



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2021 – 11:27 AM EDT

PDB ID : 1M57  
Title : Structure of cytochrome c oxidase from Rhodobacter sphaeroides (EQ(I-286 mutant))  
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.  
Deposited on : 2002-07-08  
Resolution : 3.00 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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

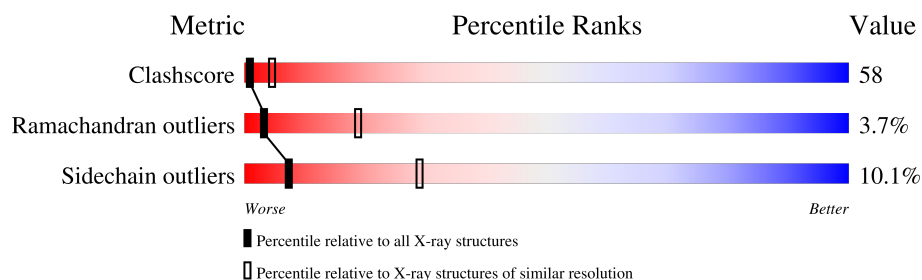
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	21% 53% 20% . .
1	G	566	20% 53% 20% . .
2	B	264	33% 48% 15% . .
2	H	264	29% 49% 19% . .
3	C	266	35% 51% 12% .
3	I	266	38% 48% 14% .
4	D	51	29% 41% 12% 18%
4	J	51	25% 47% 8% . 18%

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
8	HEA	A	1001	X	-	-	-
8	HEA	A	1002	X	-	-	-
8	HEA	G	1001	X	-	X	-
8	HEA	G	1002	X	-	-	-
9	3PE	C	2010	-	-	X	-
9	3PE	C	2013	-	-	X	-
9	3PE	G	3012	-	-	X	-
9	3PE	I	3010	-	-	X	-
9	3PE	I	3013	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18934 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4322	2892	685	714	31			
1	G	547	Total	C	N	O	S	0	0	0
			4322	2892	685	714	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLN	GLU	engineered mutation	UNP P33517
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	286	GLN	GLU	engineered mutation	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			
2	H	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			
3	I	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			
4	J	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	2	Total	Cu	0	0
			2	2		
5	G	1	Total	Cu	0	0
			1	1		
5	H	2	Total	Cu	0	0
			2	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

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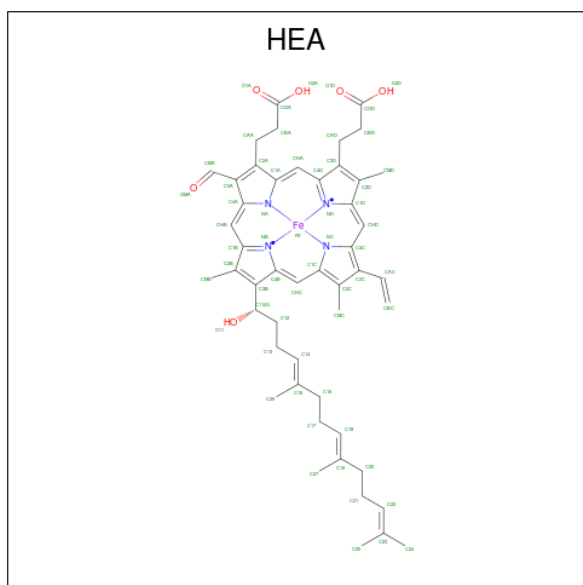
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

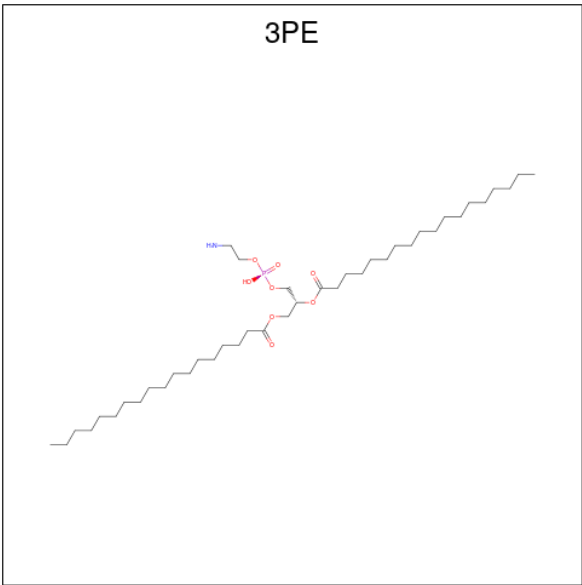
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
8	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
8	G	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
8	G	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	J	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	97	Total 97	O 97	0	0
10	B	70	Total 70	O 70	0	0
10	C	38	Total 38	O 38	0	0
10	D	13	Total 13	O 13	0	0
10	G	107	Total 107	O 107	0	0
10	H	64	Total 64	O 64	0	0
10	I	37	Total 37	O 37	0	0
10	J	10	Total 10	O 10	0	0



### 3 Residue-property plots

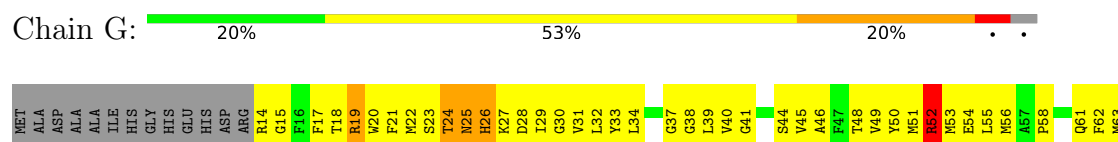
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

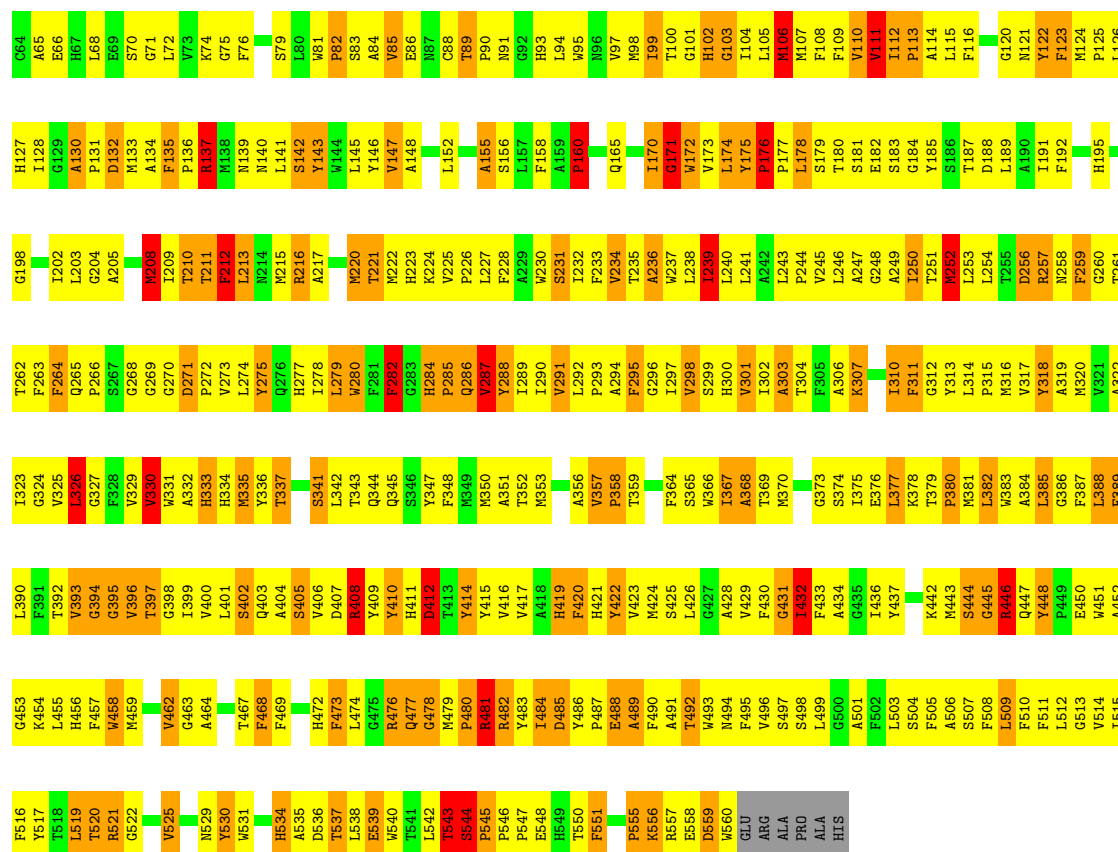
Note EDS was not executed.

#### • Molecule 1: CYTOCHROME C OXIDASE



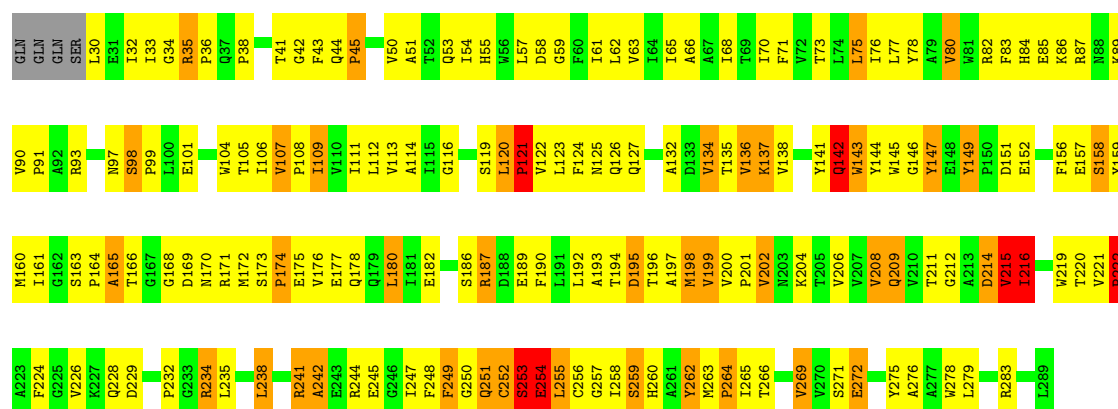
#### • Molecule 1: CYTOCHROME C OXIDASE





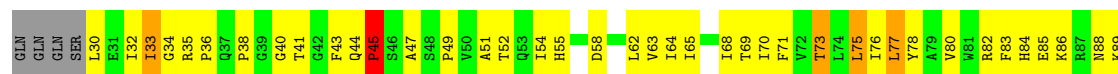
## • Molecule 2: CYTOCHROME C OXIDASE

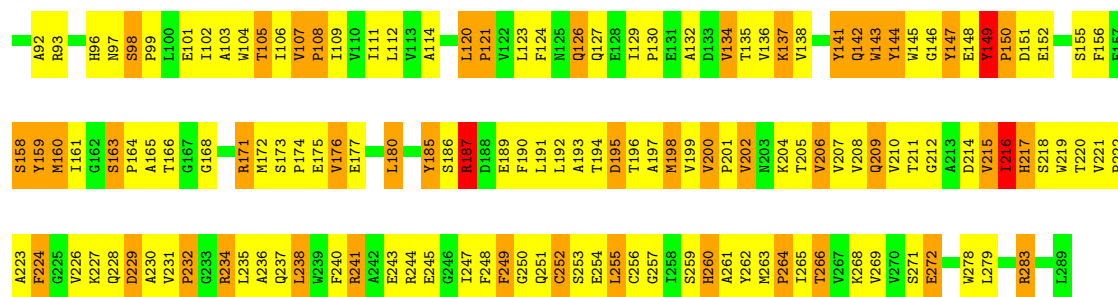
Chain B: 33% 48% 15%



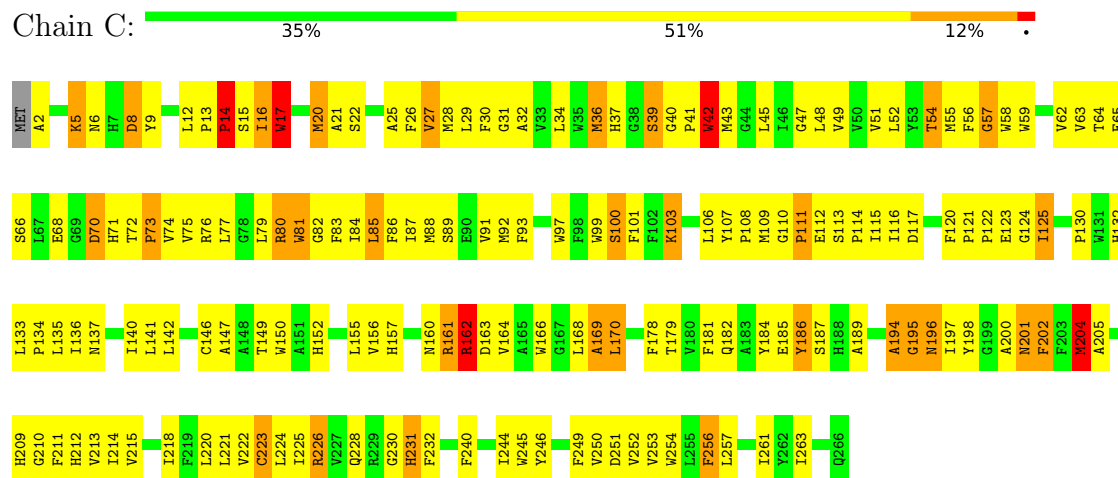
## • Molecule 2: CYTOCHROME C OXIDASE

Chain H: 29% 49% 19%

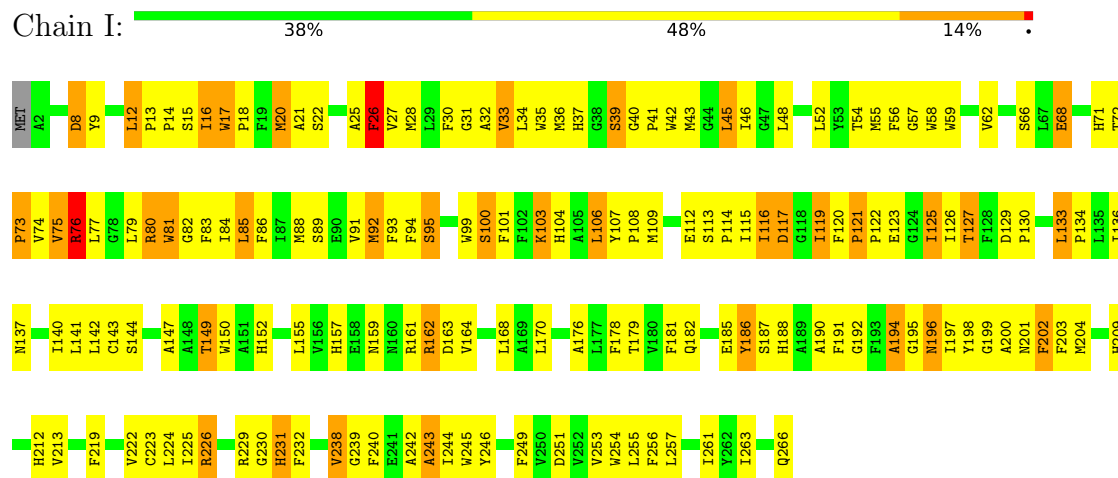




• Molecule 3: CYTOCHROME C OXIDASE



• Molecule 3: CYTOCHROME C OXIDASE

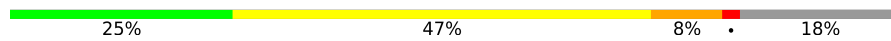


• Molecule 4: CYTOCHROME C OXIDASE



• Molecule 4: CYTOCHROME C OXIDASE

Chain J:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	340.72 Å   340.72 Å   89.76 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	4.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (4.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.293 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU, MG, CA, 3PE, HEA

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	0.73	0/4482	2.01	128/6114 (2.1%)
1	G	0.75	1/4482 (0.0%)	2.06	133/6114 (2.2%)
2	B	0.60	0/2105	1.93	56/2879 (1.9%)
2	H	0.65	0/2105	1.96	58/2879 (2.0%)
3	C	0.57	0/2232	1.66	33/3054 (1.1%)
3	I	0.59	0/2232	1.65	30/3054 (1.0%)
4	D	0.58	0/316	1.63	4/428 (0.9%)
4	J	0.60	0/316	1.63	4/428 (0.9%)
All	All	0.67	1/18270 (0.0%)	1.91	446/24950 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	G	0	16
2	B	0	6
2	H	0	3
3	C	0	5
3	I	0	7
4	D	0	1
All	All	0	57

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	112	ILE	N-CA	5.08	1.56	1.46

The worst 5 of 446 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	52	ARG	NE-CZ-NH2	-24.46	108.07	120.30
2	B	171	ARG	NE-CZ-NH1	19.39	130.00	120.30
1	A	543	THR	C-N-CA	19.24	169.80	121.70
1	G	543	THR	C-N-CA	16.53	163.02	121.70
2	H	171	ARG	NE-CZ-NH1	15.75	128.17	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	114	ALA	Mainchain
1	A	29	ILE	Mainchain
1	A	96	ASN	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4322	0	4240	609	0
1	G	4322	0	4240	621	0
2	B	2046	0	2011	219	0
2	H	2046	0	2011	231	0
3	C	2139	0	2056	224	0
3	I	2139	0	2056	214	0
4	D	311	0	319	33	0
4	J	311	0	319	40	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	120	0	108	40	0
8	G	120	0	108	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	102	0	164	38	0
9	C	153	0	246	56	0
9	D	51	0	82	17	0
9	G	102	0	164	41	0
9	I	153	0	246	59	0
9	J	51	0	82	13	0
10	A	97	0	0	26	0
10	B	70	0	0	20	0
10	C	38	0	0	8	0
10	D	13	0	0	0	0
10	G	107	0	0	30	0
10	H	64	0	0	18	0
10	I	37	0	0	7	0
10	J	10	0	0	1	0
All	All	18934	0	18452	2141	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 58.

The worst 5 of 2141 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:G:379:THR:HB	1:G:380:PRO:HD3	1.18	1.17
1:A:106:MET:HG2	8:A:1001:HEA:HAC	1.17	1.16
9:C:2010:3PE:H3E2	9:C:2010:3PE:H3I2	1.22	1.13
9:I:3010:3PE:H3E2	9:I:3010:3PE:C3I	1.78	1.13
8:A:1002:HEA:HMC1	8:A:1002:HEA:HBC1	1.30	1.11

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	545/566 (96%)	416 (76%)	106 (19%)	23 (4%)	3	16
1	G	545/566 (96%)	403 (74%)	112 (21%)	30 (6%)	2	10
2	B	258/264 (98%)	203 (79%)	47 (18%)	8 (3%)	4	23
2	H	258/264 (98%)	206 (80%)	44 (17%)	8 (3%)	4	23
3	C	263/266 (99%)	217 (82%)	41 (16%)	5 (2%)	8	36
3	I	263/266 (99%)	209 (80%)	49 (19%)	5 (2%)	8	36
4	D	40/51 (78%)	26 (65%)	13 (32%)	1 (2%)	5	28
4	J	40/51 (78%)	26 (65%)	12 (30%)	2 (5%)	2	12
All	All	2212/2294 (96%)	1706 (77%)	424 (19%)	82 (4%)	3	19

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	160	PRO
1	A	544	SER
1	A	545	PRO
2	B	254	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/459 (97%)	397 (89%)	49 (11%)	6	25
1	G	446/459 (97%)	397 (89%)	49 (11%)	6	25
2	B	216/220 (98%)	195 (90%)	21 (10%)	8	31
2	H	216/220 (98%)	196 (91%)	20 (9%)	9	33
3	C	215/216 (100%)	198 (92%)	17 (8%)	12	41
3	I	215/216 (100%)	195 (91%)	20 (9%)	9	33
4	D	30/37 (81%)	25 (83%)	5 (17%)	2	11
4	J	30/37 (81%)	27 (90%)	3 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1814/1864 (97%)	1630 (90%)	184 (10%)	7 29

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	286	GLN
2	H	63	VAL
1	G	330	VAL
1	G	443	MET
2	H	158	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	209	GLN
3	I	212	HIS
2	H	237	GLN
3	I	153	HIS
4	J	9	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	3PE	C	2010	-	50,50,50	1.53	2 (4%)	53,55,55	1.14	3 (5%)
9	3PE	J	3011	-	50,50,50	1.70	2 (4%)	53,55,55	1.51	7 (13%)
9	3PE	I	3013	-	50,50,50	1.63	3 (6%)	53,55,55	1.18	3 (5%)
9	3PE	D	2011	-	50,50,50	1.49	3 (6%)	53,55,55	1.29	7 (13%)
9	3PE	G	3009	-	50,50,50	1.49	3 (6%)	53,55,55	0.98	2 (3%)
9	3PE	C	2013	-	50,50,50	1.58	3 (6%)	53,55,55	1.29	2 (3%)
9	3PE	A	2009	-	50,50,50	1.61	3 (6%)	53,55,55	1.11	3 (5%)
8	HEA	G	1001	1	44,67,67	1.73	8 (18%)	37,103,103	2.59	19 (51%)
9	3PE	C	2008	-	50,50,50	1.58	2 (4%)	53,55,55	1.18	6 (11%)
8	HEA	G	1002	1	44,67,67	1.60	8 (18%)	37,103,103	2.04	14 (37%)
9	3PE	I	3008	-	50,50,50	1.64	2 (4%)	53,55,55	1.13	3 (5%)
9	3PE	G	3012	-	50,50,50	1.62	3 (6%)	53,55,55	1.23	5 (9%)
9	3PE	I	3010	-	50,50,50	1.60	4 (8%)	53,55,55	1.03	2 (3%)
9	3PE	A	2012	-	50,50,50	1.61	3 (6%)	53,55,55	1.39	6 (11%)
8	HEA	A	1002	1	44,67,67	1.76	8 (18%)	37,103,103	2.13	9 (24%)
8	HEA	A	1001	1	44,67,67	1.74	7 (15%)	37,103,103	2.52	21 (56%)

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
9	3PE	C	2010	-	-	23/54/54/54	-
9	3PE	J	3011	-	-	22/54/54/54	-
9	3PE	I	3013	-	-	29/54/54/54	-
9	3PE	D	2011	-	-	22/54/54/54	-
9	3PE	G	3009	-	-	29/54/54/54	-
9	3PE	C	2013	-	-	27/54/54/54	-
9	3PE	A	2009	-	-	29/54/54/54	-
8	HEA	G	1001	1	3/3/7/16	9/24/76/76	-
9	3PE	C	2008	-	-	37/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEA	G	1002	1	3/3/7/16	2/24/76/76	-
9	3PE	I	3008	-	-	34/54/54/54	-
9	3PE	G	3012	-	-	22/54/54/54	-
9	3PE	I	3010	-	-	29/54/54/54	-
9	3PE	A	2012	-	-	22/54/54/54	-
8	HEA	A	1002	1	3/3/7/16	3/24/76/76	-
8	HEA	A	1001	1	3/3/7/16	10/24/76/76	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	3011	3PE	O21-C21	8.34	1.57	1.34
9	I	3013	3PE	O31-C31	7.69	1.55	1.33
9	A	2009	3PE	O21-C21	7.64	1.55	1.34
9	I	3008	3PE	O21-C21	7.64	1.55	1.34
9	C	2010	3PE	O21-C21	7.56	1.55	1.34

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1001	HEA	CBA-CAA-C2A	6.88	125.16	112.48
9	C	2013	3PE	C2-O21-C21	-6.44	101.93	117.79
9	J	3011	3PE	C2-O21-C21	-6.23	102.44	117.79
8	A	1002	HEA	C13-C14-C15	-6.19	112.75	127.66
8	G	1002	HEA	C13-C14-C15	-5.49	114.44	127.66

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1001	HEA	ND
8	A	1001	HEA	NA
8	A	1001	HEA	NB
8	A	1002	HEA	ND
8	A	1002	HEA	NA

5 of 349 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C1A-C2A-CAA-CBA
8	A	1001	HEA	C3A-C2A-CAA-CBA

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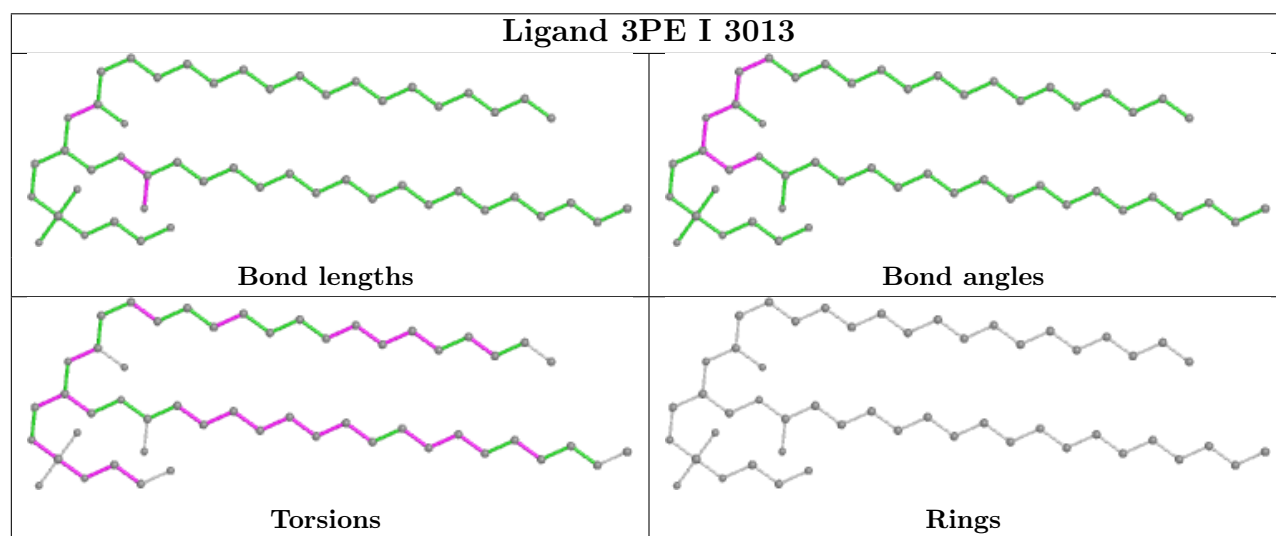
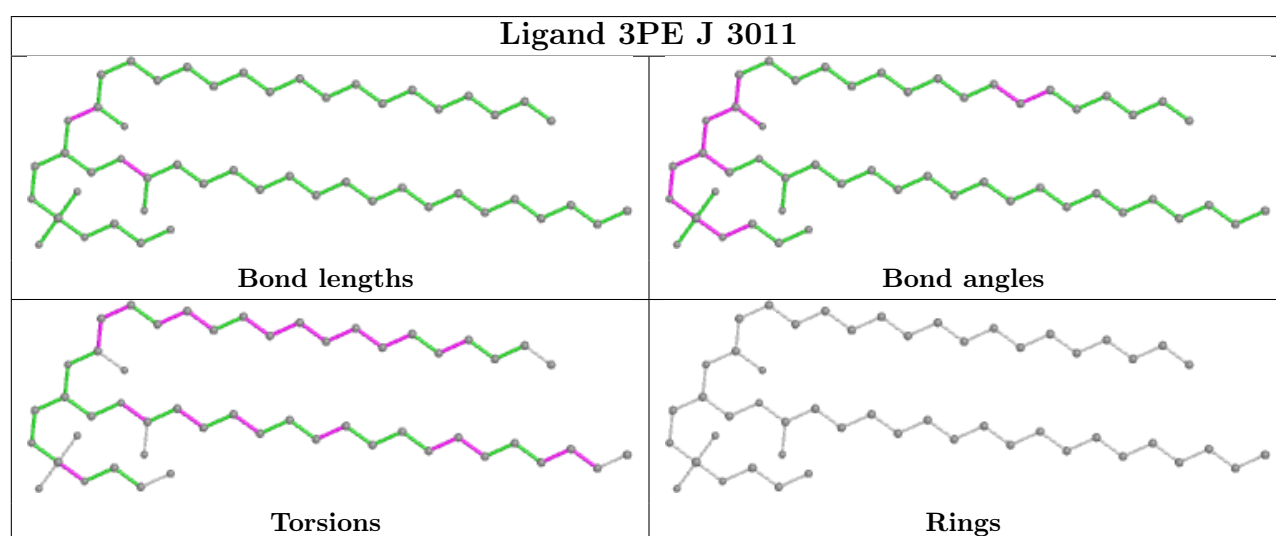
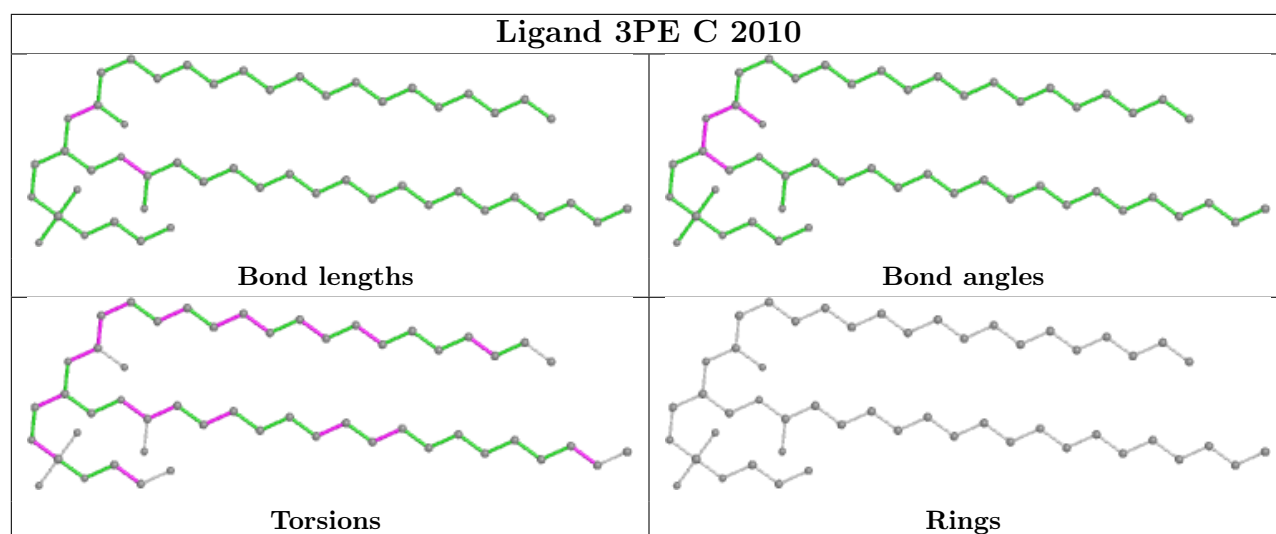
Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C3B-C11-C12-C13
8	A	1001	HEA	O11-C11-C12-C13
8	A	1001	HEA	C11-C12-C13-C14

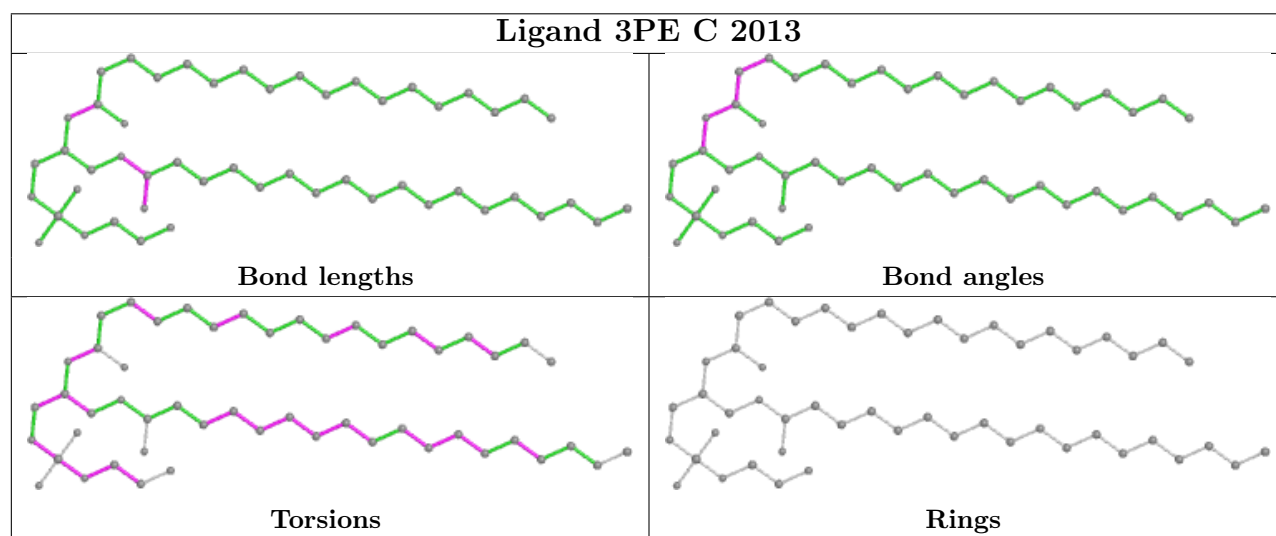
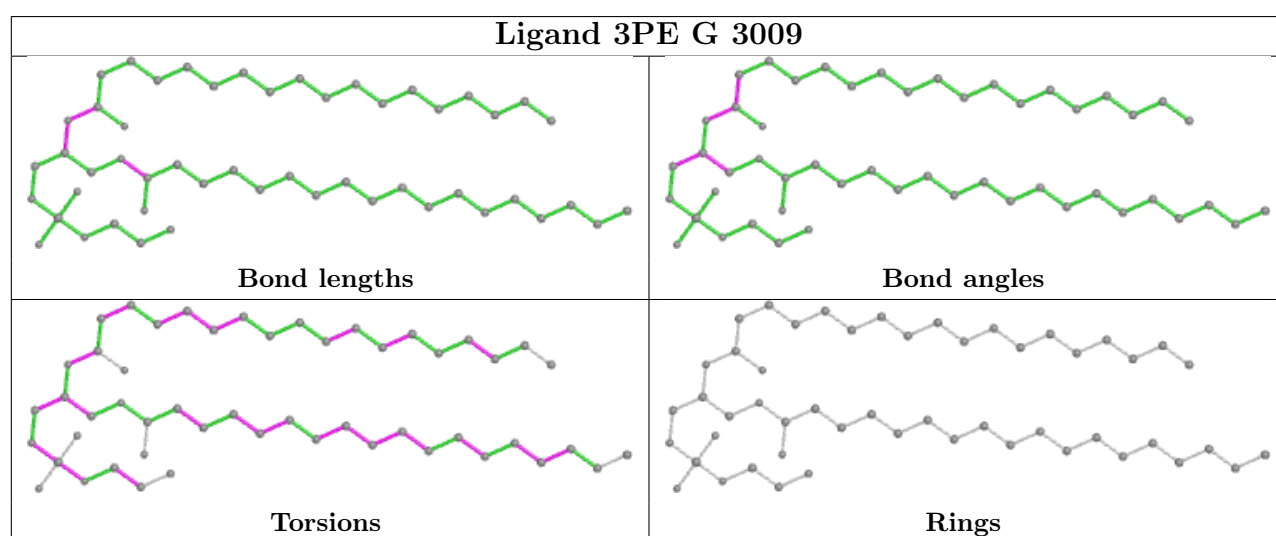
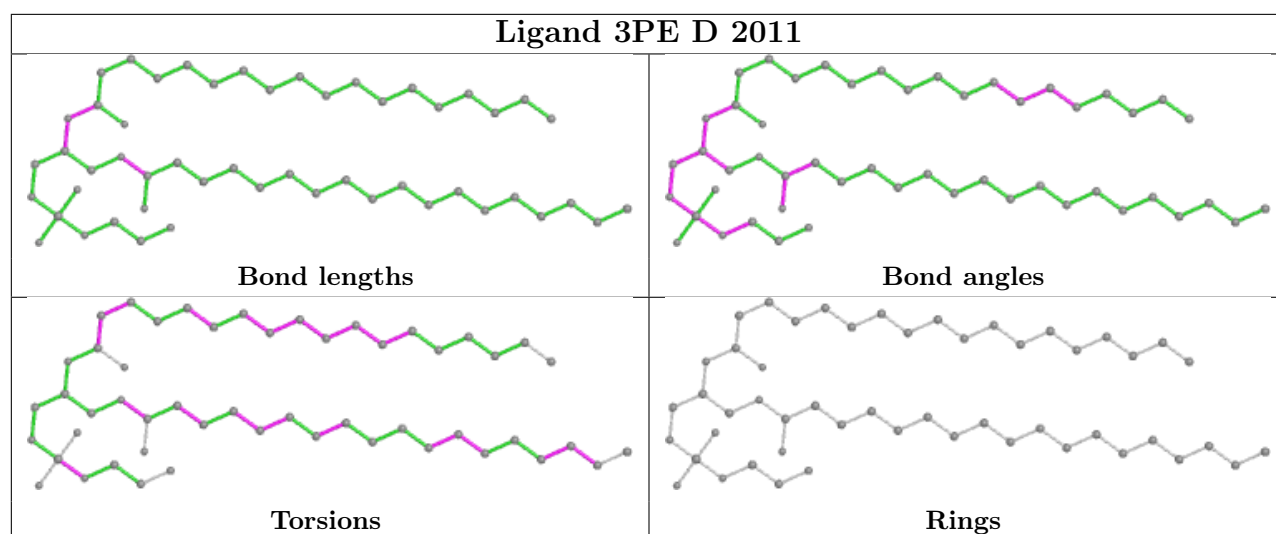
There are no ring outliers.

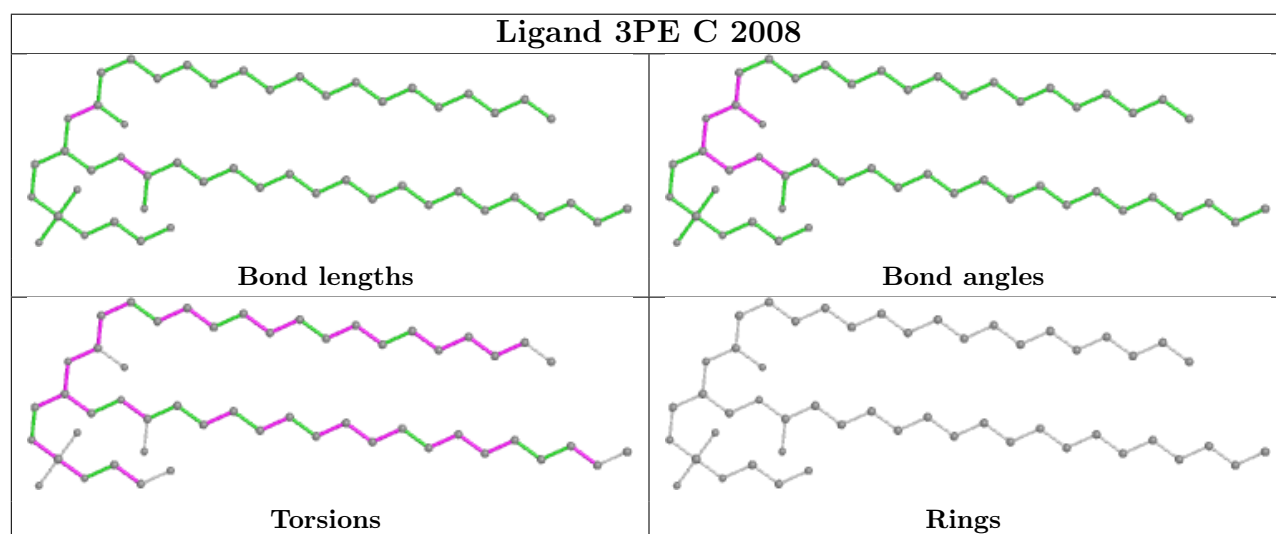
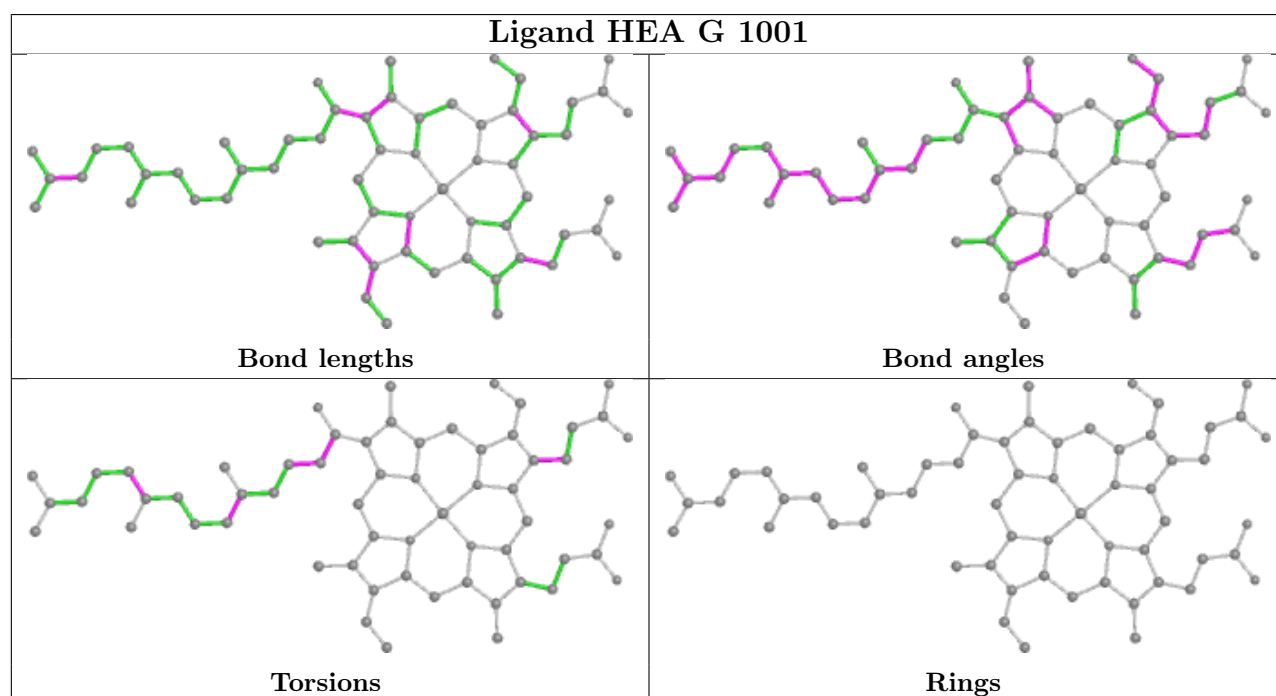
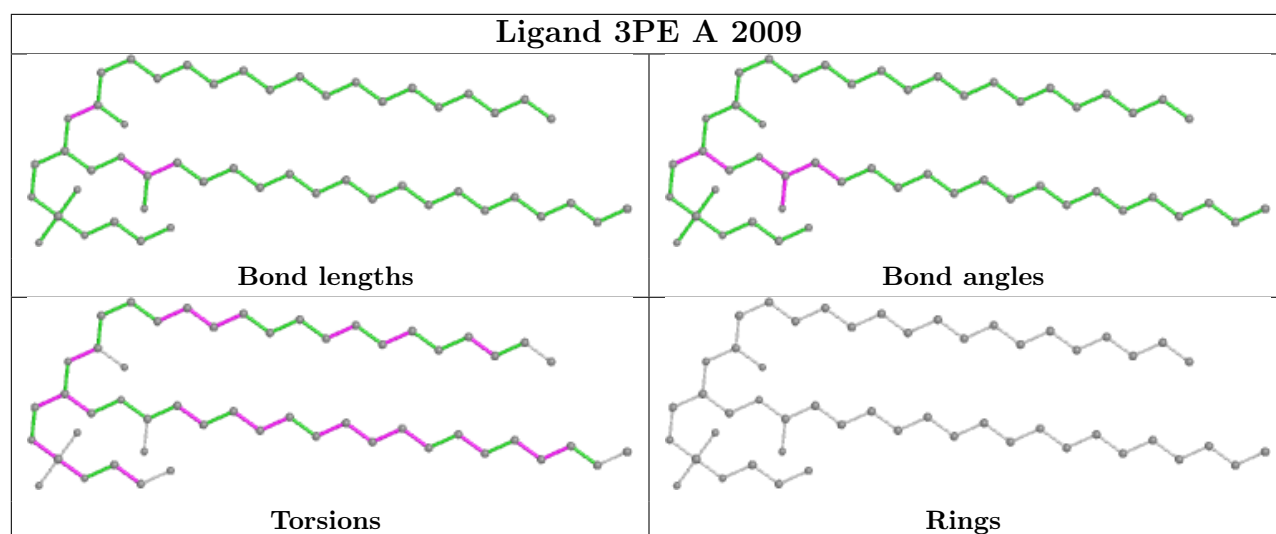
16 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2010	3PE	24	0
9	J	3011	3PE	13	0
9	I	3013	3PE	22	0
9	D	2011	3PE	17	0
9	G	3009	3PE	19	0
9	C	2013	3PE	21	0
9	A	2009	3PE	18	0
8	G	1001	HEA	23	0
9	C	2008	3PE	13	0
8	G	1002	HEA	15	0
9	I	3008	3PE	13	0
9	G	3012	3PE	22	0
9	I	3010	3PE	24	0
9	A	2012	3PE	20	0
8	A	1002	HEA	20	0
8	A	1001	HEA	20	0

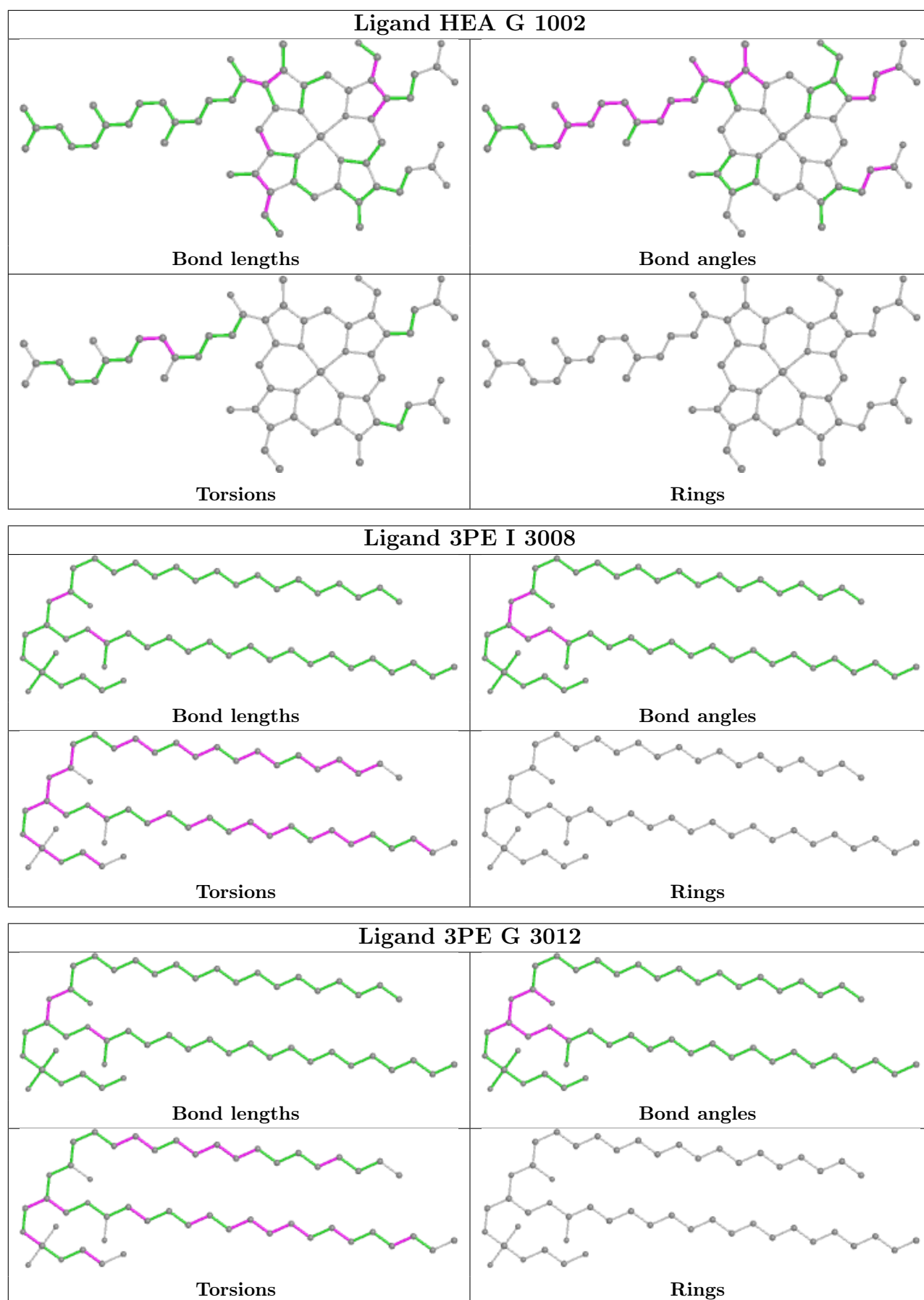
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

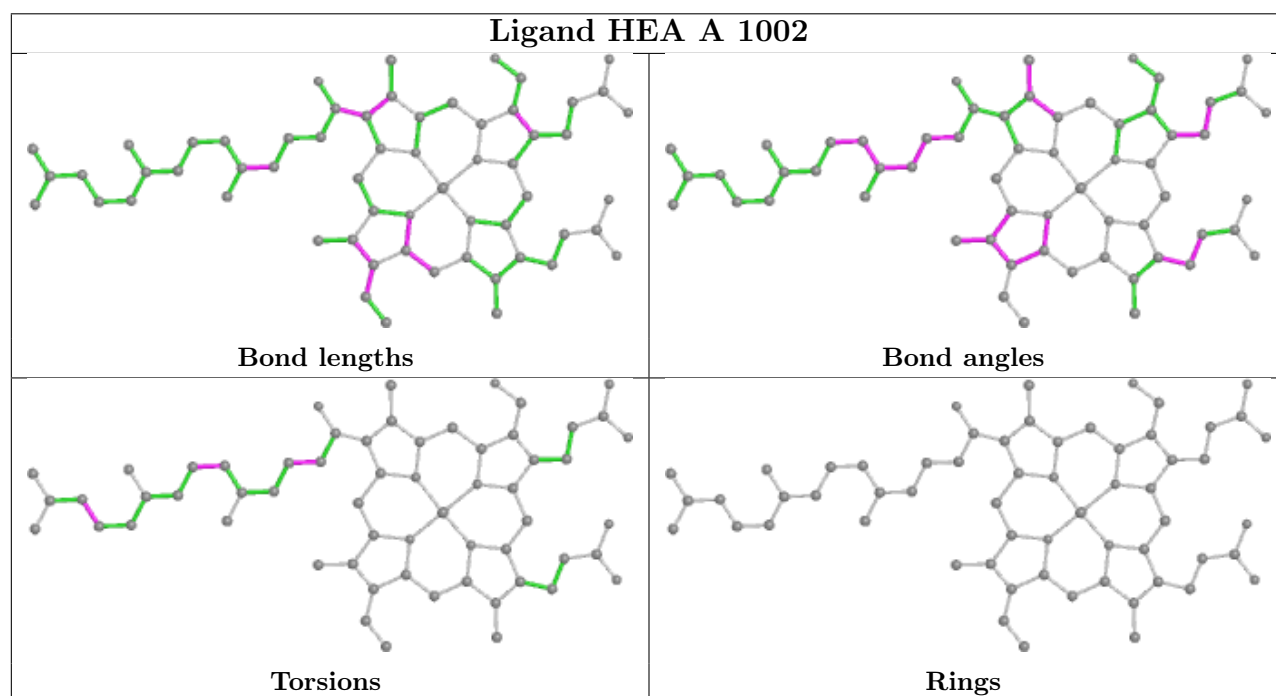
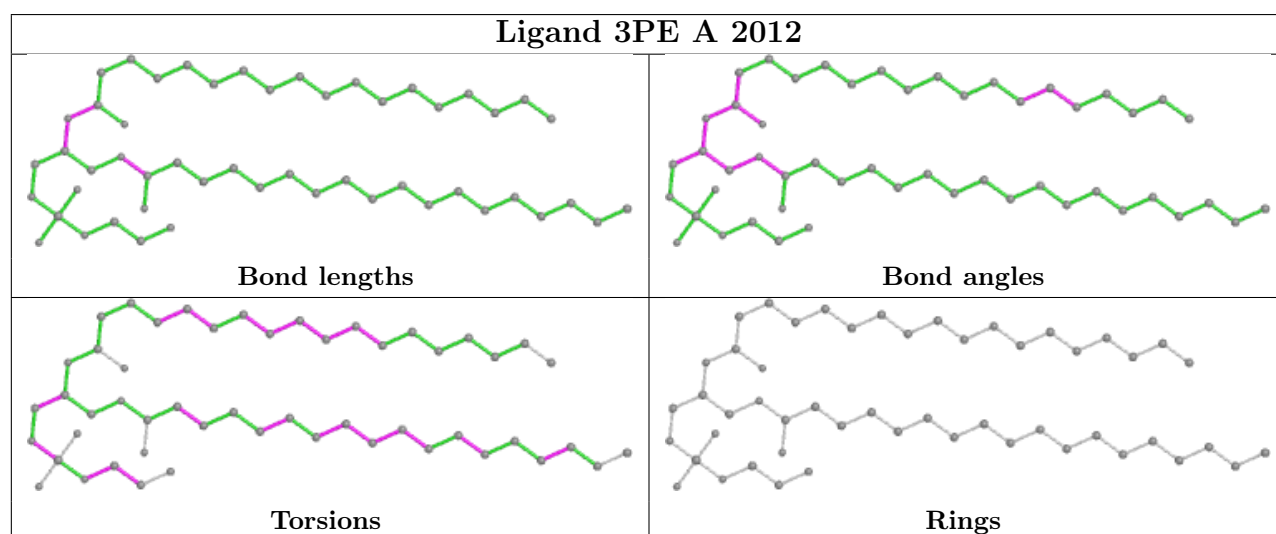
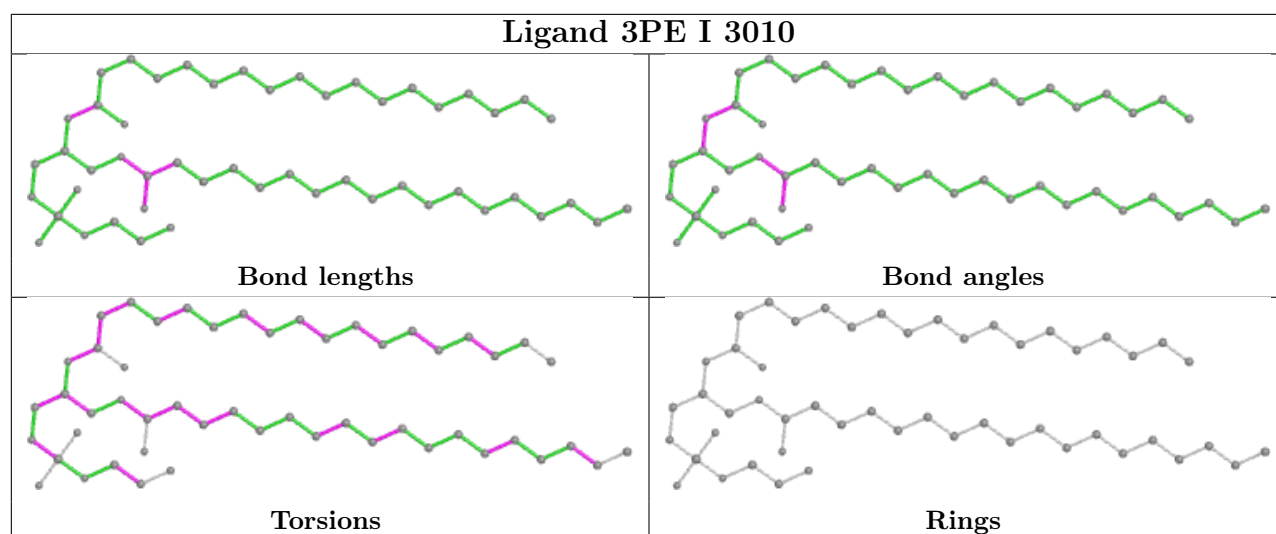


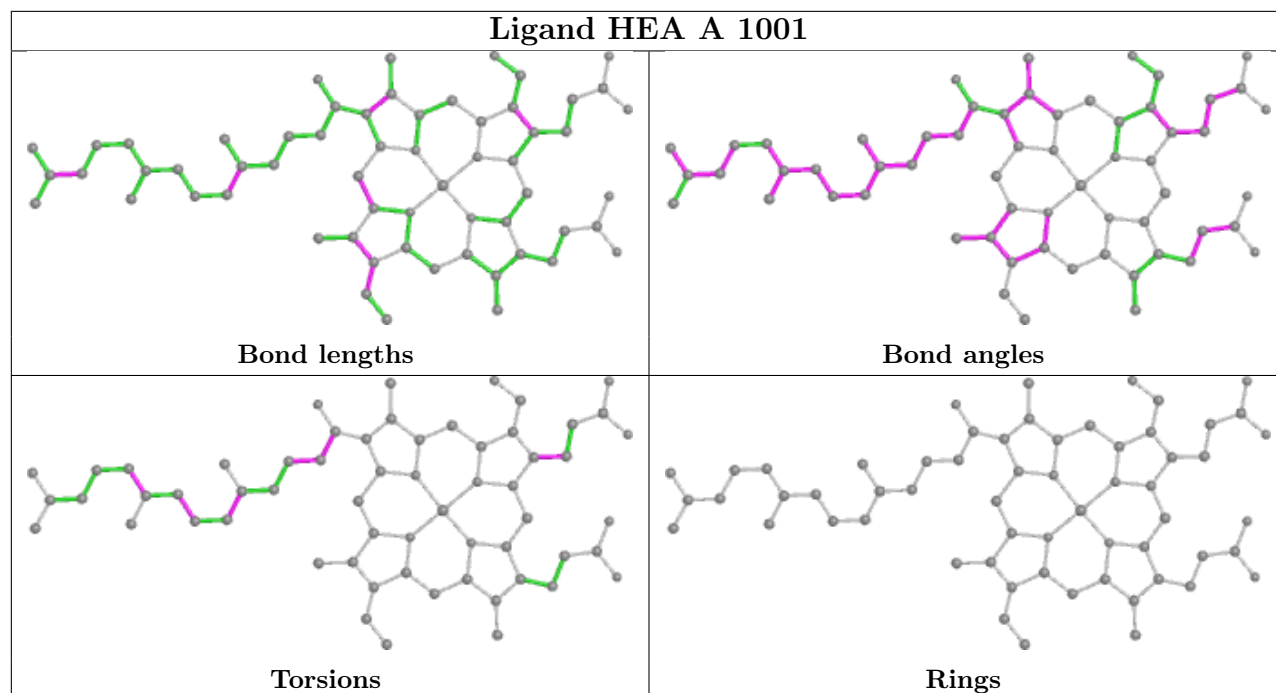












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.