



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 06:57 am BST

PDB ID : 4TL3  
Title : Mechanistic insights from the crystal structure of an inward proton-transporting Anabaena sensory rhodopsin mutant  
Authors : Dong, B.H.; Luecke, H.  
Deposited on : 2014-05-29  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

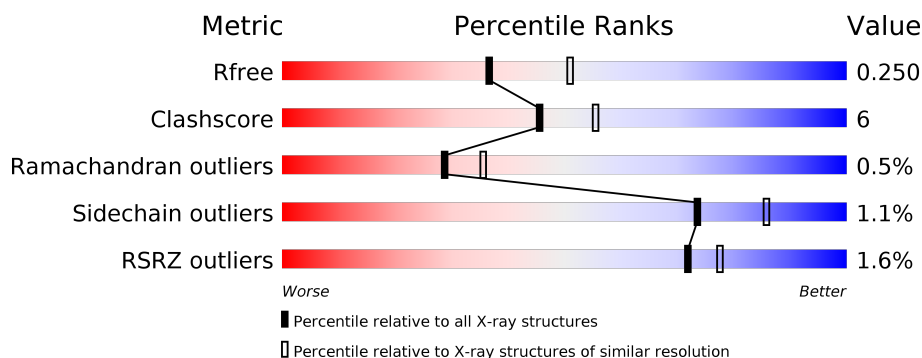
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 on 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	226	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	B	226	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div></div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEE	A	305	-	-	-	X
3	PEE	A	314	-	-	-	X
3	PEE	B	308	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4140 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.

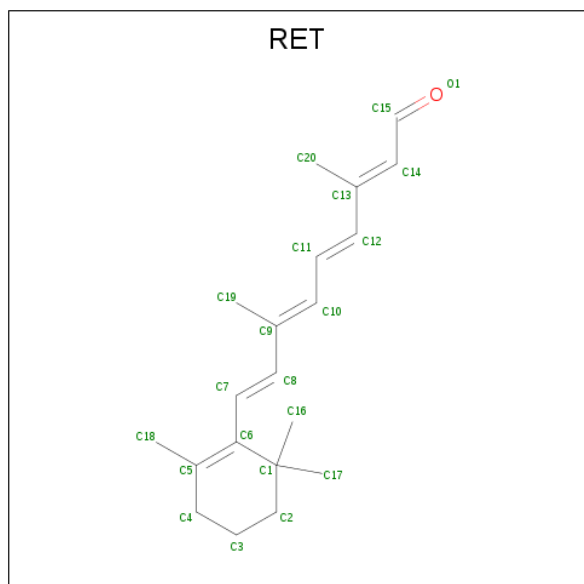
- Molecule 1 is a protein called Anabaena sensory rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1774	1195	278	290	11			
1	B	217	Total	C	N	O	S	0	0	0
			1782	1199	279	293	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLU	ASP	engineered mutation	UNP Q8YSC4
B	217	GLU	ASP	engineered mutation	UNP Q8YSC4

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



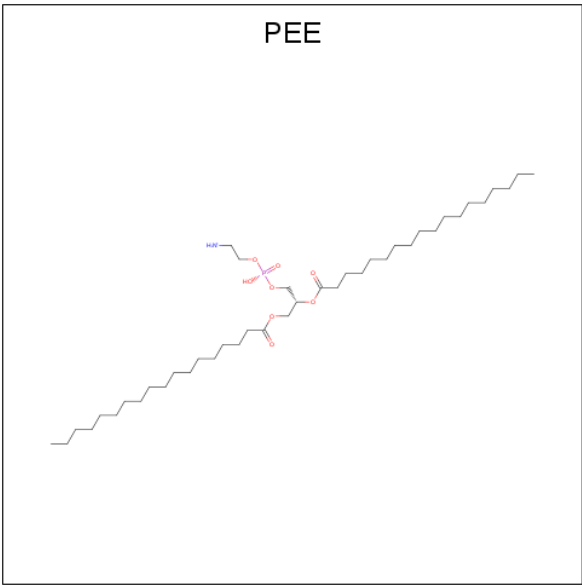
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	C	0	0
			20	20		

- Molecule 3 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>83</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			14	14		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			11	11		
3	A	1	Total	C	0	0
			17	17		
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			17	17		
3	A	1	Total	C	0	0
			17	17		
3	A	1	Total	C	0	0
			11	11		
3	A	1	Total	C	0	0
			15	15		
3	A	1	Total	C	0	0
			11	11		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 17 17	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 8 8	0	0
3	B	1	Total C 15 15	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 15 15	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 15 15	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 18 18	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 16 16	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 18 18	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 17 17	0	0

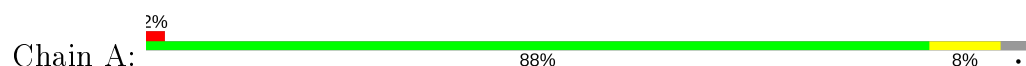
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	B	58	Total O 58 58	0	0

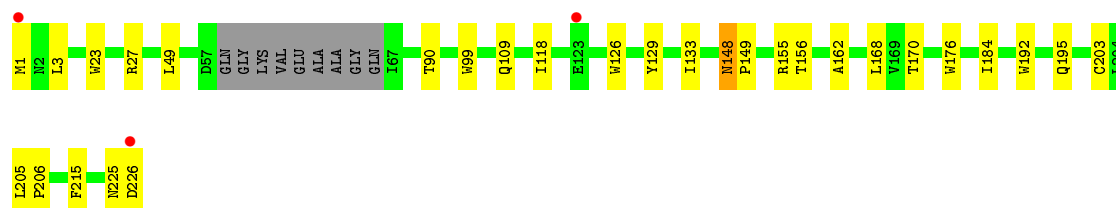
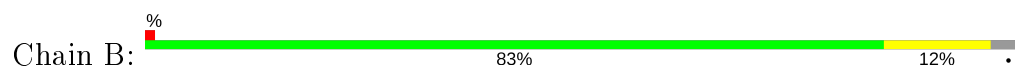
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Anabaena sensory rhodopsin



- Molecule 1: Anabaena sensory rhodopsin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.27Å 104.30Å 111.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.19 – 2.30 33.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.19-2.30) 96.6 (33.19-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.220 , 0.250 0.219 , 0.250	Depositor DCC
$R_{free}$ test set	1449 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.70 % 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 8.2860e-05. 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: PEE, RET

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	0.45	0/1834	0.56	0/2506
1	B	0.46	0/1842	0.56	0/2517
All	All	0.46	0/3676	0.56	0/5023

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	1774	0	1784	14	0
1	B	1782	0	1788	30	0
2	A	20	0	27	5	0
2	B	20	0	27	3	0
3	A	204	0	356	7	0
3	B	231	0	404	21	0
4	A	51	0	0	0	0
4	B	58	0	0	1	0
All	All	4140	0	4386	54	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 6.

The worst 5 of 54 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)
2:A:301:RET:H171	2:A:301:RET:H8	1.70	0.74
2:B:301:RET:H171	2:B:301:RET:H8	1.75	0.69
1:B:215:PHE:HE2	3:B:318:PEE:H25	1.61	0.65
1:B:225:ASN:O	1:B:226:ASP:HB2	1.99	0.63
1:A:205:LEU:HB3	1:A:206:PRO:HD3	1.81	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/226 (94%)	211 (100%)	0	1 (0%)	29	35
1	B	213/226 (94%)	212 (100%)	0	1 (0%)	29	35
All	All	425/452 (94%)	423 (100%)	0	2 (0%)	29	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	148	ASN

### 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	189/195 (97%)	188 (100%)	1 (0%)	88	95
1	B	190/195 (97%)	187 (98%)	3 (2%)	62	78
All	All	379/390 (97%)	375 (99%)	4 (1%)	73	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	B	3	LEU
1	B	156	THR
1	B	184	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	B	109	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

37 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	$\# Z  > 2$
3	PEE	A	317	-	13,13,50	0.25	0	12,12,55	0.52	0
3	PEE	B	302	-	14,14,50	0.28	0	13,13,55	0.50	0
3	PEE	B	307	-	14,14,50	0.33	0	13,13,55	0.51	0
3	PEE	A	316	-	5,5,50	0.29	0	4,4,55	0.42	0
3	PEE	B	303	-	10,10,50	0.32	0	9,9,55	0.37	0
3	PEE	B	320	-	5,5,50	0.25	0	4,4,55	0.40	0
3	PEE	A	311	-	10,10,50	0.31	0	9,9,55	0.49	0
3	PEE	B	308	-	10,10,50	0.35	0	9,9,55	0.38	0
3	PEE	A	312	-	14,14,50	0.26	0	13,13,55	0.52	0
3	PEE	B	317	-	11,11,50	0.34	0	10,10,55	0.36	0
3	PEE	B	318	-	15,15,50	0.28	0	14,14,55	0.51	0
3	PEE	A	309	-	16,16,50	0.28	0	15,15,55	0.54	0
3	PEE	A	308	-	11,11,50	0.31	0	10,10,55	0.46	0
3	PEE	A	306	-	16,16,50	0.29	0	15,15,55	0.52	0
3	PEE	B	309	-	11,11,50	0.29	0	10,10,55	0.44	0
3	PEE	B	315	-	5,5,50	0.30	0	4,4,55	0.37	0
3	PEE	B	321	-	9,9,50	0.26	0	8,8,55	0.48	0
3	PEE	B	312	-	17,17,50	0.27	0	16,16,55	0.52	0
3	PEE	A	303	-	13,13,50	0.31	0	12,12,55	0.43	0
3	PEE	A	304	-	7,7,50	0.26	0	6,6,55	0.56	0
2	RET	B	301	1	20,20,21	0.80	0	27,27,28	1.61	8 (29%)
3	PEE	A	313	-	10,10,50	0.34	0	9,9,55	0.38	0
3	PEE	B	313	-	4,4,50	0.32	0	3,3,55	0.44	0
3	PEE	B	314	-	13,13,50	0.33	0	12,12,55	0.37	0
3	PEE	A	305	-	10,10,50	0.33	0	9,9,55	0.40	0
3	PEE	B	310	-	8,8,50	0.36	0	7,7,55	0.36	0
3	PEE	A	319	-	17,17,50	0.26	0	16,16,55	0.57	0
3	PEE	B	304	-	14,14,50	0.28	0	13,13,55	0.54	0
3	PEE	B	322	-	16,16,50	0.30	0	15,15,55	0.48	0
3	PEE	A	315	-	7,7,50	0.23	0	6,6,55	0.57	0
3	PEE	B	306	-	11,11,50	0.27	0	10,10,55	0.48	0
3	PEE	A	321	-	7,7,50	0.30	0	6,6,55	0.35	0
3	PEE	B	305	-	8,8,50	0.34	0	7,7,55	0.39	0
3	PEE	A	314	-	16,16,50	0.33	0	15,15,55	0.41	0
2	RET	A	301	1	20,20,21	0.91	1 (5%)	27,27,28	1.45	6 (22%)
3	PEE	A	310	-	16,16,50	0.31	0	15,15,55	0.43	0
3	PEE	B	319	-	17,17,50	0.34	0	16,16,55	0.39	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
3	PEE	A	317	-	-	10/11/11/54	-
3	PEE	B	302	-	-	8/12/12/54	-
3	PEE	B	307	-	-	7/12/12/54	-
3	PEE	A	316	-	-	3/3/3/54	-
3	PEE	B	303	-	-	6/8/8/54	-
3	PEE	B	320	-	-	1/3/3/54	-
3	PEE	A	311	-	-	6/8/8/54	-
3	PEE	B	308	-	-	5/8/8/54	-
3	PEE	A	312	-	-	8/12/12/54	-
3	PEE	B	317	-	-	8/9/9/54	-
3	PEE	B	318	-	-	9/13/13/54	-
3	PEE	A	309	-	-	6/14/14/54	-
3	PEE	A	308	-	-	4/9/9/54	-
3	PEE	A	306	-	-	6/14/14/54	-
3	PEE	B	309	-	-	5/9/9/54	-
3	PEE	B	315	-	-	2/3/3/54	-
3	PEE	B	321	-	-	6/7/7/54	-
3	PEE	B	312	-	-	11/15/15/54	-
3	PEE	A	303	-	-	5/11/11/54	-
3	PEE	A	304	-	-	3/5/5/54	-
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
3	PEE	A	313	-	-	6/8/8/54	-
3	PEE	B	313	-	-	0/2/2/54	-
3	PEE	B	314	-	-	8/11/11/54	-
3	PEE	A	305	-	-	4/8/8/54	-
3	PEE	B	310	-	-	3/6/6/54	-
3	PEE	A	319	-	-	11/15/15/54	-
3	PEE	B	304	-	-	5/12/12/54	-
3	PEE	B	322	-	-	7/14/14/54	-
3	PEE	A	315	-	-	3/5/5/54	-
3	PEE	B	306	-	-	8/9/9/54	-
3	PEE	A	321	-	-	4/5/5/54	-
3	PEE	B	305	-	-	2/6/6/54	-
3	PEE	A	314	-	-	10/14/14/54	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	PEE	A	310	-	-	10/14/14/54	-
3	PEE	B	319	-	-	8/15/15/54	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C14-C13	2.32	1.35	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C18-C5-C6	-3.58	120.51	124.53
2	B	301	RET	C10-C11-C12	-2.75	114.62	123.22
2	A	301	RET	C7-C8-C9	-2.70	122.15	126.23
2	A	301	RET	C20-C13-C12	2.65	122.25	118.08
2	B	301	RET	C19-C9-C8	2.60	122.18	118.08

There are no chirality outliers.

5 of 208 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	PEE	C22-C23-C24-C25
3	B	302	PEE	C21-C22-C23-C24
3	B	307	PEE	C14-C15-C16-C17
3	A	312	PEE	C18-C19-C20-C21
3	B	314	PEE	C17-C18-C19-C20

There are no ring outliers.

20 monomers are involved in 35 short contacts:

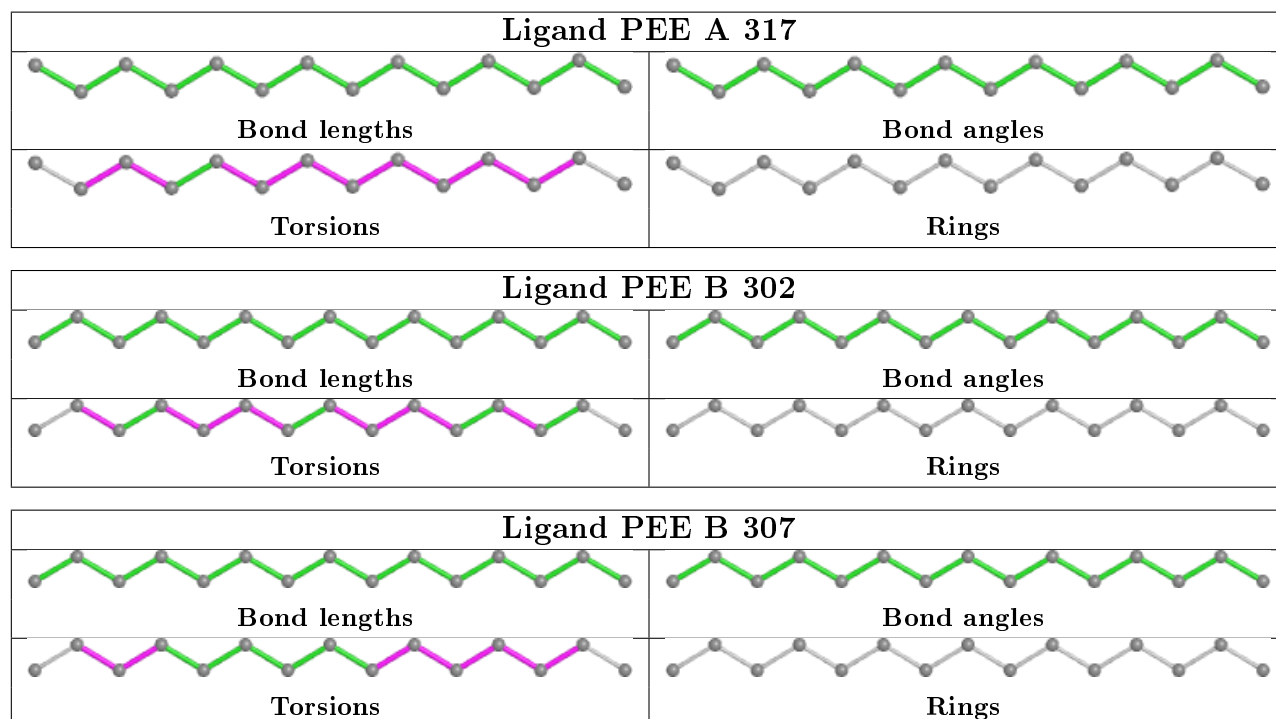
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	PEE	4	0
3	B	307	PEE	1	0
3	B	303	PEE	1	0
3	A	311	PEE	2	0
3	B	308	PEE	1	0
3	A	312	PEE	1	0
3	B	318	PEE	2	0
3	A	309	PEE	1	0

*Continued on next page...*

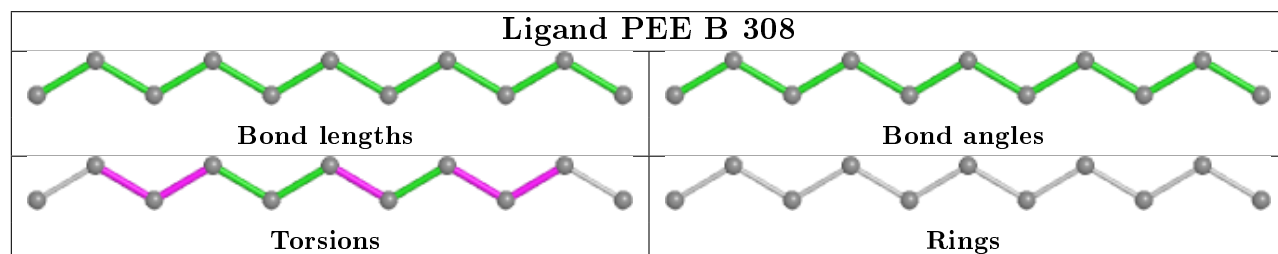
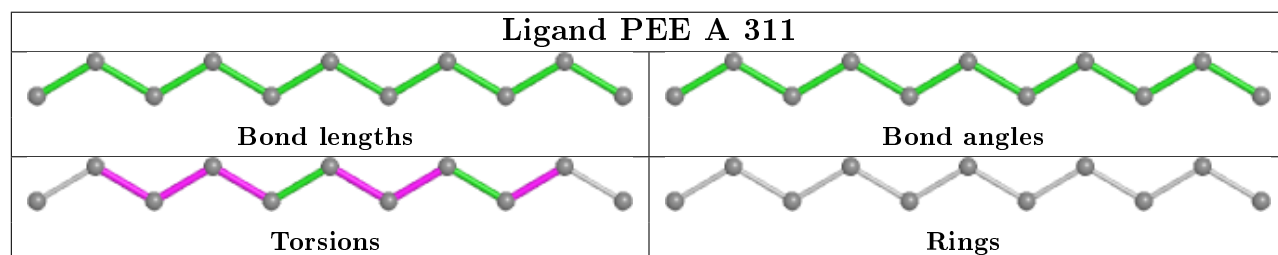
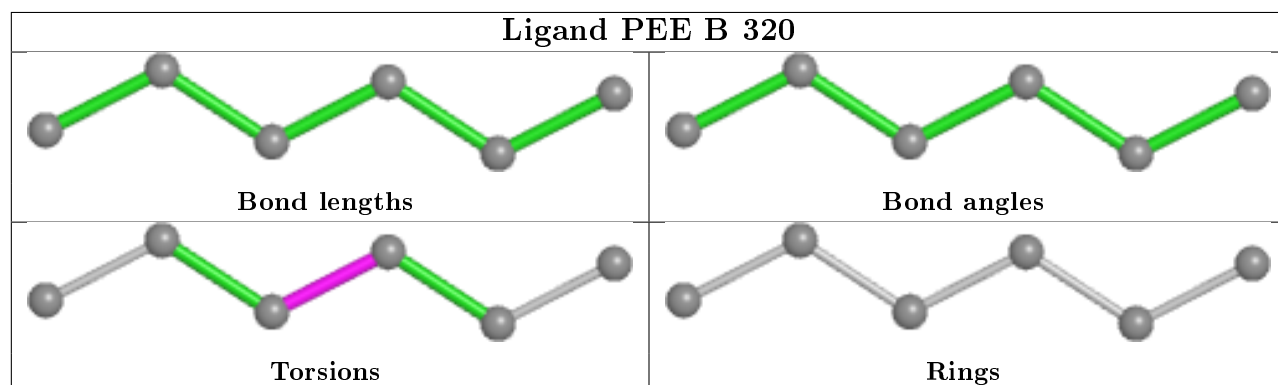
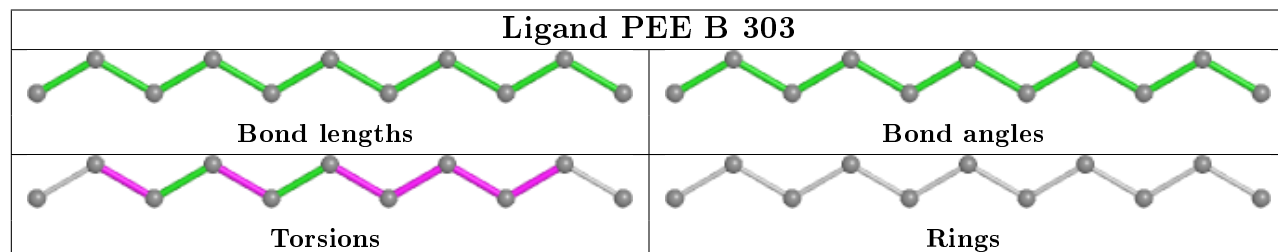
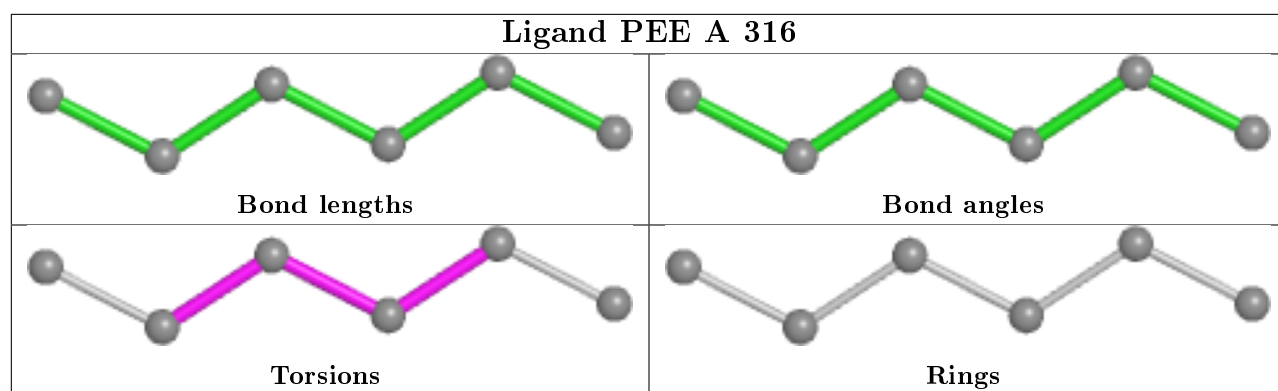
*Continued from previous page...*

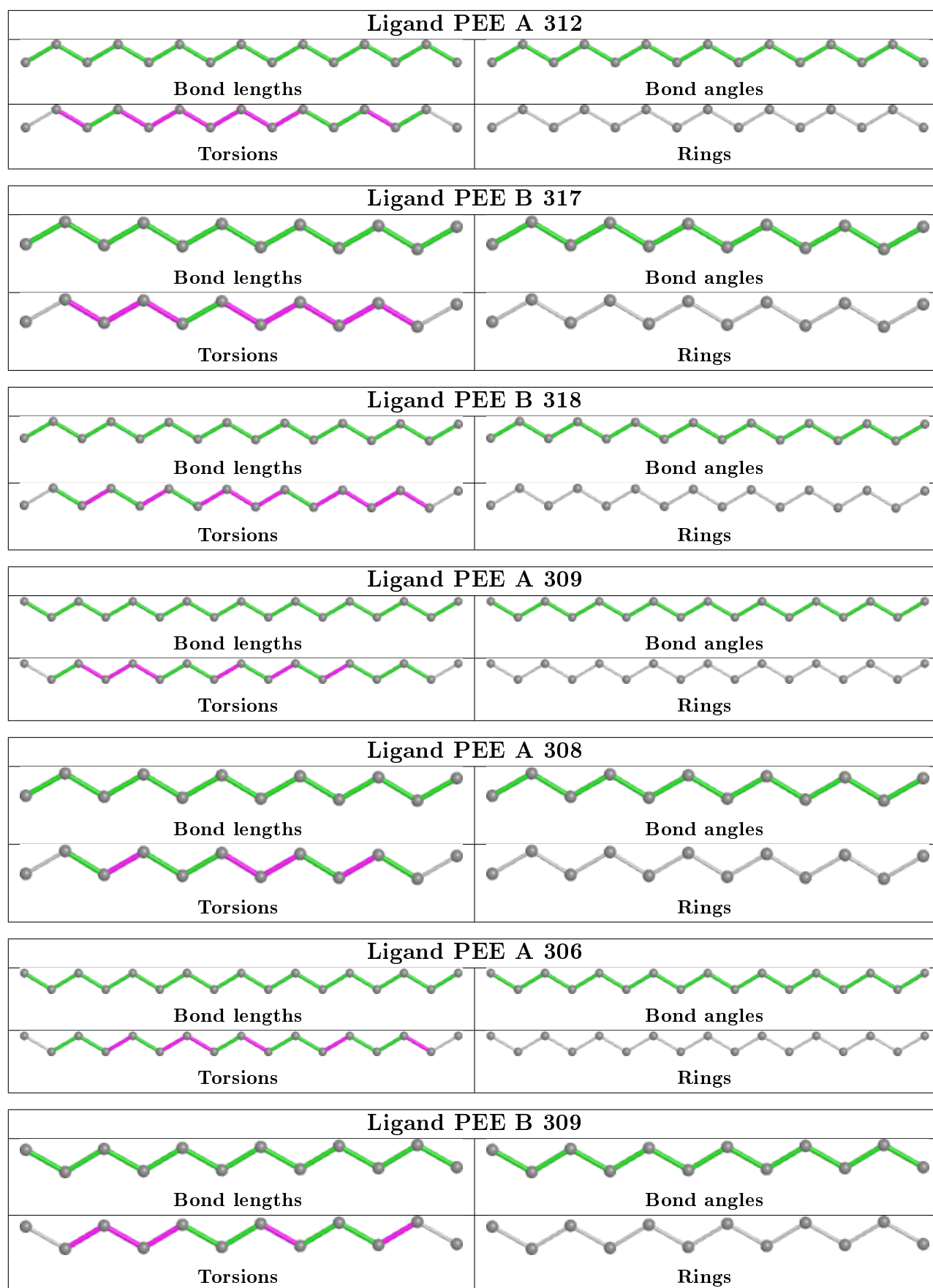
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	309	PEE	3	0
2	B	301	RET	3	0
3	B	314	PEE	1	0
3	A	319	PEE	1	0
3	B	304	PEE	3	0
3	B	322	PEE	3	0
3	A	321	PEE	1	0
3	B	305	PEE	1	0
3	A	314	PEE	1	0
2	A	301	RET	5	0
3	A	310	PEE	1	0
3	B	319	PEE	1	0

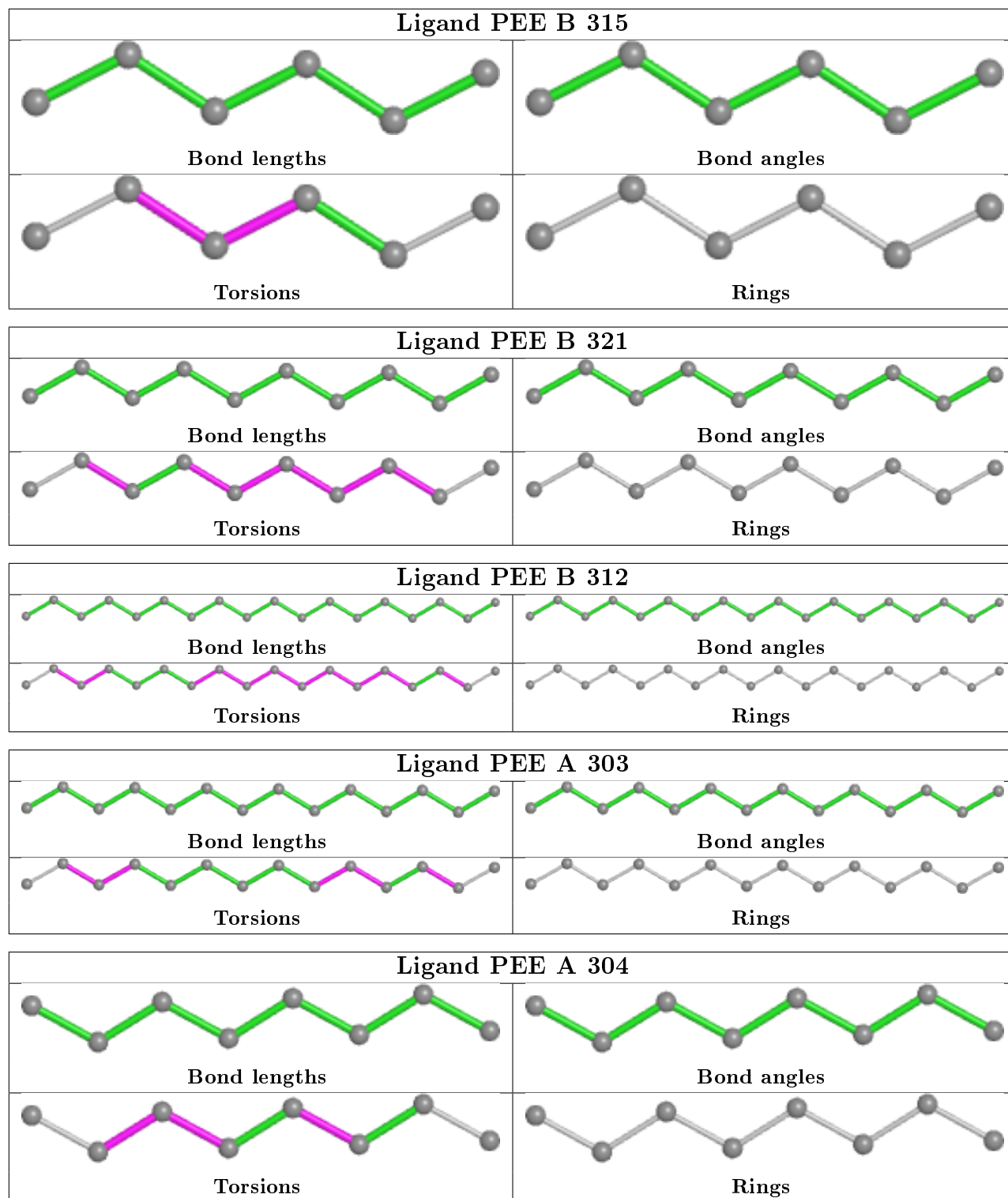
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

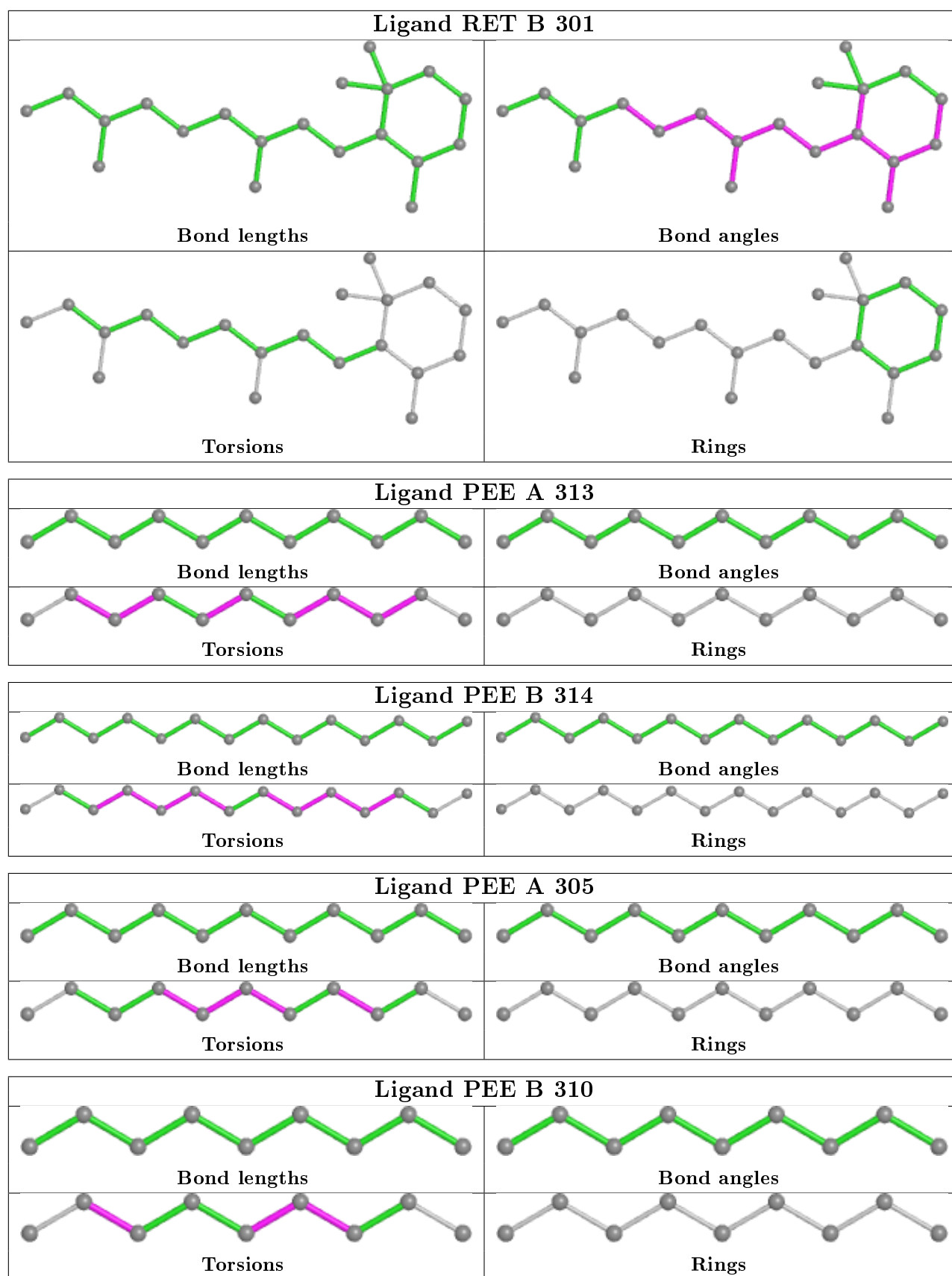


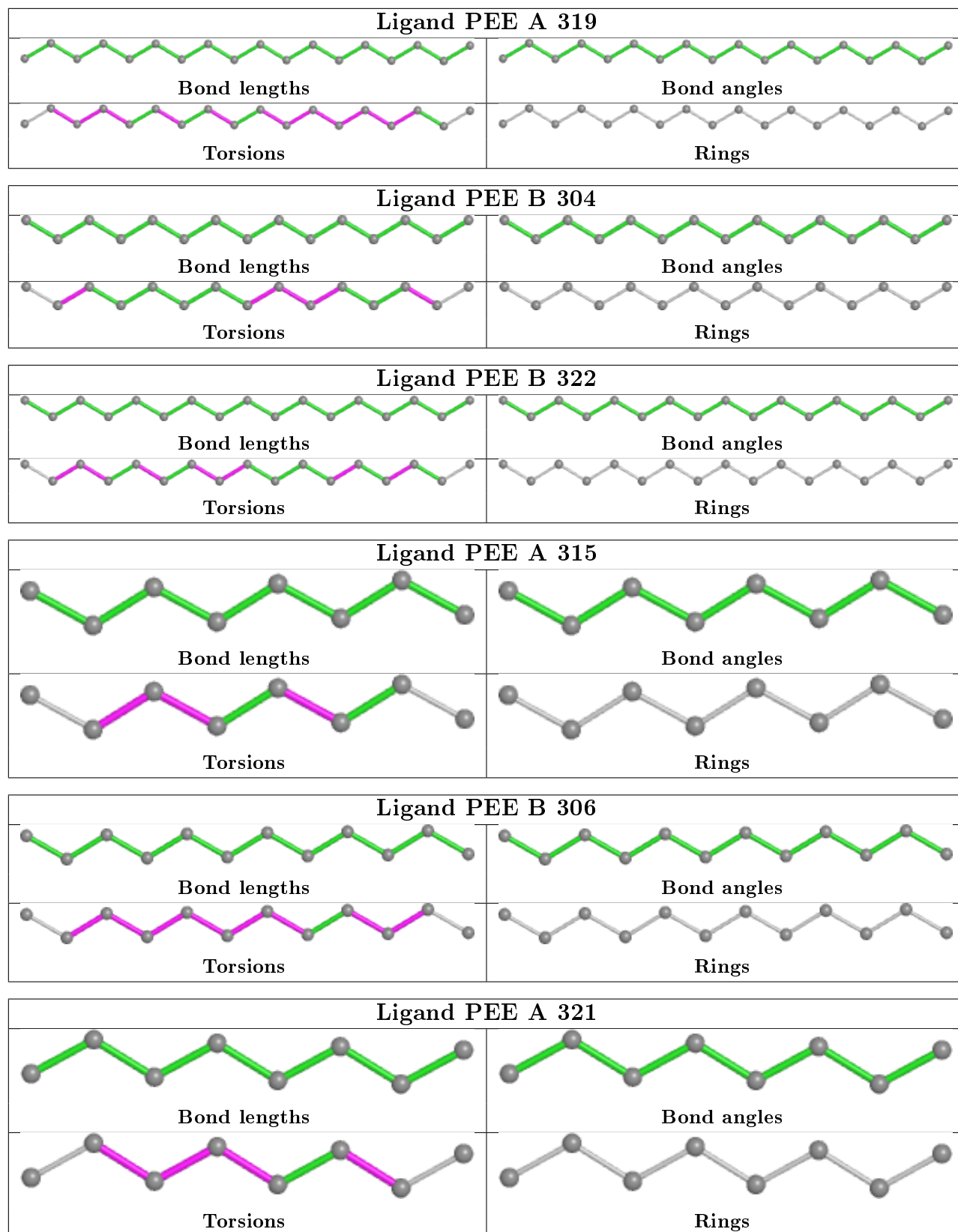


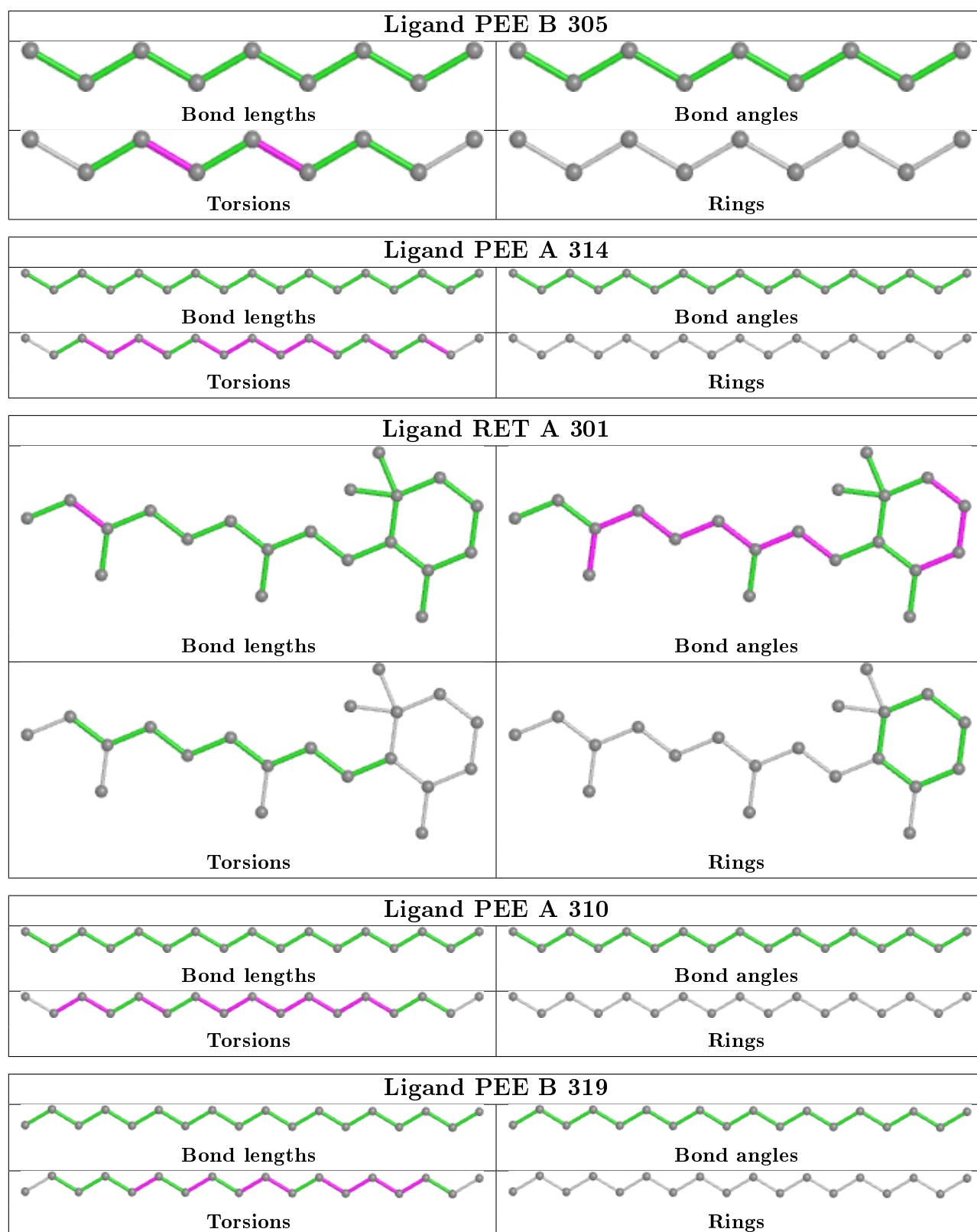












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	216/226 (95%)	-0.21	4 (1%) 66 73	16, 23, 36, 60	0
1	B	217/226 (96%)	-0.26	3 (1%) 75 80	15, 23, 37, 60	0
All	All	433/452 (95%)	-0.23	7 (1%) 72 77	15, 23, 37, 60	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.9
1	B	226	ASP	3.9
1	B	1	MET	3.1
1	A	126	TRP	2.8
1	A	2	ASN	2.7

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

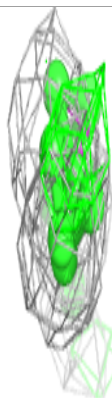
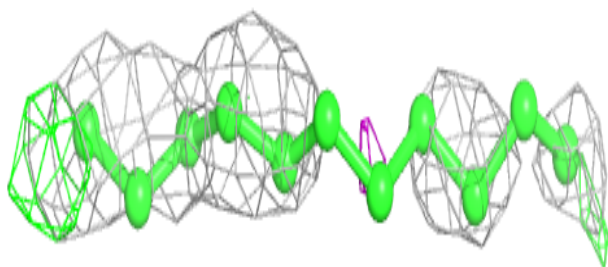
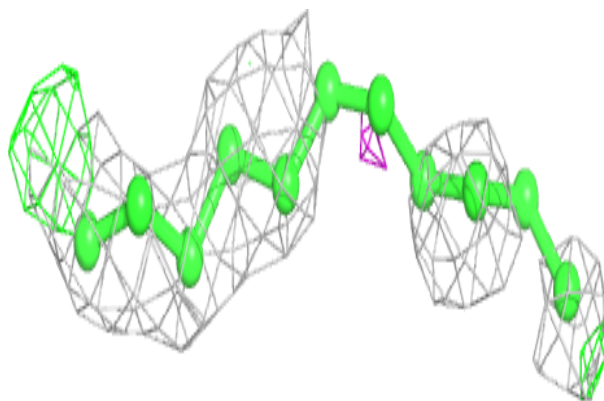


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEE	B	308	11/51	0.43	0.43	46,51,56,58	0
3	PEE	A	305	11/51	0.44	0.42	49,57,62,63	0
3	PEE	A	314	17/51	0.49	0.43	53,59,69,70	0
3	PEE	B	312	18/51	0.50	0.32	62,65,76,77	0
3	PEE	A	308	12/51	0.56	0.29	66,68,70,72	0
3	PEE	B	303	11/51	0.60	0.26	47,54,57,58	0
3	PEE	A	313	11/51	0.63	0.20	46,48,50,50	0
3	PEE	B	314	14/51	0.64	0.29	46,56,63,65	0
3	PEE	A	321	8/51	0.65	0.27	43,48,49,49	0
3	PEE	B	315	6/51	0.68	0.24	56,56,57,58	0
3	PEE	B	322	17/51	0.70	0.30	45,52,55,55	0
3	PEE	A	319	18/51	0.73	0.27	41,54,57,57	0
3	PEE	B	302	15/51	0.74	0.23	46,53,65,65	0
3	PEE	A	309	17/51	0.74	0.24	45,54,58,59	0
3	PEE	A	310	17/51	0.74	0.23	36,44,47,48	0
3	PEE	B	319	18/51	0.74	0.24	44,48,54,56	0
3	PEE	B	318	16/51	0.75	0.23	45,48,58,59	0
3	PEE	B	307	15/51	0.75	0.21	43,46,52,53	0
3	PEE	A	316	6/51	0.77	0.24	47,50,51,52	0
3	PEE	A	312	15/51	0.77	0.21	45,47,49,50	0
3	PEE	A	304	8/51	0.79	0.24	48,50,53,54	0
3	PEE	B	317	12/51	0.79	0.20	47,49,50,50	0
3	PEE	A	311	11/51	0.80	0.18	45,47,55,56	0
3	PEE	B	309	12/51	0.80	0.21	57,60,65,66	0
3	PEE	A	303	14/51	0.81	0.17	41,42,44,44	0
3	PEE	A	306	17/51	0.83	0.23	35,39,42,43	0
3	PEE	B	321	10/51	0.83	0.18	40,45,47,48	0
3	PEE	A	317	14/51	0.84	0.27	46,59,67,68	0
3	PEE	B	305	9/51	0.85	0.14	35,37,39,40	0
3	PEE	B	313	5/51	0.87	0.26	42,43,44,46	0
3	PEE	B	304	15/51	0.88	0.16	38,40,51,52	0
3	PEE	B	310	9/51	0.88	0.17	28,29,31,34	0
3	PEE	A	315	8/51	0.88	0.23	35,37,40,41	0
3	PEE	B	320	6/51	0.88	0.20	32,33,36,38	0
3	PEE	B	306	12/51	0.89	0.23	48,53,60,62	0
2	RET	A	301	20/21	0.92	0.17	17,18,24,25	0
2	RET	B	301	20/21	0.94	0.15	15,16,23,26	0

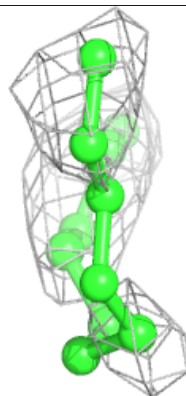
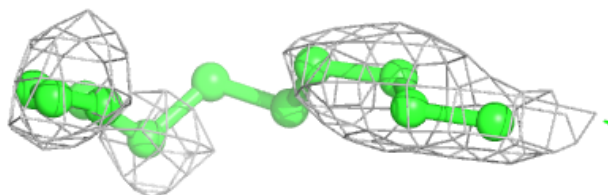
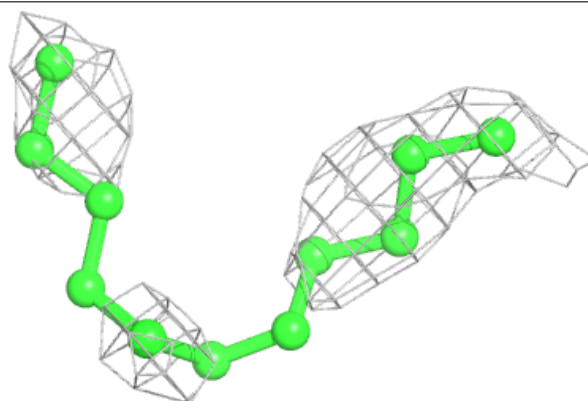
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PEE B 308:**

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

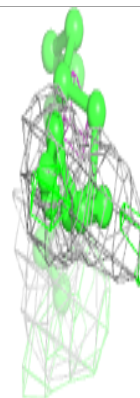
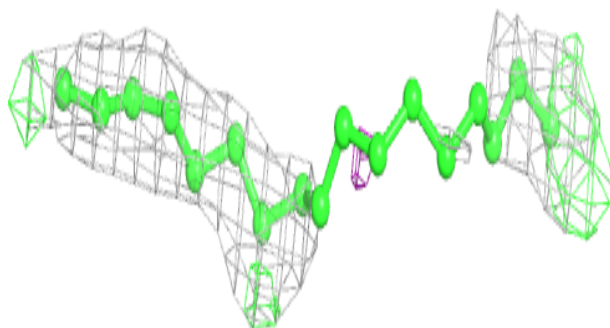
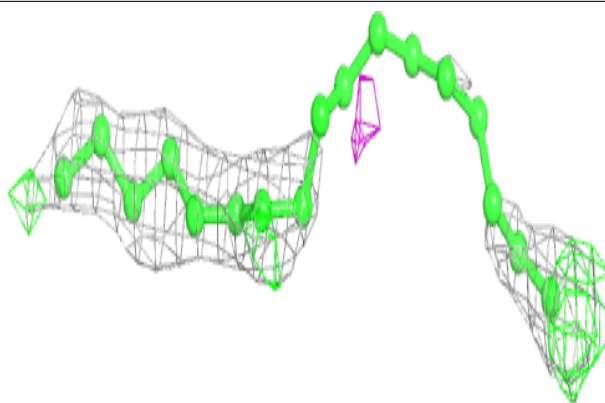
**Electron density around PEE A 305:**

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

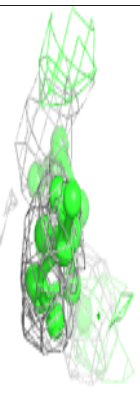
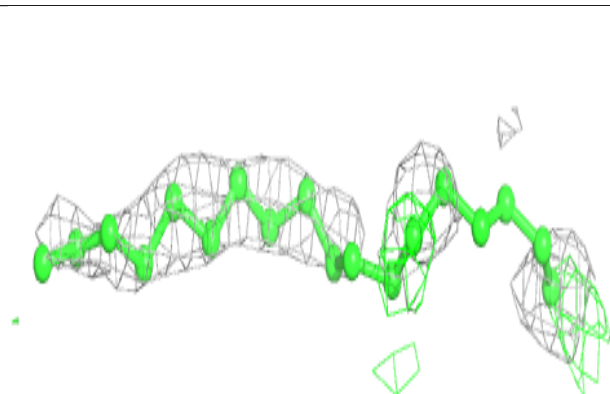
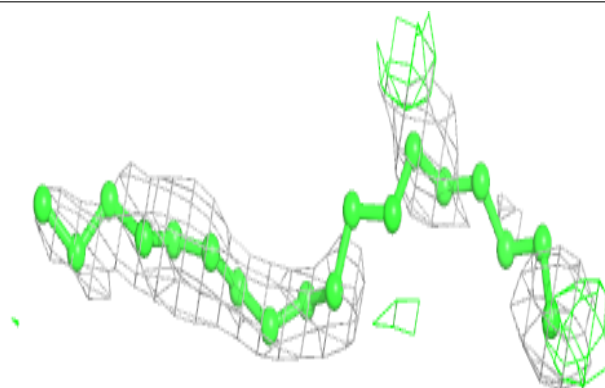


**Electron density around PEE A 314:**

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

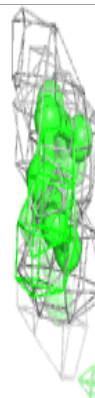
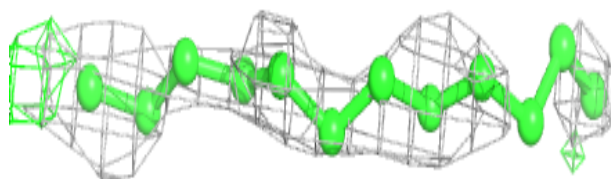
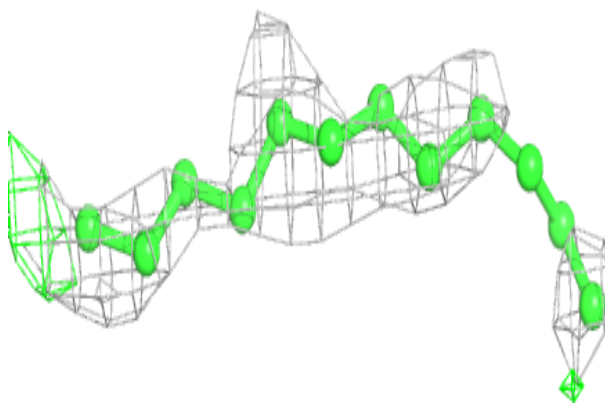
**Electron density around PEE B 312:**

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



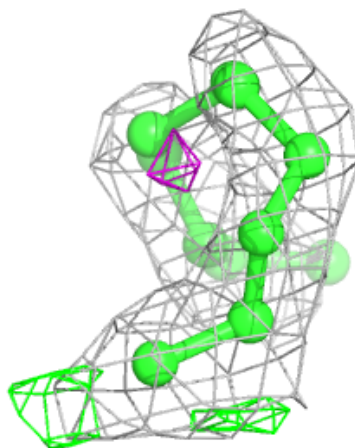
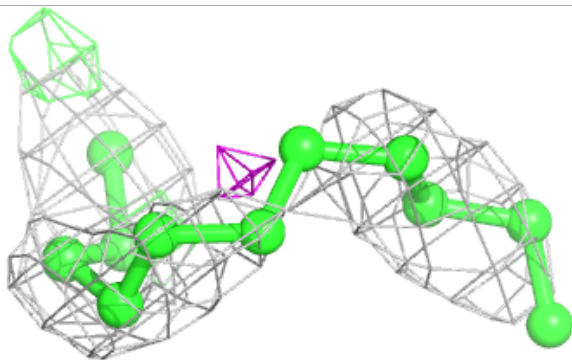
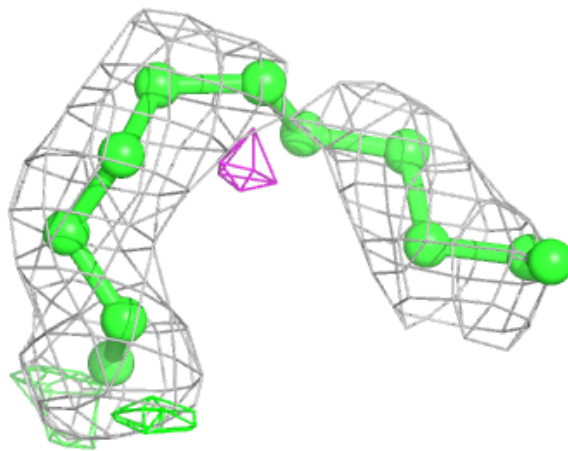
**Electron density around PEE A 308:**

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



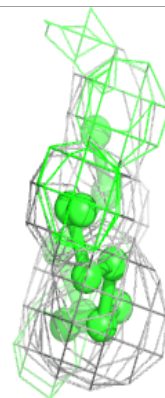
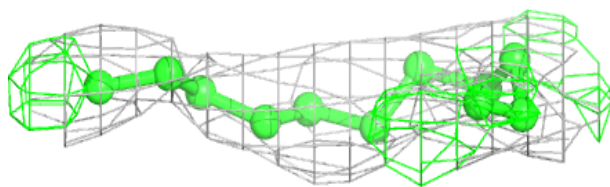
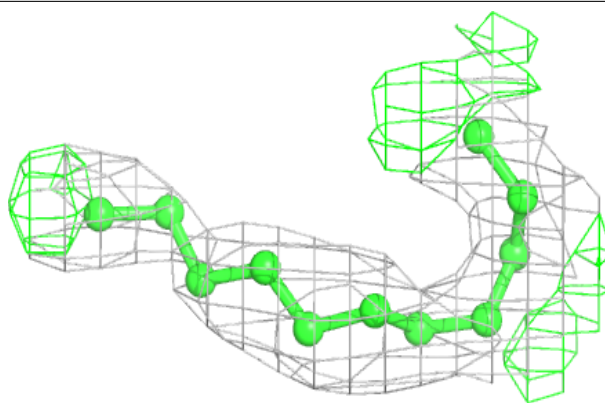
**Electron density around PEE B 303:**

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

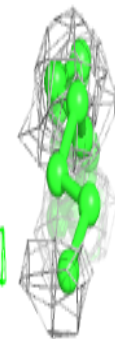
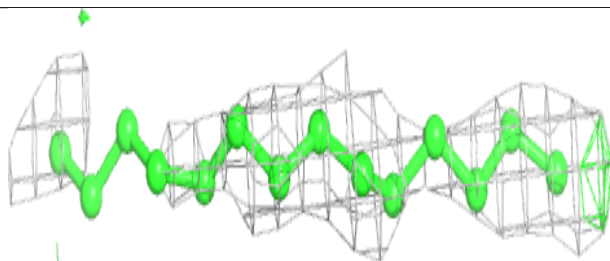
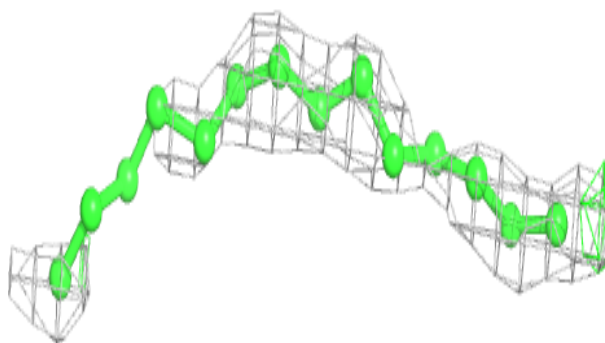


**Electron density around PEE A 313:**

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

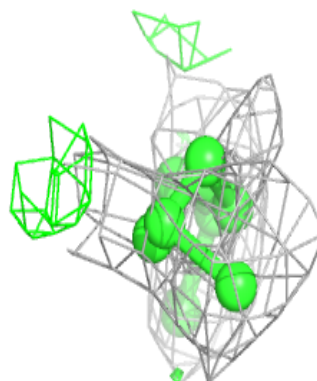
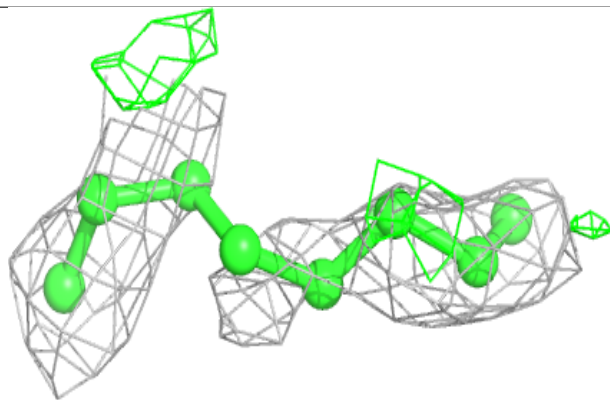
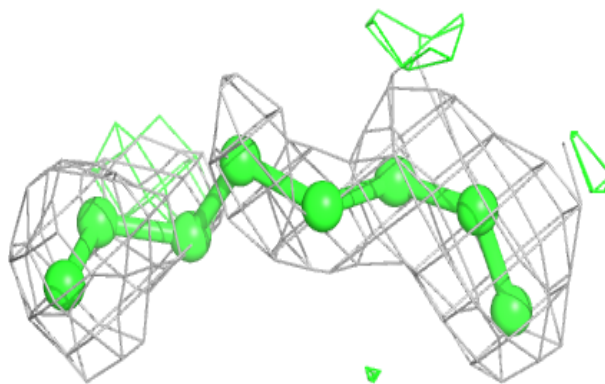
**Electron density around PEE B 314:**

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

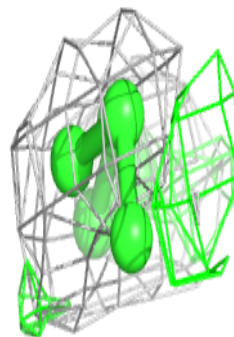
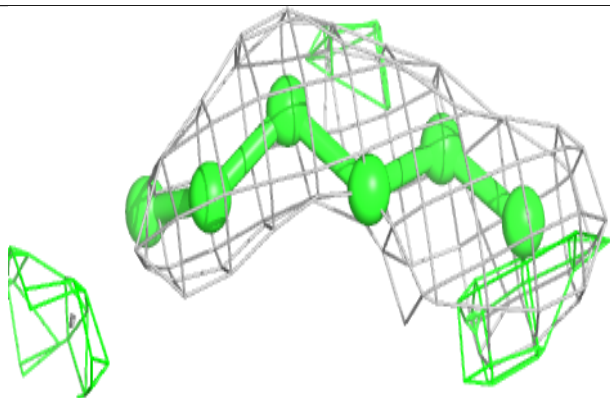
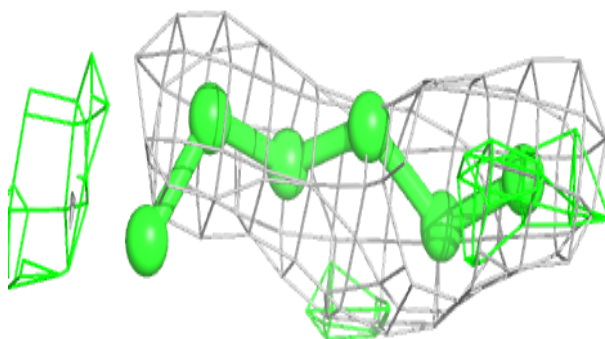


**Electron density around PEE A 321:**

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

**Electron density around PEE B 315:**

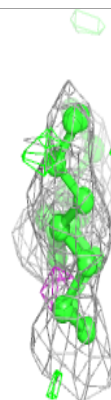
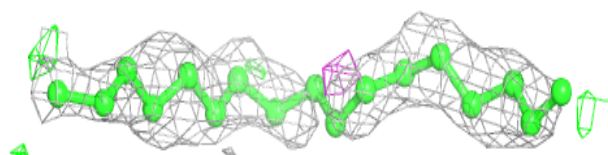
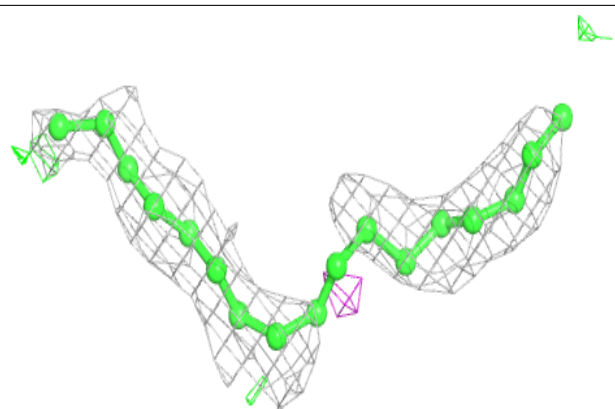
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



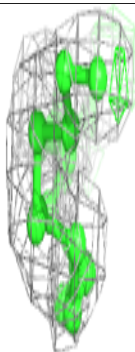
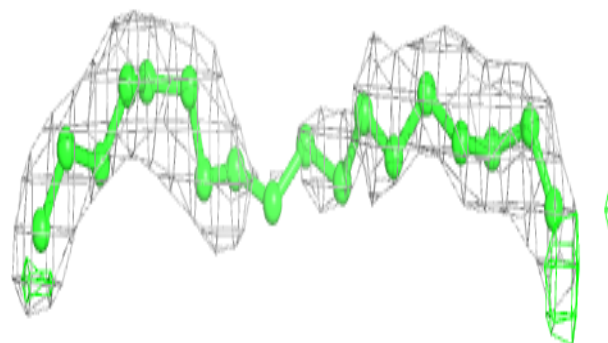
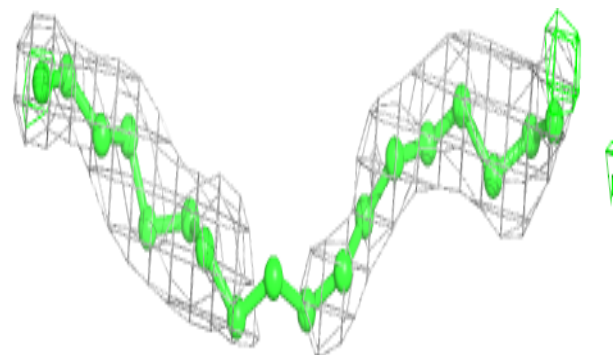


**Electron density around PEE B 322:**

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

**Electron density around PEE A 319:**

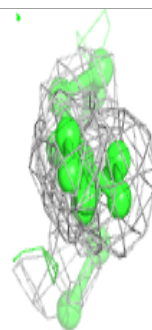
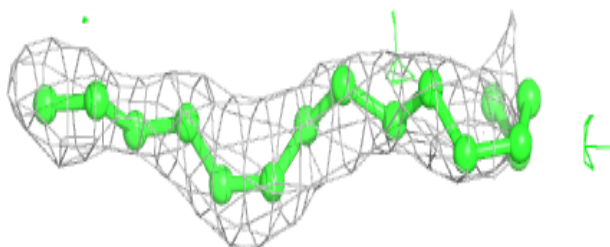
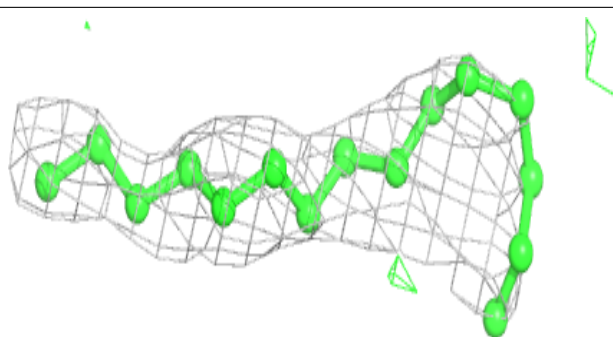
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



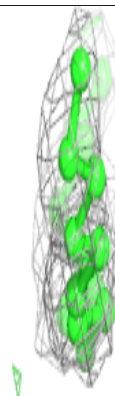
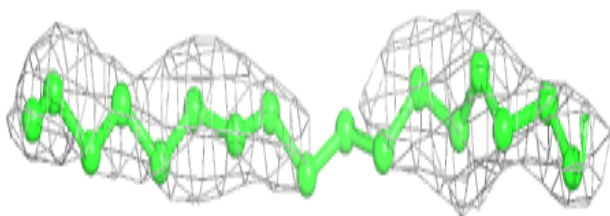
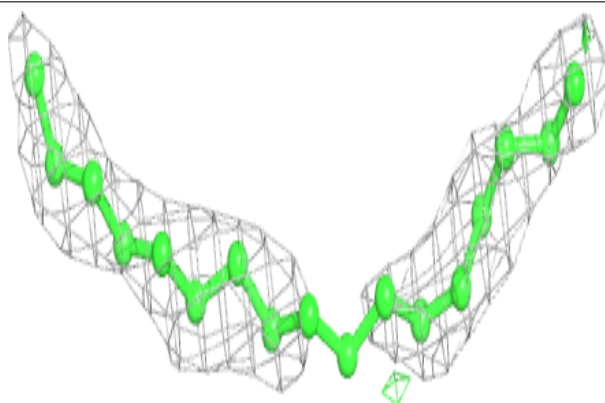


**Electron density around PEE B 302:**

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

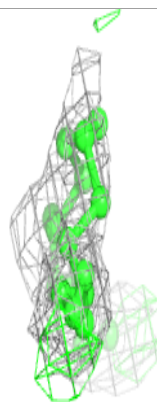
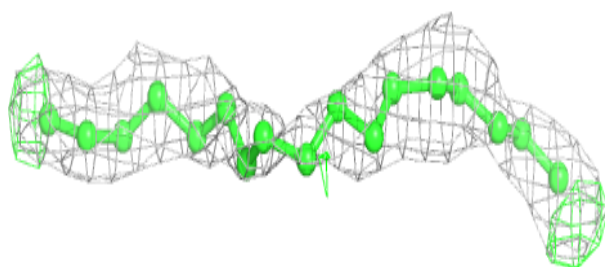
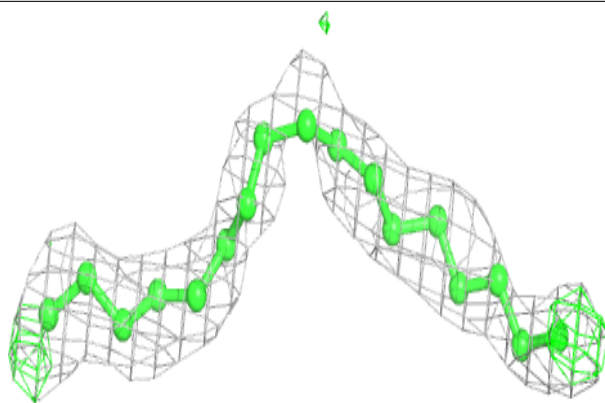
**Electron density around PEE A 309:**

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

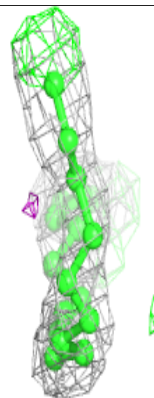
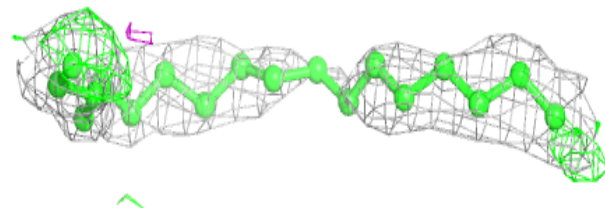
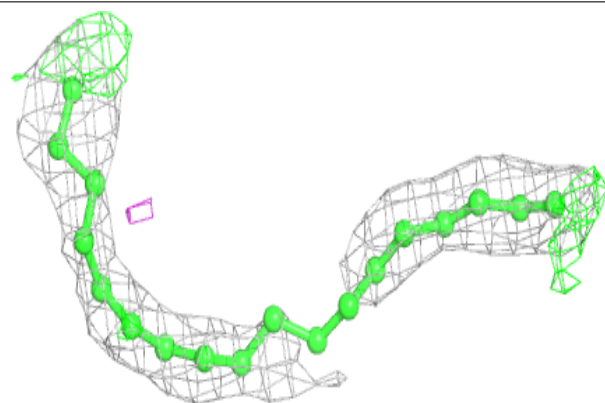


**Electron density around PEE A 310:**

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

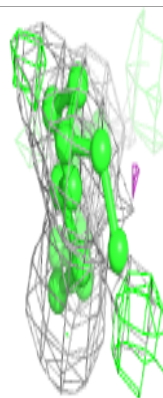
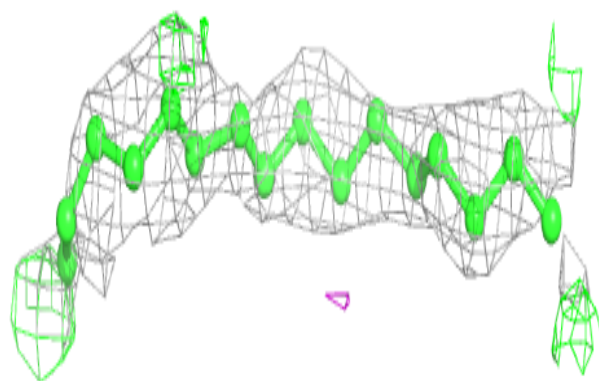
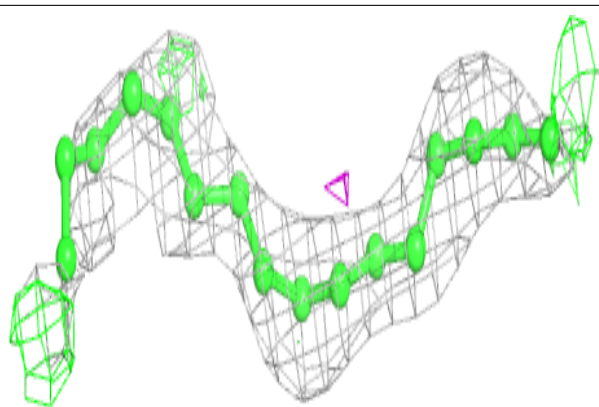
**Electron density around PEE B 319:**

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

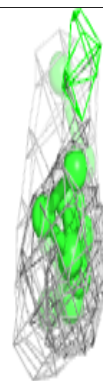
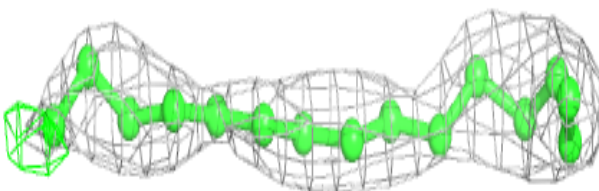
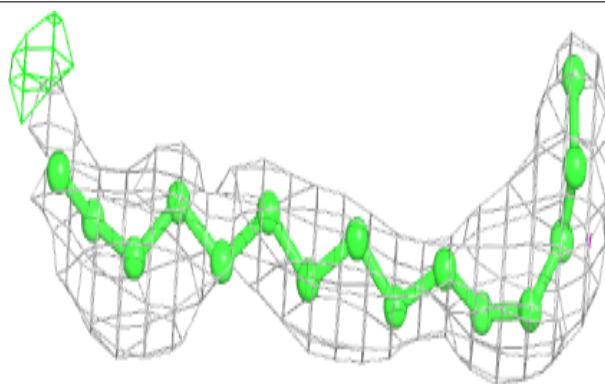


**Electron density around PEE B 318:**

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

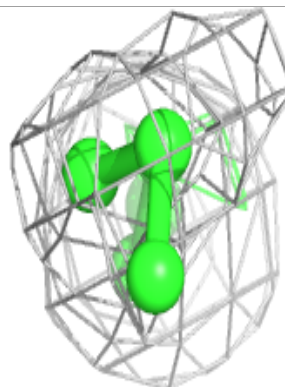
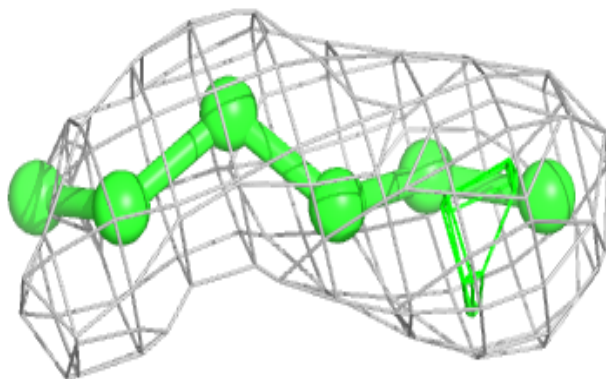
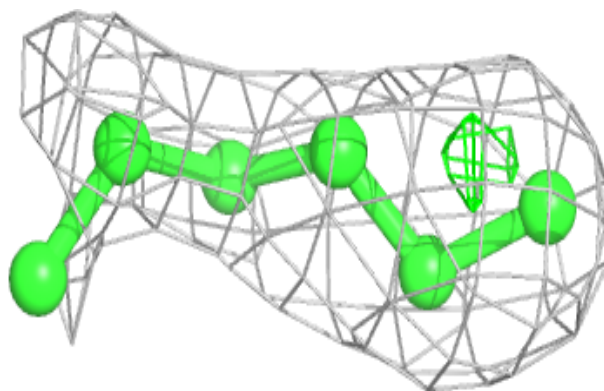
**Electron density around PEE B 307:**

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

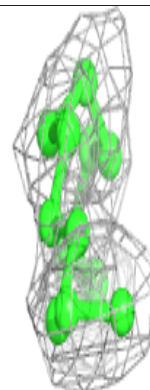
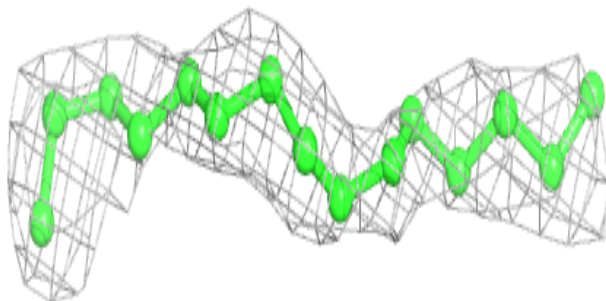
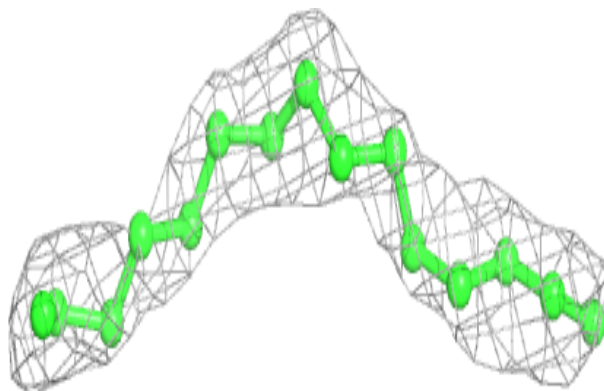


**Electron density around PEE A 316:**

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

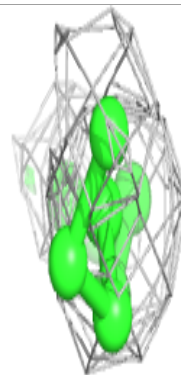
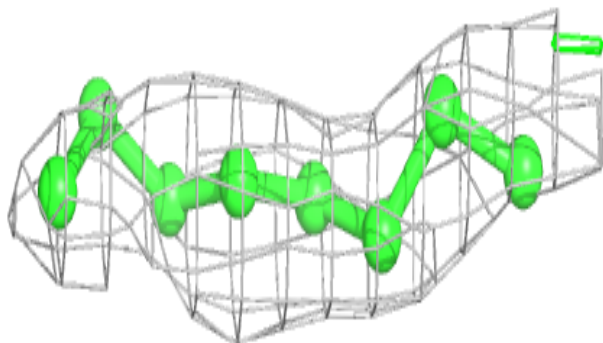
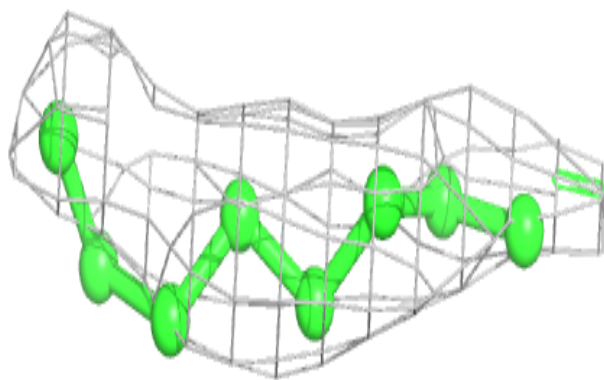
**Electron density around PEE A 312:**

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

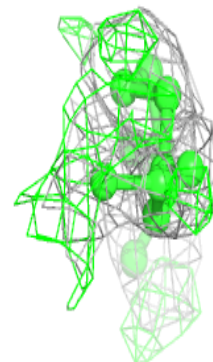
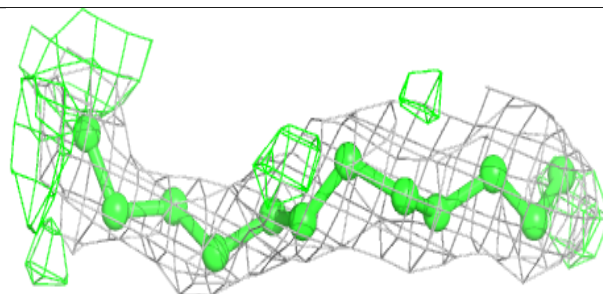
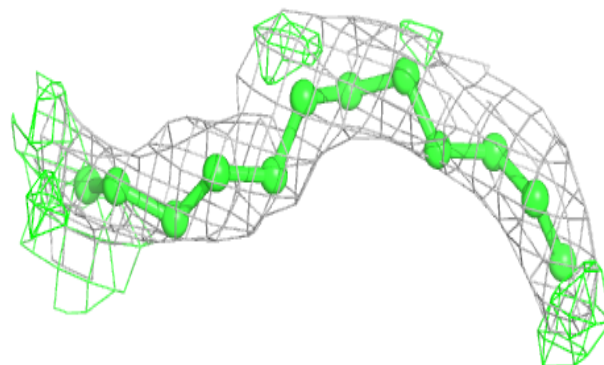


**Electron density around PEE A 304:**

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

**Electron density around PEE B 317:**

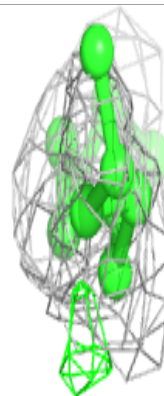
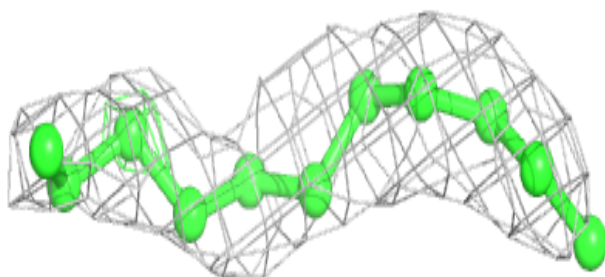
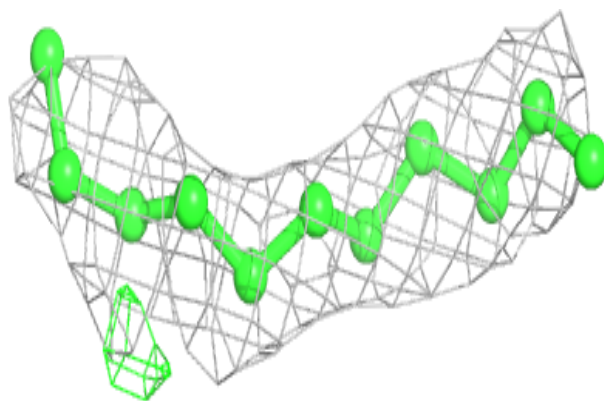
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



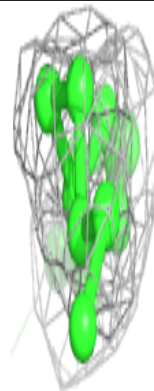
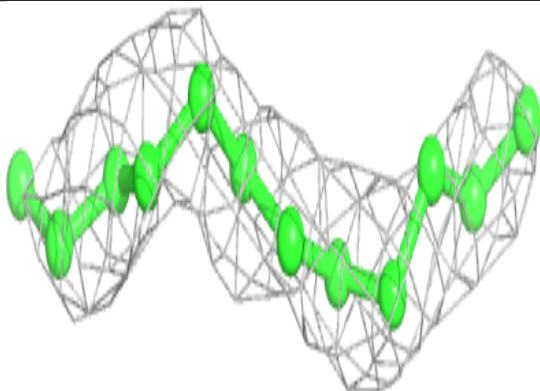
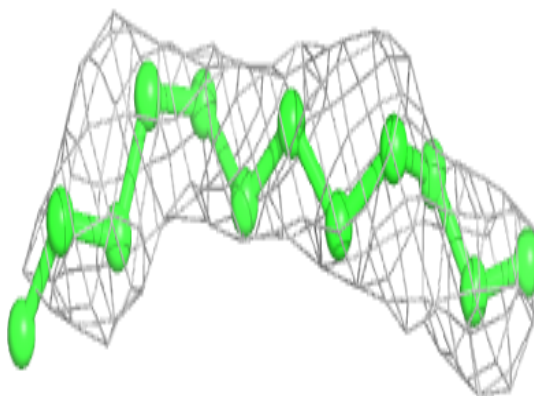


**Electron density around PEE A 311:**

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

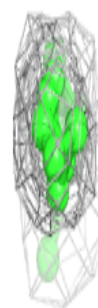
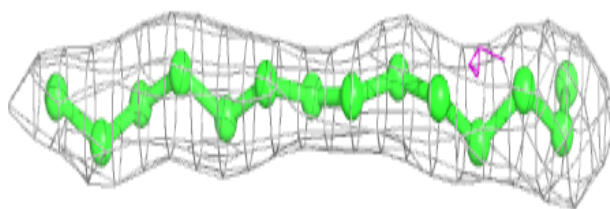
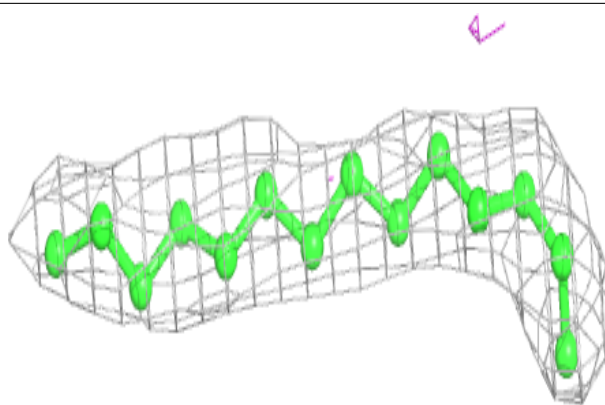
**Electron density around PEE B 309:**

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

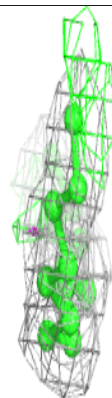
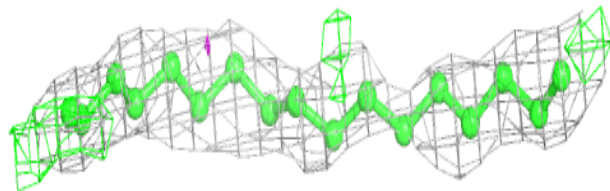
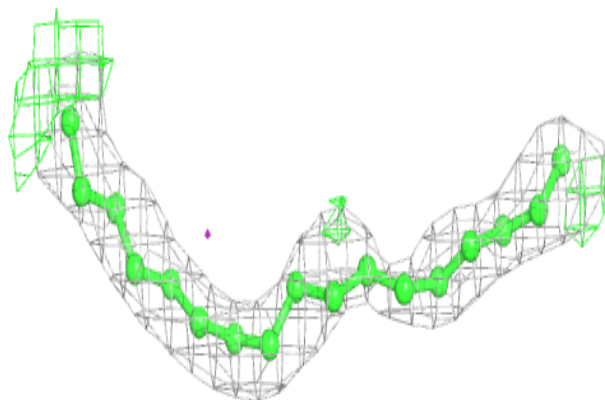


**Electron density around PEE A 303:**

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

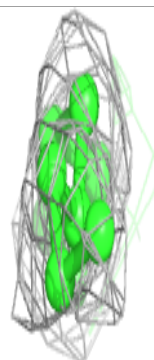
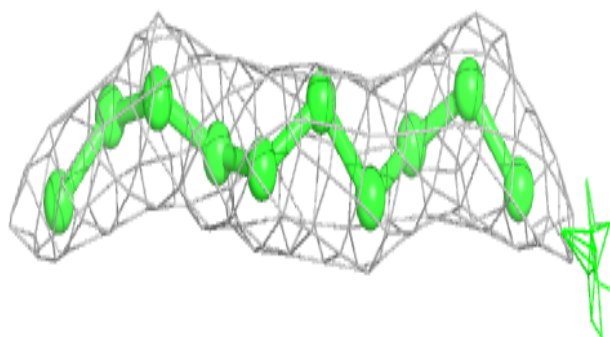
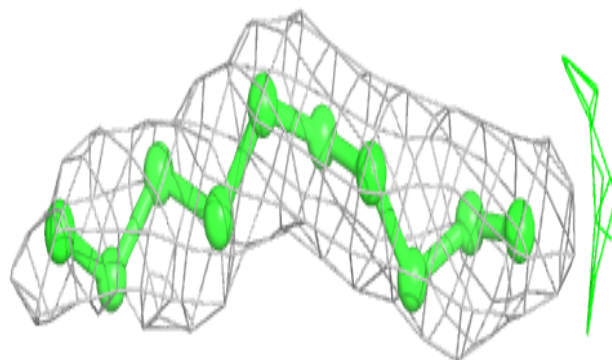
**Electron density around PEE A 306:**

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

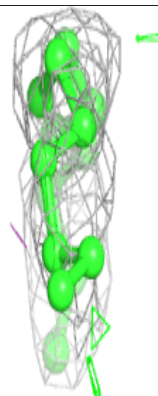
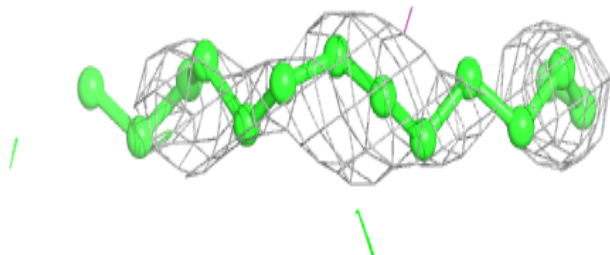
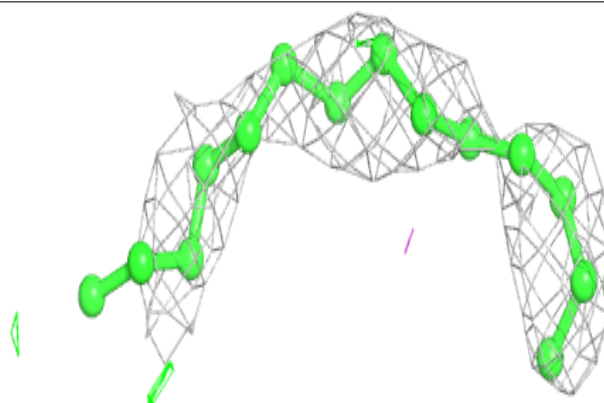


**Electron density around PEE B 321:**

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

**Electron density around PEE A 317:**

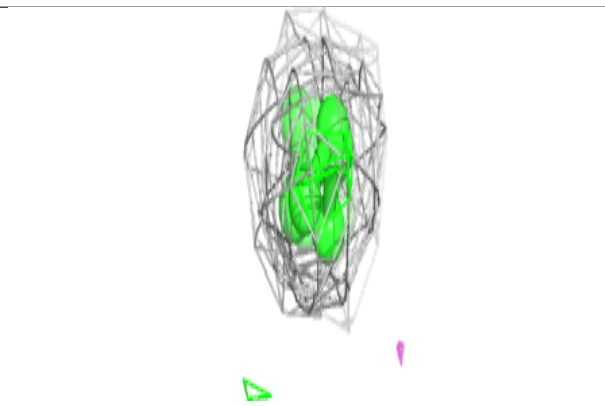
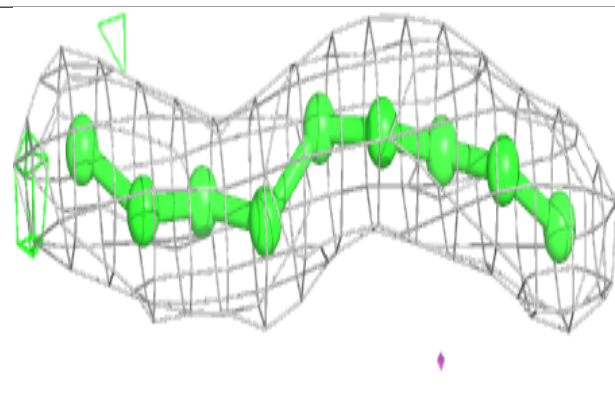
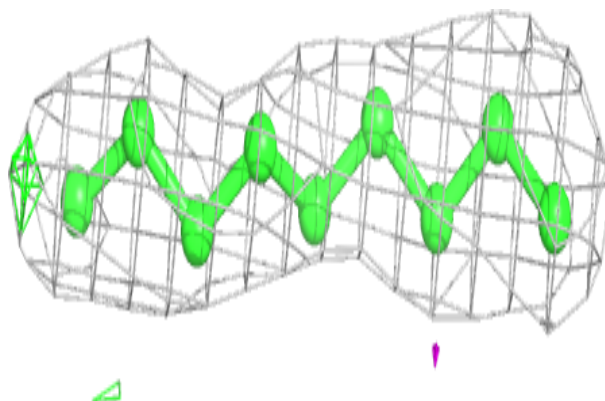
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



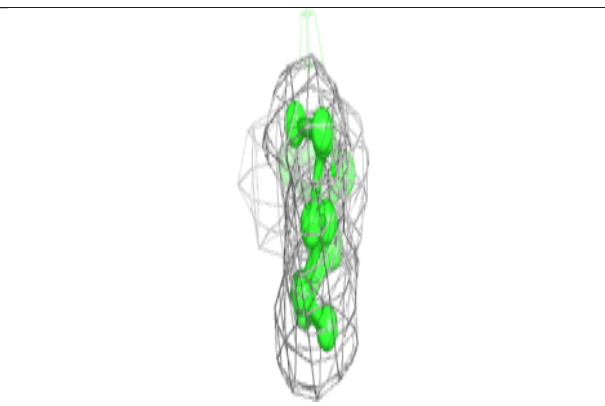
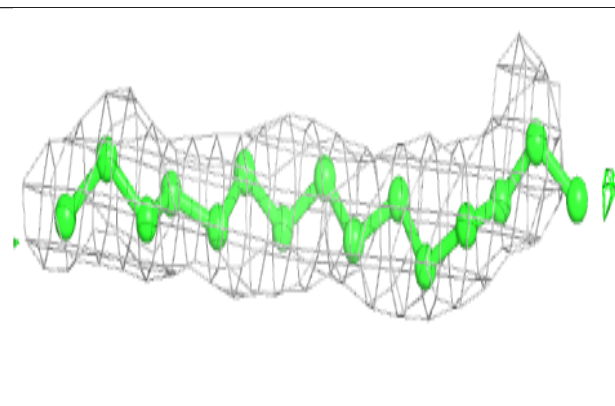
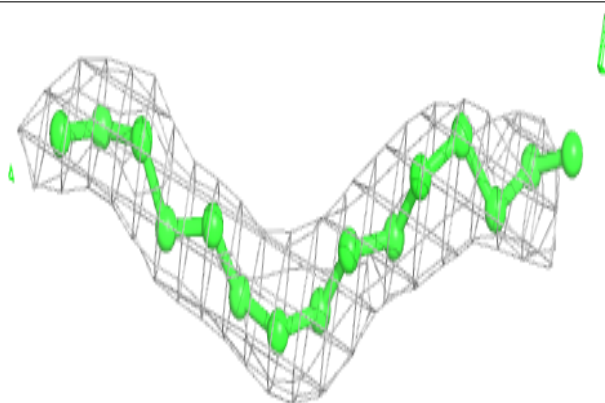


**Electron density around PEE B 305:**

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

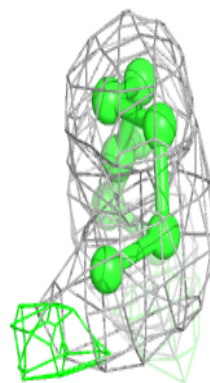
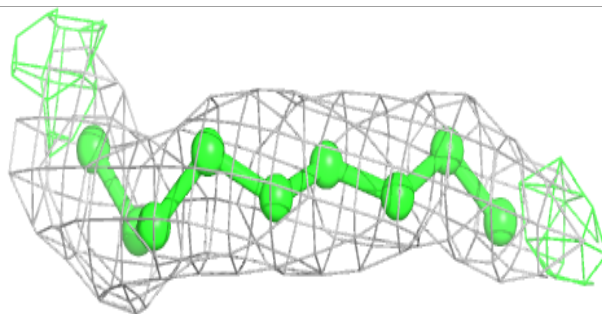
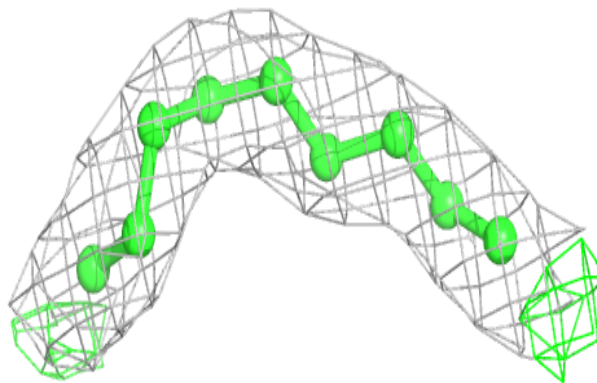
**Electron density around PEE B 304:**

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

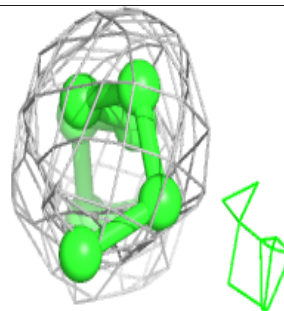
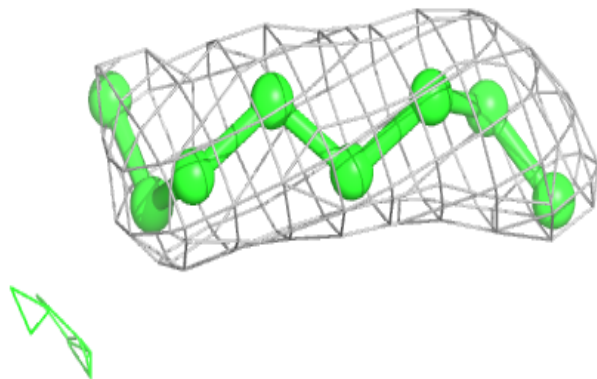
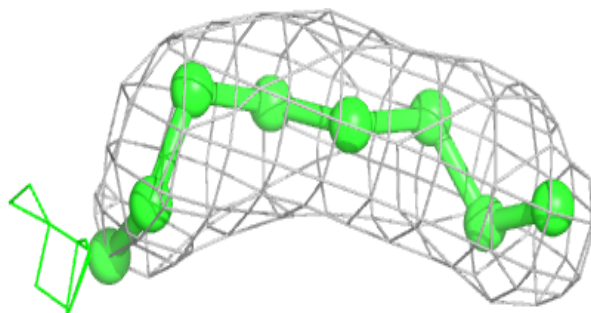


**Electron density around PEE B 310:**

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

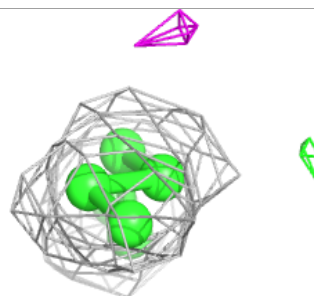
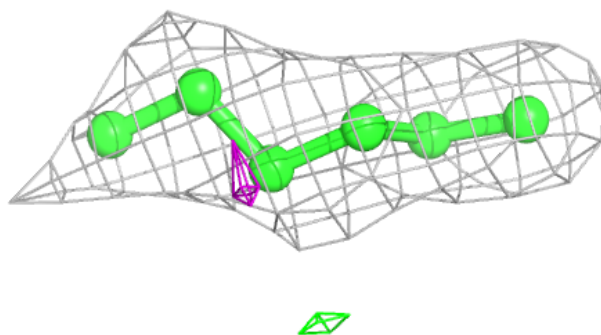
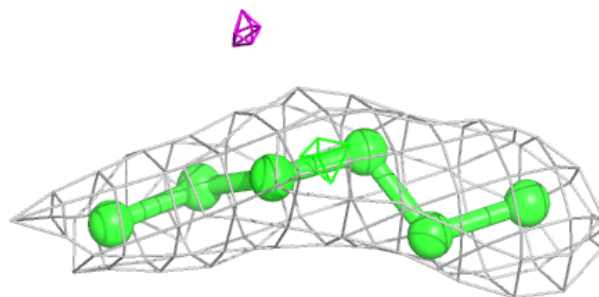
**Electron density around PEE A 315:**

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

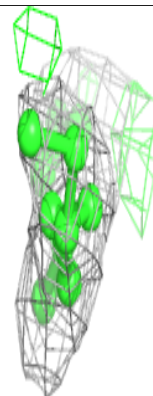
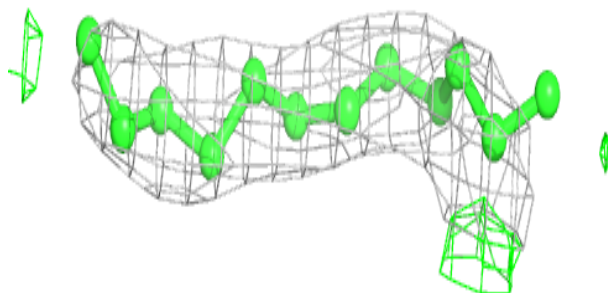
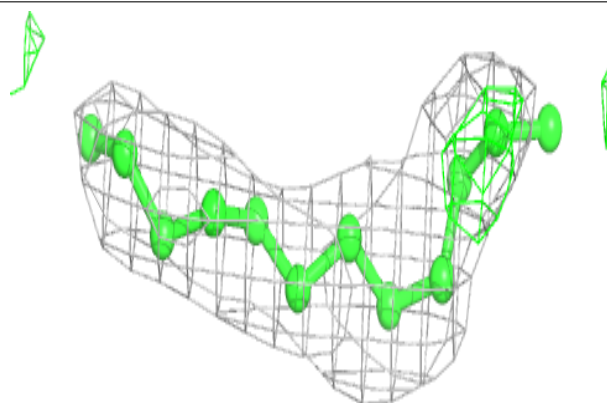


**Electron density around PEE B 320:**

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

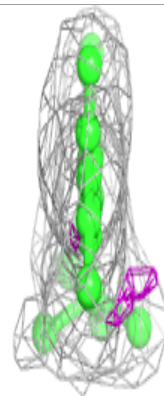
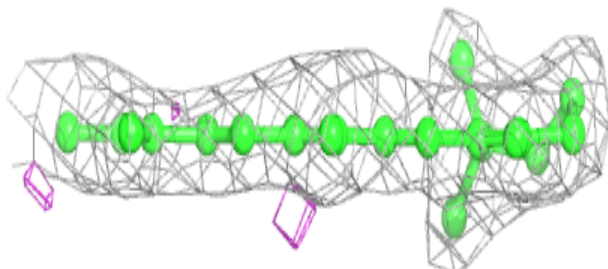
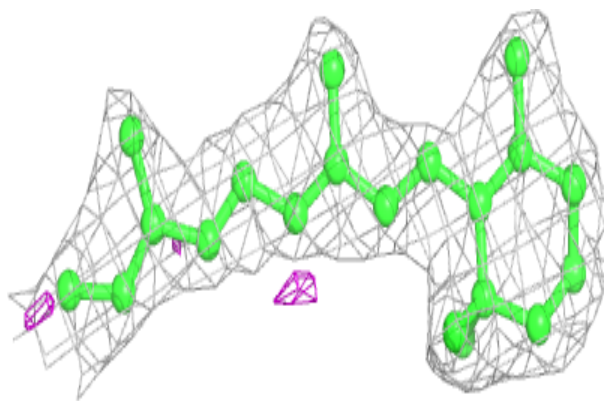
**Electron density around PEE B 306:**

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

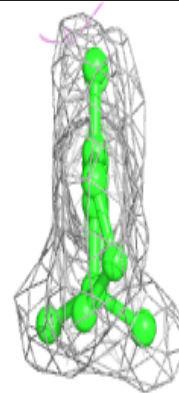
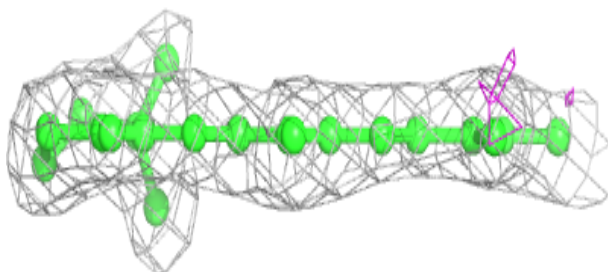
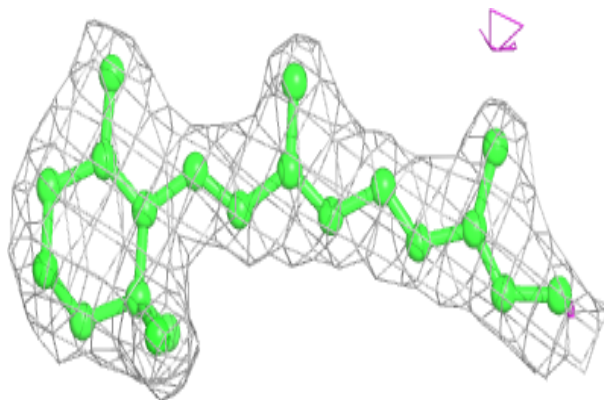


**Electron density around RET A 301:**

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

**Electron density around RET 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.