



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2022 – 01:15 pm BST

PDB ID : 7Q3T  
Title : Crystal structure of the OmpK36 D insertion chimera from Klebsiella pneumonia  
Authors : Kwong, H.; Beis, K.  
Deposited on : 2021-10-28  
Resolution : 1.79 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](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

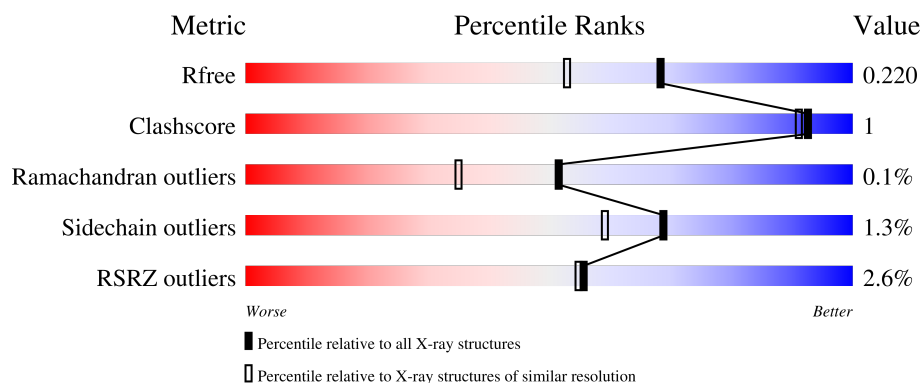
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	346	<div> <div>2%</div> <div>96%</div> <div>5%</div> <div>..</div> </div>
1	B	346	<div> <div>3%</div> <div>96%</div> <div>5%</div> <div>.</div> </div>
1	C	346	<div> <div>3%</div> <div>95%</div> <div>5%</div> <div></div> </div>
1	D	346	<div> <div>3%</div> <div>97%</div> <div>5%</div> <div>.</div> </div>
1	E	346	<div> <div>3%</div> <div>95%</div> <div>5%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	F	346	<div><div></div><div>2%</div><div>96%</div><div>.</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17772 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.

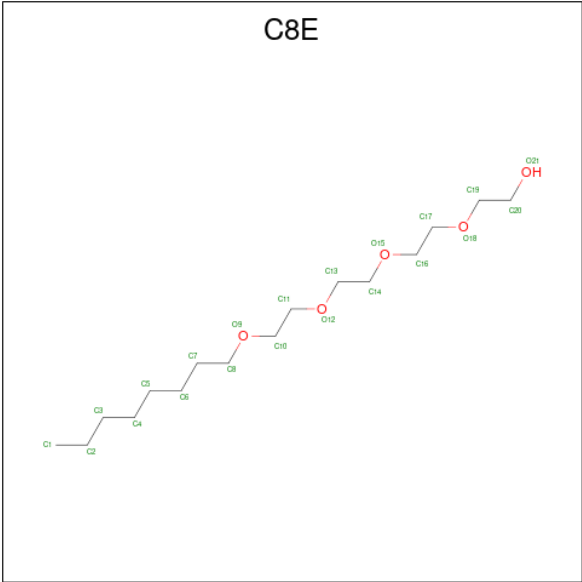
- Molecule 1 is a protein called OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	B	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	C	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	D	346	Total	C	N	O	S	0	1	0
			2711	1700	453	556	2			
1	E	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	F	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP D6QLY0
A	114	ASP	-	insertion	UNP D6QLY0
B	0	GLY	-	expression tag	UNP D6QLY0
B	114	ASP	-	insertion	UNP D6QLY0
C	0	GLY	-	expression tag	UNP D6QLY0
C	114	ASP	-	insertion	UNP D6QLY0
D	0	GLY	-	expression tag	UNP D6QLY0
D	114	ASP	-	insertion	UNP D6QLY0
E	0	GLY	-	expression tag	UNP D6QLY0
E	114	ASP	-	insertion	UNP D6QLY0
F	0	GLY	-	expression tag	UNP D6QLY0
F	114	ASP	-	insertion	UNP D6QLY0

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			11	10	1		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			17	14	3		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C		0	0
			8	8			
2	A	1	Total	C	O	0	0
			10	7	3		
2	A	1	Total	C		0	0
			6	6			
2	A	1	Total	C	O	0	0
			10	8	2		
2	A	1	Total	C	O	0	0
			15	12	3		
2	B	1	Total	C	O	0	0
			21	16	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 9 1	0	0
2	B	1	Total C O 14 12 2	0	0
2	B	1	Total C O 9 8 1	0	0
2	B	1	Total C O 16 11 5	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C O 10 9 1	0	0
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 7 4 3	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C O 15 12 3	0	0
2	C	1	Total C O 13 11 2	0	0
2	C	1	Total C O 13 11 2	0	0
2	C	1	Total C O 21 16 5	0	0
2	D	1	Total C O 11 7 4	0	0
2	D	1	Total C O 9 8 1	0	0
2	D	1	Total C O 21 16 5	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 15 12 3	0	0
2	D	1	Total C O 15 10 5	0	0
2	E	1	Total C O 20 15 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 15 12 3	0	0
2	E	1	Total C O 14 11 3	0	0
2	E	1	Total C O 19 15 4	0	0
2	F	1	Total C O 9 6 3	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C O 10 9 1	0	0
2	F	1	Total C O 9 8 1	0	0
2	F	1	Total C O 10 9 1	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C O 11 10 1	0	0
2	F	1	Total C O 13 11 2	0	0
2	F	1	Total C O 17 14 3	0	0

- Molecule 3 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Li 2 2	0	0
3	B	2	Total Li 2 2	0	0
3	C	2	Total Li 2 2	0	0
3	D	2	Total Li 2 2	0	0
3	E	2	Total Li 2 2	0	0
3	F	2	Total Li 2 2	0	0

- Molecule 4 is water.

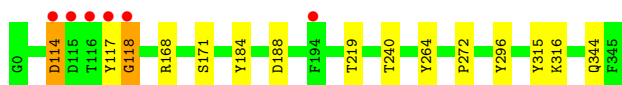
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total 177	O 177	0	0
4	B	148	Total 148	O 148	0	0
4	C	148	Total 148	O 148	0	0
4	D	162	Total 162	O 162	0	0
4	E	153	Total 153	O 153	0	0
4	F	153	Total 153	O 153	0	0



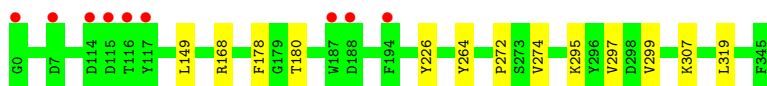
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: OmpK36



- Molecule 1: OmpK36



- Molecule 1: OmpK36



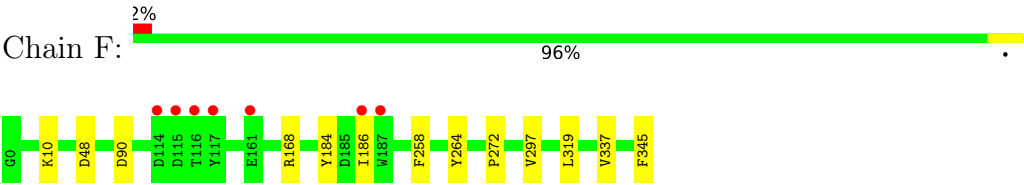
- Molecule 1: OmpK36



- Molecule 1: OmpK36



- Molecule 1: OmpK36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.02Å 73.61Å 158.66Å 91.04° 97.26° 103.16°	Depositor
Resolution (Å)	78.60 – 1.79 78.60 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.4 (78.60-1.79) 97.3 (78.60-1.79)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.78Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, $R_{free}$	0.185 , 0.213 0.190 , 0.220	Depositor DCC
$R_{free}$ test set	11110 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LI, C8E

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	0.44	0/2763	0.64	0/3741
1	B	0.44	0/2763	0.64	0/3741
1	C	0.42	0/2763	0.62	0/3741
1	D	0.42	0/2775	0.63	0/3757
1	E	0.43	0/2763	0.62	0/3741
1	F	0.42	0/2763	0.62	0/3741
All	All	0.43	0/16590	0.63	0/22462

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	2703	0	2481	6	0
1	B	2703	0	2481	10	0
1	C	2703	0	2481	9	0
1	D	2711	0	2490	7	0
1	E	2703	0	2481	10	0
1	F	2703	0	2481	4	0
2	A	162	0	259	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	119	0	192	5	0
2	C	68	0	112	2	0
2	D	82	0	127	4	0
2	E	68	0	104	7	0
2	F	94	0	157	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	177	0	0	0	0
4	B	148	0	0	0	0
4	C	148	0	0	0	0
4	D	162	0	0	0	0
4	E	153	0	0	0	0
4	F	153	0	0	0	0
All	All	17772	0	15846	48	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 1.

All (48) 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:E:180:THR:HG23	2:E:401:C8E:H52	1.73	0.71
1:E:194:PHE:HB3	2:E:401:C8E:H71	1.74	0.68
1:A:117:TYR:O	1:A:118:GLY:O	2.13	0.67
1:E:151:TYR:HD2	2:E:406:C8E:H141	1.65	0.60
1:B:178:PHE:CZ	1:B:180:THR:HG23	2.38	0.59
1:F:258:PHE:HE1	2:F:408:C8E:H32	1.69	0.56
1:D:200:LYS:HE3	2:D:508:C8E:H131	1.88	0.55
1:C:194:PHE:HB3	2:C:407:C8E:H101	1.89	0.55
1:D:149:LEU:HD23	1:D:180:THR:HG22	1.89	0.54
1:E:4:TYR:HB3	1:E:11:LEU:HB2	1.89	0.54
1:A:114:ASP:HB3	1:A:118:GLY:HA2	1.90	0.54
2:A:505:C8E:H111	2:A:506:C8E:H131	1.89	0.54
1:E:210:ALA:HB1	1:E:286:ARG:HD2	1.89	0.54
1:B:226:TYR:HB2	2:B:401:C8E:H22	1.92	0.52
1:B:149:LEU:HD23	1:B:180:THR:HG22	1.90	0.52
1:A:264:TYR:O	1:A:272:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:C8E:H132	2:E:401:C8E:H172	1.93	0.51
1:D:200:LYS:CE	2:D:508:C8E:H131	2.41	0.49
1:A:315:TYR:HB2	2:A:501:C8E:H172	1.94	0.49
1:B:297:VAL:HG11	2:B:410:C8E:H61	1.94	0.48
2:C:407:C8E:H112	1:E:184:TYR:CE1	2.49	0.48
1:A:296:TYR:CD1	1:A:316:LYS:HG3	2.49	0.47
1:C:142:VAL:HG21	2:E:401:C8E:H102	1.95	0.47
1:D:200:LYS:NZ	2:D:508:C8E:H131	2.29	0.47
1:F:337:VAL:HG21	2:F:406:C8E:H72	1.96	0.46
1:A:219:THR:HG22	1:A:240:THR:HG22	1.97	0.46
1:F:264:TYR:O	1:F:272:PRO:HD2	2.15	0.45
1:F:297:VAL:HG23	1:F:319:LEU:HD11	1.99	0.45
1:E:220:TYR:HB3	2:E:401:C8E:H101	1.99	0.45
1:E:298:ASP:OD2	1:E:314:ASP:OD1	2.35	0.45
1:E:264:TYR:O	1:E:272:PRO:HD2	2.17	0.45
1:B:274:VAL:HG13	2:B:403:C8E:H42	1.99	0.44
1:C:264:TYR:O	1:C:272:PRO:HD2	2.17	0.44
1:C:145:LEU:HD13	1:C:184:TYR:HB3	2.00	0.44
1:D:297:VAL:HG11	2:D:506:C8E:H41	1.99	0.44
1:C:22:TYR:HD2	1:C:29:VAL:HG13	1.83	0.44
1:E:239:GLN:HB2	2:E:401:C8E:H171	2.00	0.44
1:C:226:TYR:HB3	1:C:233:LEU:HB2	1.98	0.43
1:B:178:PHE:CZ	1:B:180:THR:CG2	3.01	0.43
1:C:296:TYR:CD1	1:C:316:LYS:HG3	2.53	0.43
1:C:259:GLU:HG2	1:C:277:LEU:HG	2.00	0.42
1:D:0:GLY:HA3	1:D:12:ASP:OD2	2.19	0.42
1:B:299:VAL:HG21	2:B:410:C8E:H52	2.01	0.42
1:C:4:TYR:HB3	1:C:11:LEU:HB2	2.02	0.42
1:B:272:PRO:HB3	2:B:411:C8E:H31	2.02	0.42
1:B:264:TYR:O	1:B:272:PRO:HD2	2.19	0.41
1:B:295:LYS:HG2	1:B:319:LEU:HB2	2.03	0.41
1:D:190:ILE:HG12	1:D:226:TYR:HD1	1.84	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	344/346 (99%)	325 (94%)	17 (5%)	2 (1%)	25	11
1	B	344/346 (99%)	327 (95%)	17 (5%)	0	100	100
1	C	344/346 (99%)	328 (95%)	16 (5%)	0	100	100
1	D	345/346 (100%)	326 (94%)	19 (6%)	0	100	100
1	E	344/346 (99%)	324 (94%)	20 (6%)	0	100	100
1	F	344/346 (99%)	326 (95%)	18 (5%)	0	100	100
All	All	2065/2076 (100%)	1956 (95%)	107 (5%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	114	ASP

### 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	277/277 (100%)	272 (98%)	5 (2%)	59	45
1	B	277/277 (100%)	275 (99%)	2 (1%)	84	79
1	C	277/277 (100%)	274 (99%)	3 (1%)	73	65
1	D	278/277 (100%)	275 (99%)	3 (1%)	73	65
1	E	277/277 (100%)	275 (99%)	2 (1%)	84	79
1	F	277/277 (100%)	270 (98%)	7 (2%)	47	31
All	All	1663/1662 (100%)	1641 (99%)	22 (1%)	69	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ARG
1	A	171	SER
1	A	184	TYR
1	A	188	ASP
1	A	344	GLN
1	B	168	ARG
1	B	307	LYS
1	C	143	ASP
1	C	168	ARG
1	C	239	GLN
1	D	168	ARG
1	D	188	ASP
1	D	267	ASP
1	E	168	ARG
1	E	307	LYS
1	F	10	LYS
1	F	48	ASP
1	F	90	ASP
1	F	168	ARG
1	F	184	TYR
1	F	186	ILE
1	F	345	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 59 ligands modelled in this entry, 12 are monoatomic - leaving 47 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	$\# Z  > 2$
2	C8E	D	502	-	8,8,20	0.23	0	7,7,19	0.53	0
2	C8E	A	508	-	8,8,20	0.23	0	7,7,19	0.56	0
2	C8E	A	510	-	12,12,20	0.39	0	11,11,19	0.46	0
2	C8E	B	404	-	8,8,20	0.26	0	7,7,19	0.56	0
2	C8E	F	406	-	8,8,20	0.25	0	7,7,19	0.49	0
2	C8E	D	505	-	20,20,20	0.43	0	19,19,19	0.60	0
2	C8E	B	412	-	6,6,20	0.45	0	5,5,19	0.27	0
2	C8E	B	411	-	11,11,20	0.31	0	10,10,19	0.49	0
2	C8E	A	512	-	9,9,20	0.47	0	8,8,19	0.23	0
2	C8E	A	513	-	5,5,20	0.21	0	4,4,19	0.47	0
2	C8E	D	508	-	14,14,20	0.45	0	13,13,19	0.50	0
2	C8E	A	502	-	10,10,20	0.37	0	9,9,19	0.61	0
2	C8E	B	402	-	9,9,20	0.39	0	8,8,19	0.46	0
2	C8E	F	404	-	6,6,20	0.28	0	5,5,19	0.36	0
2	C8E	F	411	-	16,16,20	0.45	0	15,15,19	0.35	0
2	C8E	B	405	-	15,15,20	0.47	0	14,14,19	0.24	0
2	C8E	A	506	-	11,11,20	0.43	0	10,10,19	0.37	0
2	C8E	F	407	-	9,9,20	0.34	0	8,8,19	0.41	0
2	C8E	B	401	-	20,20,20	0.38	0	19,19,19	0.47	0
2	C8E	A	514	-	9,9,20	0.48	0	8,8,19	0.22	0
2	C8E	F	405	-	9,9,20	0.37	0	8,8,19	0.55	0
2	C8E	E	403	-	12,12,20	0.27	0	10,10,19	0.54	0
2	C8E	B	408	-	7,7,20	0.25	0	6,6,19	0.52	0
2	C8E	B	410	-	11,11,20	0.35	0	10,10,19	0.51	0
2	C8E	A	515	-	14,14,20	0.35	0	13,13,19	0.46	0
2	C8E	C	406	-	12,12,20	0.44	0	11,11,19	0.41	0
2	C8E	D	501	-	10,10,20	0.44	0	9,9,19	0.29	0
2	C8E	E	401	-	19,19,20	0.49	0	18,18,19	0.59	0
2	C8E	E	402	-	14,14,20	0.38	0	13,13,19	0.43	0
2	C8E	F	403	-	8,8,20	0.46	0	7,7,19	0.28	0
2	C8E	D	506	-	10,10,20	0.35	0	9,9,19	0.53	0
2	C8E	D	507	-	14,14,20	0.34	0	13,13,19	0.59	0
2	C8E	C	404	-	14,14,20	0.38	0	13,13,19	0.44	0
2	C8E	B	409	-	9,9,20	0.29	0	8,8,19	0.51	0
2	C8E	B	403	-	13,13,20	0.36	0	12,12,19	0.46	0
2	C8E	F	409	-	10,10,20	0.37	0	9,9,19	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C8E	A	505	-	20,20,20	0.41	0	19,19,19	0.41	0
2	C8E	A	501	-	20,20,20	0.53	0	19,19,19	0.43	0
2	C8E	A	509	-	8,8,20	0.23	0	7,7,19	0.57	0
2	C8E	C	407	-	20,20,20	0.37	0	19,19,19	0.43	0
2	C8E	A	511	-	7,7,20	0.26	0	6,6,19	0.43	0
2	C8E	C	405	-	12,12,20	0.35	0	11,11,19	0.48	0
2	C8E	F	410	-	12,12,20	0.38	0	11,11,19	0.41	0
2	C8E	A	507	-	16,16,20	0.48	0	15,15,19	0.41	0
2	C8E	C	403	-	5,5,20	0.26	0	4,4,19	0.38	0
2	C8E	F	408	-	7,7,20	0.22	0	6,6,19	0.67	0
2	C8E	E	406	-	18,18,20	0.38	0	17,17,19	0.43	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
2	C8E	D	502	-	-	2/6/6/18	-
2	C8E	A	508	-	-	1/6/6/18	-
2	C8E	A	510	-	-	5/10/10/18	-
2	C8E	B	404	-	-	1/6/6/18	-
2	C8E	F	406	-	-	2/6/6/18	-
2	C8E	D	505	-	-	7/18/18/18	-
2	C8E	B	412	-	-	2/4/4/18	-
2	C8E	B	411	-	-	1/9/9/18	-
2	C8E	A	512	-	-	1/7/7/18	-
2	C8E	A	513	-	-	0/3/3/18	-
2	C8E	D	508	-	-	5/12/12/18	-
2	C8E	A	502	-	-	2/8/8/18	-
2	C8E	B	402	-	-	2/7/7/18	-
2	C8E	F	404	-	-	1/4/4/18	-
2	C8E	F	411	-	-	6/14/14/18	-
2	C8E	B	405	-	-	1/13/13/18	-
2	C8E	A	506	-	-	6/9/9/18	-
2	C8E	F	407	-	-	3/7/7/18	-
2	C8E	B	401	-	-	5/18/18/18	-
2	C8E	A	514	-	-	0/7/7/18	-
2	C8E	F	405	-	-	3/7/7/18	-
2	C8E	E	403	-	-	1/8/8/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	B	408	-	-	4/5/5/18	-
2	C8E	B	410	-	-	2/9/9/18	-
2	C8E	A	515	-	-	5/12/12/18	-
2	C8E	C	406	-	-	5/10/10/18	-
2	C8E	D	501	-	-	3/8/8/18	-
2	C8E	E	401	-	-	7/17/17/18	-
2	C8E	E	402	-	-	5/12/12/18	-
2	C8E	F	403	-	-	3/6/6/18	-
2	C8E	D	506	-	-	0/8/8/18	-
2	C8E	D	507	-	-	4/12/12/18	-
2	C8E	C	404	-	-	7/12/12/18	-
2	C8E	B	409	-	-	2/7/7/18	-
2	C8E	B	403	-	-	3/11/11/18	-
2	C8E	F	409	-	-	2/8/8/18	-
2	C8E	A	505	-	-	5/18/18/18	-
2	C8E	A	501	-	-	11/18/18/18	-
2	C8E	A	509	-	-	3/6/6/18	-
2	C8E	C	407	-	-	6/18/18/18	-
2	C8E	A	511	-	-	0/5/5/18	-
2	C8E	C	405	-	-	3/10/10/18	-
2	C8E	F	410	-	-	1/10/10/18	-
2	C8E	A	507	-	-	3/14/14/18	-
2	C8E	C	403	-	-	1/3/3/18	-
2	C8E	F	408	-	-	3/5/5/18	-
2	C8E	E	406	-	-	6/16/16/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	505	C8E	O12-C13-C14-O15
2	D	501	C8E	O12-C13-C14-O15
2	F	410	C8E	O9-C10-C11-O12
2	C	407	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
2	E	402	C8E	O9-C10-C11-O12
2	C	407	C8E	O12-C13-C14-O15
2	C	404	C8E	O12-C13-C14-O15
2	A	506	C8E	O15-C16-C17-O18
2	A	515	C8E	C6-C7-C8-O9
2	A	502	C8E	C6-C7-C8-O9
2	A	501	C8E	C6-C7-C8-O9
2	E	402	C8E	C6-C7-C8-O9
2	B	412	C8E	O18-C19-C20-O21
2	A	510	C8E	C6-C7-C8-O9
2	B	409	C8E	C2-C3-C4-C5
2	B	403	C8E	C3-C4-C5-C6
2	F	411	C8E	C6-C7-C8-O9
2	B	408	C8E	C4-C5-C6-C7
2	F	411	C8E	C3-C4-C5-C6
2	A	501	C8E	O9-C10-C11-O12
2	B	403	C8E	C4-C5-C6-C7
2	B	410	C8E	C2-C3-C4-C5
2	C	405	C8E	C2-C3-C4-C5
2	F	411	C8E	C4-C5-C6-C7
2	E	406	C8E	C3-C4-C5-C6
2	A	505	C8E	O18-C19-C20-O21
2	A	506	C8E	O12-C13-C14-O15
2	A	515	C8E	C2-C3-C4-C5
2	D	505	C8E	C3-C4-C5-C6
2	B	409	C8E	C3-C4-C5-C6
2	F	407	C8E	C2-C3-C4-C5
2	C	404	C8E	C5-C6-C7-C8
2	C	406	C8E	C6-C7-C8-O9
2	C	405	C8E	C6-C7-C8-O9
2	C	407	C8E	C6-C7-C8-O9
2	E	403	C8E	C3-C4-C5-C6
2	D	508	C8E	O9-C10-C11-O12
2	A	510	C8E	C2-C3-C4-C5
2	F	405	C8E	C4-C5-C6-C7
2	C	407	C8E	O15-C16-C17-O18
2	C	404	C8E	C6-C7-C8-O9
2	D	505	C8E	O18-C19-C20-O21
2	F	403	C8E	O18-C19-C20-O21
2	A	501	C8E	C5-C6-C7-C8
2	A	507	C8E	C1-C2-C3-C4
2	F	405	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	C	406	C8E	C3-C4-C5-C6
2	B	401	C8E	C3-C4-C5-C6
2	A	508	C8E	C1-C2-C3-C4
2	B	408	C8E	C5-C6-C7-C8
2	E	406	C8E	C6-C7-C8-O9
2	E	402	C8E	C1-C2-C3-C4
2	B	412	C8E	O15-C16-C17-O18
2	A	510	C8E	C1-C2-C3-C4
2	D	505	C8E	O15-C16-C17-O18
2	A	507	C8E	C3-C4-C5-C6
2	A	509	C8E	C3-C4-C5-C6
2	C	403	C8E	C2-C3-C4-C5
2	A	510	C8E	O9-C10-C11-O12
2	F	407	C8E	C5-C6-C7-C8
2	C	404	C8E	C4-C5-C6-C7
2	C	406	C8E	C10-C11-O12-C13
2	F	406	C8E	C1-C2-C3-C4
2	A	501	C8E	C3-C4-C5-C6
2	A	502	C8E	C1-C2-C3-C4
2	F	408	C8E	C2-C3-C4-C5
2	F	408	C8E	C1-C2-C3-C4
2	B	410	C8E	C1-C2-C3-C4
2	C	404	C8E	C3-C4-C5-C6
2	B	402	C8E	C2-C3-C4-C5
2	F	409	C8E	C6-C7-C8-O9
2	B	401	C8E	C16-C17-O18-C19
2	E	401	C8E	C10-C11-O12-C13
2	E	401	C8E	O15-C16-C17-O18
2	B	405	C8E	C16-C17-O18-C19
2	A	506	C8E	C14-C13-O12-C11
2	D	508	C8E	C10-C11-O12-C13
2	F	411	C8E	C10-C11-O12-C13
2	A	506	C8E	C13-C14-O15-C16
2	E	401	C8E	C11-C10-O9-C8
2	C	405	C8E	O9-C10-C11-O12
2	A	505	C8E	C5-C6-C7-C8
2	E	402	C8E	O12-C13-C14-O15
2	A	507	C8E	C6-C7-C8-O9
2	A	501	C8E	C20-C19-O18-C17
2	C	406	C8E	C11-C10-O9-C8
2	A	509	C8E	C2-C3-C4-C5
2	A	515	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	F	407	C8E	C7-C8-O9-C10
2	E	406	C8E	C11-C10-O9-C8
2	A	505	C8E	C10-C11-O12-C13
2	C	407	C8E	C7-C8-O9-C10
2	E	401	C8E	C4-C5-C6-C7
2	D	507	C8E	C2-C3-C4-C5
2	D	502	C8E	C3-C4-C5-C6
2	F	408	C8E	C4-C5-C6-C7
2	D	505	C8E	C14-C13-O12-C11
2	B	402	C8E	C3-C4-C5-C6
2	B	404	C8E	C5-C6-C7-C8
2	F	406	C8E	C3-C4-C5-C6
2	F	411	C8E	C14-C13-O12-C11
2	B	411	C8E	C2-C3-C4-C5
2	F	405	C8E	C7-C8-O9-C10
2	F	411	C8E	O12-C13-C14-O15
2	F	404	C8E	C3-C4-C5-C6
2	D	502	C8E	C1-C2-C3-C4
2	C	406	C8E	O9-C10-C11-O12
2	E	402	C8E	C7-C8-O9-C10
2	A	506	C8E	O18-C19-C20-O21
2	A	515	C8E	C5-C6-C7-C8
2	E	406	C8E	C16-C17-O18-C19
2	D	501	C8E	C14-C13-O12-C11
2	E	401	C8E	C17-C16-O15-C14
2	C	404	C8E	C2-C3-C4-C5
2	A	506	C8E	C17-C16-O15-C14
2	B	401	C8E	C13-C14-O15-C16
2	E	401	C8E	C6-C7-C8-O9
2	C	407	C8E	C4-C5-C6-C7
2	A	501	C8E	C10-C11-O12-C13
2	A	501	C8E	O15-C16-C17-O18
2	A	509	C8E	C1-C2-C3-C4
2	A	510	C8E	C11-C10-O9-C8
2	B	401	C8E	O15-C16-C17-O18
2	B	408	C8E	C3-C4-C5-C6
2	B	408	C8E	C2-C3-C4-C5
2	D	505	C8E	C1-C2-C3-C4
2	D	505	C8E	O9-C10-C11-O12
2	A	505	C8E	O12-C13-C14-O15
2	F	409	C8E	C7-C8-O9-C10
2	A	505	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	D	508	C8E	C11-C10-O9-C8
2	A	501	C8E	C2-C3-C4-C5
2	A	501	C8E	C11-C10-O9-C8
2	A	512	C8E	O9-C10-C11-O12
2	D	507	C8E	O9-C10-C11-O12
2	B	401	C8E	O18-C19-C20-O21
2	D	507	C8E	O12-C13-C14-O15
2	D	501	C8E	O15-C16-C17-O18
2	A	501	C8E	C16-C17-O18-C19
2	E	406	C8E	O9-C10-C11-O12
2	E	406	C8E	O12-C13-C14-O15
2	C	404	C8E	O9-C10-C11-O12
2	A	515	C8E	C11-C10-O9-C8
2	B	403	C8E	O9-C10-C11-O12
2	D	507	C8E	C1-C2-C3-C4
2	F	403	C8E	C13-C14-O15-C16
2	A	501	C8E	O12-C13-C14-O15
2	D	508	C8E	C14-C13-O12-C11
2	D	508	C8E	O15-C16-C17-O18
2	E	401	C8E	O12-C13-C14-O15
2	F	403	C8E	O15-C16-C17-O18

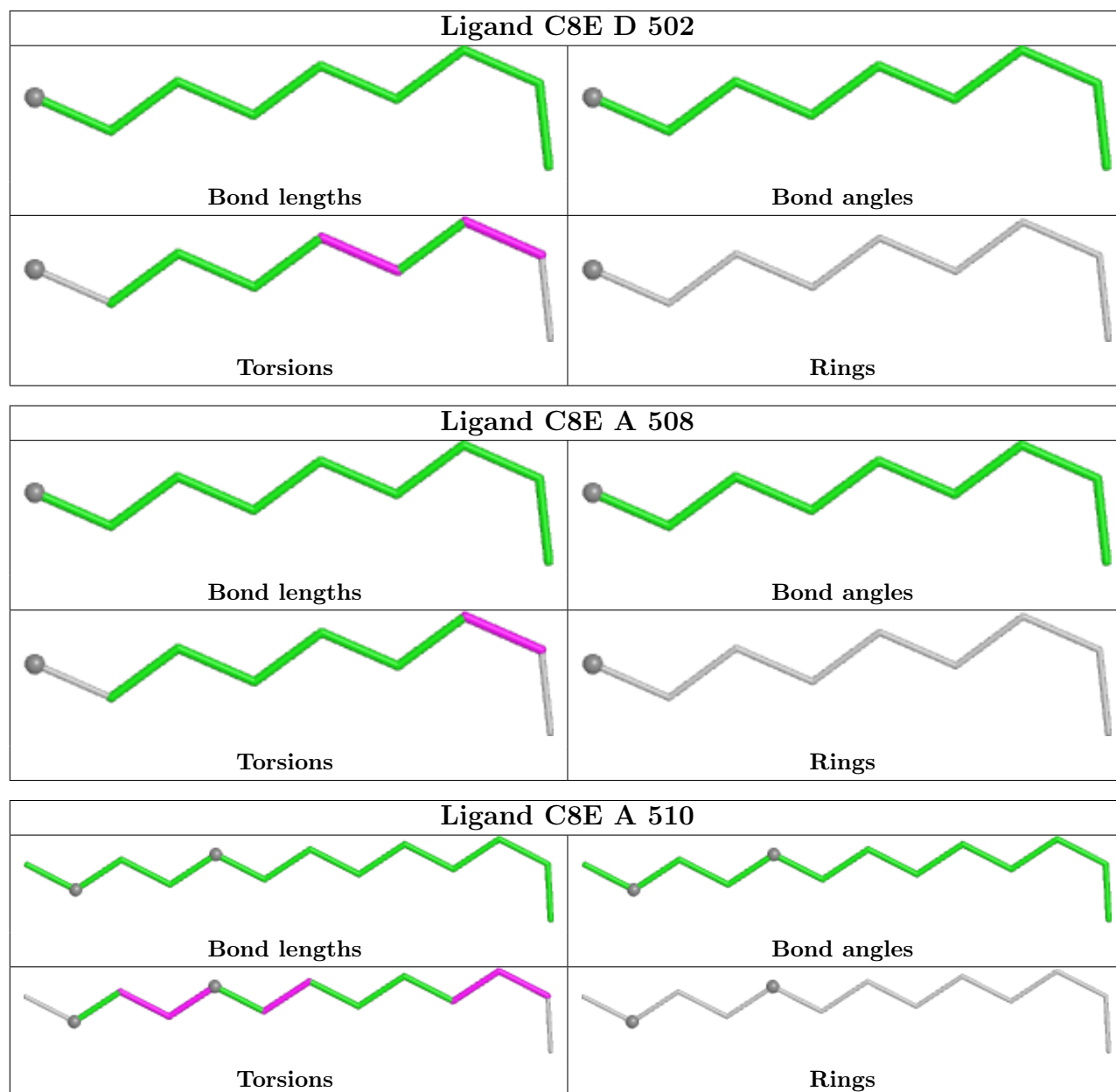
There are no ring outliers.

14 monomers are involved in 22 short contacts:

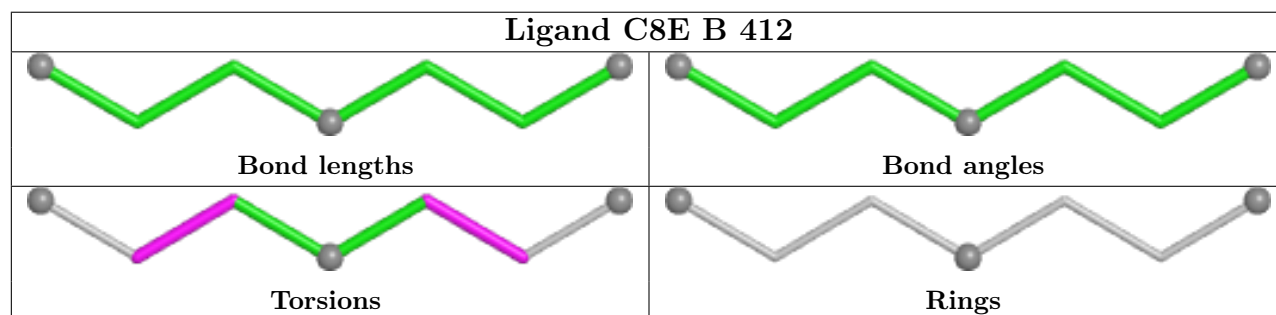
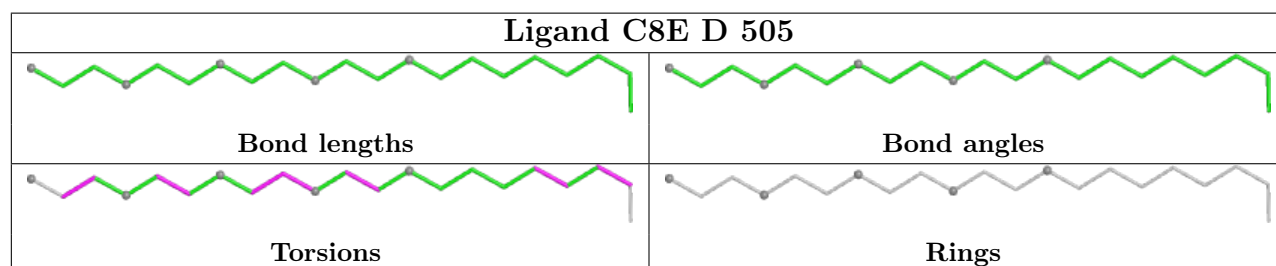
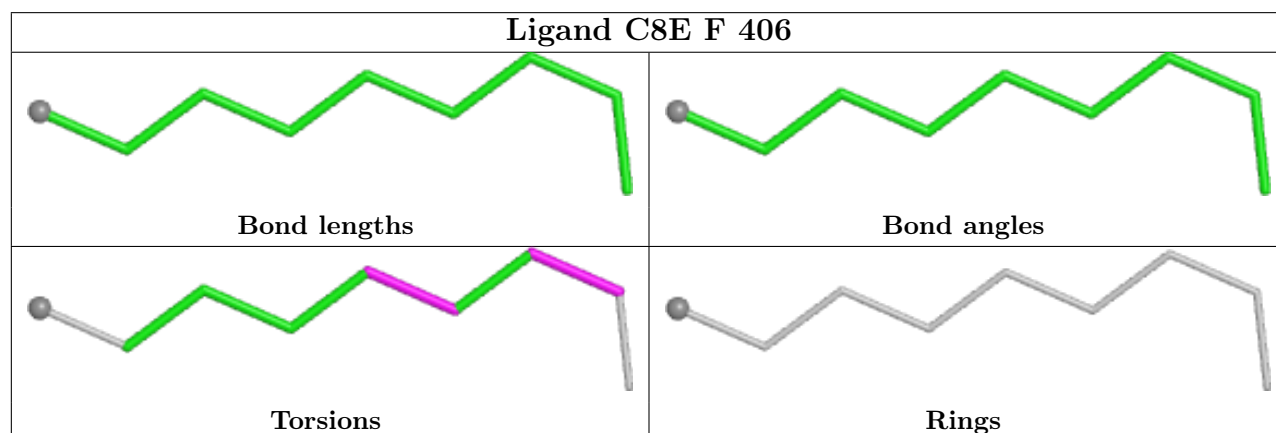
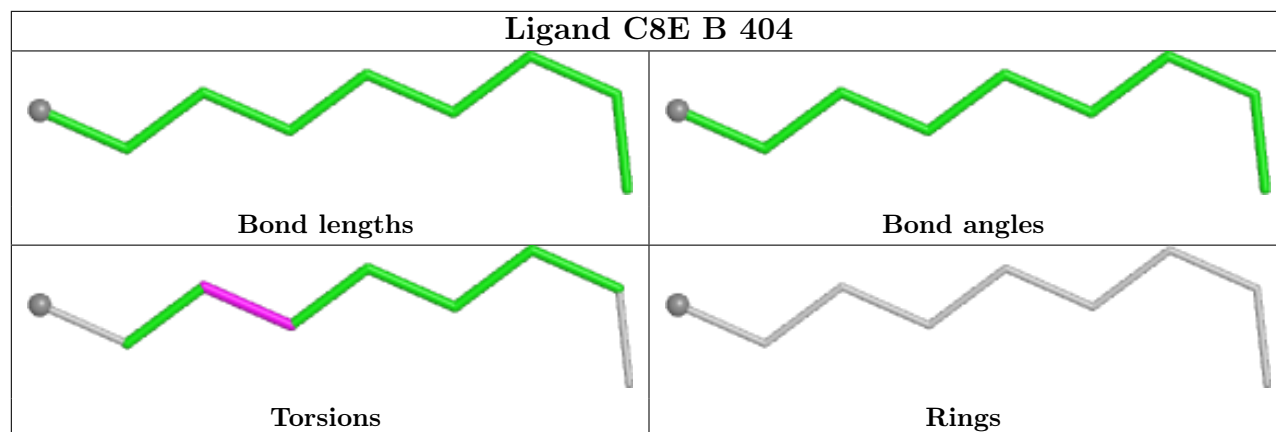
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	406	C8E	1	0
2	B	411	C8E	1	0
2	D	508	C8E	3	0
2	A	506	C8E	1	0
2	B	401	C8E	1	0
2	B	410	C8E	2	0
2	E	401	C8E	6	0
2	D	506	C8E	1	0
2	B	403	C8E	1	0
2	A	505	C8E	1	0
2	A	501	C8E	1	0
2	C	407	C8E	2	0
2	F	408	C8E	1	0
2	E	406	C8E	1	0

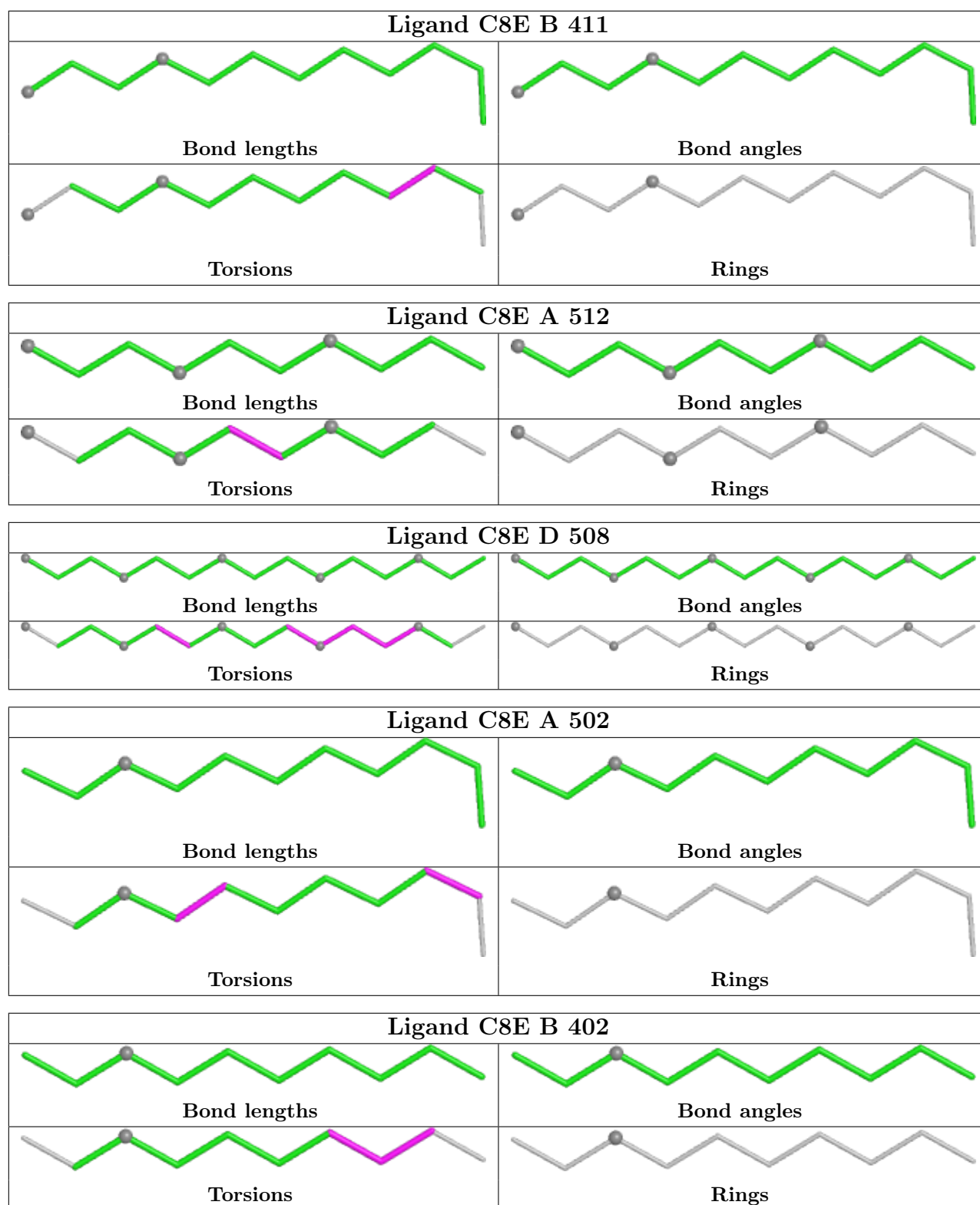
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

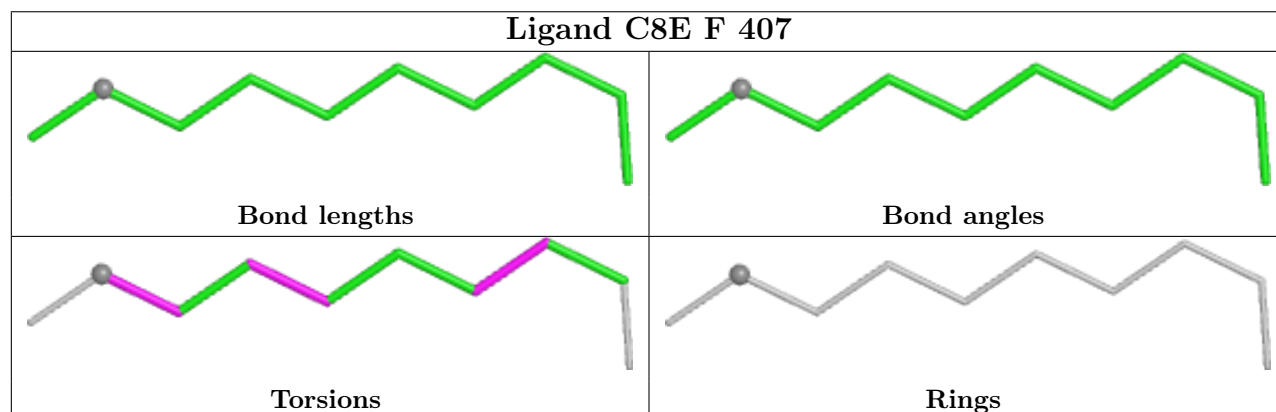
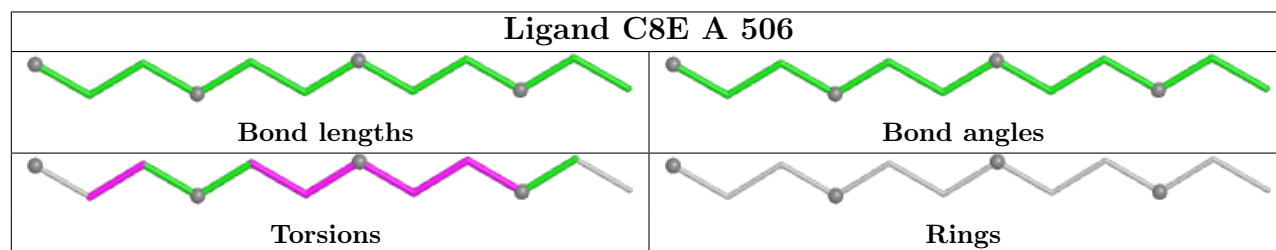
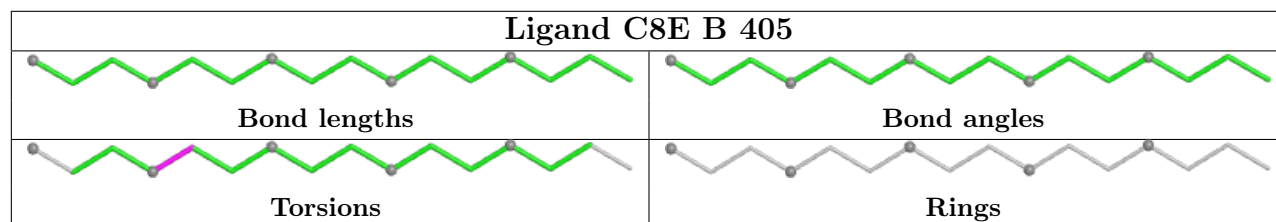
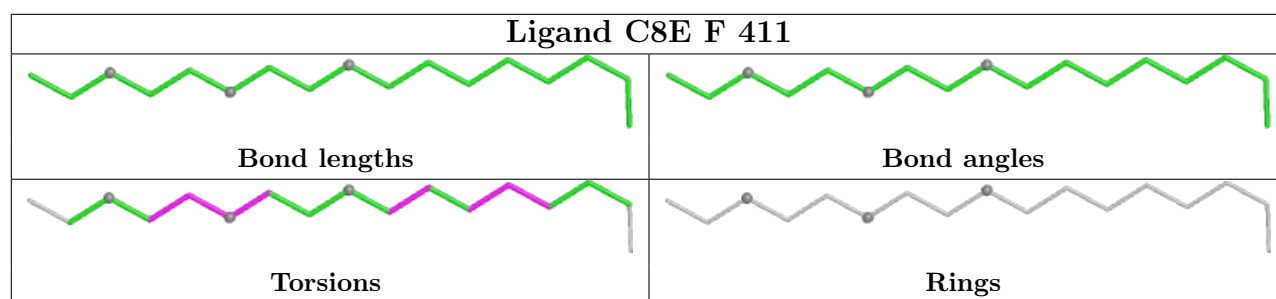
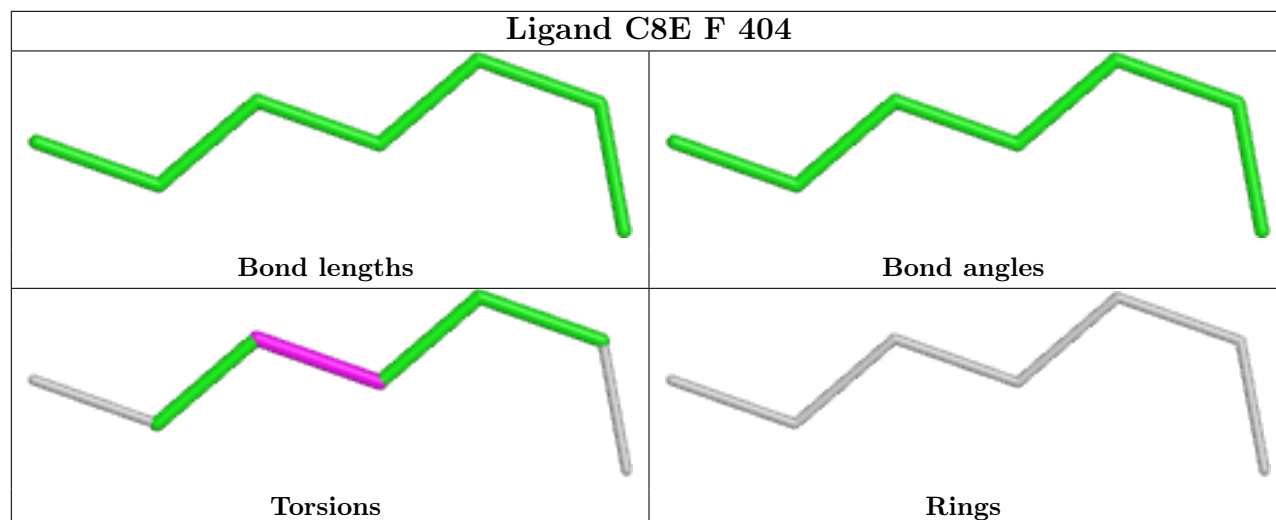
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

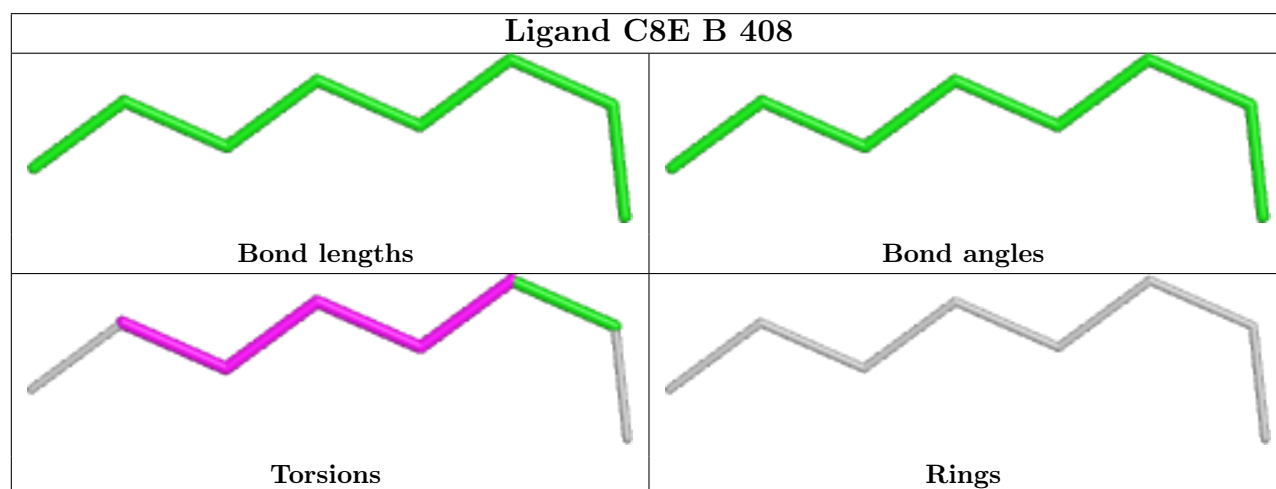
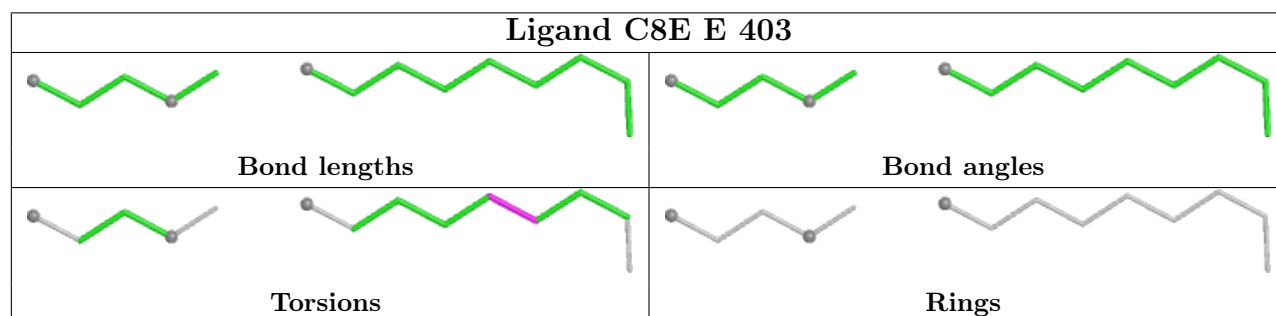
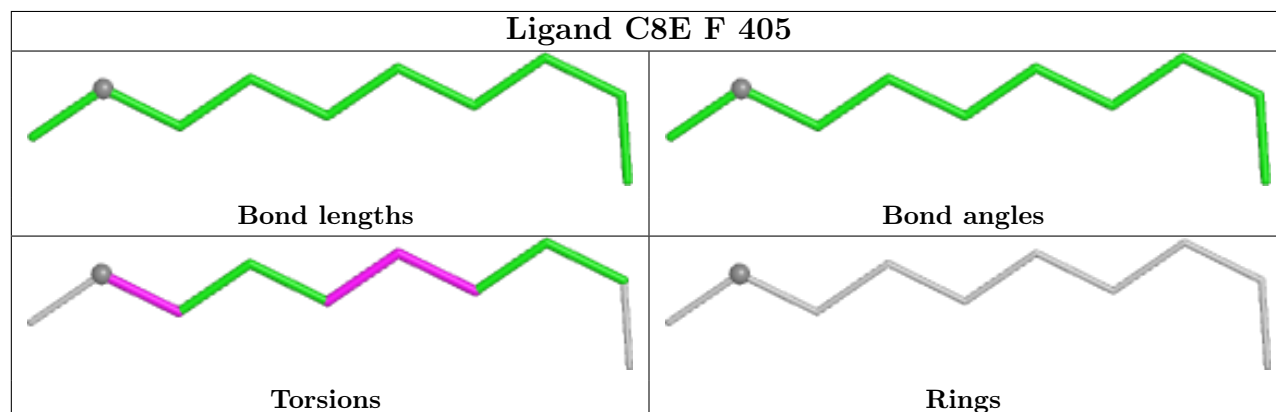
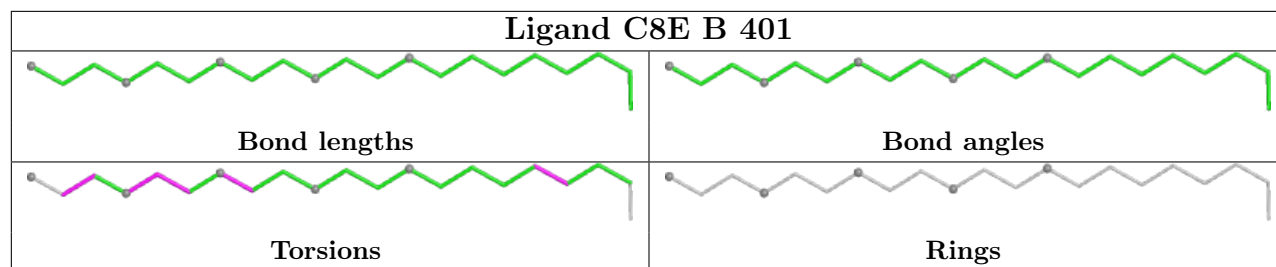


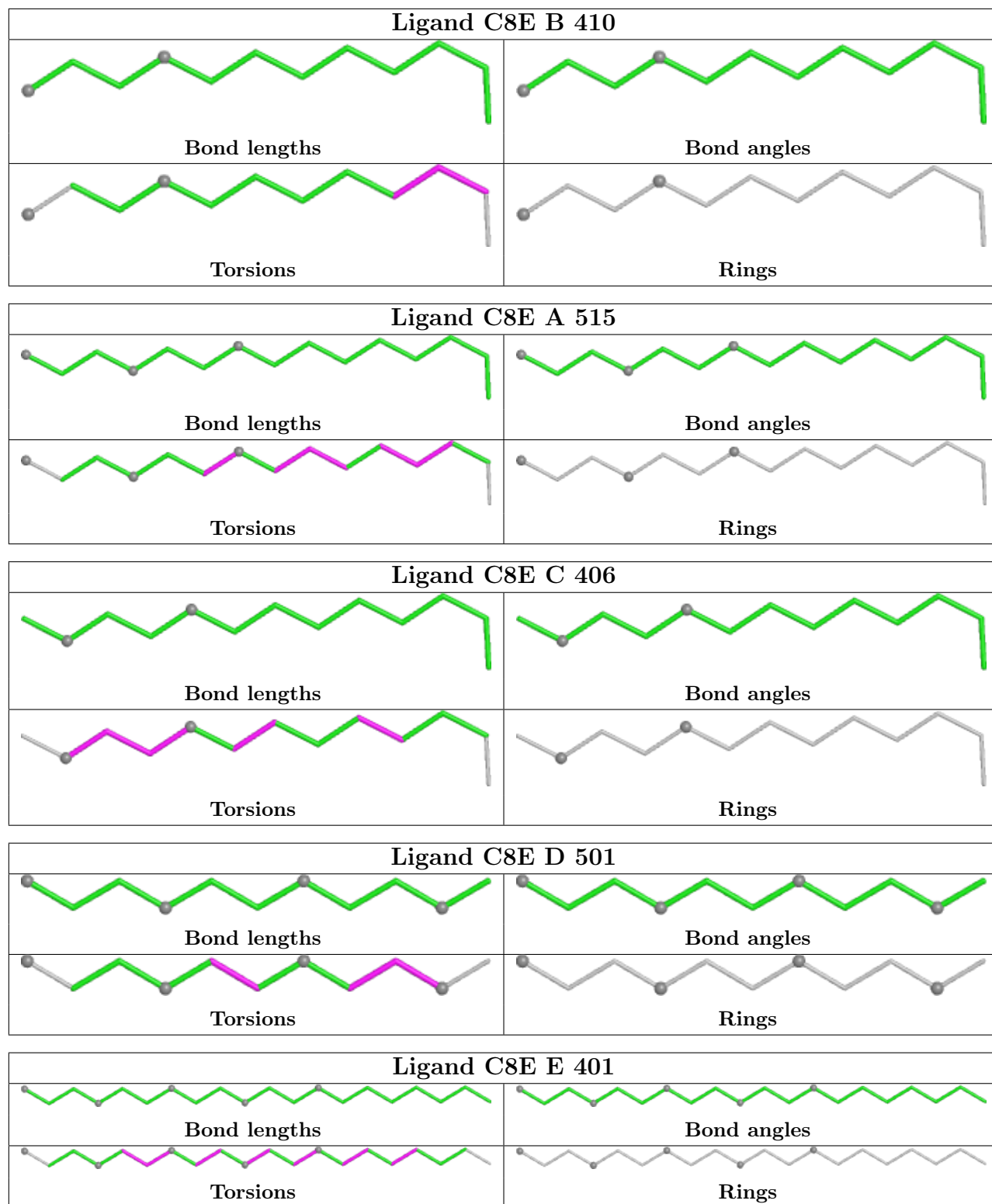


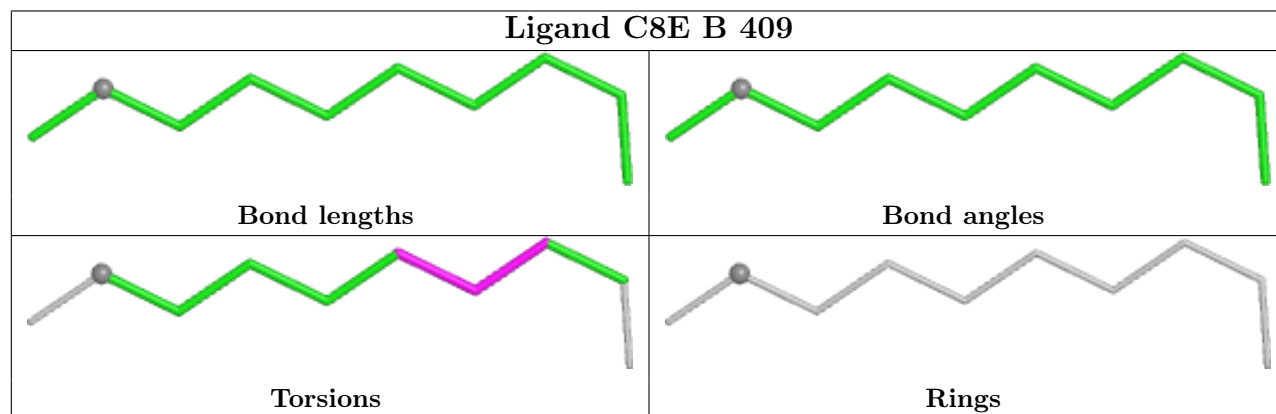
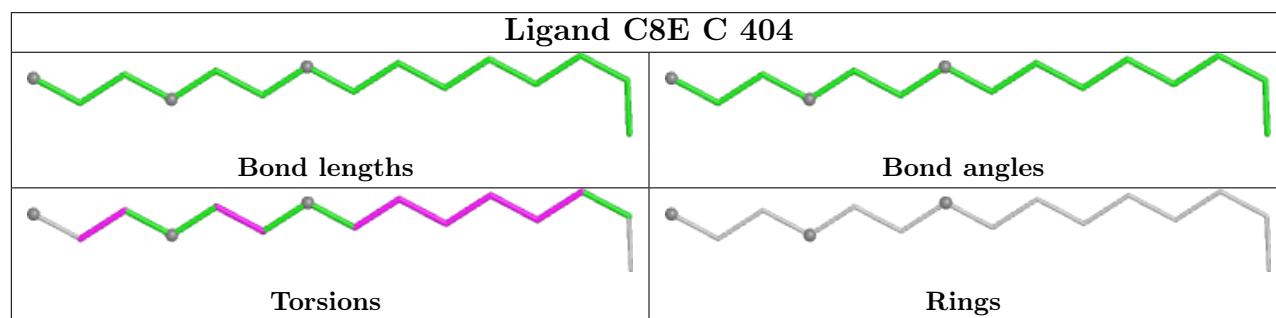
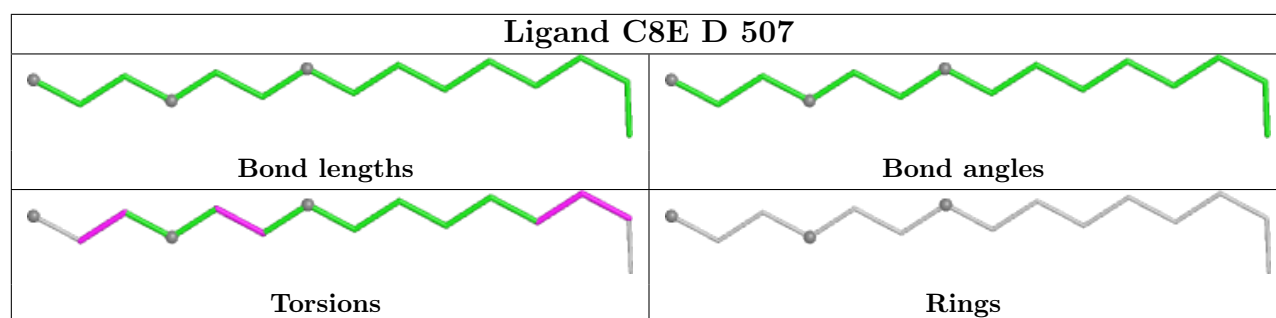
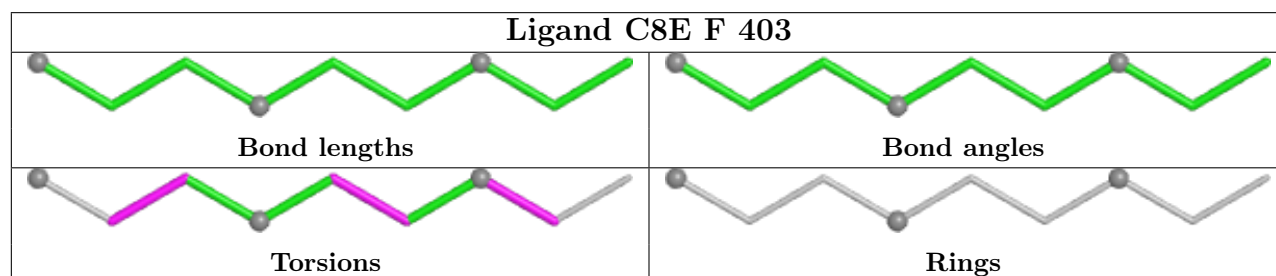
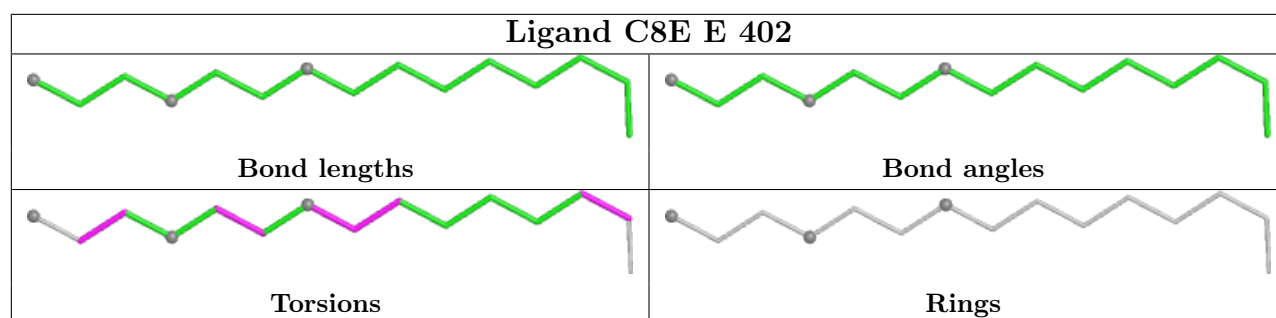


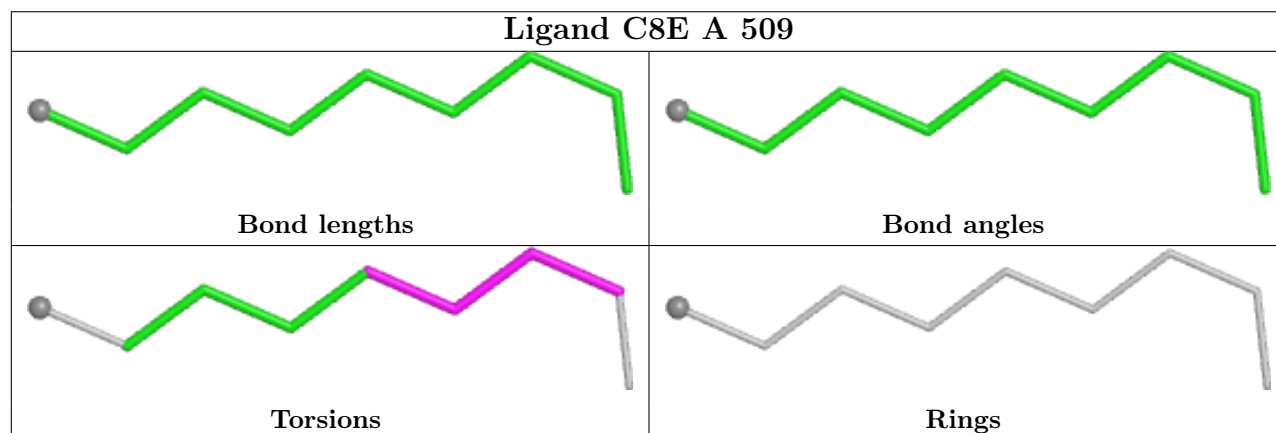
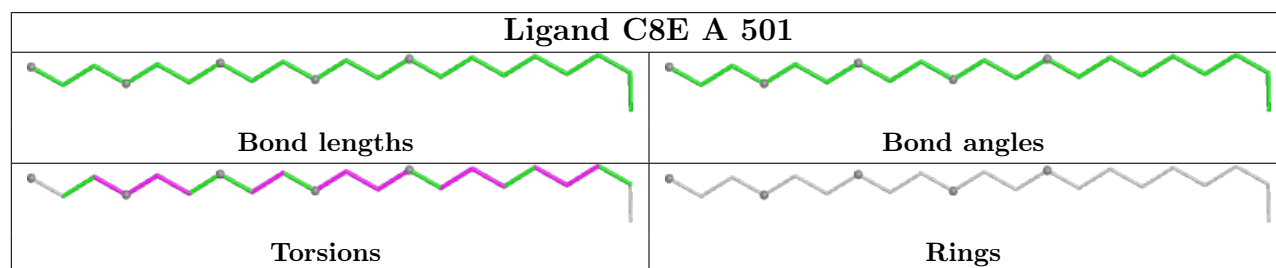
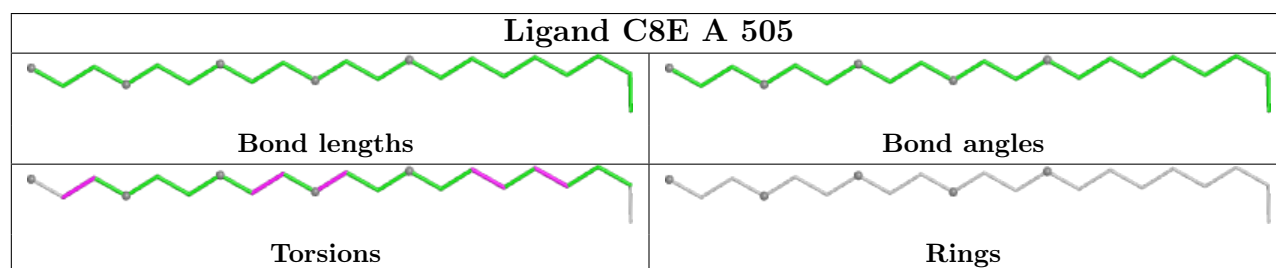
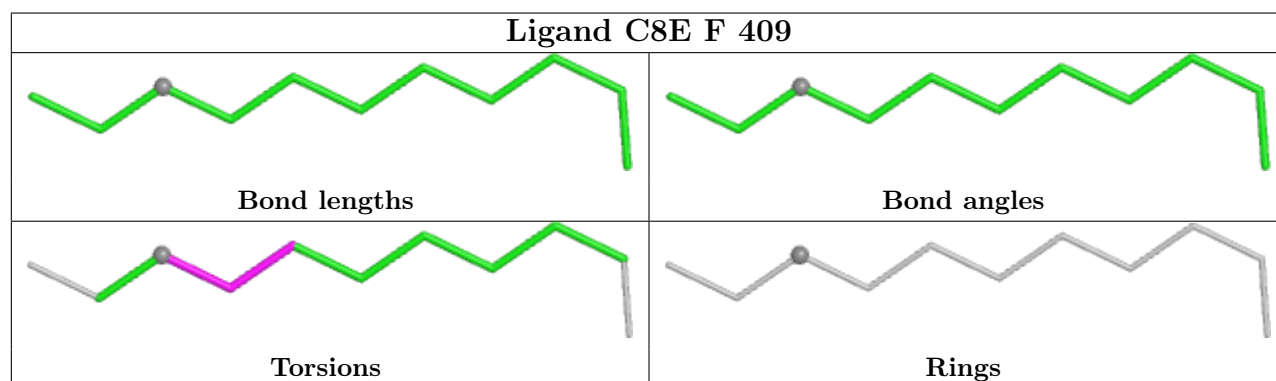
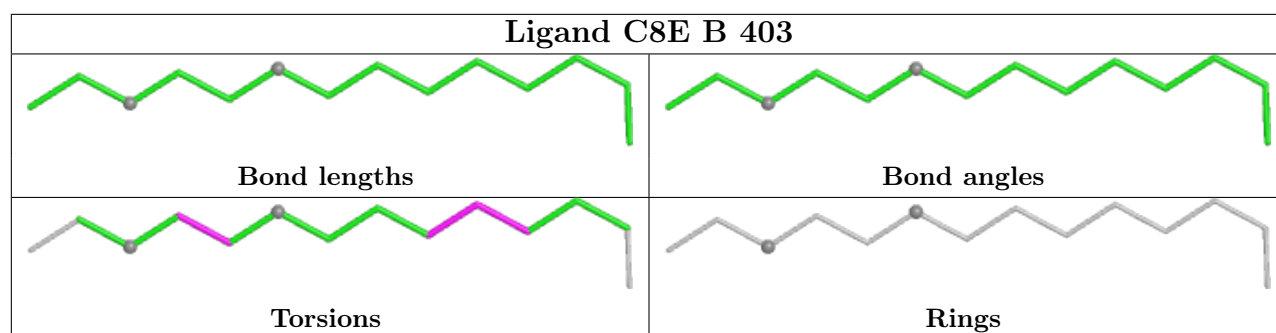


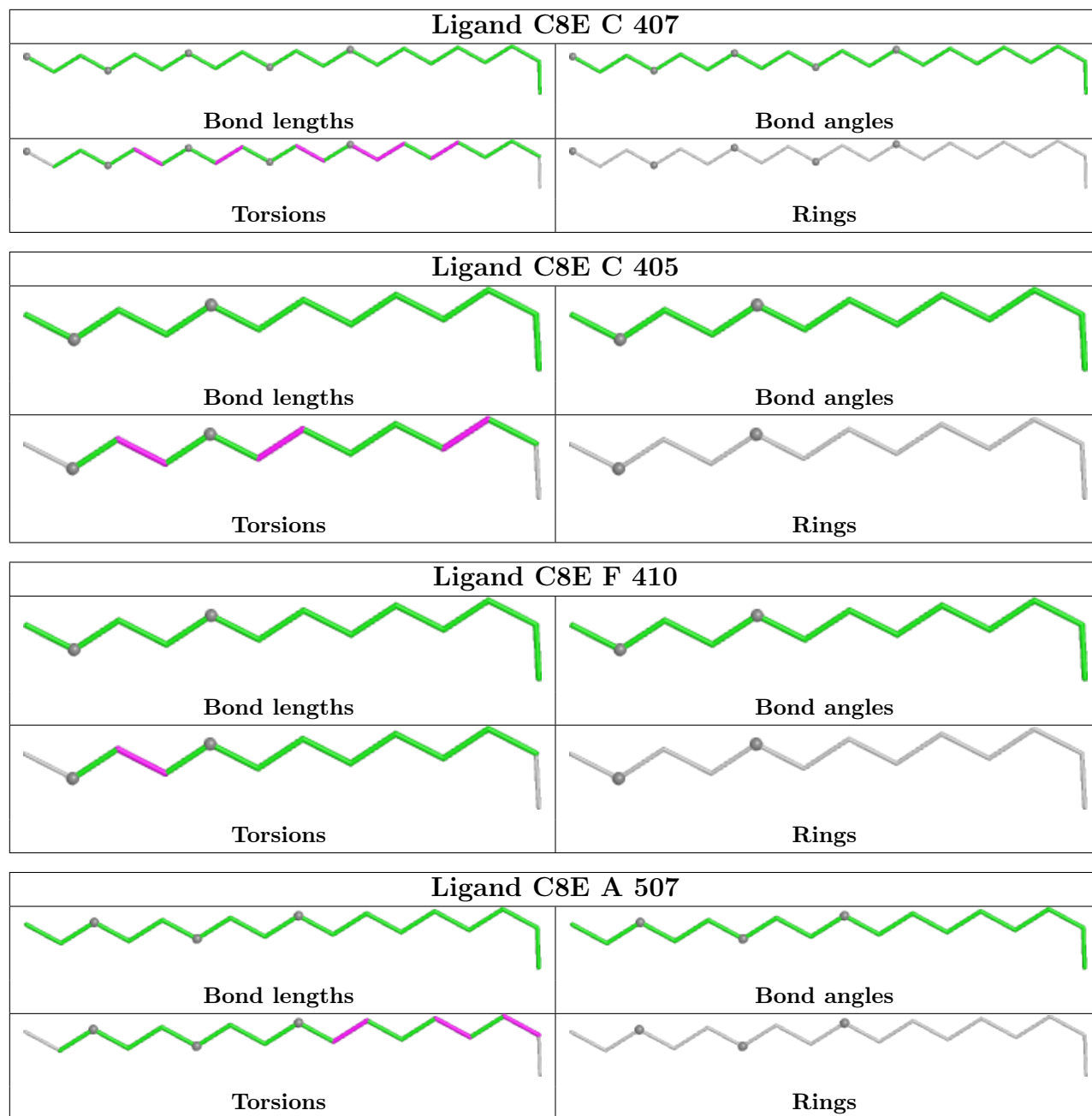




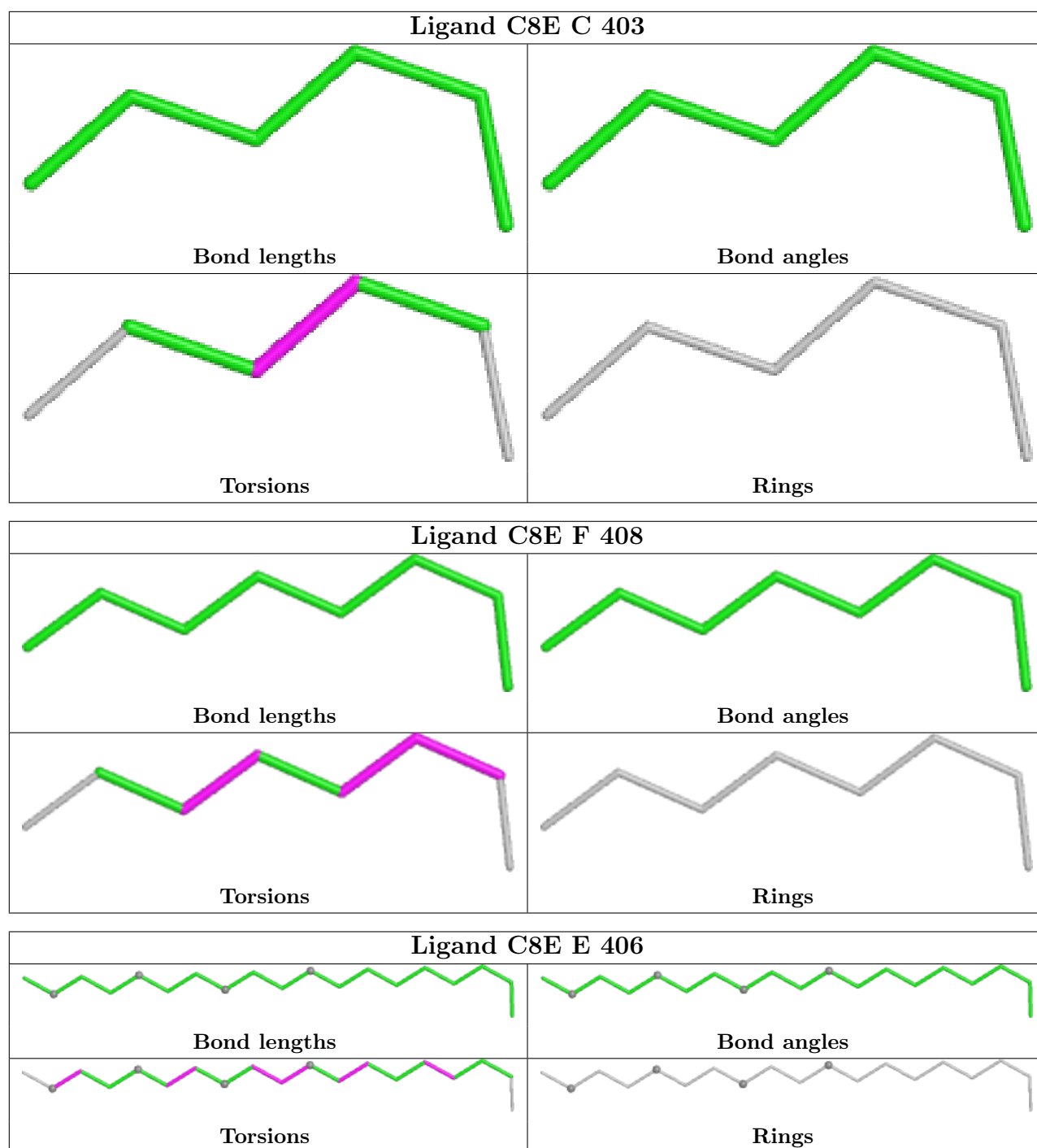












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	346/346 (100%)	-0.07	6 (1%) 70 70	14, 19, 30, 56	0
1	B	346/346 (100%)	-0.07	9 (2%) 56 55	12, 20, 34, 53	0
1	C	346/346 (100%)	-0.01	9 (2%) 56 55	13, 21, 34, 56	0
1	D	346/346 (100%)	-0.06	12 (3%) 44 42	13, 20, 35, 58	0
1	E	346/346 (100%)	-0.01	12 (3%) 44 42	14, 20, 37, 52	0
1	F	346/346 (100%)	-0.02	7 (2%) 65 65	14, 21, 34, 52	0
All	All	2076/2076 (100%)	-0.04	55 (2%) 56 55	12, 20, 35, 58	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	TYR	13.8
1	D	187	TRP	11.5
1	A	115	ASP	10.3
1	A	117	TYR	9.9
1	F	116	THR	8.5
1	E	116	THR	8.3
1	C	116	THR	7.9
1	A	116	THR	7.5
1	E	117	TYR	7.5
1	B	115	ASP	7.1
1	B	117	TYR	6.7
1	C	117	TYR	6.7
1	D	116	THR	6.6
1	C	187	TRP	6.4
1	B	116	THR	5.8
1	A	118	GLY	5.7
1	F	187	TRP	5.4
1	D	117	TYR	5.2
1	C	115	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	115	ASP	5.0
1	D	186	ILE	4.9
1	B	187	TRP	4.8
1	D	115	ASP	4.8
1	E	86	ALA	4.6
1	C	186	ILE	4.5
1	E	115	ASP	4.1
1	E	114	ASP	3.9
1	D	188	ASP	3.8
1	B	188	ASP	3.5
1	D	7	ASP	3.3
1	B	114	ASP	3.2
1	C	114	ASP	3.1
1	B	7	ASP	3.0
1	A	114	ASP	2.8
1	D	114	ASP	2.8
1	E	188	ASP	2.7
1	D	118	GLY	2.7
1	E	187	TRP	2.7
1	E	141	LEU	2.6
1	E	85	ASP	2.6
1	F	186	ILE	2.5
1	C	147	PHE	2.5
1	F	114	ASP	2.3
1	C	113	GLY	2.3
1	E	84	GLY	2.3
1	B	0	GLY	2.2
1	B	194	PHE	2.2
1	D	12	ASP	2.2
1	A	194	PHE	2.1
1	E	7	ASP	2.1
1	F	161	GLU	2.1
1	D	267	ASP	2.1
1	D	83[A]	PHE	2.1
1	E	118	GLY	2.0
1	C	118	GLY	2.0

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	C8E	A	512	10/21	0.45	0.22	57,58,59,59	0
2	C8E	F	411	17/21	0.62	0.21	42,49,50,50	0
2	C8E	F	410	13/21	0.63	0.21	47,50,53,53	0
2	C8E	B	401	21/21	0.64	0.24	53,57,60,60	0
2	C8E	B	404	9/21	0.67	0.24	46,47,49,49	0
2	C8E	C	406	13/21	0.67	0.18	41,45,47,47	0
2	C8E	F	406	9/21	0.69	0.14	54,54,54,54	0
2	C8E	B	405	16/21	0.70	0.21	55,57,57,57	0
2	C8E	F	409	11/21	0.70	0.26	43,44,44,44	0
2	C8E	A	501	21/21	0.71	0.18	41,47,49,50	0
2	C8E	D	505	21/21	0.71	0.19	39,44,52,52	0
2	C8E	A	515	15/21	0.72	0.20	53,54,56,56	0
2	C8E	A	514	10/21	0.72	0.18	49,50,51,51	0
2	C8E	A	507	17/21	0.73	0.17	33,38,43,43	0
2	C8E	B	412	7/21	0.74	0.16	47,47,48,48	0
2	C8E	F	405	10/21	0.75	0.20	32,33,36,36	0
2	C8E	F	403	9/21	0.76	0.16	56,56,57,57	0
2	C8E	E	401	20/21	0.77	0.17	37,39,46,46	0
2	C8E	A	510	13/21	0.78	0.17	38,41,44,44	0
2	C8E	D	506	11/21	0.80	0.16	47,48,49,49	0
2	C8E	C	407	21/21	0.81	0.20	47,48,49,49	0
2	C8E	B	410	12/21	0.81	0.15	44,44,47,47	0
2	C8E	E	406	19/21	0.81	0.16	41,46,51,51	0
2	C8E	A	511	8/21	0.82	0.19	37,37,37,37	0
2	C8E	A	506	12/21	0.83	0.20	40,41,44,45	0
2	C8E	C	404	15/21	0.83	0.14	45,46,51,52	0
2	C8E	E	403	14/21	0.84	0.14	39,40,53,53	0
2	C8E	F	407	10/21	0.84	0.15	40,40,41,41	0
2	C8E	F	408	8/21	0.84	0.16	39,41,42,43	0
2	C8E	F	404	7/21	0.85	0.13	38,38,40,40	0
2	C8E	C	405	13/21	0.85	0.12	45,48,50,51	0
2	C8E	B	408	8/21	0.86	0.11	41,42,42,42	0

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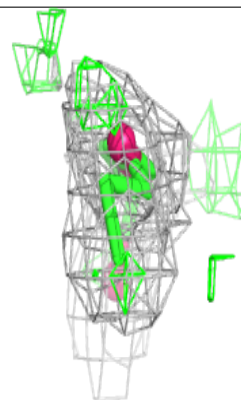
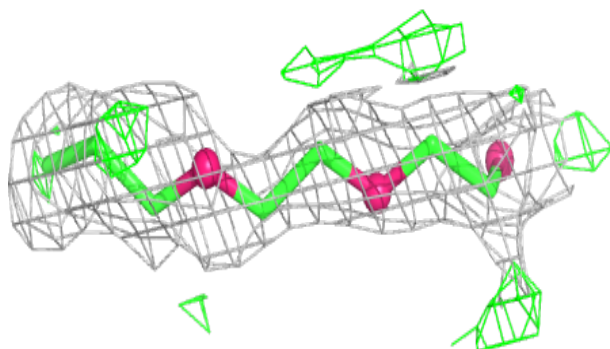
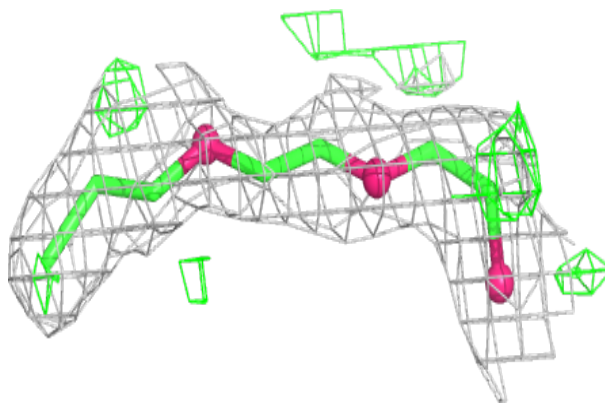
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C8E	A	505	21/21	0.86	0.16	33,38,40,41	0
2	C8E	A	509	9/21	0.86	0.17	44,44,46,46	0
2	C8E	D	507	15/21	0.86	0.15	43,43,45,45	0
2	C8E	E	402	15/21	0.87	0.15	41,42,45,45	0
2	C8E	A	502	11/21	0.87	0.15	33,34,36,37	0
2	C8E	D	502	9/21	0.87	0.12	44,45,46,47	0
2	C8E	B	409	10/21	0.88	0.13	34,38,42,42	0
2	C8E	B	403	14/21	0.88	0.14	41,41,44,45	0
2	C8E	B	402	10/21	0.88	0.16	41,41,42,42	0
2	C8E	C	403	6/21	0.89	0.15	34,34,35,35	0
2	C8E	D	508	15/21	0.89	0.15	38,40,43,43	0
2	C8E	B	411	12/21	0.89	0.15	43,43,44,44	0
2	C8E	A	508	9/21	0.90	0.13	35,35,37,38	0
2	C8E	D	501	11/21	0.92	0.12	44,44,46,46	0
3	LI	C	401	1/1	0.92	0.34	8,8,8,8	0
3	LI	E	404	1/1	0.92	0.32	4,4,4,4	0
2	C8E	A	513	6/21	0.93	0.11	31,31,31,31	0
3	LI	B	407	1/1	0.94	0.44	3,3,3,3	0
3	LI	A	504	1/1	0.94	0.46	3,3,3,3	0
3	LI	B	406	1/1	0.94	0.26	4,4,4,4	0
3	LI	F	401	1/1	0.94	0.41	3,3,3,3	0
3	LI	A	503	1/1	0.96	0.42	3,3,3,3	0
3	LI	F	402	1/1	0.96	0.21	3,3,3,3	0
3	LI	D	504	1/1	0.97	0.43	3,3,3,3	0
3	LI	C	402	1/1	0.98	0.47	3,3,3,3	0
3	LI	E	405	1/1	0.98	0.43	3,3,3,3	0
3	LI	D	503	1/1	0.99	0.38	3,3,3,3	0

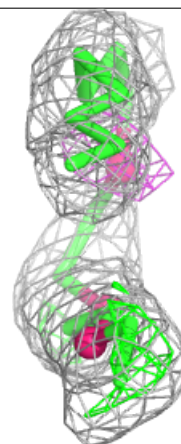
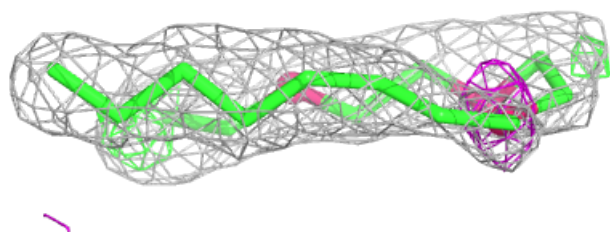
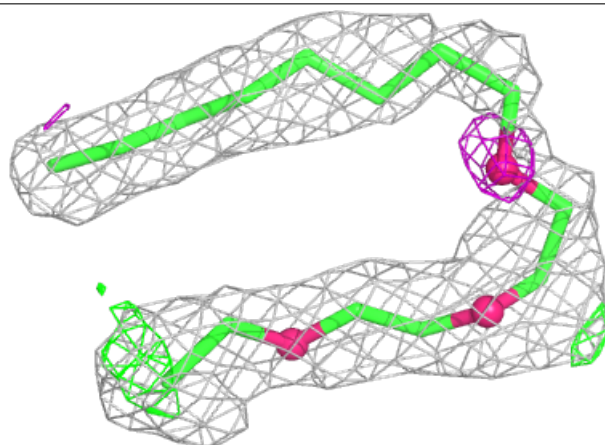
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around C8E A 512:**

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

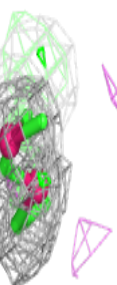
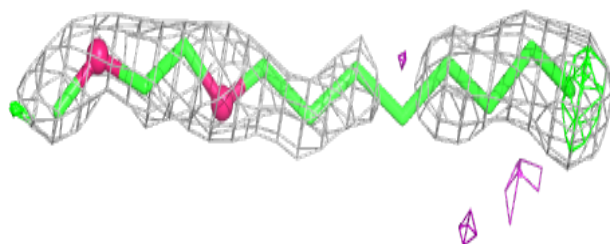
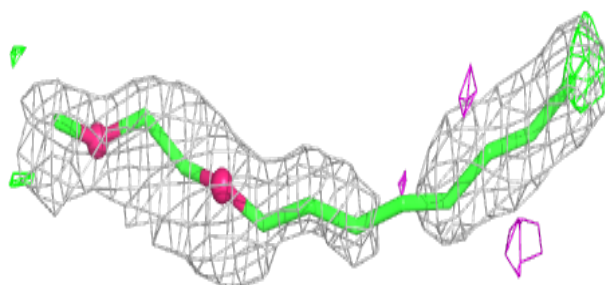
**Electron density around C8E F 411:**

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

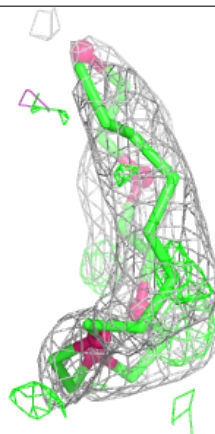
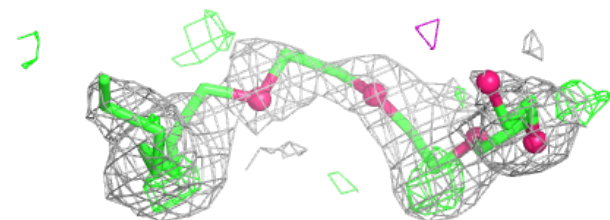
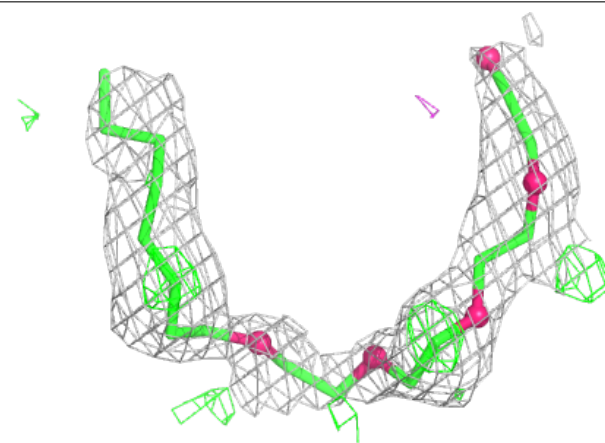


**Electron density around C8E F 410:**

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

**Electron density around C8E B 401:**

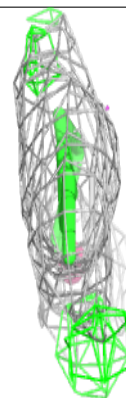
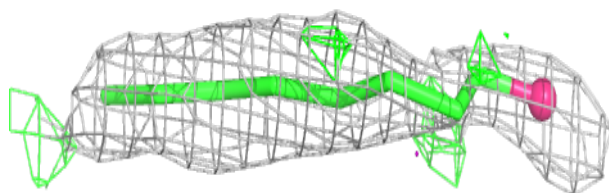
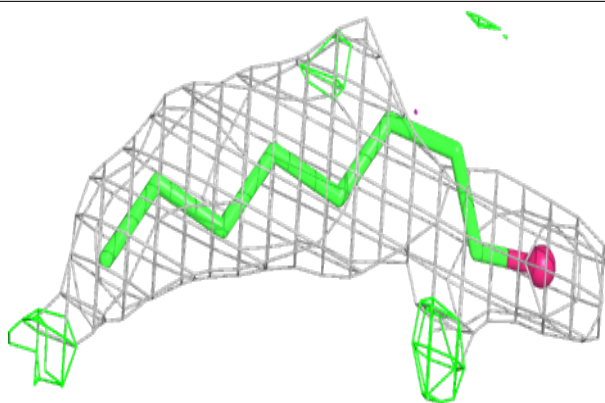
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



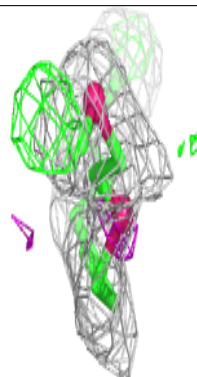
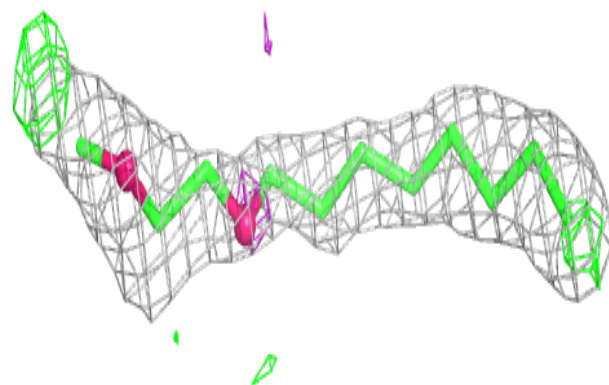
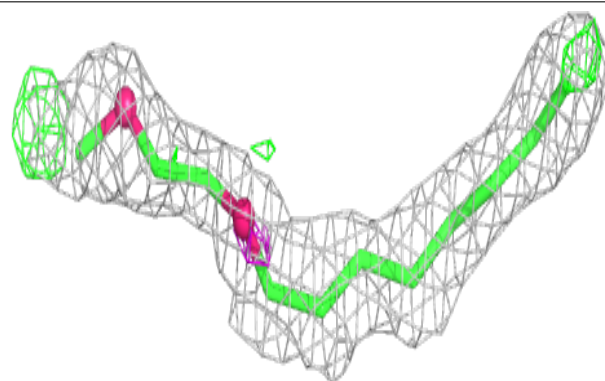


**Electron density around C8E B 404:**

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

**Electron density around C8E C 406:**

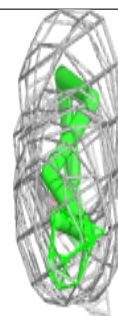
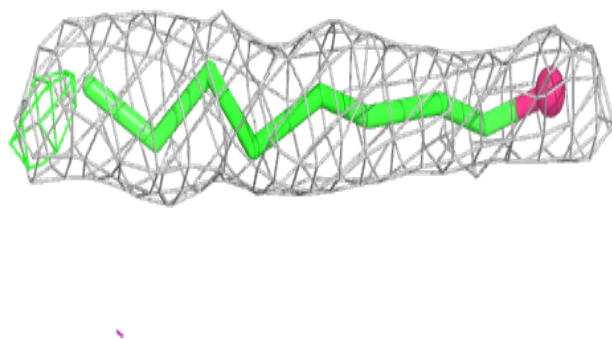
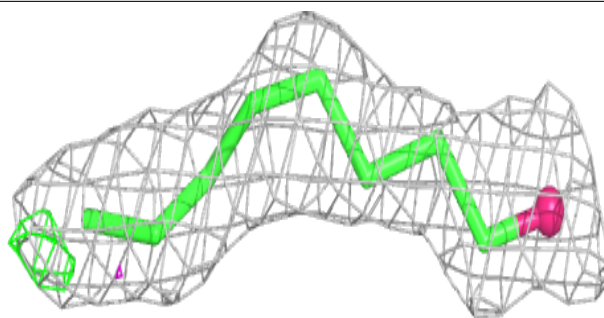
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



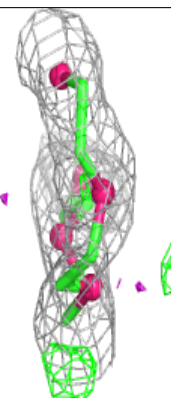
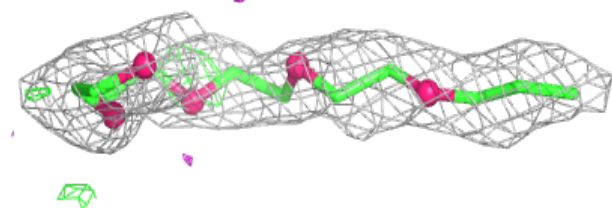
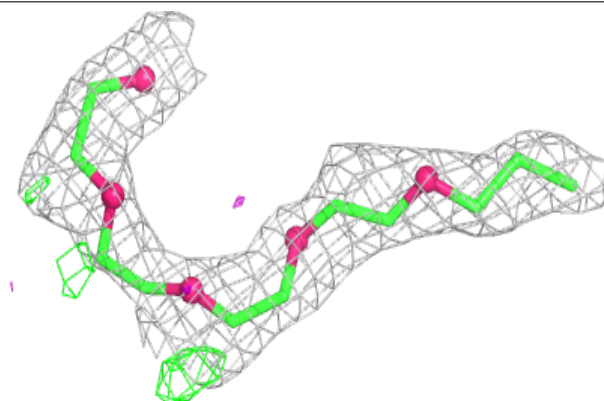


**Electron density around C8E F 406:**

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

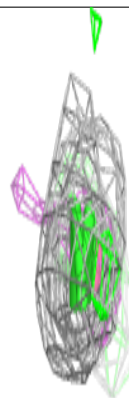
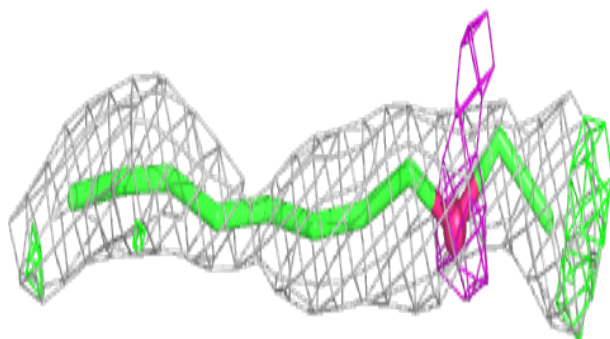
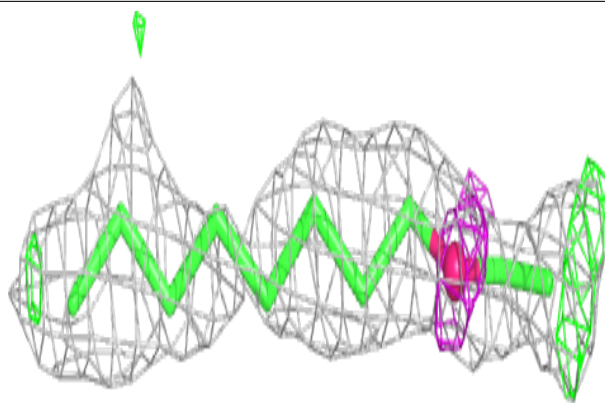
**Electron density around C8E B 405:**

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

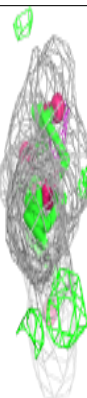
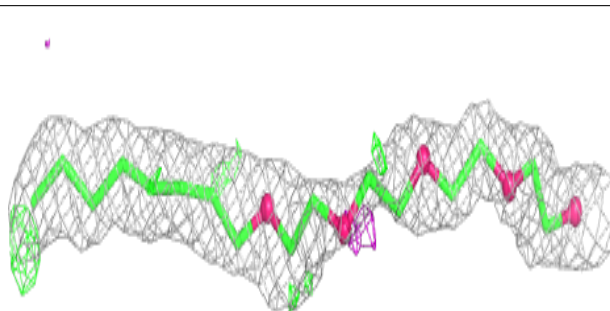
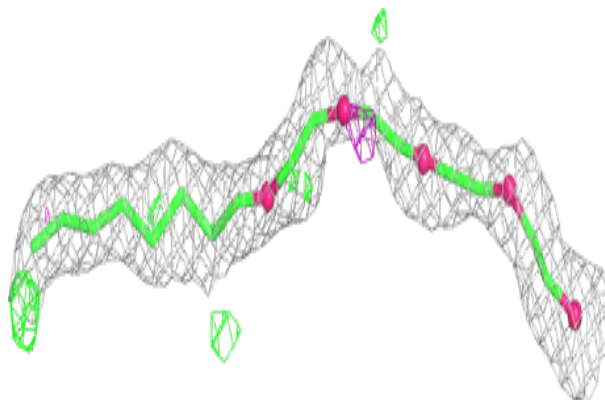


**Electron density around C8E F 409:**

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

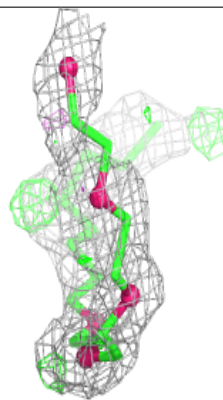
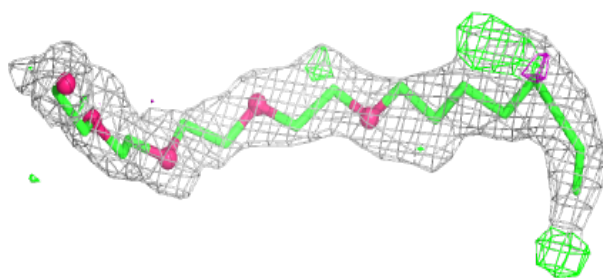
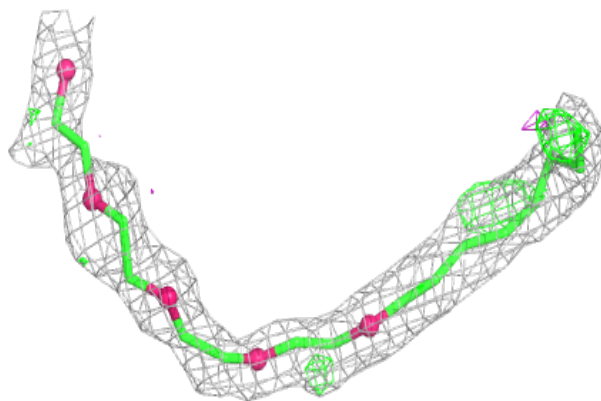
**Electron density around C8E A 501:**

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

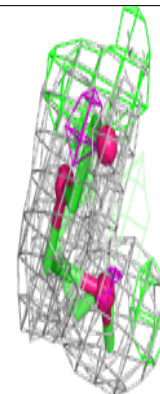
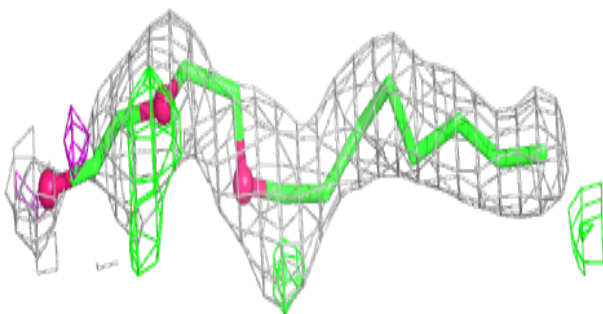
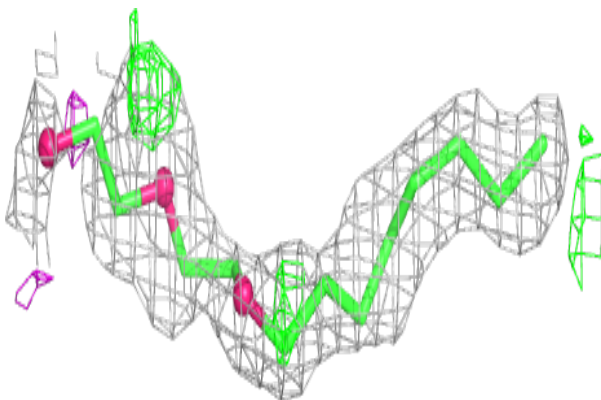


**Electron density around C8E D 505:**

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

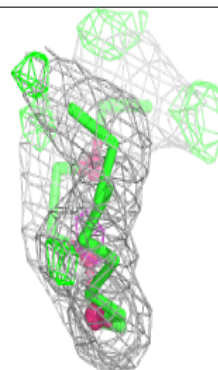
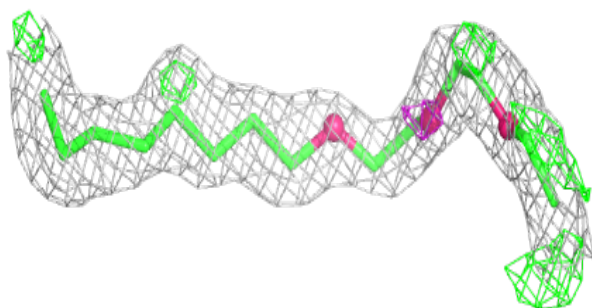
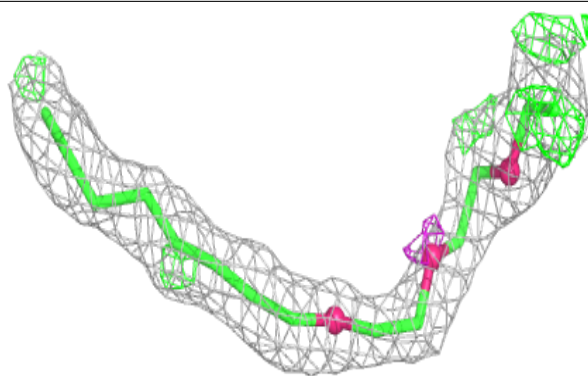
**Electron density around C8E A 515:**

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

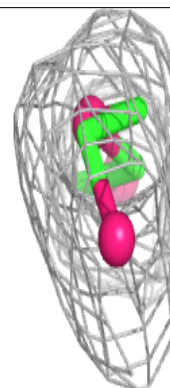
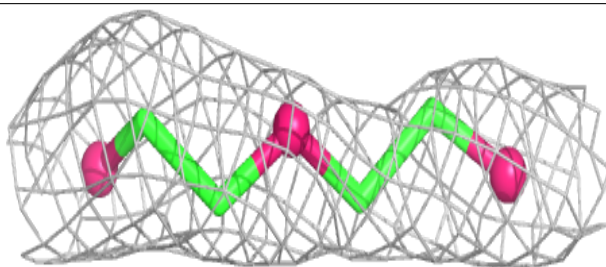
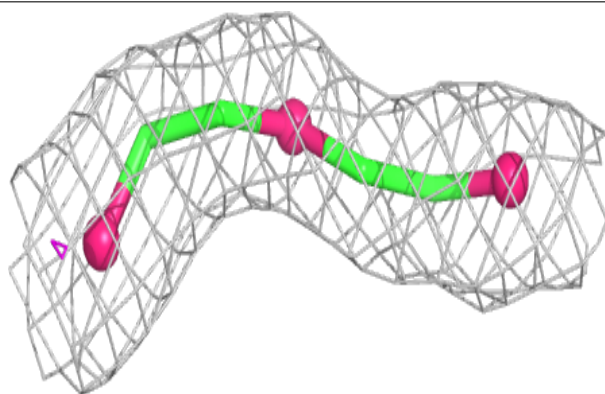


**Electron density around C8E A 507:**

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

**Electron density around C8E B 412:**

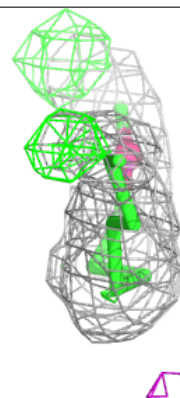
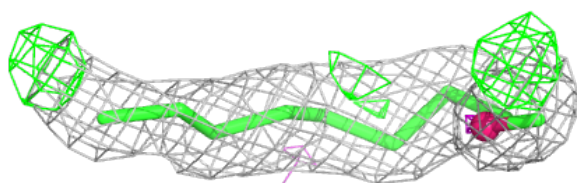
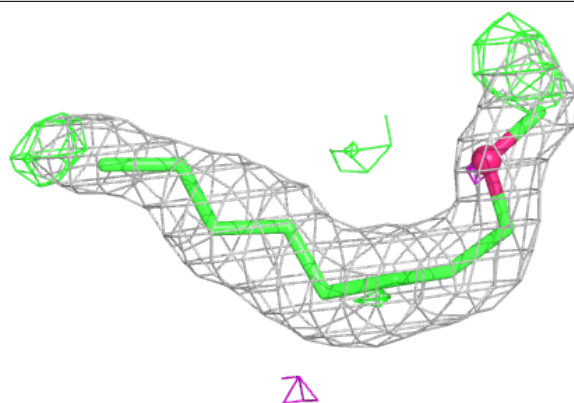
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



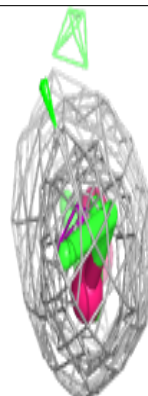
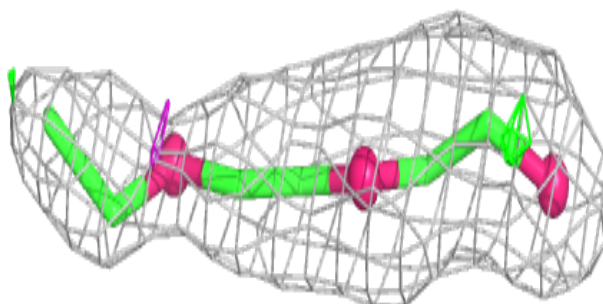
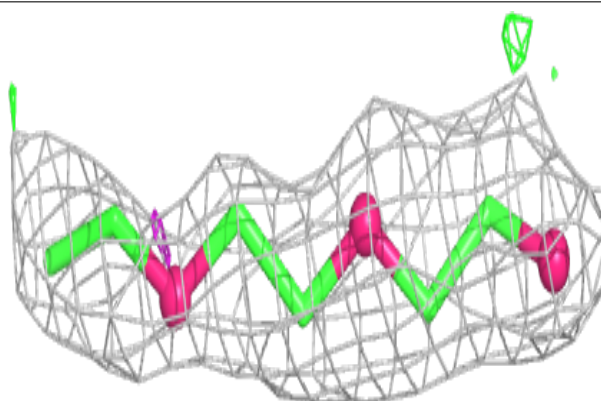


**Electron density around C8E F 405:**

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

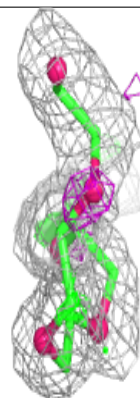
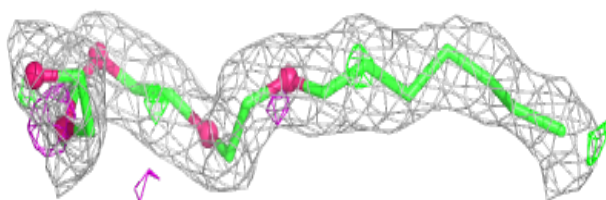
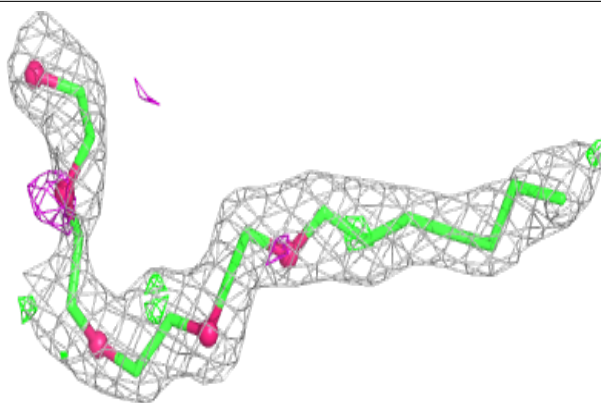
**Electron density around C8E F 403:**

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

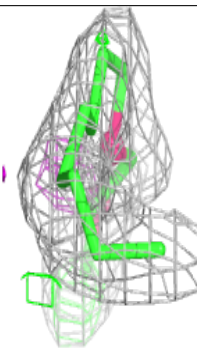
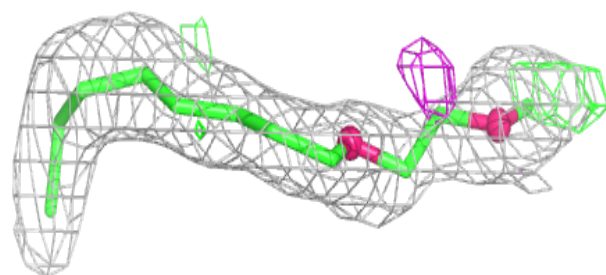


**Electron density around C8E E 401:**

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

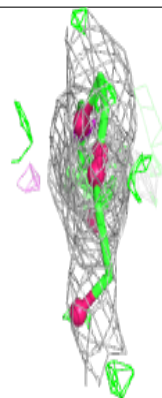
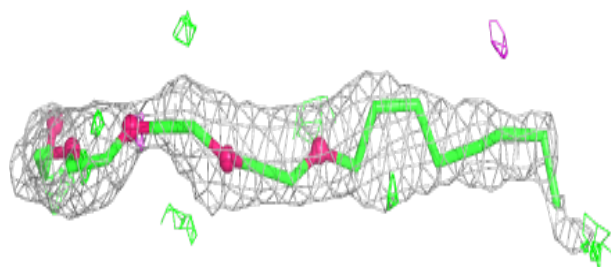
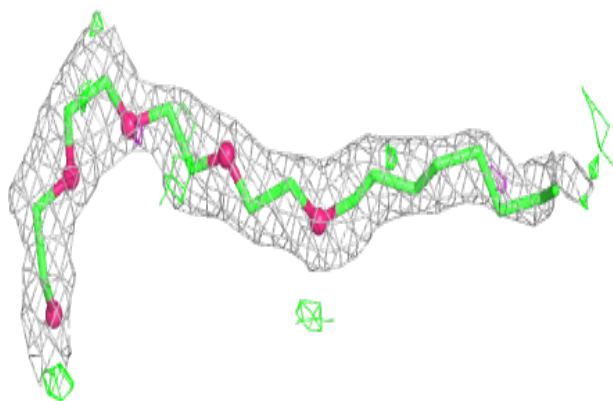
**Electron density around C8E A 510:**

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

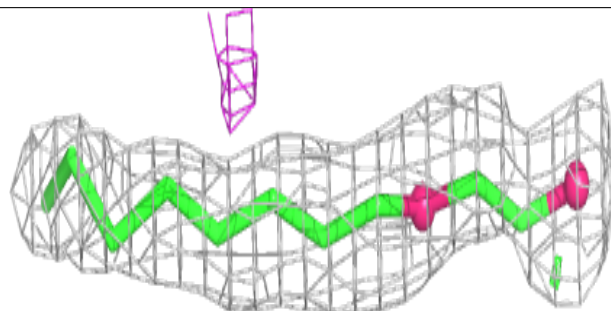
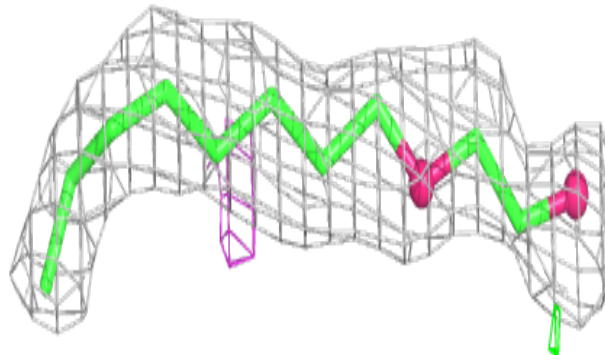


**Electron density around C8E C 407:**

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

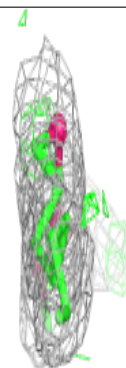
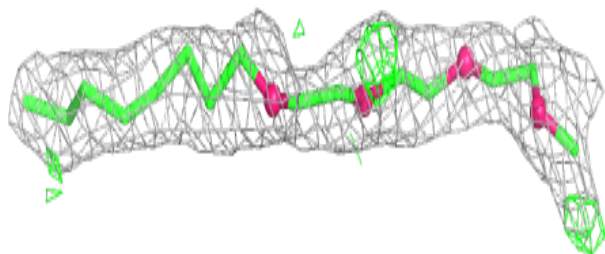
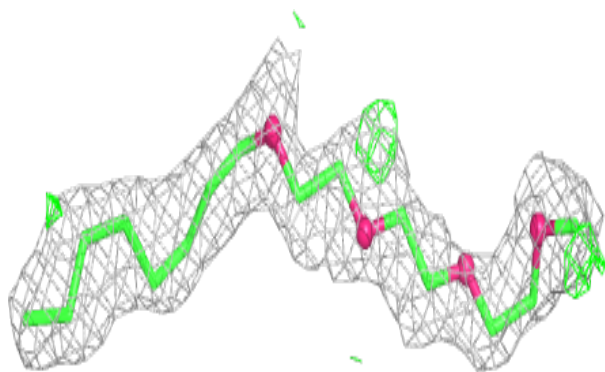
**Electron density around C8E B 410:**

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

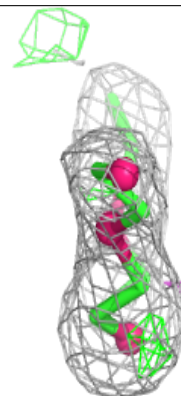
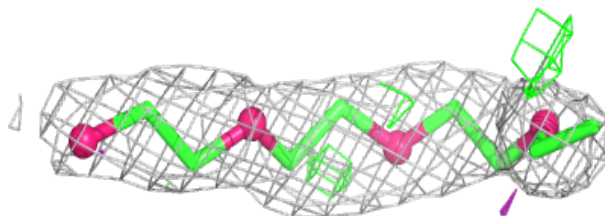
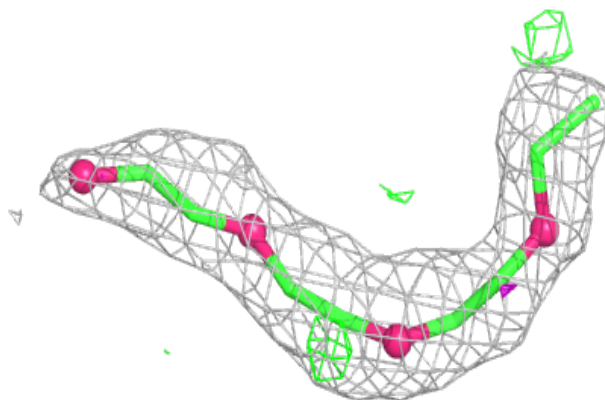


**Electron density around C8E E 406:**

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

**Electron density around C8E A 506:**

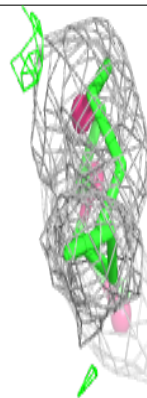
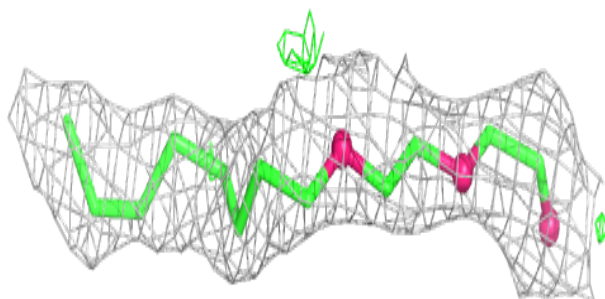
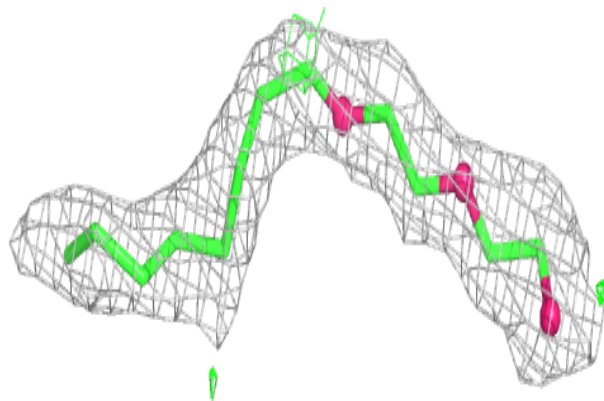
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



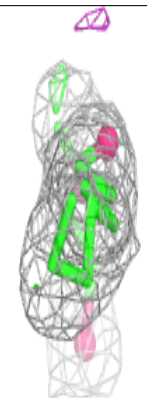
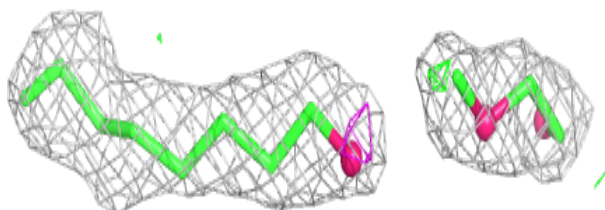
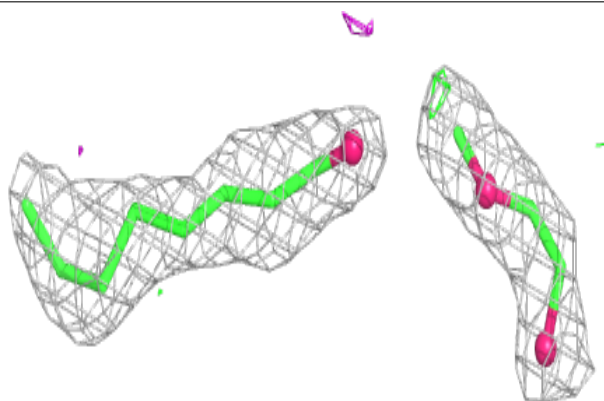


**Electron density around C8E C 404:**

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

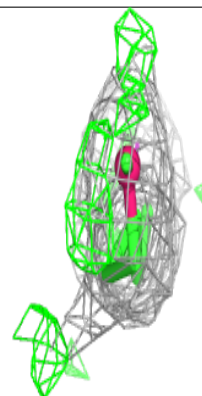
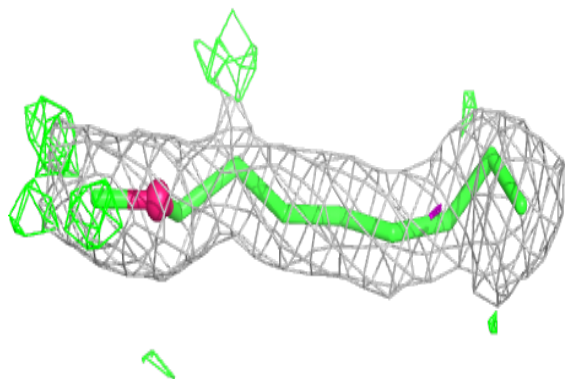
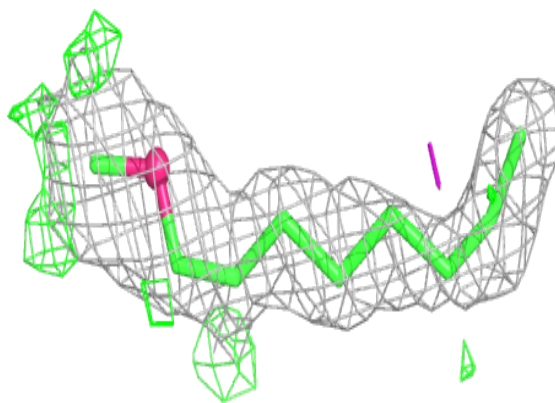
**Electron density around C8E E 403:**

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

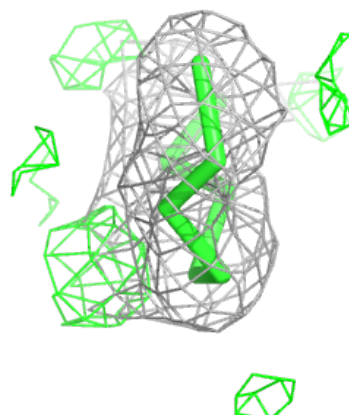
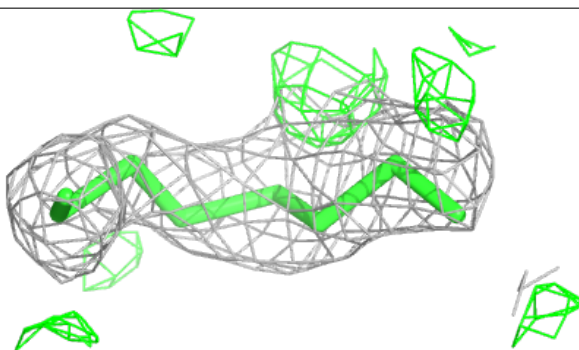
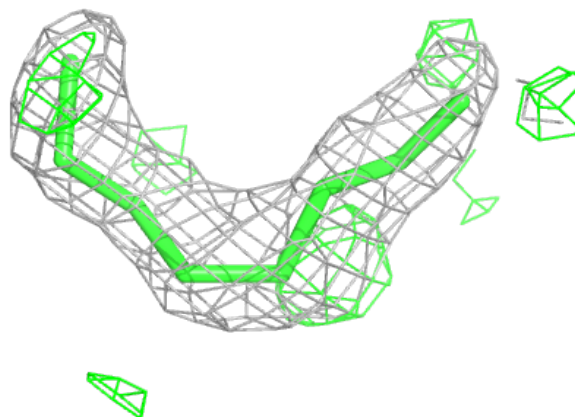


**Electron density around C8E F 407:**

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

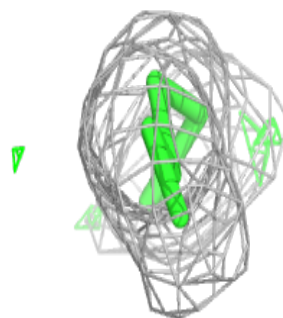
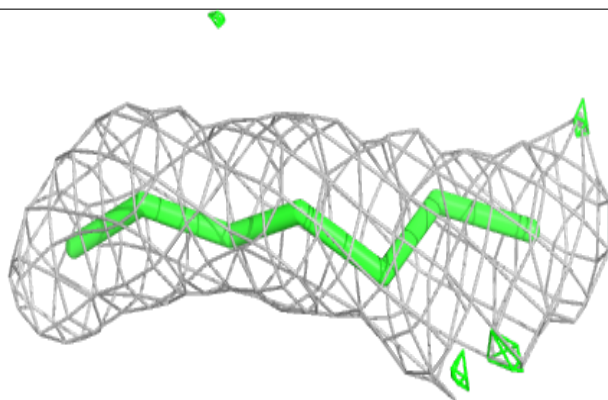
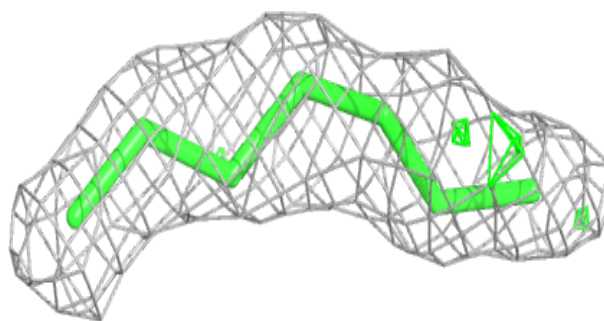
**Electron density around C8E F 408:**

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

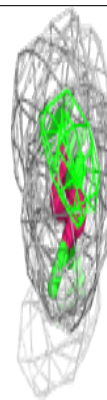
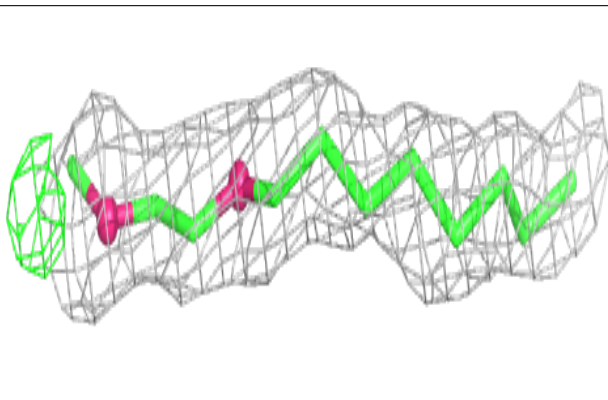
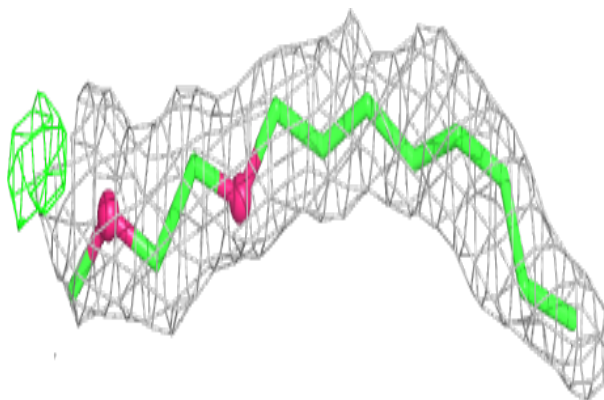


**Electron density around C8E F 404:**

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

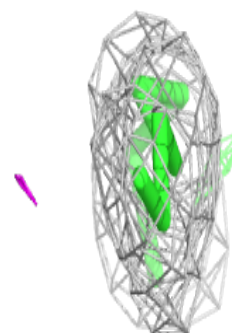
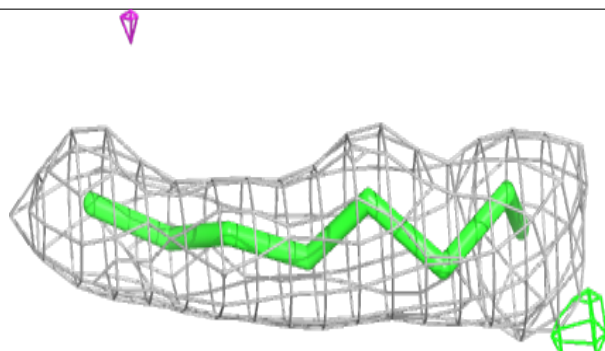
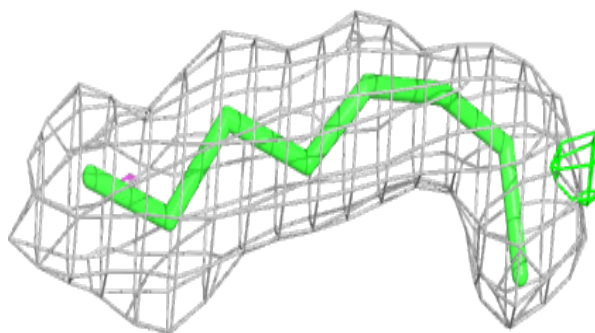
**Electron density around C8E C 405:**

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

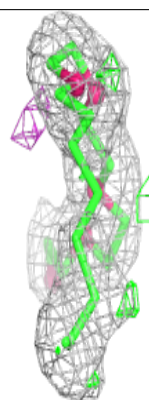
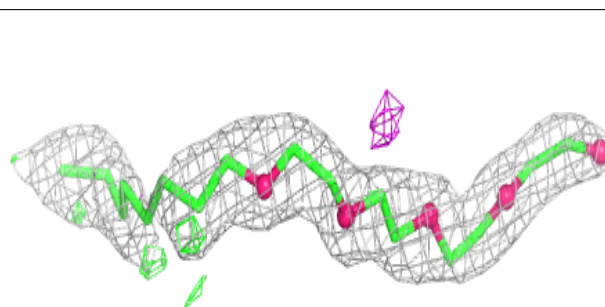
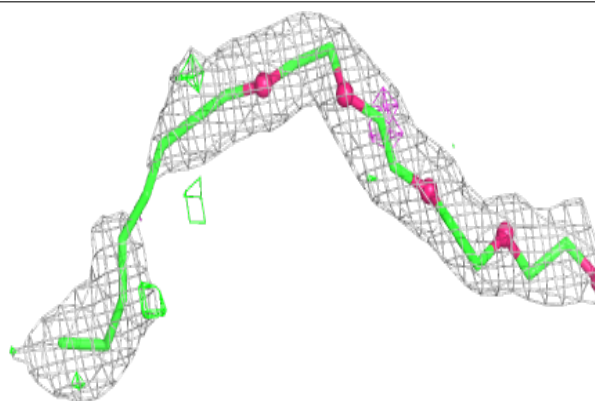


**Electron density around C8E B 408:**

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

**Electron density around C8E A 505:**

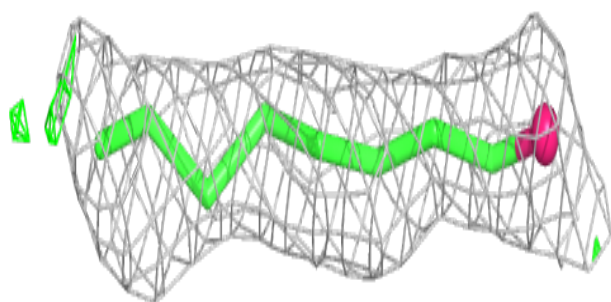
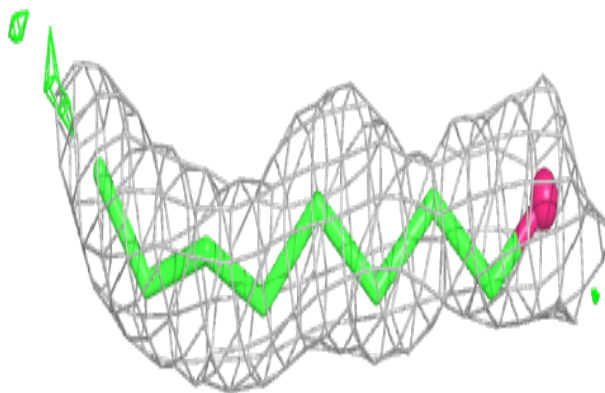
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



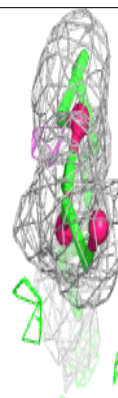
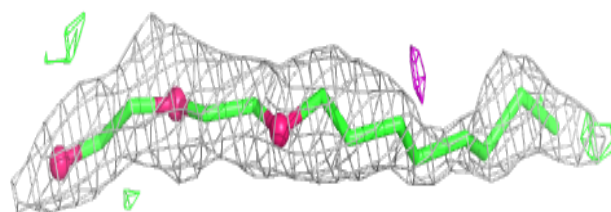
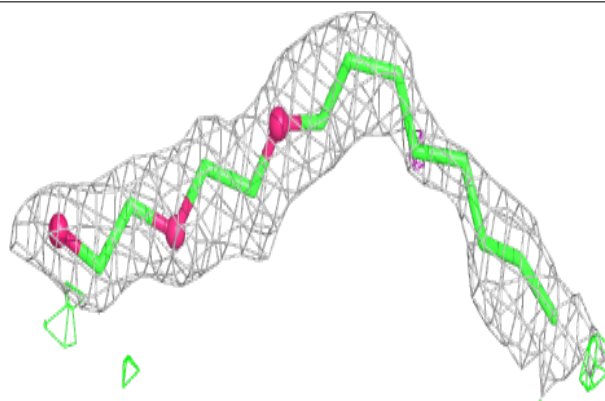


**Electron density around C8E A 509:**

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

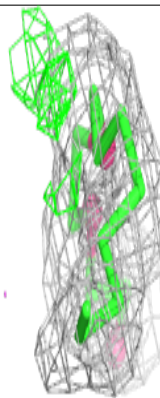
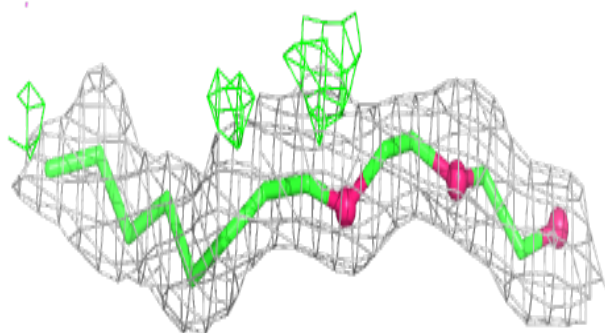
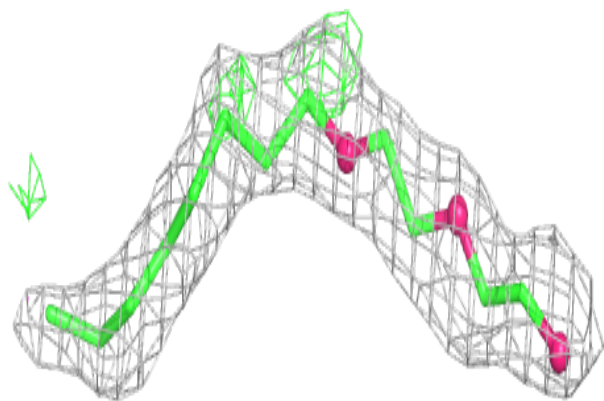
**Electron density around C8E D 507:**

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

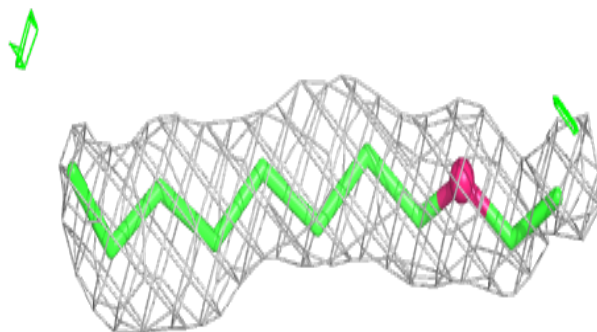
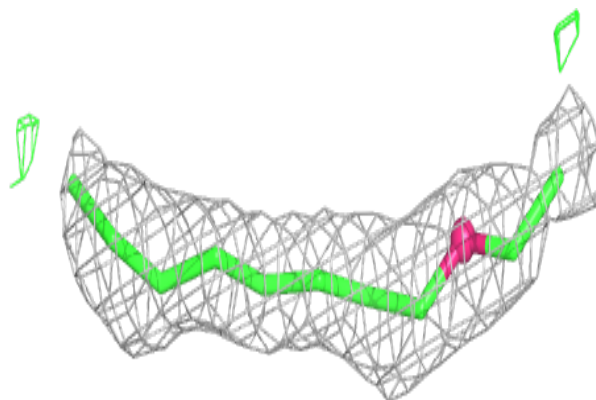


**Electron density around C8E E 402:**

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

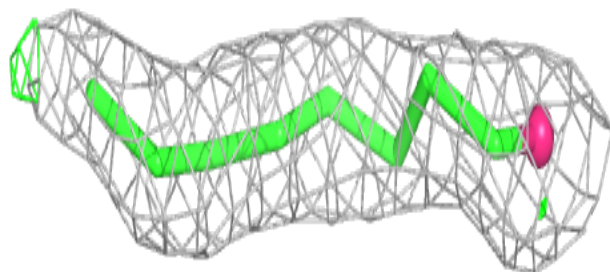
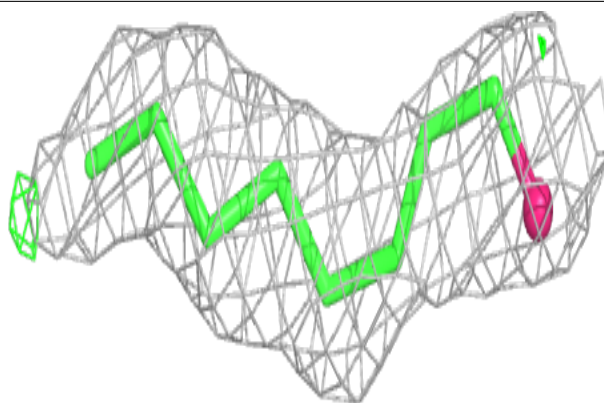
**Electron density around C8E A 502:**

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

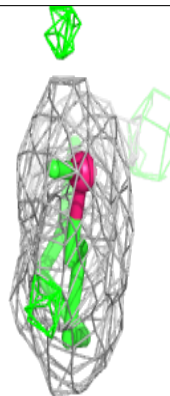
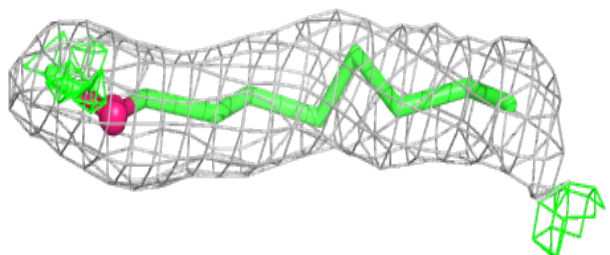
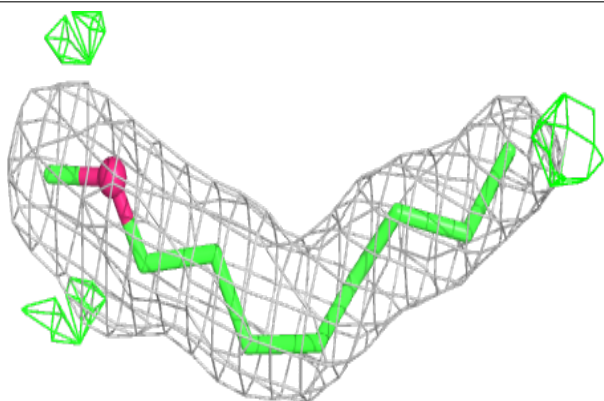


**Electron density around C8E D 502:**

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

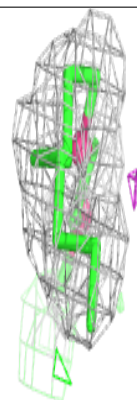
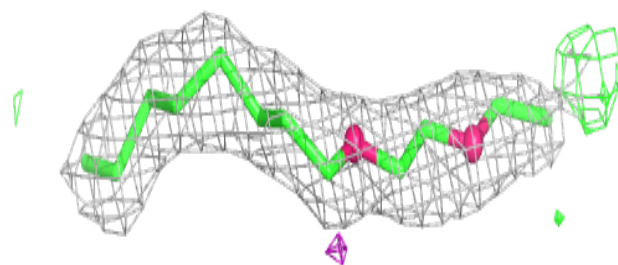
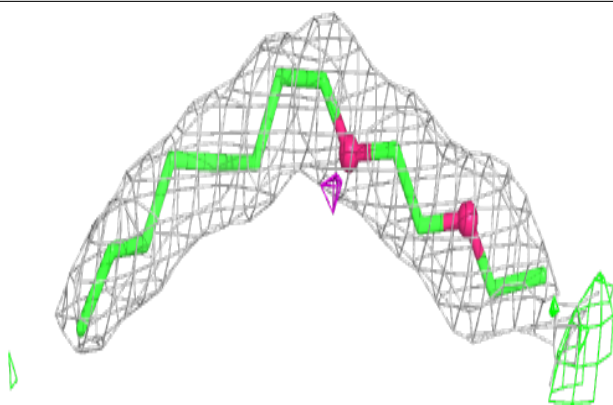
**Electron density around C8E B 409:**

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

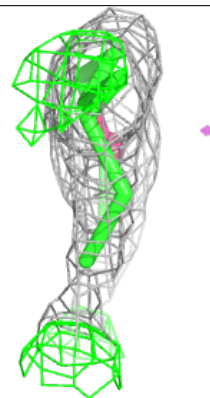
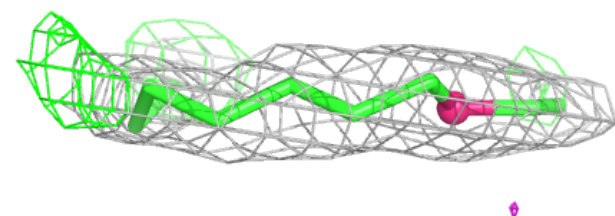
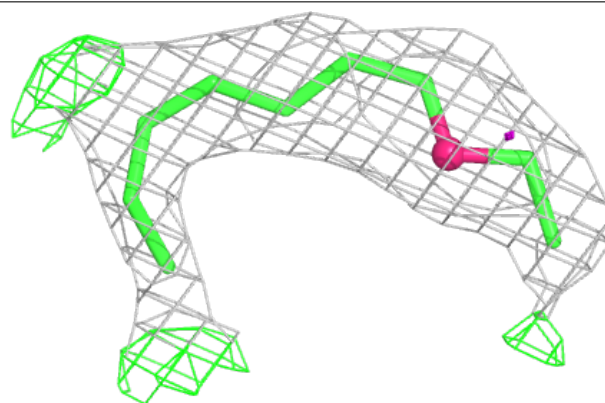


**Electron density around C8E B 403:**

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

**Electron density around C8E B 402:**

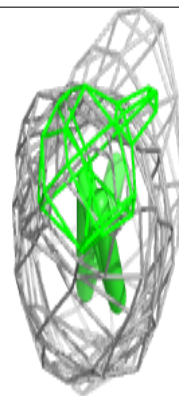
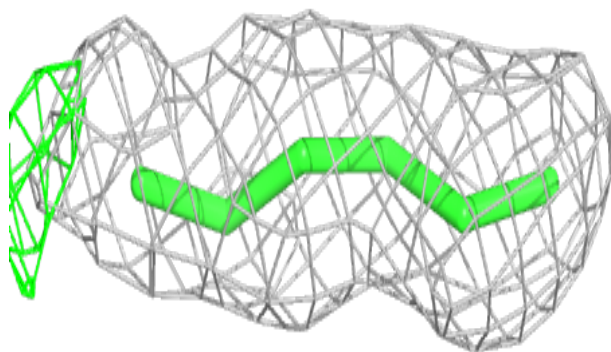
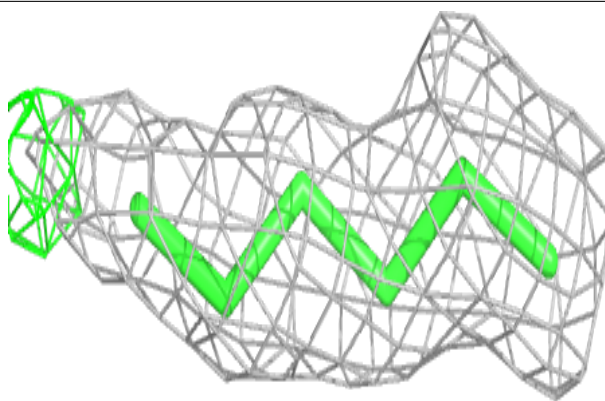
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



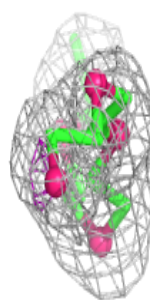
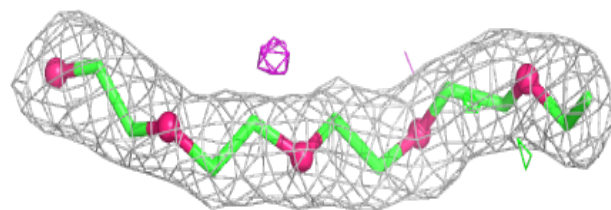
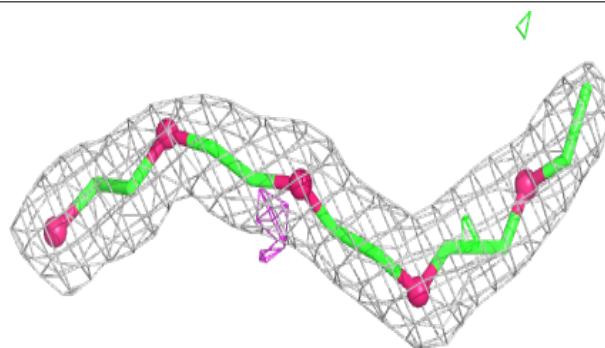


**Electron density around C8E C 403:**

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

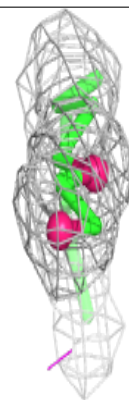
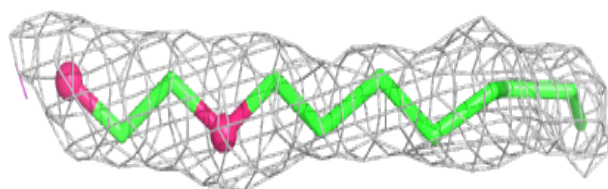
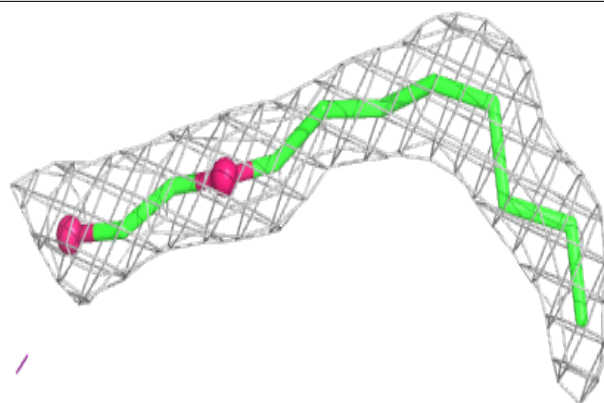
**Electron density around C8E D 508:**

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

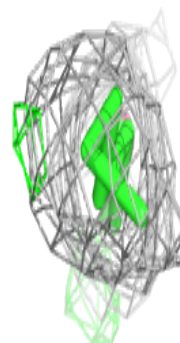
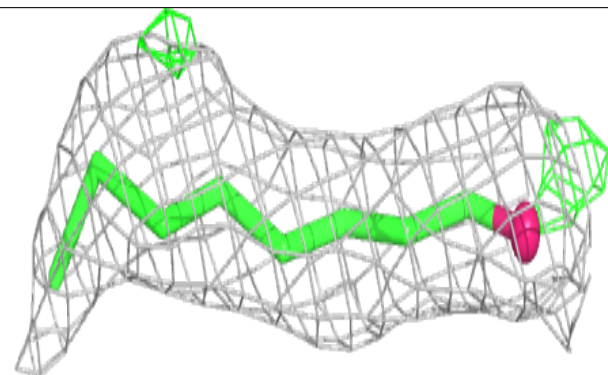
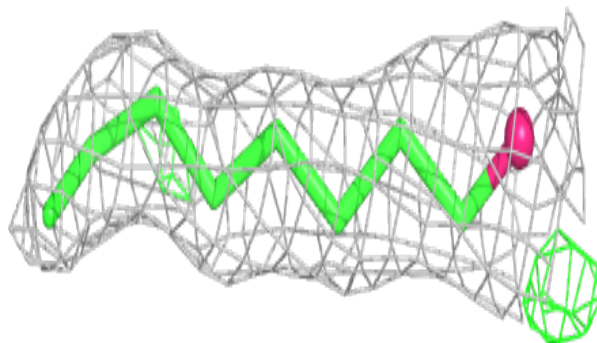


**Electron density around C8E B 411:**

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

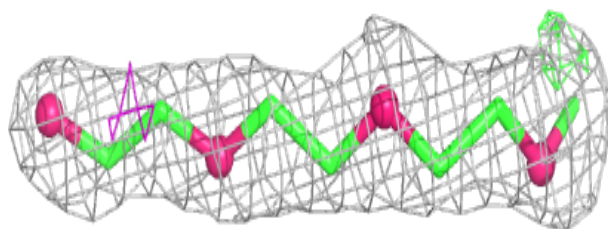
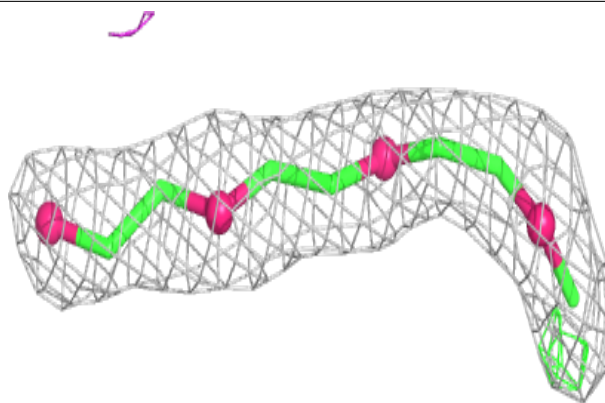
**Electron density around C8E A 508:**

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



**Electron density around C8E D 501:**

$2mF_o-DF_c$  (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.