4	1.00	0	6,6,6	0.42	0
3	PO4	A	1203	-	4,4,4	0.92	0	6,6,6	0.45	0
4	OLC	A	1211	-	24,24,24	0.94	1 (4%)	25,25,25	0.87	1 (4%)
4	OLC	A	1207	-	24,24,24	0.92	1 (4%)	25,25,25	0.87	1 (4%)
2	D2U	A	1201	-	43,47,47	1.52	4 (9%)	55,66,66	1.02	2 (3%)
4	OLC	A	1209	-	24,24,24	0.93	1 (4%)	25,25,25	0.93	2 (8%)

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	OLC	A	1212	-	-	5/15/17/24	-
4	OLC	A	1206	-	-	8/20/20/24	-
4	OLC	A	1208	-	-	11/24/24/24	-
4	OLC	A	1213	-	-	5/15/17/24	-
4	OLC	A	1210	-	-	10/24/24/24	-
4	OLC	A	1211	-	-	8/24/24/24	-
4	OLC	A	1207	-	-	6/24/24/24	-
2	D2U	A	1201	-	-	3/31/36/36	0/5/5/5
4	OLC	A	1209	-	-	11/24/24/24	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	D2U	C9-N10	5.82	1.46	1.34
2	A	1201	D2U	C27-N29	5.47	1.46	1.34
4	A	1210	OLC	O20-C1	4.38	1.46	1.33
4	A	1211	OLC	O20-C1	4.36	1.46	1.33
4	A	1207	OLC	O20-C1	4.30	1.45	1.33
4	A	1206	OLC	O20-C1	4.29	1.45	1.33
4	A	1209	OLC	O20-C1	4.29	1.45	1.33
4	A	1208	OLC	O20-C1	4.27	1.45	1.33
2	A	1201	D2U	C3-C9	2.51	1.54	1.50
2	A	1201	D2U	O28-C27	-2.11	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	D2U	O26-C9-N10	-3.51	118.25	122.61
4	A	1206	OLC	O20-C1-C2	3.17	121.85	111.91
4	A	1208	OLC	O20-C1-C2	3.16	121.84	111.91
4	A	1210	OLC	O20-C1-C2	3.07	121.55	111.91
4	A	1209	OLC	O20-C1-C2	2.96	121.20	111.91
4	A	1211	OLC	O20-C1-C2	2.63	120.16	111.91
4	A	1207	OLC	O20-C1-C2	2.61	120.10	111.91
2	A	1201	D2U	C12-C11-N10	2.32	116.45	112.69
4	A	1206	OLC	O20-C1-O19	-2.22	117.98	123.59
4	A	1209	OLC	O20-C1-O19	-2.07	118.38	123.59

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1206	OLC	O20-C21-C22-O23
4	A	1210	OLC	C10-C11-C12-C13
4	A	1207	OLC	O20-C21-C22-C24
4	A	1208	OLC	O20-C21-C22-C24
4	A	1207	OLC	O20-C21-C22-O23
4	A	1208	OLC	C1-C2-C3-C4
4	A	1210	OLC	C12-C13-C14-C15
4	A	1206	OLC	O20-C21-C22-C24
4	A	1212	OLC	C11-C12-C13-C14
4	A	1211	OLC	C21-C22-C24-O25
4	A	1208	OLC	O20-C21-C22-O23
4	A	1206	OLC	C1-C2-C3-C4
4	A	1212	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	A	1207	OLC	C1-C2-C3-C4
4	A	1209	OLC	C4-C5-C6-C7
4	A	1206	OLC	C2-C3-C4-C5
4	A	1211	OLC	C10-C11-C12-C13
4	A	1212	OLC	C5-C6-C7-C8
4	A	1213	OLC	C4-C5-C6-C7
4	A	1213	OLC	C6-C7-C8-C9
4	A	1213	OLC	C2-C3-C4-C5
4	A	1210	OLC	C2-C1-O20-C21
4	A	1207	OLC	C4-C5-C6-C7
4	A	1211	OLC	C1-C2-C3-C4
4	A	1213	OLC	C5-C6-C7-C8
4	A	1210	OLC	O19-C1-O20-C21
4	A	1211	OLC	O23-C22-C24-O25
4	A	1209	OLC	C15-C16-C17-C18
4	A	1208	OLC	C2-C1-O20-C21
4	A	1208	OLC	O19-C1-O20-C21
4	A	1213	OLC	C13-C14-C15-C16
4	A	1209	OLC	C21-C22-C24-O25
4	A	1212	OLC	C12-C13-C14-C15
4	A	1208	OLC	C3-C4-C5-C6
4	A	1208	OLC	O23-C22-C24-O25
2	A	1201	D2U	C11-C12-C13-C14
4	A	1210	OLC	C7-C8-C9-C10
4	A	1209	OLC	C2-C3-C4-C5
4	A	1209	OLC	C3-C4-C5-C6
4	A	1210	OLC	C15-C16-C17-C18
4	A	1208	OLC	C12-C13-C14-C15
4	A	1209	OLC	O20-C21-C22-O23
4	A	1206	OLC	C11-C12-C13-C14
2	A	1201	D2U	C11-C12-C13-C18
4	A	1209	OLC	C5-C6-C7-C8
4	A	1206	OLC	C6-C7-C8-C9
4	A	1209	OLC	C12-C13-C14-C15
4	A	1208	OLC	C21-C22-C24-O25
4	A	1206	OLC	C5-C6-C7-C8
4	A	1212	OLC	C9-C10-C11-C12
2	A	1201	D2U	C30-C32-C33-C34
4	A	1209	OLC	O23-C22-C24-O25
4	A	1206	OLC	C3-C4-C5-C6
4	A	1211	OLC	C2-C3-C4-C5
4	A	1210	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	1210	OLC	C4-C5-C6-C7
4	A	1211	OLC	C2-C1-O20-C21
4	A	1211	OLC	C9-C10-C11-C12
4	A	1207	OLC	C5-C6-C7-C8
4	A	1207	OLC	C9-C10-C11-C12
4	A	1208	OLC	C10-C11-C12-C13
4	A	1209	OLC	C2-C1-O20-C21
4	A	1210	OLC	C6-C7-C8-C9
4	A	1209	OLC	O19-C1-O20-C21
4	A	1210	OLC	C2-C3-C4-C5
4	A	1208	OLC	C7-C8-C9-C10
4	A	1211	OLC	O19-C1-O20-C21

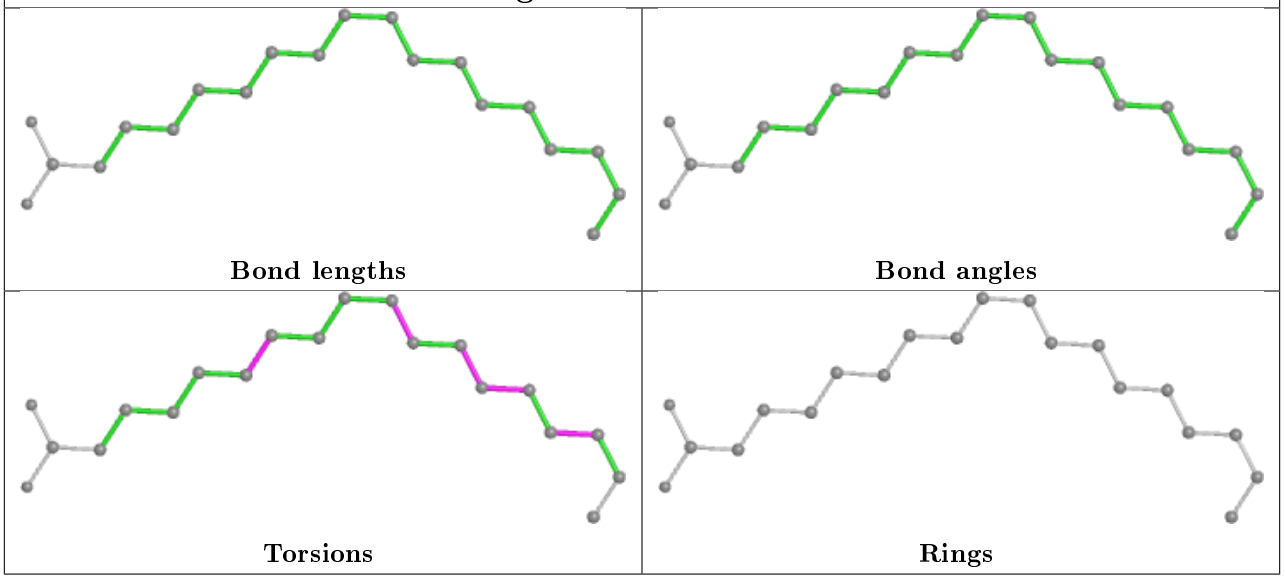
There are no ring outliers.

7 monomers are involved in 13 short contacts:

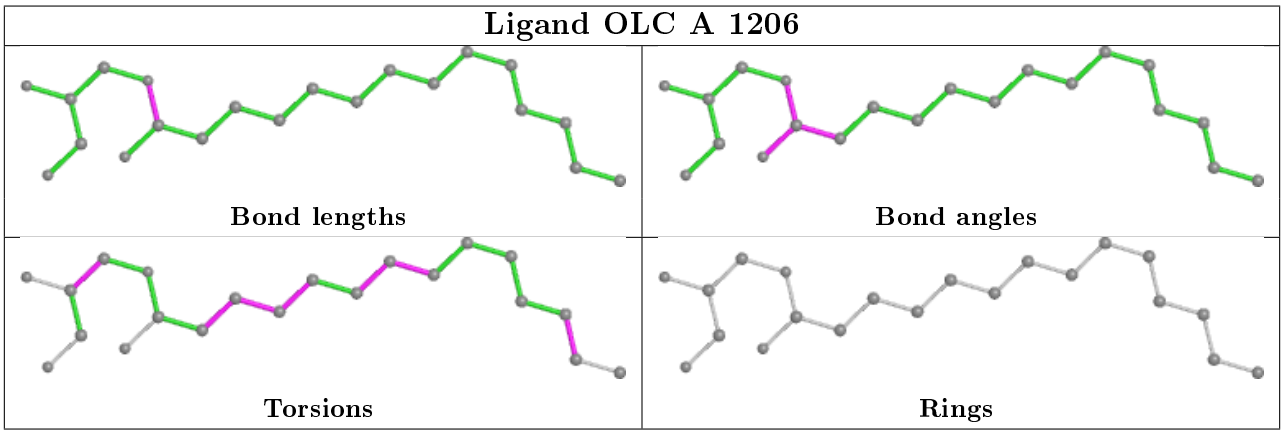
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1212	OLC	2	0
4	A	1206	OLC	2	0
4	A	1208	OLC	2	0
4	A	1210	OLC	3	0
4	A	1211	OLC	4	0
4	A	1207	OLC	1	0
2	A	1201	D2U	2	0

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.

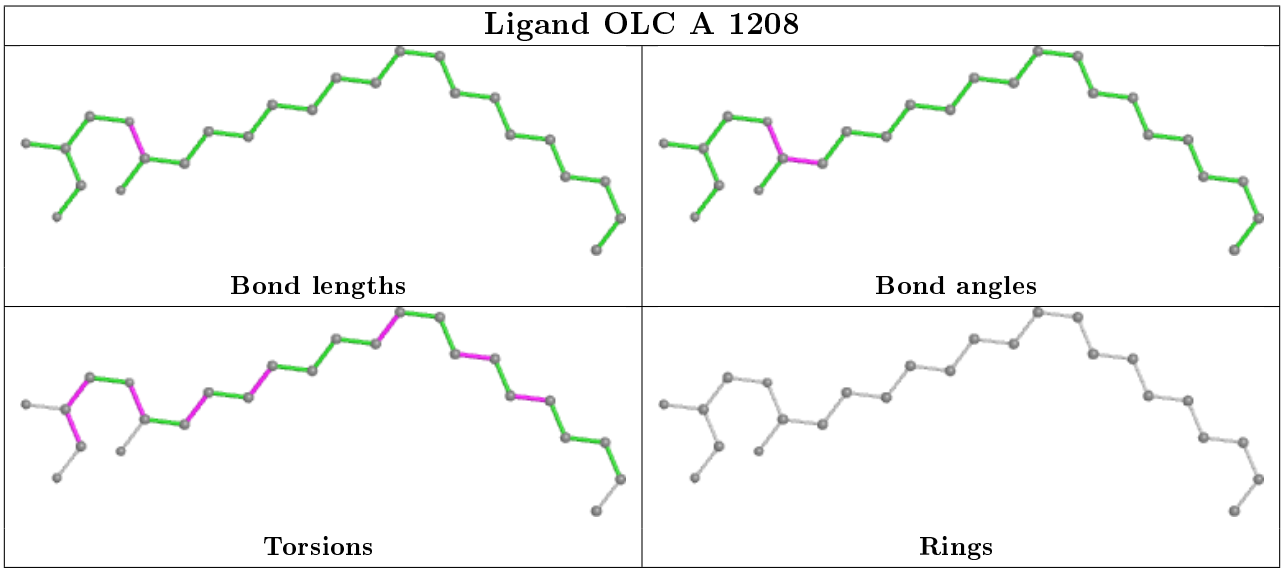
Ligand OLC A 1212



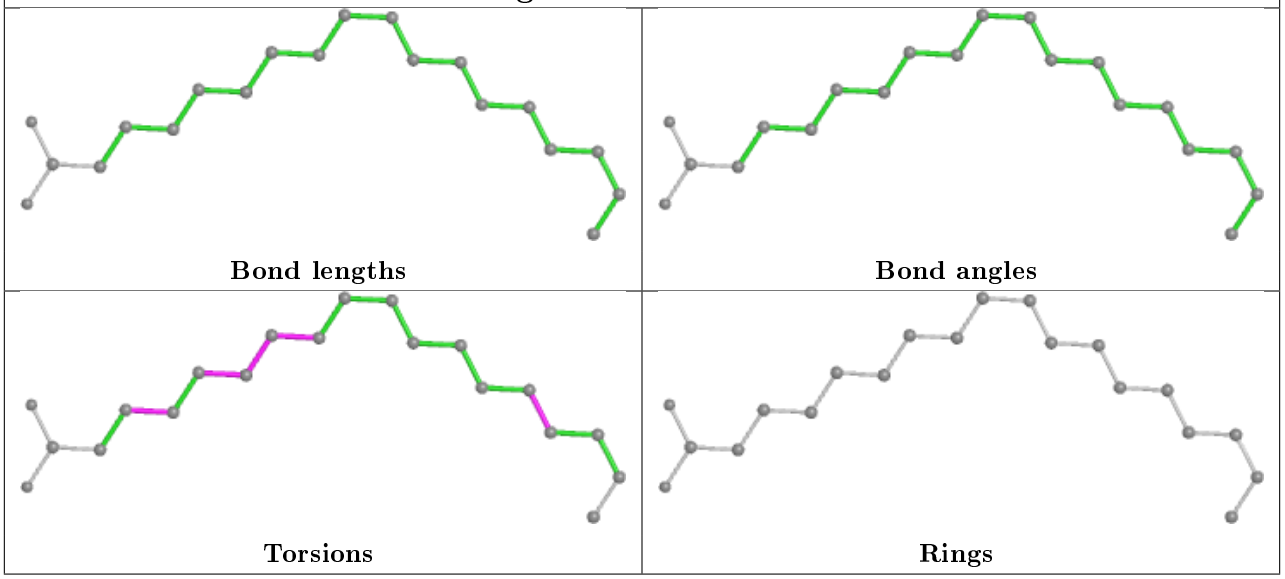
Ligand OLC A 1206



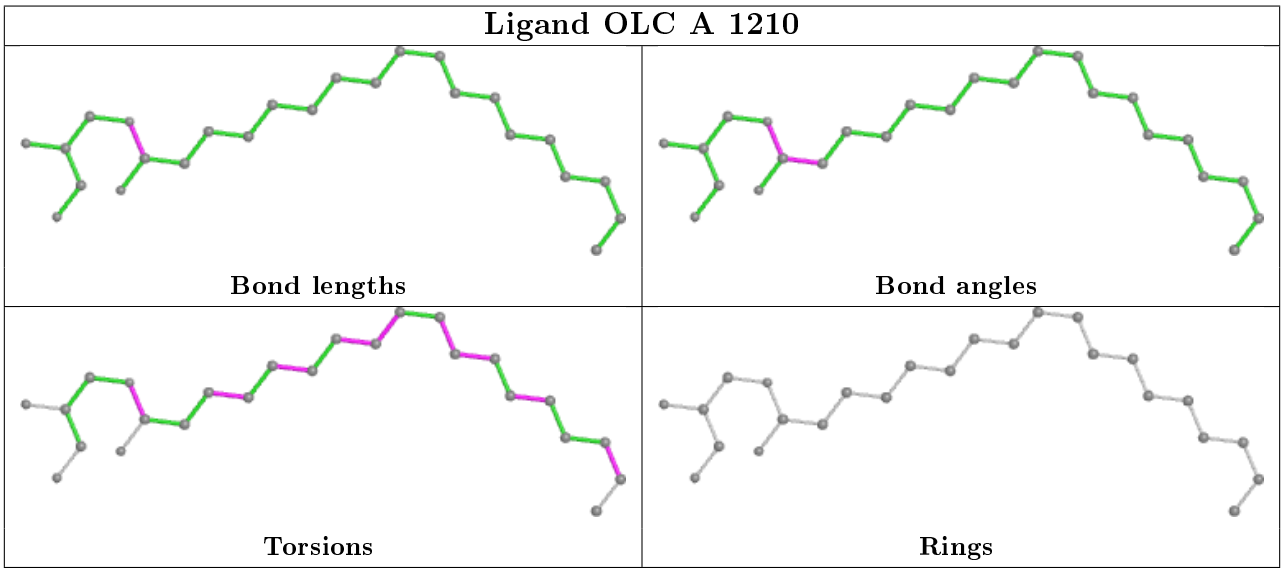
Ligand OLC A 1208



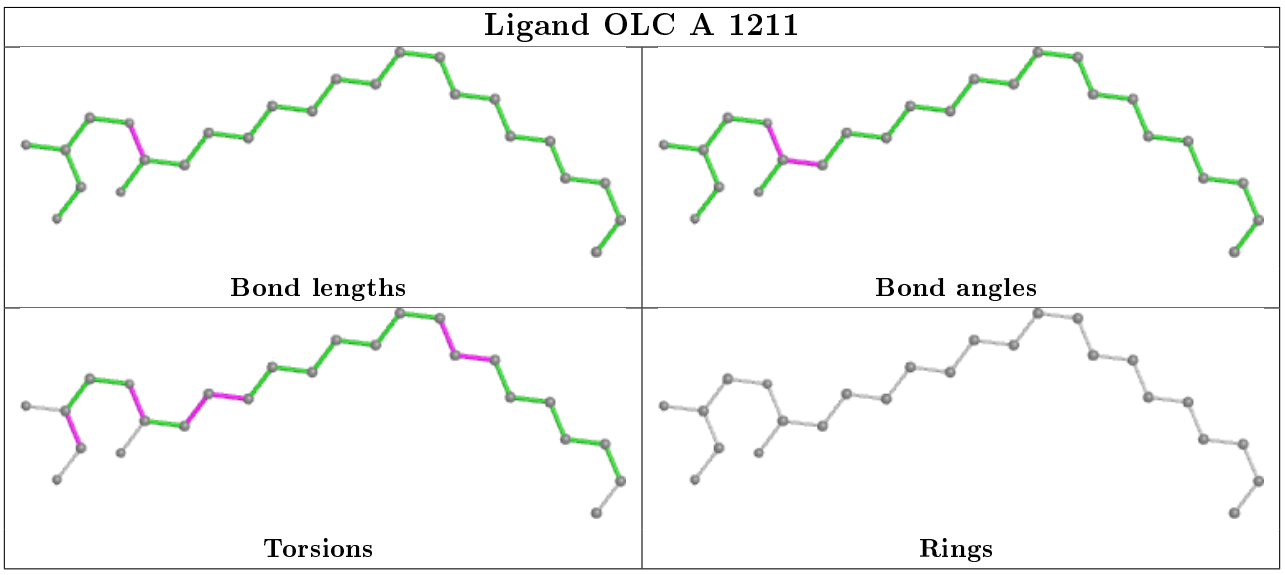
Ligand OLC A 1213



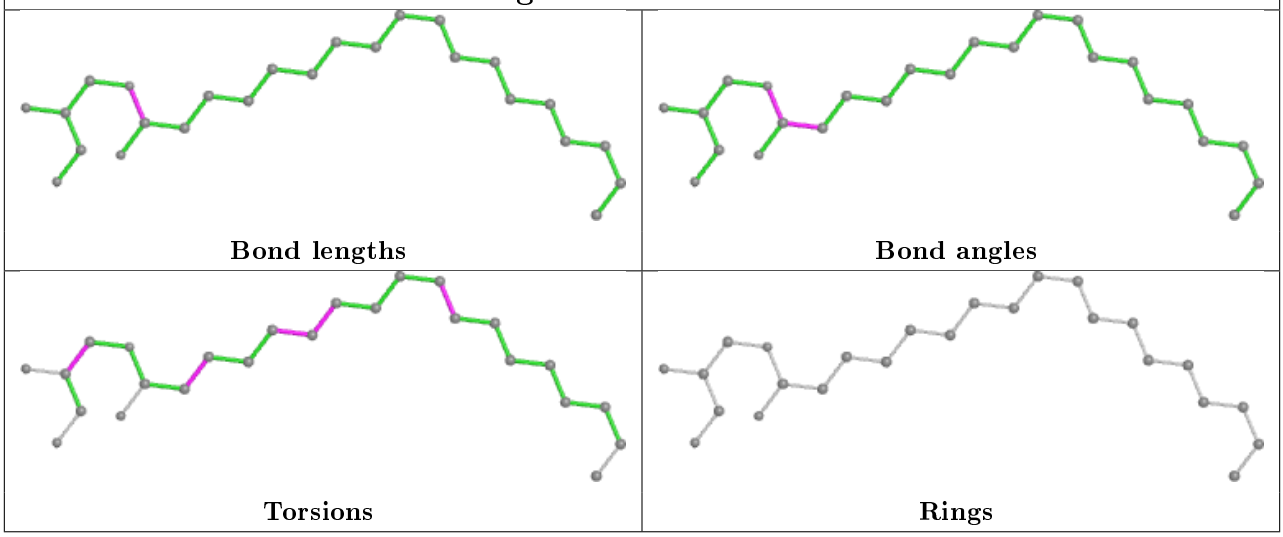
Ligand OLC A 1210



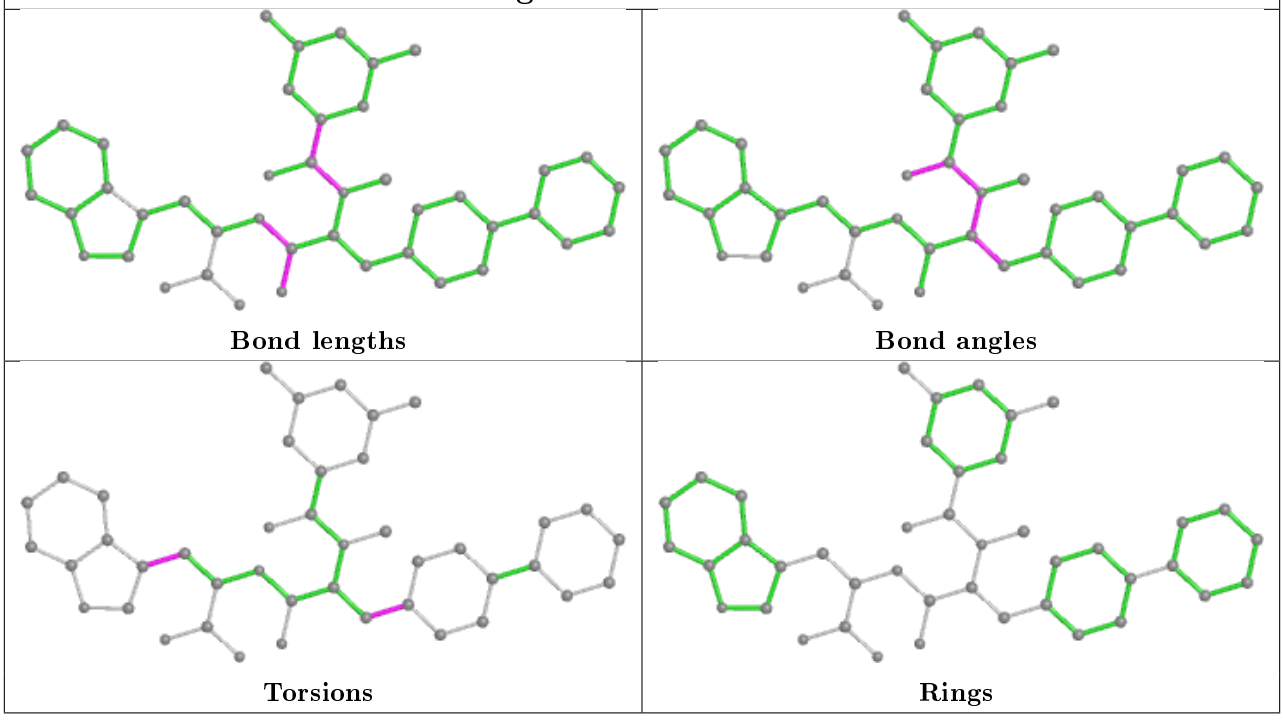
Ligand OLC A 1211



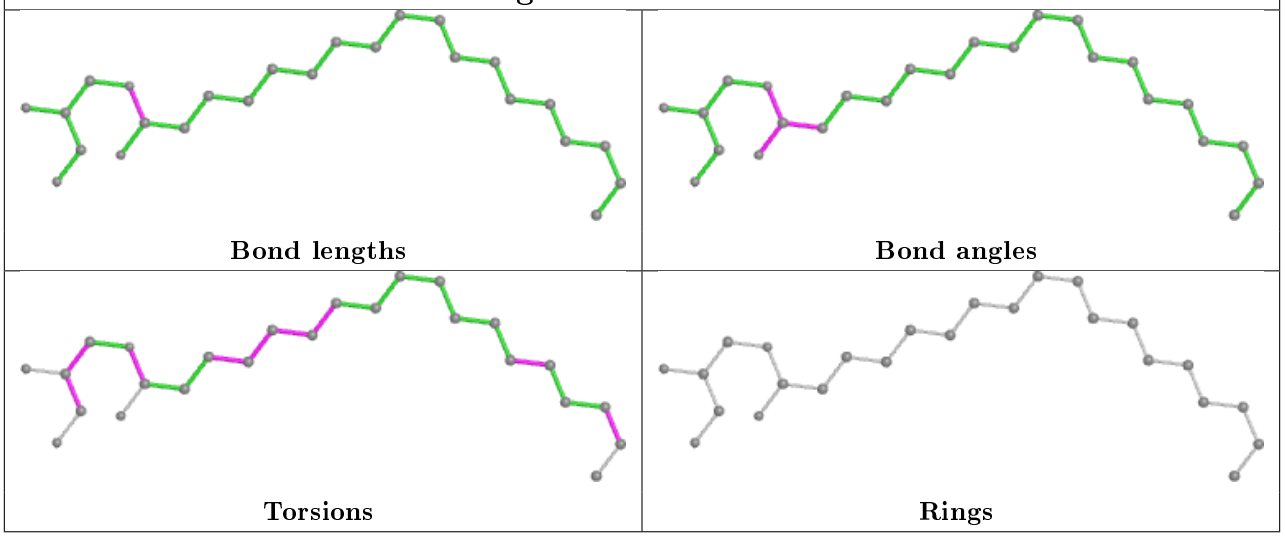
Ligand OLC A 1207



Ligand D2U A 1201



Ligand OLC A 1209



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	410/464 (88%)	0.43	24 (5%)	22	21	42, 72, 142, 230	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	TYR	5.6
1	A	354	ASP	4.6
1	A	205	SER	4.3
1	A	207	SER	4.2
1	A	355	PRO	4.2
1	A	214	VAL	3.2
1	A	360	LEU	3.0
1	A	1087	ARG	2.8
1	A	1090	ASN	2.8
1	A	204	ALA	2.7
1	A	1091	GLN	2.7
1	A	92	GLY	2.6
1	A	1004	PHE	2.6
1	A	206	TRP	2.4
1	A	1085	LYS	2.3
1	A	200	TYR	2.2
1	A	217	TRP	2.2
1	A	95	GLU	2.2
1	A	347	LEU	2.2
1	A	96	ILE	2.2
1	A	127	TYR	2.1
1	A	94	ILE	2.1
1	A	216	LYS	2.0
1	A	314	HIS	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 carbohydrates in this entry.

6.4 Ligands (i)

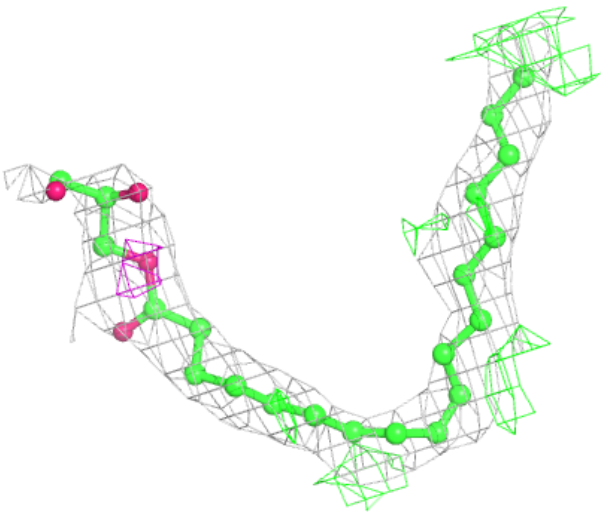
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

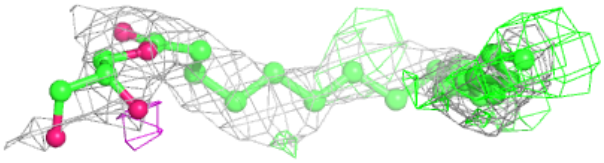
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	1211	25/25	0.61	0.42	94,99,103,107	0
3	PO4	A	1203	5/5	0.64	0.44	152,156,158,159	0
3	PO4	A	1205	5/5	0.72	0.17	219,219,220,220	0
3	PO4	A	1202	5/5	0.72	0.42	146,147,151,152	0
4	OLC	A	1208	25/25	0.76	0.36	85,97,116,117	0
4	OLC	A	1212	20/25	0.76	0.42	87,94,105,110	0
4	OLC	A	1207	25/25	0.79	0.42	99,108,121,125	0
4	OLC	A	1210	25/25	0.81	0.33	69,100,118,119	0
4	OLC	A	1206	21/25	0.86	0.34	51,68,94,97	0
3	PO4	A	1204	5/5	0.87	0.38	104,108,109,117	0
4	OLC	A	1209	25/25	0.88	0.29	69,83,106,108	0
4	OLC	A	1213	20/25	0.91	0.31	57,73,85,88	0
2	D2U	A	1201	43/43	0.97	0.20	36,48,63,67	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 OLC A 1211:

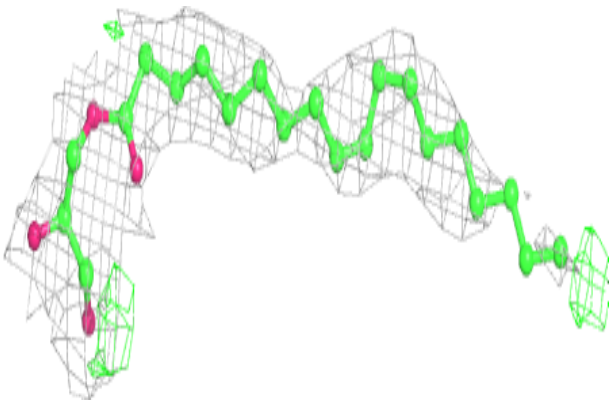
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

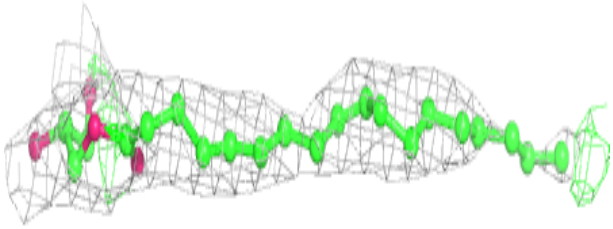


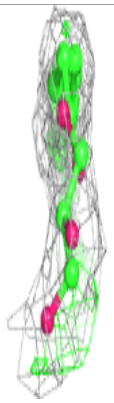


Electron density around OLC A 1208:

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

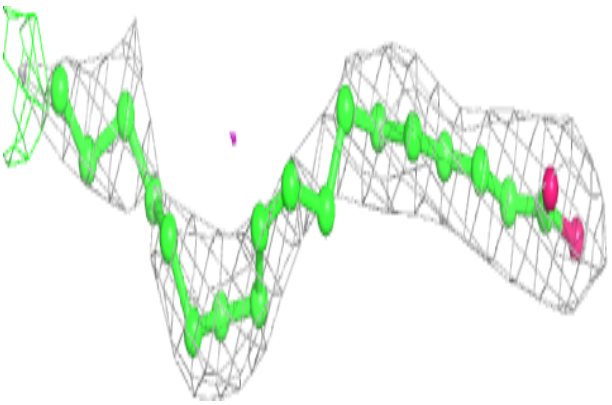


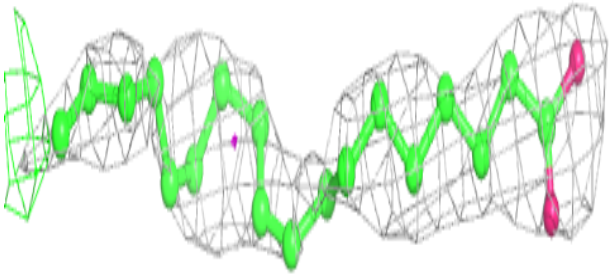


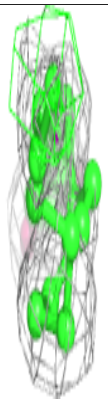


Electron density around OLC A 1212:

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

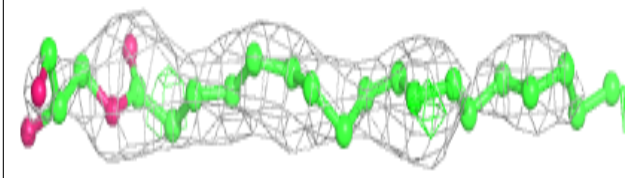


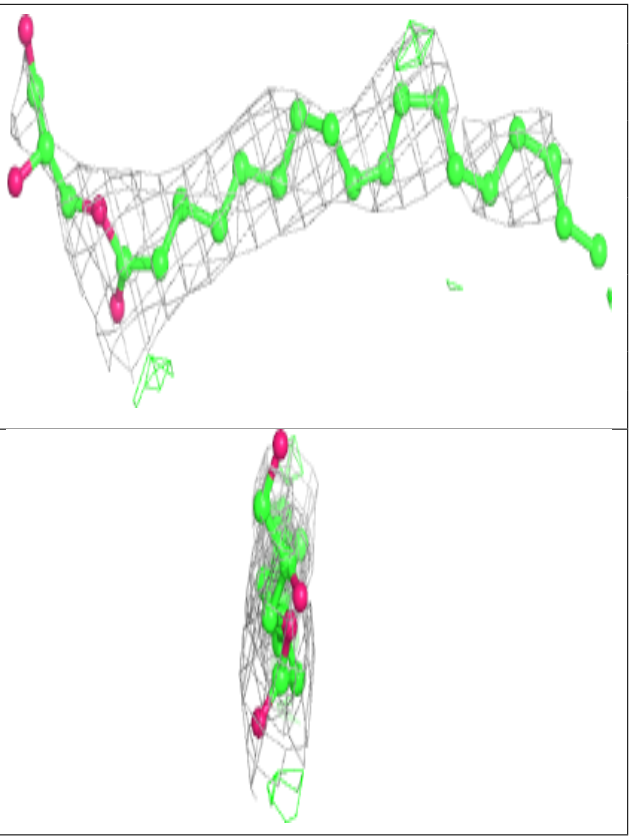




Electron density around OLC A 1207:

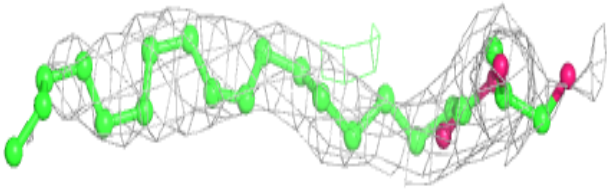
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

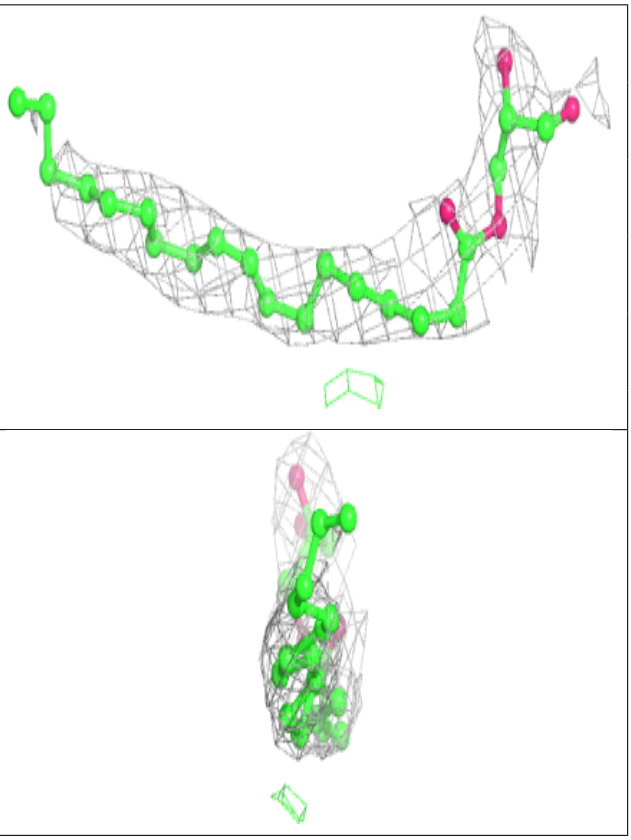




Electron density around OLC A 1210:

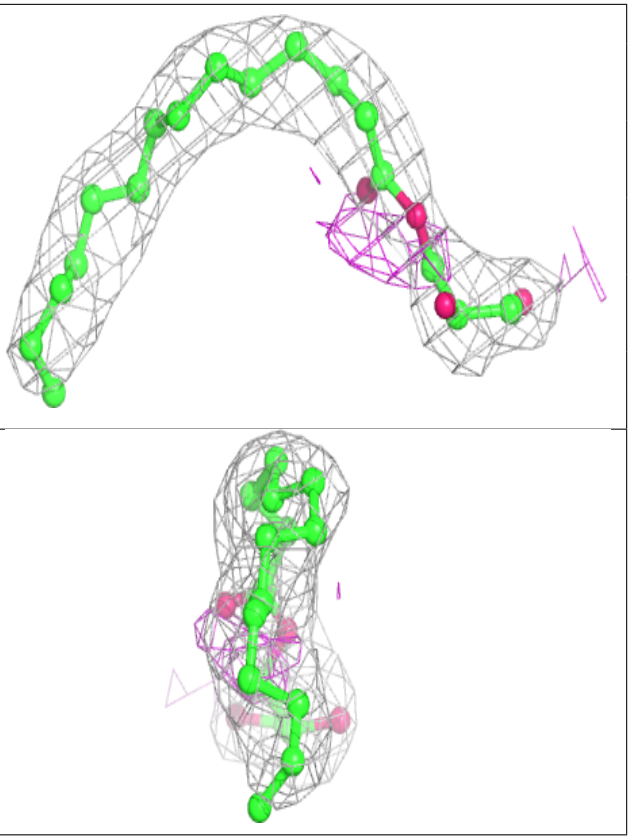
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





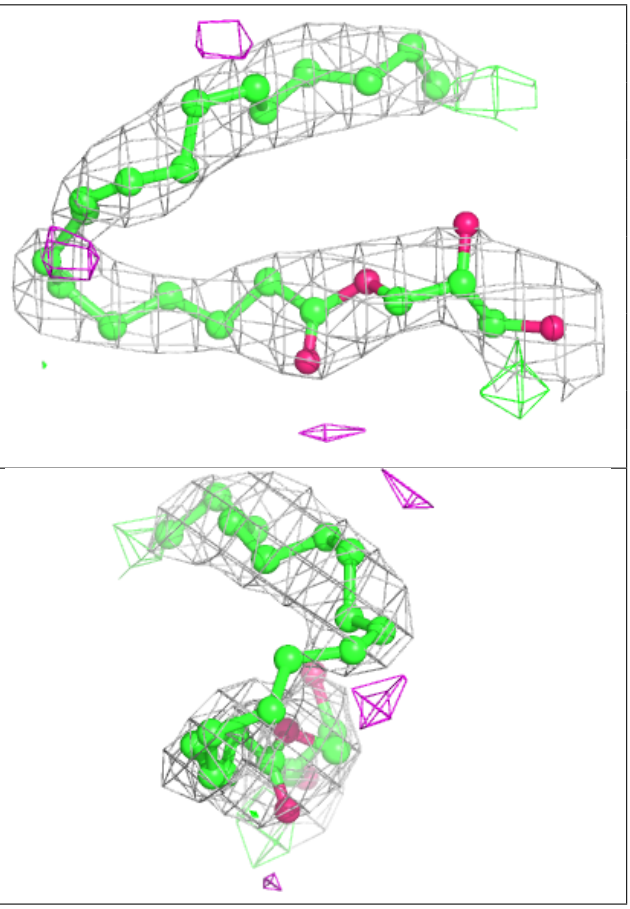
Electron density around OLC A 1206:

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



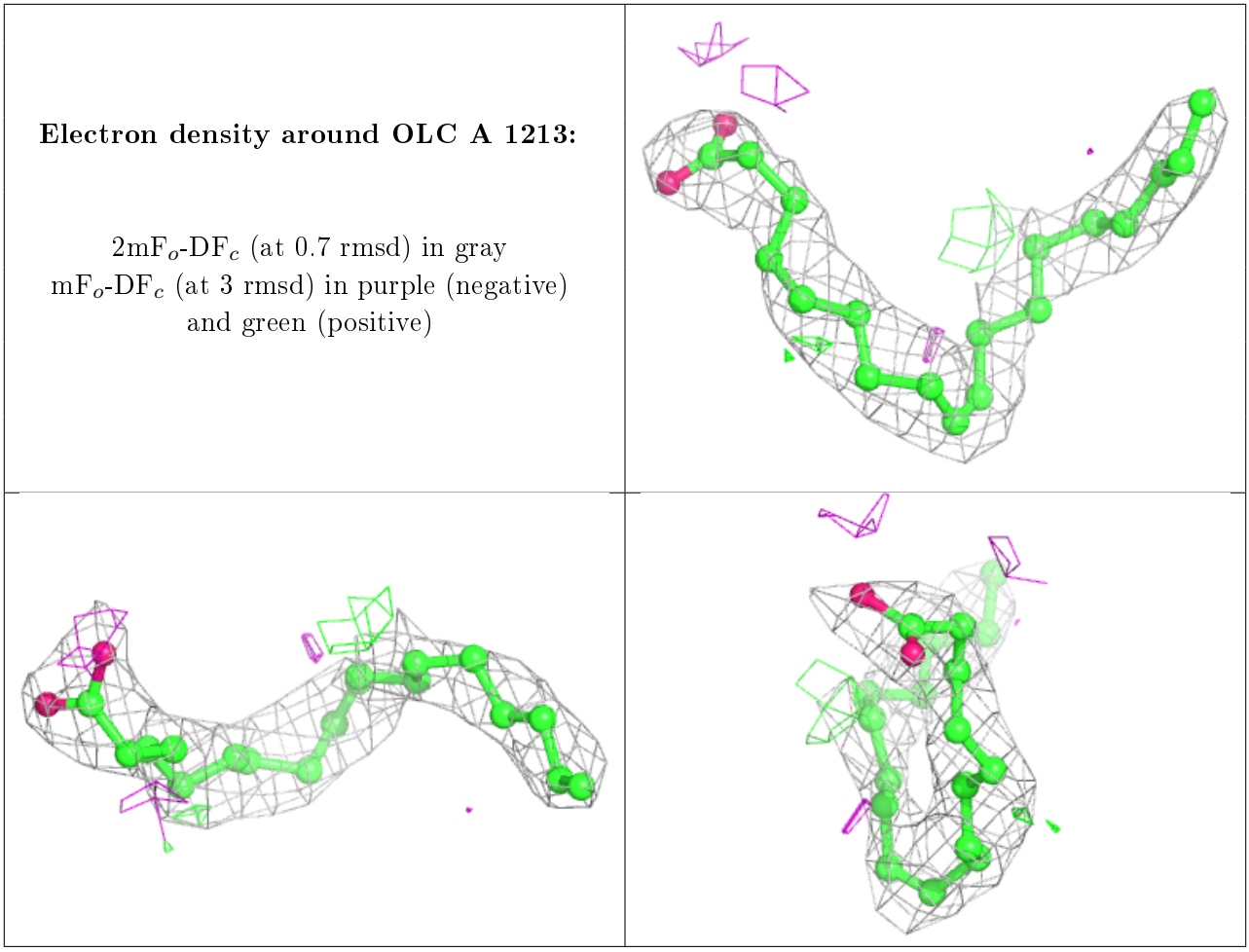
Electron density around OLC A 1209:

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



Electron density around OLC 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 D2U A 1201:

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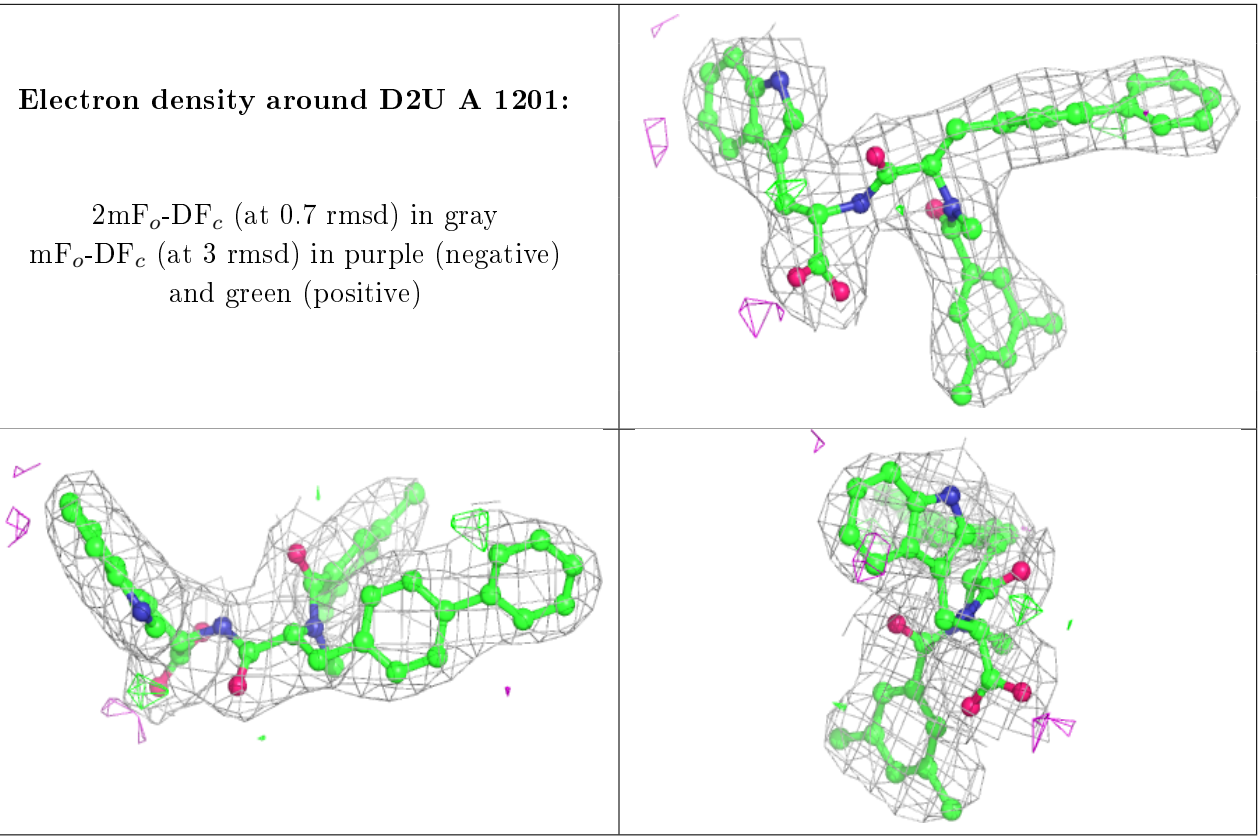
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.