



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 03:01 PM BST

PDB ID : 6WMV
Title : Structure of a phosphatidylinositol-phosphate synthase (PIPS) from Mycobacterium kansasii with evidence of substrate binding
Authors : Belcher Dufrisne, M.; Jorge, C.D.; Timoteo, C.G.; Petrou, V.I.; Ashraf, K.U.; Banerjee, S.; Clarke, O.B.; Santos, H.; Mancia, F.
Deposited on : 2020-04-21
Resolution : 2.14 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 : 2.14.2
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) : 2.14.2

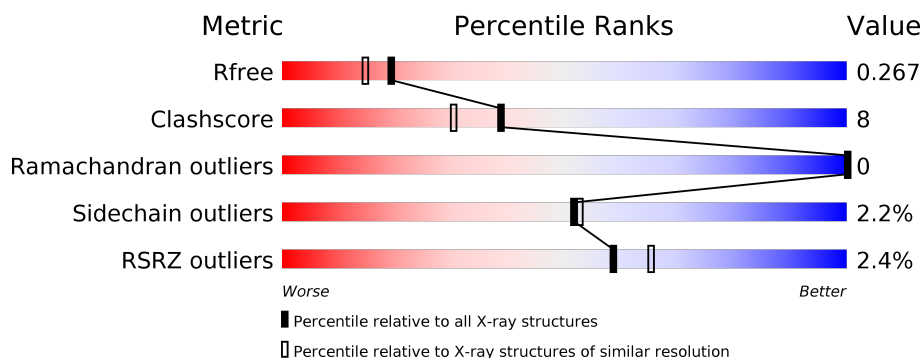
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 $\leq 5\%$. 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	370	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
1	C	370	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5322 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.

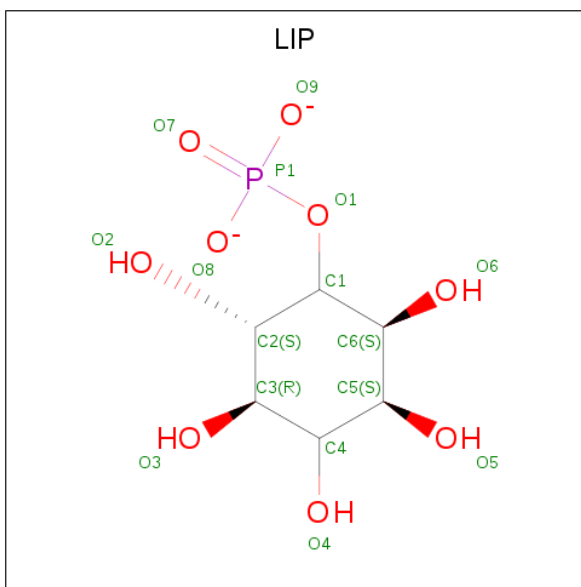
- Molecule 1 is a protein called AfCTD-Phosphatidylinositol-phosphate synthase (PIPS) fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2510	1641	415	445	9			
1	C	336	Total	C	N	O	S	0	0	0
			2517	1642	416	451	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	linker	UNP A0A101DFK9
A	-1	SER	-	linker	UNP A0A101DFK9
A	0	GLY	-	linker	UNP A0A101DFK9
A	1	SER	-	linker	UNP A0A101DFK9
A	17	LEU	ASP	engineered mutation	UNP U5WZP7
A	77	LEU	GLN	engineered mutation	UNP U5WZP7
A	79	SER	GLY	engineered mutation	UNP U5WZP7
C	-2	GLY	-	linker	UNP A0A101DFK9
C	-1	SER	-	linker	UNP A0A101DFK9
C	0	GLY	-	linker	UNP A0A101DFK9
C	1	SER	-	linker	UNP A0A101DFK9
C	17	LEU	ASP	engineered mutation	UNP U5WZP7
C	77	LEU	GLN	engineered mutation	UNP U5WZP7
C	79	SER	GLY	engineered mutation	UNP U5WZP7

- Molecule 2 is L-MYO-INOSITOL-1-PHOSPHATE (three-letter code: LIP) (formula: C₆H₁₁O₉P) (labeled as "Ligand of Interest" by author).

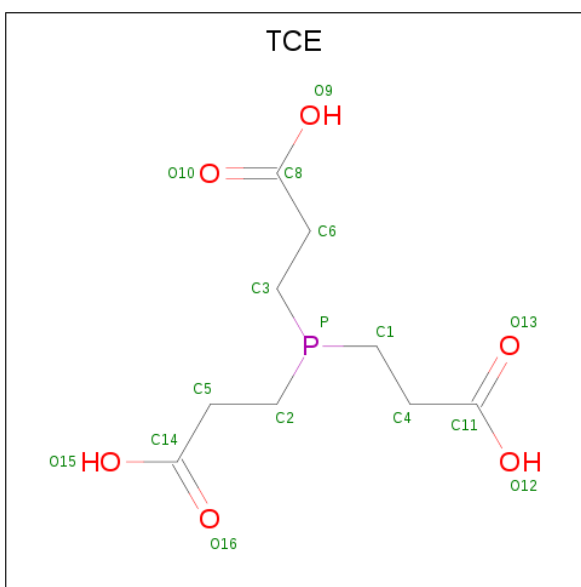


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is 3,3',3''-phosphanetriyltripropanoic acid (three-letter code: TCE) (formula: C₉H₁₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			16	9	6	1		

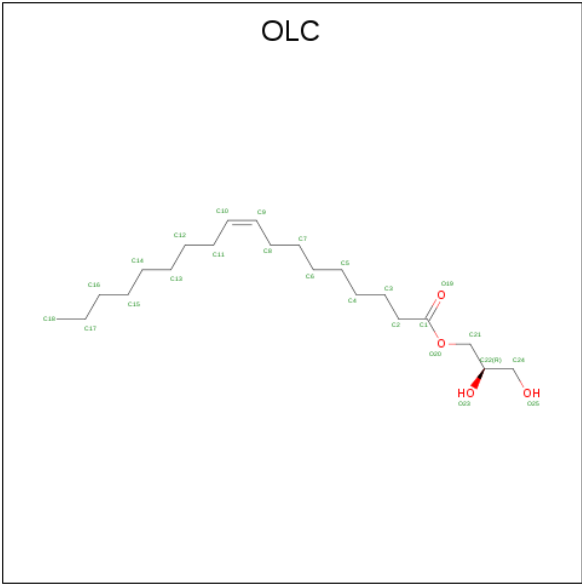
- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			8	5	3		

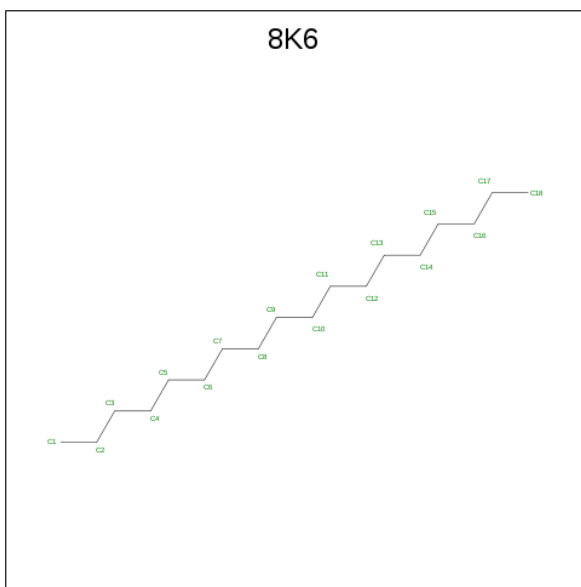
- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC)

(formula: C₂₁H₄₀O₄).



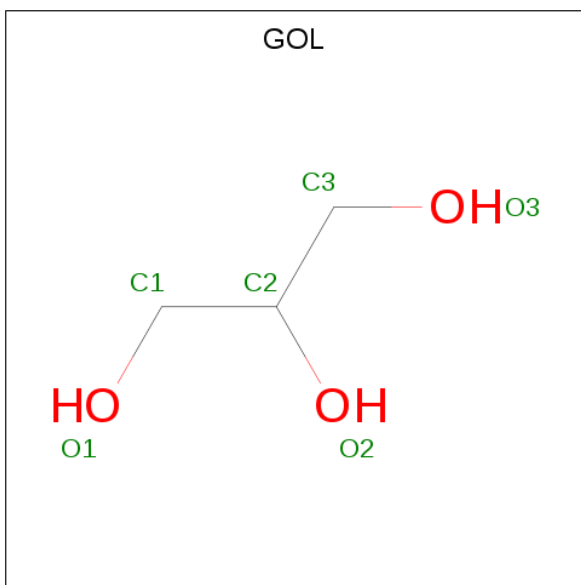
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	18	4		
6	A	1	Total	C	O	0	0
			12	8	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			12	8	4		
6	C	1	Total	C	O	0	0
			11	7	4		
6	C	1	Total	C	O	0	0
			25	21	4		
6	C	1	Total	C	O	0	0
			13	9	4		

- Molecule 7 is Octadecane (three-letter code: 8K6) (formula: C₁₈H₃₈).



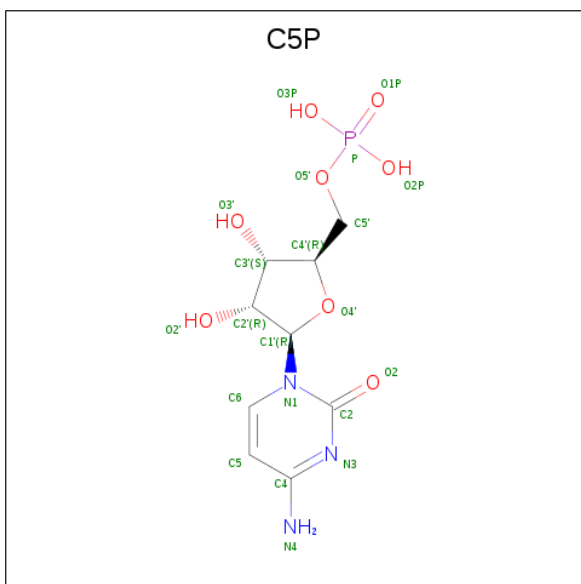
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 15 15	0	0
7	A	1	Total C 5 5	0	0
7	A	1	Total C 10 10	0	0
7	A	1	Total C 8 8	0	0
7	C	1	Total C 7 7	0	0
7	C	1	Total C 15 15	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



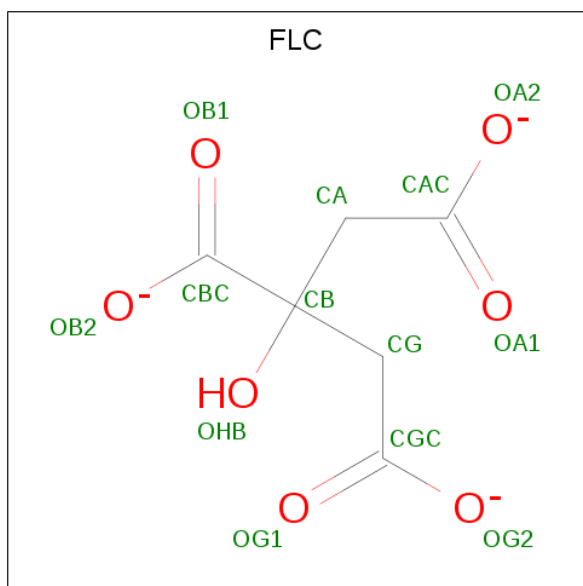
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 10 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			13	6	7		

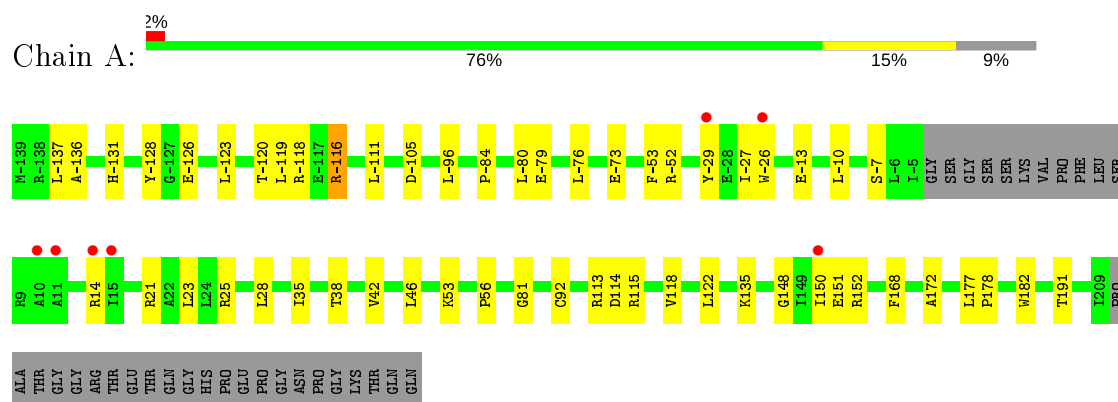
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	16	Total	O	0	0
			16	16		
11	C	11	Total	O	0	0
			11	11		

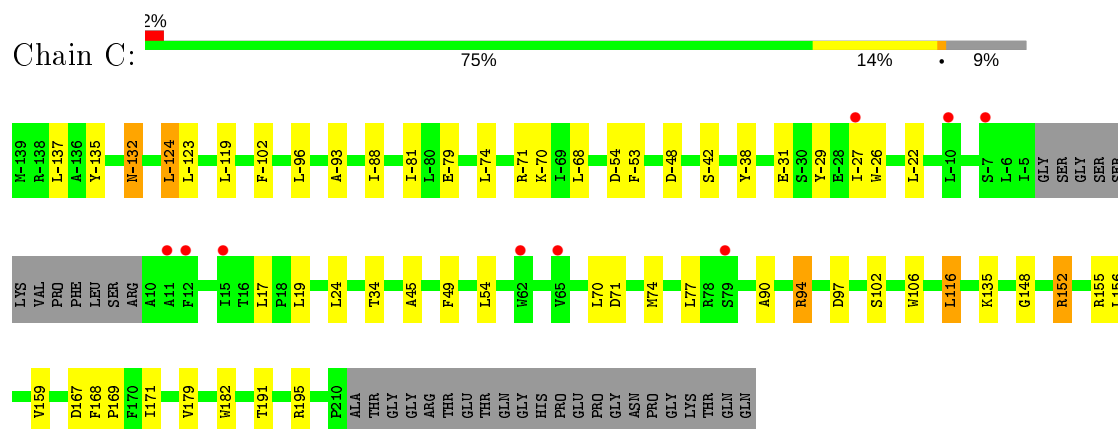
3 Residue-property plots

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: AfCTD-Phosphatidylinositol-phosphate synthase (PIPS) fusion



- Molecule 1: AfCTD-Phosphatidylinositol-phosphate synthase (PIPS) fusion



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.09Å 60.86Å 85.42Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	78.08 – 2.14 85.41 – 2.14	Depositor EDS
% Data completeness (in resolution range)	58.5 (78.08-2.14) 58.6 (85.41-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.223 , 0.270 0.225 , 0.267	Depositor DCC
R_{free} test set	1298 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, OLC, C5P, NA, 1PE, LIP, FLC, TCE, 8K6

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	0.35	0/2561	0.51	0/3494
1	C	0.34	0/2568	0.51	0/3501
All	All	0.35	0/5129	0.51	0/6995

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	2510	0	2504	39	0
1	C	2517	0	2523	38	0
2	A	16	0	11	3	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
4	A	16	0	12	1	0
5	A	7	0	9	0	0
5	C	8	0	9	0	0
6	A	44	0	53	1	0
6	C	61	0	79	3	0
7	A	38	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	22	0	42	4	0
8	A	6	0	8	0	0
8	C	12	0	16	1	0
9	C	21	0	12	0	0
10	C	13	0	5	3	0
11	A	16	0	0	0	0
11	C	11	0	0	0	0
All	All	5322	0	5355	80	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 8.

All (80) 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:-116:ARG:NH1	1:A:-10:LEU:HD21	1.60	1.12
1:A:81:GLY:HA3	4:A:305:TCE:H5A	1.61	0.82
1:A:-116:ARG:HH12	1:A:-10:LEU:HD21	1.42	0.81
1:A:-116:ARG:NH1	1:A:-10:LEU:CD2	2.43	0.81
1:C:195:ARG:HH22	10:C:302:FLC:HA1	1.47	0.80
1:A:-116:ARG:HH11	1:A:-10:LEU:HD21	1.45	0.80
1:C:179:VAL:HG12	6:C:308:OLC:H5A	1.64	0.79
1:C:135:LYS:HD3	10:C:302:FLC:OHB	1.89	0.72
1:C:97:ASP:OD2	1:C:152:ARG:NH1	2.24	0.71
1:A:35:ILE:HD11	7:A:310:8K6:H112	1.71	0.70
1:A:-79:GLU:OE2	1:A:-27:ILE:HG13	1.94	0.68
1:A:-116:ARG:HH11	1:A:-10:LEU:CD2	2.05	0.68
7:A:310:8K6:H122	7:C:309:8K6:H182	1.76	0.68
1:A:-128:TYR:HB3	1:A:-118:ARG:HB2	1.75	0.67
1:A:46:LEU:HD22	6:A:307:OLC:H6A	1.77	0.65
1:A:-123:LEU:HD21	1:A:-13:GLU:HG3	1.81	0.63
1:A:182:TRP:HE1	7:A:312:8K6:H183	1.65	0.61
1:C:19:LEU:HD13	1:C:70:LEU:HD11	1.82	0.61
7:A:310:8K6:H91C	7:C:309:8K6:H151	1.84	0.59
1:C:-123:LEU:HD13	1:C:77:LEU:HD22	1.83	0.59
1:C:-70:LYS:NZ	1:C:-31:GLU:OE2	2.36	0.59
6:C:307:OLC:H5A	8:C:311:GOL:H31	1.85	0.59
1:C:-119:LEU:HD13	1:C:-22:LEU:HD13	1.85	0.58
1:A:151:GLU:HB3	2:A:301:LIP:O4	2.04	0.58
1:C:195:ARG:NH2	10:C:302:FLC:HA1	2.20	0.57
1:A:-137:LEU:HD23	1:A:-105:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HB3	1:A:56:PRO:HG2	1.88	0.56
1:C:168:PHE:CD2	1:C:169:PRO:HD2	2.40	0.56
1:A:-96:LEU:HD23	1:A:-52:ARG:HA	1.88	0.56
1:A:114:ASP:O	1:A:118:VAL:HG13	2.06	0.55
1:C:-124:LEU:HD22	1:C:-119:LEU:HD21	1.89	0.54
1:A:152:ARG:N	2:A:301:LIP:O4	2.39	0.53
7:A:310:8K6:H102	7:C:309:8K6:H151	1.89	0.53
1:A:-118:ARG:HH11	1:A:-118:ARG:HG2	1.73	0.52
1:A:38:THR:O	1:A:42:VAL:HG13	2.10	0.52
1:C:-132:ASN:ND2	1:C:-102:PHE:HB3	2.24	0.52
1:C:34:THR:OG1	1:C:71:ASP:OD2	2.26	0.51
1:A:-126:GLU:HB3	1:A:-119:LEU:HD12	1.93	0.51
1:A:115:ARG:O	1:A:118:VAL:HG22	2.11	0.50
1:A:23:LEU:HD22	1:A:28:LEU:HD12	1.94	0.49
1:C:155:ARG:O	1:C:159:VAL:HG12	2.12	0.49
1:C:148:GLY:HA3	1:C:191:THR:HG23	1.93	0.49
1:C:45:ALA:O	1:C:49:PHE:HB2	2.13	0.49
1:C:-135:TYR:HB2	1:C:-88:ILE:HD13	1.95	0.49
1:A:21:ARG:O	1:A:25:ARG:HD3	2.14	0.48
1:A:38:THR:OG1	1:A:92:CYS:HB3	2.14	0.48
1:C:168:PHE:CG	1:C:169:PRO:HD2	2.48	0.47
1:C:152:ARG:NH1	1:C:156:LEU:HD11	2.29	0.47
1:C:171:ILE:O	1:C:171:ILE:HG13	2.14	0.47
1:C:24:LEU:HG	1:C:74:MET:HG2	1.98	0.46
1:A:-136:ALA:HB1	1:A:-111:LEU:HD13	1.98	0.46
1:A:135:LYS:NZ	2:A:301:LIP:O2	2.45	0.45
7:A:310:8K6:H122	7:C:309:8K6:C18	2.43	0.45
1:C:-74:LEU:HD21	1:C:-68:LEU:HD21	1.98	0.45
1:C:17:LEU:HA	1:C:17:LEU:HD23	1.82	0.44
1:C:-137:LEU:HD12	1:C:-93:ALA:HB2	2.00	0.44
1:A:115:ARG:HB3	1:C:106:TRP:CH2	2.53	0.44
1:A:-131:HIS:NE2	1:A:-84:PRO:HD3	2.32	0.44
1:C:-79:GLU:HG3	1:C:-27:ILE:HG13	2.00	0.44
1:C:-79:GLU:HG2	1:C:-26:TRP:HB3	2.00	0.44
1:A:-29:TYR:CE1	1:A:14:ARG:HD3	2.53	0.44
1:C:116:LEU:HD22	1:C:182:TRP:CZ2	2.52	0.44
1:A:177:LEU:HB3	1:A:178:PRO:HD3	1.99	0.43
1:A:148:GLY:HA3	1:A:191:THR:HG23	2.00	0.43
1:C:-54:ASP:N	1:C:-54:ASP:OD2	2.51	0.43
1:C:90:ALA:O	1:C:94:ARG:HG2	2.18	0.43
1:A:115:ARG:NH1	6:C:307:OLC:H22	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-71:ARG:HD3	1:C:-38:TYR:OH	2.18	0.43
1:C:-81:ILE:HG23	1:C:-27:ILE:HD11	2.00	0.43
1:C:54:LEU:HB2	1:C:167:ASP:HB2	1.99	0.43
1:C:-124:LEU:HA	1:C:-124:LEU:HD12	1.85	0.43
1:C:-48:ASP:OD1	1:C:-42:SER:OG	2.37	0.43
1:A:168:PHE:O	1:A:172:ALA:HB2	2.19	0.42
1:A:122:LEU:HD13	1:C:102:SER:HB3	2.01	0.42
1:A:-131:HIS:CD2	1:A:-84:PRO:HD3	2.54	0.42
1:A:-96:LEU:HD21	1:A:-53:PHE:CD2	2.55	0.42
1:A:150:ILE:HD13	1:A:150:ILE:HA	1.86	0.42
1:C:-96:LEU:HD11	1:C:-53:PHE:CD1	2.55	0.41
1:C:-68:LEU:HD23	1:C:-29:TYR:HB3	2.01	0.41
1:A:-80:LEU:HB2	1:A:-26[B]:TRP:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/370 (90%)	323 (97%)	10 (3%)	0	100	100
1	C	332/370 (90%)	323 (97%)	9 (3%)	0	100	100
All	All	665/740 (90%)	646 (97%)	19 (3%)	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	248/300 (83%)	242 (98%)	6 (2%)	49	49
1	C	253/300 (84%)	248 (98%)	5 (2%)	55	57
All	All	501/600 (84%)	490 (98%)	11 (2%)	52	53

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

Mol	Chain	Res	Type
1	A	-120	THR
1	A	-116	ARG
1	A	-76	LEU
1	A	-73	GLU
1	A	-7	SER
1	A	113	ARG
1	C	-132	ASN
1	C	-124	LEU
1	C	94	ARG
1	C	116	LEU
1	C	152	ARG

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

Mol	Chain	Res	Type
1	C	-132	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

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$
7	8K6	A	311	-	4,4,17	0.35	0	3,3,16	0.55	0
9	C5P	C	301	-	19,22,22	0.77	0	24,33,33	1.18	1 (4%)
8	GOL	A	314	-	5,5,5	0.35	0	5,5,5	0.25	0
7	8K6	A	310	-	14,14,17	0.13	0	13,13,16	0.12	0
7	8K6	A	313	-	7,7,17	0.11	0	6,6,16	0.10	0
6	OLC	A	309	-	9,9,24	1.50	1 (11%)	10,10,25	1.33	1 (10%)
6	OLC	A	307	-	21,21,24	1.04	1 (4%)	22,22,25	0.92	1 (4%)
7	8K6	A	312	-	9,9,17	0.14	0	8,8,16	0.09	0
6	OLC	C	306	-	10,10,24	1.44	1 (10%)	11,11,25	1.00	1 (9%)
7	8K6	C	310	-	14,14,17	0.17	0	13,13,16	0.11	0
5	1PE	A	306	-	6,6,15	0.44	0	5,5,14	0.31	0
2	LIP	A	301	-	16,16,16	1.08	1 (6%)	24,25,25	0.70	1 (4%)
8	GOL	C	312	-	5,5,5	0.37	0	5,5,5	0.26	0
6	OLC	C	305	-	11,11,24	1.40	1 (9%)	12,12,25	1.13	1 (8%)
7	8K6	C	309	-	6,6,17	0.12	0	5,5,16	0.13	0
10	FLC	C	302	-	3,12,12	1.06	0	3,17,17	0.59	0
8	GOL	C	311	-	5,5,5	0.35	0	5,5,5	0.24	0
6	OLC	C	307	-	24,24,24	0.94	1 (4%)	25,25,25	0.85	1 (4%)
5	1PE	C	304	-	7,7,15	0.49	0	6,6,14	0.25	0
6	OLC	A	308	-	11,11,24	1.36	1 (9%)	12,12,25	0.99	1 (8%)
4	TCE	A	305	3	6,15,15	0.90	0	9,18,18	3.49	3 (33%)
6	OLC	C	308	-	12,12,24	1.32	1 (8%)	13,13,25	0.99	1 (7%)

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
7	8K6	A	311	-	-	0/2/2/15	-
9	C5P	C	301	-	-	2/8/26/26	0/2/2/2
8	GOL	A	314	-	-	0/4/4/4	-
7	8K6	A	310	-	-	4/12/12/15	-
7	8K6	A	313	-	-	2/5/5/15	-
6	OLC	A	309	-	-	0/9/9/24	-
6	OLC	A	307	-	-	4/21/21/24	-
7	8K6	A	312	-	-	2/7/7/15	-
6	OLC	C	306	-	-	2/10/10/24	-
7	8K6	C	310	-	-	2/12/12/15	-
5	1PE	A	306	-	-	0/4/4/13	-
2	LIP	A	301	-	-	1/5/29/29	0/1/1/1
8	GOL	C	312	-	-	2/4/4/4	-
6	OLC	C	305	-	-	1/11/11/24	-
7	8K6	C	309	-	-	4/4/4/15	-
10	FLC	C	302	-	-	3/6/16/16	-
8	GOL	C	311	-	-	2/4/4/4	-
6	OLC	C	307	-	-	6/24/24/24	-
5	1PE	C	304	-	-	1/5/5/13	-
6	OLC	A	308	-	-	0/11/11/24	-
4	TCE	A	305	3	-	5/9/15/15	-
6	OLC	C	308	-	-	0/12/12/24	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	307	OLC	O20-C1	4.53	1.46	1.33
6	C	305	OLC	O20-C1	4.48	1.46	1.33
6	C	308	OLC	O20-C1	4.37	1.46	1.33
6	A	309	OLC	O20-C1	4.36	1.46	1.33
6	C	306	OLC	O20-C1	4.35	1.46	1.33
6	A	308	OLC	O20-C1	4.32	1.46	1.33
6	C	307	OLC	O20-C1	4.30	1.45	1.33
2	A	301	LIP	P1-O1	2.71	1.64	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	TCE	C1-P-C3	6.04	120.19	100.95
4	A	305	TCE	C1-P-C2	5.96	119.93	100.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	TCE	C3-P-C2	5.94	119.88	100.95
9	C	301	C5P	C2-N3-C4	4.63	121.04	116.34
6	A	309	OLC	O20-C1-C2	3.40	120.28	111.38
6	C	305	OLC	O20-C1-C2	2.81	120.72	111.91
6	A	307	OLC	O20-C1-C2	2.62	120.14	111.91
6	C	307	OLC	O20-C1-C2	2.57	119.96	111.91
6	C	308	OLC	O20-C1-C2	2.46	119.64	111.91
6	A	308	OLC	O20-C1-C2	2.42	119.49	111.91
6	C	306	OLC	O20-C1-C2	2.17	118.70	111.91
2	A	301	LIP	C6-C1-C2	2.11	113.89	110.85

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	312	GOL	O1-C1-C2-O2
8	C	312	GOL	O1-C1-C2-C3
4	A	305	TCE	C5-C2-P-C1
4	A	305	TCE	C6-C3-P-C1
4	A	305	TCE	C4-C1-P-C2
4	A	305	TCE	P-C1-C4-C11
7	A	310	8K6	C11-C12-C13-C14
6	A	307	OLC	O20-C21-C22-C24
6	A	307	OLC	O20-C21-C22-O23
6	C	307	OLC	C3-C4-C5-C6
7	C	309	8K6	C14-C15-C16-C17
7	A	310	8K6	C11-C10-C9-C8
6	C	307	OLC	C21-C22-C24-O25
7	A	310	8K6	C5-C6-C7-C8
7	C	310	8K6	C6-C7-C8-C9
9	C	301	C5P	C3'-C4'-C5'-O5'
10	C	302	FLC	CAC-CA-CB-OHB
6	C	307	OLC	C6-C7-C8-C9
7	A	313	8K6	C13-C14-C15-C16
7	A	312	8K6	C15-C16-C17-C18
10	C	302	FLC	CAC-CA-CB-CG
7	C	309	8K6	C15-C16-C17-C18
6	C	306	OLC	C2-C1-O20-C21
7	C	309	8K6	C13-C14-C15-C16
6	C	307	OLC	C2-C3-C4-C5
2	A	301	LIP	C1-O1-P1-O7
4	A	305	TCE	P-C2-C5-C14

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Mol	Chain	Res	Type	Atoms
9	C	301	C5P	O4'-C4'-C5'-O5'
7	A	310	8K6	C1-C2-C3-C4
7	C	309	8K6	C12-C13-C14-C15
6	C	306	OLC	O19-C1-O20-C21
10	C	302	FLC	CAC-CA-CB-CBC
7	C	310	8K6	C10-C11-C12-C13
7	A	313	8K6	C12-C13-C14-C15
8	C	311	GOL	O1-C1-C2-C3
8	C	311	GOL	O1-C1-C2-O2
6	C	307	OLC	O23-C22-C24-O25
6	C	305	OLC	C2-C3-C4-C5
6	A	307	OLC	C9-C10-C11-C12
6	A	307	OLC	C7-C8-C9-C10
7	A	312	8K6	C12-C13-C14-C15
5	C	304	1PE	OH4-C13-C23-OH3
6	C	307	OLC	C7-C8-C9-C10

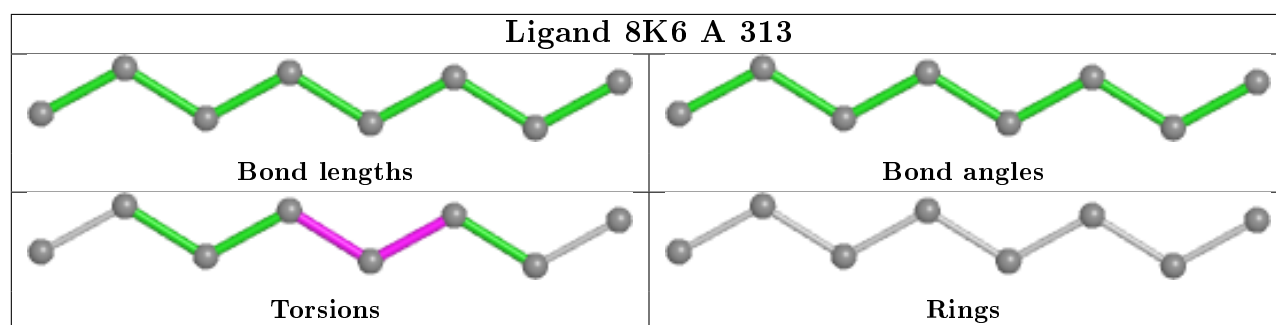
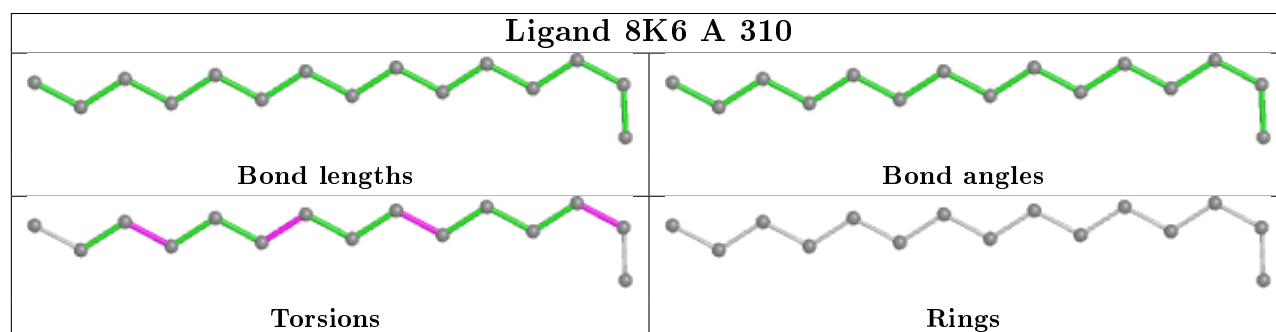
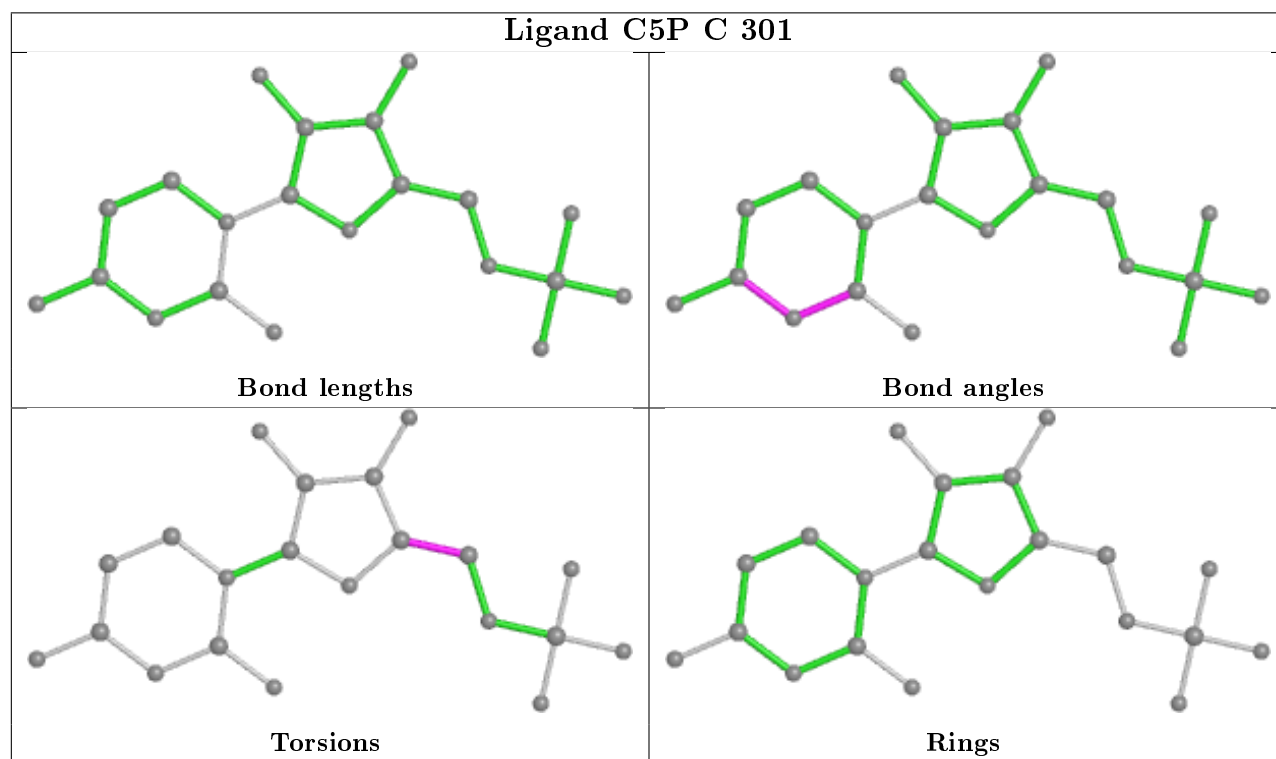
There are no ring outliers.

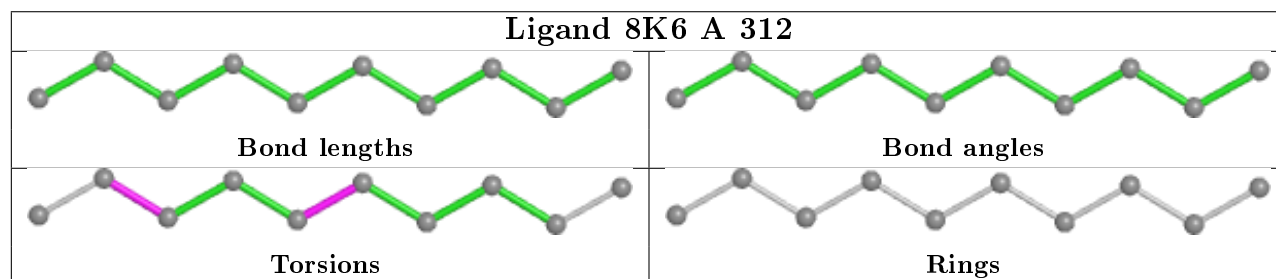
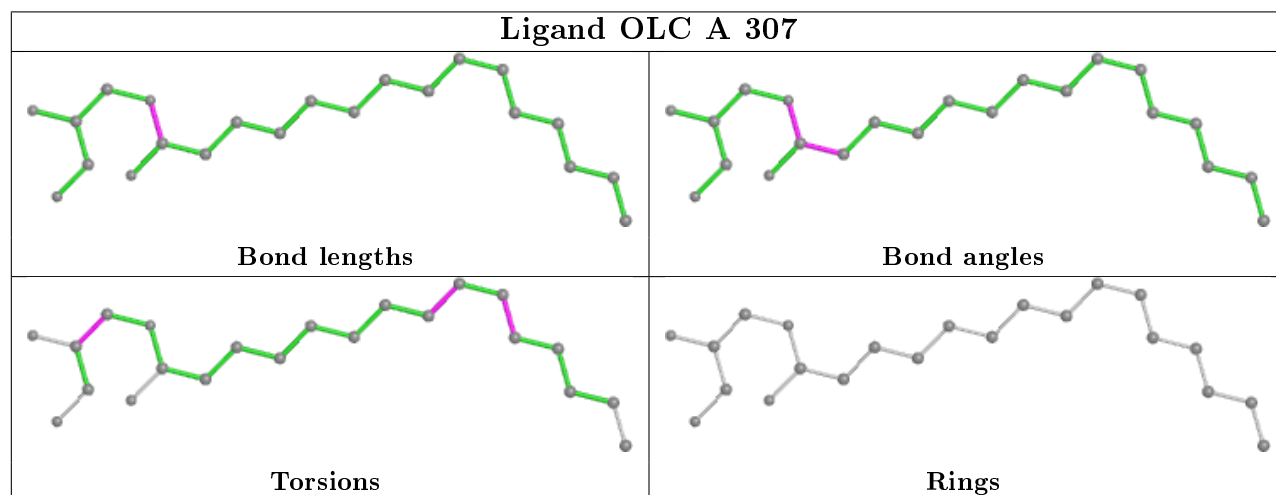
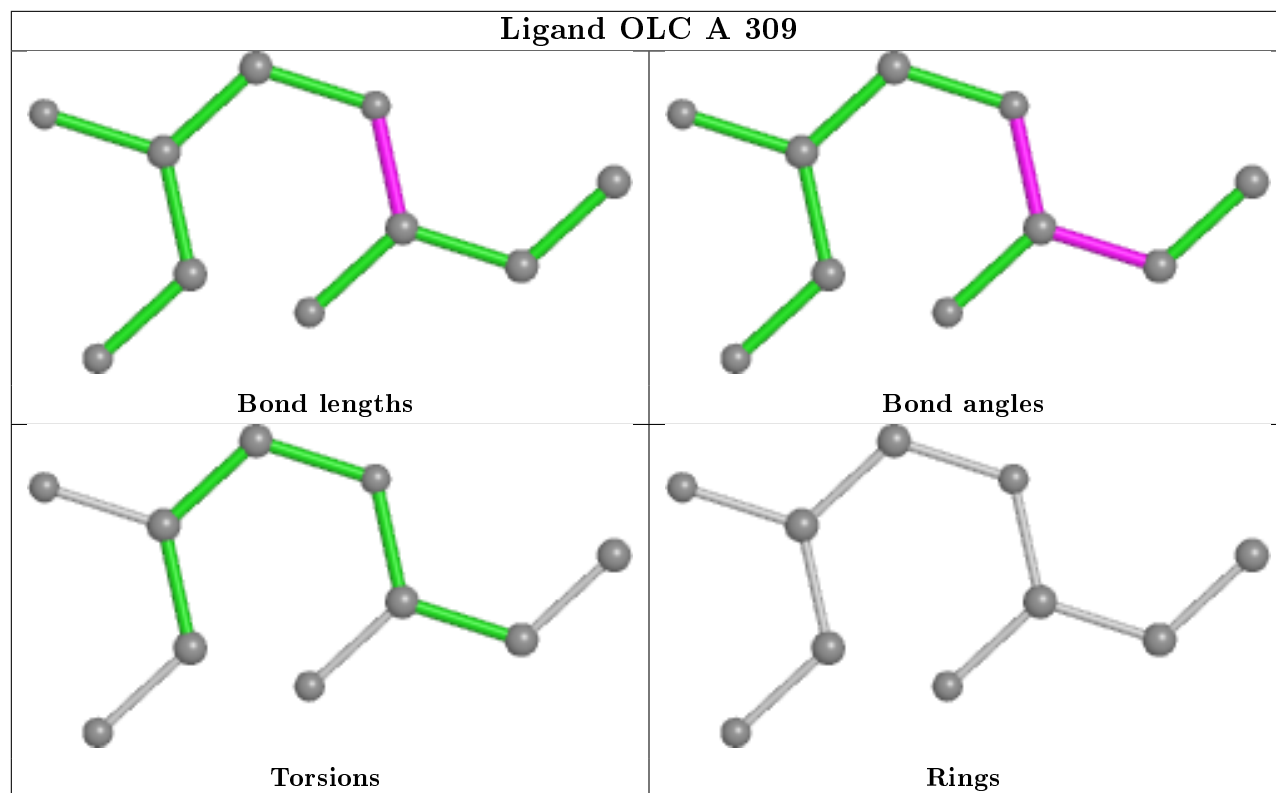
10 monomers are involved in 17 short contacts:

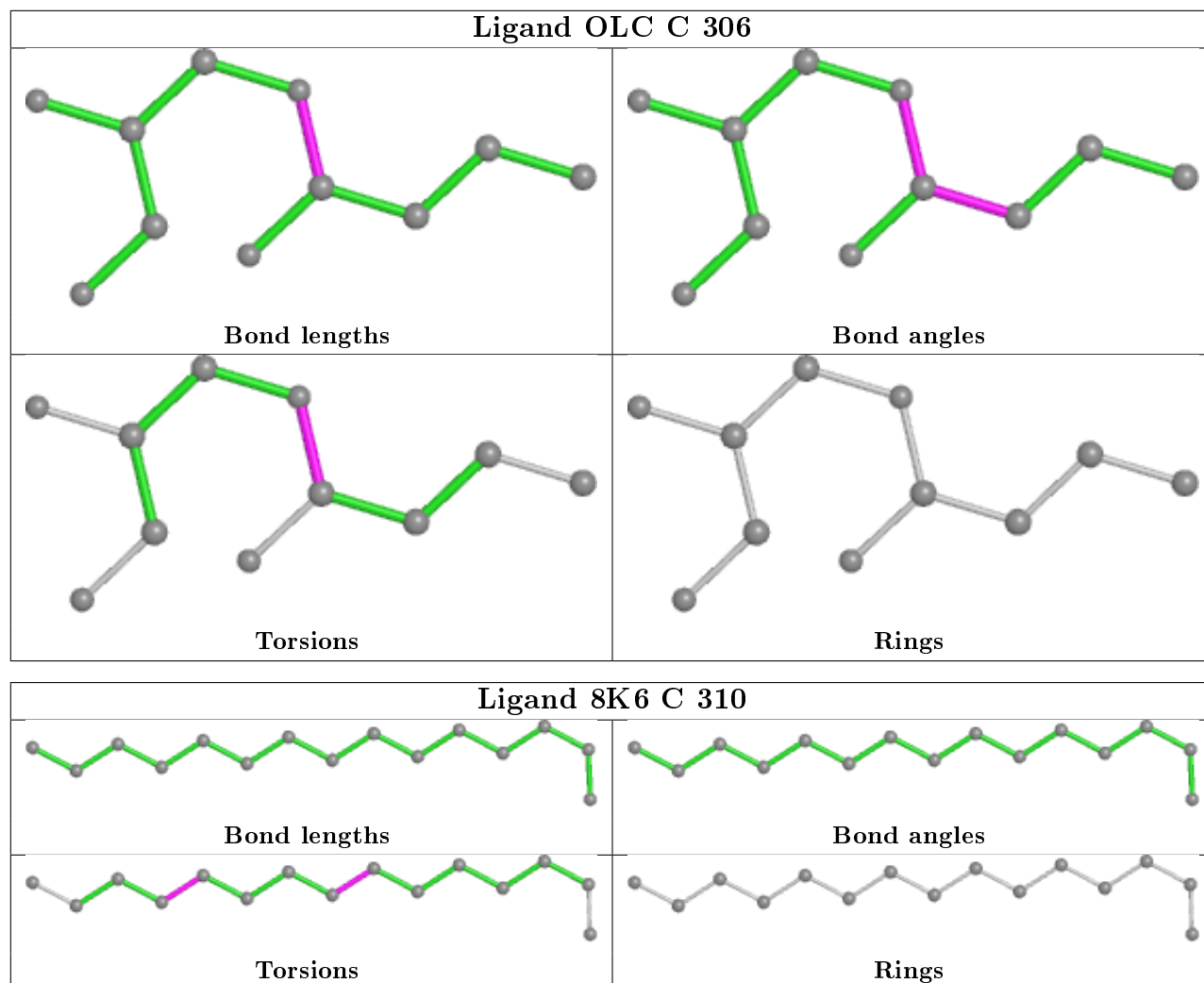
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	310	8K6	5	0
6	A	307	OLC	1	0
7	A	312	8K6	1	0
2	A	301	LIP	3	0
7	C	309	8K6	4	0
10	C	302	FLC	3	0
8	C	311	GOL	1	0
6	C	307	OLC	2	0
4	A	305	TCE	1	0
6	C	308	OLC	1	0

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.

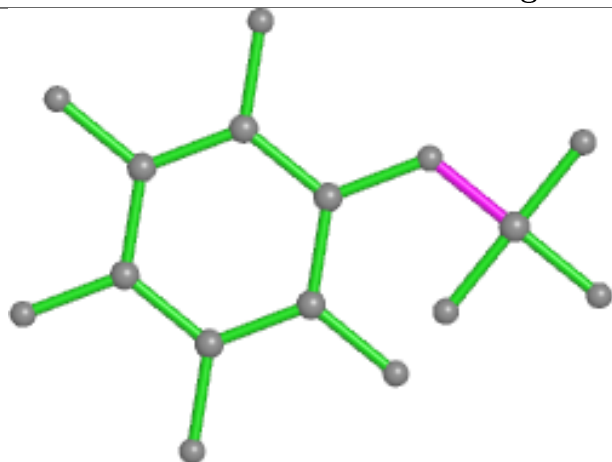
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



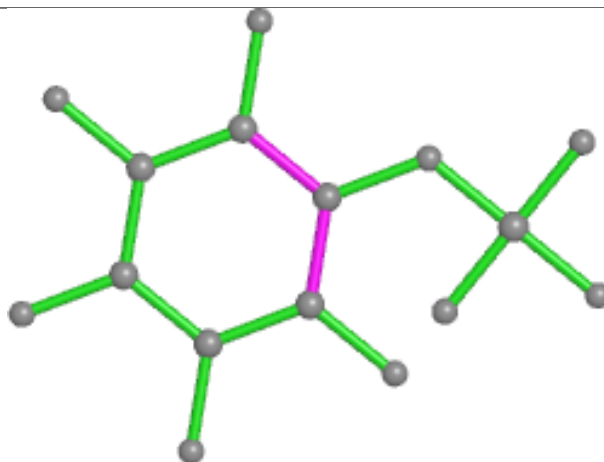




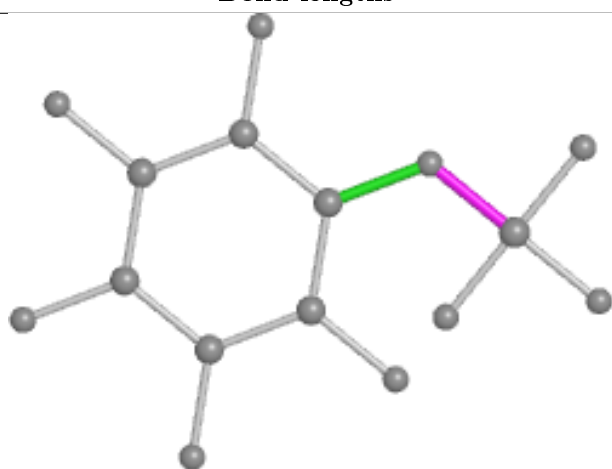
Ligand LIP A 301



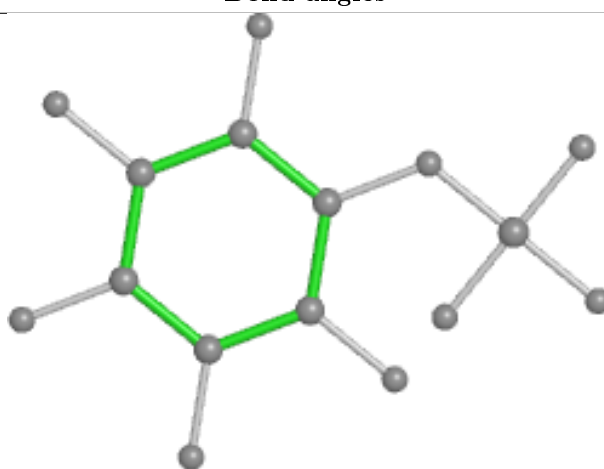
Bond lengths



Bond angles

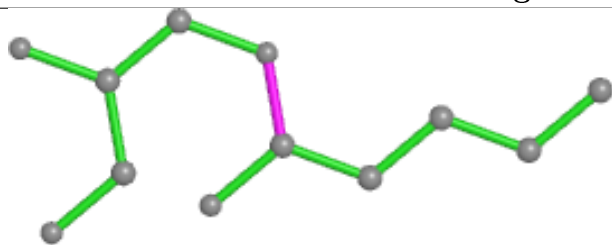


Torsions

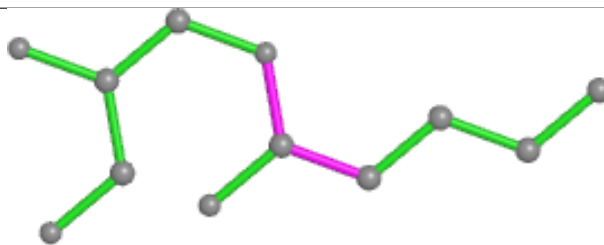


Rings

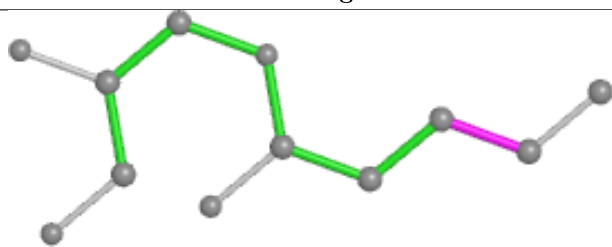
Ligand OLC C 305



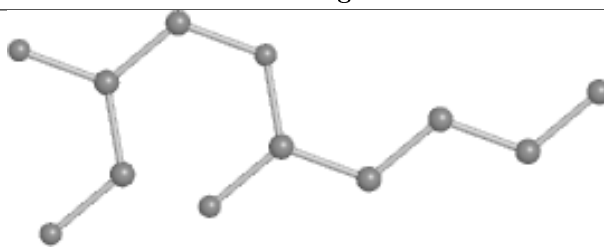
Bond lengths



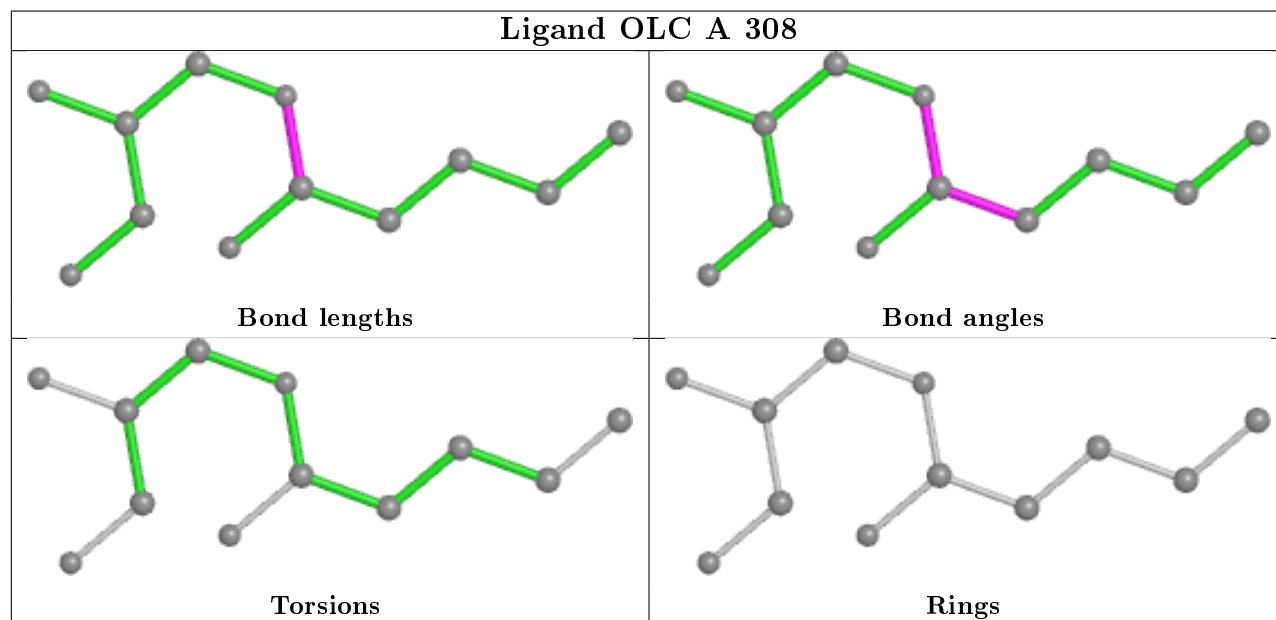
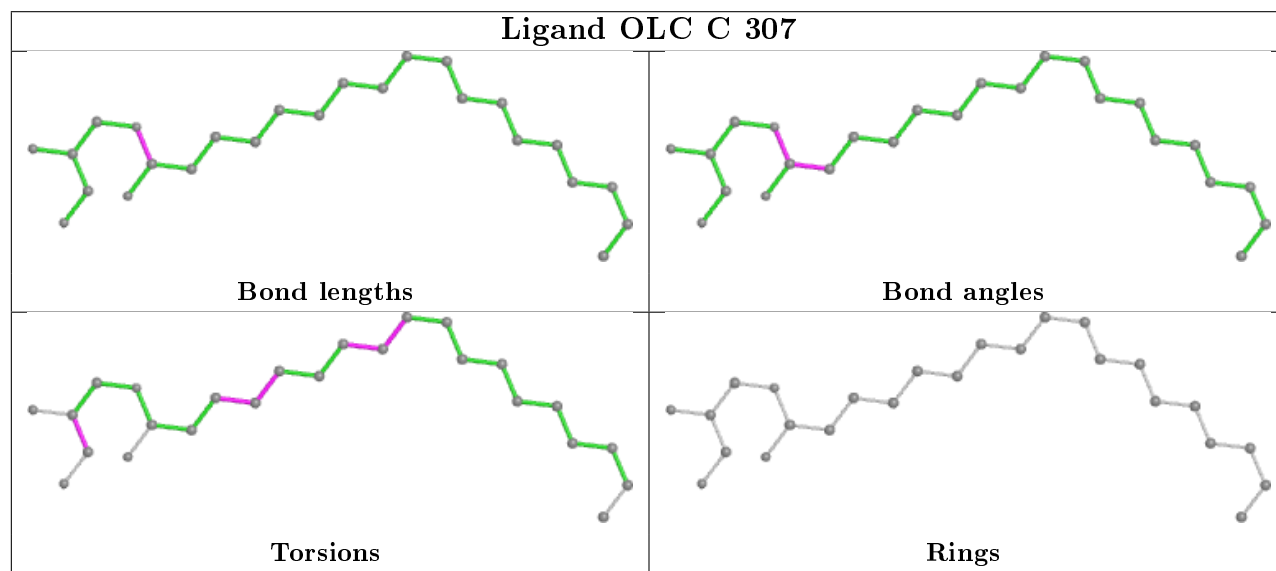
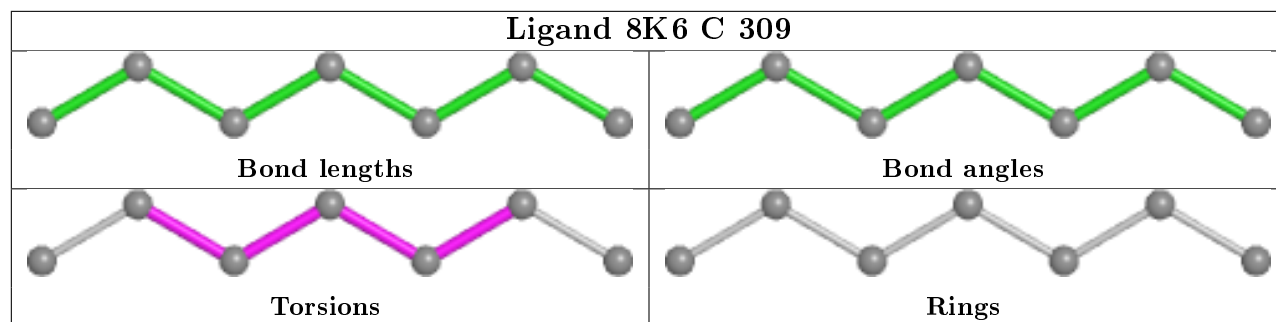
Bond angles

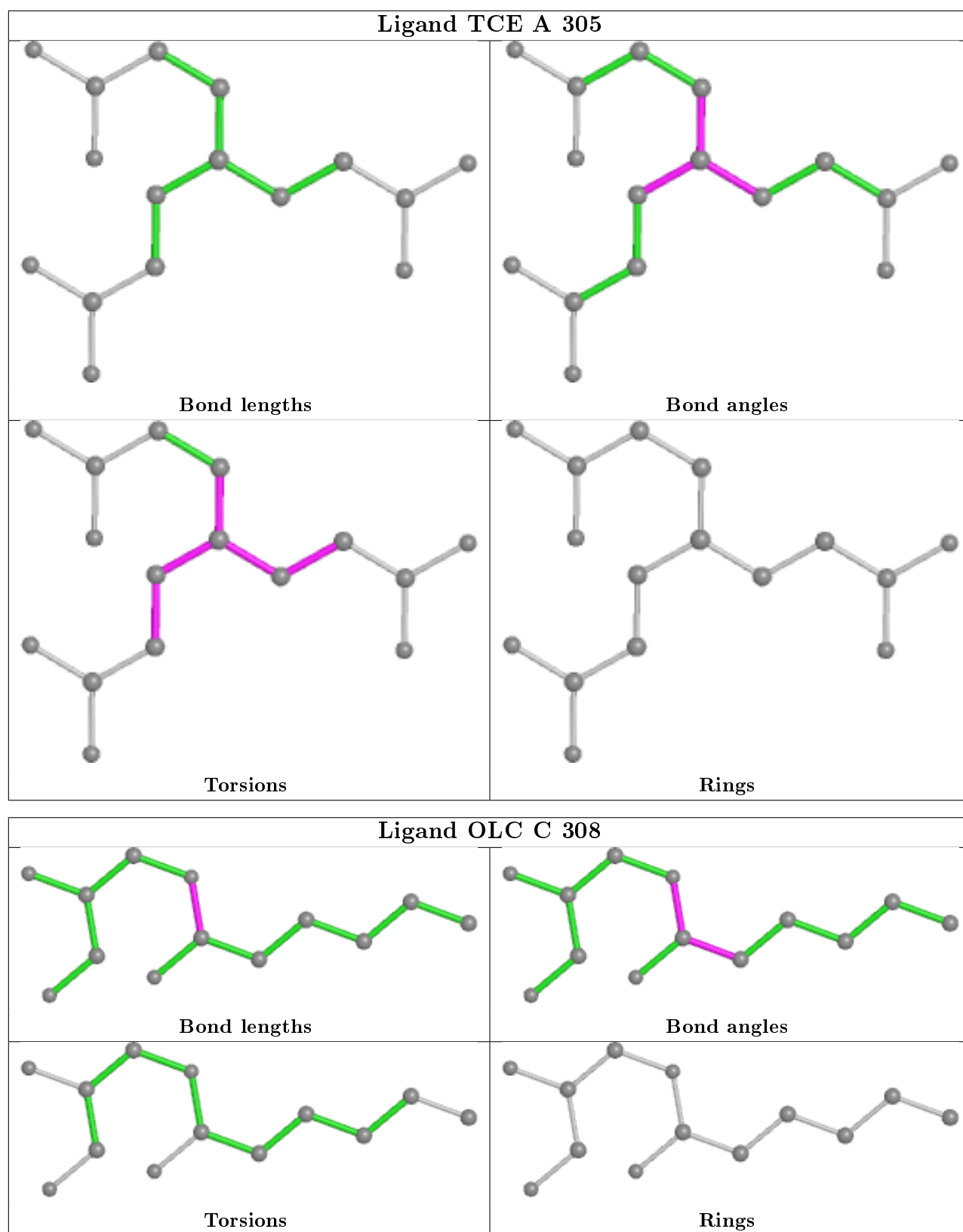


Torsions



Rings





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 [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	336/370 (90%)	0.15	7 (2%) 63 69	24, 43, 67, 77	0
1	C	336/370 (90%)	0.22	9 (2%) 54 61	26, 42, 65, 74	0
All	All	672/740 (90%)	0.18	16 (2%) 59 65	24, 42, 67, 77	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	79	SER	7.1
1	A	-26[A]	TRP	5.6
1	C	15	ILE	5.5
1	C	11	ALA	4.8
1	C	65	VAL	3.5
1	A	11	ALA	3.4
1	A	10	ALA	3.4
1	C	62	TRP	2.9
1	C	12	PHE	2.8
1	C	-27	ILE	2.7
1	A	15	ILE	2.4
1	C	-7	SER	2.4
1	A	14	ARG	2.3
1	C	-10	LEU	2.2
1	A	-29	TYR	2.1
1	A	150	ILE	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

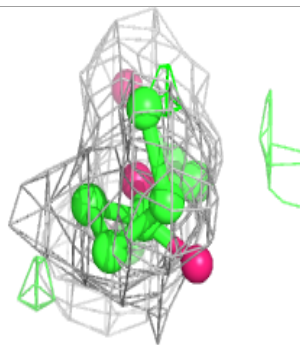
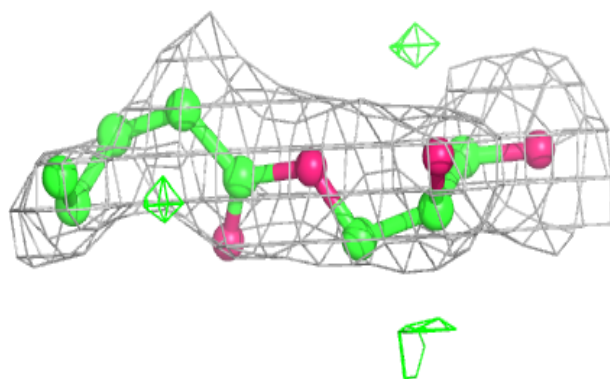
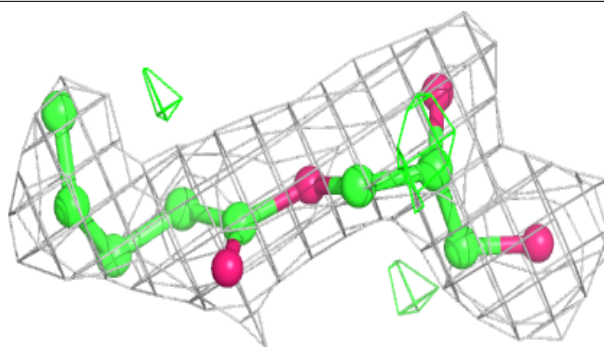
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	OLC	C	305	12/25	0.73	0.15	58,69,79,81	0
10	FLC	C	302	13/13	0.76	0.18	58,70,76,76	0
6	OLC	C	306	11/25	0.77	0.16	45,65,69,73	0
9	C5P	C	301	21/21	0.80	0.20	49,67,81,94	0
2	LIP	A	301	16/16	0.80	0.15	56,69,108,116	0
7	8K6	A	312	10/18	0.83	0.27	36,42,46,48	0
4	TCE	A	305	16/16	0.85	0.16	54,82,100,101	0
6	OLC	A	307	22/25	0.86	0.19	22,39,52,67	0
3	NA	A	303	1/1	0.86	0.09	43,43,43,43	0
8	GOL	C	311	6/6	0.86	0.20	59,65,65,68	0
5	1PE	A	306	7/16	0.86	0.16	56,59,62,63	0
5	1PE	C	304	8/16	0.87	0.13	33,46,55,55	0
7	8K6	A	310	15/18	0.87	0.15	22,35,42,47	0
6	OLC	A	309	10/25	0.88	0.15	39,53,61,67	0
6	OLC	C	308	13/25	0.88	0.16	30,51,62,62	0
3	NA	A	302	1/1	0.89	0.18	53,53,53,53	0
7	8K6	C	310	15/18	0.89	0.25	28,40,45,46	0
6	OLC	C	307	25/25	0.90	0.14	27,43,60,63	0
8	GOL	C	312	6/6	0.91	0.27	51,55,68,69	0
7	8K6	A	313	8/18	0.92	0.15	29,34,40,41	0
3	NA	A	304	1/1	0.92	0.09	45,45,45,45	0
7	8K6	C	309	7/18	0.93	0.11	33,36,41,46	0
8	GOL	A	314	6/6	0.93	0.13	44,47,54,58	0
6	OLC	A	308	12/25	0.93	0.15	35,47,56,65	0
7	8K6	A	311	5/18	0.94	0.11	24,28,31,32	0
3	NA	C	303	1/1	0.97	0.30	54,54,54,54	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.

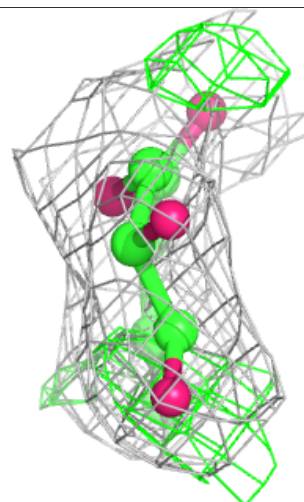
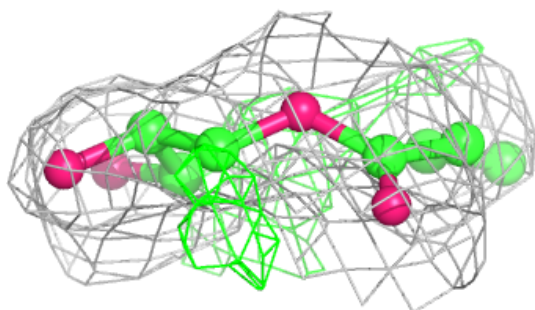
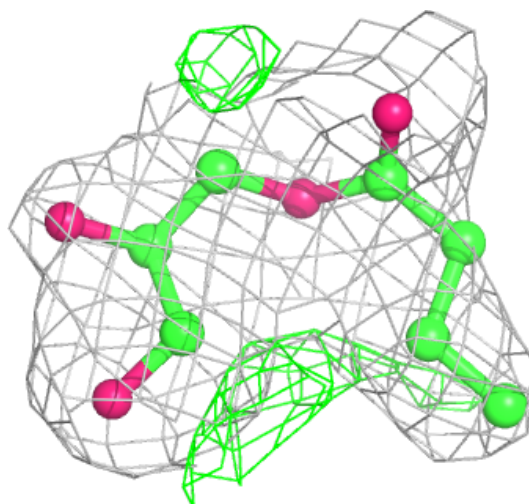
Electron density around OLC C 305:

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



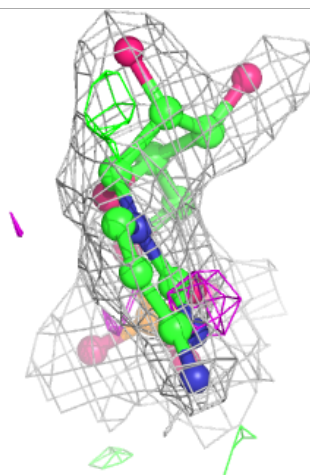
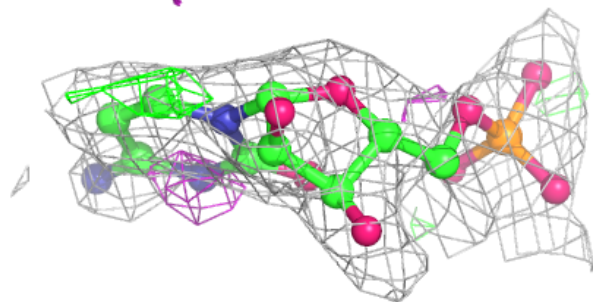
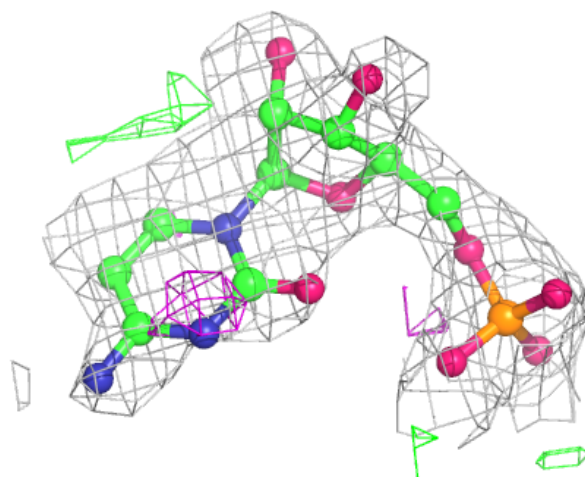
Electron density around OLC C 306:

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



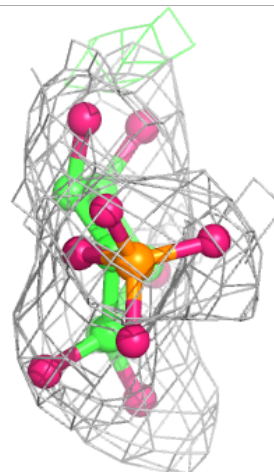
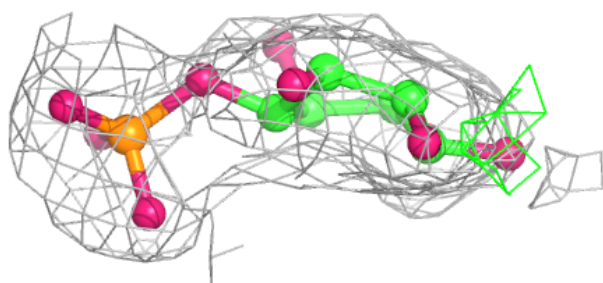
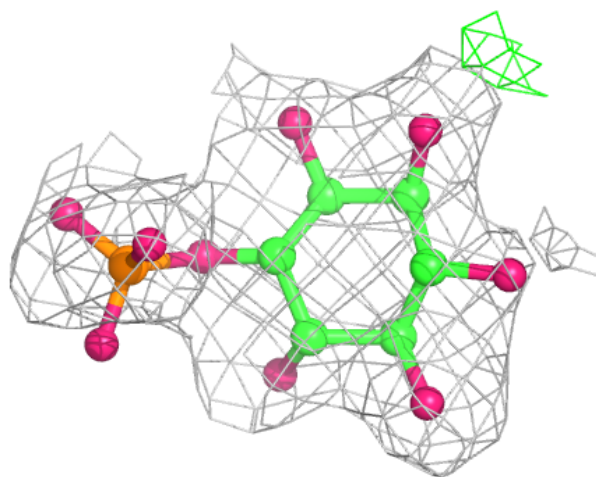
Electron density around C5P C 301:

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



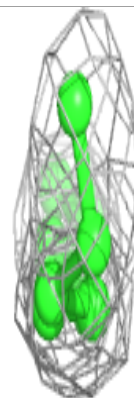
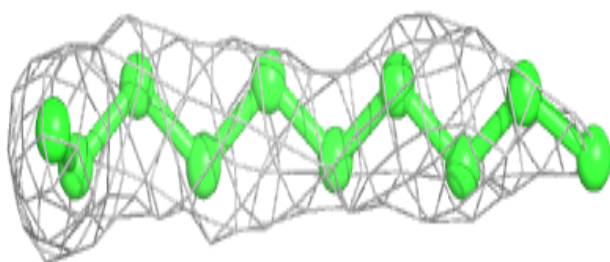
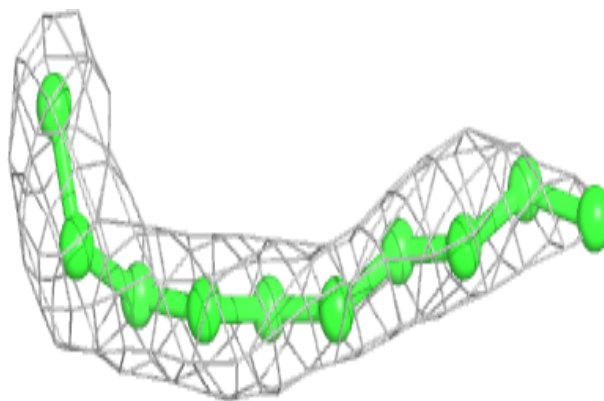
Electron density around LIP A 301:

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



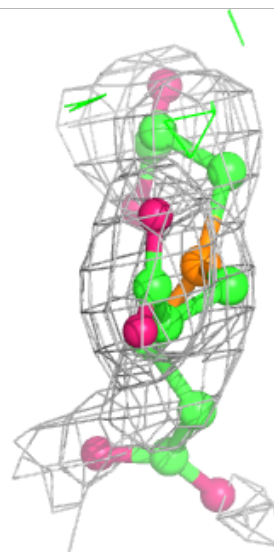
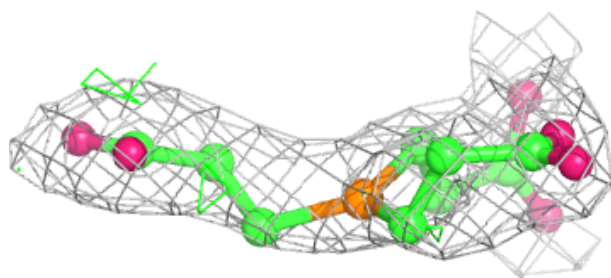
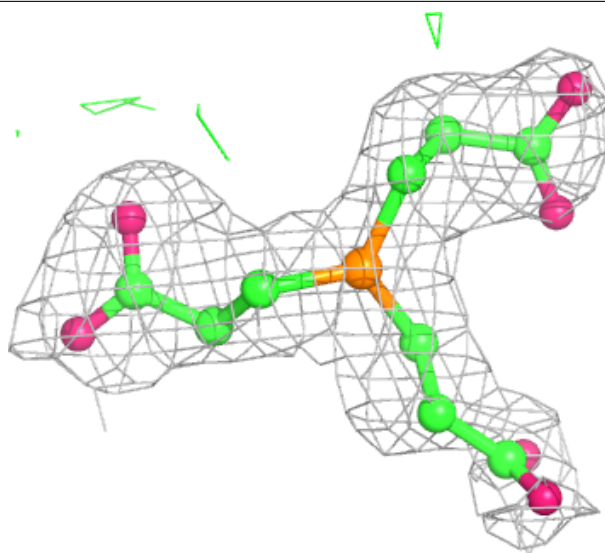
Electron density around 8K6 A 312:

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



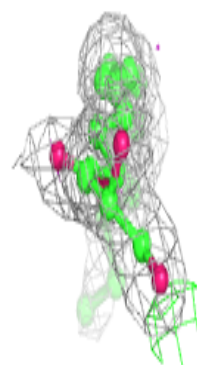
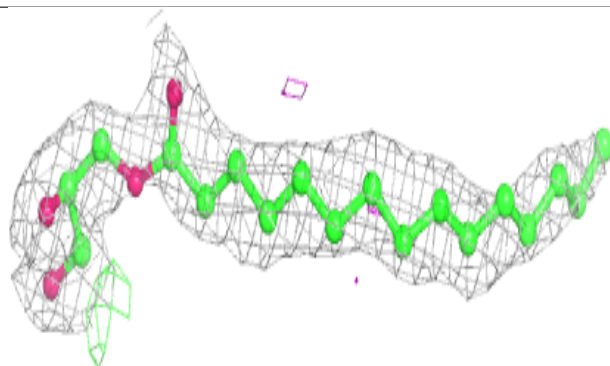
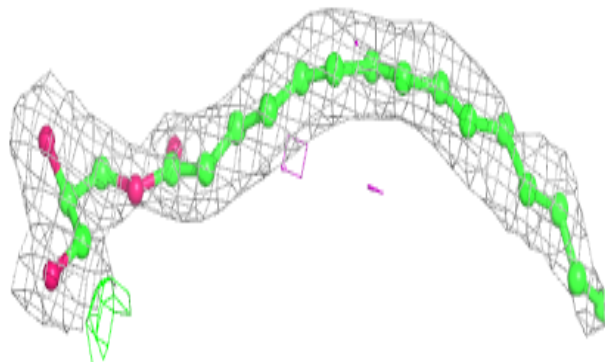
Electron density around TCE A 305:

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

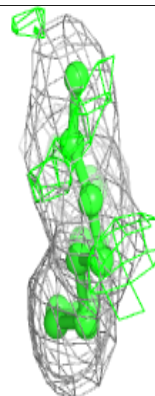
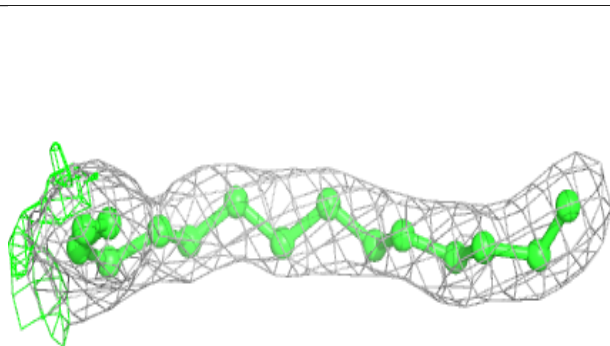
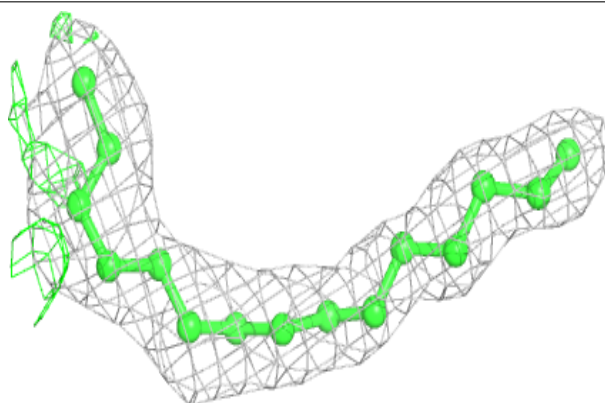


Electron density around OLC A 307:

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

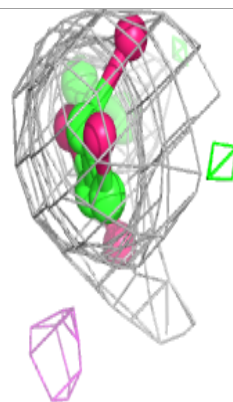
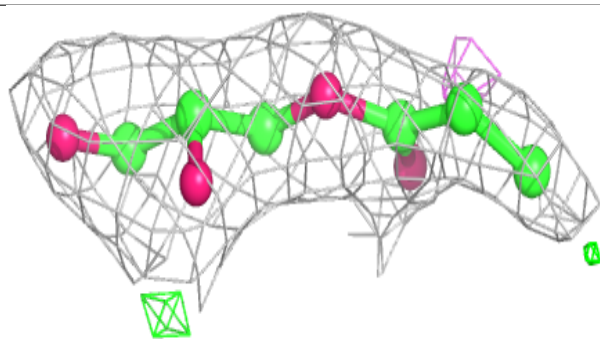
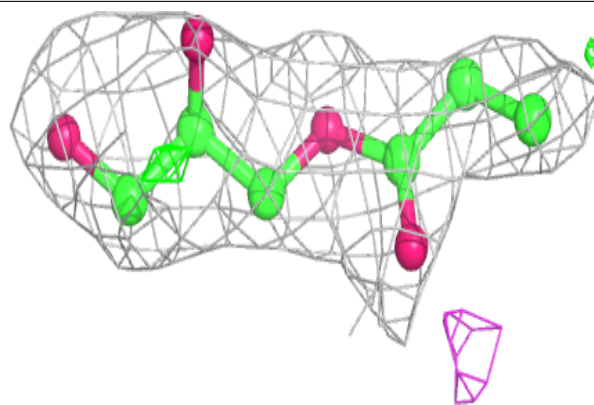
**Electron density around 8K6 A 310:**

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

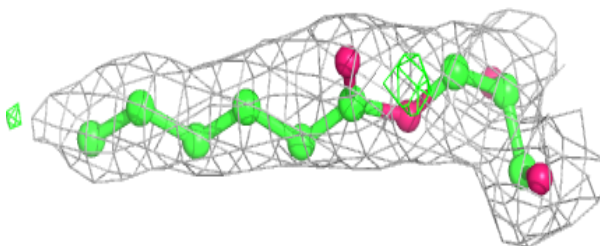
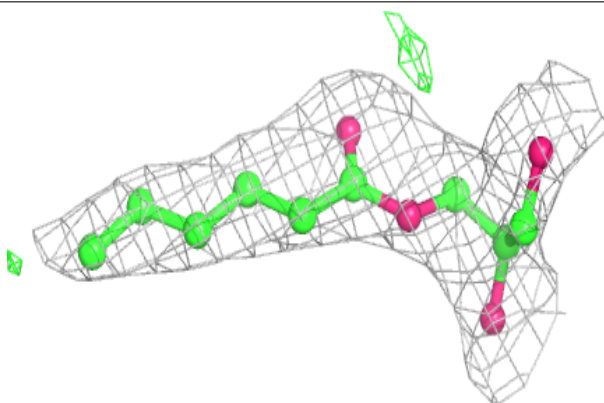


Electron density around OLC A 309:

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

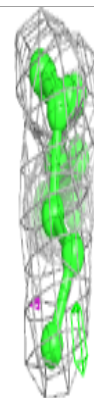
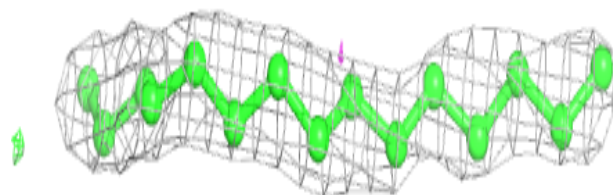
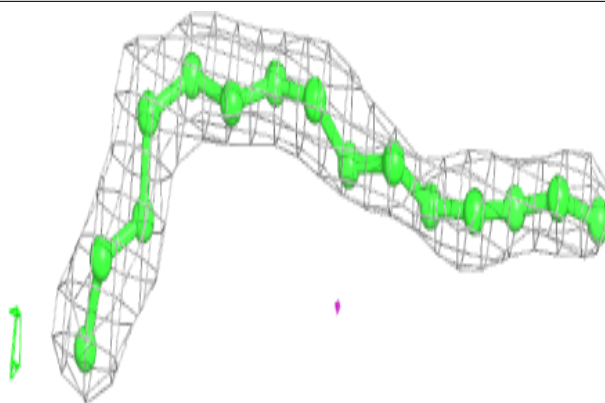
**Electron density around OLC C 308:**

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

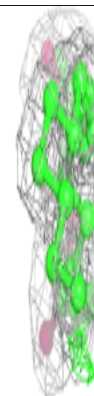
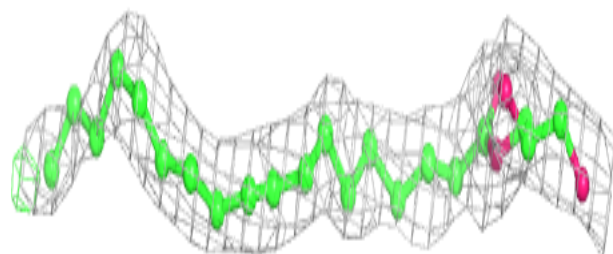
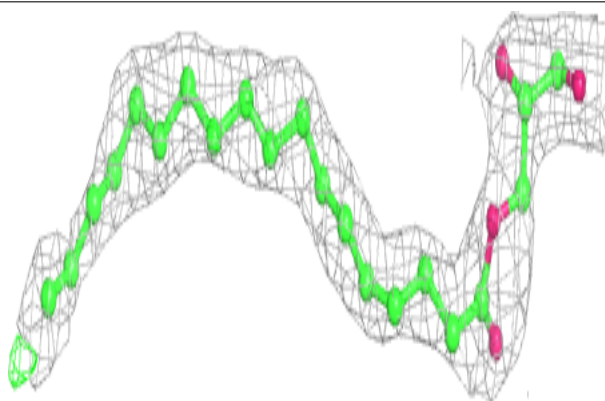


Electron density around 8K6 C 310:

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

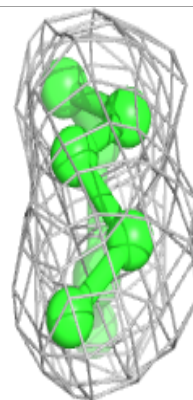
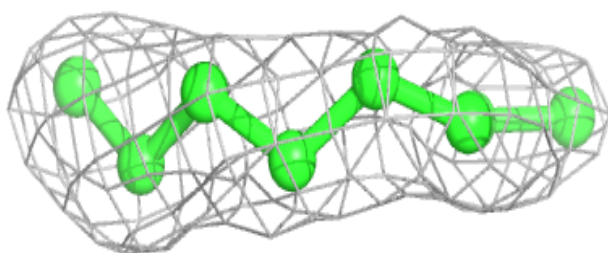
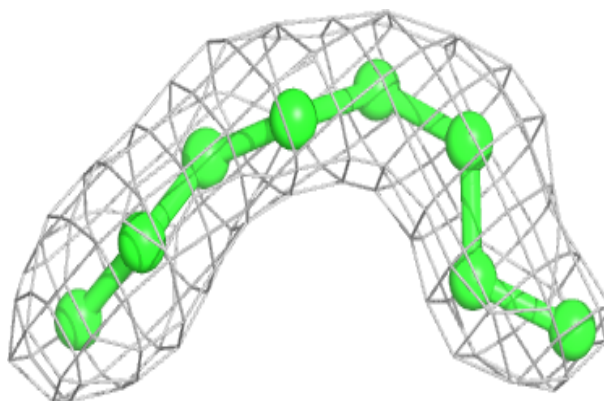
**Electron density around OLC C 307:**

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

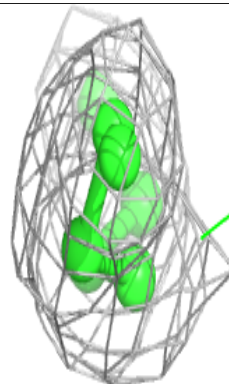
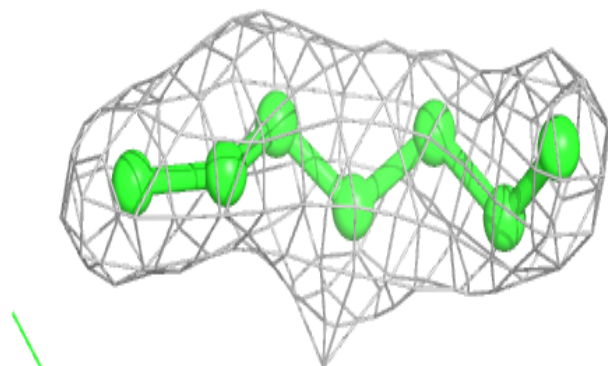
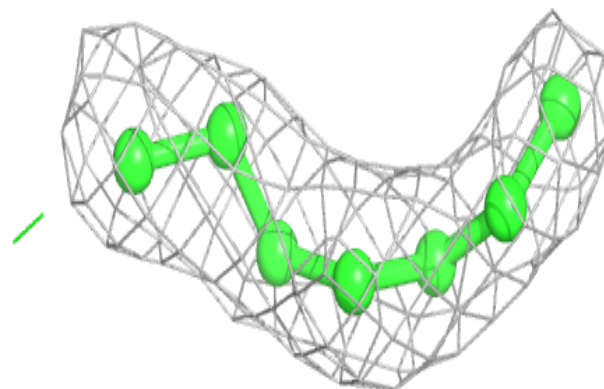


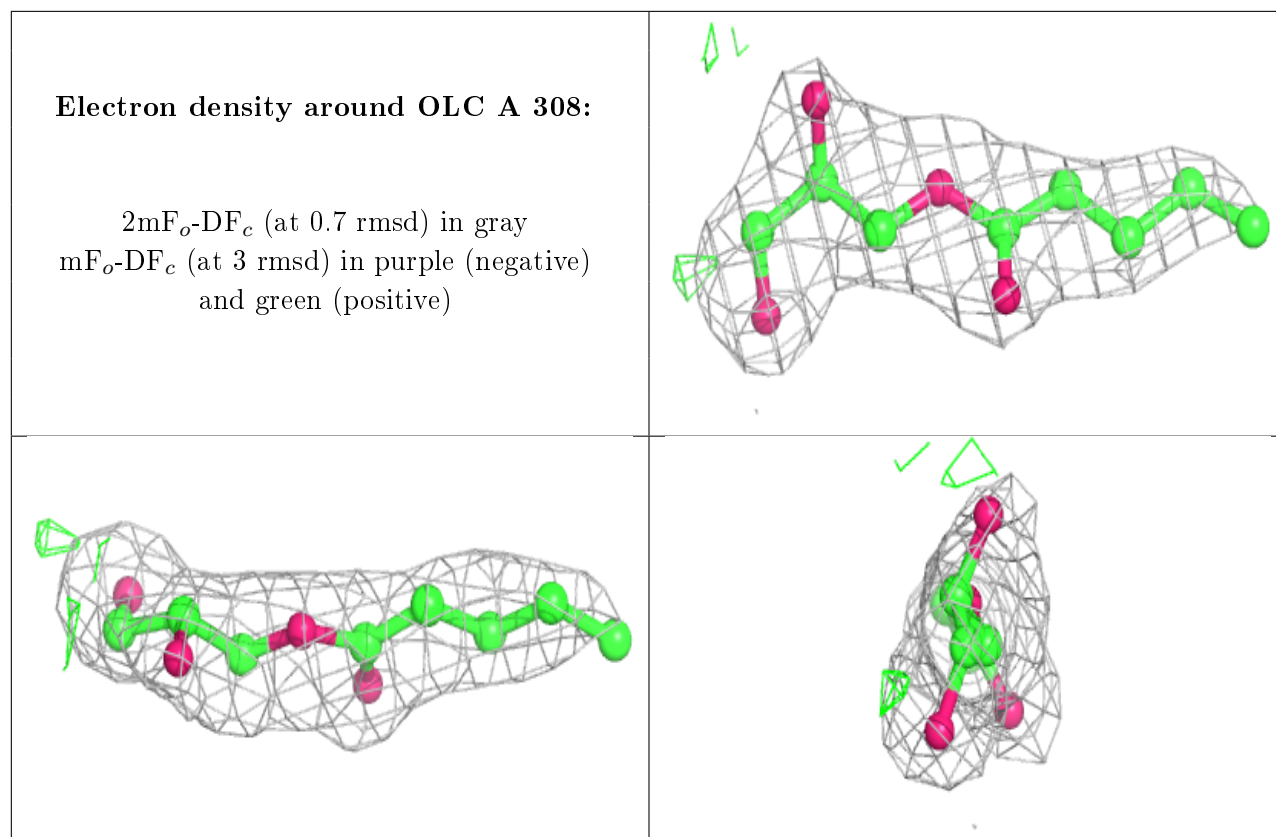
Electron density around 8K6 A 313:

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

**Electron density around 8K6 C 309:**

$2mF_o-DF_c$ (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.