



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 09:39 PM EST

PDB ID : 4RL8  
Title : Crystal structure of the COG4313 outer membrane channel from *Pseudomonas putida* F1  
Authors : van den Berg, B.  
Deposited on : 2014-10-16  
Resolution : 2.30 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)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

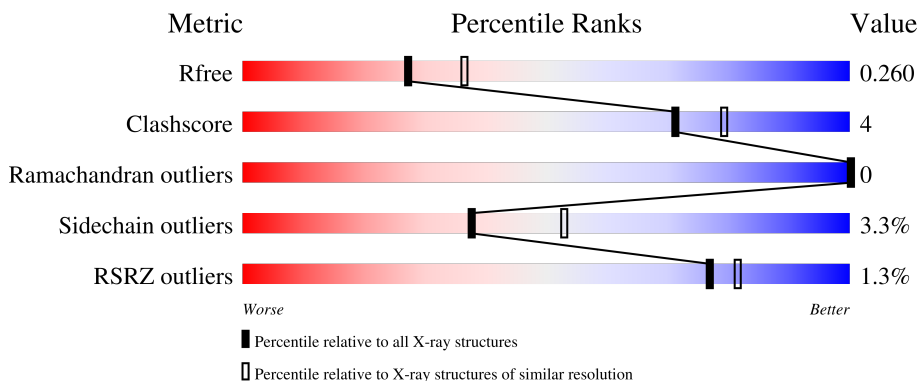
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	275	 3% 87% 9% ..
1	B	275	 % 86% 11% .
1	C	275	 % 90% 7% .
1	D	275	 86% 11% ..

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8823 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 Protein involved in meta-pathway of phenol degradation-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2002	1268	343	389	2	0	0	0
1	B	267	2021	1275	348	396	2	0	0	0
1	C	268	2045	1288	351	404	2	0	1	0
1	D	268	2042	1286	350	404	2	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

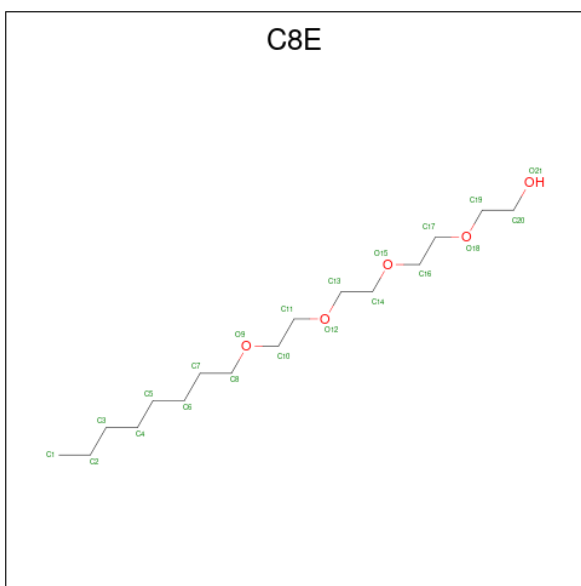
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A5W3Z9
A	269	HIS	-	expression tag	UNP A5W3Z9
A	270	HIS	-	expression tag	UNP A5W3Z9
A	271	HIS	-	expression tag	UNP A5W3Z9
A	272	HIS	-	expression tag	UNP A5W3Z9
A	273	HIS	-	expression tag	UNP A5W3Z9
A	274	HIS	-	expression tag	UNP A5W3Z9
B	0	MET	-	expression tag	UNP A5W3Z9
B	269	HIS	-	expression tag	UNP A5W3Z9
B	270	HIS	-	expression tag	UNP A5W3Z9
B	271	HIS	-	expression tag	UNP A5W3Z9
B	272	HIS	-	expression tag	UNP A5W3Z9
B	273	HIS	-	expression tag	UNP A5W3Z9
B	274	HIS	-	expression tag	UNP A5W3Z9
C	0	MET	-	expression tag	UNP A5W3Z9
C	269	HIS	-	expression tag	UNP A5W3Z9
C	270	HIS	-	expression tag	UNP A5W3Z9
C	271	HIS	-	expression tag	UNP A5W3Z9
C	272	HIS	-	expression tag	UNP A5W3Z9
C	273	HIS	-	expression tag	UNP A5W3Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	274	HIS	-	expression tag	UNP A5W3Z9
D	0	MET	-	expression tag	UNP A5W3Z9
D	269	HIS	-	expression tag	UNP A5W3Z9
D	270	HIS	-	expression tag	UNP A5W3Z9
D	271	HIS	-	expression tag	UNP A5W3Z9
D	272	HIS	-	expression tag	UNP A5W3Z9
D	273	HIS	-	expression tag	UNP A5W3Z9
D	274	HIS	-	expression tag	UNP A5W3Z9

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



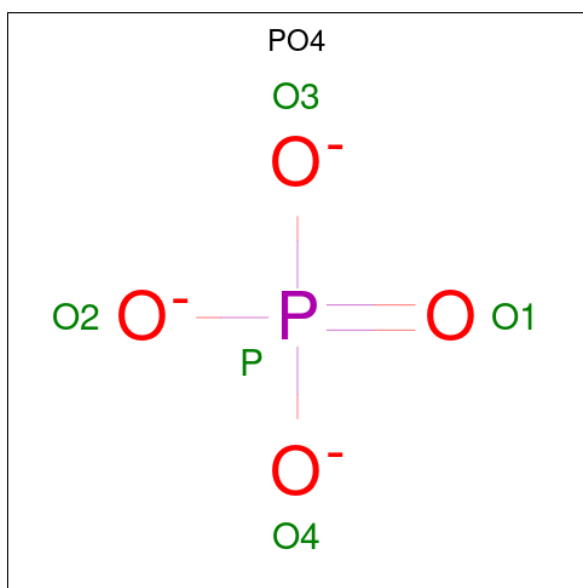
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	5	3		
2	A	1	Total	C	O	0	0
			5	4	1		
2	A	1	Total	C	O	0	0
			9	7	2		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C		0	0
			5	5			
2	A	1	Total	C	O	0	0
			10	7	3		
2	A	1	Total	C	O	0	0
			14	9	5		

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

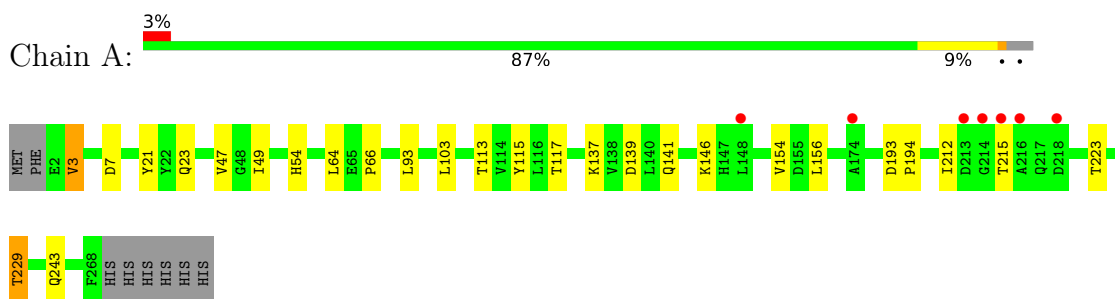
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	97	Total	O	0	0
			97	97		
4	C	111	Total	O	0	0
			111	111		
4	D	110	Total	O	0	0
			110	110		

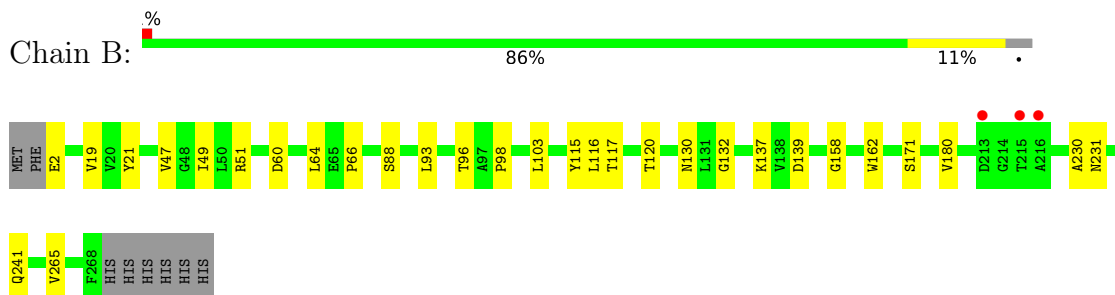
### 3 Residue-property plots [i](#)

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.

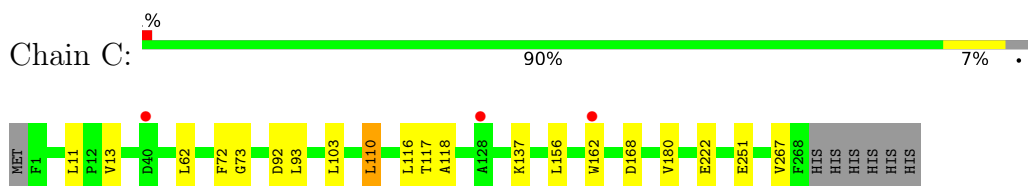
- Molecule 1: Protein involved in meta-pathway of phenol degradation-like protein



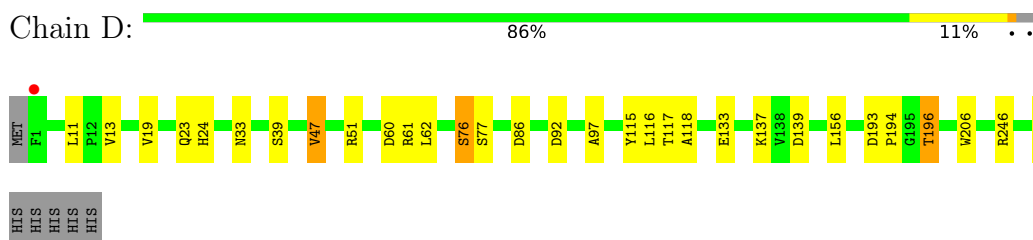
- Molecule 1: Protein involved in meta-pathway of phenol degradation-like protein



- Molecule 1: Protein involved in meta-pathway of phenol degradation-like protein



- Molecule 1: Protein involved in meta-pathway of phenol degradation-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.05Å 120.31Å 131.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 48.10 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-2.30) 94.4 (48.10-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.213 , 0.253 0.217 , 0.260	Depositor DCC
$R_{free}$ test set	3660 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.437	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9623e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: C8E, PO4

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	0/2044	0.54	0/2788
1	B	0.34	0/2063	0.52	0/2812
1	C	0.34	0/2091	0.52	0/2851
1	D	0.34	0/2083	0.53	0/2837
All	All	0.34	0/8281	0.53	0/11288

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	2002	0	1871	16	0
1	B	2021	0	1908	17	0
1	C	2045	0	1924	9	0
1	D	2042	0	1933	17	1
2	A	94	0	120	6	0
2	B	65	0	92	5	0
2	C	78	0	106	1	0
2	D	71	0	101	4	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	82	0	0	1	0
4	B	97	0	0	1	0
4	C	111	0	0	0	1
4	D	110	0	0	2	0
All	All	8823	0	8055	58	1

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 4.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:HB	1:A:243:GLN:HG3	1.64	0.78
2:A:309:C8E:H71	1:C:73:GLY:HA2	1.73	0.69
1:B:103:LEU:HD13	2:B:302:C8E:H31	1.80	0.63
1:D:117:THR:HB	1:D:137:LYS:HB2	1.82	0.62
1:A:3:VAL:HG23	1:A:7:ASP:HB2	1.82	0.61
1:D:265:VAL:HG11	2:D:305:C8E:H71	1.83	0.61
2:A:309:C8E:H51	1:C:72:PHE:CE2	2.38	0.58
1:D:97:ALA:O	2:D:303:C8E:H31	2.04	0.57
1:A:103:LEU:HD13	2:A:301:C8E:H161	1.84	0.57
1:A:115:TYR:HB2	1:A:139:ASP:HB3	1.86	0.57
1:C:117:THR:HB	1:C:137:LYS:HB2	1.87	0.57
1:A:229:THR:HG21	1:A:243:GLN:HE21	1.71	0.56
1:D:23:GLN:HB2	1:D:47:VAL:HG22	1.89	0.54
1:B:19:VAL:HB	1:B:51:ARG:HB3	1.91	0.53
1:C:103:LEU:HD21	1:C:110:LEU:HD13	1.91	0.52
1:D:193:ASP:HB2	1:D:194:PRO:HD2	1.91	0.52
1:C:156:LEU:HG	2:C:305:C8E:H71	1.92	0.52
1:B:117:THR:HB	1:B:137:LYS:HB2	1.90	0.52
1:B:2:GLU:OE1	1:B:2:GLU:N	2.45	0.50
1:B:115:TYR:HB2	1:B:139:ASP:HB3	1.94	0.50
1:D:77:SER:O	4:D:483:HOH:O	2.20	0.49
1:B:265:VAL:HG11	2:B:301:C8E:H171	1.94	0.49
4:A:415:HOH:O	1:D:196:THR:HG21	2.13	0.49
1:A:156:LEU:HG	2:A:308:C8E:H81	1.94	0.48
1:B:158:GLY:HA3	2:B:302:C8E:H192	1.95	0.48
1:A:193:ASP:HB2	1:A:194:PRO:HD2	1.96	0.47
1:D:206:TRP:HH2	2:D:301:C8E:H102	1.79	0.47
1:D:76:SER:HB3	1:D:86:ASP:OD2	2.15	0.47
1:D:133:GLU:OE1	1:D:137:LYS:NZ	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:VAL:HG23	4:B:461:HOH:O	2.14	0.47
1:B:64:LEU:HG	1:B:66:PRO:HD3	1.97	0.46
1:B:120:THR:HB	1:D:24:HIS:CE1	2.51	0.46
1:A:117:THR:HB	1:A:137:LYS:HB2	1.98	0.45
1:D:115:TYR:HB2	1:D:139:ASP:HB3	1.97	0.45
1:B:21:TYR:HB2	1:B:49:ILE:HB	1.97	0.45
1:D:60:ASP:OD1	1:D:61:ARG:HG3	2.16	0.45
1:B:130:ASN:HB3	1:B:132:GLY:O	2.16	0.45
1:D:19:VAL:HB	1:D:51:ARG:HB3	1.98	0.45
1:A:113:THR:HG22	1:A:141:GLN:HB3	1.99	0.44
1:A:212:ILE:O	1:A:215:THR:HG22	2.17	0.44
2:A:309:C8E:H51	1:C:72:PHE:HE2	1.79	0.44
1:B:162:TRP:CD1	1:B:180:VAL:HG22	2.52	0.44
1:A:21:TYR:HB2	1:A:49:ILE:HB	2.00	0.44
1:A:23:GLN:HB2	1:A:47:VAL:HG12	2.00	0.44
1:A:229:THR:CB	1:A:243:GLN:HG3	2.43	0.43
1:A:54:HIS:CE1	2:A:310:C8E:H32	2.53	0.43
1:D:246:ARG:NH1	4:D:466:HOH:O	2.38	0.43
1:D:156:LEU:HG	2:D:301:C8E:H51	2.01	0.43
1:C:162[A]:TRP:CD1	1:C:180:VAL:HG22	2.54	0.42
1:C:222:GLU:HB3	1:C:251:GLU:HB2	2.00	0.42
1:B:96:THR:HG23	1:B:98:PRO:HD3	2.01	0.42
1:C:92:ASP:HB3	1:C:118:ALA:O	2.19	0.42
1:B:230:ALA:HB1	2:B:303:C8E:H172	2.02	0.42
1:A:64:LEU:HG	1:A:66:PRO:HD3	2.02	0.41
1:D:92:ASP:HB3	1:D:118:ALA:O	2.19	0.41
1:A:146:LYS:HB3	1:A:154:VAL:HG13	2.02	0.41
1:B:231:ASN:HB3	1:B:241:GLN:HB2	2.03	0.41
1:B:158:GLY:CA	2:B:302:C8E:H192	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ASN:OD1	4:C:510:HOH:O[2_555]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/275 (96%)	263 (99%)	2 (1%)	0	100	100
1	B	265/275 (96%)	261 (98%)	4 (2%)	0	100	100
1	C	267/275 (97%)	265 (99%)	2 (1%)	0	100	100
1	D	266/275 (97%)	262 (98%)	4 (2%)	0	100	100
All	All	1063/1100 (97%)	1051 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/226 (86%)	191 (98%)	4 (2%)	53	70
1	B	203/226 (90%)	197 (97%)	6 (3%)	41	57
1	C	206/226 (91%)	198 (96%)	8 (4%)	32	46
1	D	206/226 (91%)	197 (96%)	9 (4%)	28	39
All	All	810/904 (90%)	783 (97%)	27 (3%)	38	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	223	THR
1	A	229	THR
1	B	47	VAL
1	B	60	ASP
1	B	88	SER
1	B	93	LEU
1	B	116	LEU
1	B	171	SER
1	C	11	LEU
1	C	13	VAL
1	C	62	LEU
1	C	93	LEU
1	C	110	LEU
1	C	116	LEU
1	C	168	ASP
1	C	267	VAL
1	D	11	LEU
1	D	13	VAL
1	D	39	SER
1	D	47	VAL
1	D	62	LEU
1	D	76	SER
1	D	116	LEU
1	D	196	THR
1	D	267	VAL

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

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C8E	A	306	-	9,9,20	0.50	0	8,8,19	0.38	0
2	C8E	A	303	-	8,8,20	0.37	0	7,7,19	0.34	0
2	C8E	A	307	-	12,12,20	0.38	0	10,10,19	0.29	0
2	C8E	D	305	-	11,11,20	0.33	0	10,10,19	0.47	0
2	C8E	B	304	-	7,7,20	0.35	0	5,5,19	0.31	0
2	C8E	D	307	-	10,10,20	0.42	0	9,9,19	0.29	0
2	C8E	D	302	-	4,4,20	0.29	0	3,3,19	0.45	0
2	C8E	A	308	-	8,8,20	0.32	0	6,6,19	0.35	0
2	C8E	A	301	-	7,7,20	0.38	0	6,6,19	0.21	0
2	C8E	C	304	-	14,14,20	0.33	0	11,11,19	0.47	0
2	C8E	D	304	-	5,5,20	0.48	0	4,4,19	0.30	0
2	C8E	C	301	-	12,12,20	0.39	0	10,10,19	0.43	0
2	C8E	A	309	-	9,9,20	0.31	0	8,8,19	0.46	0
2	C8E	B	303	-	14,14,20	0.40	0	12,12,19	0.24	0
2	C8E	A	304	-	12,12,20	0.47	0	11,11,19	0.29	0
2	C8E	D	306	-	12,12,20	0.38	0	9,9,19	0.33	0
2	C8E	C	305	-	10,10,20	0.40	0	8,8,19	0.38	0
2	C8E	C	302	-	13,13,20	0.42	0	12,12,19	0.23	0
2	C8E	D	303	-	9,9,20	0.40	0	8,8,19	0.34	0
2	C8E	B	302	-	15,15,20	0.35	0	13,13,19	0.42	0
2	C8E	A	302	-	4,4,20	0.30	0	3,3,19	0.29	0
2	C8E	A	305	-	4,4,20	0.29	0	3,3,19	0.36	0
2	C8E	B	301	-	9,9,20	0.40	0	8,8,19	0.35	0
2	C8E	B	305	-	12,12,20	0.38	0	11,11,19	0.39	0
2	C8E	C	306	-	8,8,20	0.33	0	6,6,19	0.58	0
2	C8E	A	310	-	8,8,20	0.33	0	6,6,19	0.41	0
3	PO4	A	311	-	4,4,4	0.94	0	6,6,6	0.44	0
2	C8E	C	303	-	10,10,20	0.36	0	9,9,19	0.51	0
2	C8E	D	301	-	11,11,20	0.32	0	10,10,19	0.51	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	A	306	-	-	4/7/7/18	-
2	C8E	A	303	-	-	4/6/6/18	-
2	C8E	A	307	-	-	6/8/8/18	-
2	C8E	D	305	-	-	5/9/9/18	-
2	C8E	B	304	-	-	3/3/3/18	-
2	C8E	D	307	-	-	4/8/8/18	-
2	C8E	D	302	-	-	1/2/2/18	-
2	C8E	A	308	-	-	1/4/4/18	-
2	C8E	A	301	-	-	4/5/5/18	-
2	C8E	C	304	-	-	4/8/8/18	-
2	C8E	D	304	-	-	3/3/3/18	-
2	C8E	C	301	-	-	6/8/8/18	-
2	C8E	A	309	-	-	6/7/7/18	-
2	C8E	B	303	-	-	9/10/10/18	-
2	C8E	A	304	-	-	5/10/10/18	-
2	C8E	D	306	-	-	5/6/6/18	-
2	C8E	C	305	-	-	2/6/6/18	-
2	C8E	C	302	-	-	5/11/11/18	-
2	C8E	D	303	-	-	3/7/7/18	-
2	C8E	B	302	-	-	7/11/11/18	-
2	C8E	A	302	-	-	0/2/2/18	-
2	C8E	A	305	-	-	1/2/2/18	-
2	C8E	B	301	-	-	5/7/7/18	-
2	C8E	B	305	-	-	6/10/10/18	-
2	C8E	C	306	-	-	0/4/4/18	-
2	C8E	A	310	-	-	3/4/4/18	-
2	C8E	C	303	-	-	4/8/8/18	-
2	C8E	D	301	-	-	5/9/9/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	305	C8E	C3-C4-C5-C6
2	D	307	C8E	O15-C16-C17-O18
2	A	306	C8E	O12-C13-C14-O15
2	D	307	C8E	O12-C13-C14-O15
2	A	306	C8E	O9-C10-C11-O12
2	B	301	C8E	O18-C19-C20-O21
2	B	303	C8E	O18-C19-C20-O21
2	D	304	C8E	O12-C13-C14-O15
2	D	307	C8E	O18-C19-C20-O21
2	B	301	C8E	O15-C16-C17-O18
2	A	304	C8E	O18-C19-C20-O21
2	A	307	C8E	O18-C19-C20-O21
2	A	303	C8E	C6-C7-C8-O9
2	B	305	C8E	C6-C7-C8-O9
2	D	305	C8E	C6-C7-C8-O9
2	A	309	C8E	C6-C7-C8-O9
2	A	307	C8E	O15-C16-C17-O18
2	B	302	C8E	O18-C19-C20-O21
2	D	303	C8E	C3-C4-C5-C6
2	D	306	C8E	O15-C16-C17-O18
2	D	301	C8E	C2-C3-C4-C5
2	A	309	C8E	C4-C5-C6-C7
2	C	303	C8E	C2-C3-C4-C5
2	C	301	C8E	O12-C13-C14-O15
2	D	306	C8E	O18-C19-C20-O21
2	A	310	C8E	O9-C10-C11-O12
2	B	304	C8E	O9-C10-C11-O12
2	A	309	C8E	C7-C8-O9-C10
2	C	304	C8E	C7-C8-O9-C10
2	B	303	C8E	O9-C10-C11-O12
2	C	303	C8E	C3-C4-C5-C6
2	B	303	C8E	C5-C6-C7-C8
2	D	305	C8E	C2-C3-C4-C5
2	A	309	C8E	C3-C4-C5-C6
2	B	303	C8E	C6-C7-C8-O9
2	B	304	C8E	C2-C3-C4-C5
2	A	301	C8E	O18-C19-C20-O21
2	A	307	C8E	O9-C10-C11-O12
2	B	301	C8E	O12-C13-C14-O15
2	C	304	C8E	C2-C3-C4-C5
2	B	302	C8E	C2-C3-C4-C5
2	A	308	C8E	C4-C5-C6-C7
2	D	301	C8E	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	C	301	C8E	C7-C8-O9-C10
2	B	305	C8E	C10-C11-O12-C13
2	B	302	C8E	C1-C2-C3-C4
2	A	310	C8E	C2-C3-C4-C5
2	A	305	C8E	C1-C2-C3-C4
2	B	305	C8E	O9-C10-C11-O12
2	C	304	C8E	O12-C13-C14-O15
2	D	306	C8E	C2-C3-C4-C5
2	D	301	C8E	C3-C4-C5-C6
2	C	302	C8E	O9-C10-C11-O12
2	A	309	C8E	C5-C6-C7-C8
2	B	303	C8E	C20-C19-O18-C17
2	C	301	C8E	C14-C13-O12-C11
2	C	302	C8E	C14-C13-O12-C11
2	B	301	C8E	C20-C19-O18-C17
2	B	302	C8E	C13-C14-O15-C16
2	A	301	C8E	C17-C16-O15-C14
2	D	304	C8E	C10-C11-O12-C13
2	C	302	C8E	C17-C16-O15-C14
2	D	305	C8E	C4-C5-C6-C7
2	C	303	C8E	C7-C8-O9-C10
2	C	301	C8E	C10-C11-O12-C13
2	D	306	C8E	C16-C17-O18-C19
2	A	304	C8E	C20-C19-O18-C17
2	A	307	C8E	C11-C10-O9-C8
2	A	309	C8E	C2-C3-C4-C5
2	C	304	C8E	C3-C4-C5-C6
2	C	301	C8E	C11-C10-O9-C8
2	D	303	C8E	C2-C3-C4-C5
2	B	303	C8E	C10-C11-O12-C13
2	A	304	C8E	C17-C16-O15-C14
2	D	303	C8E	C5-C6-C7-C8
2	B	302	C8E	O12-C13-C14-O15
2	C	302	C8E	O15-C16-C17-O18
2	A	301	C8E	C16-C17-O18-C19
2	A	303	C8E	C7-C8-O9-C10
2	A	303	C8E	C10-C11-O12-C13
2	A	304	C8E	O15-C16-C17-O18
2	D	301	C8E	C4-C5-C6-C7
2	A	306	C8E	C11-C10-O9-C8
2	B	305	C8E	C7-C8-O9-C10
2	B	303	C8E	C4-C5-C6-C7

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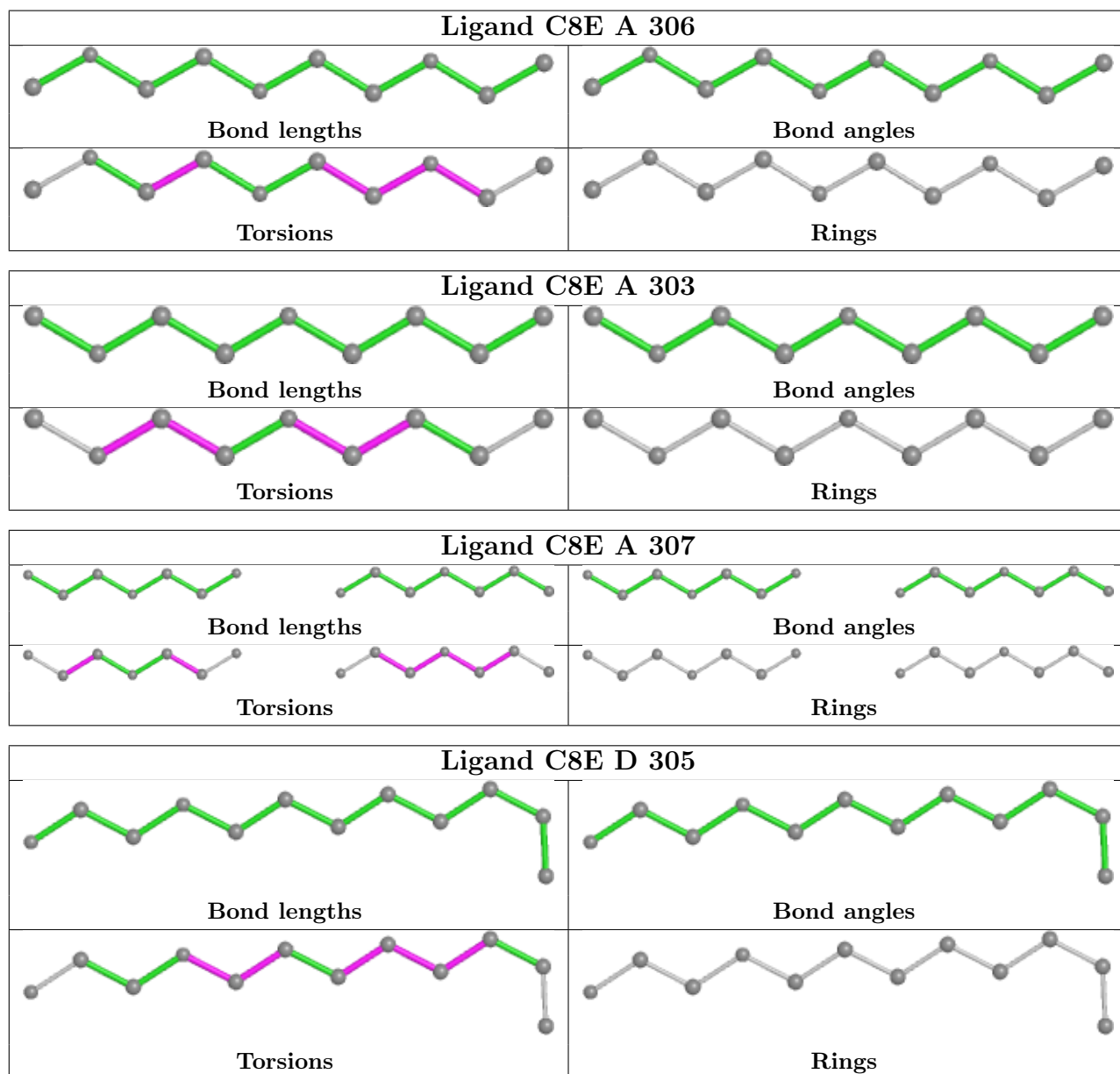
Mol	Chain	Res	Type	Atoms
2	B	301	C8E	C13-C14-O15-C16
2	A	307	C8E	C7-C8-O9-C10
2	B	303	C8E	C7-C8-O9-C10
2	B	305	C8E	C4-C5-C6-C7
2	C	305	C8E	C13-C14-O15-C16
2	D	307	C8E	C14-C13-O12-C11
2	D	301	C8E	C7-C8-O9-C10
2	A	303	C8E	O9-C10-C11-O12
2	A	301	C8E	O15-C16-C17-O18
2	D	302	C8E	C2-C3-C4-C5
2	A	307	C8E	C6-C7-C8-O9
2	C	303	C8E	C4-C5-C6-C7
2	D	306	C8E	C1-C2-C3-C4
2	B	303	C8E	C16-C17-O18-C19
2	A	310	C8E	C1-C2-C3-C4
2	C	302	C8E	C10-C11-O12-C13
2	D	305	C8E	C7-C8-O9-C10
2	C	305	C8E	C6-C7-C8-O9
2	C	301	C8E	O9-C10-C11-O12
2	A	304	C8E	C10-C11-O12-C13
2	B	304	C8E	C1-C2-C3-C4
2	A	306	C8E	C7-C8-O9-C10
2	B	302	C8E	C16-C17-O18-C19
2	B	302	C8E	C4-C5-C6-C7
2	D	305	C8E	C3-C4-C5-C6
2	D	304	C8E	C14-C13-O12-C11

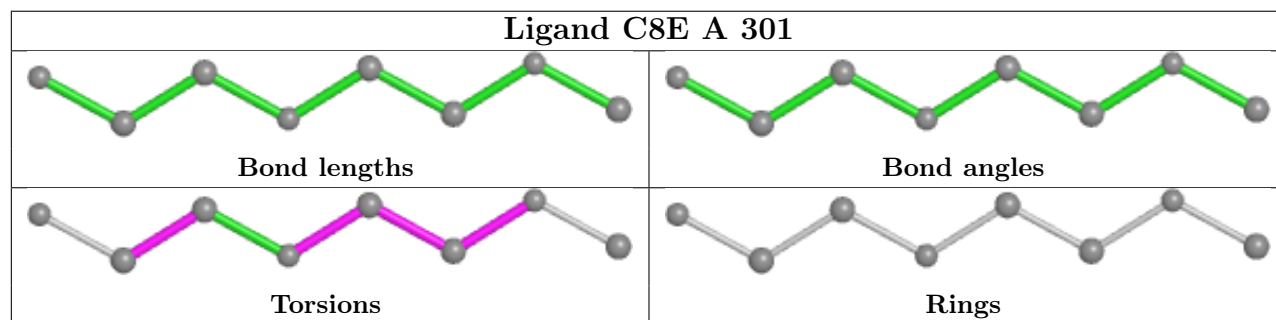
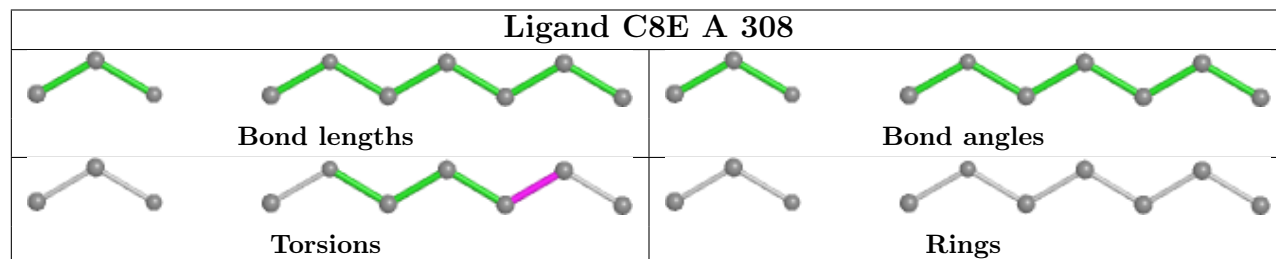
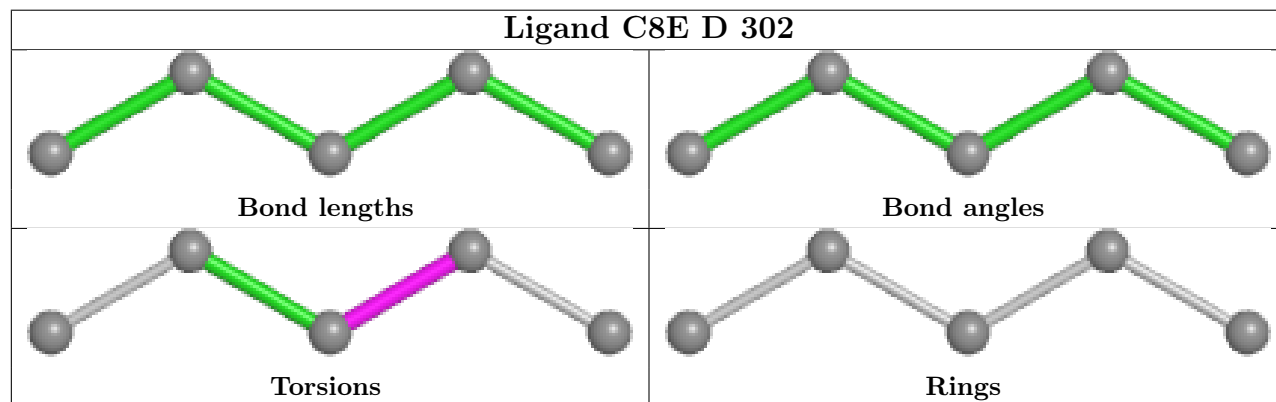
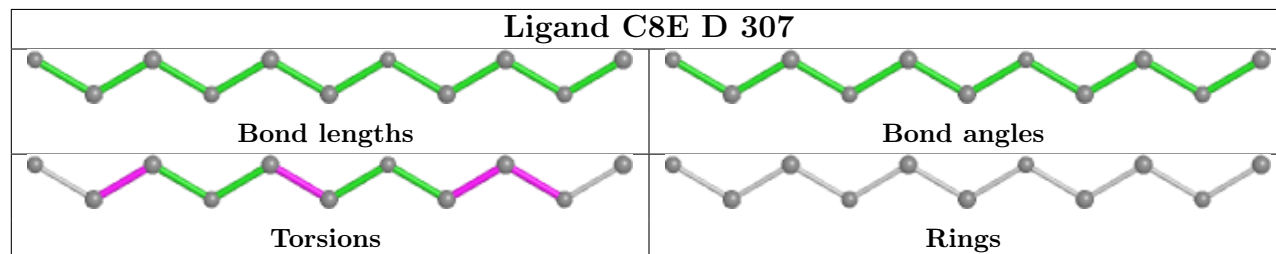
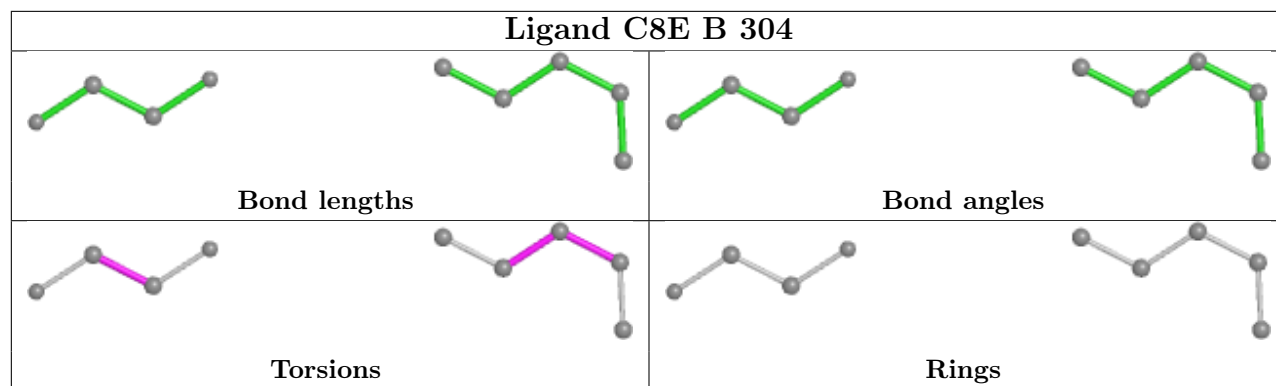
There are no ring outliers.

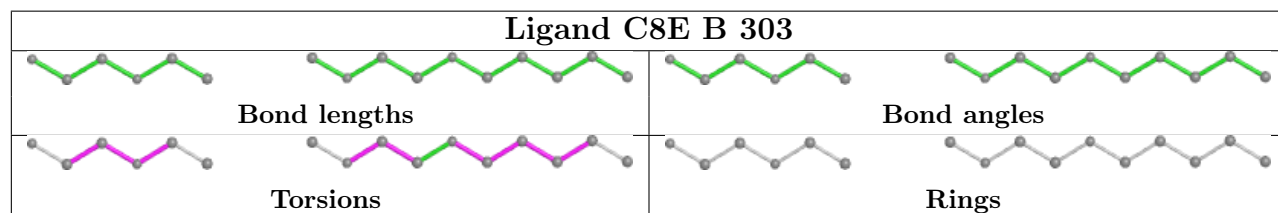
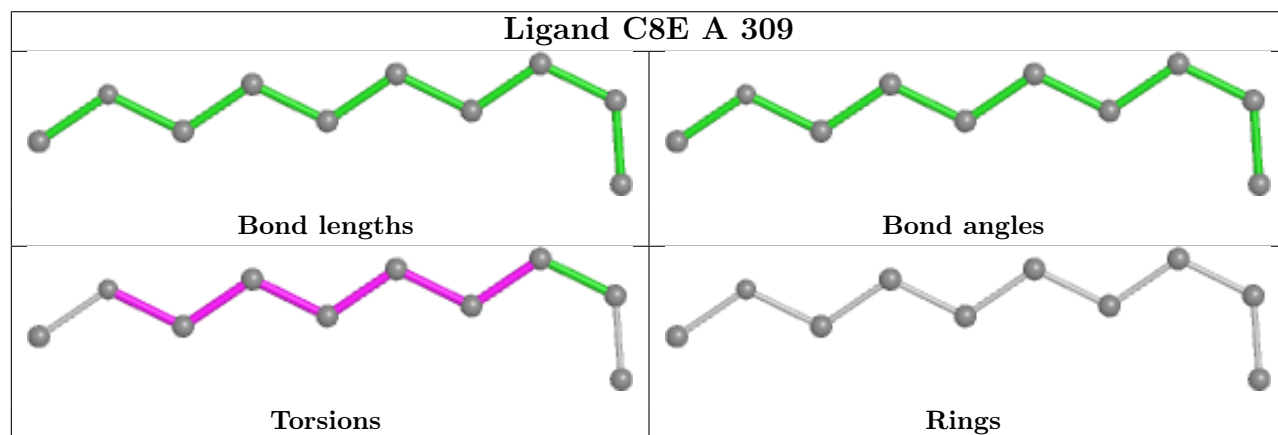
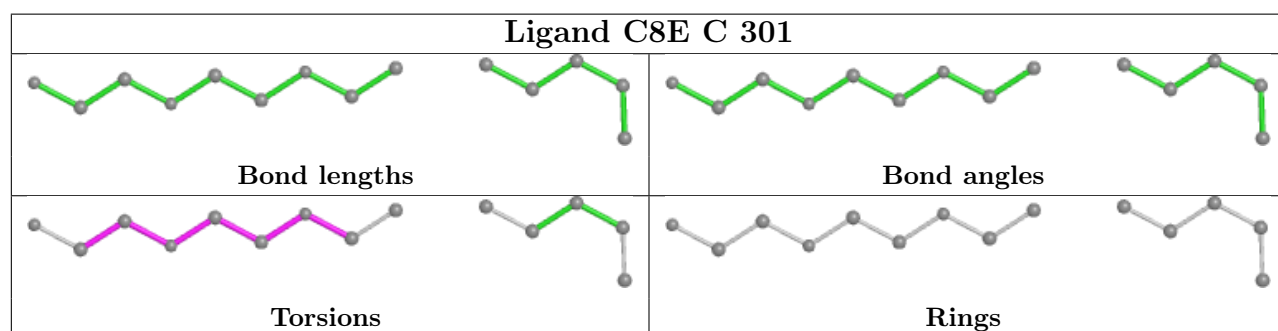
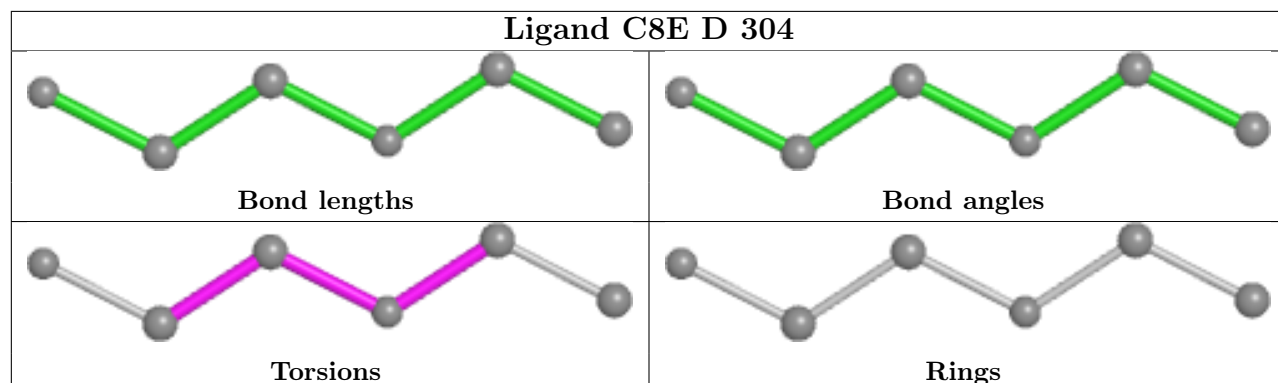
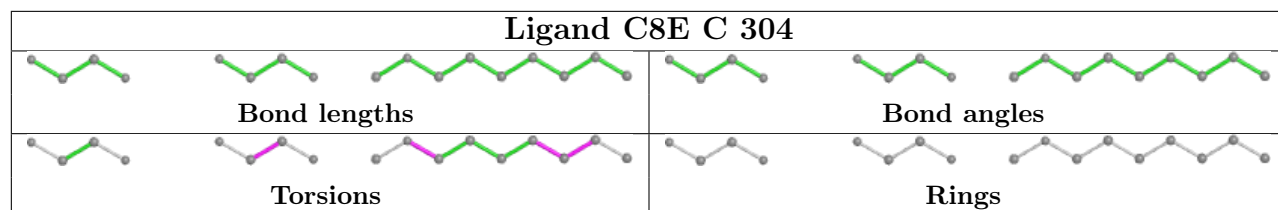
11 monomers are involved in 16 short contacts:

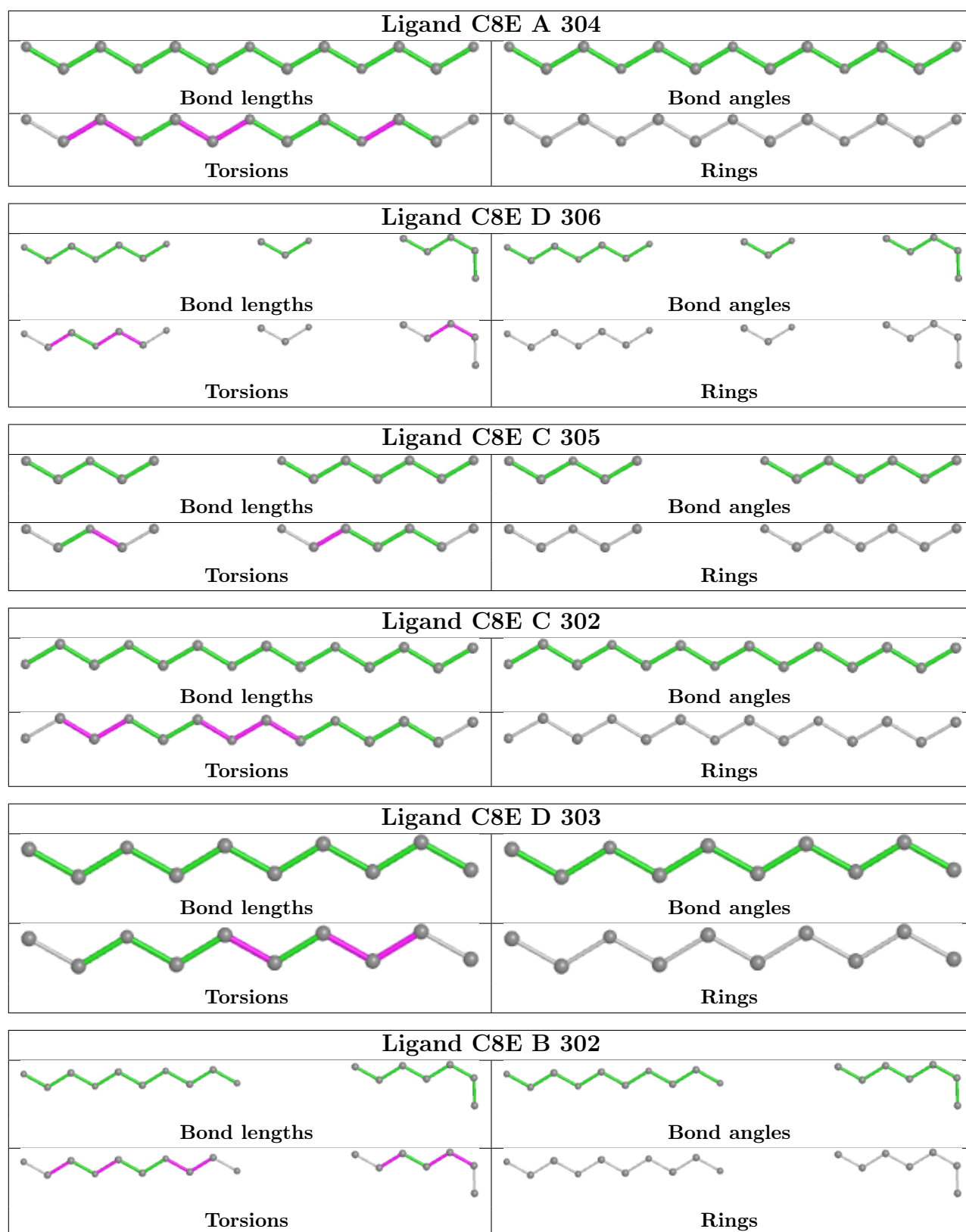
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	305	C8E	1	0
2	A	308	C8E	1	0
2	A	301	C8E	1	0
2	A	309	C8E	3	0
2	B	303	C8E	1	0
2	C	305	C8E	1	0
2	D	303	C8E	1	0
2	B	302	C8E	3	0
2	B	301	C8E	1	0
2	A	310	C8E	1	0
2	D	301	C8E	2	0

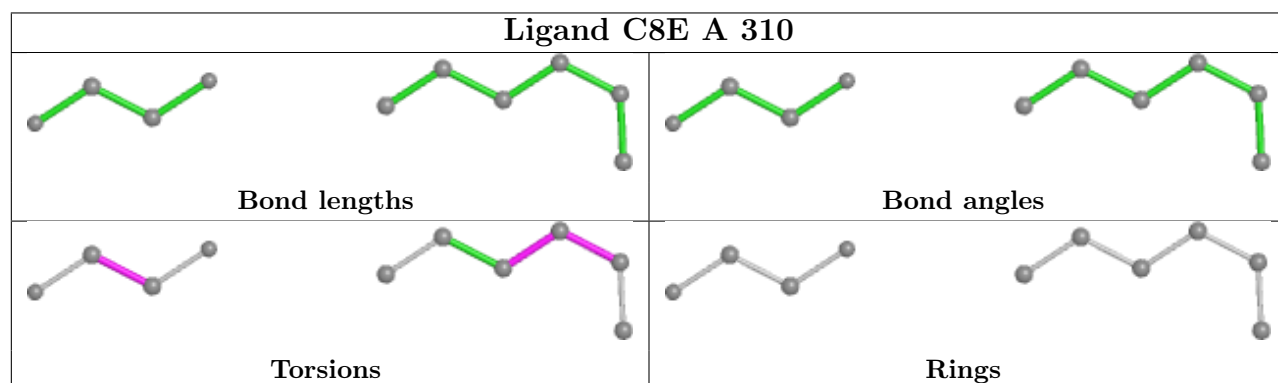
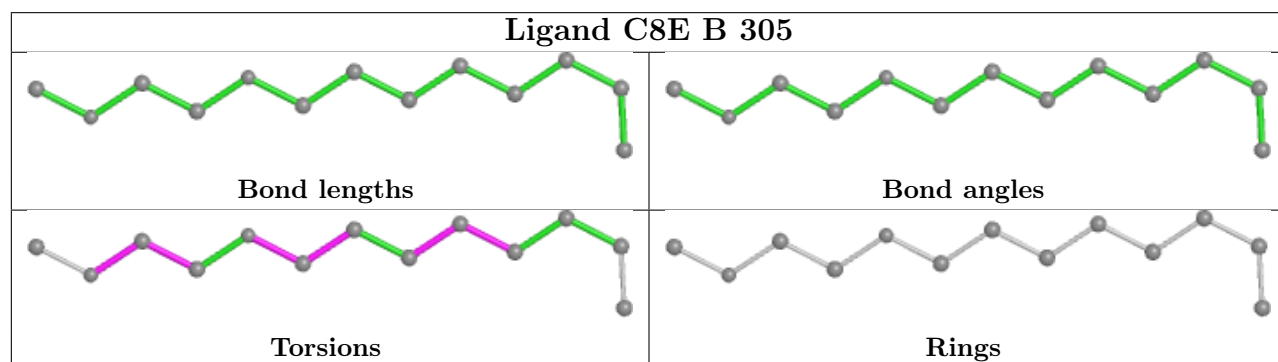
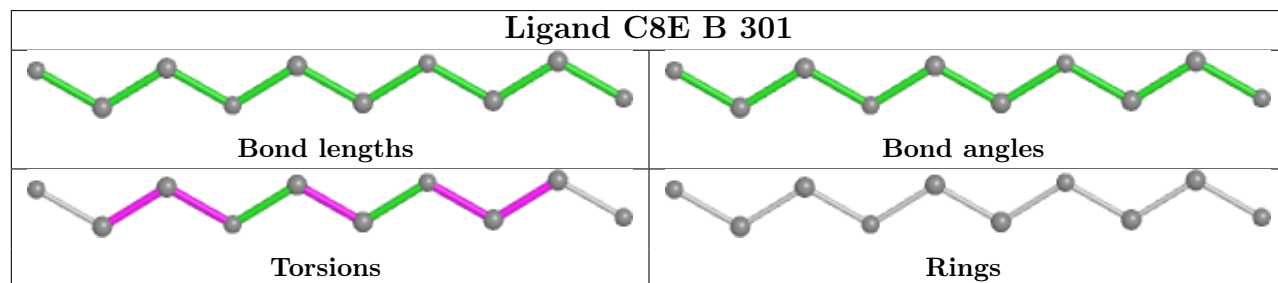
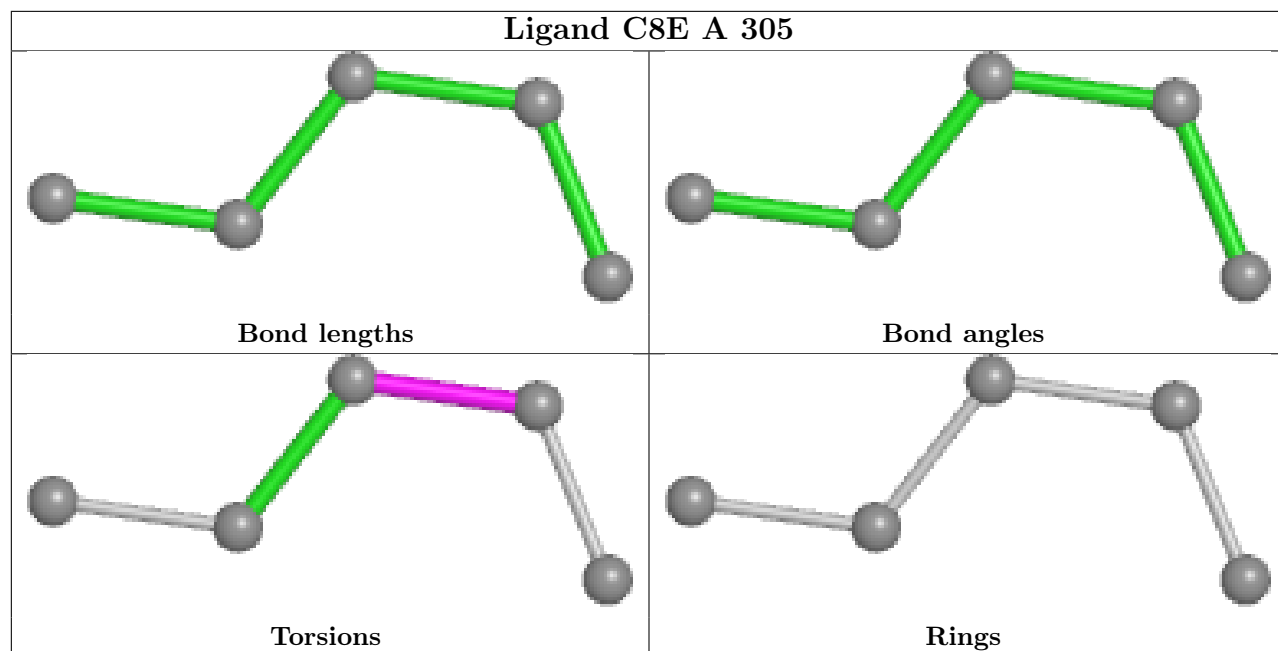
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

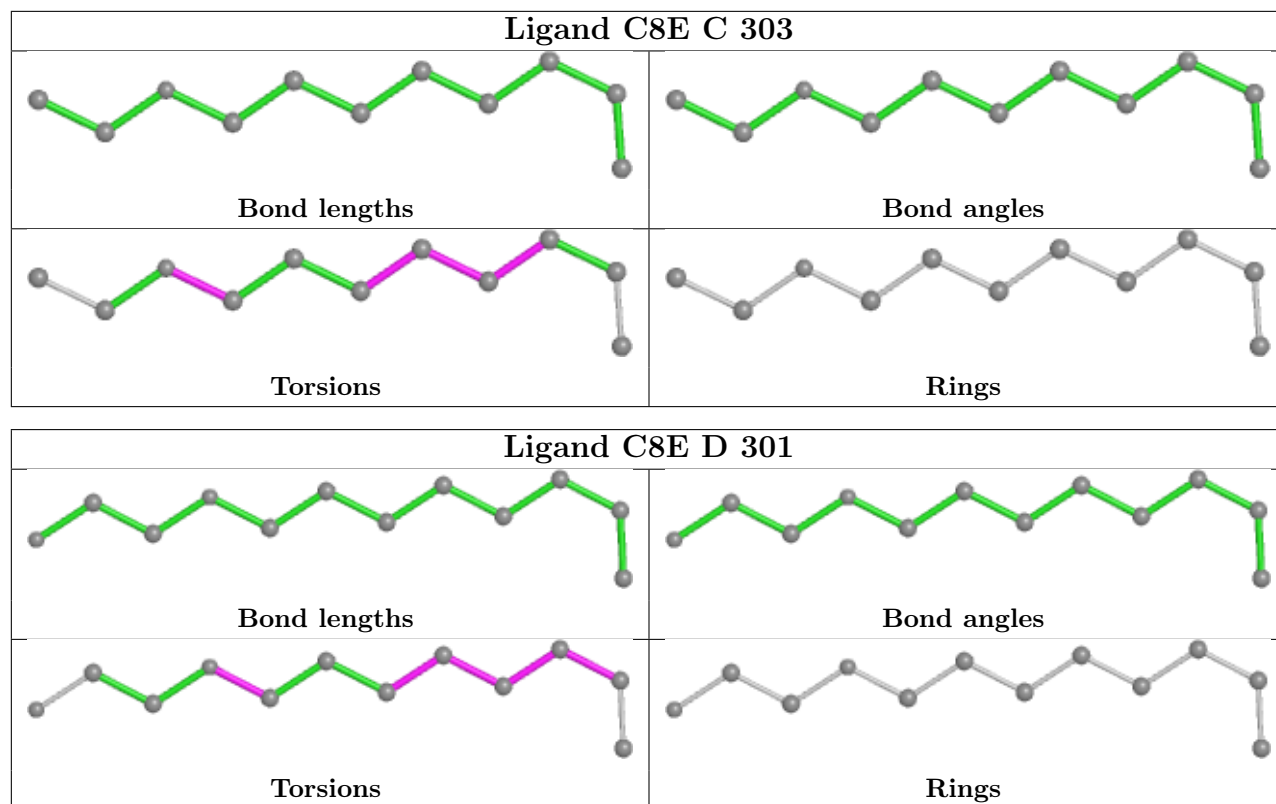












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	267/275 (97%)	-0.14	7 (2%) 56 63	19, 27, 42, 65	0
1	B	267/275 (97%)	-0.19	3 (1%) 80 85	18, 26, 38, 47	0
1	C	268/275 (97%)	-0.18	3 (1%) 80 85	18, 26, 39, 53	0
1	D	268/275 (97%)	-0.20	1 (0%) 92 95	19, 26, 37, 52	0
All	All	1070/1100 (97%)	-0.18	14 (1%) 77 81	18, 26, 39, 65	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	6.9
1	A	213	ASP	4.5
1	C	128	ALA	3.8
1	A	216	ALA	3.4
1	A	218	ASP	3.2
1	B	216	ALA	3.1
1	D	1	PHE	3.1
1	C	162[A]	TRP	2.9
1	A	215	THR	2.8
1	A	174	ALA	2.7
1	B	213	ASP	2.5
1	B	215	THR	2.2
1	A	148	LEU	2.2
1	C	40	ASP	2.1

### 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, 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.

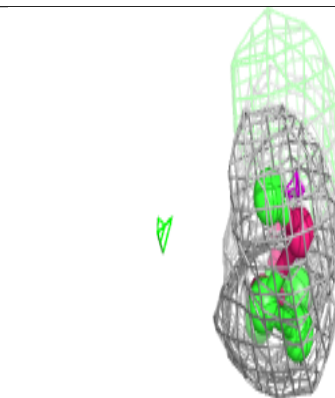
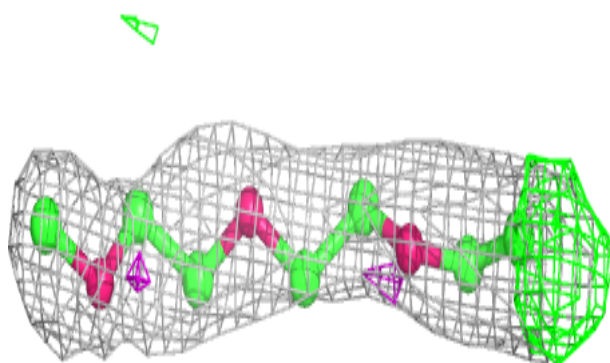
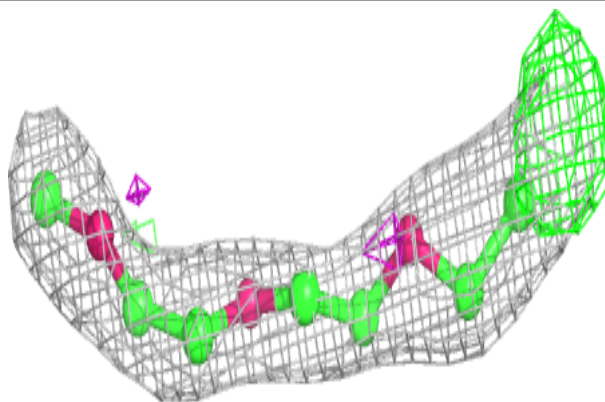
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	C8E	A	306	10/21	0.78	0.23	30,43,48,50	0
2	C8E	C	301	14/21	0.78	0.28	28,39,49,51	0
2	C8E	C	302	14/21	0.79	0.23	35,44,52,53	0
2	C8E	D	306	15/21	0.80	0.25	25,33,48,52	0
2	C8E	D	302	5/21	0.81	0.32	33,36,41,49	0
2	C8E	B	305	13/21	0.81	0.18	32,40,50,52	0
2	C8E	D	301	12/21	0.82	0.22	32,40,50,56	0
2	C8E	A	304	13/21	0.83	0.20	40,44,51,60	0
2	C8E	A	302	5/21	0.83	0.22	35,36,43,45	0
2	C8E	A	310	10/21	0.83	0.17	32,38,46,51	0
2	C8E	D	307	11/21	0.83	0.19	42,50,61,63	0
2	C8E	A	309	10/21	0.84	0.17	30,39,45,47	0
2	C8E	D	305	12/21	0.84	0.18	31,41,49,50	0
2	C8E	C	305	12/21	0.84	0.26	24,38,46,46	0
2	C8E	B	302	17/21	0.84	0.16	22,35,45,47	0
2	C8E	C	306	10/21	0.85	0.17	30,38,50,55	0
2	C8E	C	304	17/21	0.85	0.20	33,38,45,51	0
2	C8E	D	303	10/21	0.86	0.18	28,38,40,41	0
2	C8E	A	301	8/21	0.88	0.17	29,41,49,49	0
2	C8E	A	303	9/21	0.88	0.15	29,36,42,49	0
2	C8E	A	308	10/21	0.88	0.14	29,34,42,45	0
2	C8E	A	305	5/21	0.90	0.23	25,25,29,32	0
2	C8E	B	301	10/21	0.90	0.16	30,43,46,52	0
2	C8E	A	307	14/21	0.90	0.18	29,39,48,52	0
2	C8E	B	303	16/21	0.90	0.27	25,39,47,48	0
2	C8E	C	303	11/21	0.91	0.21	35,41,45,45	0
2	C8E	B	304	9/21	0.92	0.21	25,30,44,51	0
2	C8E	D	304	6/21	0.93	0.26	24,30,42,45	0
3	PO4	A	311	5/5	0.97	0.18	46,46,47,55	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

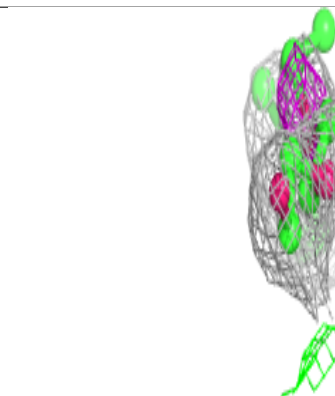
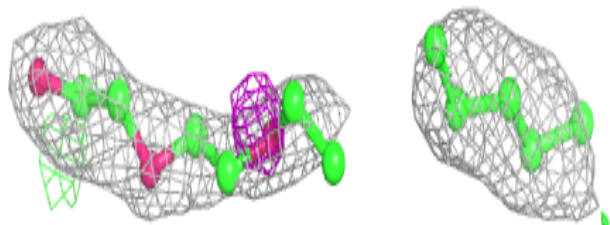
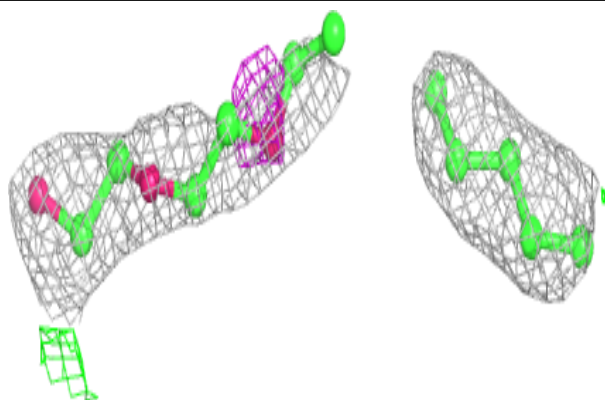
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around C8E A 306:**

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

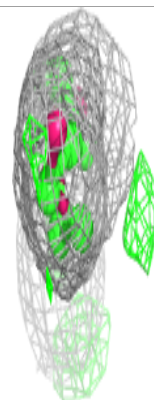
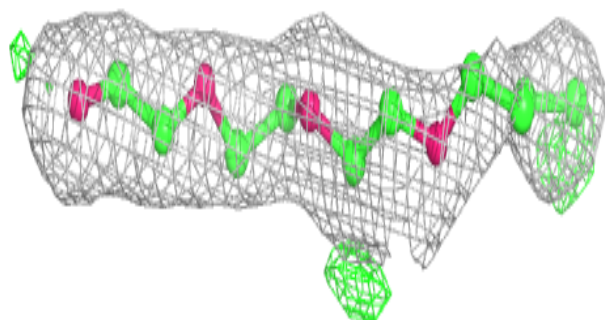
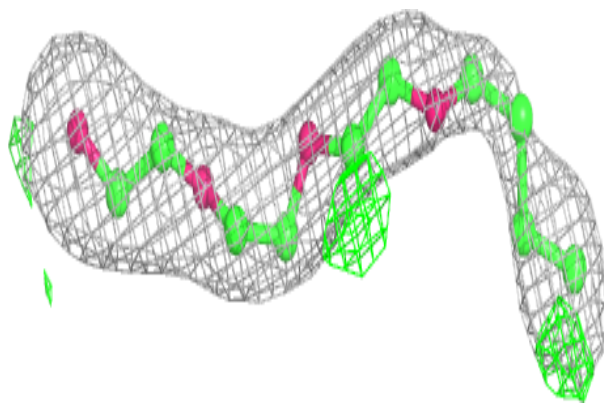
**Electron density around C8E C 301:**

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

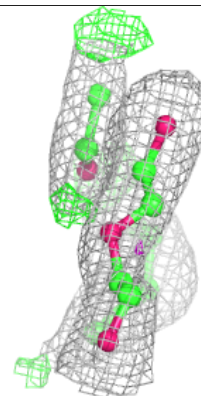
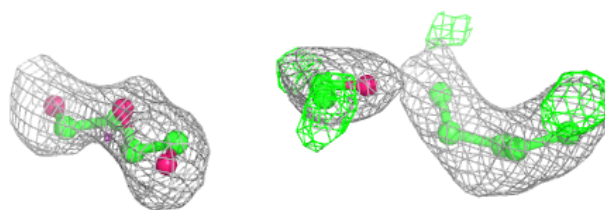
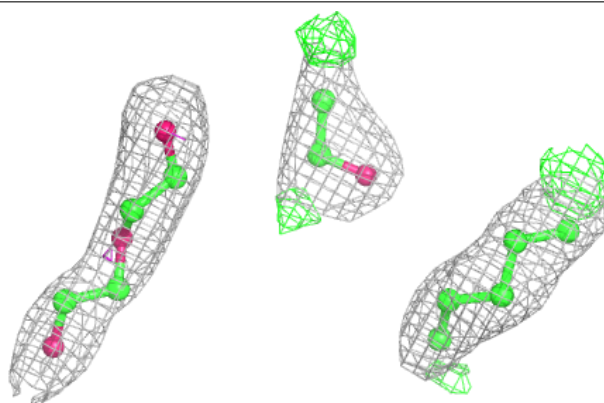


**Electron density around C8E C 302:**

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

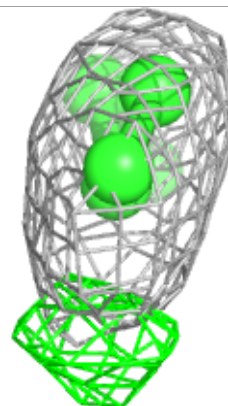
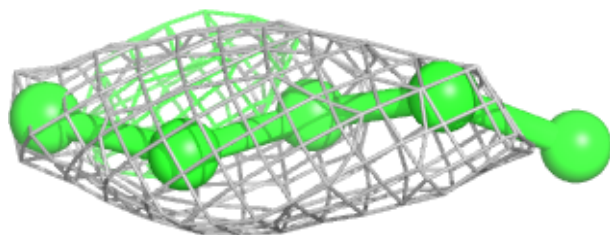
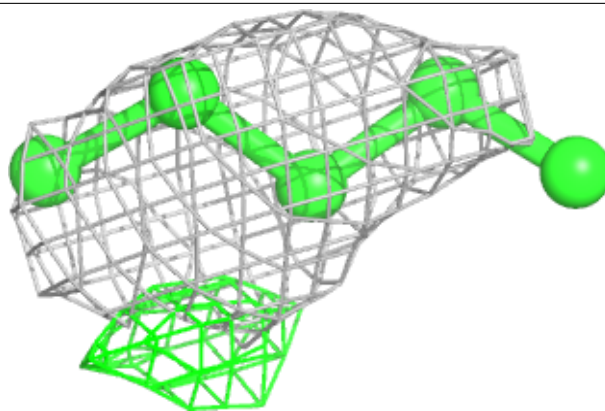
**Electron density around C8E D 306:**

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

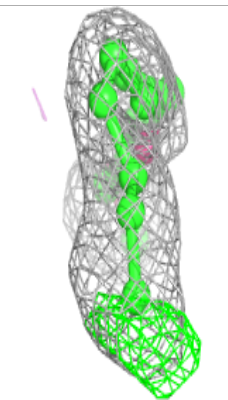
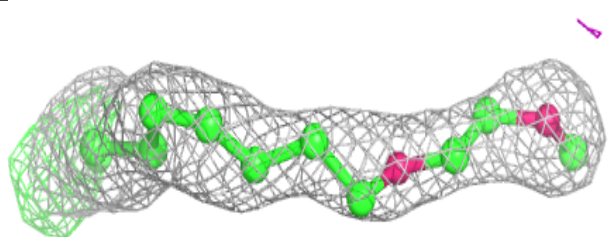
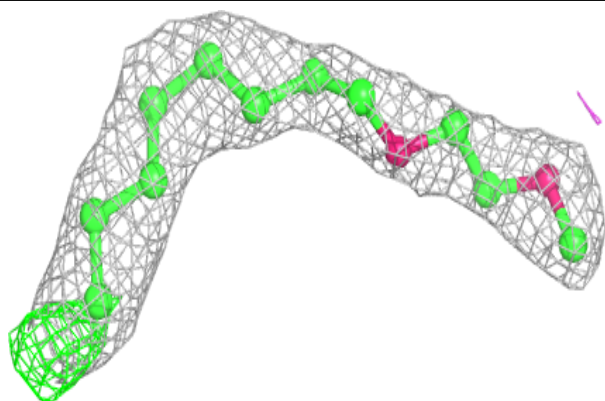


**Electron density around C8E D 302:**

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

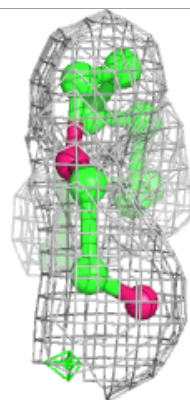
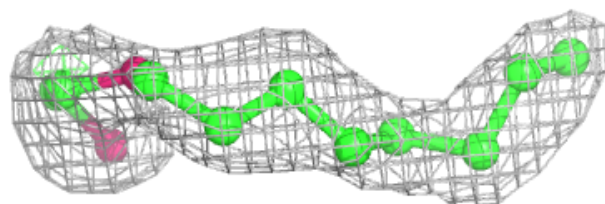
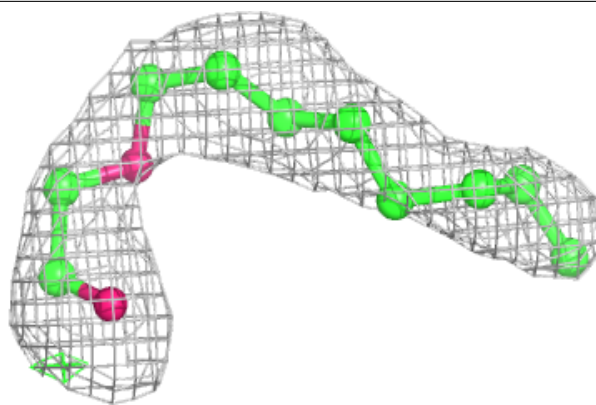
**Electron density around C8E B 305:**

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

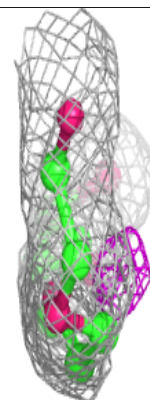
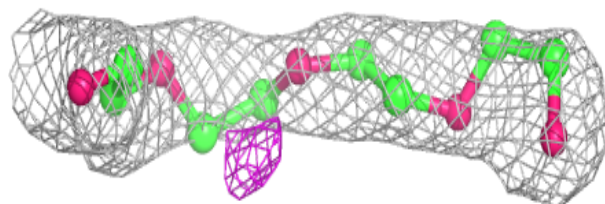
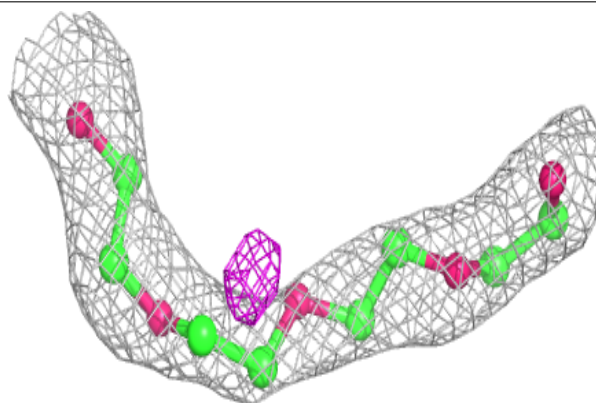


**Electron density around C8E D 301:**

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

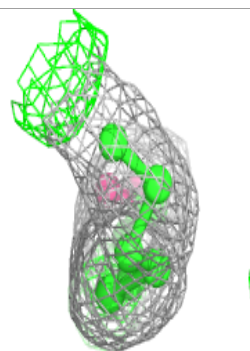
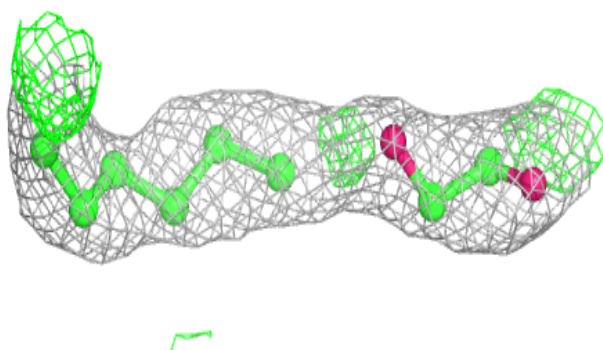
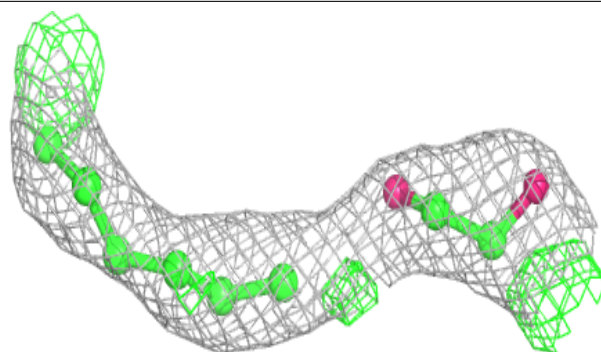
**Electron density around C8E A 304:**

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

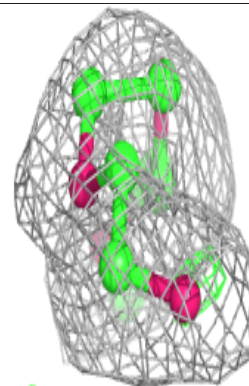
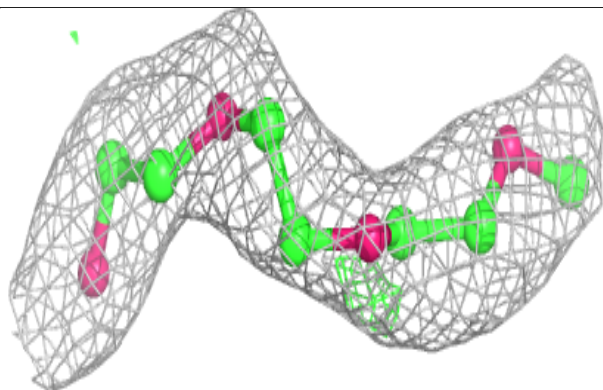
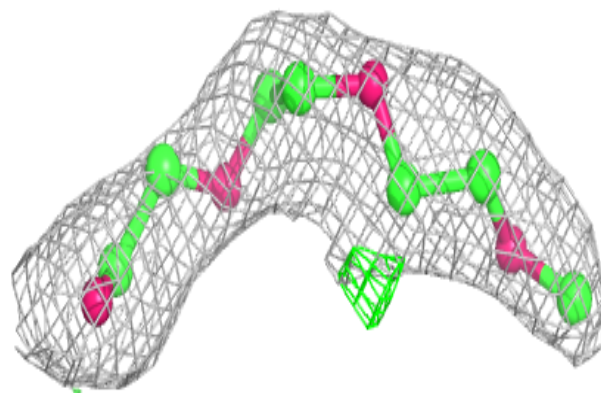


**Electron density around C8E A 310:**

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

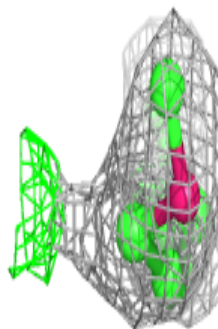
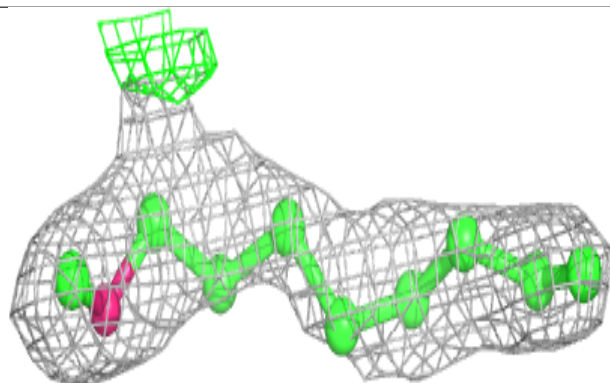
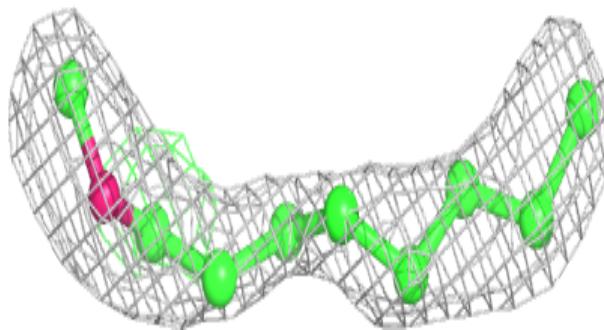
**Electron density around C8E D 307:**

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

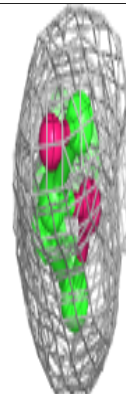
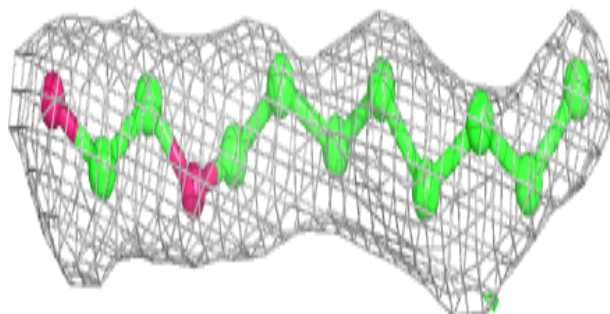
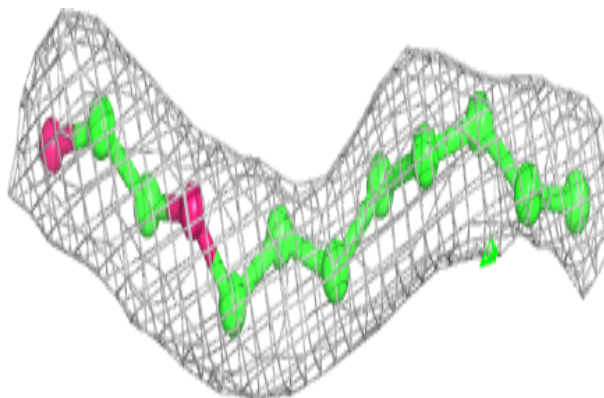


**Electron density around C8E A 309:**

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

**Electron density around C8E D 305:**

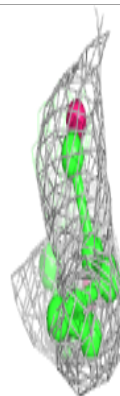
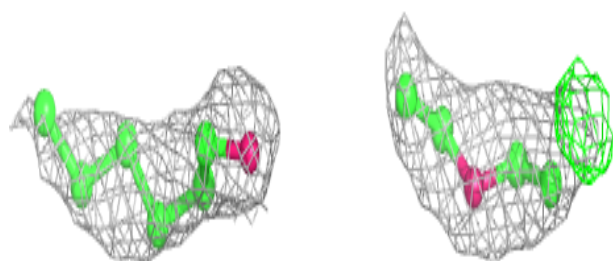
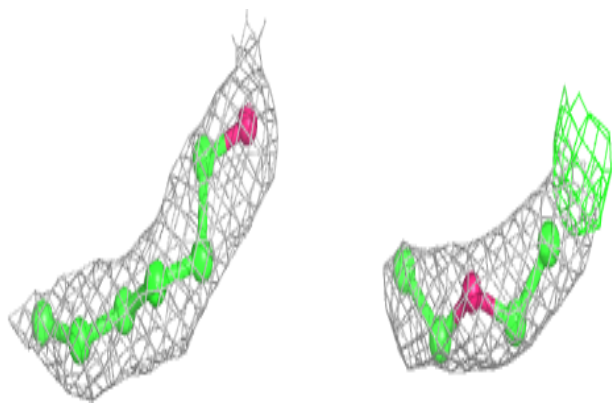
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



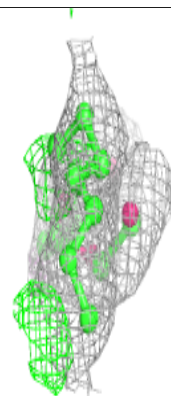
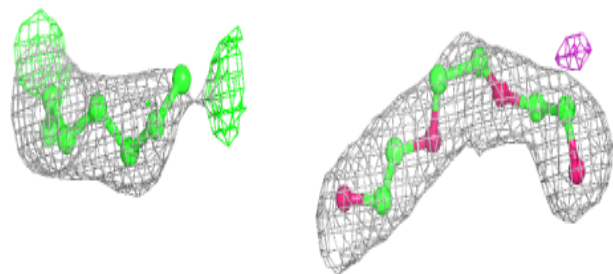
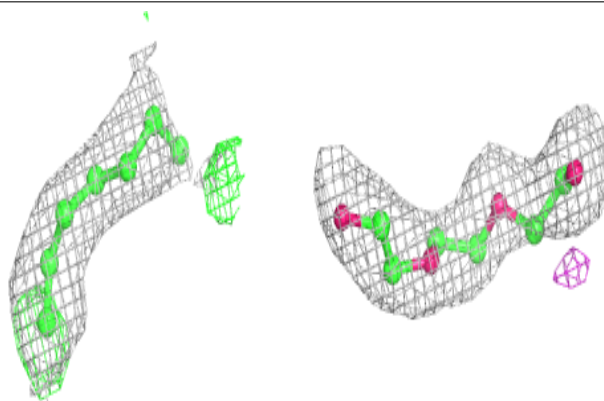


**Electron density around C8E C 305:**

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

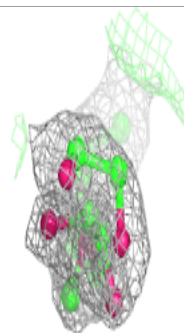
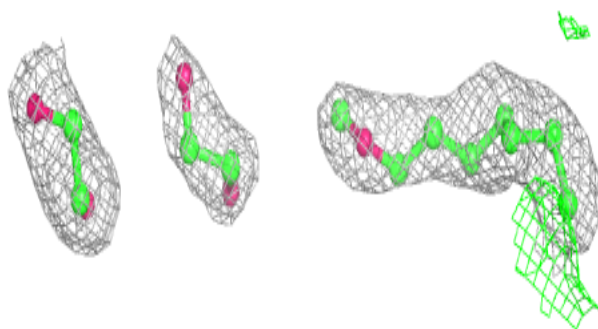
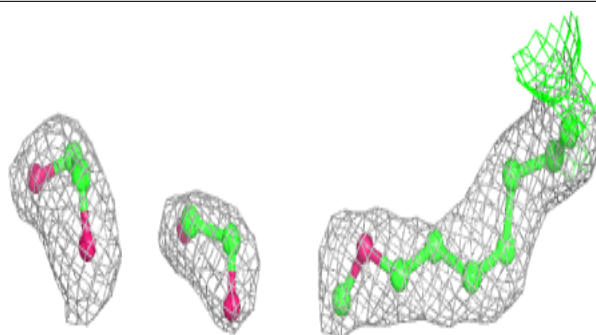
**Electron density around C8E B 302:**

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

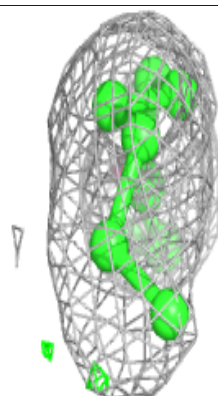
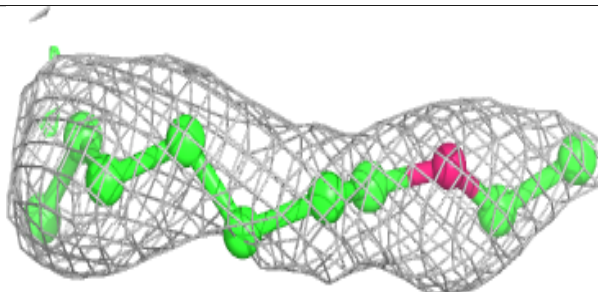
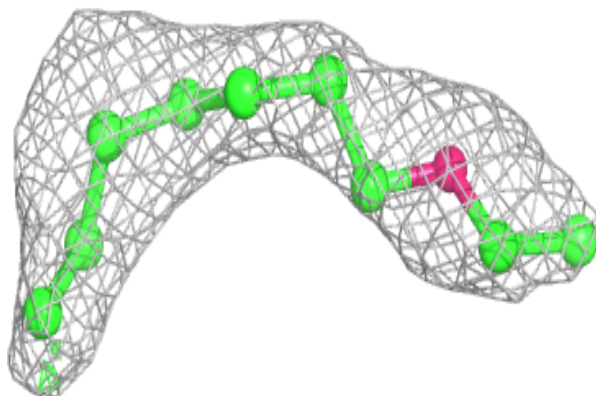


**Electron density around C8E C 304:**

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

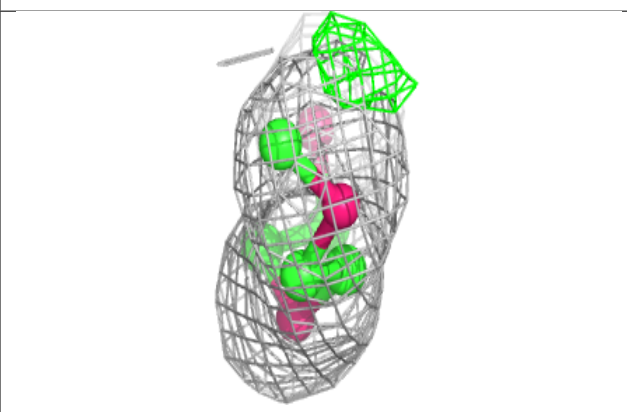
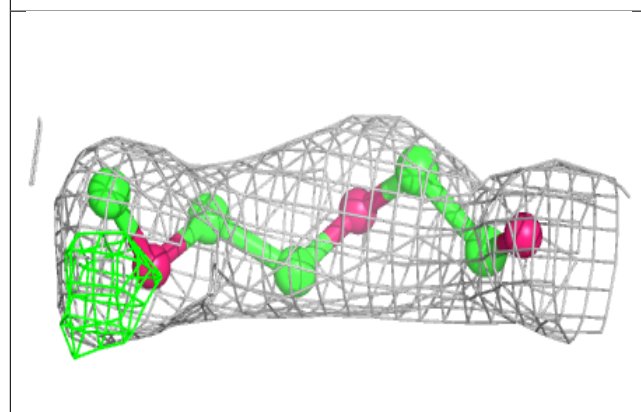
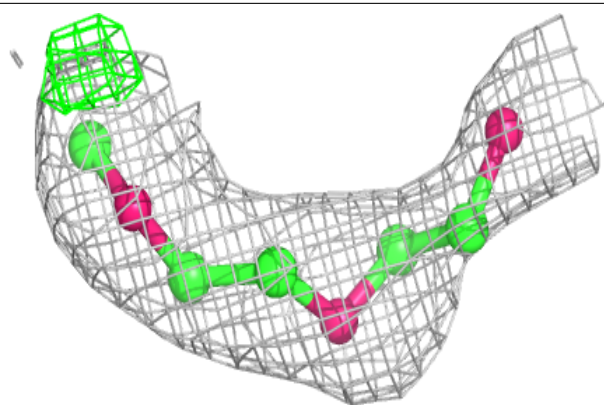
**Electron density around C8E D 303:**

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

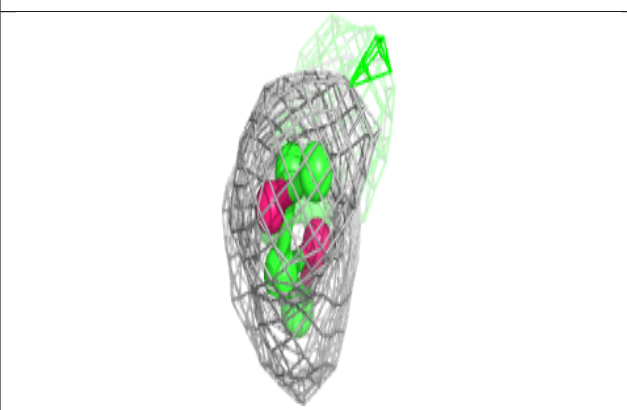
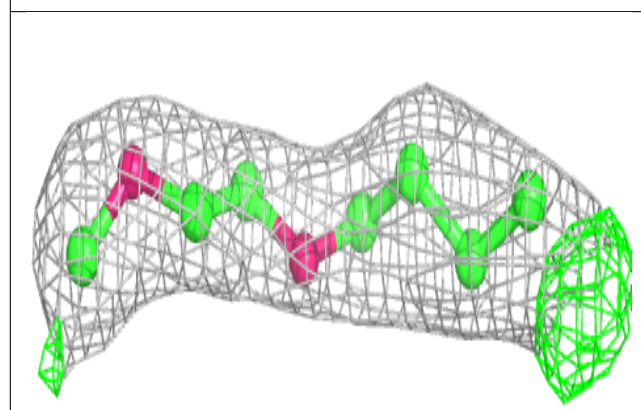
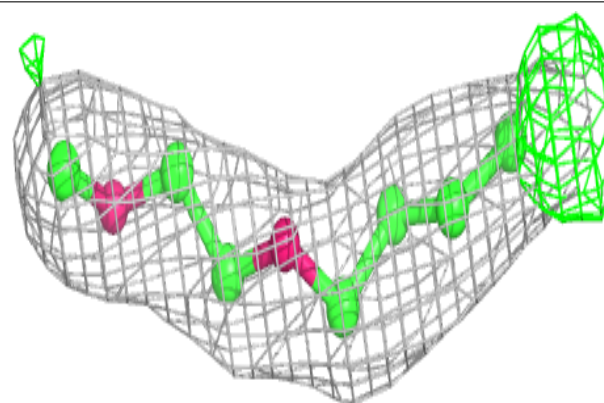


**Electron density around C8E A 301:**

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

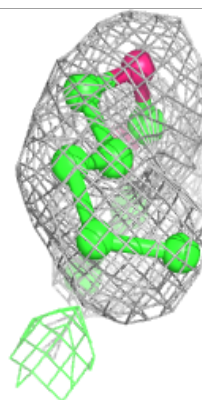
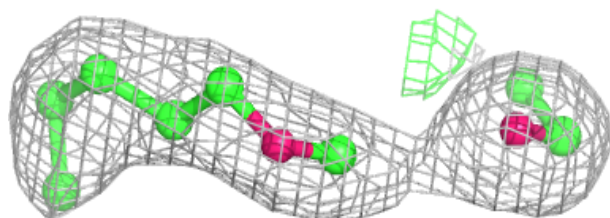
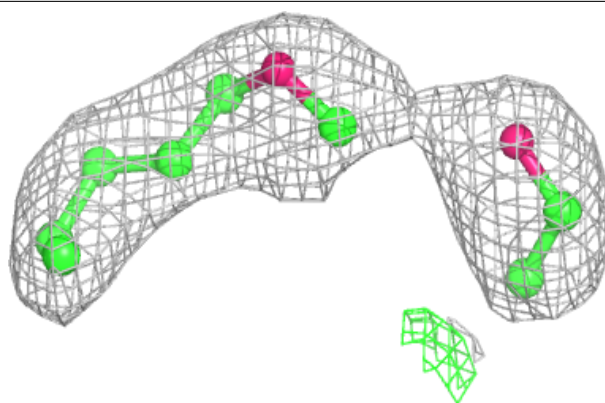
**Electron density around C8E A 303:**

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

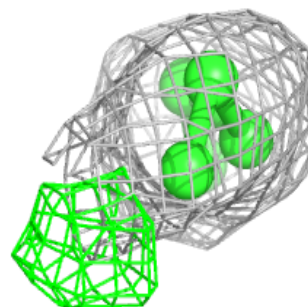
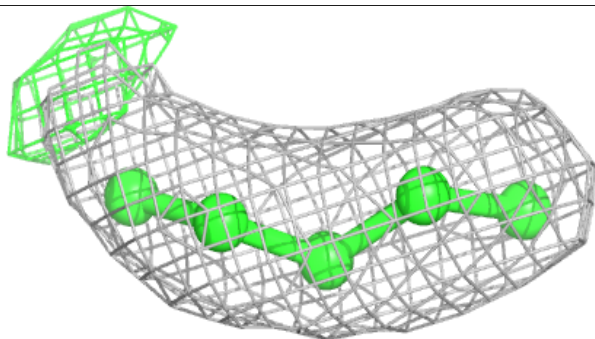
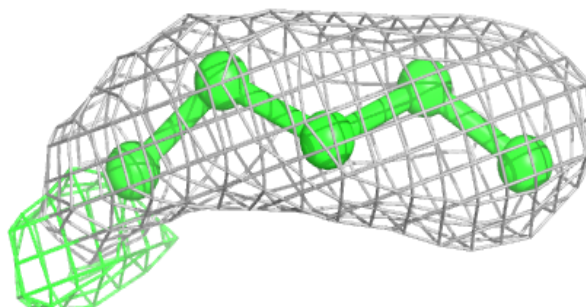


**Electron density around C8E A 308:**

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

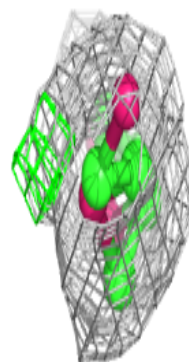
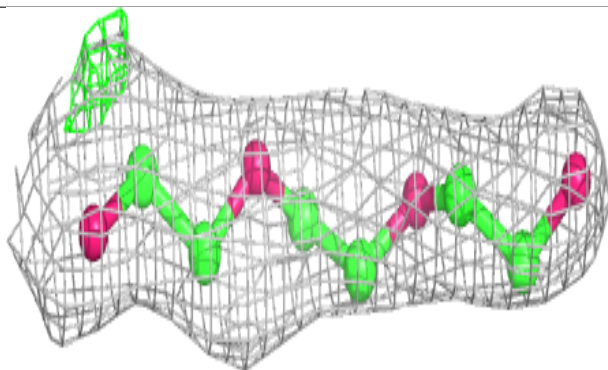
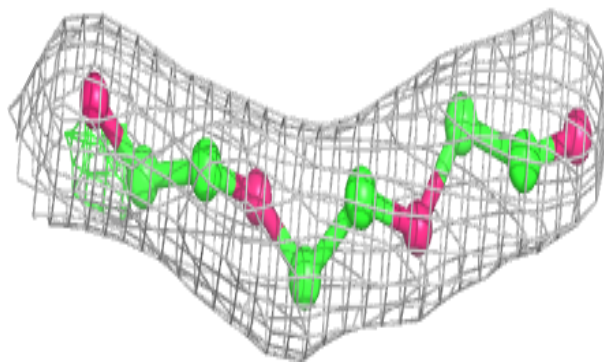
**Electron density around C8E A 305:**

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

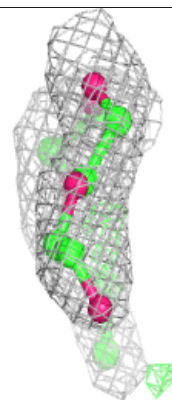
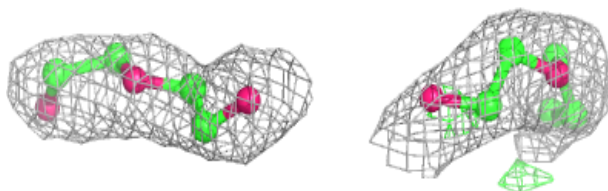
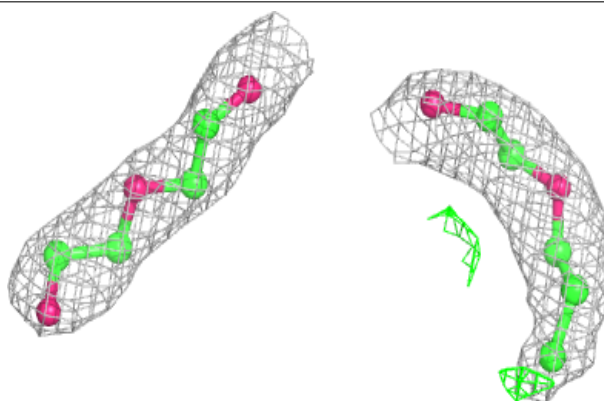


**Electron density around C8E B 301:**

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

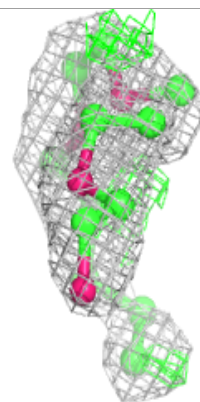
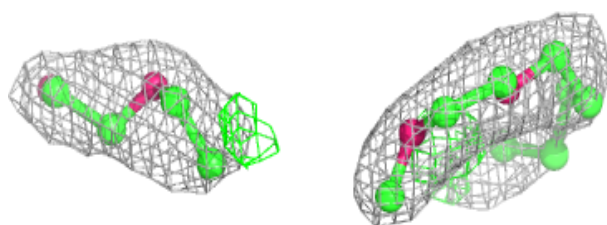
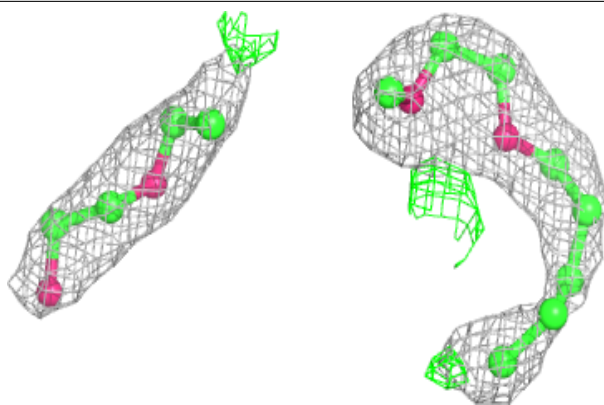
**Electron density around C8E A 307:**

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

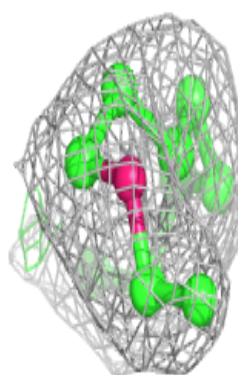
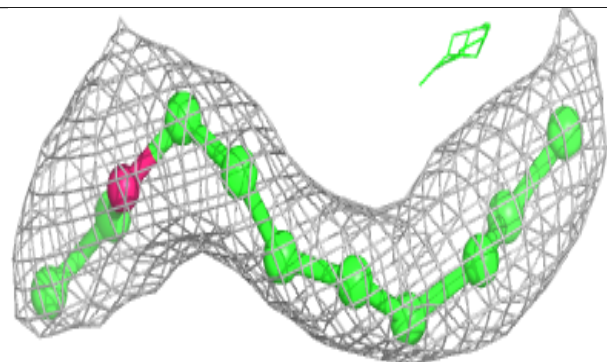
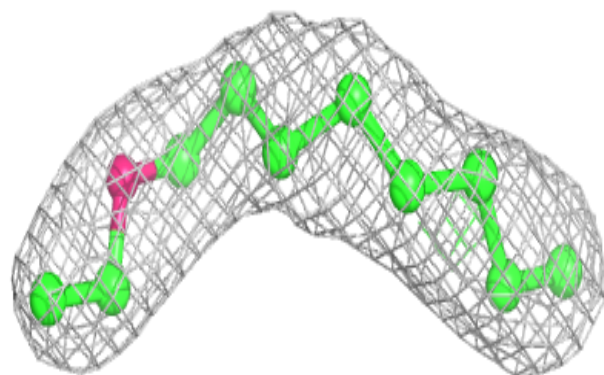


**Electron density around C8E B 303:**

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

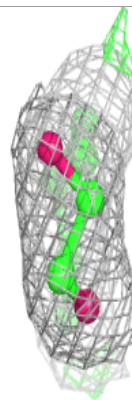
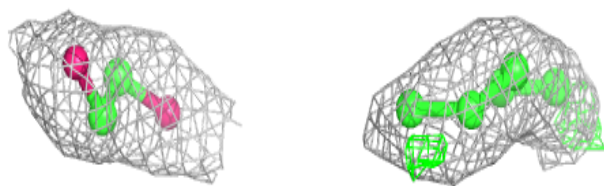
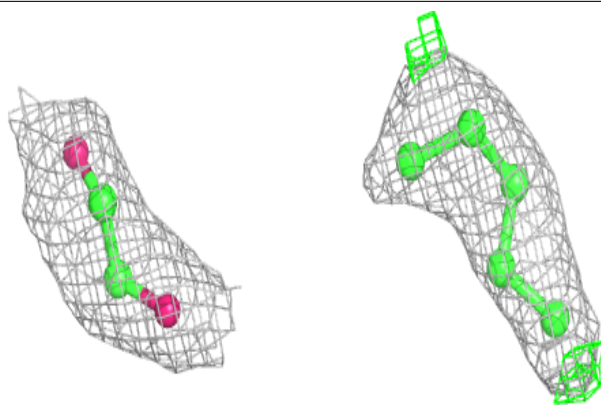
**Electron density around C8E C 303:**

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

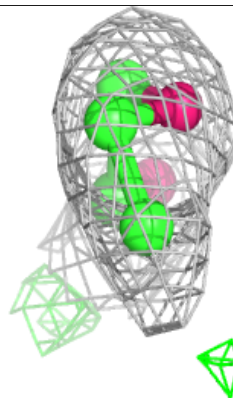
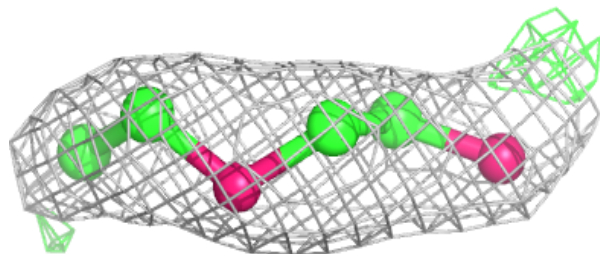
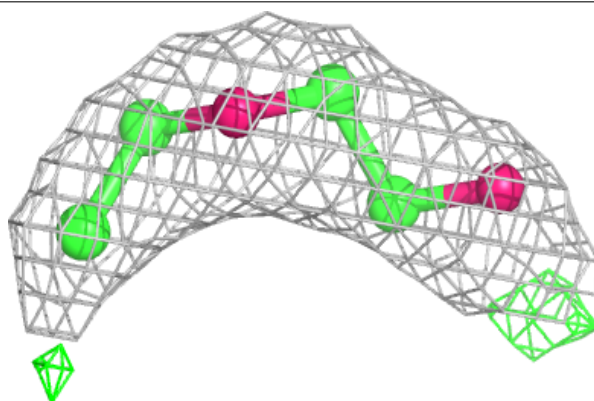


**Electron density around C8E B 304:**

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

**Electron density around C8E D 304:**

$2mF_o-DF_c$  (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.