



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 03:03 PM BST

PDB ID : 6WM5
Title : Structure of a phosphatidylinositol-phosphate synthase (PIPS) from *Mycobacterium kansasii*
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.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2020-04-20
Resolution : 1.96 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

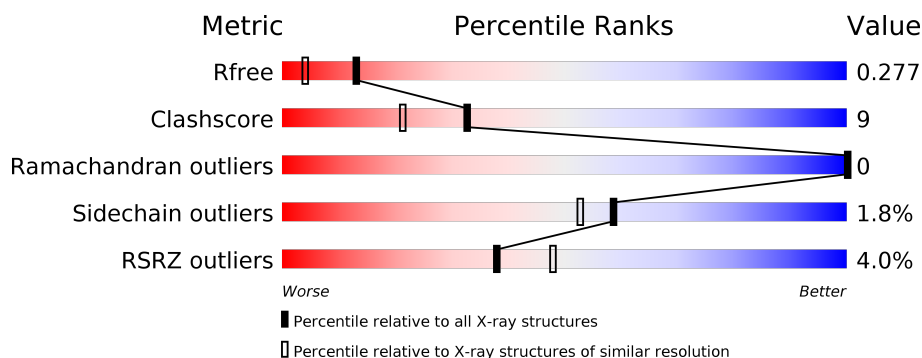
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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>5%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	C	370	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 9%</div> </div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5682 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	337	Total	C	N	O	S	0	7	0
			2588	1691	436	451	10			
1	C	335	Total	C	N	O	S	0	4	0
			2531	1650	422	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 CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

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

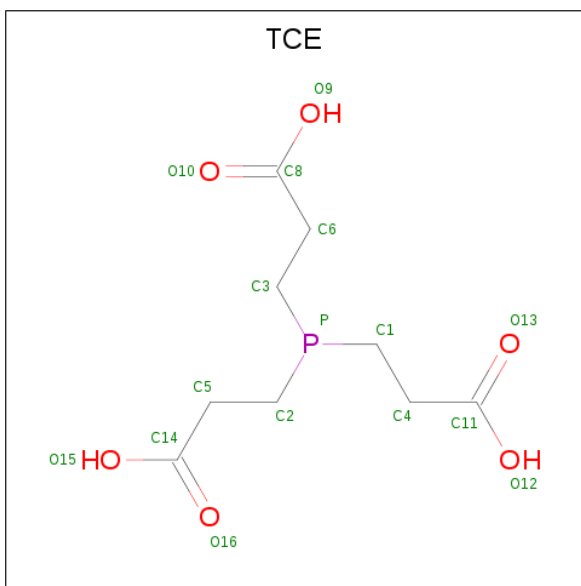
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Na	0	0
			4	4		
3	C	3	Total	Na	0	0
			3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



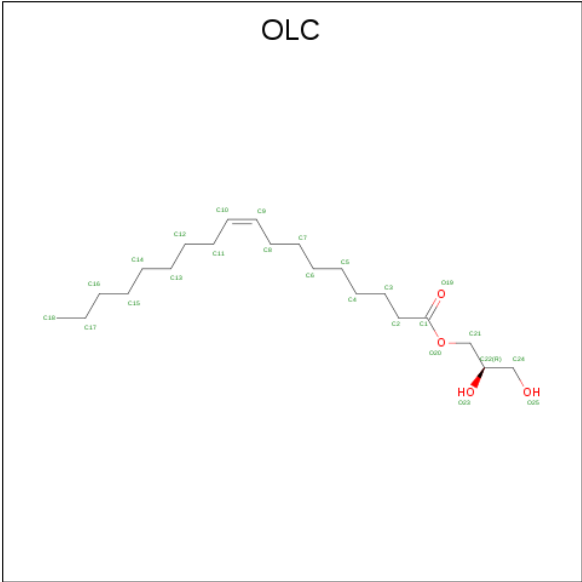
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	1
			5	4	1		

- Molecule 5 is 3,3',3''-phosphanetriyltripropanoic acid (three-letter code: TCE) (formula: C₉H₁₅O₆P).



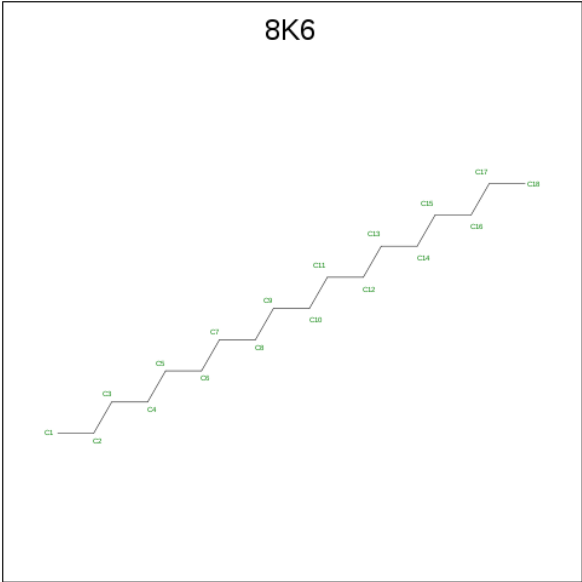
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			16	9	6	1		

- 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
			10	6	4		
6	A	1	Total	C	O	0	0
			17	13	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			19	15	4		
6	C	1	Total	C	O	0	0
			16	12	4		
6	C	1	Total	C	O	0	0
			25	21	4		
6	C	1	Total	C	O	0	0
			9	5	4		
6	C	1	Total	C	O	0	0
			25	21	4		

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



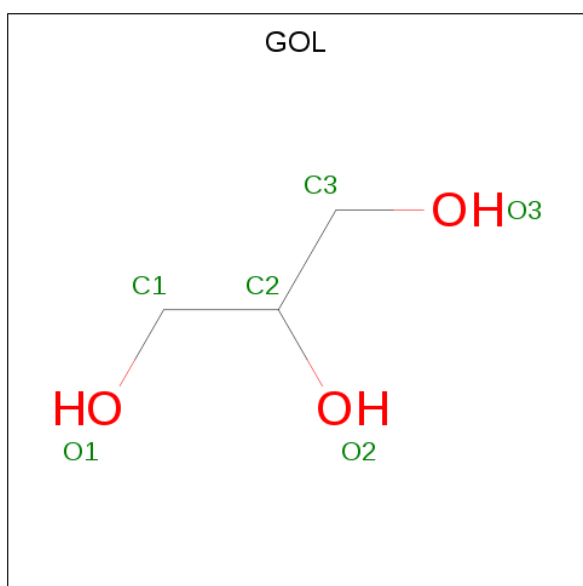
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 17 17	0	0
7	A	1	Total C 10 10	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 5 5	0	0
7	A	1	Total C 5 5	0	0
7	A	1	Total C 5 5	0	0
7	A	1	Total C 5 5	0	0
7	A	1	Total C 5 5	0	0
7	A	1	Total C 8 8	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 14 14	0	0
7	A	1	Total C 9 9	0	0
7	A	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 12 12	0	0
7	A	1	Total C 7 7	0	0
7	C	1	Total C 9 9	0	0
7	C	1	Total C 8 8	0	0
7	C	1	Total C 8 8	0	0
7	C	1	Total C 7 7	0	0
7	C	1	Total C 8 8	0	0
7	C	1	Total C 7 7	0	0
7	C	1	Total C 8 8	0	0
7	C	1	Total C 5 5	0	0

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



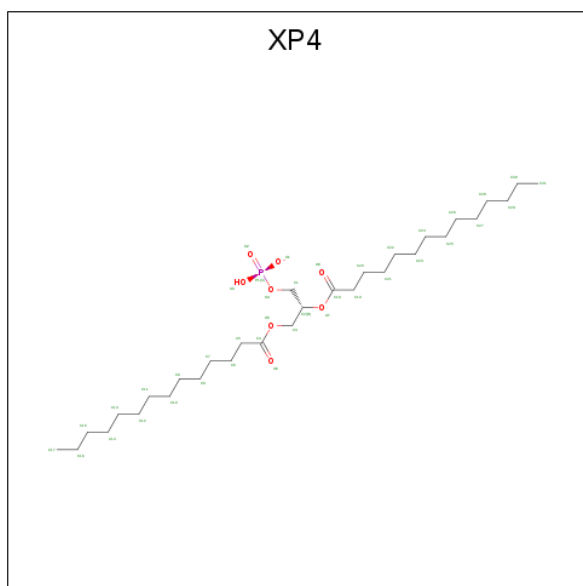
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
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 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: XP4) (formula: $C_{31}H_{60}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	P	0	0
			40	31	8	1		

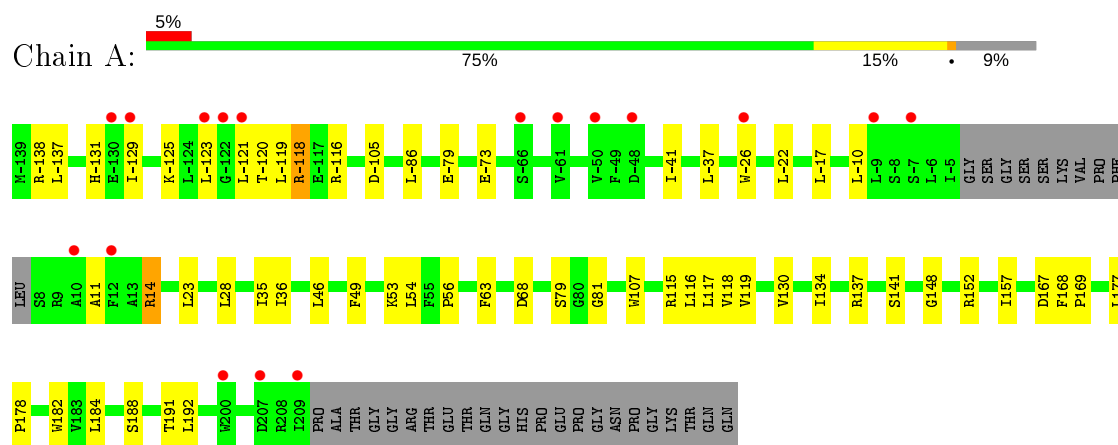
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	51	Total	O	0	0
			51	51		
10	C	52	Total	O	0	0
			52	52		

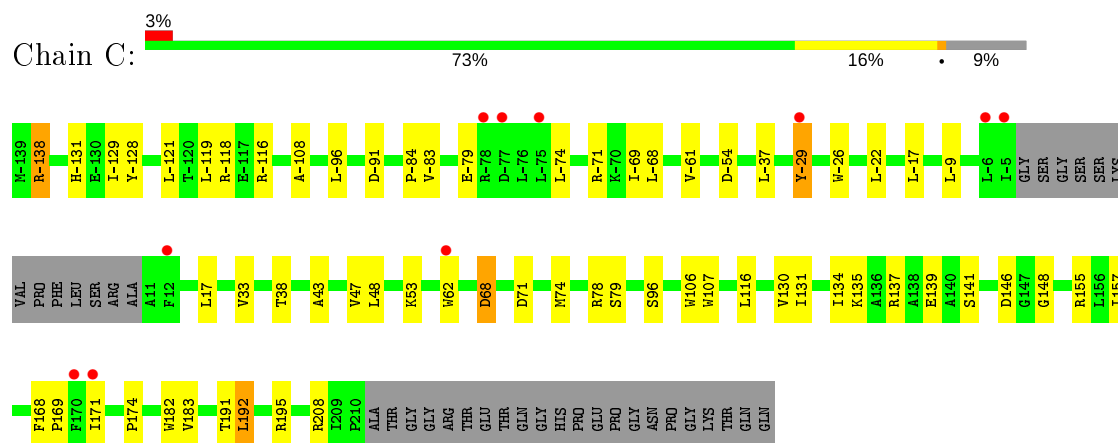
3 Residue-property plots

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	78.34Å 60.24Å 85.38Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.22 – 1.96 49.22 – 1.96	Depositor EDS
% Data completeness (in resolution range)	65.4 (49.22-1.96) 65.4 (49.22-1.96)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.235 , 0.277 0.235 , 0.277	Depositor DCC
R_{free} test set	1930 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 74.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5682	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: GOL, OLC, NA, PO4, FLC, TCE, 8K6, XP4

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	0.33	0/2643	0.48	0/3599
1	C	0.33	0/2582	0.49	0/3520
All	All	0.33	0/5225	0.48	0/7119

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	2588	0	2618	48	0
1	C	2531	0	2535	50	0
2	A	13	0	5	1	0
2	C	13	0	5	0	0
3	A	4	0	0	0	0
3	C	3	0	0	0	0
4	A	5	0	0	0	0
5	A	16	0	12	0	0
6	A	64	0	79	7	0
6	C	75	0	108	11	0
7	A	131	0	237	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	60	0	112	7	0
8	A	24	0	32	0	0
8	C	12	0	16	1	0
9	A	40	0	60	1	0
10	A	51	0	0	3	0
10	C	52	0	0	1	0
All	All	5682	0	5819	99	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 9.

All (99) 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:C:62:TRP:CD2	7:C:315:8K6:H181	2.18	0.78
1:A:182:TRP:HE1	6:A:310:OLC:H21A	1.50	0.77
1:A:54:LEU:HD22	6:A:309:OLC:H2	1.70	0.73
1:A:168:PHE:CD2	1:A:169:PRO:HD2	2.26	0.69
1:C:62:TRP:CE2	7:C:315:8K6:H181	2.27	0.69
1:C:106:TRP:HE1	6:C:308:OLC:H3A	1.56	0.69
1:A:35:ILE:HD11	7:A:312:8K6:H111	1.75	0.68
1:A:-119:LEU:HD13	1:A:-22:LEU:HD13	1.77	0.67
1:A:177:LEU:HB3	1:A:178:PRO:HD3	1.76	0.66
1:C:107:TRP:HZ2	6:C:306:OLC:H24	1.61	0.65
1:C:-79:GLU:HG3	1:C:-26:TRP:HB3	1.80	0.63
1:A:81:GLY:HA3	2:A:301:FLC:HG1	1.81	0.62
1:C:-119:LEU:HD13	1:C:-22:LEU:HD13	1.81	0.62
1:C:171:ILE:O	1:C:171:ILE:HG23	2.00	0.62
1:C:47:VAL:HG21	7:C:316:8K6:H12C	1.82	0.61
1:C:-138[B]:ARG:NH1	1:C:-91:ASP:OD2	2.34	0.59
1:C:-138[A]:ARG:NH1	1:C:-108:ALA:O	2.34	0.59
1:A:-129:ILE:HD13	1:A:-22:LEU:HB3	1.83	0.59
1:A:-131:HIS:NE2	1:A:-86:LEU:O	2.29	0.58
1:A:-118[B]:ARG:NH1	10:A:402:HOH:O	2.35	0.58
1:A:11:ALA:HA	1:A:14:ARG:HH21	1.69	0.58
1:A:-129:ILE:HD11	1:A:-17:LEU:HD21	1.86	0.56
1:A:35:ILE:HD11	7:A:312:8K6:H131	1.86	0.56
1:C:-9:LEU:HD21	1:C:17:LEU:HD13	1.86	0.55
1:C:155:ARG:NH1	10:C:402:HOH:O	2.38	0.55
1:C:47:VAL:HG23	1:C:48:LEU:HG	1.89	0.55
1:A:148:GLY:HA3	1:A:191:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:NZ	1:C:139:GLU:OE1	2.33	0.54
1:C:116:LEU:HD23	6:C:305:OLC:H21A	1.90	0.54
1:C:174:PRO:HB3	6:C:306:OLC:H6A	1.90	0.53
1:A:53:LYS:HB3	1:A:56:PRO:HG2	1.92	0.52
1:C:68:ASP:O	1:C:71:ASP:OD2	2.27	0.52
1:A:116:LEU:HD23	6:A:310:OLC:H21	1.90	0.52
1:A:115:ARG:HB3	1:C:106:TRP:CH2	2.45	0.51
1:C:-129:ILE:HD11	1:C:-17:LEU:HD21	1.93	0.50
1:A:35:ILE:CD1	7:A:312:8K6:H131	2.42	0.50
1:A:-123:LEU:HD12	1:A:-10:LEU:HD23	1.94	0.50
1:C:130:VAL:HG12	1:C:192:LEU:HD21	1.94	0.50
1:C:106:TRP:NE1	6:C:308:OLC:H3A	2.26	0.49
1:C:53:LYS:NZ	8:C:318:GOL:O3	2.31	0.49
1:C:135:LYS:HE2	1:C:146:ASP:HB3	1.94	0.49
7:C:310:8K6:H183	7:C:311:8K6:H181	1.93	0.49
1:A:-138[B]:ARG:NH2	10:A:408:HOH:O	2.45	0.49
1:A:117:LEU:HB2	6:A:310:OLC:H22	1.95	0.48
1:C:78:ARG:HB3	1:C:79:SER:H	1.48	0.47
1:C:-128:TYR:HB3	1:C:-118:ARG:HB2	1.97	0.47
1:A:79:SER:O	1:C:208:ARG:NH1	2.47	0.47
1:A:192:LEU:HD13	7:A:314:8K6:H62C	1.96	0.47
1:A:-121:LEU:HB2	1:A:-116:ARG:HH21	1.78	0.46
1:A:130:VAL:O	1:A:134:ILE:HG13	2.14	0.46
1:A:-125:LYS:HA	1:A:-120:THR:HA	1.96	0.46
1:A:-79:GLU:HG3	1:A:-26[A]:TRP:HB3	1.98	0.45
1:A:137:ARG:NH1	1:A:141:SER:OG	2.45	0.45
6:C:306:OLC:H14A	7:C:312:8K6:H171	1.97	0.45
1:C:130:VAL:O	1:C:134:ILE:HG13	2.17	0.45
1:A:115:ARG:HB3	1:C:106:TRP:HH2	1.81	0.44
1:C:148:GLY:HA3	1:C:191:THR:HG23	2.00	0.44
1:C:131:ILE:HG23	1:C:195:ARG:HD2	1.99	0.44
1:A:36:ILE:HD11	7:A:323:8K6:H111	1.98	0.44
1:C:-128:TYR:HA	1:C:-119:LEU:HB2	1.99	0.44
1:C:131:ILE:HG13	1:C:192:LEU:HD23	2.00	0.44
1:A:119:VAL:HG22	6:C:308:OLC:H11A	2.00	0.44
1:C:-74:LEU:HD11	1:C:-68:LEU:HD21	2.00	0.43
1:C:-121:LEU:HB2	1:C:-116:ARG:HH21	1.83	0.43
1:C:33:VAL:HG21	1:C:74:MET:SD	2.59	0.43
1:A:157:ILE:HD12	7:A:326:8K6:H181	2.00	0.43
1:C:183:VAL:HA	7:C:313:8K6:H141	2.01	0.43
1:A:49:PHE:O	1:A:107:TRP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:TRP:CE3	6:C:305:OLC:H5A	2.55	0.42
1:A:-137:LEU:HD23	1:A:-105:ASP:HB3	2.01	0.42
7:A:331:8K6:H61C	6:C:308:OLC:H15A	2.02	0.42
1:A:23:LEU:HD22	1:A:28:LEU:HD12	2.00	0.42
1:C:43:ALA:O	1:C:47:VAL:HG22	2.19	0.42
1:C:-69:ILE:HD11	1:C:-37:LEU:HD22	2.02	0.42
1:A:167:ASP:O	6:A:311:OLC:O25	2.37	0.42
1:C:62:TRP:CG	7:C:315:8K6:H171	2.53	0.42
1:C:38:THR:HG23	1:C:96[B]:SER:OG	2.19	0.42
1:C:-68:LEU:HD23	1:C:-29:TYR:HB3	2.02	0.42
6:C:306:OLC:H4	6:C:306:OLC:H7	1.65	0.42
1:A:-118[A]:ARG:HB2	1:A:-118[A]:ARG:HH21	1.84	0.42
1:C:137:ARG:NH1	1:C:141:SER:OG	2.52	0.42
1:A:182:TRP:CE3	6:A:310:OLC:H7A	2.55	0.41
1:C:168:PHE:CD2	1:C:169:PRO:HD2	2.55	0.41
1:A:46:LEU:HD22	9:A:330:XP4:H39	2.01	0.41
1:C:-96:LEU:HD23	1:C:-96:LEU:HA	1.89	0.41
1:A:63:PHE:CG	6:A:311:OLC:H10	2.55	0.41
1:A:115:ARG:O	1:A:118[A]:VAL:HG22	2.21	0.41
1:A:11:ALA:HA	1:A:14:ARG:HD2	2.03	0.41
1:A:28:LEU:HD21	7:A:323:8K6:H122	2.01	0.41
1:A:-41:ILE:O	1:A:-37:LEU:HG	2.21	0.41
1:C:-54:ASP:N	1:C:-54:ASP:OD2	2.53	0.41
1:C:-131:HIS:CE1	1:C:-84:PRO:HD3	2.56	0.41
1:C:-83:VAL:HG21	1:C:-61:VAL:HG13	2.03	0.41
1:A:184:LEU:O	1:A:188:SER:N	2.52	0.40
1:A:152:ARG:NH2	10:A:401:HOH:O	2.29	0.40
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.92	0.40
1:C:174:PRO:HB3	6:C:306:OLC:H3A	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	339/370 (92%)	335 (99%)	4 (1%)	0	100	100
1	C	335/370 (90%)	327 (98%)	8 (2%)	0	100	100
All	All	674/740 (91%)	662 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/300 (87%)	255 (98%)	5 (2%)	57	50
1	C	255/300 (85%)	249 (98%)	6 (2%)	49	40
All	All	515/600 (86%)	504 (98%)	11 (2%)	59	46

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

Mol	Chain	Res	Type
1	A	-118[A]	ARG
1	A	-118[B]	ARG
1	A	-73	GLU
1	A	14	ARG
1	A	68	ASP
1	C	-138[A]	ARG
1	C	-138[B]	ARG
1	C	-71	ARG
1	C	-29	TYR
1	C	68	ASP
1	C	192	LEU

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

Mol	Chain	Res	Type
1	A	129	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 7 are monoatomic - leaving 43 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	331	-	6,6,17	0.15	0	5,5,16	0.09	0
7	8K6	C	314	-	6,6,17	0.14	0	5,5,16	0.10	0
5	TCE	A	307	-	6,15,15	1.27	0	9,18,18	3.91	6 (66%)
7	8K6	C	309	-	8,8,17	0.13	0	7,7,16	0.09	0
6	OLC	A	309	-	16,16,24	1.15	1 (6%)	17,17,25	1.17	2 (11%)
2	FLC	C	301	3	3,12,12	0.78	0	3,17,17	1.02	0
8	GOL	A	328	-	5,5,5	0.35	0	5,5,5	0.38	0
6	OLC	C	306	-	24,24,24	0.94	1 (4%)	25,25,25	0.83	1 (4%)
7	8K6	A	318	-	4,4,17	0.32	0	3,3,16	0.54	0
7	8K6	A	312	-	16,16,17	0.09	0	15,15,16	0.09	0
7	8K6	A	326	-	11,11,17	0.14	0	10,10,16	0.08	0
7	8K6	C	312	-	6,6,17	0.14	0	5,5,16	0.10	0
8	GOL	A	327	-	5,5,5	0.34	0	5,5,5	0.28	0
7	8K6	A	314	-	6,6,17	0.13	0	5,5,16	0.09	0
7	8K6	A	320	-	7,7,17	0.16	0	6,6,16	0.08	0
7	8K6	A	317	-	4,4,17	0.33	0	3,3,16	0.52	0
7	8K6	C	315	-	7,7,17	0.15	0	6,6,16	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	8K6	C	311	-	7,7,17	0.15	0	6,6,16	0.11	0
6	OLC	C	308	-	24,24,24	0.96	1 (4%)	25,25,25	0.92	2 (8%)
7	8K6	A	321	-	6,6,17	0.18	0	5,5,16	0.11	0
8	GOL	C	318	-	5,5,5	0.35	0	5,5,5	0.29	0
7	8K6	A	322	-	6,6,17	0.14	0	5,5,16	0.09	0
6	OLC	C	307	-	8,8,24	1.03	1 (12%)	9,9,25	0.94	0
7	8K6	C	313	-	7,7,17	0.14	0	6,6,16	0.10	0
7	8K6	A	313	-	9,9,17	0.14	0	8,8,16	0.10	0
7	8K6	C	310	-	7,7,17	0.13	0	6,6,16	0.10	0
8	GOL	A	332	-	5,5,5	0.37	0	5,5,5	0.20	0
7	8K6	A	323	-	13,13,17	0.10	0	12,12,16	0.07	0
6	OLC	A	311	-	18,18,24	1.04	1 (5%)	18,19,25	0.99	1 (5%)
7	8K6	A	316	-	4,4,17	0.34	0	3,3,16	0.53	0
6	OLC	A	308	-	9,9,24	1.49	1 (11%)	10,10,25	1.47	1 (10%)
6	OLC	A	310	-	17,17,24	1.09	1 (5%)	18,18,25	1.12	2 (11%)
7	8K6	C	316	-	4,4,17	0.32	0	3,3,16	0.51	0
8	GOL	A	329	-	5,5,5	0.36	0	5,5,5	0.23	0
7	8K6	A	319	-	4,4,17	0.34	0	3,3,16	0.53	0
7	8K6	A	325	-	7,7,17	0.13	0	6,6,16	0.09	0
4	PO4	A	306[A]	-	4,4,4	0.88	0	6,6,6	0.34	0
7	8K6	A	324	-	8,8,17	0.12	0	7,7,16	0.10	0
6	OLC	C	305	-	15,15,24	1.18	1 (6%)	16,16,25	0.99	1 (6%)
2	FLC	A	301	-	3,12,12	0.80	0	3,17,17	0.63	0
9	XP4	A	330	-	39,39,39	1.02	2 (5%)	43,44,44	1.18	3 (6%)
7	8K6	A	315	-	4,4,17	0.15	0	3,3,16	0.23	0
8	GOL	C	317	-	5,5,5	0.40	0	5,5,5	0.27	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
7	8K6	A	331	-	-	1/4/4/15	-
7	8K6	C	314	-	-	2/4/4/15	-
5	TCE	A	307	-	-	4/9/15/15	-
7	8K6	C	309	-	-	1/6/6/15	-
6	OLC	A	309	-	-	5/16/16/24	-
2	FLC	C	301	3	-	3/6/16/16	-
8	GOL	A	328	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLC	C	306	-	-	5/24/24/24	-
7	8K6	A	318	-	-	0/2/2/15	-
7	8K6	A	312	-	-	5/14/14/15	-
7	8K6	A	326	-	-	6/9/9/15	-
7	8K6	C	312	-	-	1/4/4/15	-
8	GOL	A	327	-	-	2/4/4/4	-
7	8K6	A	314	-	-	3/4/4/15	-
7	8K6	A	320	-	-	1/5/5/15	-
7	8K6	A	317	-	-	0/2/2/15	-
7	8K6	C	315	-	-	2/5/5/15	-
7	8K6	C	311	-	-	2/5/5/15	-
6	OLC	C	308	-	-	7/24/24/24	-
8	GOL	C	318	-	-	2/4/4/4	-
7	8K6	A	322	-	-	1/4/4/15	-
6	OLC	C	307	-	-	4/7/7/24	-
7	8K6	C	313	-	-	1/5/5/15	-
7	8K6	A	313	-	-	2/7/7/15	-
7	8K6	C	310	-	-	3/5/5/15	-
8	GOL	A	332	-	-	2/4/4/4	-
7	8K6	A	323	-	-	6/11/11/15	-
6	OLC	A	311	-	-	2/18/18/24	-
7	8K6	A	316	-	-	1/2/2/15	-
6	OLC	A	308	-	-	0/9/9/24	-
6	OLC	A	310	-	-	7/17/17/24	-
7	8K6	C	316	-	-	2/2/2/15	-
8	GOL	A	329	-	-	2/4/4/4	-
7	8K6	A	319	-	-	0/2/2/15	-
7	8K6	A	325	-	-	3/5/5/15	-
7	8K6	A	321	-	-	1/4/4/15	-
7	8K6	A	324	-	-	2/6/6/15	-
6	OLC	C	305	-	-	2/15/15/24	-
2	FLC	A	301	-	-	3/6/16/16	-
9	XP4	A	330	-	-	20/41/41/41	-
7	8K6	A	315	-	-	0/2/2/15	-
8	GOL	C	317	-	-	4/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	305	OLC	O20-C1	4.38	1.46	1.33
6	C	308	OLC	O20-C1	4.38	1.46	1.33
6	C	306	OLC	O20-C1	4.35	1.46	1.33
6	A	308	OLC	O20-C1	4.33	1.46	1.33
6	A	309	OLC	O20-C1	4.33	1.46	1.33
6	A	310	OLC	O20-C1	4.29	1.45	1.33
6	A	311	OLC	O20-C1	4.17	1.45	1.33
9	A	330	XP4	O7-C18	3.95	1.45	1.34
9	A	330	XP4	O5-C4	3.95	1.44	1.33
6	C	307	OLC	O20-C1	2.61	1.46	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	307	TCE	C1-P-C3	6.17	120.59	100.95
5	A	307	TCE	C3-P-C2	6.00	120.08	100.95
5	A	307	TCE	C1-P-C2	5.77	119.32	100.95
9	A	330	XP4	O7-C18-C19	4.78	121.81	111.50
6	A	308	OLC	O20-C1-C2	3.68	121.03	111.38
6	A	309	OLC	O20-C1-C2	3.23	122.06	111.91
6	C	308	OLC	O20-C1-C2	3.14	121.78	111.91
5	A	307	TCE	P-C3-C6	-3.09	110.05	113.67
5	A	307	TCE	P-C1-C4	-3.07	110.07	113.67
5	A	307	TCE	P-C2-C5	-3.05	110.10	113.67
6	A	310	OLC	O20-C1-C2	2.99	121.28	111.91
9	A	330	XP4	O5-C4-C5	2.89	120.98	111.91
6	C	305	OLC	O20-C1-C2	2.79	120.66	111.91
6	A	311	OLC	O20-C1-C2	2.56	119.94	111.91
6	A	309	OLC	O20-C1-O19	-2.33	117.72	123.59
6	C	308	OLC	O20-C1-O19	-2.23	117.97	123.59
6	A	310	OLC	O20-C1-O19	-2.18	118.09	123.59
6	C	306	OLC	O20-C1-C2	2.15	118.66	111.91
9	A	330	XP4	O5-C4-O6	-2.02	118.51	123.59

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	307	TCE	C5-C2-P-C3
5	A	307	TCE	C6-C3-P-C1
5	A	307	TCE	C4-C1-P-C3
2	C	301	FLC	CA-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
2	C	301	FLC	CBC-CB-CG-CGC
2	C	301	FLC	OHB-CB-CG-CGC
8	A	328	GOL	O1-C1-C2-C3
8	A	327	GOL	O1-C1-C2-C3
8	A	332	GOL	O1-C1-C2-C3
6	A	310	OLC	O20-C21-C22-C24
8	A	329	GOL	O1-C1-C2-C3
9	A	330	XP4	C1-O4-P1-O1
9	A	330	XP4	C1-O4-P1-O3
8	C	317	GOL	C1-C2-C3-O3
9	A	330	XP4	O6-C4-O5-C3
9	A	330	XP4	C5-C4-O5-C3
6	A	310	OLC	C2-C1-O20-C21
6	A	310	OLC	O20-C21-C22-O23
6	A	310	OLC	O19-C1-O20-C21
6	C	306	OLC	O20-C21-C22-C24
9	A	330	XP4	C26-C27-C28-C29
6	C	306	OLC	C1-C2-C3-C4
8	A	327	GOL	O1-C1-C2-O2
6	A	309	OLC	C1-C2-C3-C4
6	C	306	OLC	O20-C21-C22-O23
7	C	315	8K6	C12-C13-C14-C15
6	C	305	OLC	C2-C3-C4-C5
9	A	330	XP4	C19-C20-C21-C22
6	C	307	OLC	O20-C21-C22-C24
9	A	330	XP4	C13-C14-C15-C16
9	A	330	XP4	C18-C19-C20-C21
2	A	301	FLC	CA-CB-CG-CGC
7	A	314	8K6	C5-C6-C7-C8
6	A	309	OLC	C2-C3-C4-C5
7	A	313	8K6	C3-C4-C5-C6
7	A	326	8K6	C11-C10-C9-C8
6	A	309	OLC	C4-C5-C6-C7
7	A	326	8K6	C12-C13-C14-C15
6	A	309	OLC	C21-C22-C24-O25
8	A	328	GOL	C1-C2-C3-O3
8	C	318	GOL	O1-C1-C2-C3
8	C	317	GOL	O1-C1-C2-C3
6	C	307	OLC	O20-C21-C22-O23
6	C	308	OLC	C14-C15-C16-C17
6	C	306	OLC	C4-C5-C6-C7
6	C	308	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	A	323	8K6	C11-C12-C13-C14
7	C	315	8K6	C13-C14-C15-C16
7	A	325	8K6	C13-C14-C15-C16
9	A	330	XP4	C21-C22-C23-C24
7	A	314	8K6	C4-C5-C6-C7
8	A	332	GOL	O1-C1-C2-O2
8	C	317	GOL	O2-C2-C3-O3
7	A	323	8K6	C7-C8-C9-C10
7	C	310	8K6	C12-C13-C14-C15
7	A	323	8K6	C6-C7-C8-C9
7	A	321	8K6	C14-C15-C16-C17
7	A	323	8K6	C11-C10-C9-C8
7	A	312	8K6	C10-C11-C12-C13
9	A	330	XP4	C11-C10-C9-C8
7	A	326	8K6	C15-C16-C17-C18
7	C	310	8K6	C11-C12-C13-C14
9	A	330	XP4	C28-C29-C30-C31
8	A	328	GOL	O1-C1-C2-O2
8	C	318	GOL	O1-C1-C2-O2
8	A	329	GOL	O1-C1-C2-O2
8	C	317	GOL	O1-C1-C2-O2
7	A	325	8K6	C15-C16-C17-C18
9	A	330	XP4	C1-O4-P1-O2
7	C	316	8K6	C1-C2-C3-C4
7	C	314	8K6	C14-C15-C16-C17
7	A	325	8K6	C11-C12-C13-C14
7	A	312	8K6	C14-C15-C16-C17
7	C	312	8K6	C12-C13-C14-C15
7	A	326	8K6	C11-C12-C13-C14
7	A	322	8K6	C14-C15-C16-C17
6	C	306	OLC	C2-C3-C4-C5
9	A	330	XP4	C20-C21-C22-C23
7	C	314	8K6	C13-C14-C15-C16
6	C	307	OLC	C2-C1-O20-C21
8	A	328	GOL	O2-C2-C3-O3
6	A	310	OLC	C2-C3-C4-C5
7	A	324	8K6	C15-C16-C17-C18
9	A	330	XP4	C24-C25-C26-C27
9	A	330	XP4	C25-C26-C27-C28
7	A	323	8K6	C12-C13-C14-C15
2	A	301	FLC	OHB-CB-CG-CGC
5	A	307	TCE	P-C1-C4-C11

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Mol	Chain	Res	Type	Atoms
7	C	311	8K6	C13-C14-C15-C16
9	A	330	XP4	C27-C28-C29-C30
7	C	309	8K6	C6-C7-C8-C9
9	A	330	XP4	C10-C11-C12-C13
7	A	326	8K6	C14-C15-C16-C17
7	A	314	8K6	C3-C4-C5-C6
2	A	301	FLC	CBC-CB-CG-CGC
6	C	305	OLC	C4-C5-C6-C7
7	A	331	8K6	C3-C4-C5-C6
7	C	313	8K6	C14-C15-C16-C17
9	A	330	XP4	C5-C6-C7-C8
6	C	308	OLC	C5-C6-C7-C8
7	A	320	8K6	C13-C14-C15-C16
7	A	323	8K6	C10-C11-C12-C13
7	C	316	8K6	C2-C3-C4-C5
9	A	330	XP4	C1-C2-C3-O5
7	C	310	8K6	C15-C16-C17-C18
7	C	311	8K6	C12-C13-C14-C15
7	A	312	8K6	C11-C10-C9-C8
6	A	311	OLC	C5-C6-C7-C8
6	C	307	OLC	O19-C1-O20-C21
6	C	308	OLC	C7-C8-C9-C10
6	C	308	OLC	C15-C16-C17-C18
7	A	316	8K6	C1-C2-C3-C4
6	C	308	OLC	O20-C1-C2-C3
6	A	310	OLC	C7-C8-C9-C10
7	A	326	8K6	C10-C11-C12-C13
6	A	311	OLC	C7-C8-C9-C10
9	A	330	XP4	C14-C15-C16-C17
7	A	312	8K6	C2-C3-C4-C5
7	A	313	8K6	C6-C7-C8-C9
6	A	309	OLC	O23-C22-C24-O25
6	C	308	OLC	O19-C1-C2-C3
6	A	310	OLC	C4-C5-C6-C7
7	A	324	8K6	C11-C12-C13-C14
7	A	312	8K6	C7-C8-C9-C10

There are no ring outliers.

20 monomers are involved in 34 short contacts:

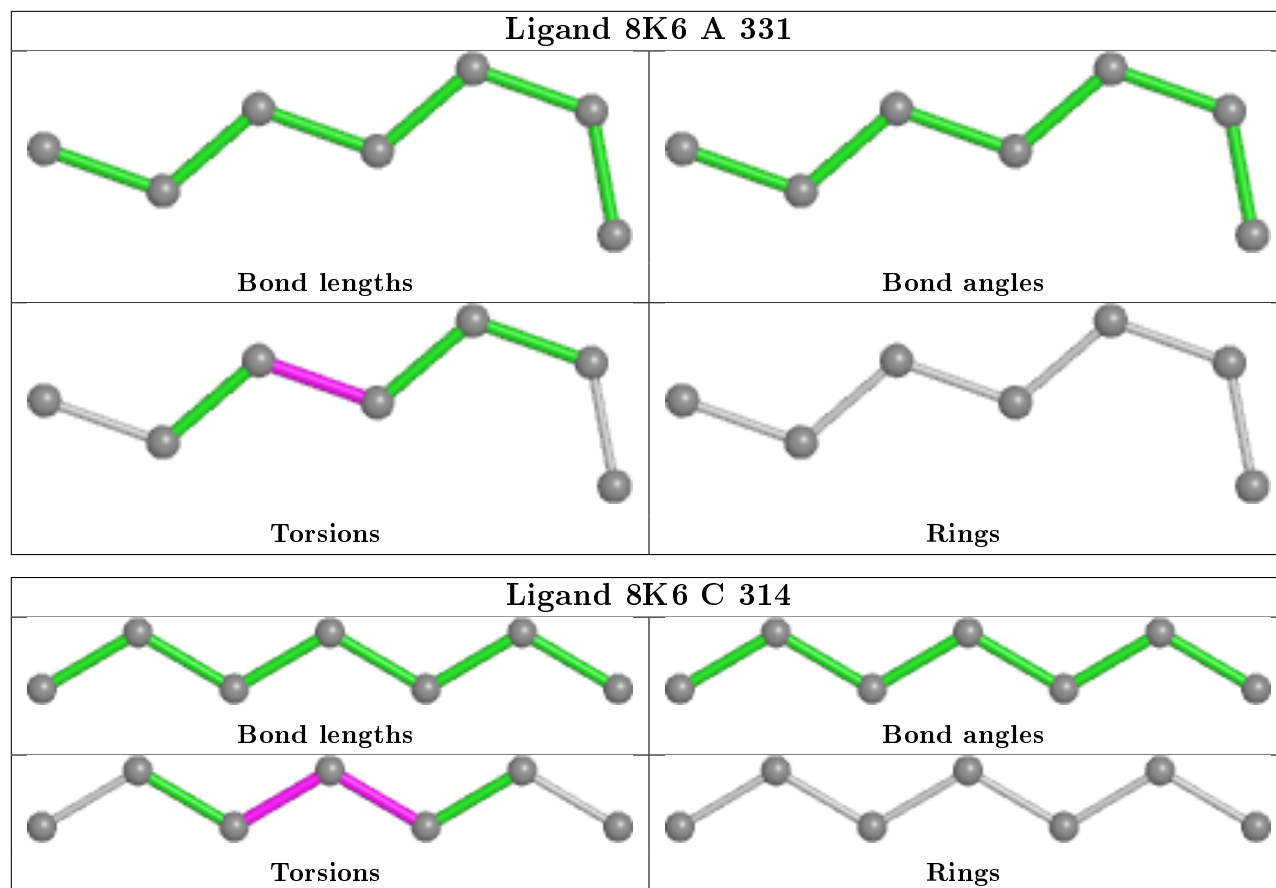
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	331	8K6	1	0

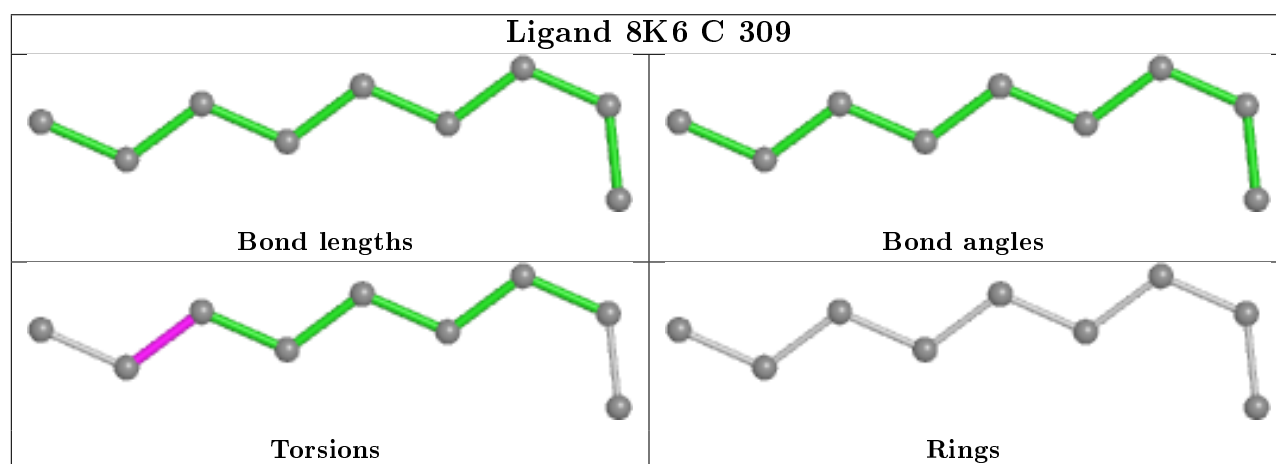
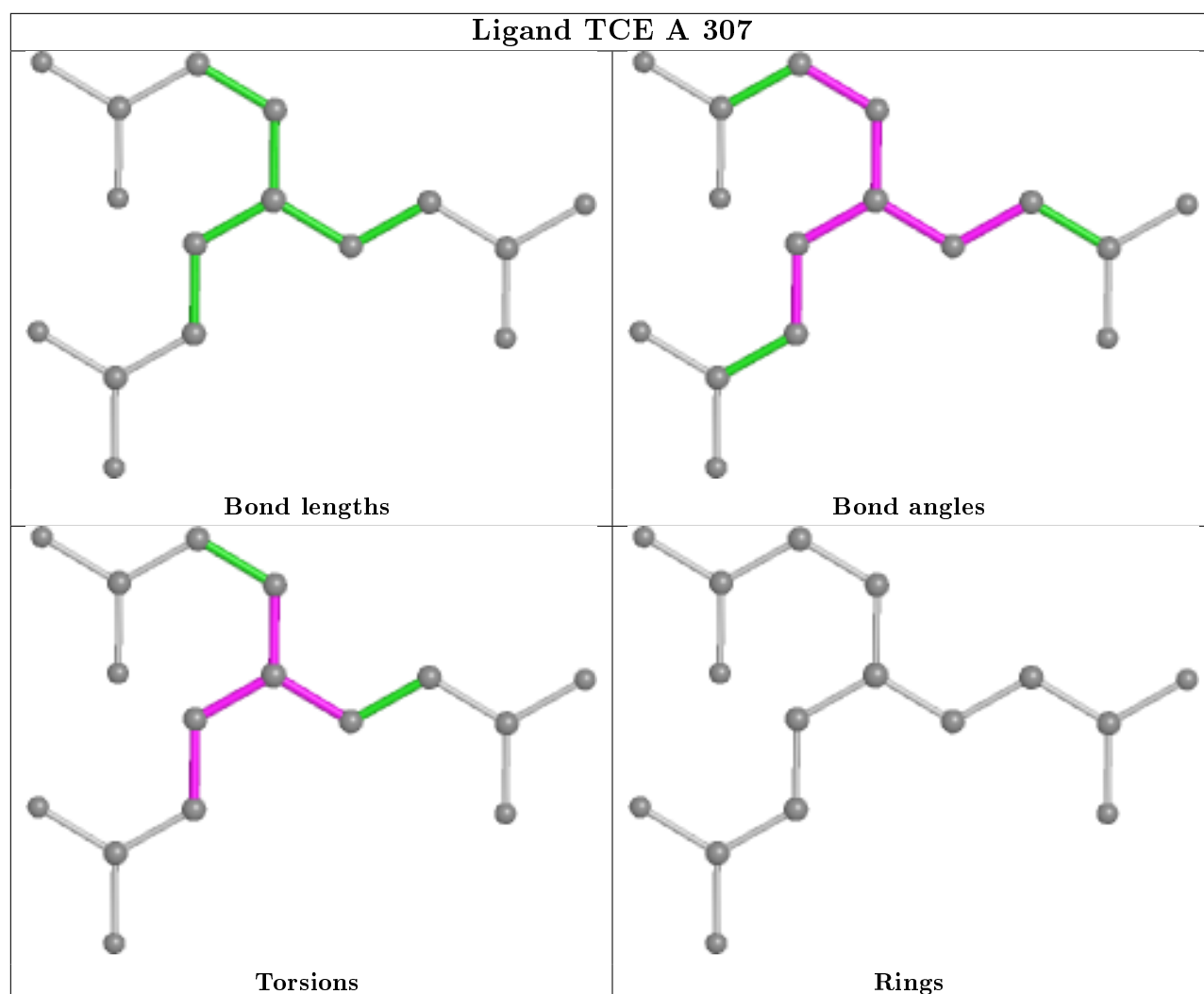
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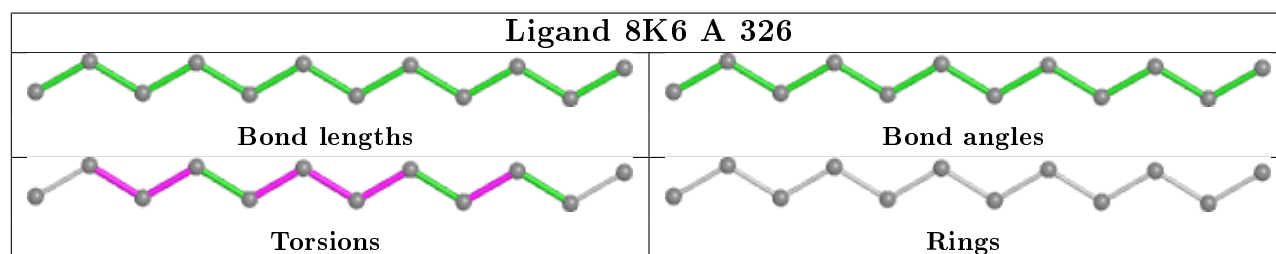
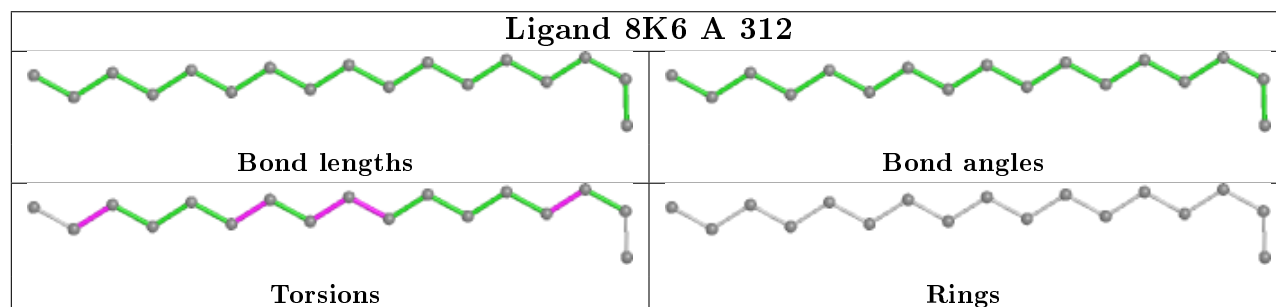
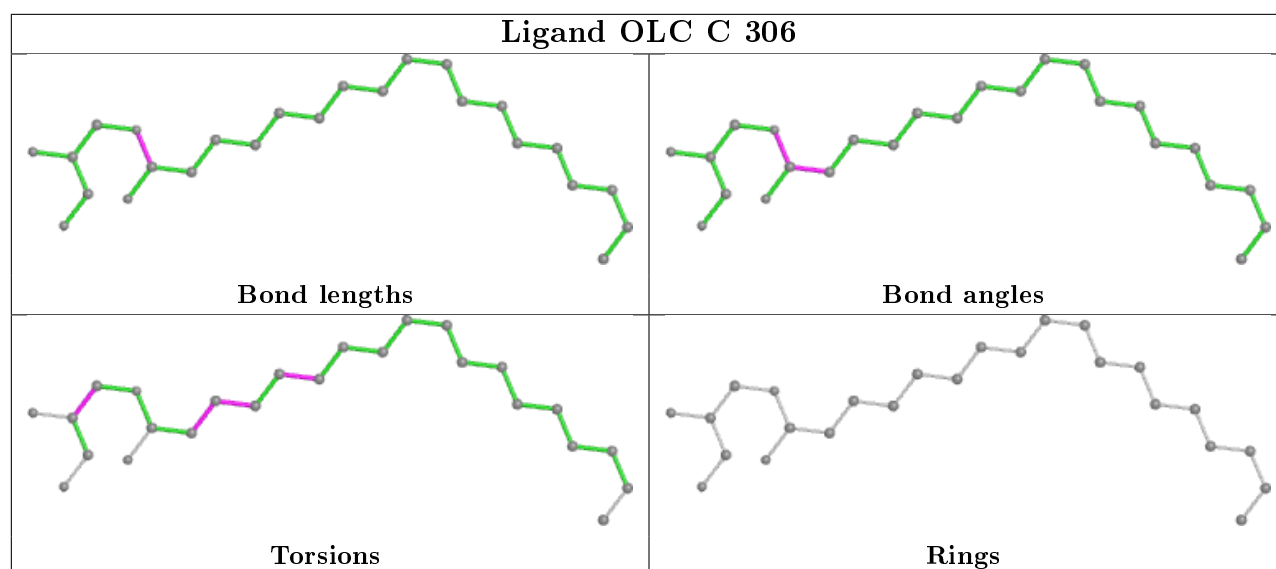
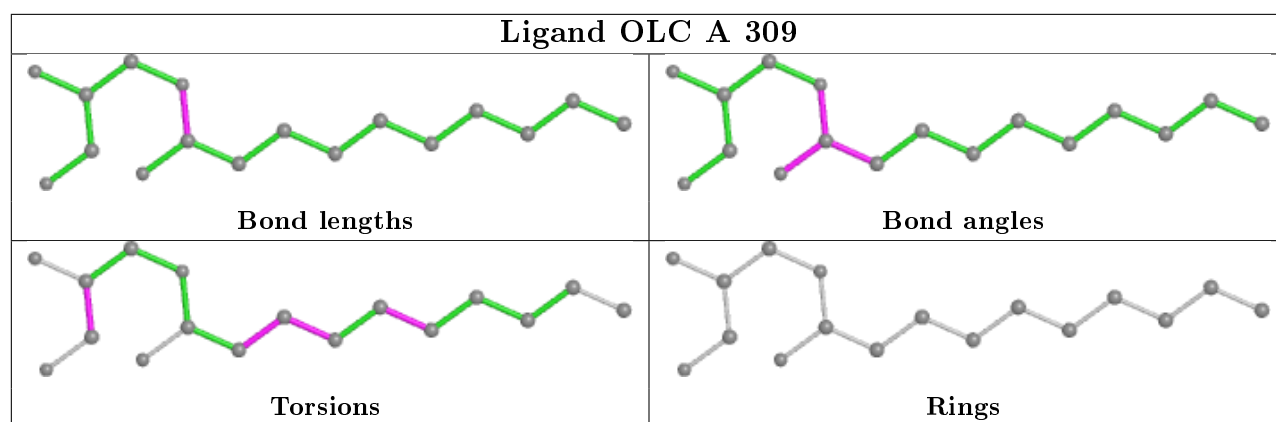
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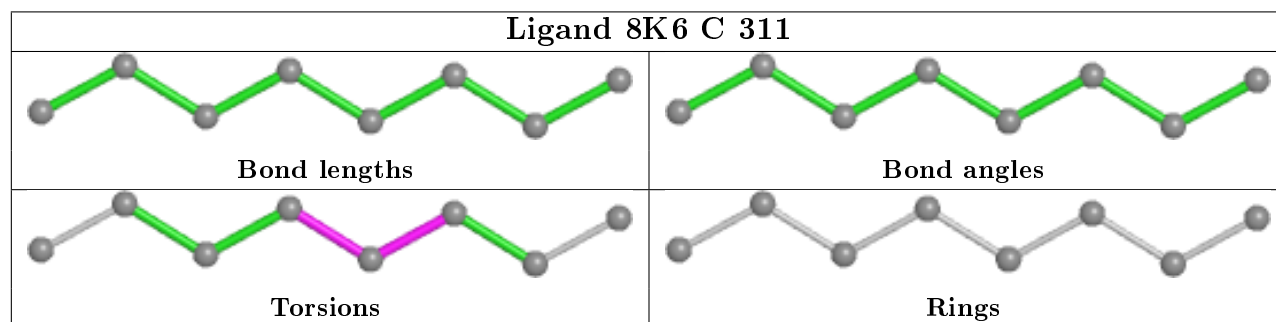
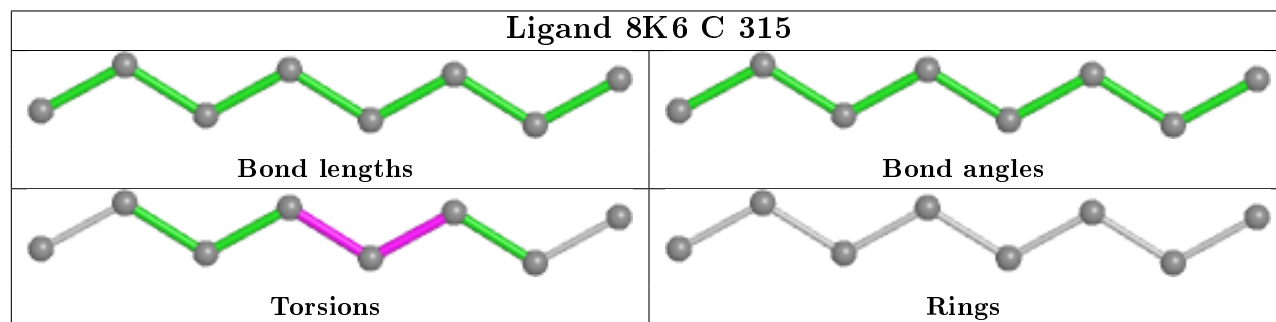
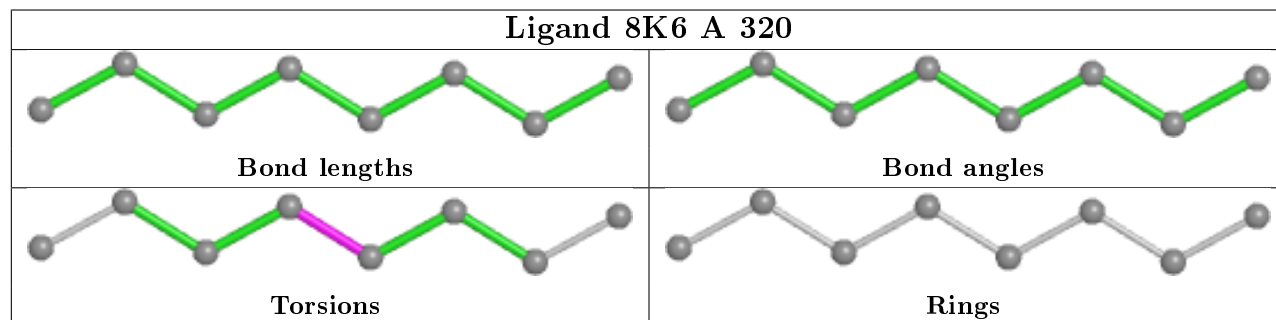
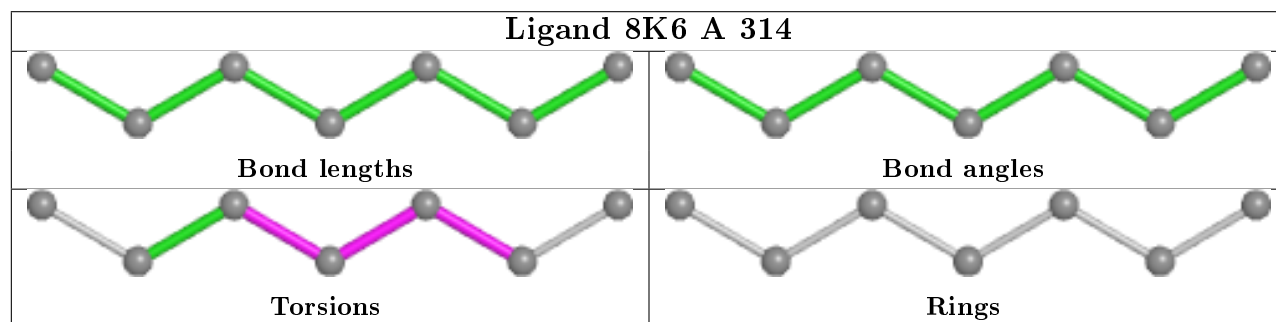
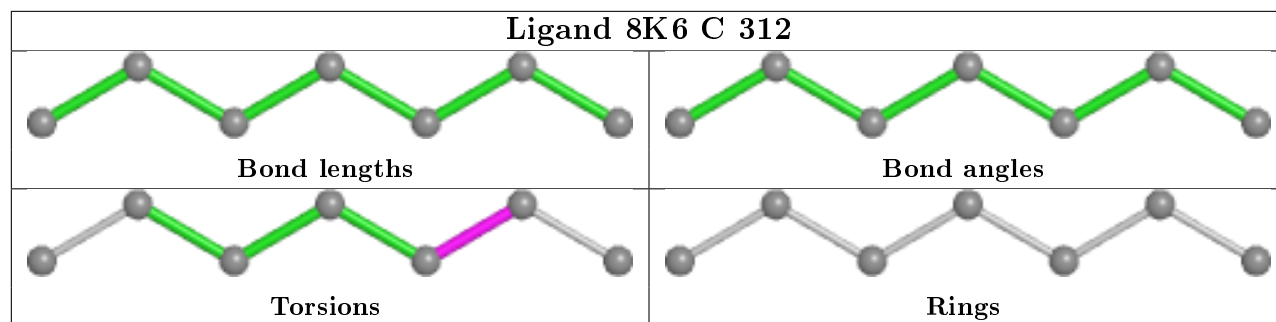
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	309	OLC	1	0
6	C	306	OLC	5	0
7	A	312	8K6	3	0
7	A	326	8K6	1	0
7	C	312	8K6	1	0
7	A	314	8K6	1	0
7	C	315	8K6	3	0
7	C	311	8K6	1	0
6	C	308	OLC	4	0
8	C	318	GOL	1	0
7	C	313	8K6	1	0
7	C	310	8K6	1	0
7	A	323	8K6	2	0
6	A	311	OLC	2	0
6	A	310	OLC	4	0
7	C	316	8K6	1	0
6	C	305	OLC	2	0
2	A	301	FLC	1	0
9	A	330	XP4	1	0

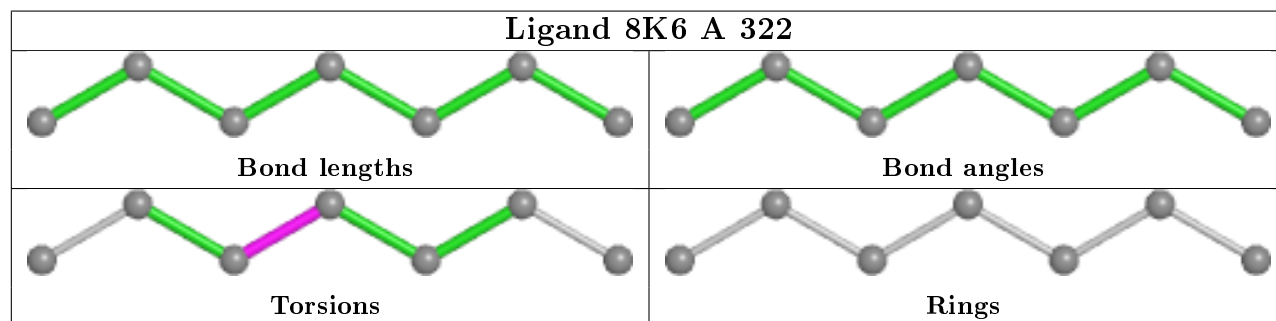
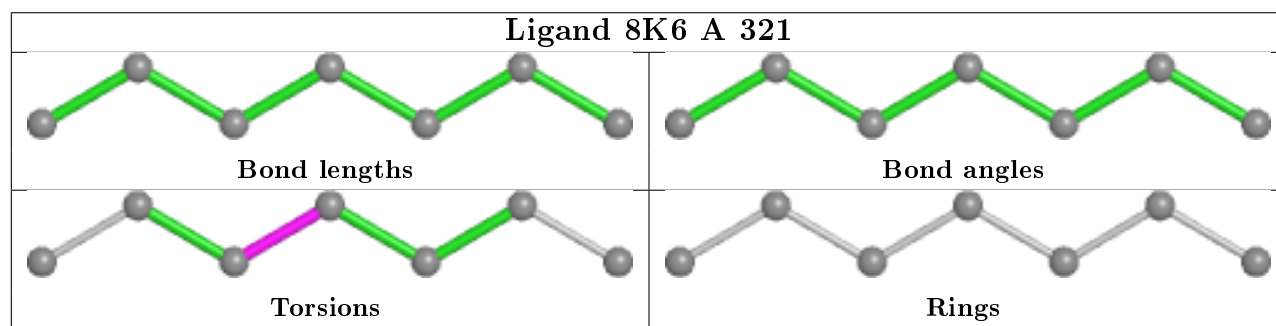
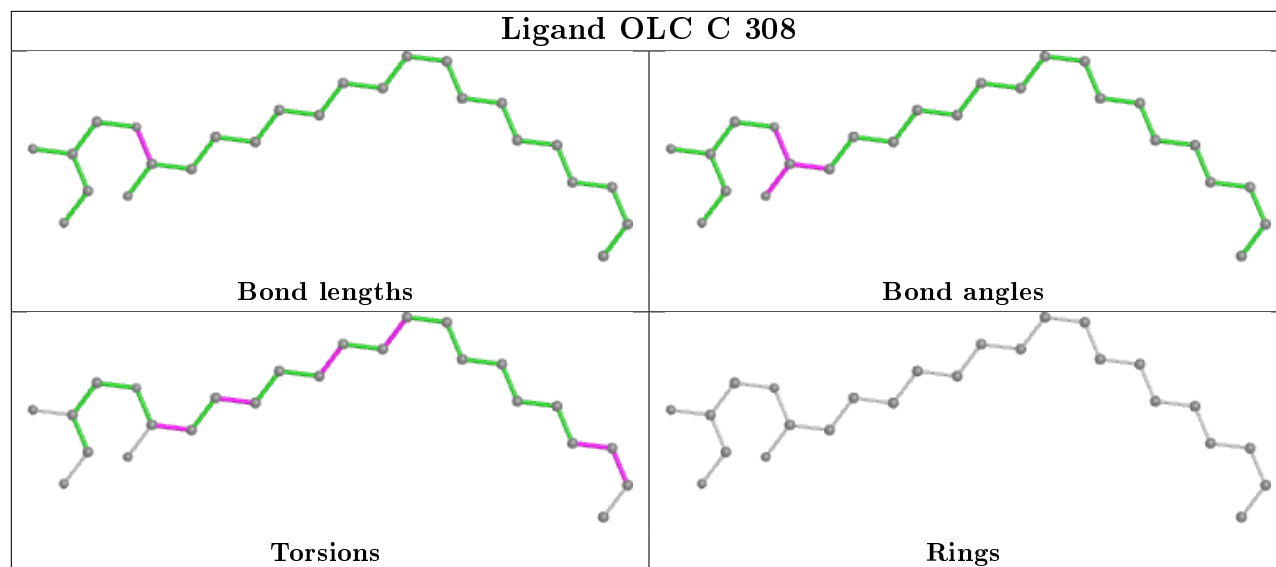
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

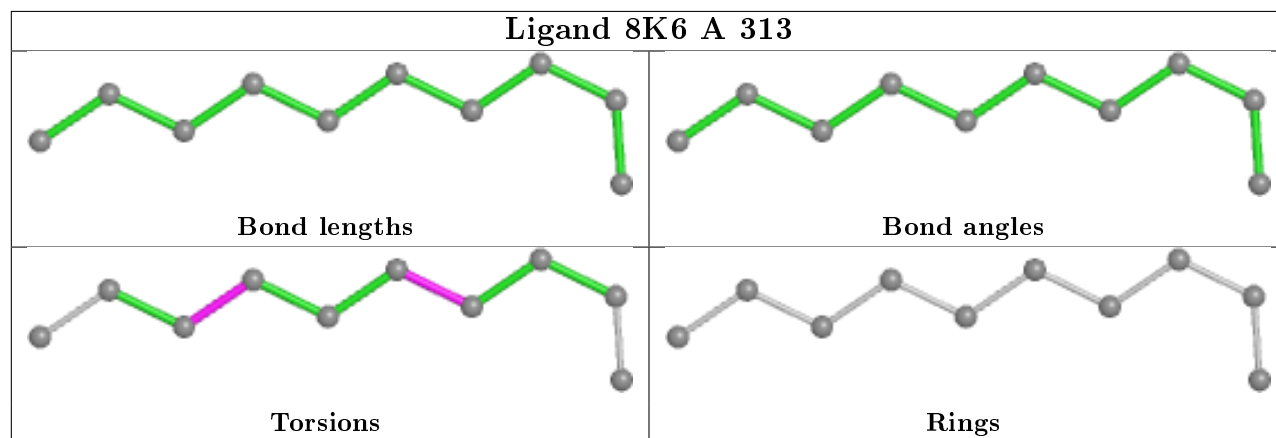
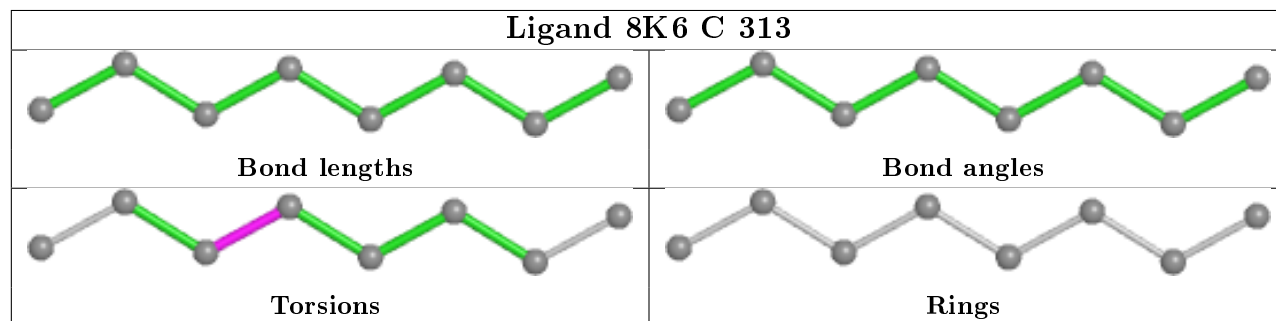
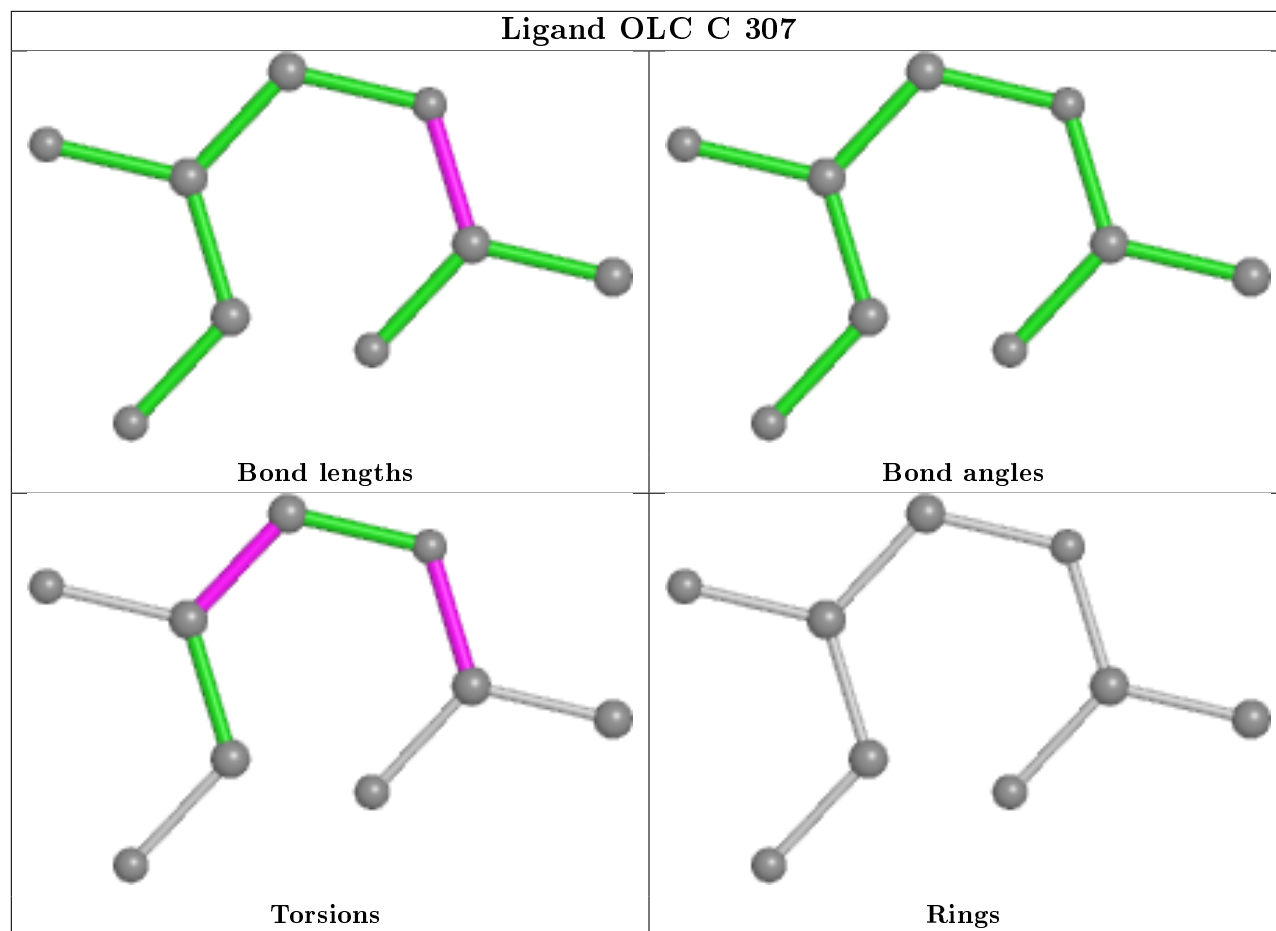


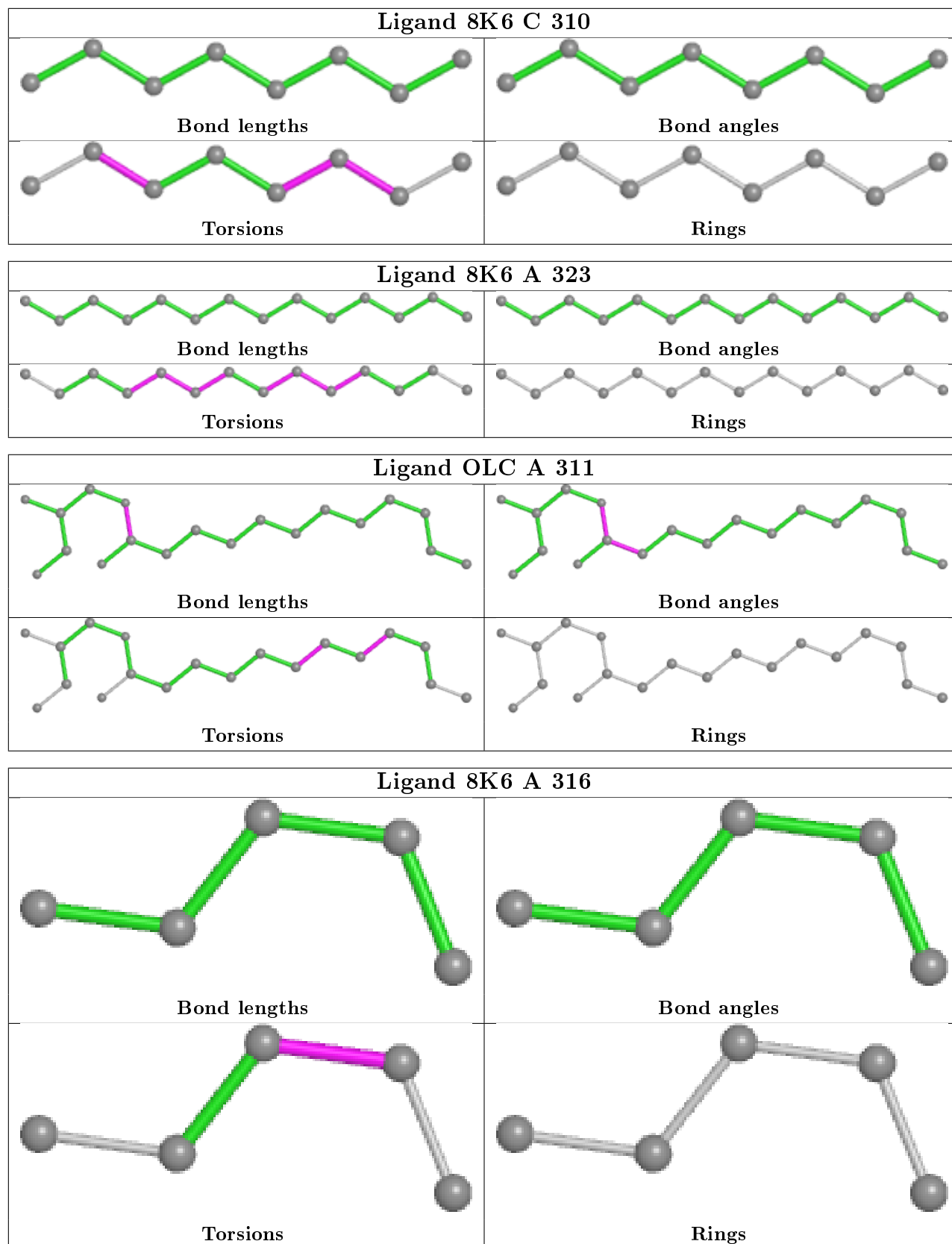


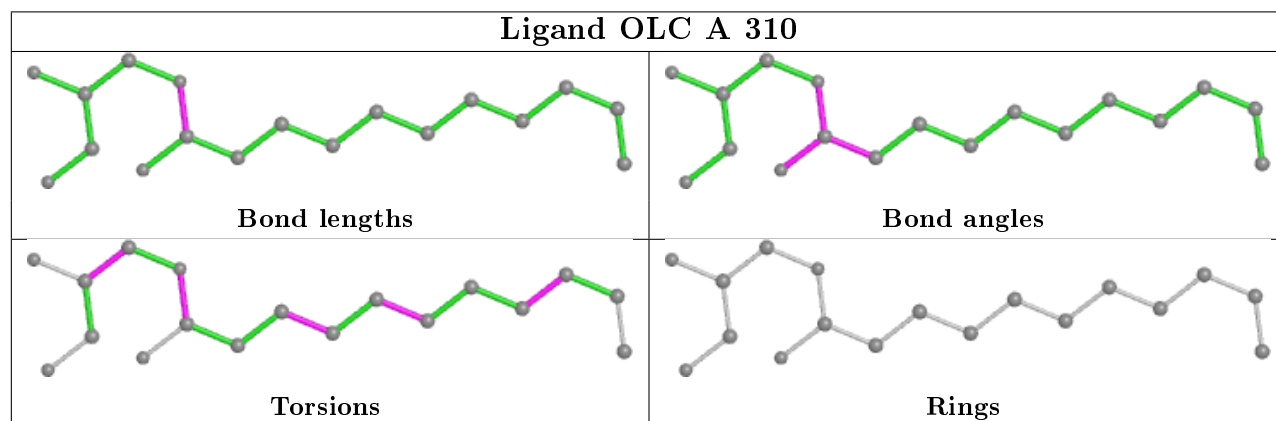
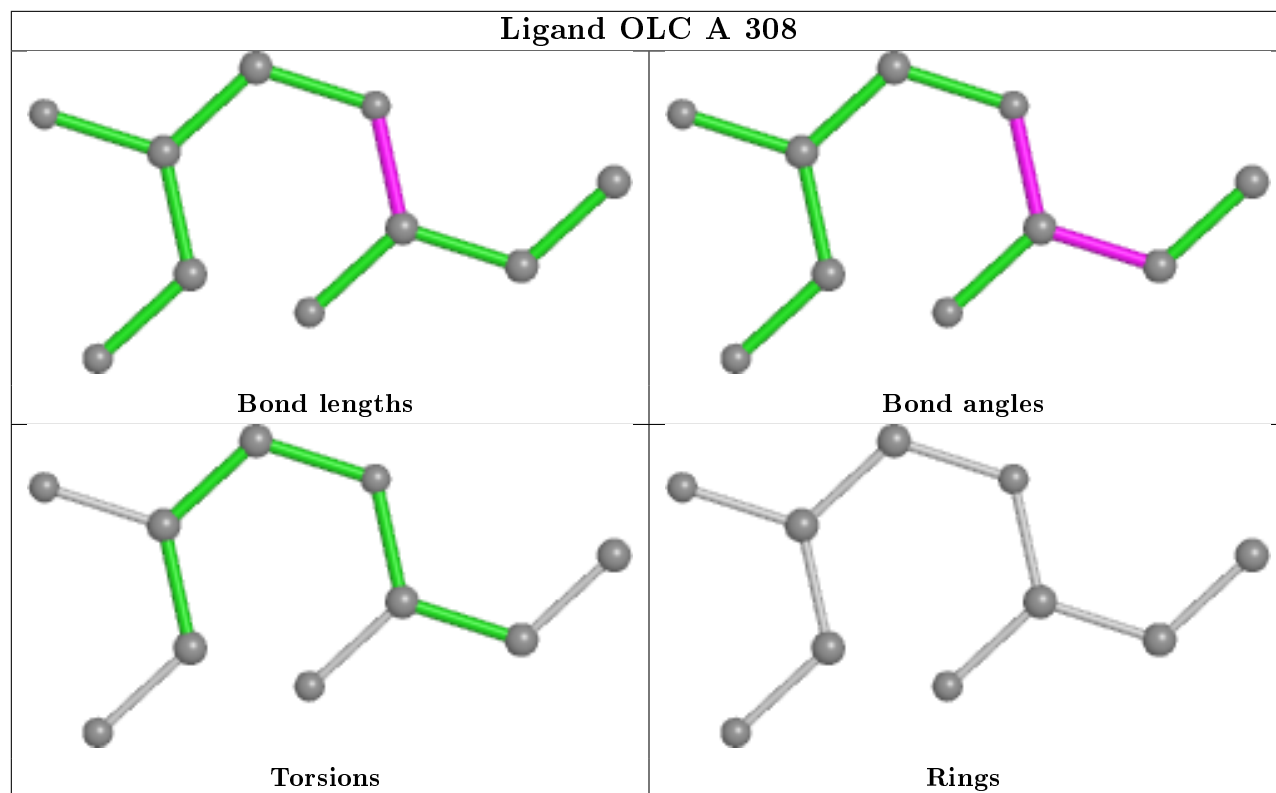


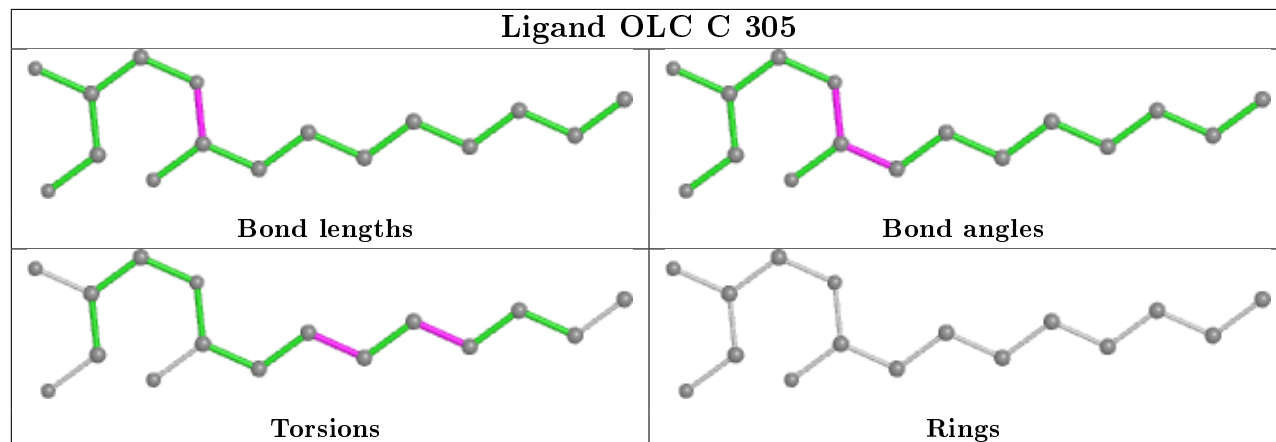
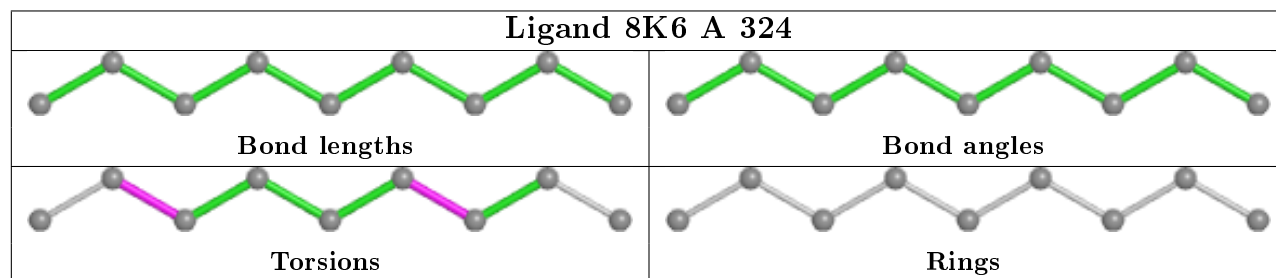
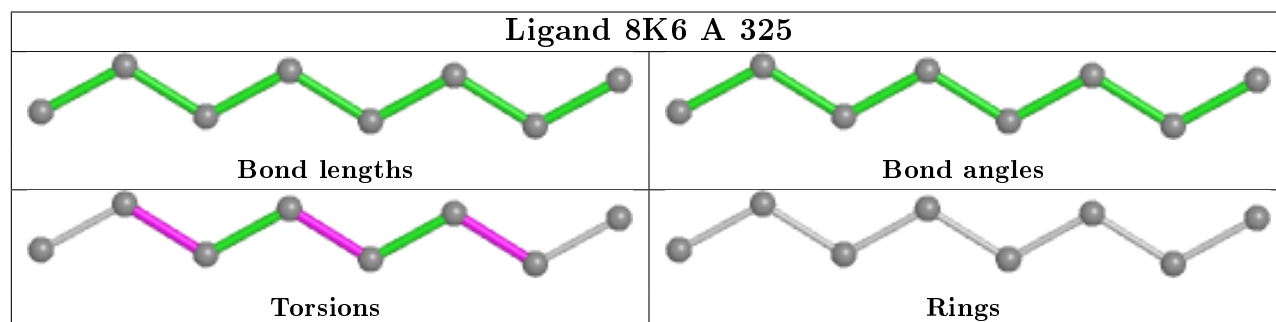
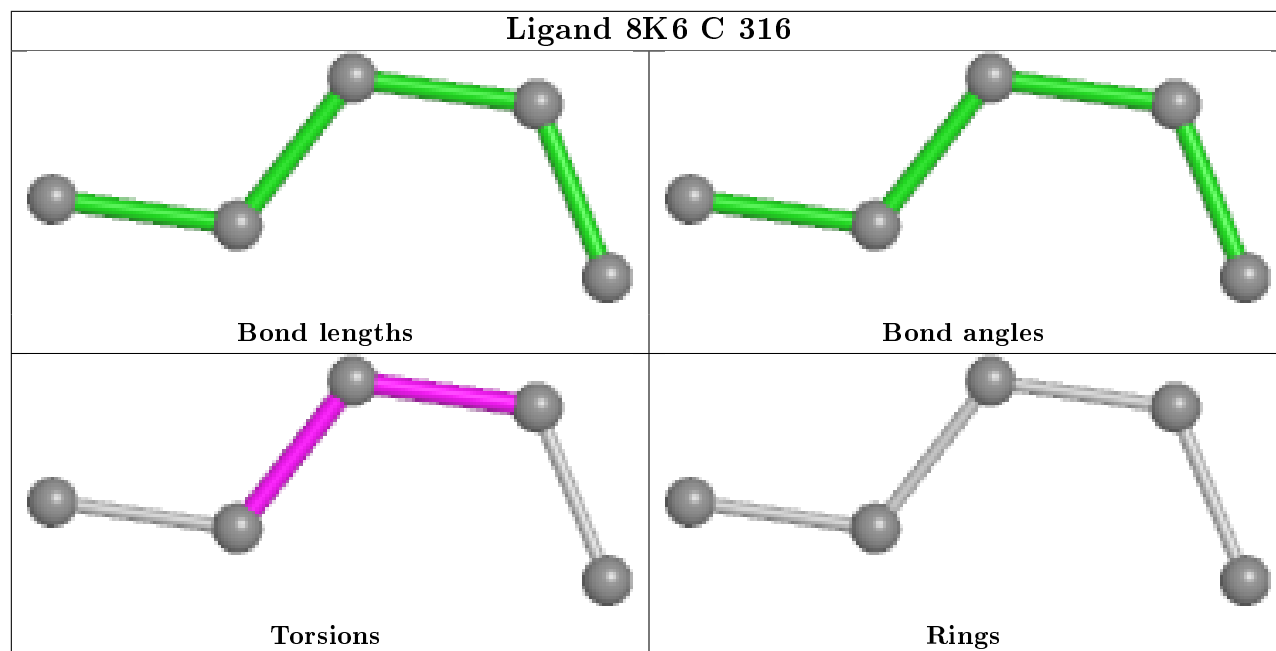


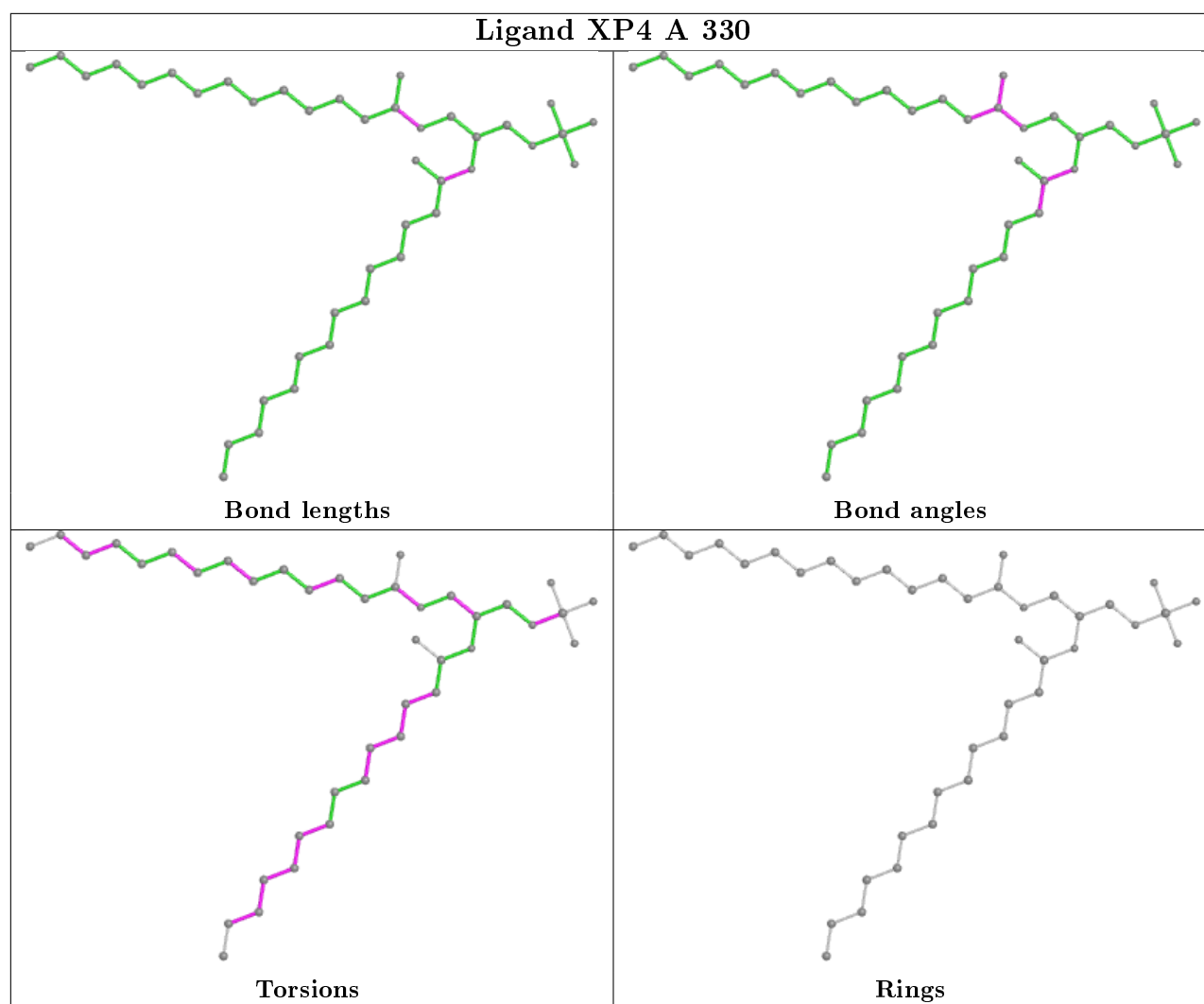












5.7 Other polymers [i](#)

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	337/370 (91%)	0.30	17 (5%) 28 39	13, 31, 58, 71	0
1	C	335/370 (90%)	0.25	10 (2%) 50 59	14, 32, 51, 65	0
All	All	672/740 (90%)	0.28	27 (4%) 38 48	13, 31, 55, 71	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	4.0
1	C	-5	ILE	3.8
1	C	-6	LEU	3.7
1	C	-29	TYR	3.6
1	A	-26[A]	TRP	3.6
1	A	-121	LEU	3.3
1	A	209	ILE	3.0
1	A	200	TRP	2.9
1	A	-66	SER	2.8
1	A	-9	LEU	2.7
1	A	12	PHE	2.7
1	C	-78	ARG	2.6
1	A	-123	LEU	2.6
1	A	-122	GLY	2.5
1	C	-77	ASP	2.5
1	A	207	ASP	2.5
1	A	-61	VAL	2.5
1	A	-50	VAL	2.4
1	C	-75	LEU	2.3
1	C	12	PHE	2.2
1	A	-7	SER	2.1
1	C	170	PHE	2.1
1	A	-48	ASP	2.1
1	C	62	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	-129	ILE	2.1
1	C	171	ILE	2.0
1	A	-130	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	TCE	A	307	16/16	0.59	0.24	49,53,64,74	0
8	GOL	A	329	6/6	0.65	0.16	48,57,60,62	0
6	OLC	C	307	9/25	0.82	0.12	42,50,62,64	0
7	8K6	A	318	5/18	0.82	0.22	29,31,34,37	0
8	GOL	A	327	6/6	0.83	0.12	39,43,48,55	0
2	FLC	A	301	13/13	0.83	0.22	33,45,55,57	0
6	OLC	A	309	17/25	0.84	0.18	21,42,56,60	0
7	8K6	A	331	7/18	0.84	0.15	27,32,36,36	0
6	OLC	C	306	25/25	0.84	0.18	28,40,52,55	0
7	8K6	A	321	7/18	0.85	0.17	32,38,43,47	0
6	OLC	A	308	10/25	0.85	0.15	28,37,51,52	0
8	GOL	C	317	6/6	0.85	0.22	31,39,43,51	0
7	8K6	A	316	5/18	0.86	0.19	24,25,33,39	0
3	NA	C	302	1/1	0.87	0.13	43,43,43,43	0
7	8K6	A	326	12/18	0.87	0.15	22,31,39,44	0
4	PO4	A	306[A]	5/5	0.87	0.21	28,30,31,32	5
6	OLC	C	305	16/25	0.87	0.15	37,43,49,50	0
6	OLC	A	311	19/25	0.87	0.17	26,38,50,52	0
7	8K6	A	315	5/18	0.87	0.26	33,37,40,45	0
6	OLC	C	308	25/25	0.87	0.14	15,33,46,51	0

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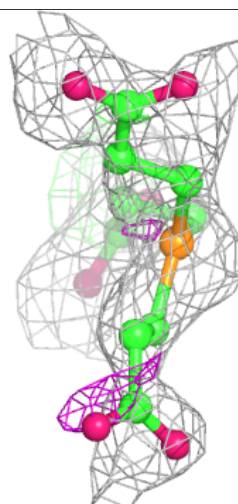
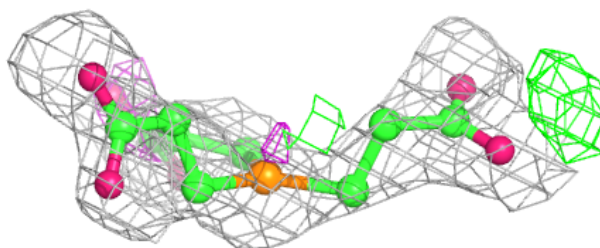
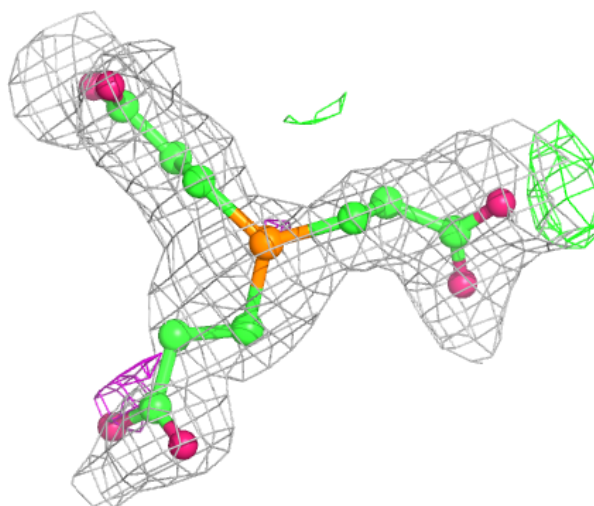
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FLC	C	301	13/13	0.88	0.21	38,46,57,58	0
6	OLC	A	310	18/25	0.88	0.24	36,41,51,54	0
3	NA	A	305	1/1	0.88	0.13	38,38,38,38	0
7	8K6	A	319	5/18	0.88	0.13	31,34,38,41	0
3	NA	C	303	1/1	0.88	0.10	33,33,33,33	0
7	8K6	A	313	10/18	0.89	0.17	20,32,38,43	0
7	8K6	A	320	8/18	0.89	0.15	26,30,41,42	0
7	8K6	A	325	8/18	0.90	0.18	27,32,37,42	0
7	8K6	C	312	7/18	0.90	0.12	29,32,35,43	0
3	NA	A	302	1/1	0.90	0.27	41,41,41,41	0
7	8K6	C	310	8/18	0.90	0.12	30,34,39,43	0
8	GOL	C	318	6/6	0.90	0.16	49,50,52,53	0
7	8K6	A	323	14/18	0.90	0.16	17,28,40,41	0
7	8K6	C	309	9/18	0.90	0.12	22,27,35,37	0
7	8K6	C	311	8/18	0.91	0.10	33,36,43,44	0
7	8K6	C	313	8/18	0.91	0.12	21,31,39,41	0
9	XP4	A	330	40/40	0.91	0.15	20,40,66,78	0
7	8K6	A	317	5/18	0.91	0.12	24,29,37,39	0
7	8K6	A	322	7/18	0.91	0.12	18,22,28,35	0
7	8K6	C	315	8/18	0.92	0.12	26,31,39,42	0
8	GOL	A	332	6/6	0.92	0.33	43,46,56,57	0
8	GOL	A	328	6/6	0.92	0.18	22,33,43,45	0
7	8K6	A	314	7/18	0.94	0.20	29,35,38,39	0
7	8K6	C	314	7/18	0.94	0.13	18,22,27,30	0
7	8K6	A	312	17/18	0.95	0.10	16,28,39,42	0
3	NA	C	304	1/1	0.95	0.13	37,37,37,37	0
7	8K6	A	324	9/18	0.95	0.10	23,30,35,35	0
7	8K6	C	316	5/18	0.95	0.11	17,20,21,26	0
3	NA	A	303	1/1	0.99	0.07	21,21,21,21	0
3	NA	A	304	1/1	0.99	0.04	24,24,24,24	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.

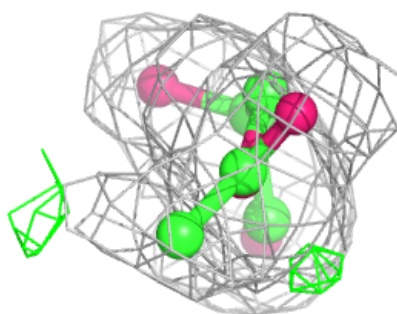
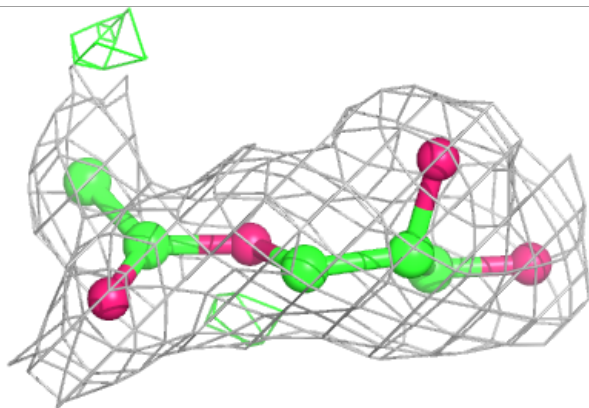
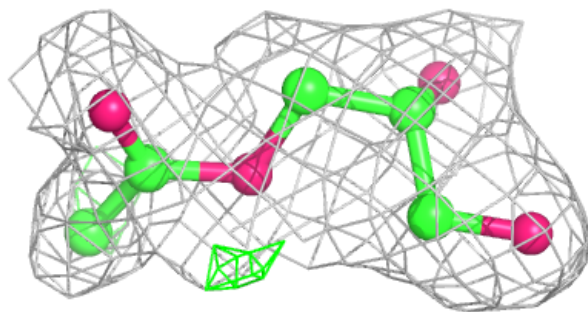
Electron density around TCE A 307:

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



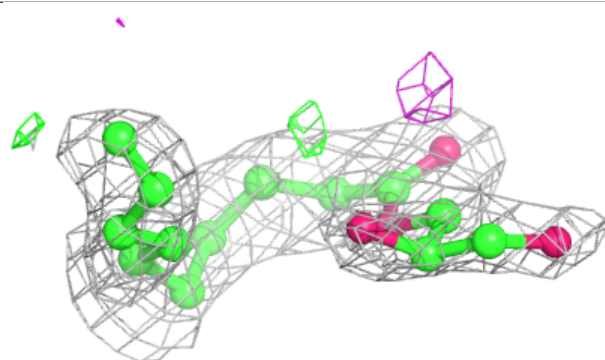
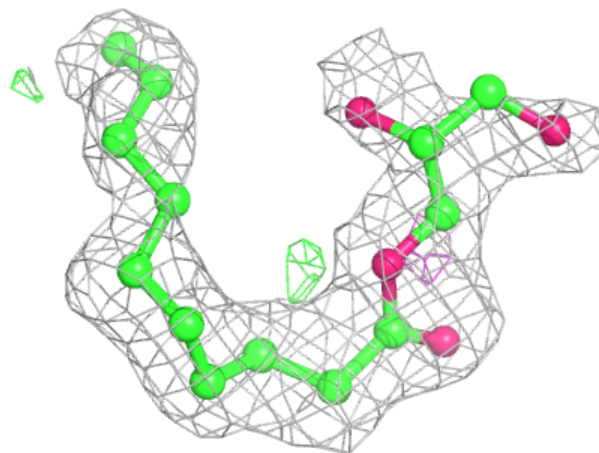
Electron density around OLC C 307:

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



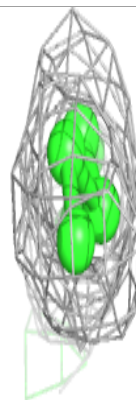
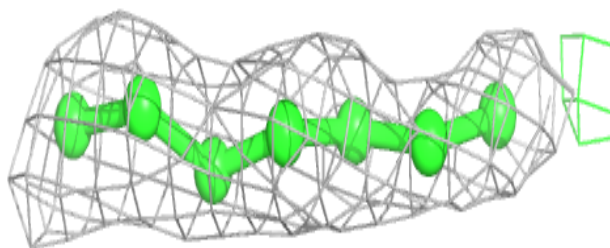
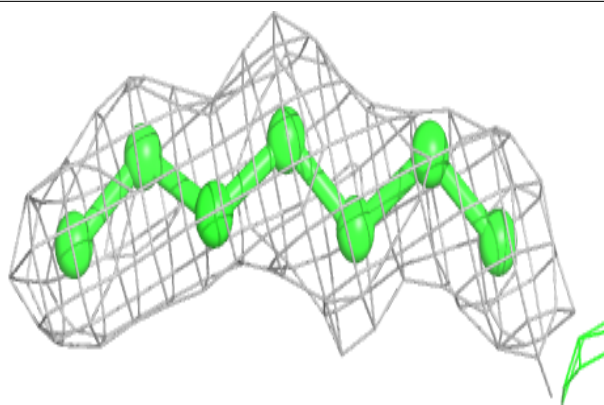
Electron density around OLC A 309:

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

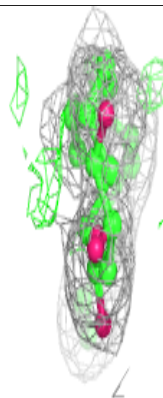
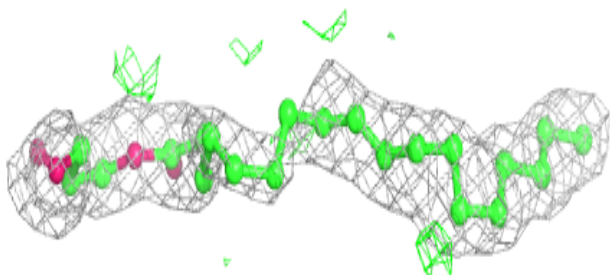
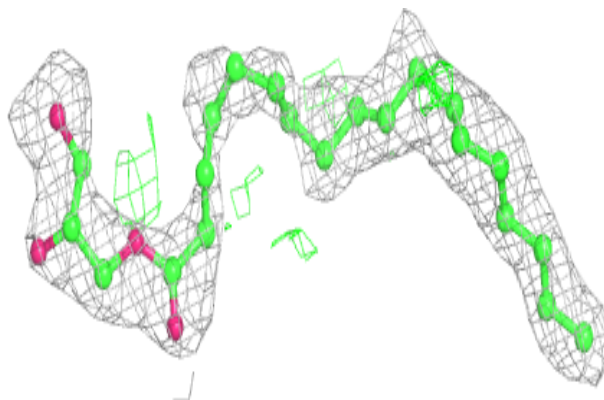


Electron density around 8K6 A 331:

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

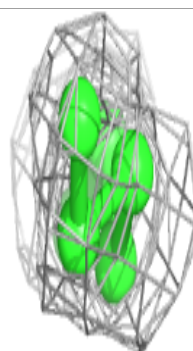
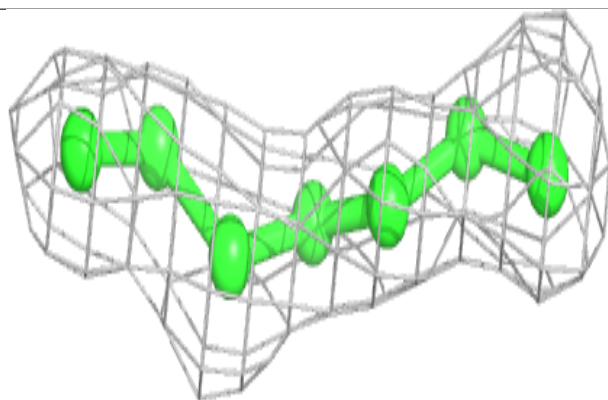
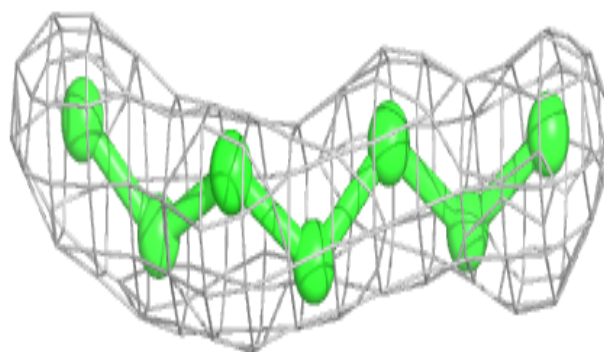
**Electron density around OLC C 306:**

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

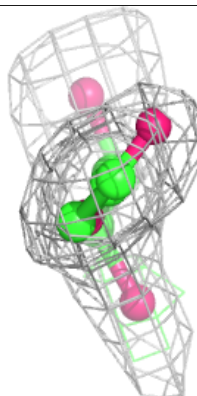
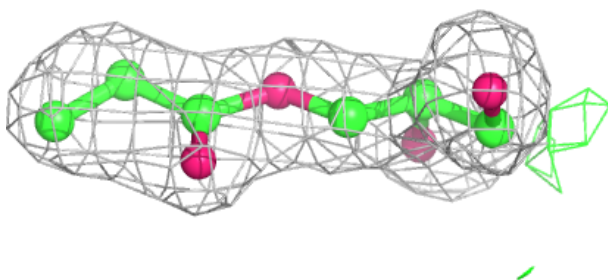
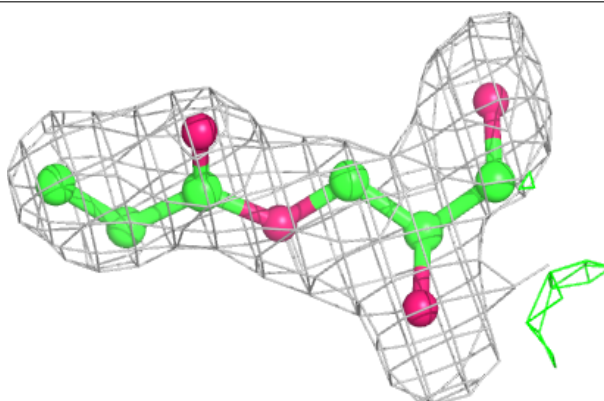


Electron density around 8K6 A 321:

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

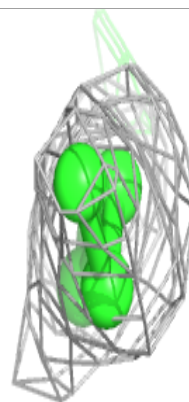
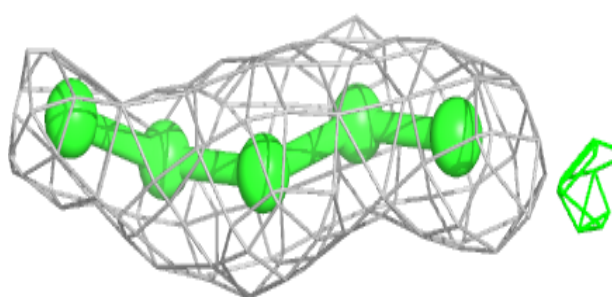
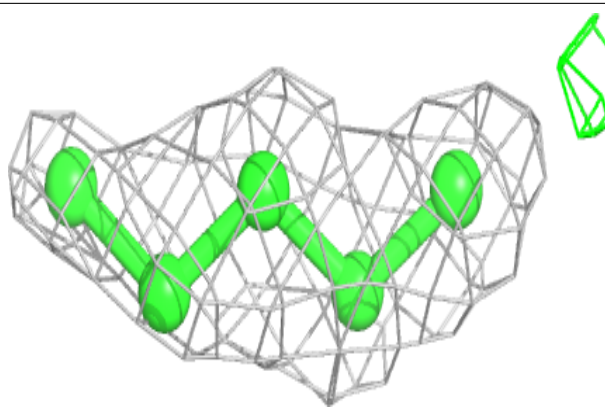
**Electron density around OLC A 308:**

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



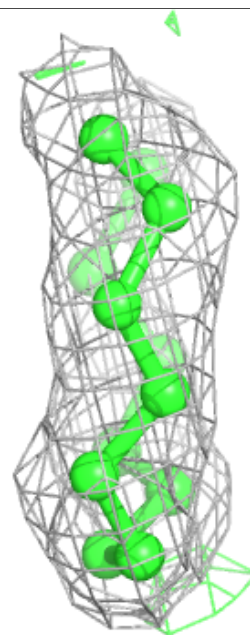
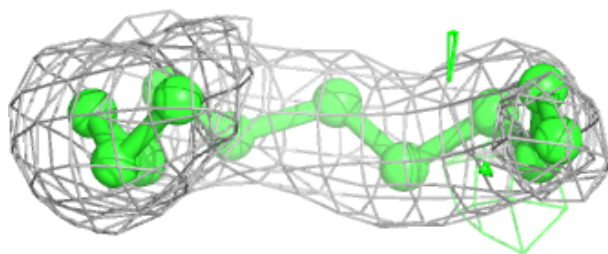
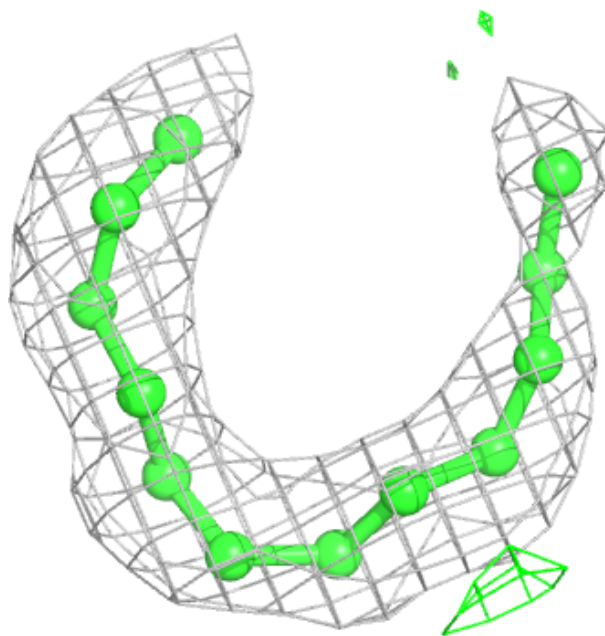
Electron density around 8K6 A 316:

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



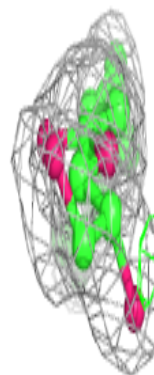
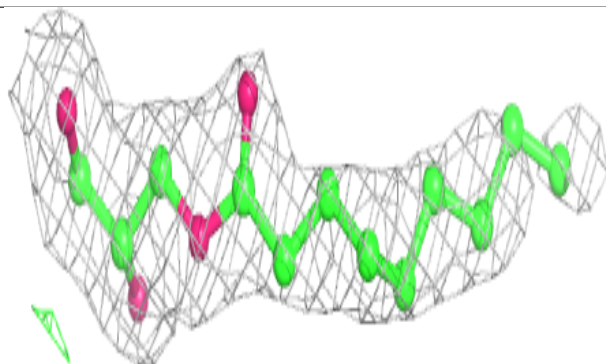
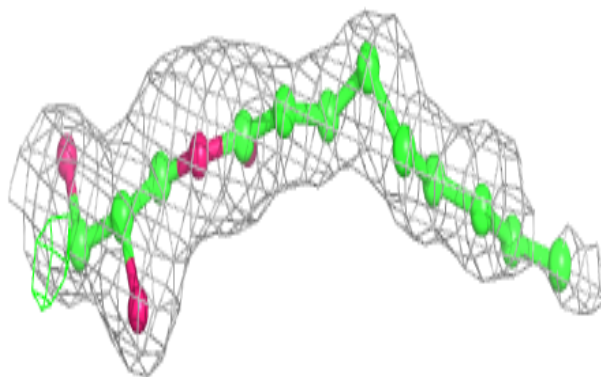
Electron density around 8K6 A 326:

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

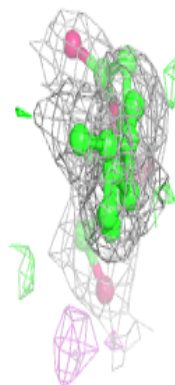
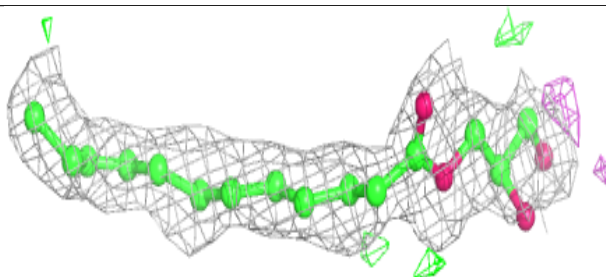
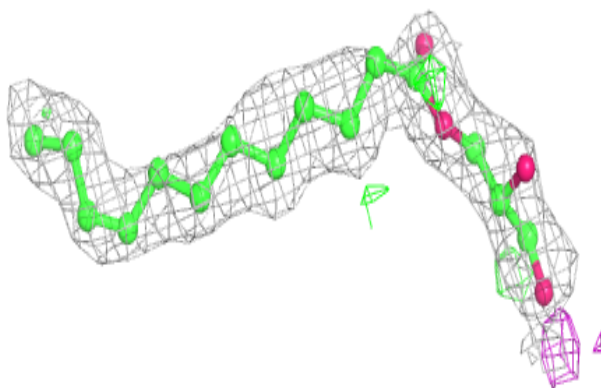


Electron density around OLC C 305:

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

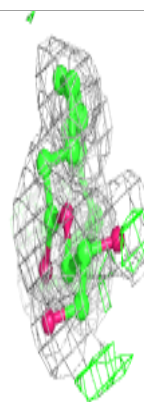
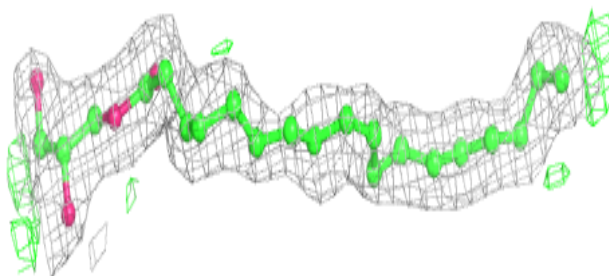
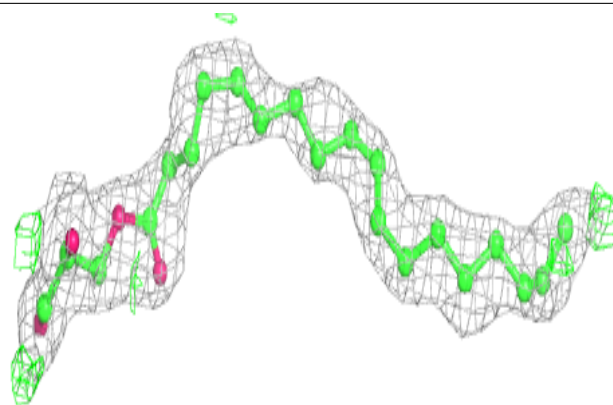
**Electron density around OLC A 311:**

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

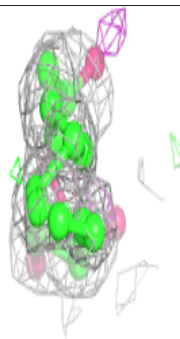
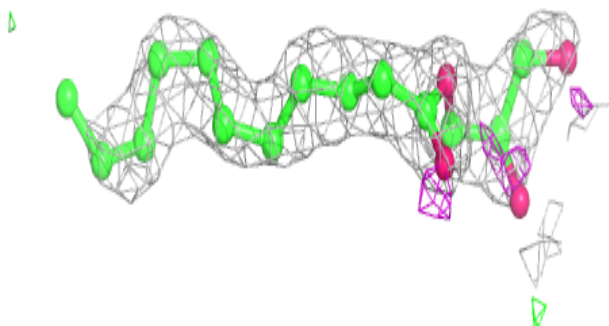
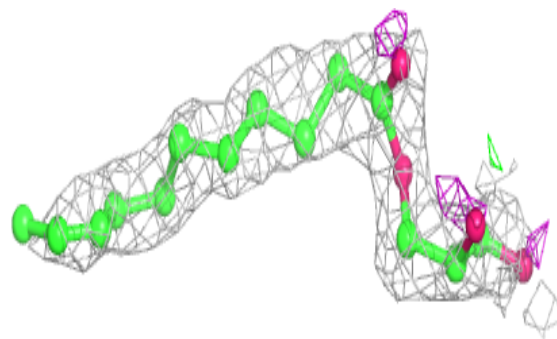


Electron density around OLC C 308:

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

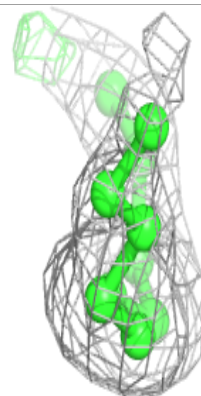
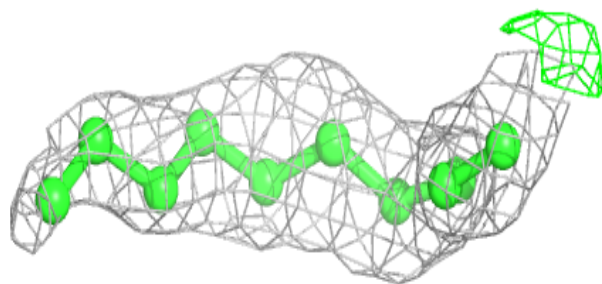
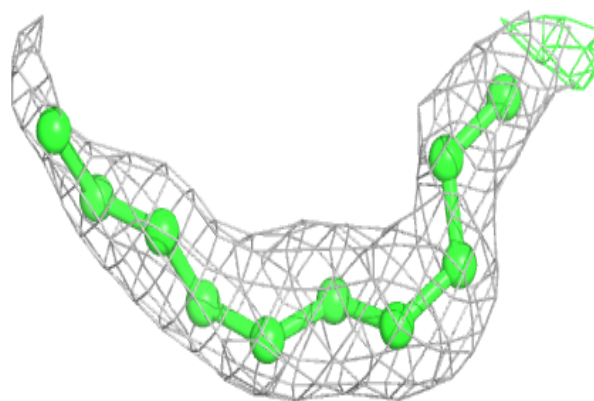
**Electron density around OLC A 310:**

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

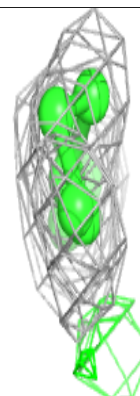
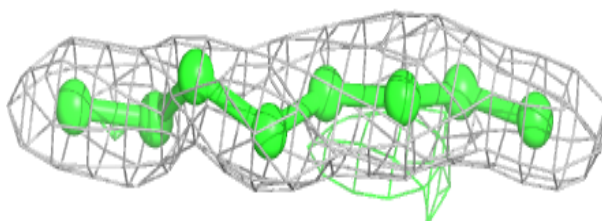
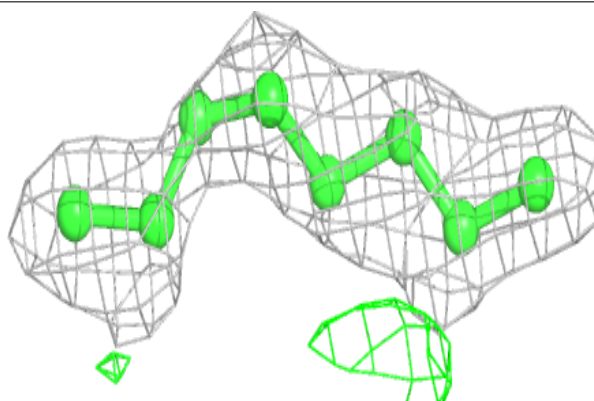


Electron density around 8K6 A 313:

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

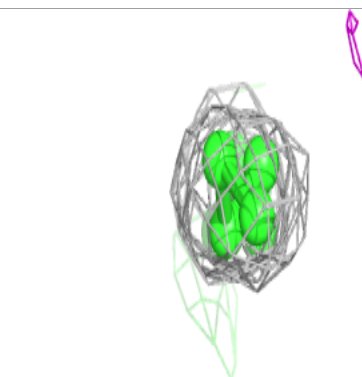
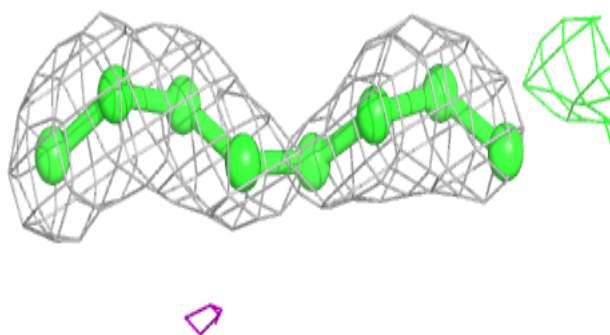
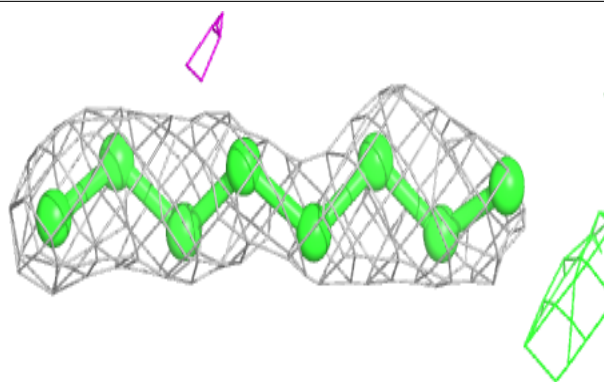
**Electron density around 8K6 A 320:**

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

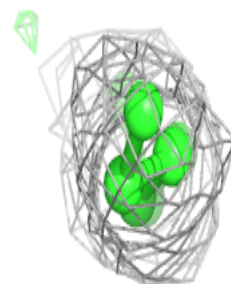
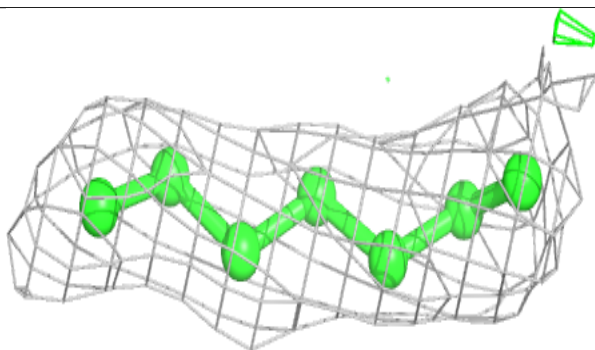
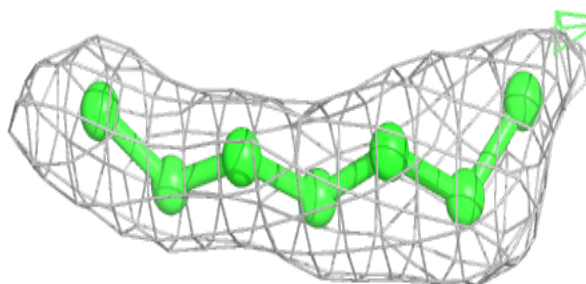


Electron density around 8K6 A 325:

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

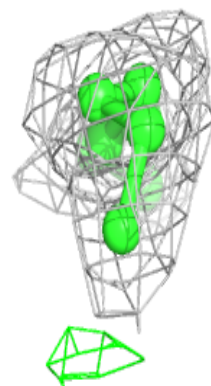
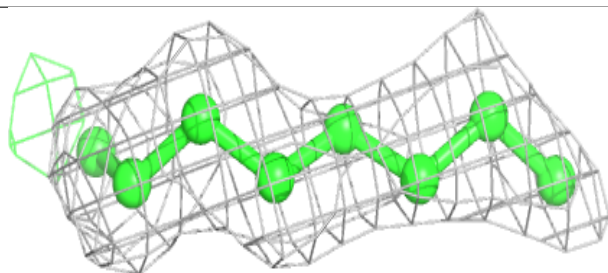
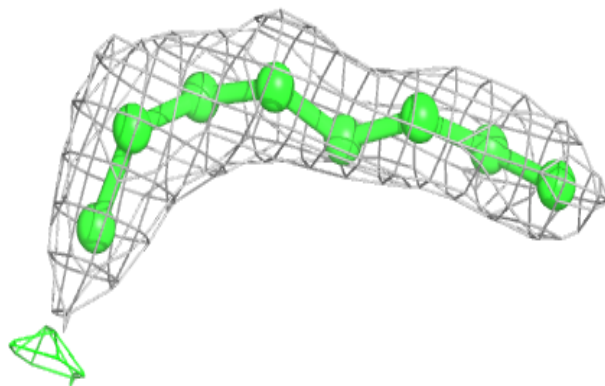
**Electron density around 8K6 C 312:**

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

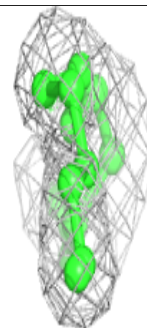
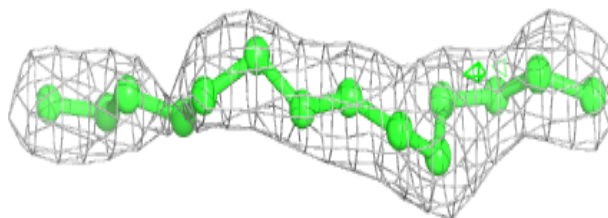
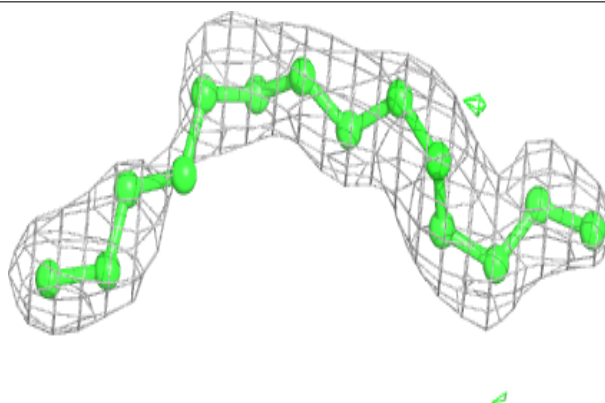


Electron density around 8K6 C 310:

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

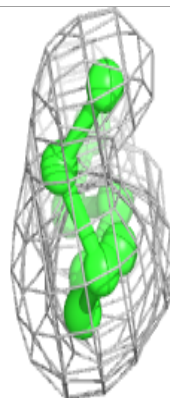
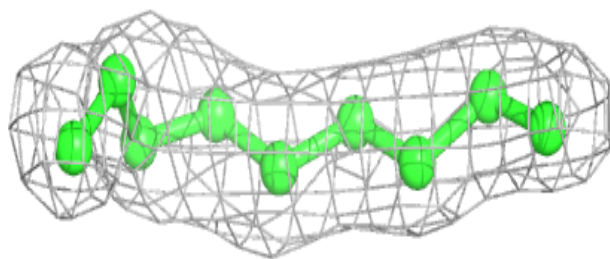
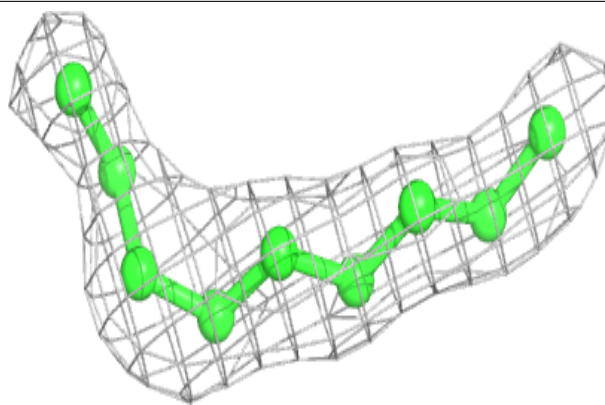
**Electron density around 8K6 A 323:**

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

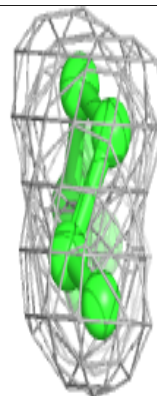
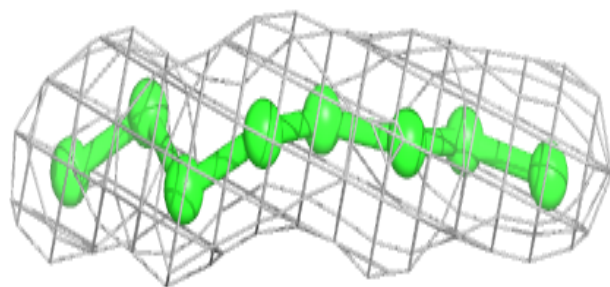
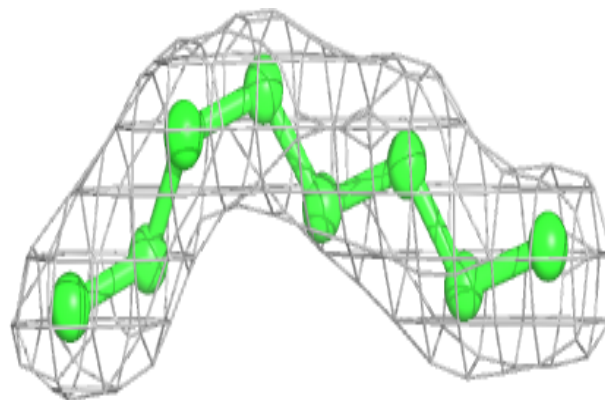


Electron density around 8K6 C 309:

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

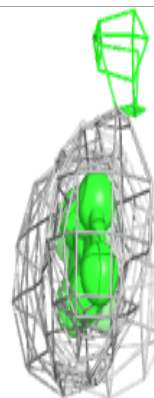
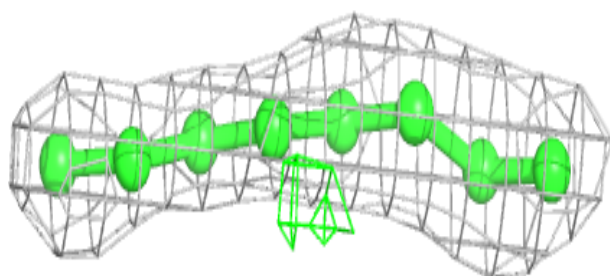
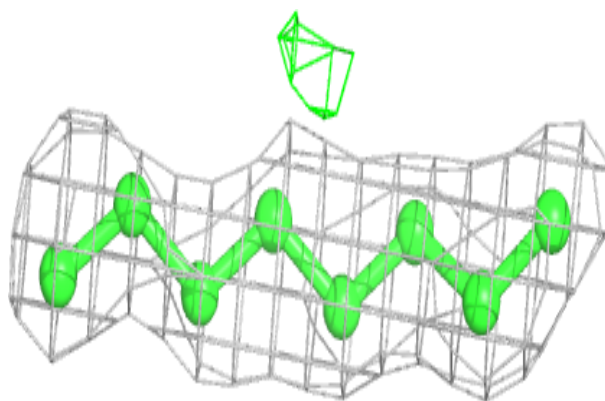
**Electron density around 8K6 C 311:**

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

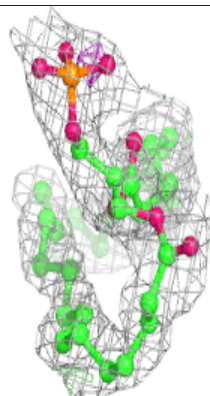
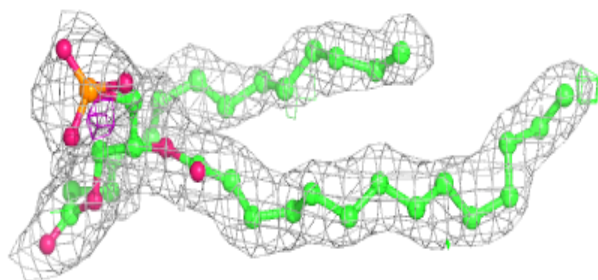
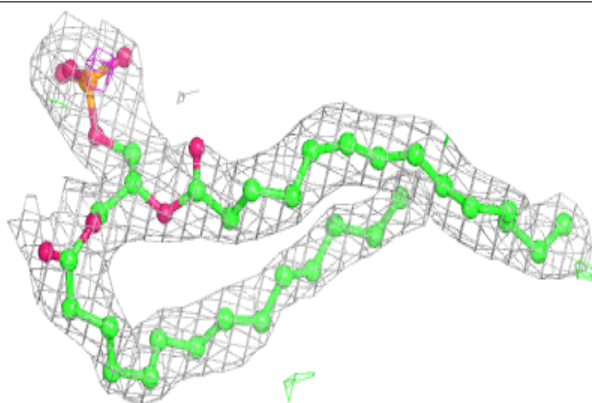


Electron density around 8K6 C 313:

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

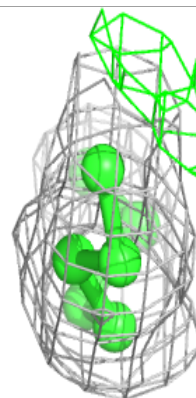
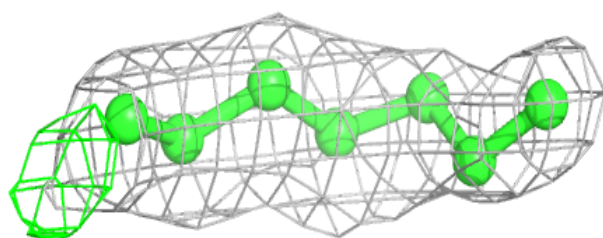
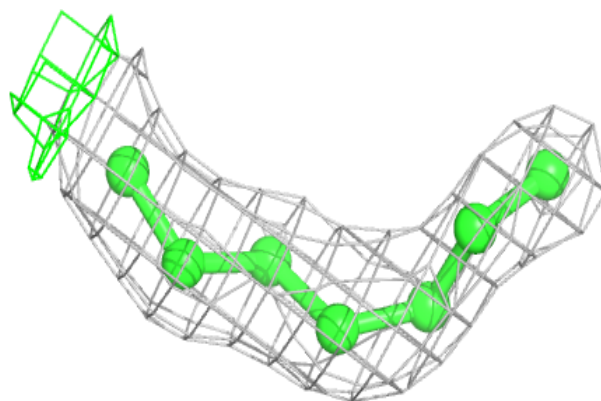
**Electron density around XP4 A 330:**

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

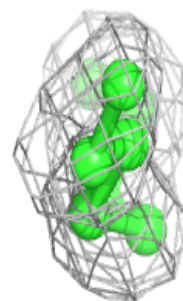
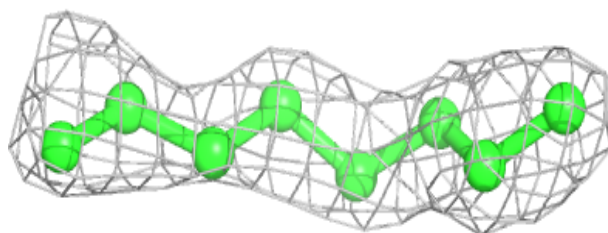
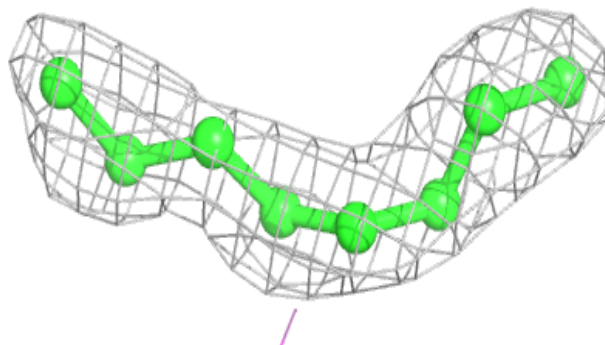


Electron density around 8K6 A 322:

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

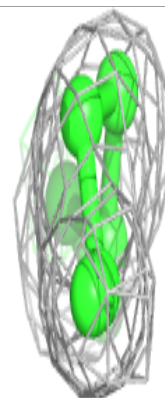
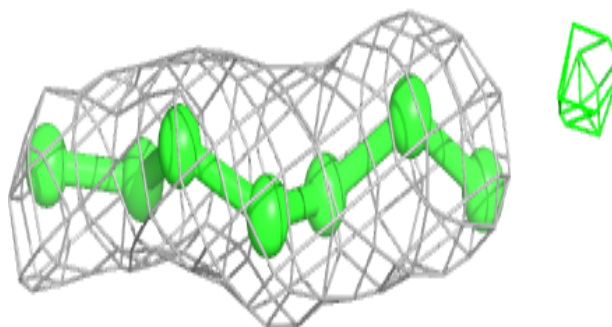
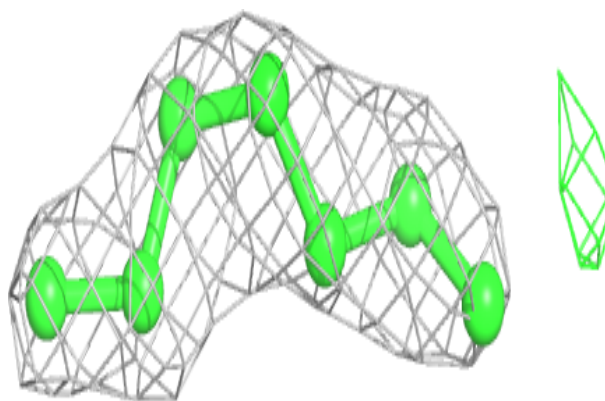
**Electron density around 8K6 C 315:**

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

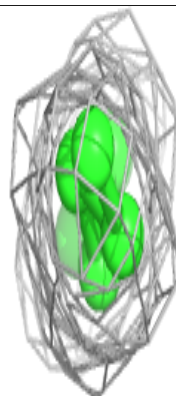
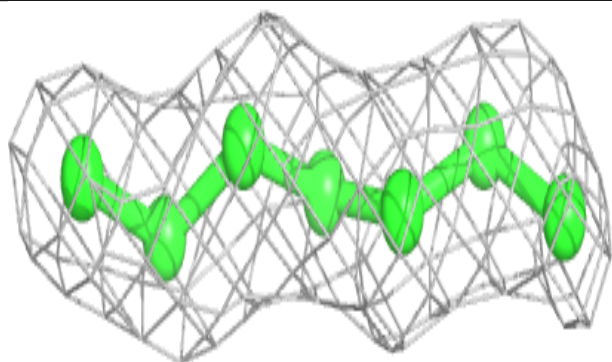
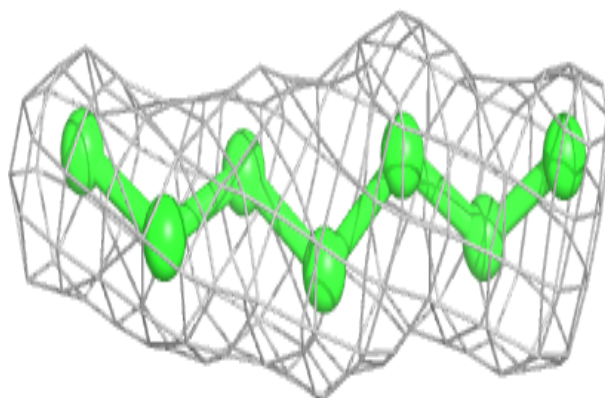


Electron density around 8K6 A 314:

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

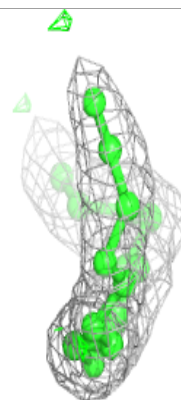
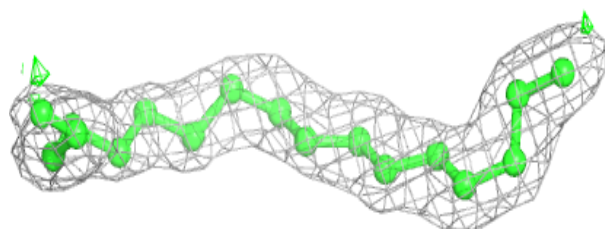
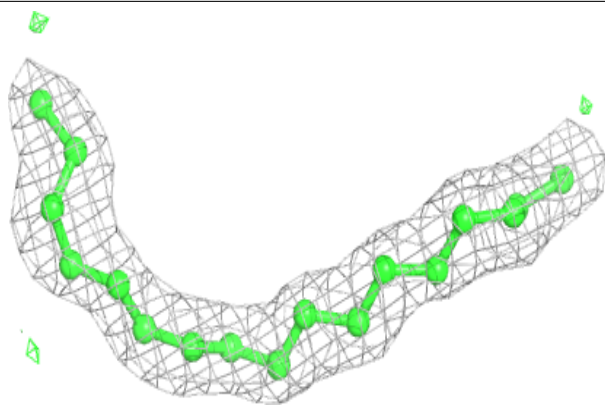
**Electron density around 8K6 C 314:**

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

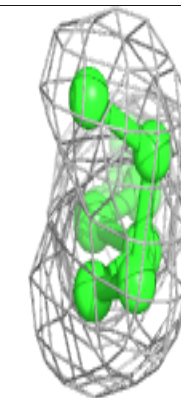
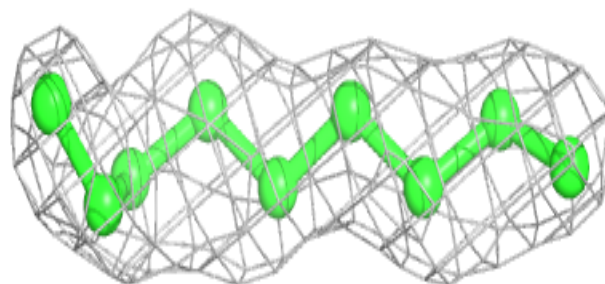
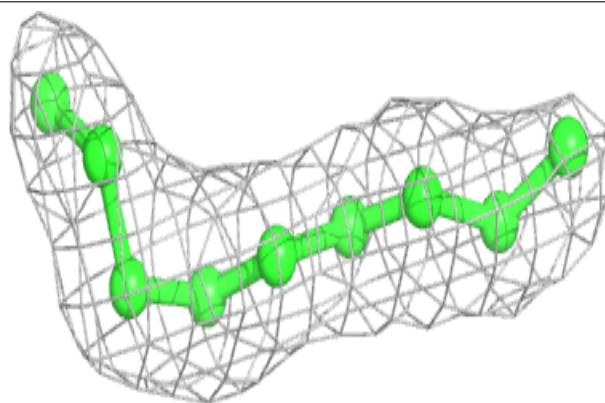


Electron density around 8K6 A 312:

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

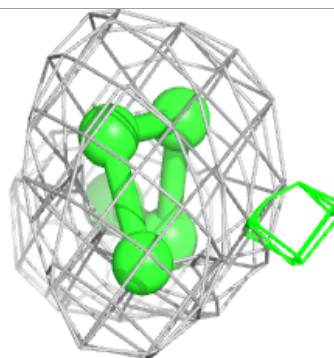
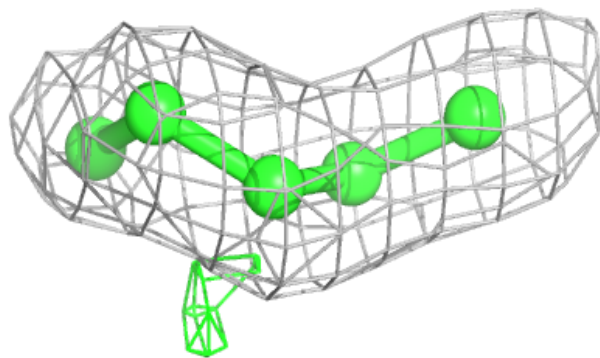
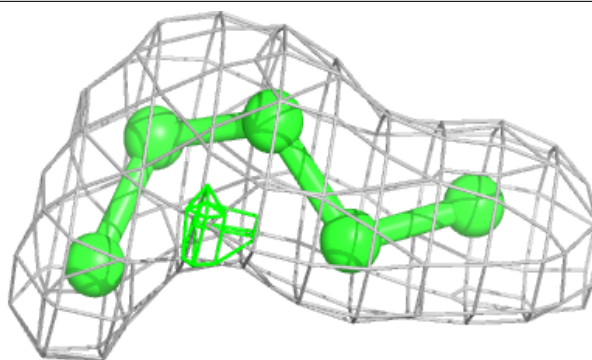
**Electron density around 8K6 A 324:**

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



Electron density around 8K6 C 316:

$2mF_o-DF_c$ (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.