



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:44 pm BST

PDB ID : 3H1J  
Title : Stigmatellin-bound cytochrome bc1 complex from chicken  
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.;  
Crofts, A.R.; Berry, E.A.; Kim, S.-H.  
Deposited on : 2009-04-12  
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) : 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

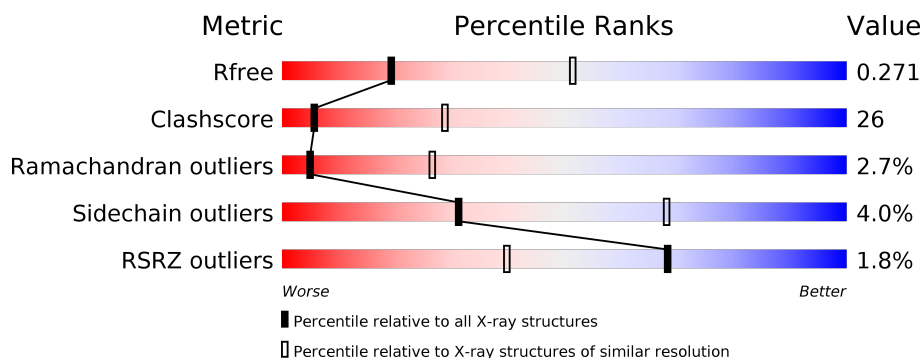
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	446	<div> <div>56%</div> <div>38%</div> <div>5%</div> </div>
1	N	446	<div> <div>53%</div> <div>41%</div> <div>5%</div> </div>
2	B	441	<div> <div>43%</div> <div>47%</div> <div>5%</div> <div>5%</div> </div>
2	O	441	<div> <div>48%</div> <div>42%</div> <div>5%</div> </div>
3	C	380	<div> <div>63%</div> <div>36%</div> </div>
3	P	380	<div> <div>59%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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
11	UNL	C	2010	-	-	-	X
11	UNL	C	2104	-	-	-	X
11	UNL	C	3015	-	-	-	X
11	UNL	E	3103	-	-	-	X
11	UNL	P	3010	-	-	-	X
11	UNL	P	3104	-	-	-	X
11	UNL	R	2103	-	-	-	X
15	PEE	N	3008	-	X	-	-

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32679 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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	2			

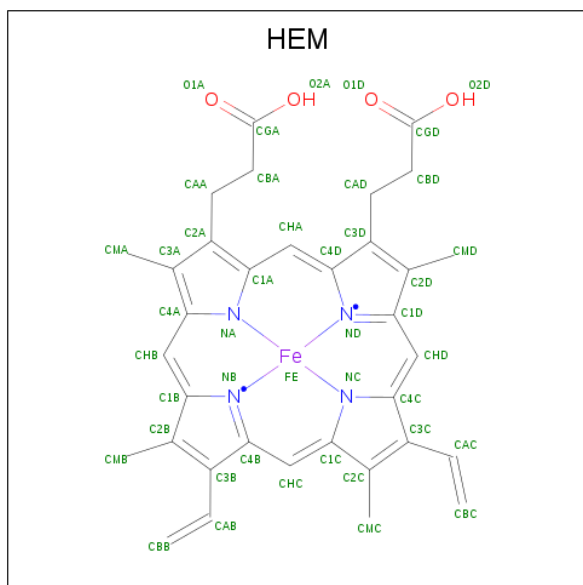
- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	3	Total	O	0	0
			3	3		
11	R	1	Total	O	0	0
			1	1		
11	A	1	Total	O	0	0
			1	1		
11	C	3	Total	O	0	0
			3	3		
11	E	2	Total	O	0	0
			2	2		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



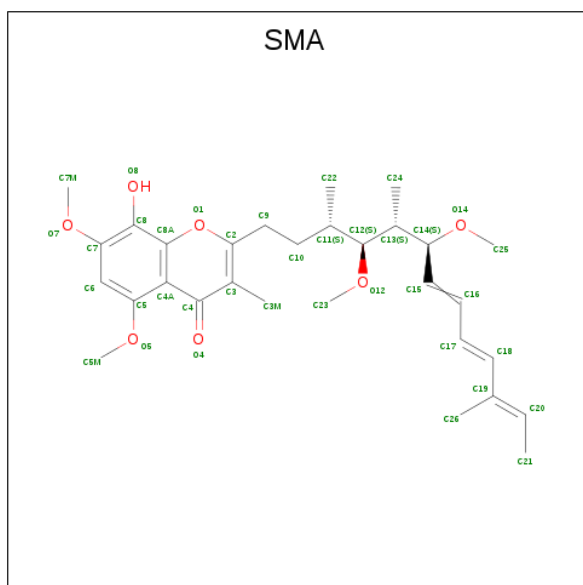
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

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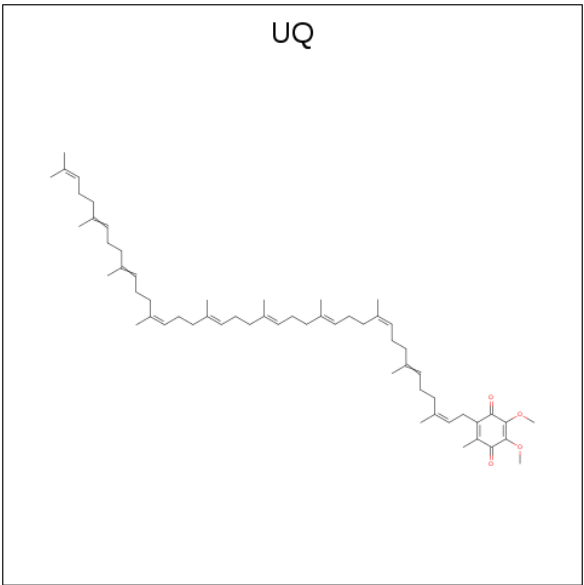
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 13 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).



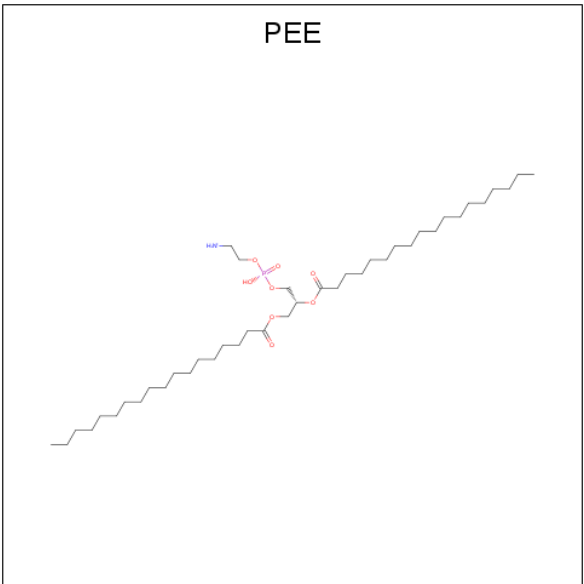
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O		
			37	30	7		
13	P	1	Total	C	O		
			37	30	7		

- Molecule 14 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 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
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

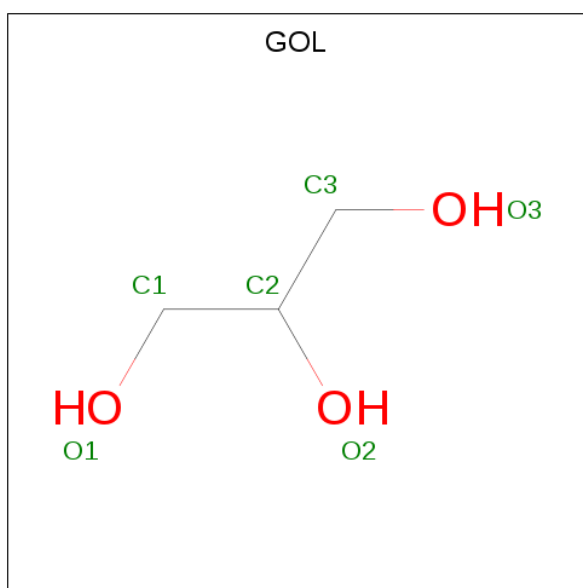
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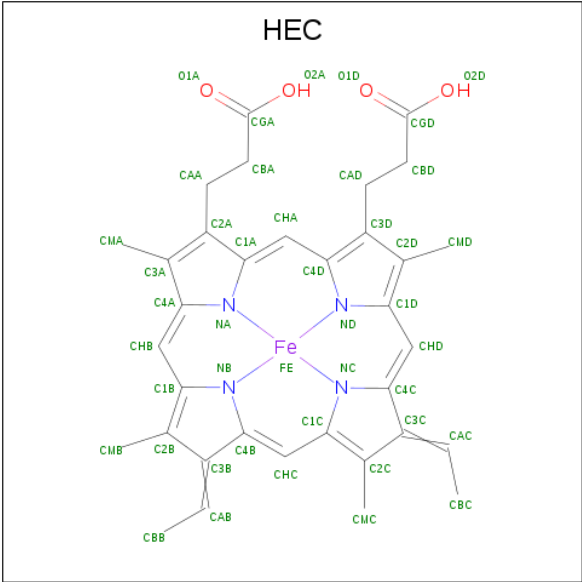
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	N	1	Total	O	P			0	0
			5	4	1				
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



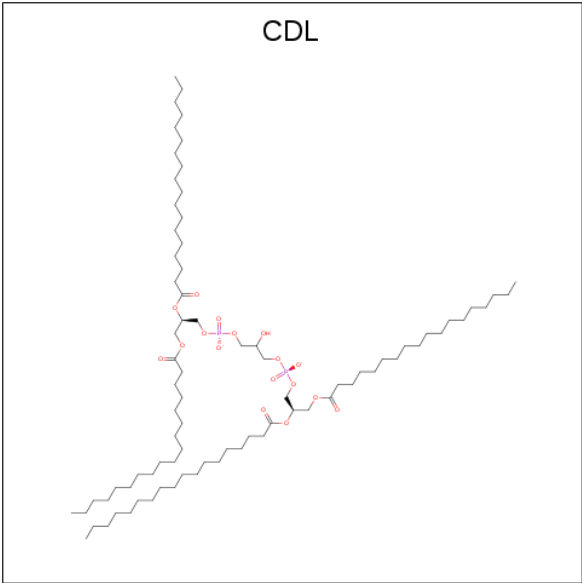
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



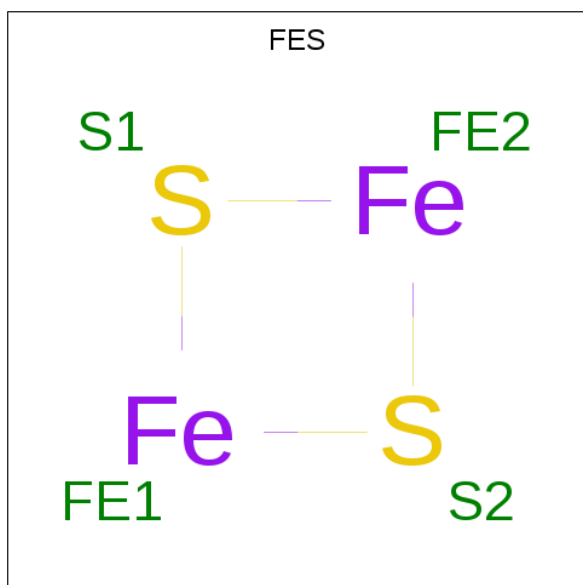
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			50	31	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		

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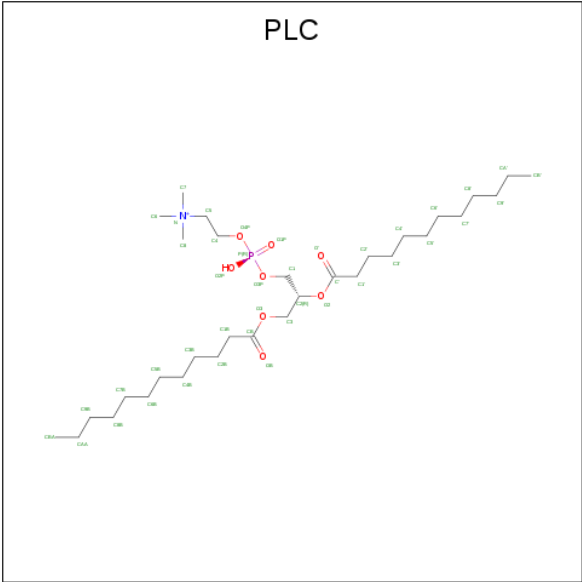
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			40	21	17	2		
18	S	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	E	1	Total	Fe	S	0	0
			4	2	2		
19	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

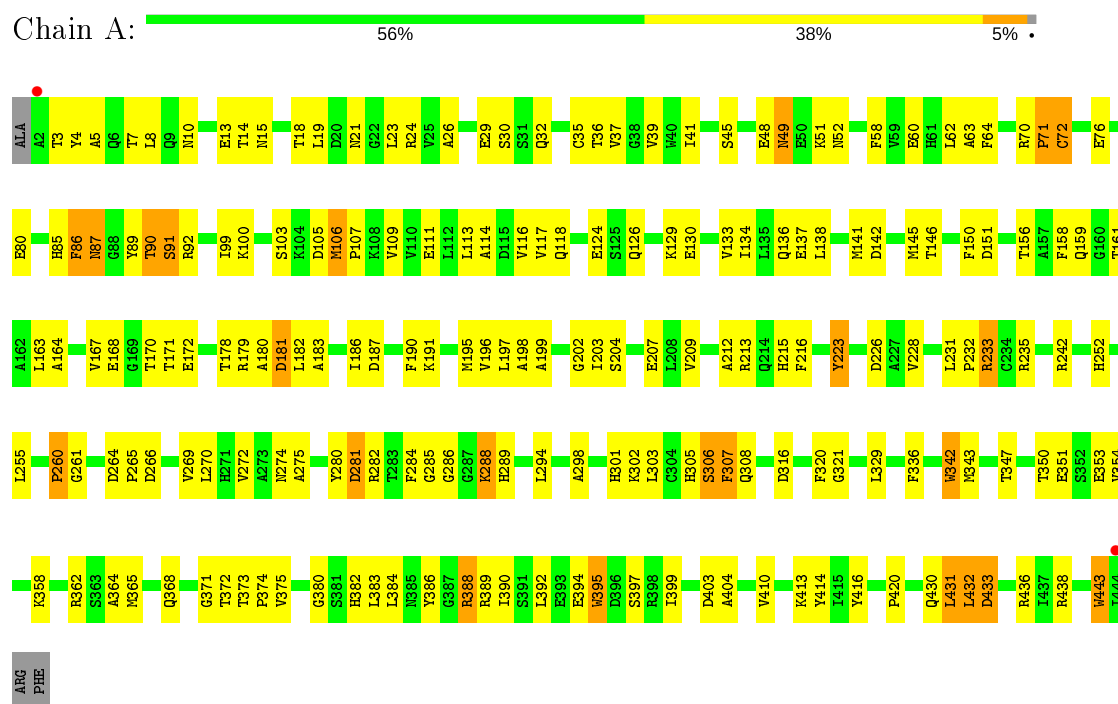
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	O	0	0
			1	1		
21	C	6	Total	O	0	0
			6	6		
21	P	6	Total	O	0	0
			6	6		
21	U	1	Total	O	0	0
			1	1		

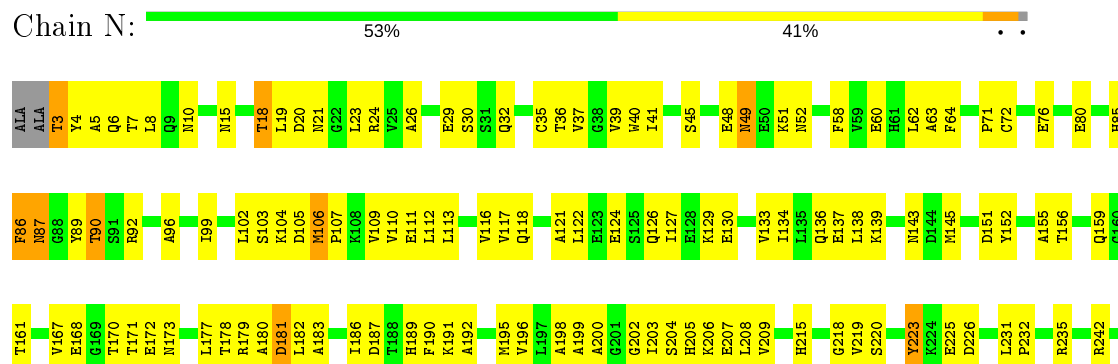
### 3 Residue-property plots [i](#)

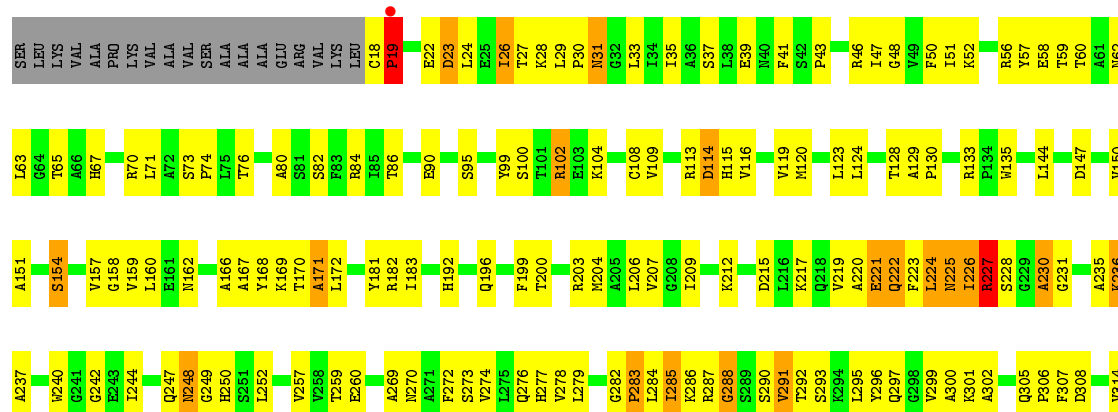
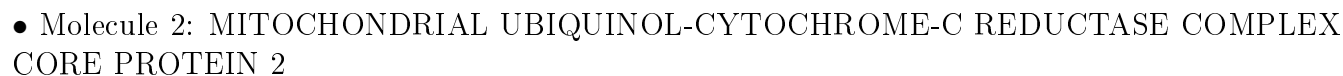
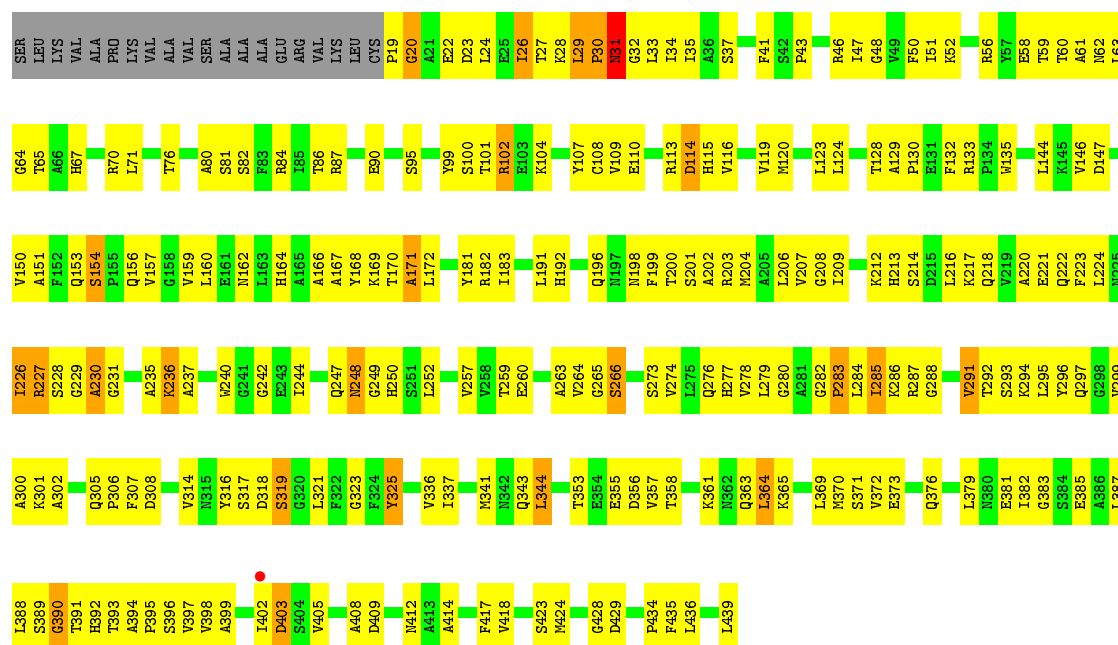
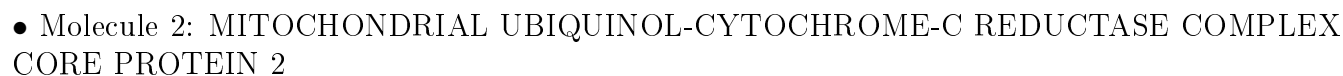
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $RSRZ > 2$ ). 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.

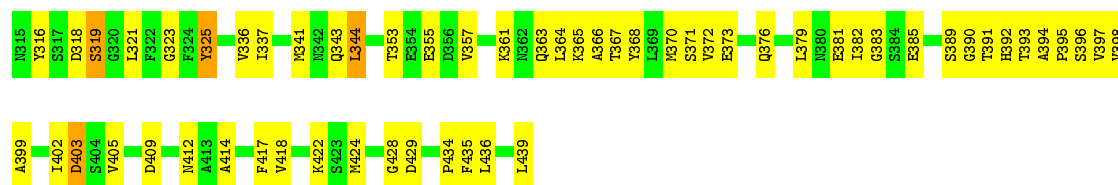
#### • Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I



#### • Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

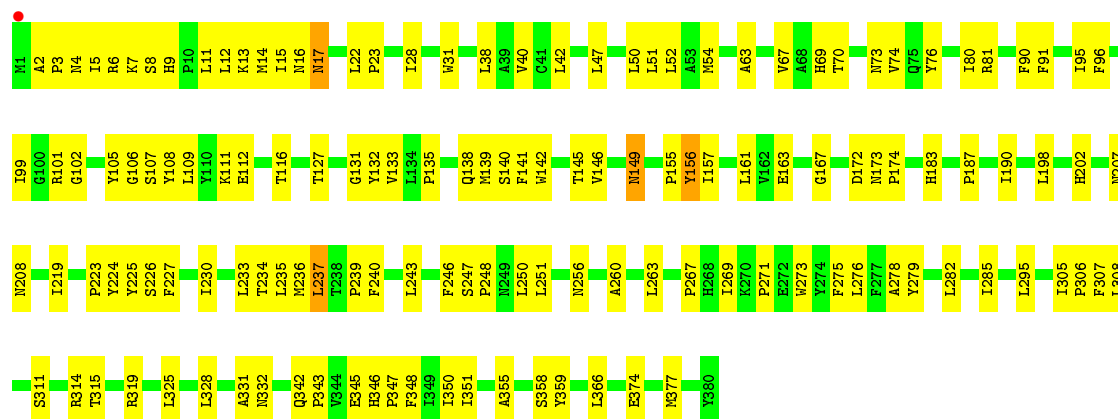






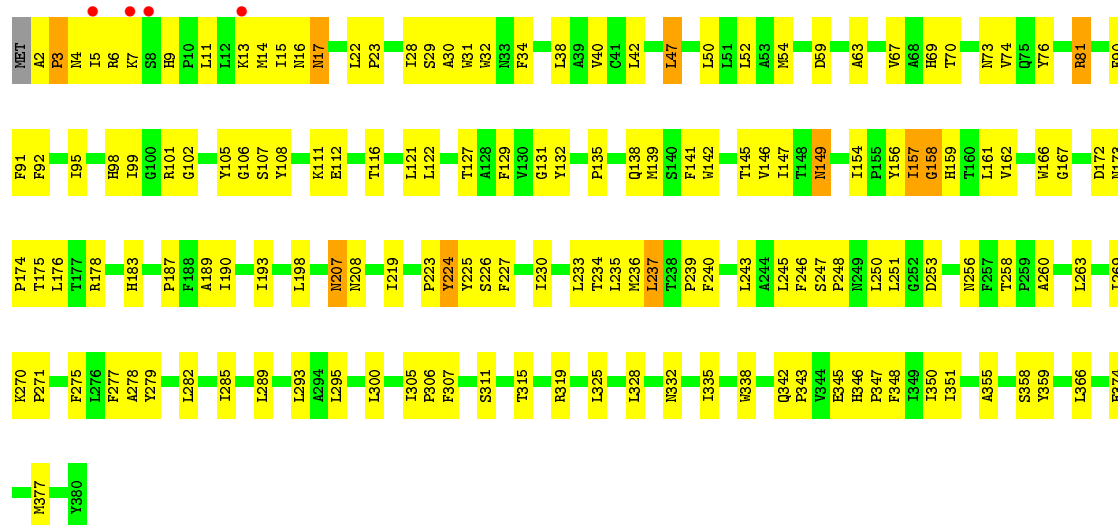
• Molecule 3: Cytochrome b

Chain C: 63% 36%



• Molecule 3: Cytochrome b

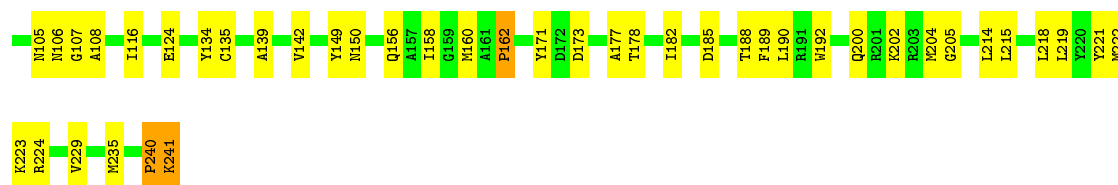
Chain P: 59% 38%



• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

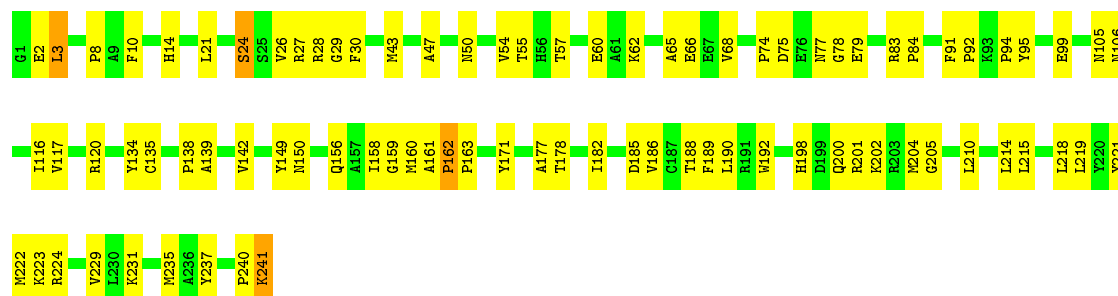
Chain D: 68% 31%





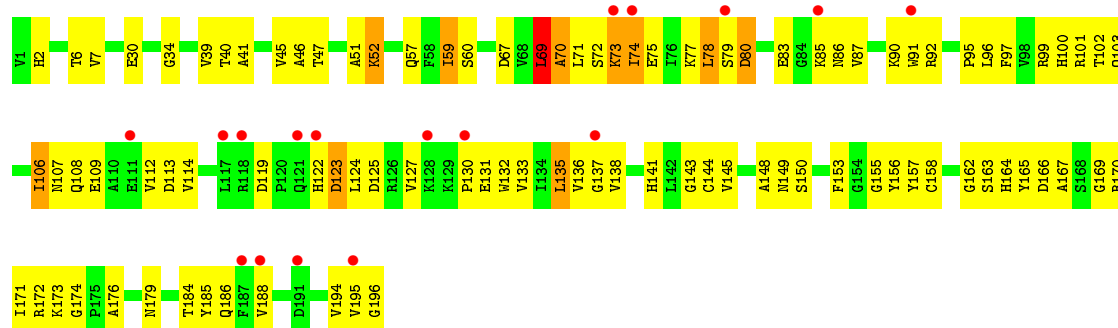
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q: 65% 34%



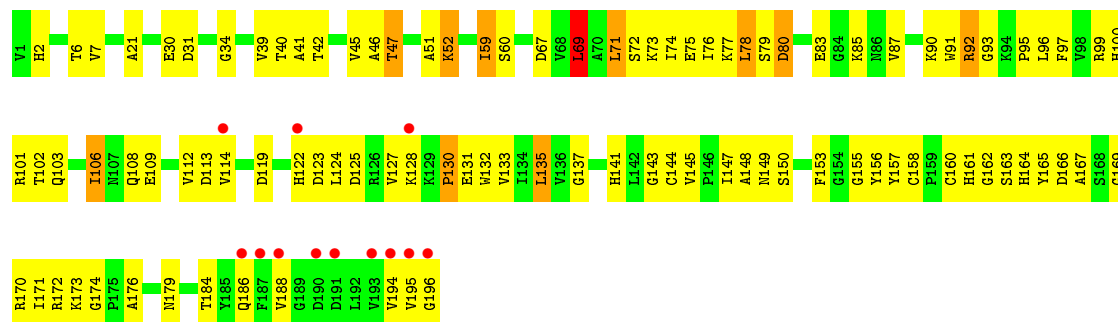
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 9% 51% 44% 5%



• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

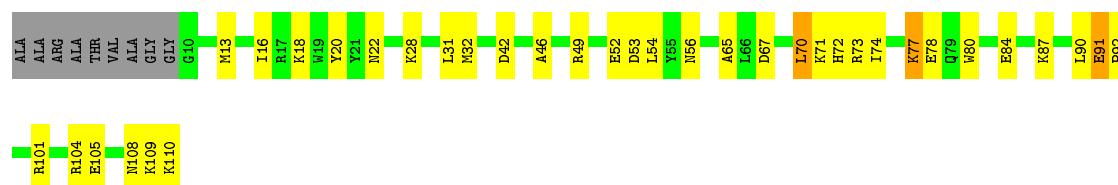
Chain R: 6% 49% 45% 5%



• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

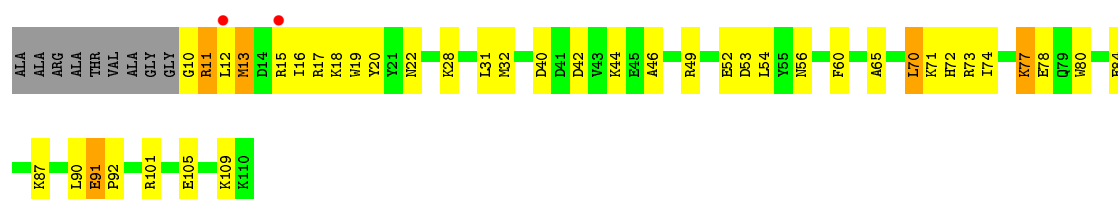


Chain F: 



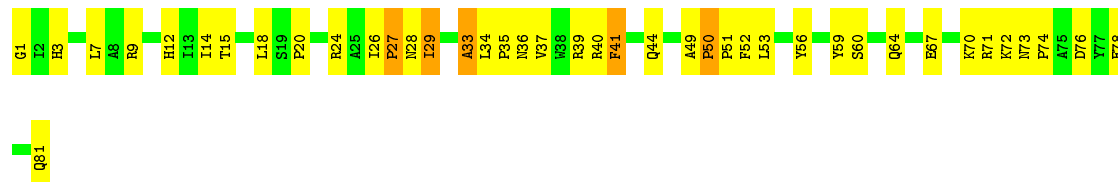
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S: 



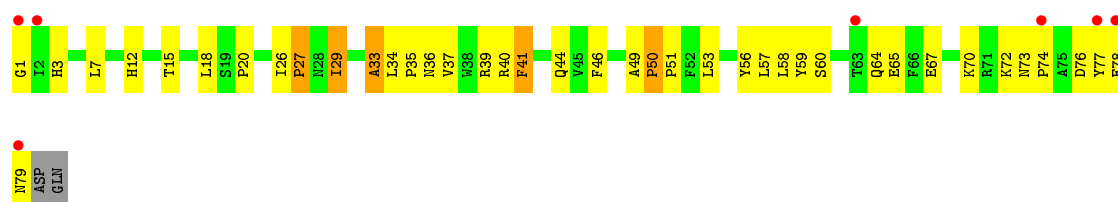
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T: 



- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H: 



L77  
K78

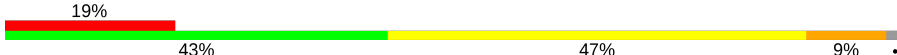
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U: 

LEU ARG GLY SER GLY GLU GLU GLU E12 L13 L14 D15 P16 L17 T18 T19 I20 R21 R22 H23 H24 C24 E25 Q26 T27 E28 V31 K32 A33 R34 E35 R36 L37 E38 L39 C40 D41 A42 R43 V44 R47 S48 R49 T50 E51 E52 Q53 C54 T55 E56 E57 L58 F61 R65 D66

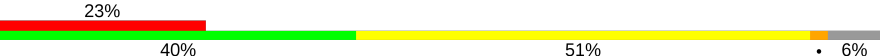
H67 C68 V69 A70 K71 K72 L73 L74 N75 L76 L77 K78

- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 

K28 X31 X32 X33 X34 X35 X38 X39 X40 R47 P48 L49 L50 C51 R52 E53 R54 M55 S56 G57 R58 S59 A60 R61 R62 D63 L64 V65 A66 G67 I68 S69 L70 A72 P73 N71 L76 R77 TYR

- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V: 

UNK UNK X28 X29 X30 X31 X32 X36 P48 L49 L50 C51 R52 E53 R54 M55 S56 G57 R58 S59 A60 R61 R62 D63 L64 V65 I68 S69 L70 A72 P73 V76 R77 TYR

- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J: 

A4 R7 Q8 A9 Y10 R16 L22 V25 L26 R33 Q37 Q38 A39 D40 A41 F42 F43 E44 H45 L46 G49 N52 K53 H54 I55 K56 H57 K58 Y59 S62 E63 E64

- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain W: 

A4 R7 Y10 F14 F20 A21 L22 L26 G27 A28 R33 Q37 Q38 A39 D40 A41 I42 F43 E44 H45 L46 G49 H52 K53 H54 I55 K56 H57 K58 Y59 E60 A61 S62 GLU GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.68-3.00) 92.5 (42.68-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.277 0.234 , 0.271	Depositor DCC
$R_{free}$ test set	2796 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, UNL, UQ, PLC, FES, HEC, HEM, PEE, SMA

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	0.43	0/3511	0.65	0/4757
1	N	0.43	0/3508	0.65	1/4753 (0.0%)
2	B	0.38	0/3196	0.63	0/4334
2	O	0.40	0/3202	0.63	0/4343
3	C	0.52	0/3122	0.67	0/4273
3	P	0.46	0/3114	0.65	0/4263
4	D	0.45	0/1956	0.64	0/2658
4	Q	0.40	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.64	1/2103 (0.0%)
5	R	0.39	0/1547	0.68	2/2103 (0.1%)
6	F	0.52	0/911	0.71	0/1219
6	S	0.43	0/911	0.63	0/1219
7	G	0.50	0/698	0.68	0/946
7	T	0.44	0/680	0.65	0/923
8	H	0.47	0/582	0.59	0/779
8	U	0.34	0/561	0.57	0/751
9	I	0.40	0/218	0.65	0/293
9	V	0.41	0/218	0.66	0/293
10	J	0.44	0/508	0.63	0/682
10	W	0.41	0/489	0.61	0/658
All	All	0.43	0/32435	0.65	4/44008 (0.0%)

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
3	P	0	1
4	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	E	143	GLY	N-CA-C	6.29	128.82	113.10
5	R	143	GLY	N-CA-C	6.28	128.80	113.10
1	N	218	GLY	N-CA-C	-5.19	100.11	113.10
5	R	71	LEU	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	33	TYR	Sidechain
3	P	224	TYR	Sidechain

## 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	3440	0	3353	169	0
1	N	3437	0	3349	192	0
2	B	3141	0	3142	255	0
2	O	3147	0	3146	228	0
3	C	3020	0	3070	136	0
3	P	3012	0	3058	152	0
4	D	1898	0	1846	63	0
4	Q	1898	0	1846	83	0
5	E	1513	0	1478	91	0
5	R	1513	0	1478	93	0
6	F	891	0	893	36	0
6	S	891	0	893	40	0
7	G	676	0	659	46	0
7	T	658	0	647	46	0
8	H	574	0	548	31	0
8	U	553	0	535	46	0
9	I	285	0	237	50	0
9	V	275	0	238	42	0
10	J	497	0	490	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	478	0	478	29	0
11	A	1	0	0	0	0
11	C	3	0	0	0	0
11	E	2	0	0	0	0
11	P	3	0	0	0	0
11	R	1	0	0	0	0
12	C	86	0	60	11	0
12	P	86	0	60	11	0
13	C	37	0	42	4	0
13	P	37	0	42	4	0
14	C	19	0	17	5	0
14	P	19	0	17	1	0
15	C	70	0	85	1	0
15	E	50	0	77	4	0
15	N	5	0	0	0	0
15	P	49	0	72	1	0
15	R	50	0	77	4	0
16	C	6	0	8	0	0
16	P	6	0	8	1	0
17	D	43	0	30	1	0
17	Q	43	0	30	1	0
18	D	50	0	44	1	0
18	G	40	0	24	1	0
18	P	40	0	24	3	0
18	S	50	0	44	2	0
19	E	4	0	0	0	0
19	R	4	0	0	1	0
20	E	32	0	38	3	0
20	R	32	0	38	2	0
21	B	1	0	0	0	0
21	C	6	0	0	0	0
21	P	6	0	0	1	0
21	U	1	0	0	1	0
All	All	32679	0	32221	1656	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 26.

The worst 5 of 1656 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:B:353:THR:HG22	2:B:355:GLU:H	1.15	1.08
3:C:17:ASN:HD21	7:G:1:GLY:HA2	0.98	1.07
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.35	1.06
2:O:353:THR:HG22	2:O:355:GLU:H	1.19	1.06
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.37	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	393 (89%)	40 (9%)	8 (2%)	8	37
1	N	440/446 (99%)	397 (90%)	36 (8%)	7 (2%)	9	40
2	B	419/441 (95%)	339 (81%)	63 (15%)	17 (4%)	3	16
2	O	420/441 (95%)	336 (80%)	66 (16%)	18 (4%)	2	15
3	C	378/380 (100%)	358 (95%)	18 (5%)	2 (0%)	29	68
3	P	377/380 (99%)	349 (93%)	24 (6%)	4 (1%)	14	50
4	D	239/241 (99%)	217 (91%)	20 (8%)	2 (1%)	19	57
4	Q	239/241 (99%)	214 (90%)	22 (9%)	3 (1%)	12	45
5	E	194/196 (99%)	157 (81%)	24 (12%)	13 (7%)	1	6
5	R	194/196 (99%)	161 (83%)	21 (11%)	12 (6%)	1	8
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	15	53
7	G	79/81 (98%)	66 (84%)	9 (11%)	4 (5%)	2	12
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	2	12
8	H	68/77 (88%)	57 (84%)	8 (12%)	3 (4%)	2	15
8	U	65/77 (84%)	48 (74%)	16 (25%)	1 (2%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	29/47 (62%)	19 (66%)	7 (24%)	3 (10%)	0	2
9	V	29/47 (62%)	20 (69%)	7 (24%)	2 (7%)	1	6
10	J	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	9	39
10	W	57/61 (93%)	45 (79%)	8 (14%)	4 (7%)	1	6
All	All	4002/4160 (96%)	3475 (87%)	418 (10%)	109 (3%)	5	26

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	114	ASP
2	B	171	ALA

### 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	365/368 (99%)	344 (94%)	21 (6%)	20	55
1	N	365/368 (99%)	344 (94%)	21 (6%)	20	55
2	B	332/347 (96%)	318 (96%)	14 (4%)	30	66
2	O	333/347 (96%)	319 (96%)	14 (4%)	30	66
3	C	329/329 (100%)	323 (98%)	6 (2%)	59	85
3	P	328/329 (100%)	321 (98%)	7 (2%)	53	82
4	D	200/200 (100%)	196 (98%)	4 (2%)	55	83
4	Q	200/200 (100%)	196 (98%)	4 (2%)	55	83
5	E	166/166 (100%)	157 (95%)	9 (5%)	22	57
5	R	166/166 (100%)	157 (95%)	9 (5%)	22	57
6	F	93/96 (97%)	90 (97%)	3 (3%)	39	74
6	S	93/96 (97%)	89 (96%)	4 (4%)	29	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	71/71 (100%)	68 (96%)	3 (4%)	30	66
7	T	69/71 (97%)	66 (96%)	3 (4%)	29	66
8	H	65/71 (92%)	63 (97%)	2 (3%)	40	75
8	U	63/71 (89%)	61 (97%)	2 (3%)	39	74
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	66
9	V	23/26 (88%)	22 (96%)	1 (4%)	29	66
10	J	49/49 (100%)	45 (92%)	4 (8%)	11	39
10	W	47/49 (96%)	44 (94%)	3 (6%)	17	51
All	All	3380/3446 (98%)	3245 (96%)	135 (4%)	31	68

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	26	GLN
1	N	124	GLU
6	S	77	LYS
9	I	71	ASN
1	N	18	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	64	GLN
1	N	143	ASN
6	S	56	ASN
7	G	81	GLN
1	N	49	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 10 are unknown - leaving 26 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$
15	PEE	N	3008	-	4,4,50	3.52	4 (100%)	6,6,55	0.61	0
20	PLC	E	2009	-	31,31,41	1.67	6 (19%)	37,39,49	0.65	0
15	PEE	R	3005	-	49,49,50	1.43	9 (18%)	52,54,55	0.94	5 (9%)
17	HEC	Q	501	4	26,50,50	2.01	3 (11%)	18,82,82	1.63	3 (16%)
20	PLC	R	3009	-	31,31,41	1.61	7 (22%)	37,39,49	0.62	0
12	HEM	P	502	3	27,50,50	1.84	6 (22%)	17,82,82	1.69	6 (35%)
12	HEM	C	502	3	27,50,50	1.86	8 (29%)	17,82,82	1.90	7 (41%)
15	PEE	P	3007	-	48,48,50	1.32	7 (14%)	51,53,55	0.92	4 (7%)
12	HEM	P	501	3	27,50,50	1.87	5 (18%)	17,82,82	1.49	4 (23%)
17	HEC	D	501	4	26,50,50	2.00	5 (19%)	18,82,82	1.84	3 (16%)
16	GOL	P	3011	-	5,5,5	1.46	1 (20%)	5,5,5	0.68	0
15	PEE	C	2007	-	48,48,50	1.34	8 (16%)	51,53,55	0.97	5 (9%)
18	CDL	D	2003	-	49,49,99	1.14	2 (4%)	55,61,111	1.00	2 (3%)
14	UQ	C	2002	-	19,19,63	2.67	9 (47%)	23,26,79	1.11	2 (8%)
15	PEE	C	2008	-	20,20,50	1.73	6 (30%)	23,25,55	0.62	0
18	CDL	S	3003	-	49,49,99	1.13	2 (4%)	55,61,111	1.00	2 (3%)
18	CDL	P	3004	-	39,39,99	1.24	3 (7%)	45,51,111	1.14	4 (8%)
16	GOL	C	2011	-	5,5,5	1.28	0	5,5,5	0.56	0
13	SMA	P	3001	-	35,38,38	1.69	9 (25%)	46,52,52	1.81	7 (15%)
14	UQ	P	3002	-	19,19,63	2.64	10 (52%)	23,26,79	1.11	2 (8%)
12	HEM	C	501	3	27,50,50	1.96	9 (33%)	17,82,82	1.80	4 (23%)
13	SMA	C	2001	-	35,38,38	1.73	9 (25%)	46,52,52	1.87	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	PEE	E	2005	-	49,49,50	1.41	10 (20%)	52,54,55	0.95	5 (9%)
19	FES	E	501	5	0,4,4	0.00	-	-		
18	CDL	G	2004	-	39,39,99	1.33	5 (12%)	45,51,111	1.13	4 (8%)
19	FES	R	501	5	0,4,4	0.00	-	-		

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
20	PLC	E	2009	-	-	15/35/35/45	-
15	PEE	R	3005	-	-	24/53/53/54	-
17	HEC	Q	501	4	-	2/6/54/54	-
20	PLC	R	3009	-	-	14/35/35/45	-
12	HEM	P	502	3	-	2/6/54/54	-
12	HEM	C	502	3	-	2/6/54/54	-
15	PEE	P	3007	-	-	28/52/52/54	-
12	HEM	P	501	3	-	0/6/54/54	-
17	HEC	D	501	4	-	2/6/54/54	-
16	GOL	P	3011	-	-	0/4/4/4	-
15	PEE	C	2007	-	-	24/52/52/54	-
18	CDL	D	2003	-	-	25/59/59/110	-
14	UQ	C	2002	-	-	3/11/35/87	0/1/1/1
15	PEE	C	2008	-	-	9/24/24/54	-
18	CDL	S	3003	-	-	25/59/59/110	-
18	CDL	P	3004	-	-	21/49/49/110	-
16	GOL	C	2011	-	-	2/4/4/4	-
13	SMA	P	3001	-	-	4/33/34/34	0/2/2/2
14	UQ	P	3002	-	-	3/11/35/87	0/1/1/1
12	HEM	C	501	3	-	0/6/54/54	-
13	SMA	C	2001	-	-	3/33/34/34	0/2/2/2
15	PEE	E	2005	-	-	24/53/53/54	-
19	FES	E	501	5	-	-	0/1/1/1
18	CDL	G	2004	-	-	21/49/49/110	-
19	FES	R	501	5	-	-	0/1/1/1

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3B-C2B	-7.62	1.32	1.40
17	D	501	HEC	C3B-C2B	-6.34	1.34	1.40
14	P	3002	UQ	C7-C6	5.44	1.60	1.51
14	P	3002	UQ	C6-C5	5.17	1.44	1.35
13	C	2001	SMA	C7-C8	5.13	1.47	1.40

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	3001	SMA	C9-C2-C3	6.58	129.72	120.39
13	C	2001	SMA	C9-C2-C3	6.55	129.68	120.39
17	D	501	HEC	CBA-CAA-C2A	5.89	123.33	112.48
17	Q	501	HEC	CBA-CAA-C2A	5.27	122.19	112.48
13	C	2001	SMA	C3-C4-C4A	-5.17	115.38	120.58

There are no chirality outliers.

5 of 253 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	E	2009	PLC	O4P-C4-C5-N
20	E	2009	PLC	C1'-C'-O2-C2
17	Q	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
20	R	3009	PLC	O4P-C4-C5-N

There are no ring outliers.

22 monomers are involved in 62 short contacts:

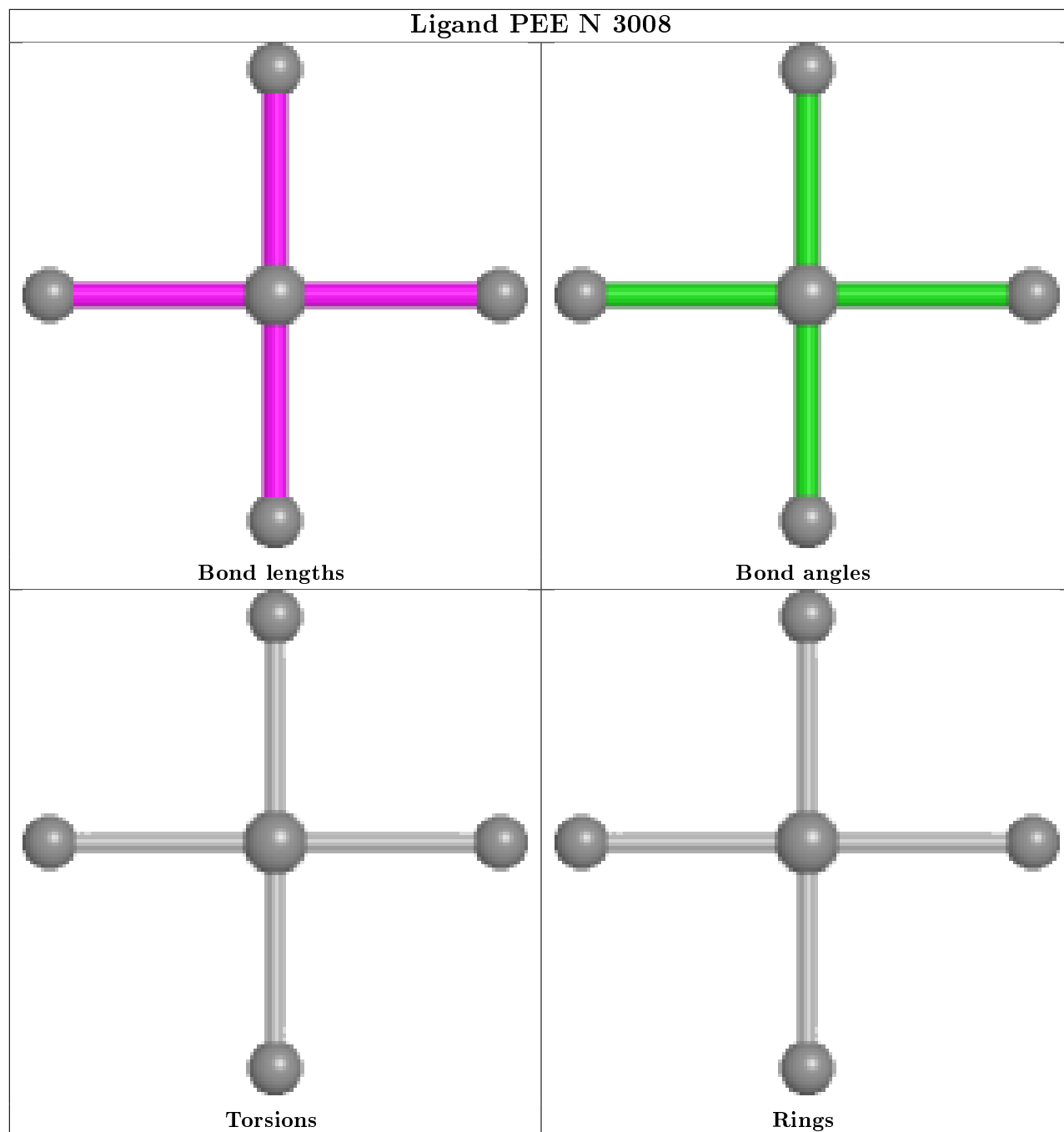
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	E	2009	PLC	3	0
15	R	3005	PEE	4	0
17	Q	501	HEC	1	0
20	R	3009	PLC	2	0
12	P	502	HEM	6	0
12	C	502	HEM	6	0
15	P	3007	PEE	1	0
12	P	501	HEM	5	0
17	D	501	HEC	1	0
16	P	3011	GOL	1	0
15	C	2007	PEE	1	0
18	D	2003	CDL	1	0
14	C	2002	UQ	5	0

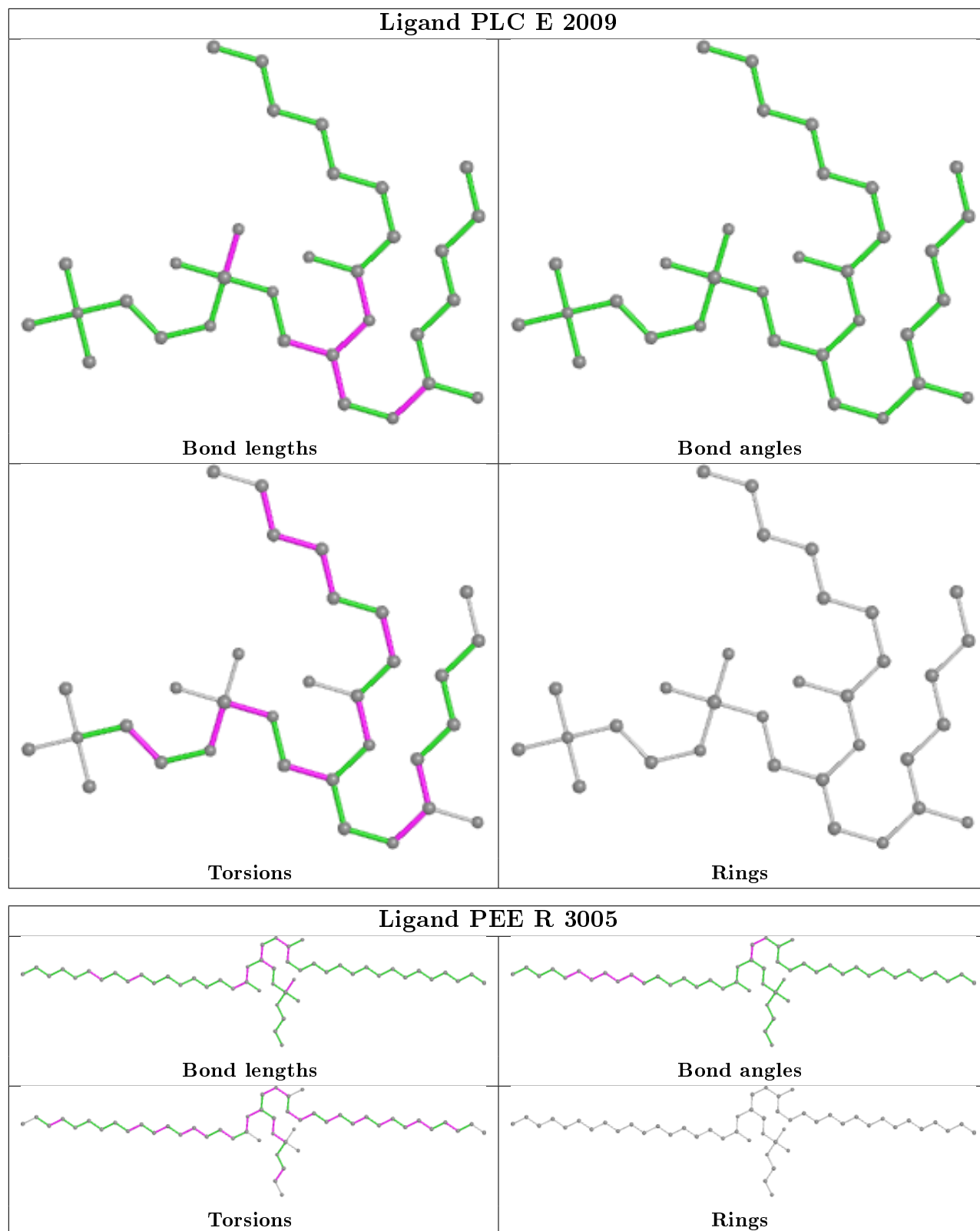
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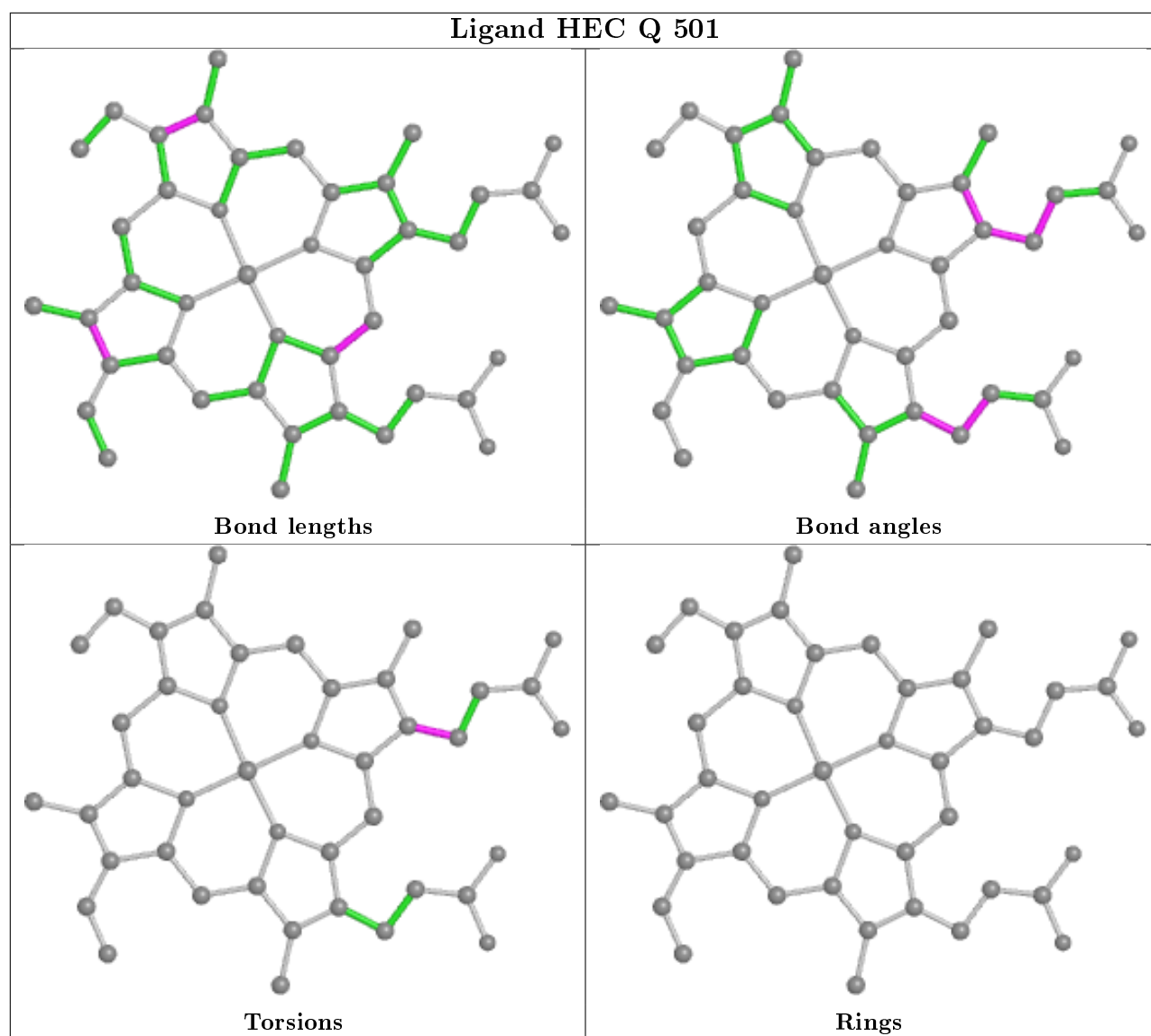
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	S	3003	CDL	2	0
18	P	3004	CDL	3	0
13	P	3001	SMA	4	0
14	P	3002	UQ	1	0
12	C	501	HEM	5	0
13	C	2001	SMA	4	0
15	E	2005	PEE	4	0
18	G	2004	CDL	1	0
19	R	501	FES	1	0

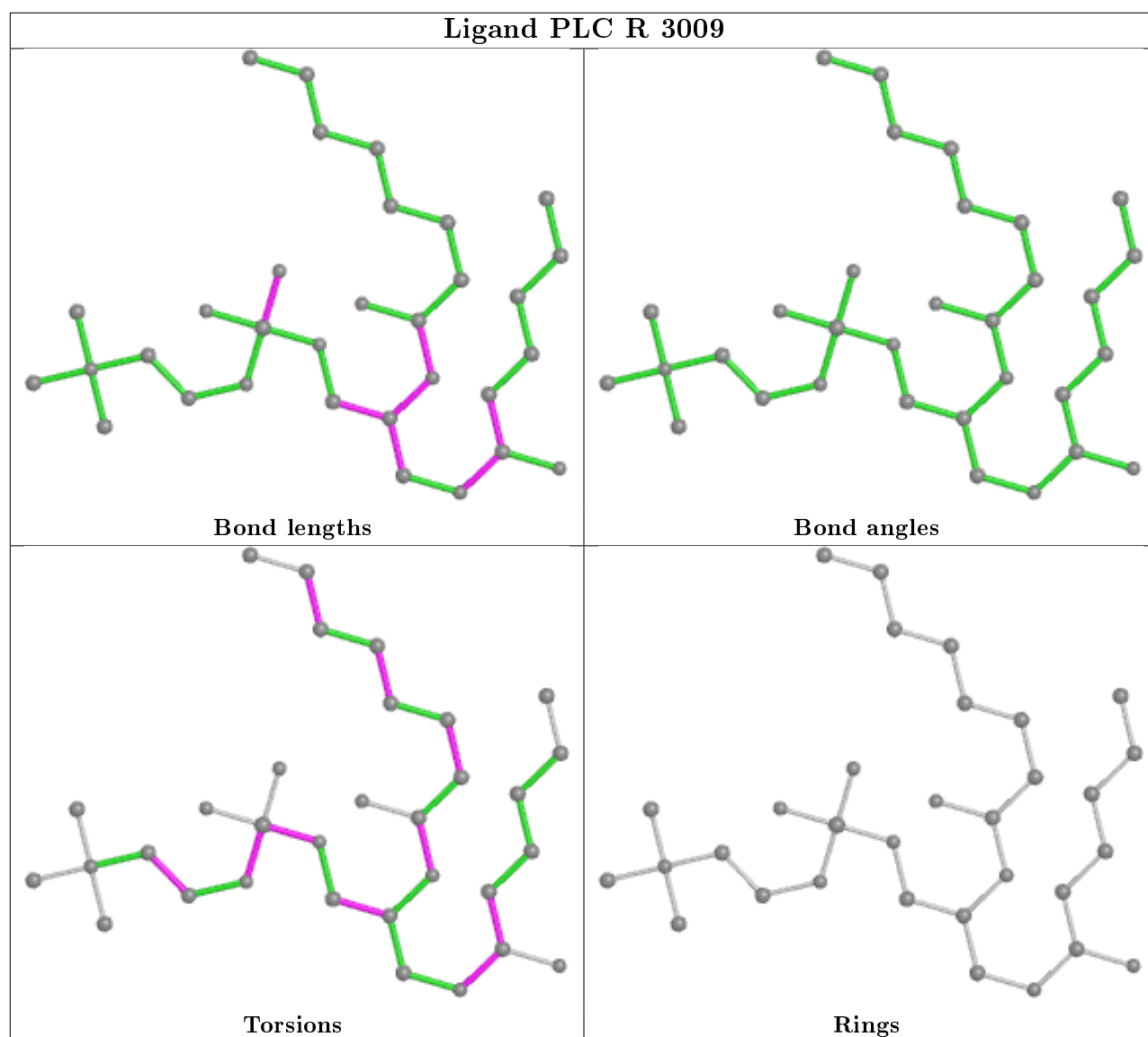
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

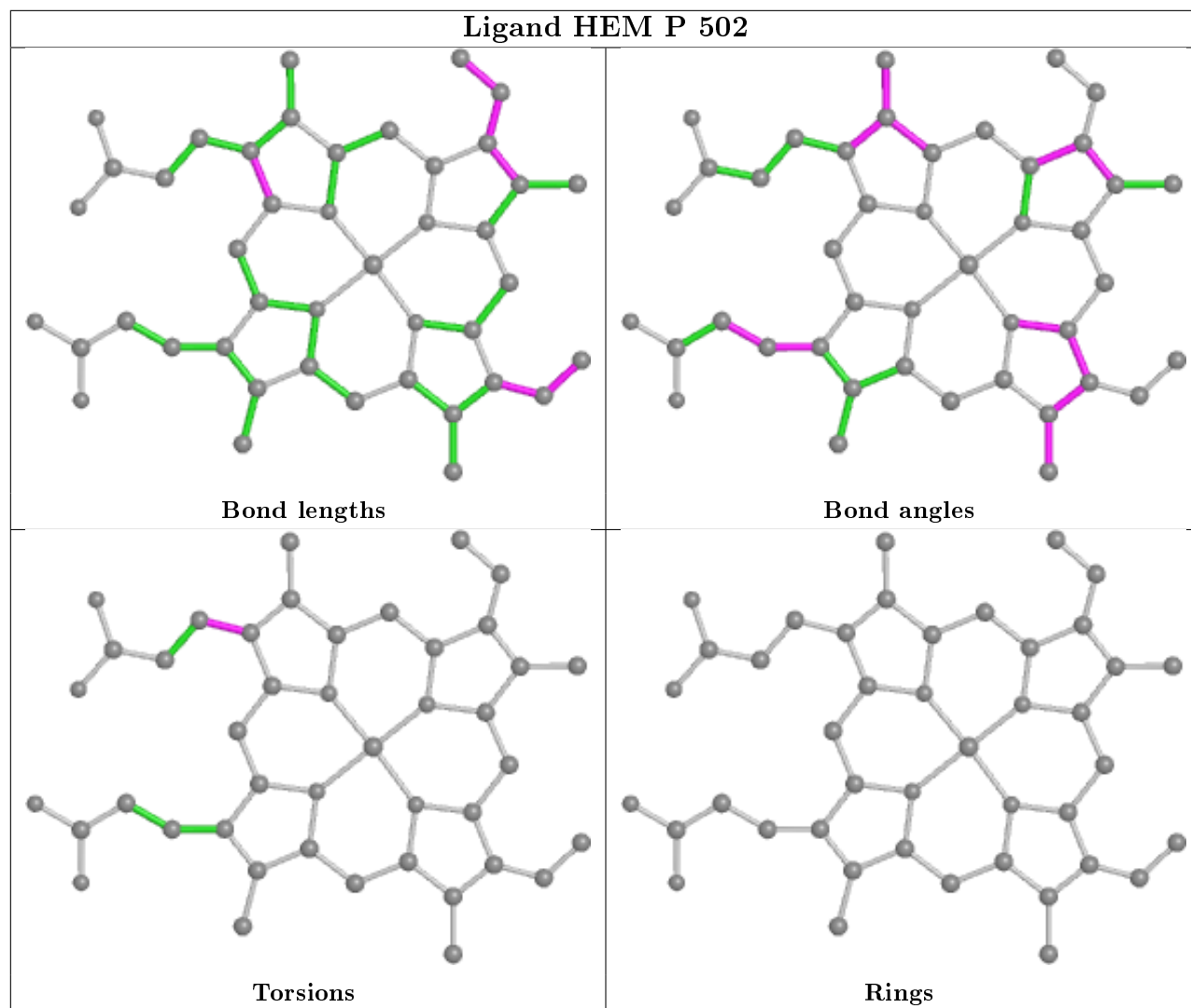


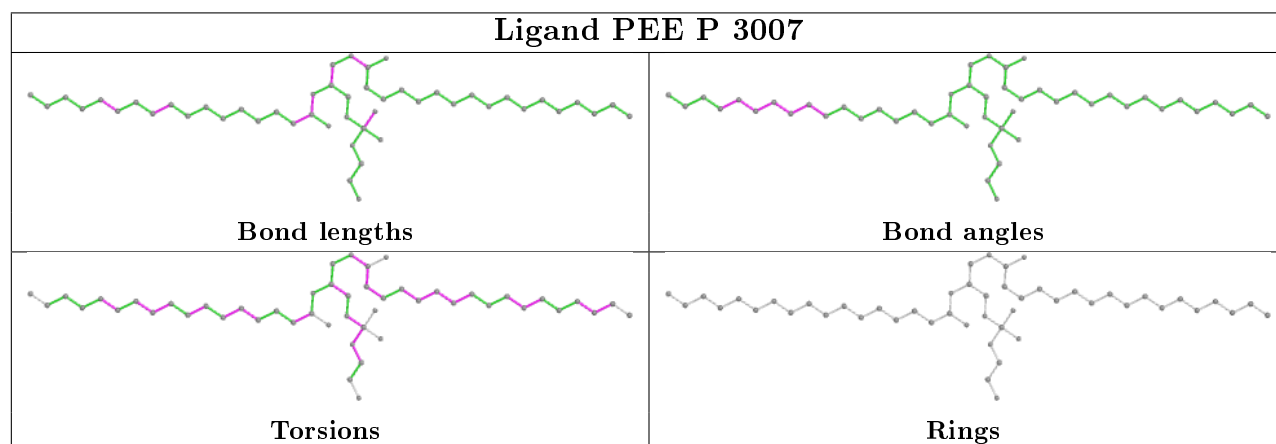
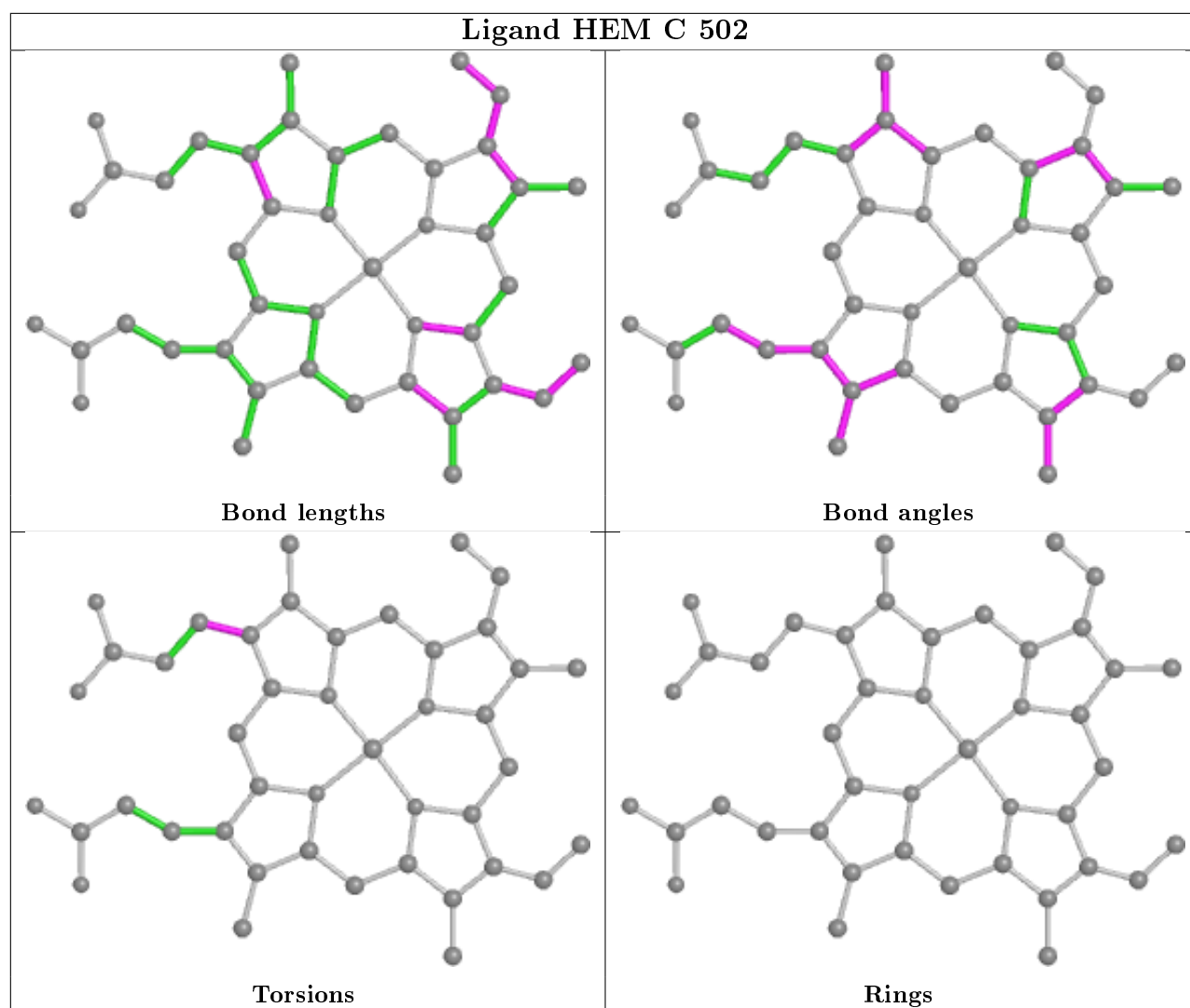


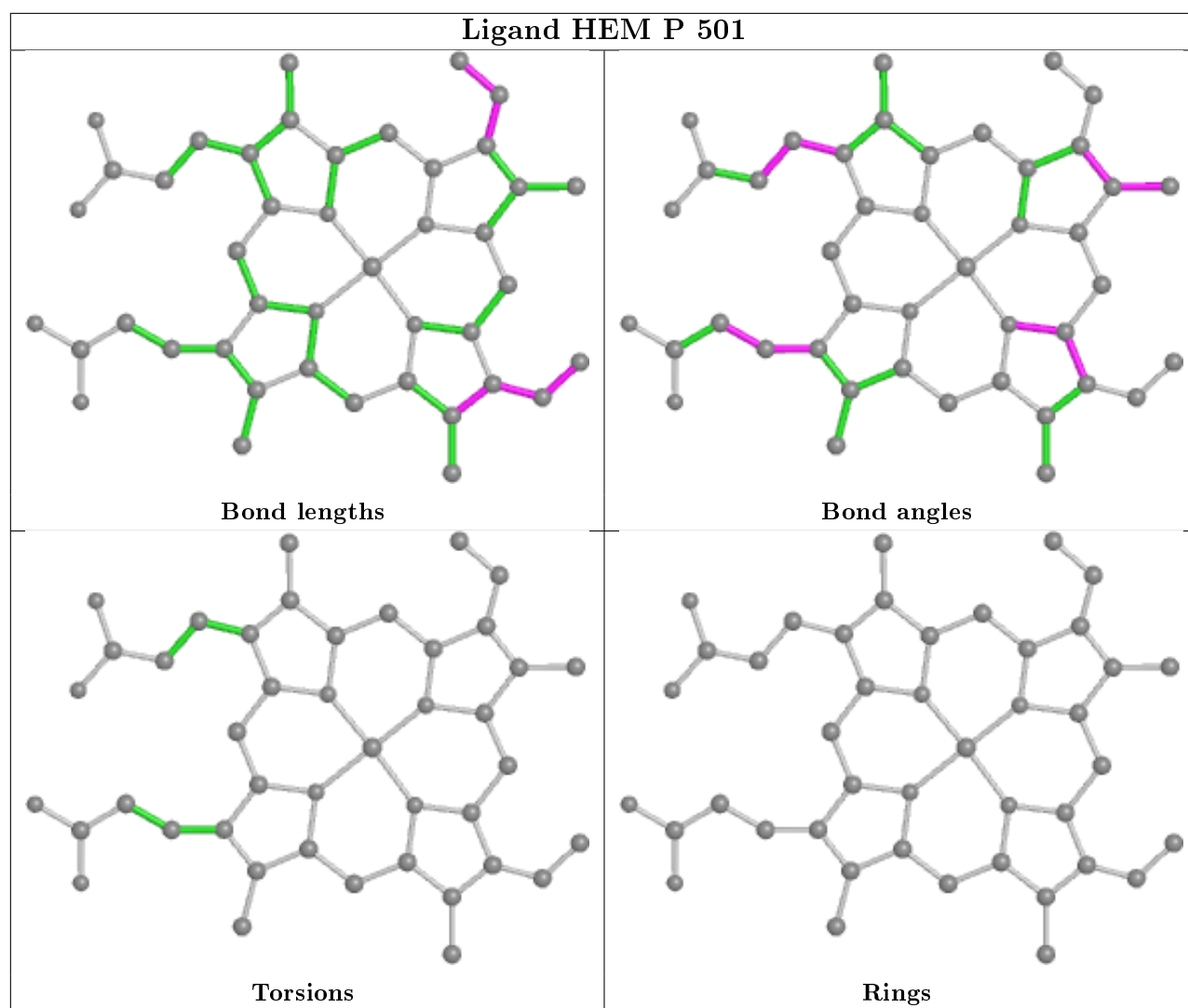


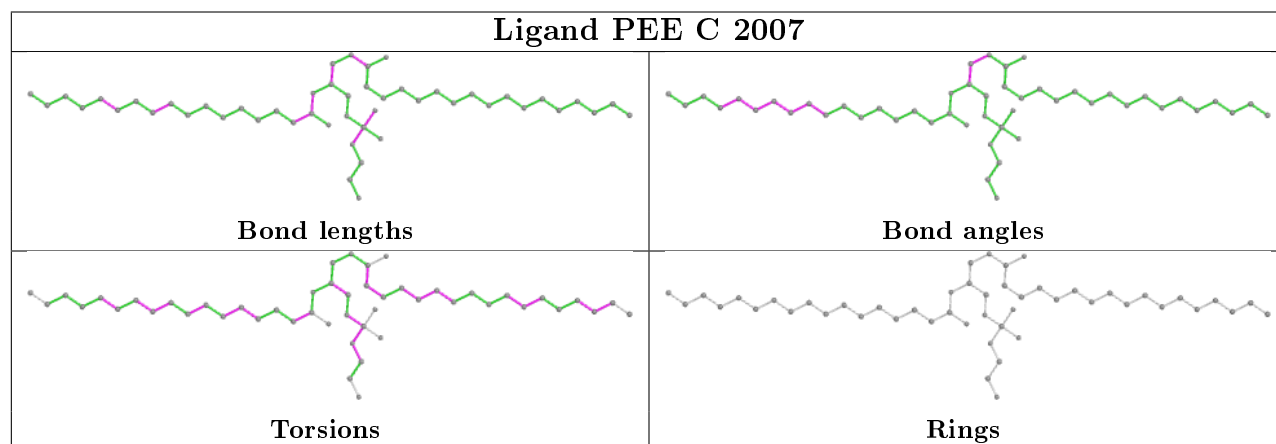
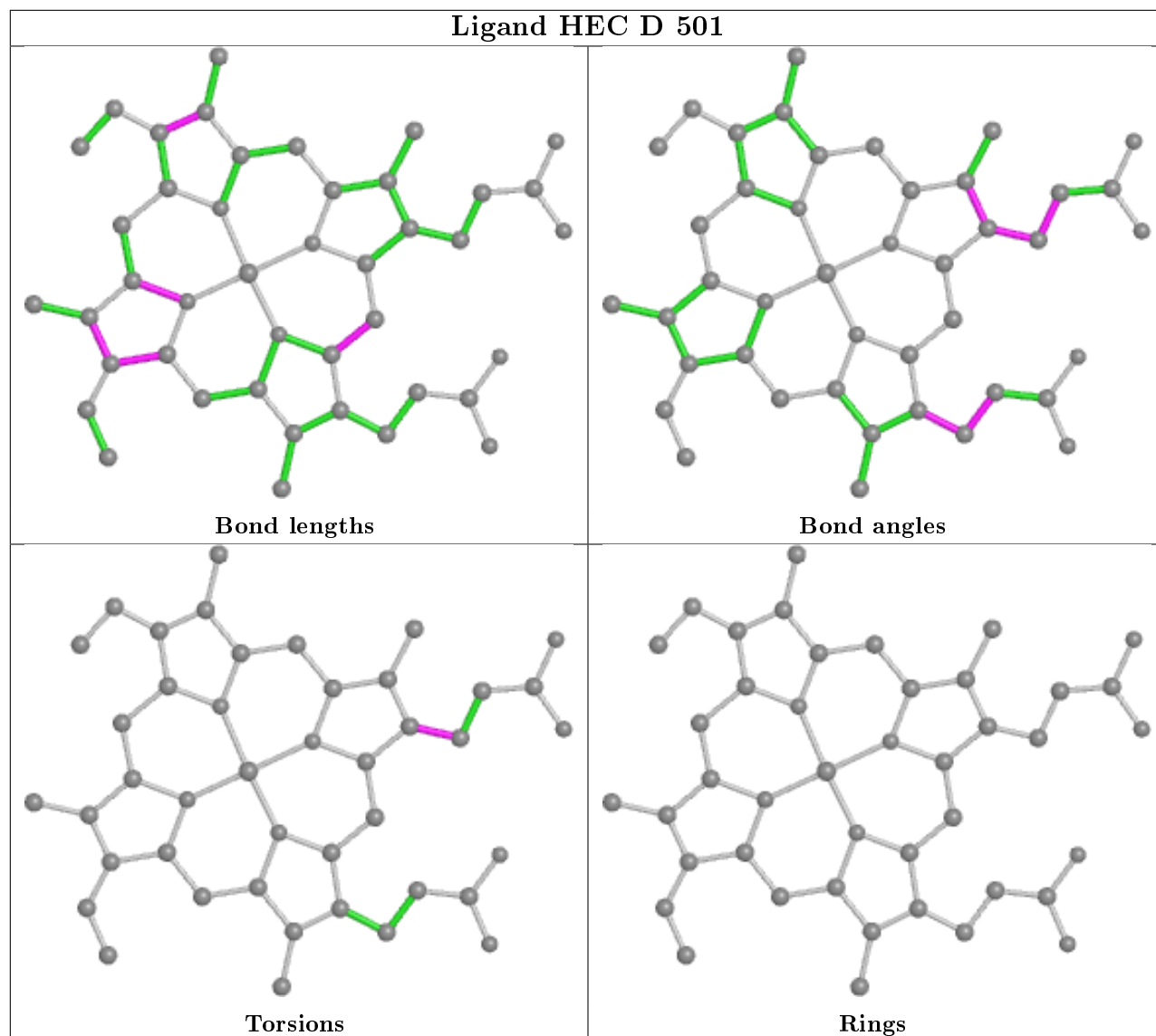


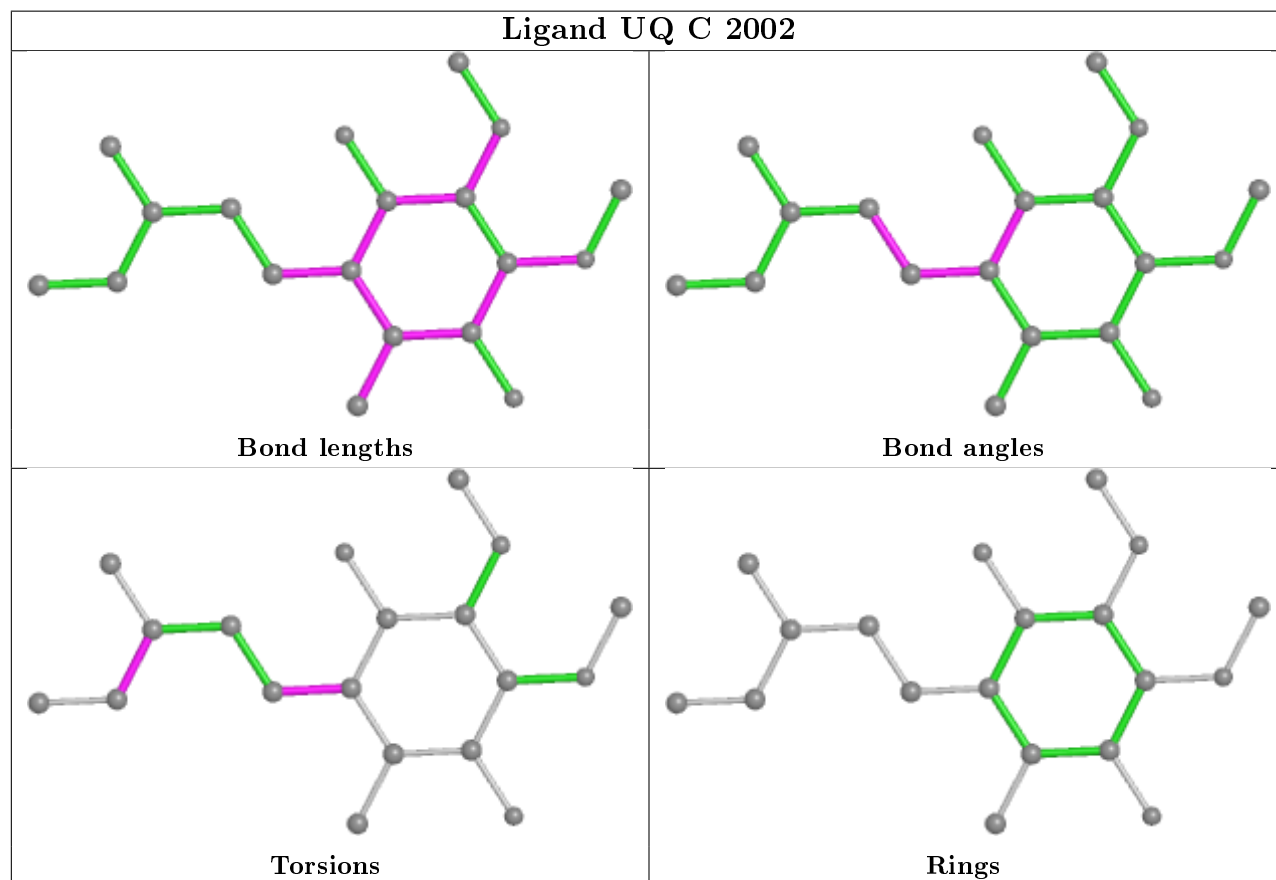
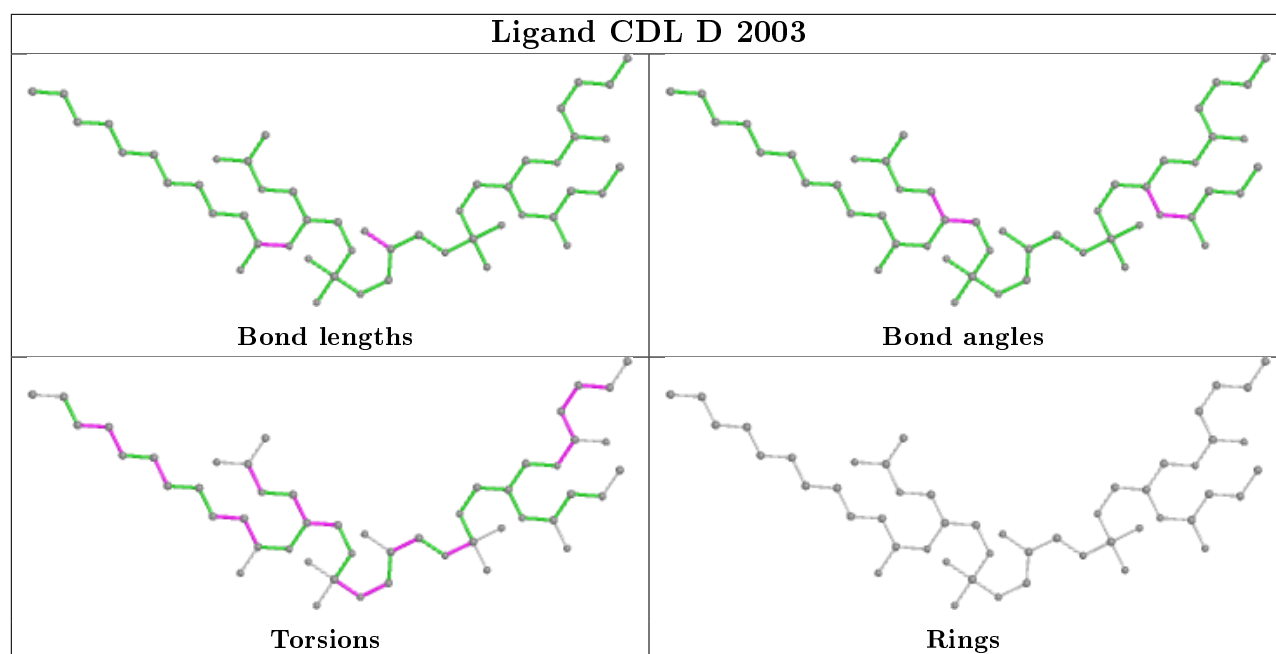


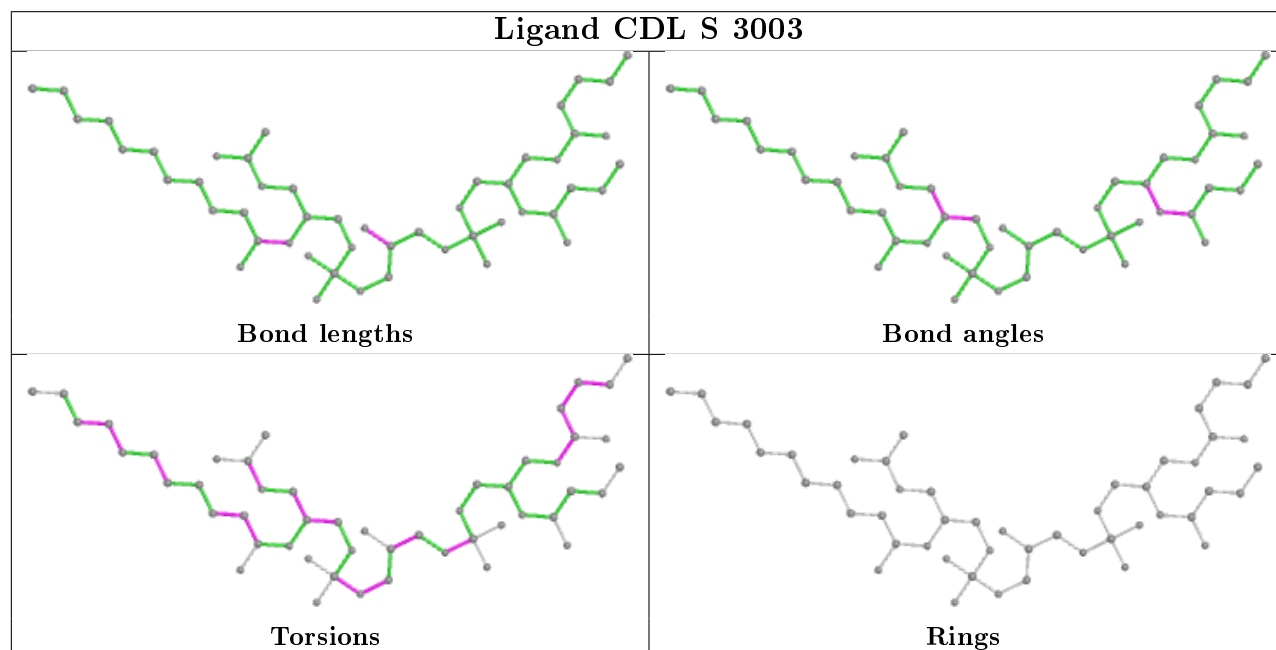
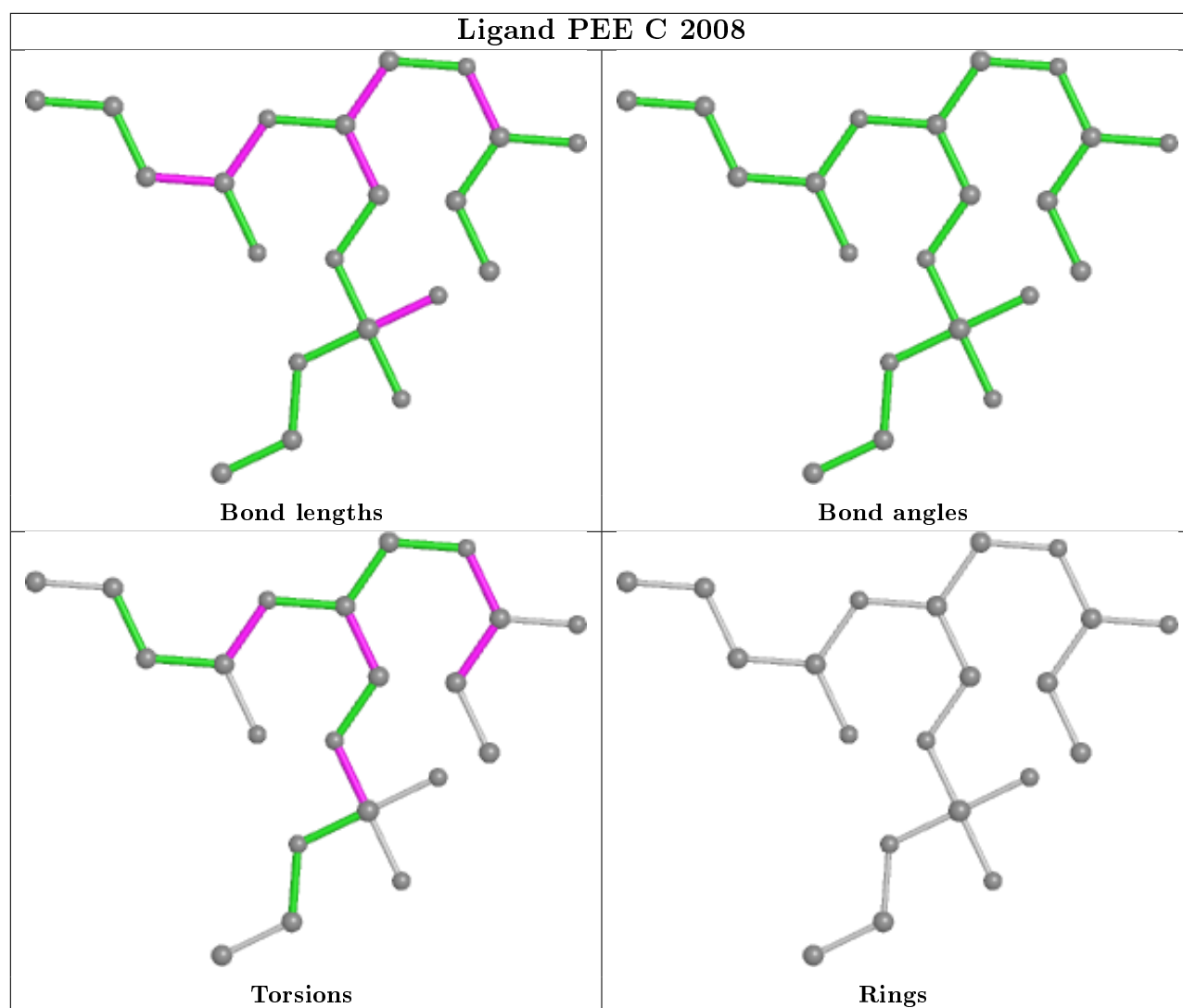


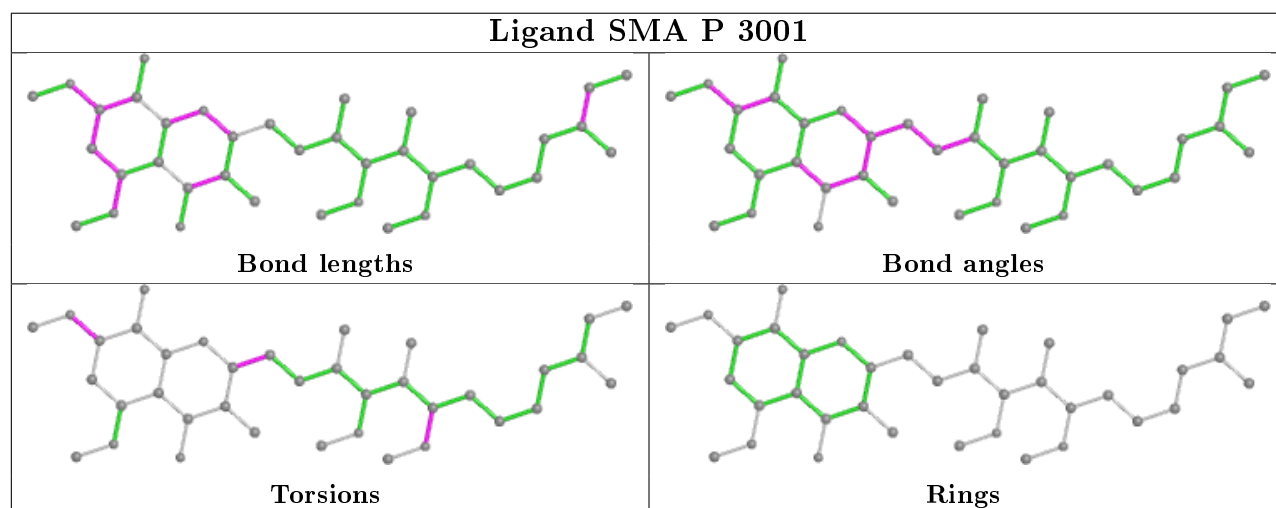
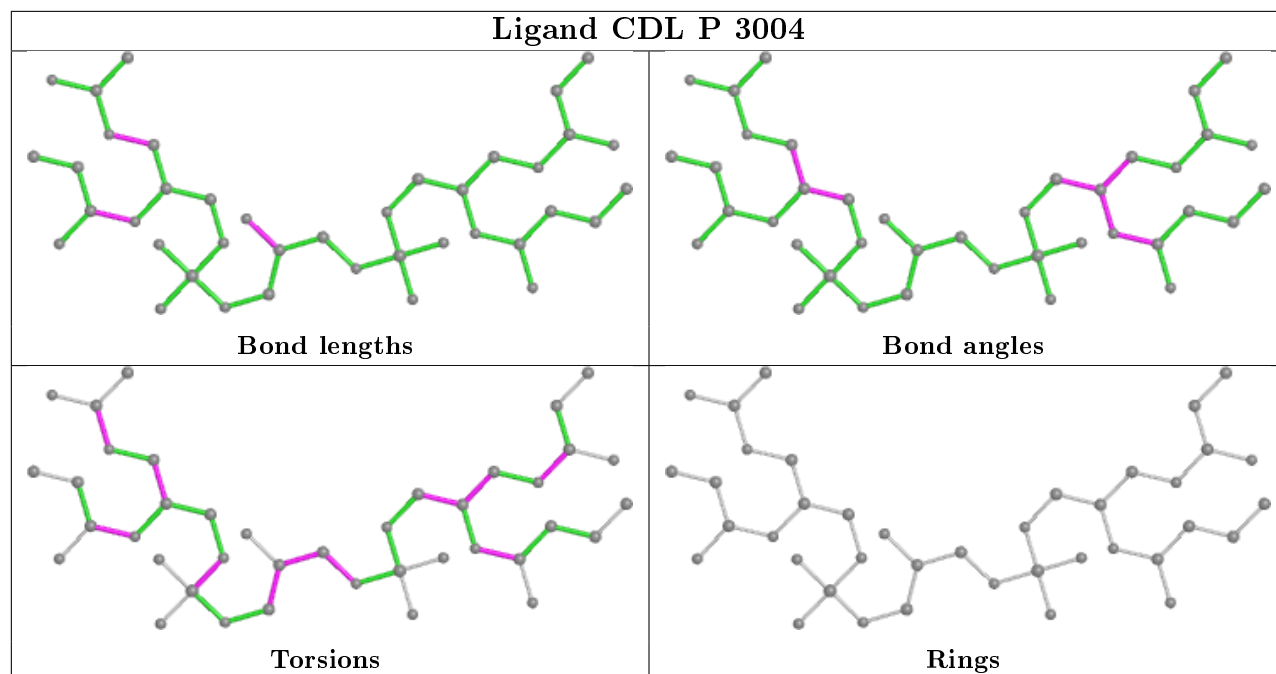




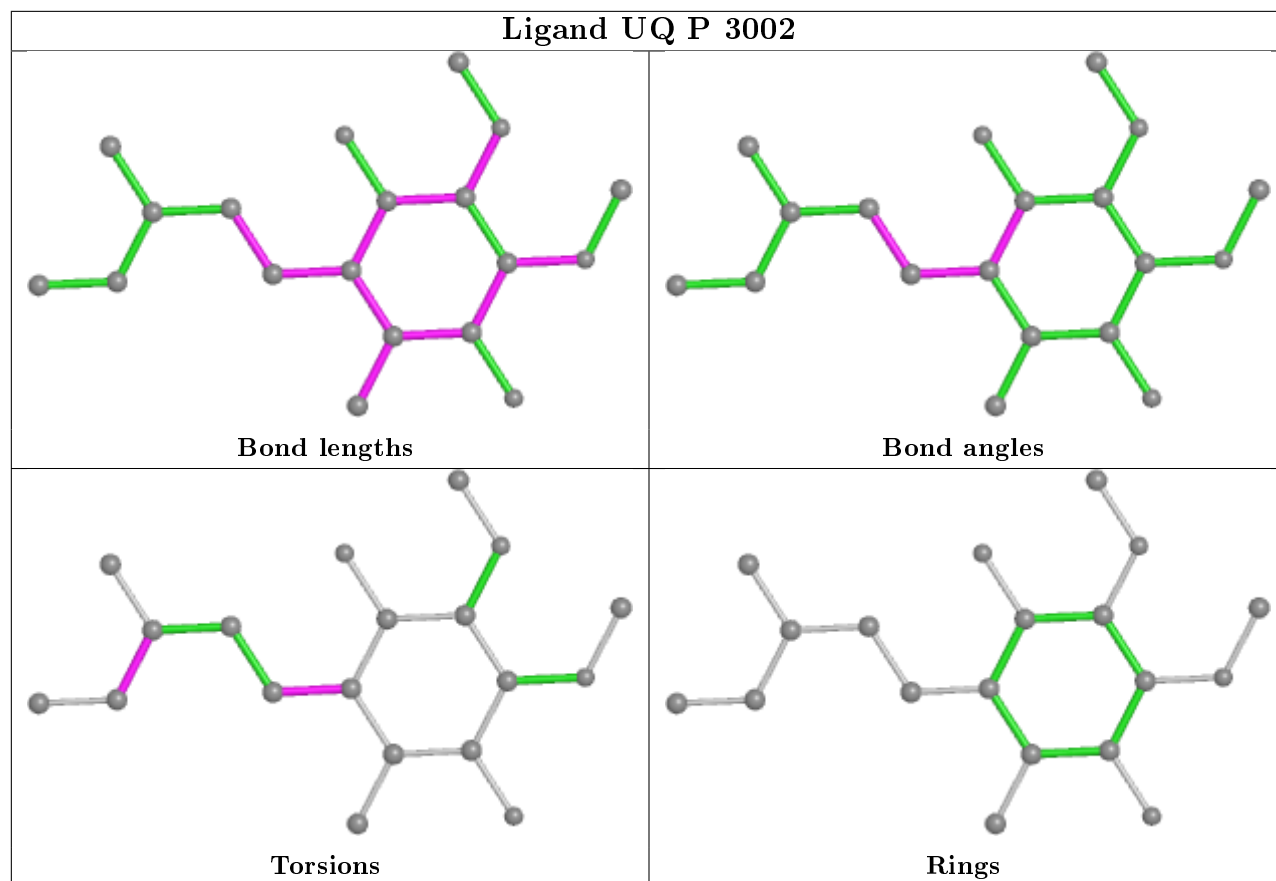


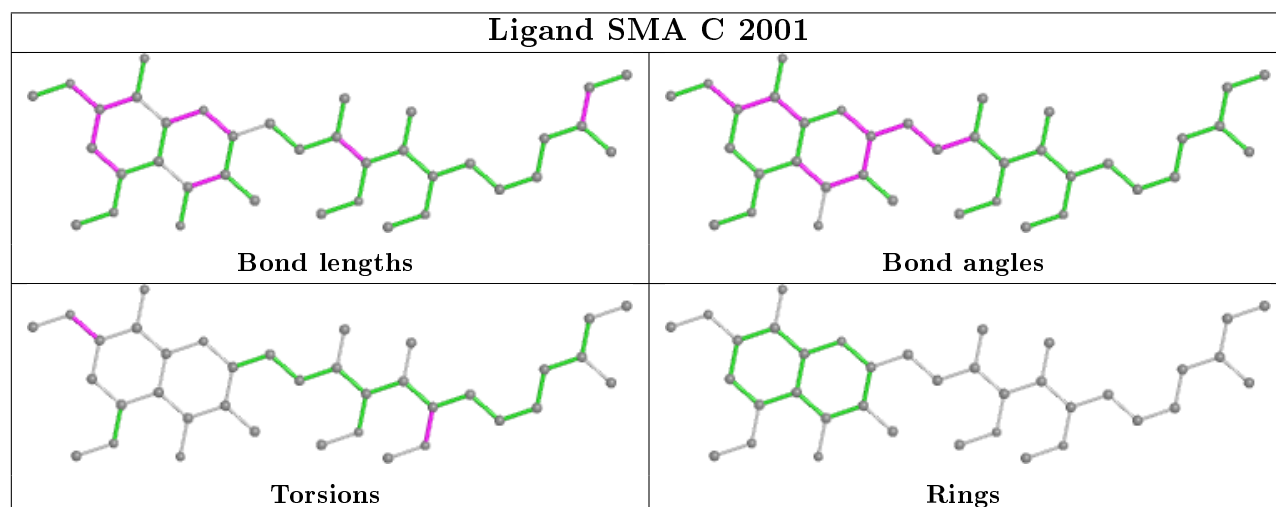
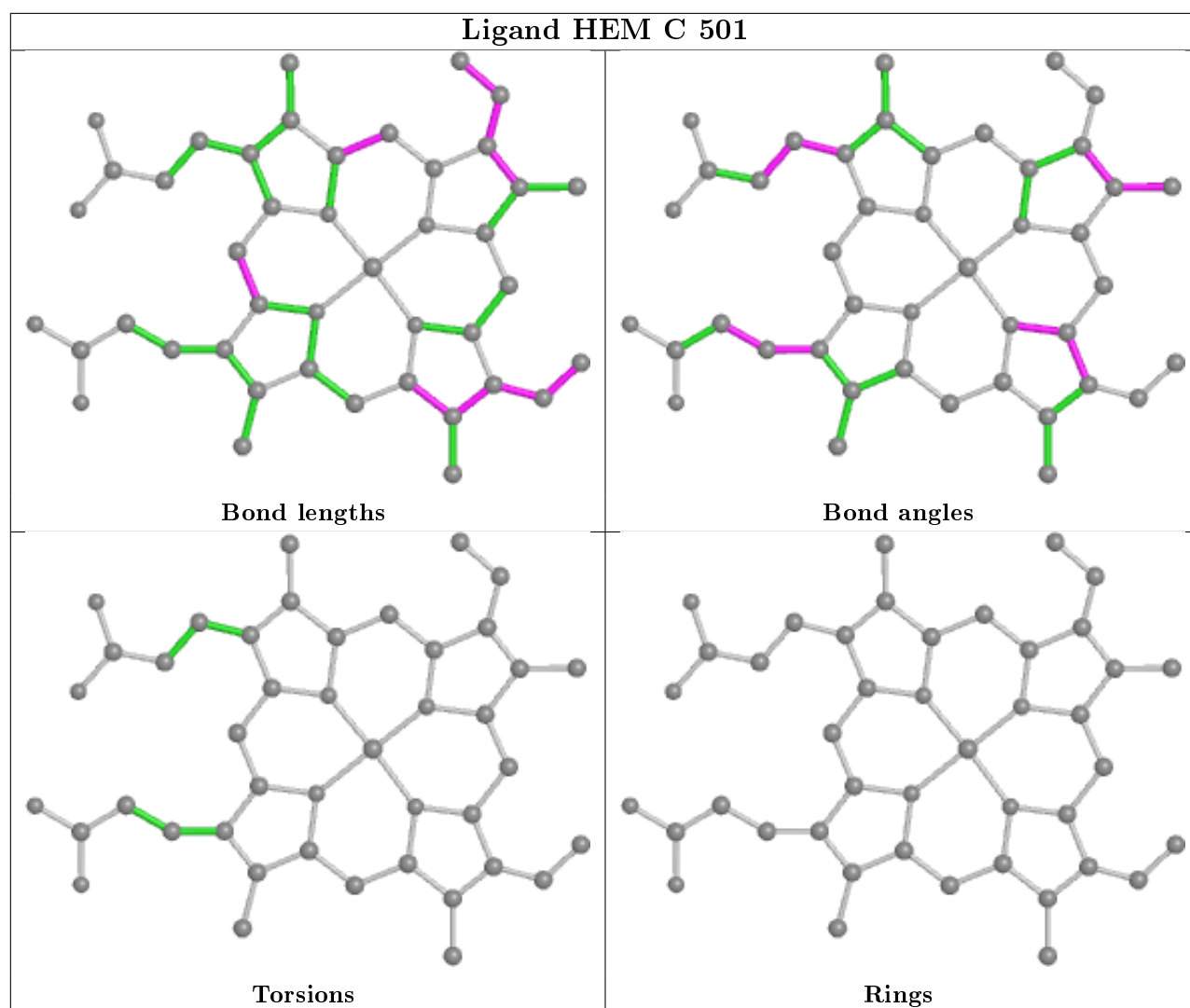


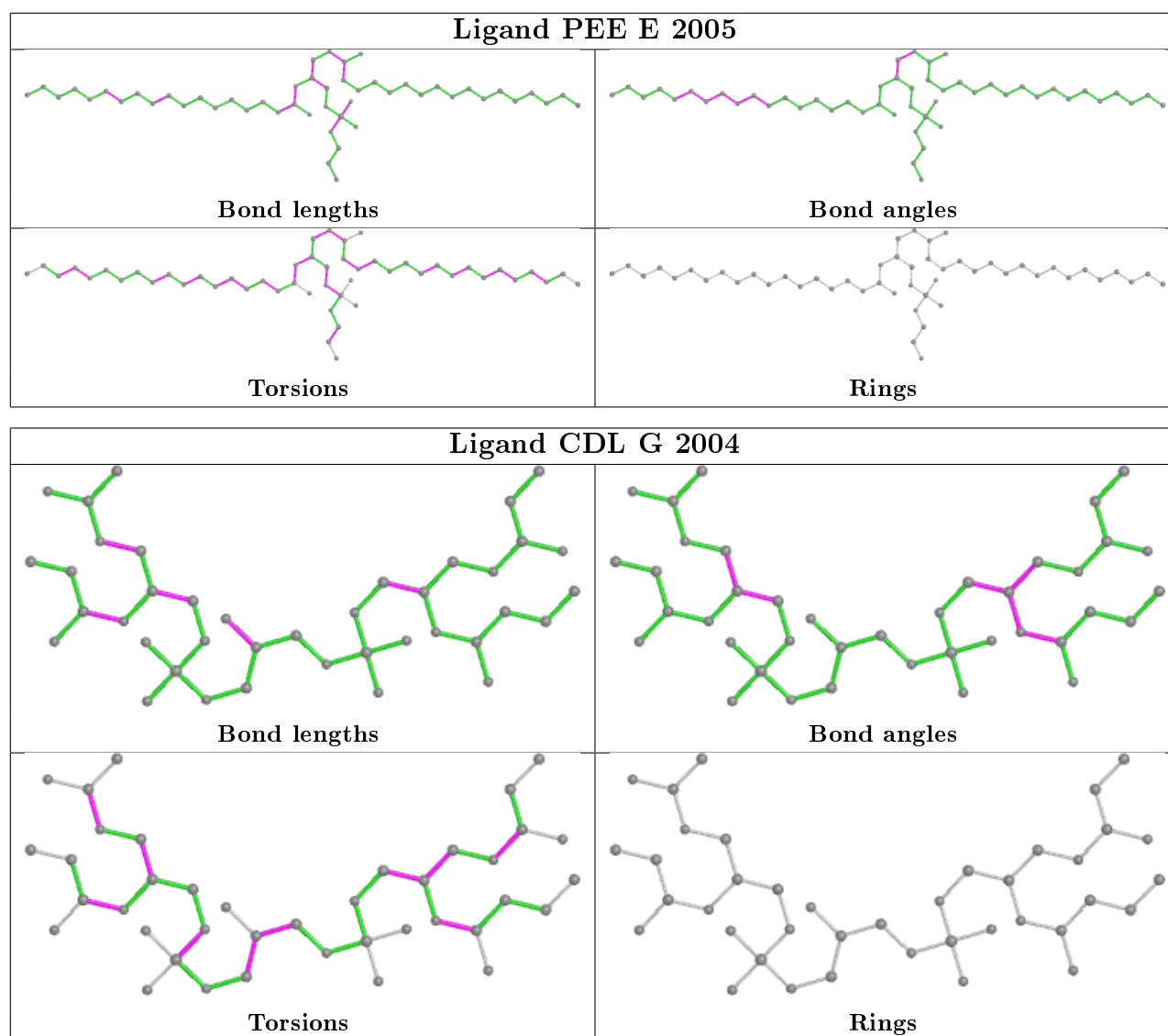












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	443/446 (99%)	-0.34	2 (0%) 91 75	44, 77, 105, 114	0
1	N	442/446 (99%)	-0.31	0 100 100	54, 80, 102, 110	0
2	B	421/441 (95%)	-0.26	1 (0%) 95 87	66, 93, 122, 140	0
2	O	422/441 (95%)	-0.29	1 (0%) 95 87	52, 85, 111, 124	0
3	C	380/380 (100%)	-0.49	1 (0%) 94 84	33, 49, 84, 140	0
3	P	379/380 (99%)	-0.31	4 (1%) 80 56	44, 75, 99, 119	0
4	D	241/241 (100%)	-0.51	0 100 100	42, 55, 86, 114	0
4	Q	241/241 (100%)	-0.25	0 100 100	59, 86, 112, 127	0
5	E	196/196 (100%)	0.28	17 (8%) 10 3	48, 114, 165, 172	0
5	R	196/196 (100%)	0.05	12 (6%) 21 7	54, 85, 134, 151	0
6	F	101/110 (91%)	-0.64	0 100 100	37, 53, 67, 99	0
6	S	101/110 (91%)	-0.24	2 (1%) 65 36	64, 84, 112, 141	0
7	G	81/81 (100%)	-0.27	0 100 100	48, 62, 94, 113	0
7	T	79/81 (97%)	0.18	7 (8%) 9 3	69, 95, 147, 164	0
8	H	70/77 (90%)	-0.44	0 100 100	48, 73, 90, 133	0
8	U	67/77 (87%)	0.18	3 (4%) 33 12	102, 125, 148, 154	0
9	I	31/47 (65%)	1.32	9 (29%) 0 0	94, 127, 172, 178	0
9	V	31/47 (65%)	1.59	11 (35%) 0 0	93, 125, 184, 184	0
10	J	61/61 (100%)	-0.43	1 (1%) 72 44	57, 71, 109, 151	0
10	W	59/61 (96%)	-0.01	1 (1%) 70 41	69, 85, 101, 117	0
All	All	4042/4160 (97%)	-0.25	72 (1%) 68 40	33, 79, 125, 184	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	GLY	5.7
8	U	50	THR	5.3
9	V	51	CYS	5.3
7	T	78	GLU	4.8
7	T	2	ILE	4.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

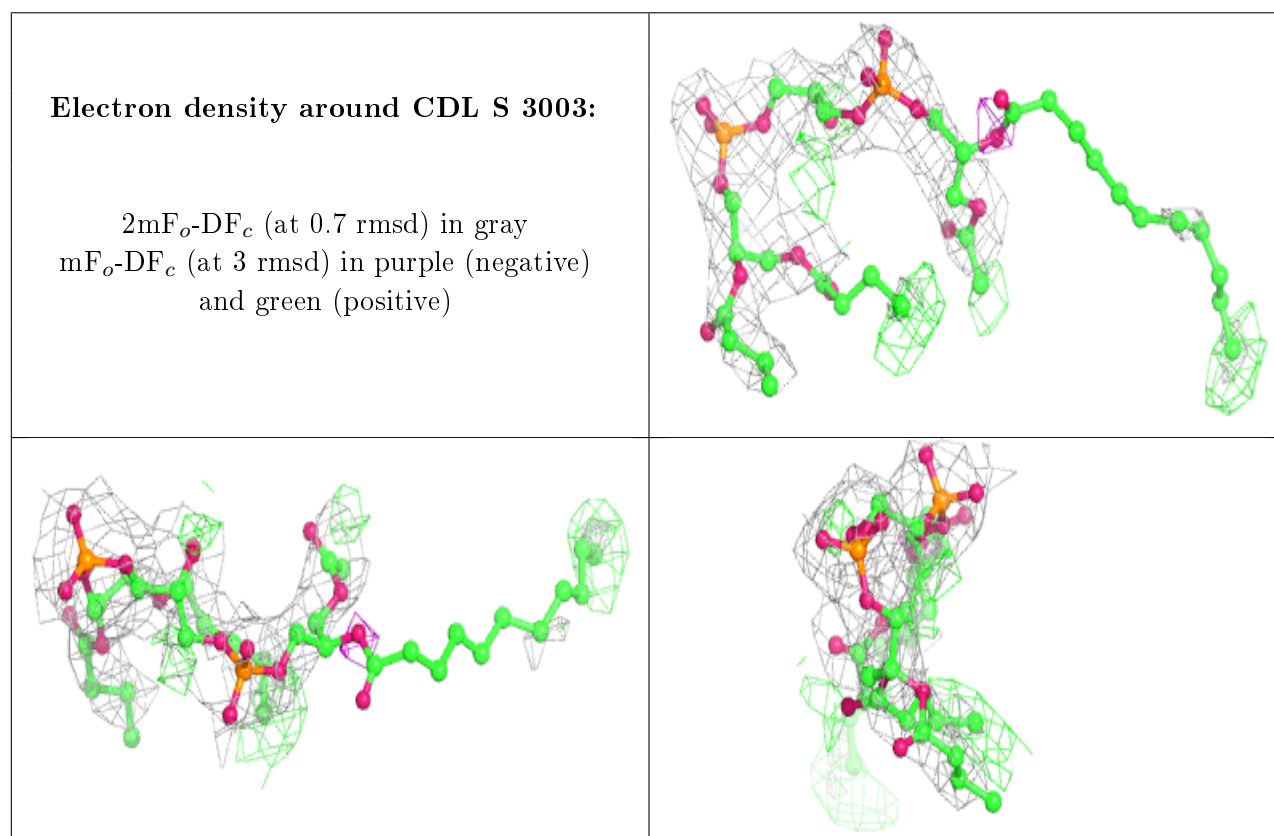
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	UNL	E	2105	1/-	0.51	0.38	62,62,62,62	0
11	UNL	C	2010	1/-	0.59	1.52	53,53,53,53	0
11	UNL	E	3103	1/-	0.65	0.43	45,45,45,45	0
11	UNL	P	3010	1/-	0.65	0.89	67,67,67,67	0
11	UNL	C	2104	1/-	0.67	0.62	71,71,71,71	0
11	UNL	P	2015	1/-	0.71	0.39	33,33,33,33	0
11	UNL	C	3015	1/-	0.73	0.48	47,47,47,47	0
11	UNL	A	3016	1/-	0.75	0.40	55,55,55,55	0
18	CDL	S	3003	50/100	0.76	0.38	126,140,153,153	0
11	UNL	P	3104	1/-	0.76	0.54	59,59,59,59	0
15	PEE	C	2008	21/51	0.76	0.33	139,142,144,144	0
15	PEE	R	3005	50/51	0.78	0.38	95,108,116,119	0
15	PEE	E	2005	50/51	0.79	0.34	76,90,95,95	0
11	UNL	R	2103	1/-	0.80	0.61	45,45,45,45	0
20	PLC	E	2009	32/42	0.82	0.32	67,83,97,98	0
20	PLC	R	3009	32/42	0.82	0.35	91,99,116,116	0
15	PEE	N	3008	5/51	0.82	0.34	135,135,136,136	0
16	GOL	C	2011	6/6	0.84	0.35	79,81,82,83	0
14	UQ	C	2002	19/63	0.84	0.28	85,88,90,91	0

*Continued on next page...*

*Continued from previous page...*

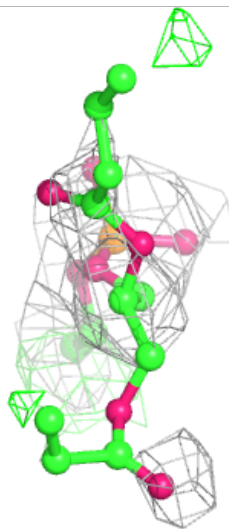
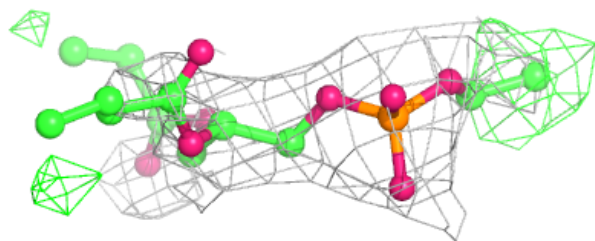
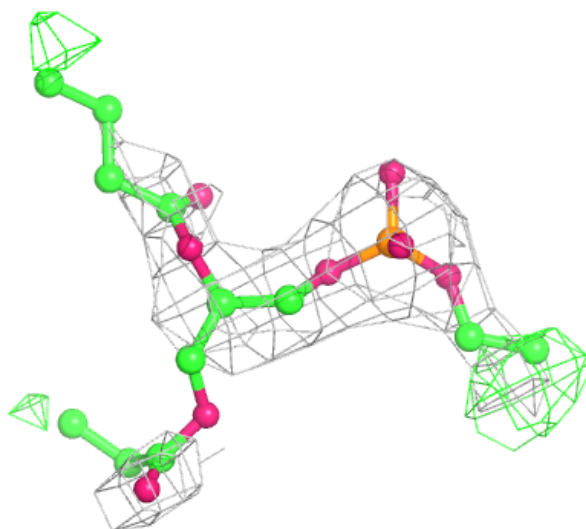
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CDL	P	3004	40/100	0.85	0.27	106,114,120,121	0
18	CDL	D	2003	50/100	0.85	0.27	79,112,130,131	0
14	UQ	P	3002	19/63	0.85	0.30	116,121,122,122	0
15	PEE	P	3007	49/51	0.87	0.34	73,98,107,108	0
18	CDL	G	2004	40/100	0.90	0.26	81,90,97,98	0
16	GOL	P	3011	6/6	0.92	0.27	69,71,72,72	0
15	PEE	C	2007	49/51	0.92	0.28	52,68,87,89	0
13	SMA	P	3001	37/37	0.94	0.23	67,73,75,78	0
17	HEC	Q	501	43/43	0.96	0.19	67,71,76,78	0
13	SMA	C	2001	37/37	0.97	0.20	41,44,46,52	0
12	HEM	C	501	43/43	0.98	0.20	44,48,50,53	0
17	HEC	D	501	43/43	0.98	0.17	44,46,50,53	0
19	FES	E	501	4/4	0.98	0.15	92,93,95,95	0
12	HEM	P	501	43/43	0.98	0.21	56,61,69,75	0
12	HEM	C	502	43/43	0.99	0.19	34,40,50,54	0
12	HEM	P	502	43/43	0.99	0.20	59,63,71,77	0
19	FES	R	501	4/4	1.00	0.16	52,54,56,57	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.



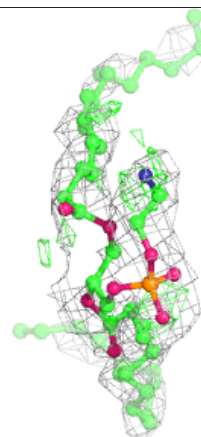
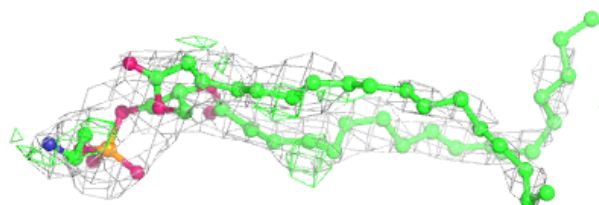
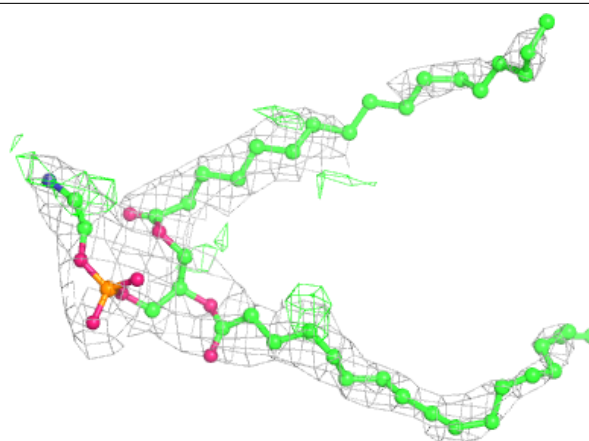
**Electron density around PEE C 2008:**

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



**Electron density around PEE R 3005:**

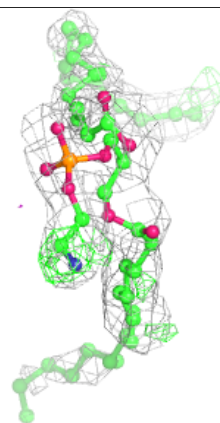
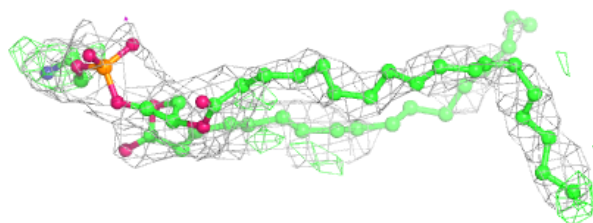
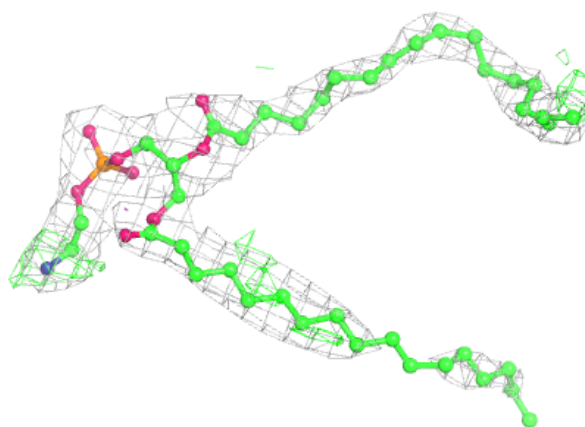
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



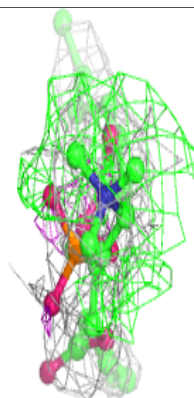
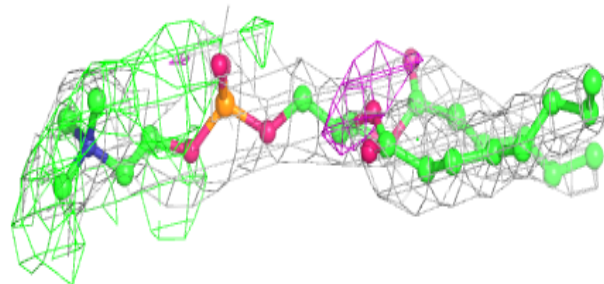
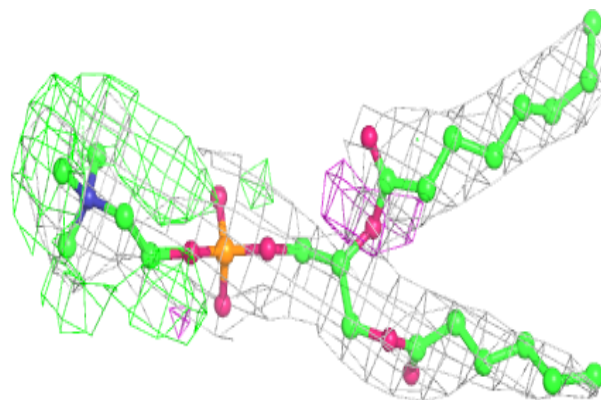


**Electron density around PEE E 2005:**

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and green (positive)

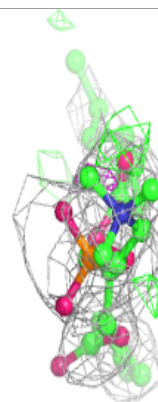
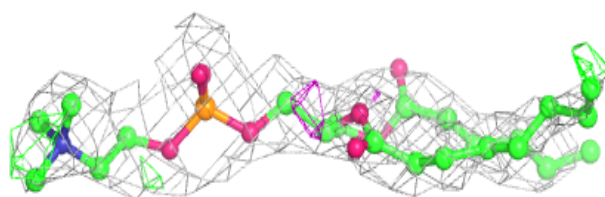
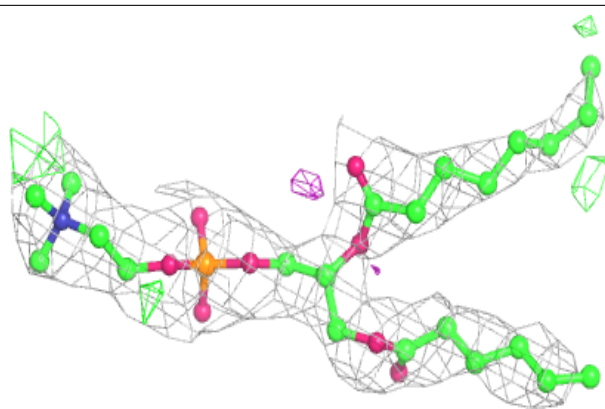
**Electron density around PLC E 2009:**

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and green (positive)



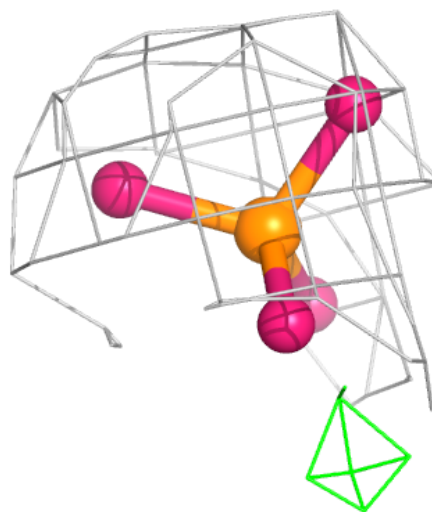
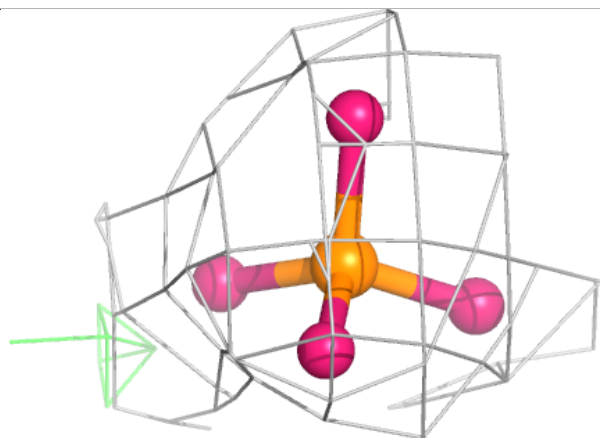
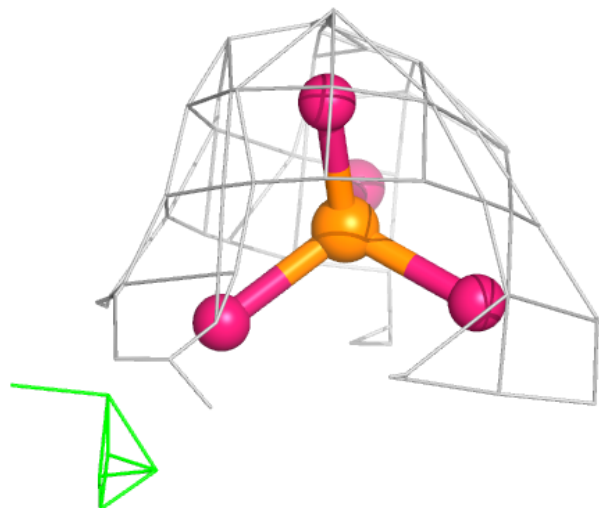
**Electron density around PLC R 3009:**

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



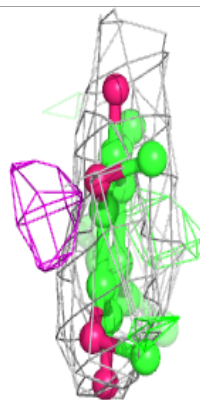
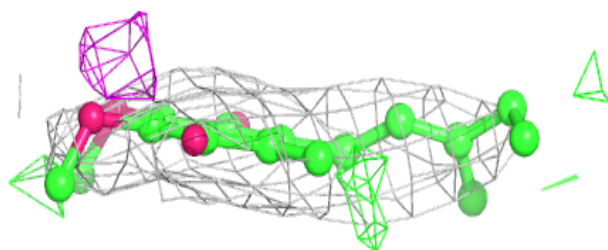
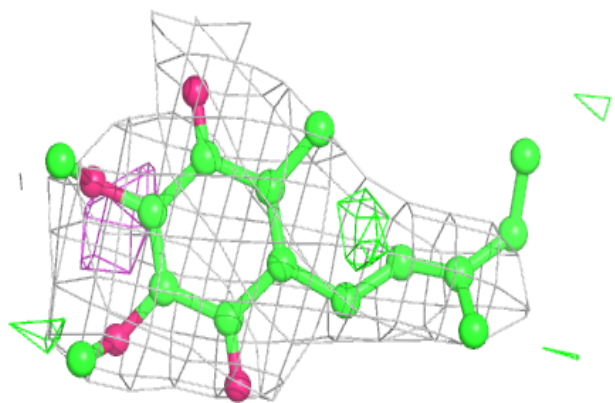
**Electron density around PEE N 3008:**

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



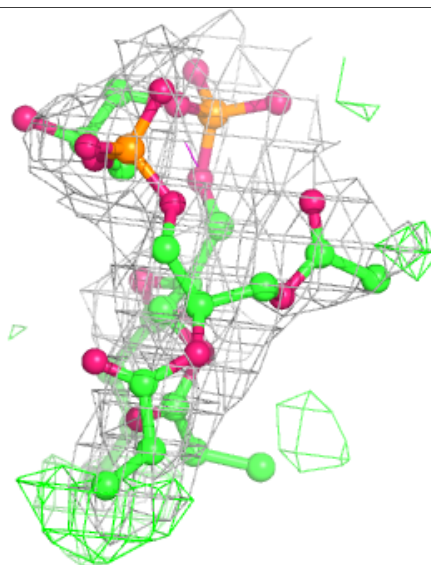
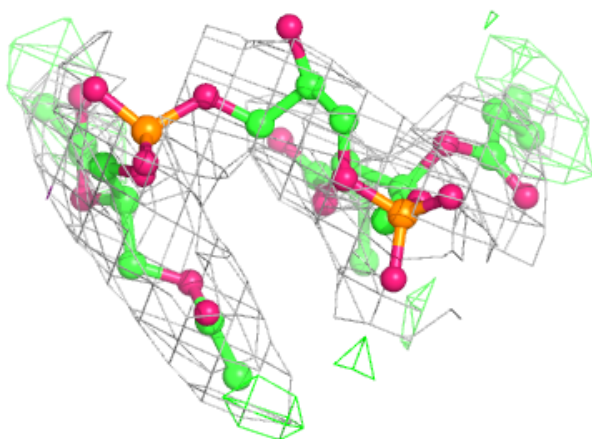
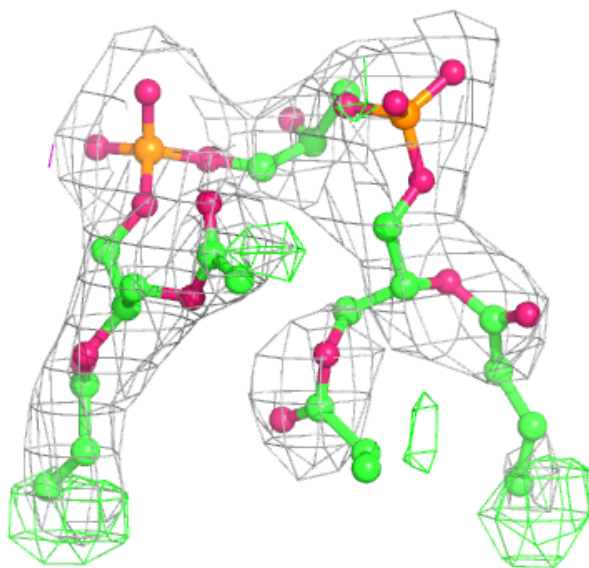
**Electron density around UQ C 2002:**

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and green (positive)



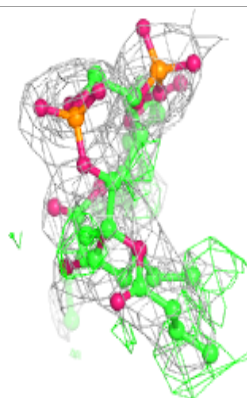
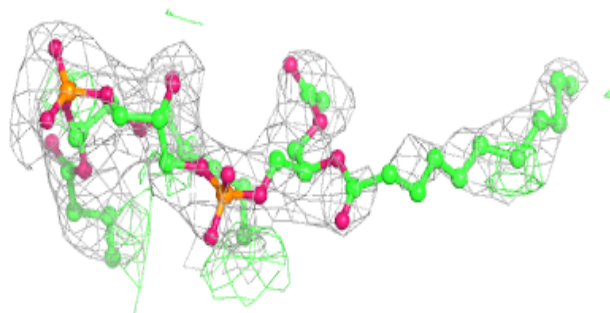
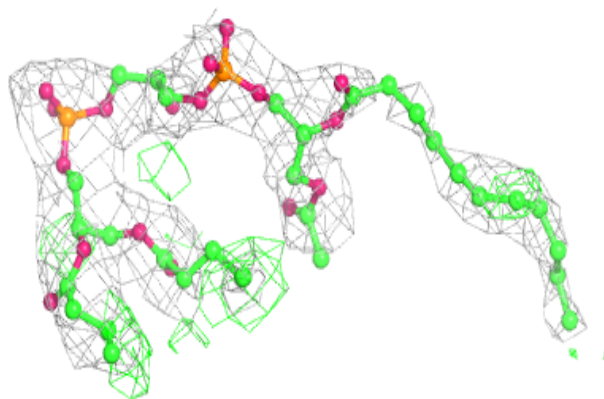
**Electron density around CDL P 3004:**

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

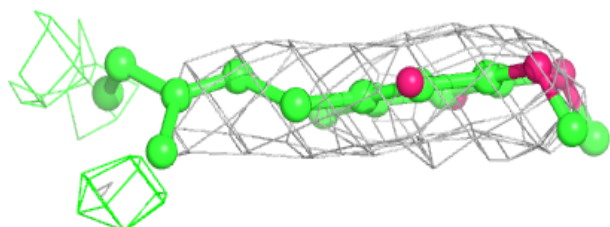
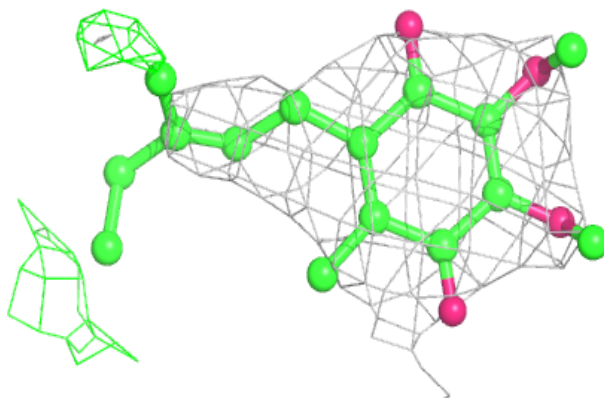


**Electron density around CDL D 2003:**

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

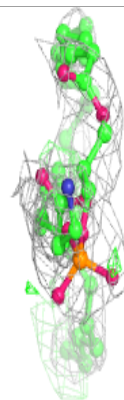
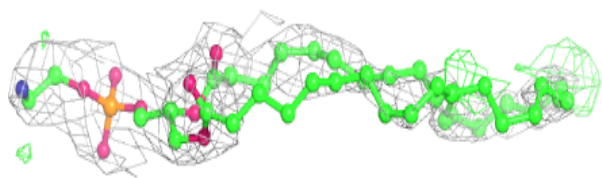
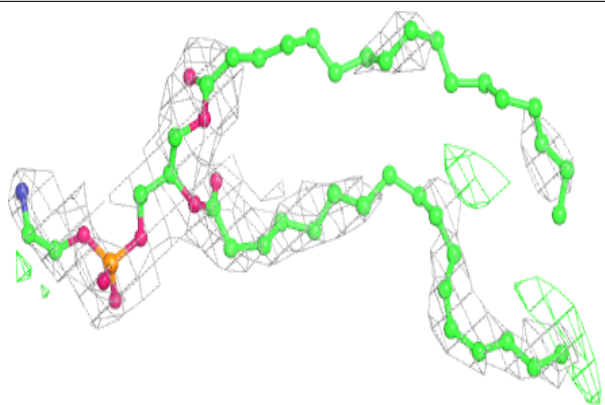
**Electron density around UQ P 3002:**

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



**Electron density around PEE P 3007:**

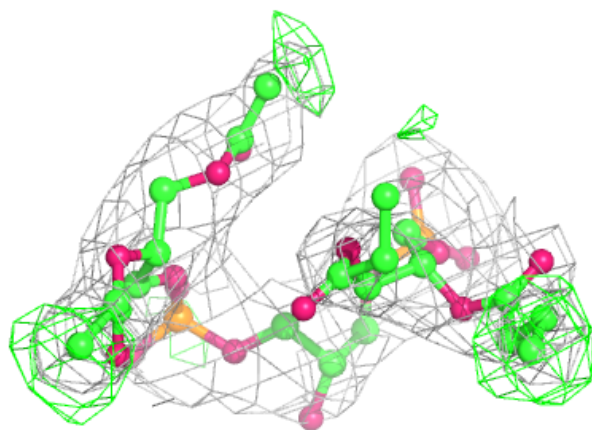
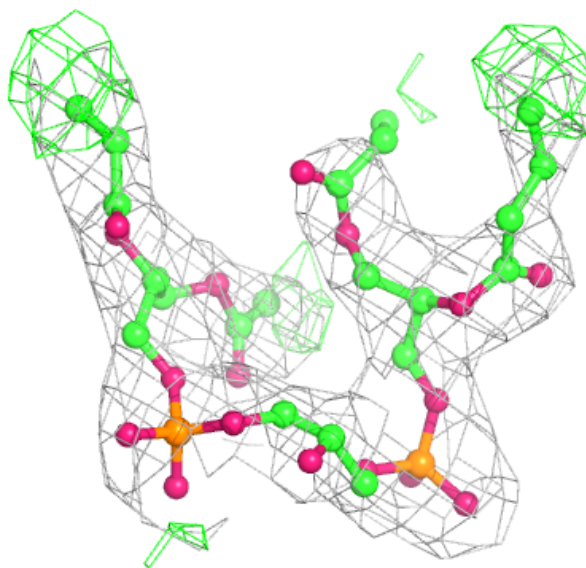
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CDL G 2004:**

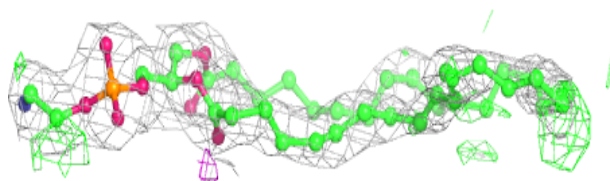
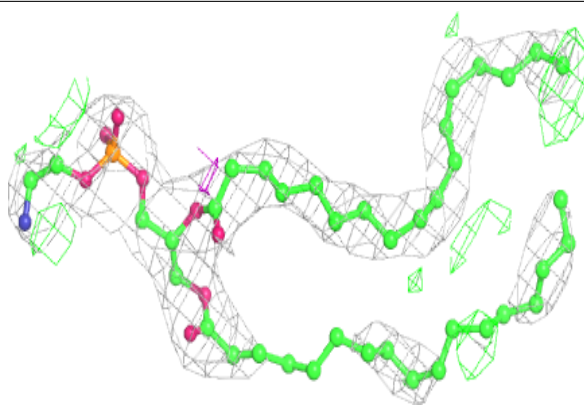
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



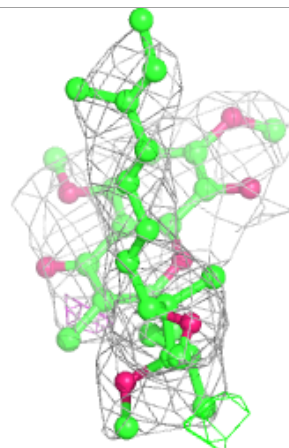
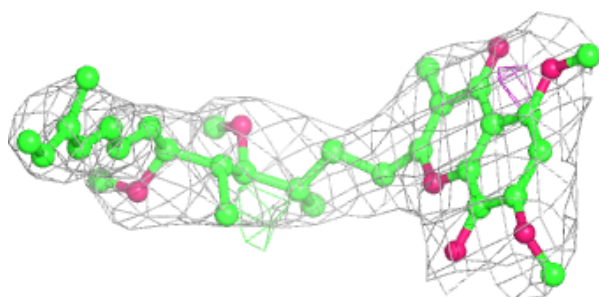
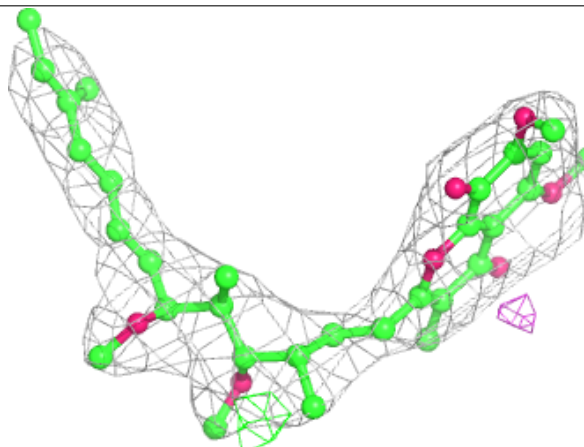


**Electron density around PEE C 2007:**

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

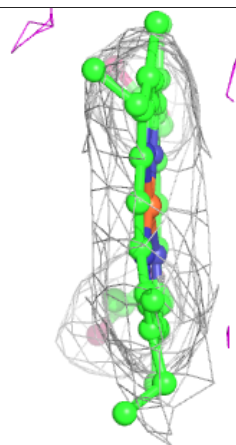
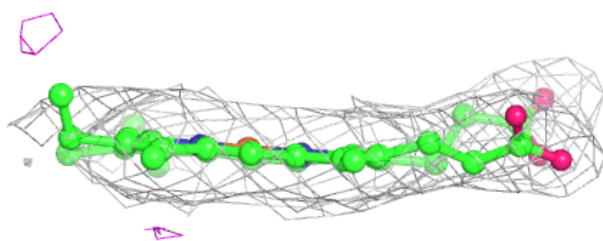
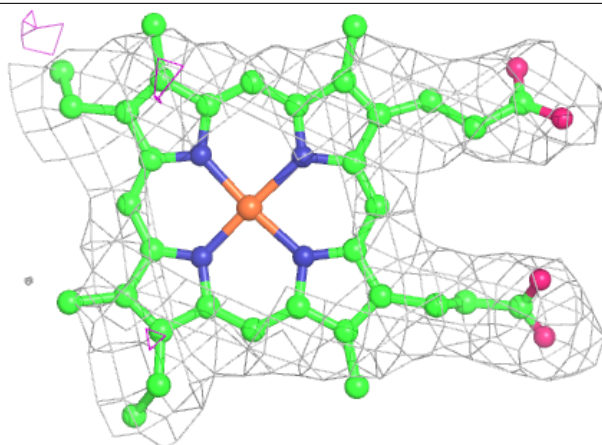
**Electron density around SMA P 3001:**

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

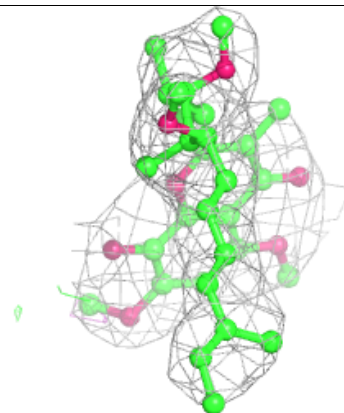
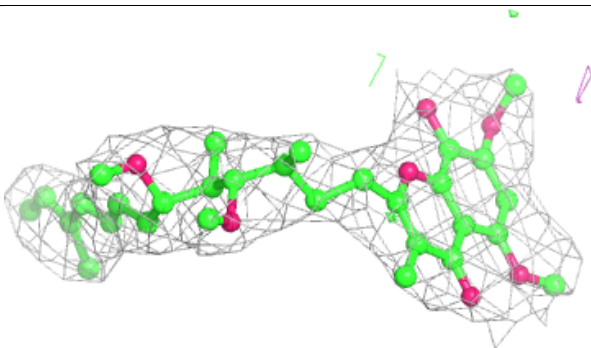
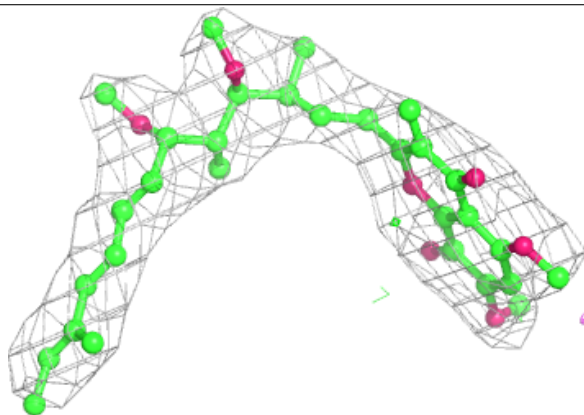


**Electron density around HEC Q 501:**

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

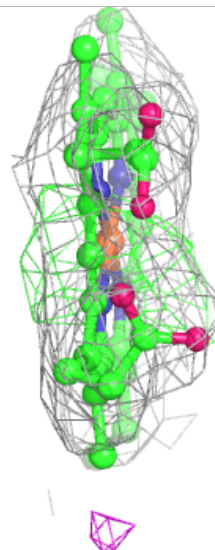
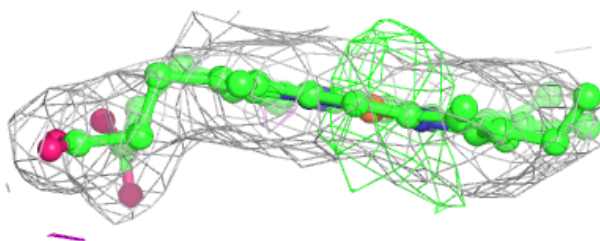
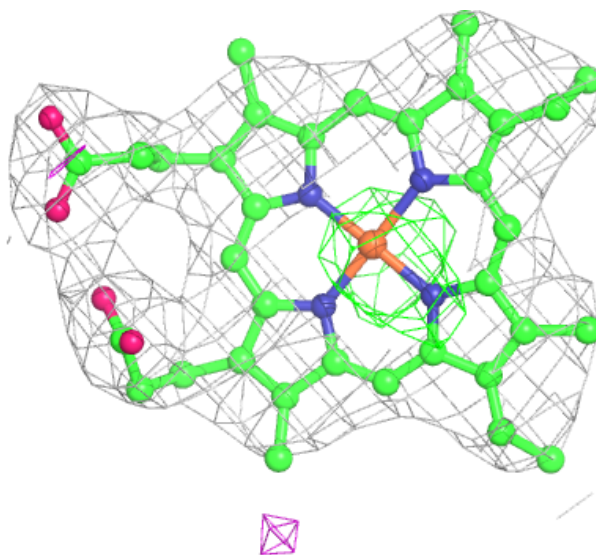
**Electron density around SMA C 2001:**

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



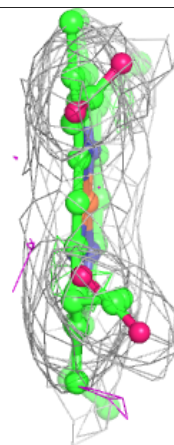
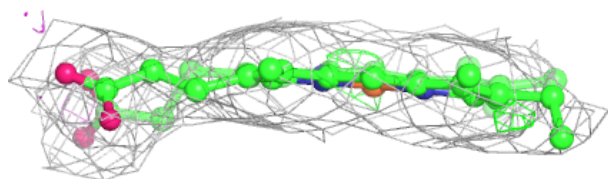
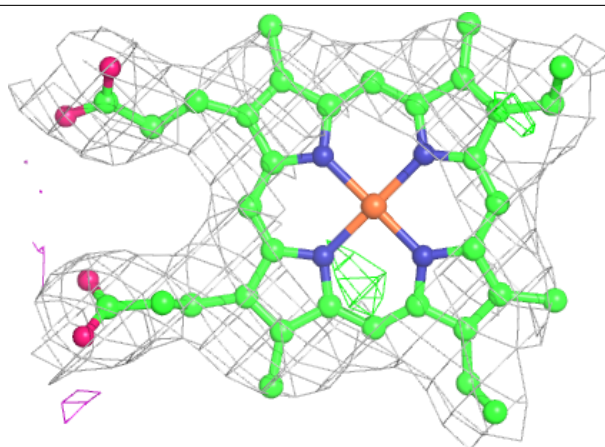
**Electron density around HEM C 501:**

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



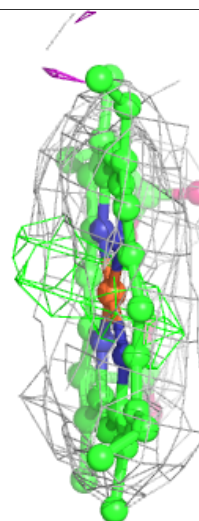
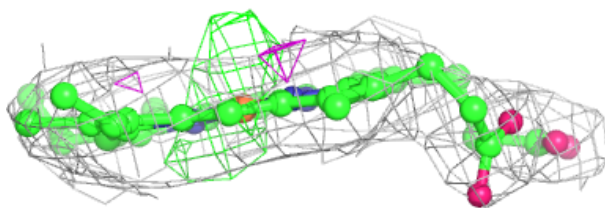
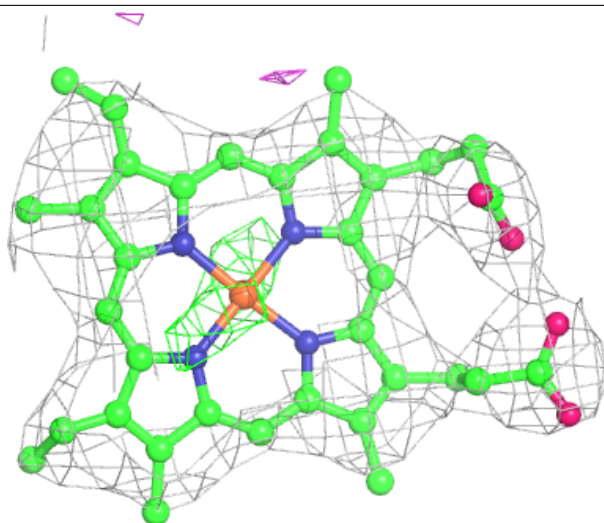
**Electron density around HEC D 501:**

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



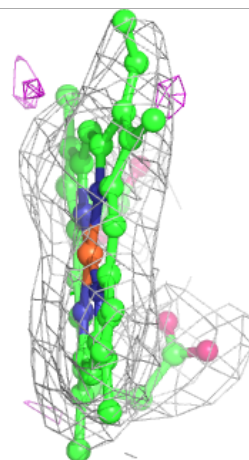
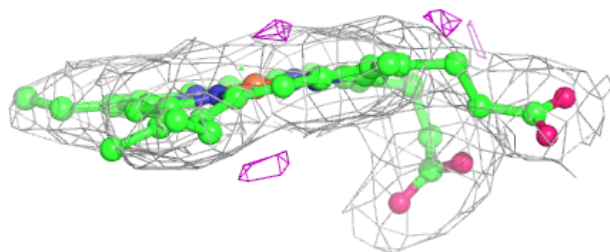
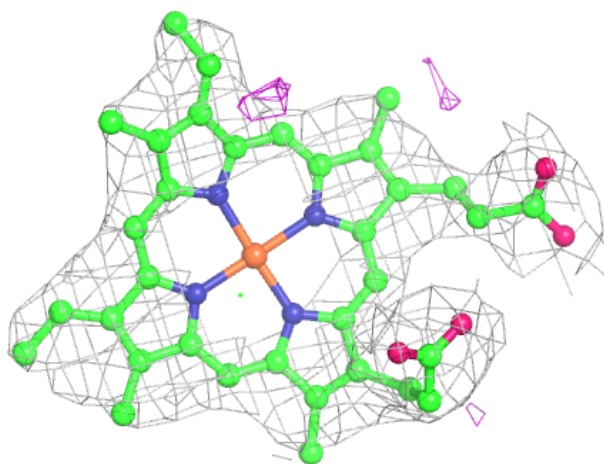
**Electron density around HEM P 501:**

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

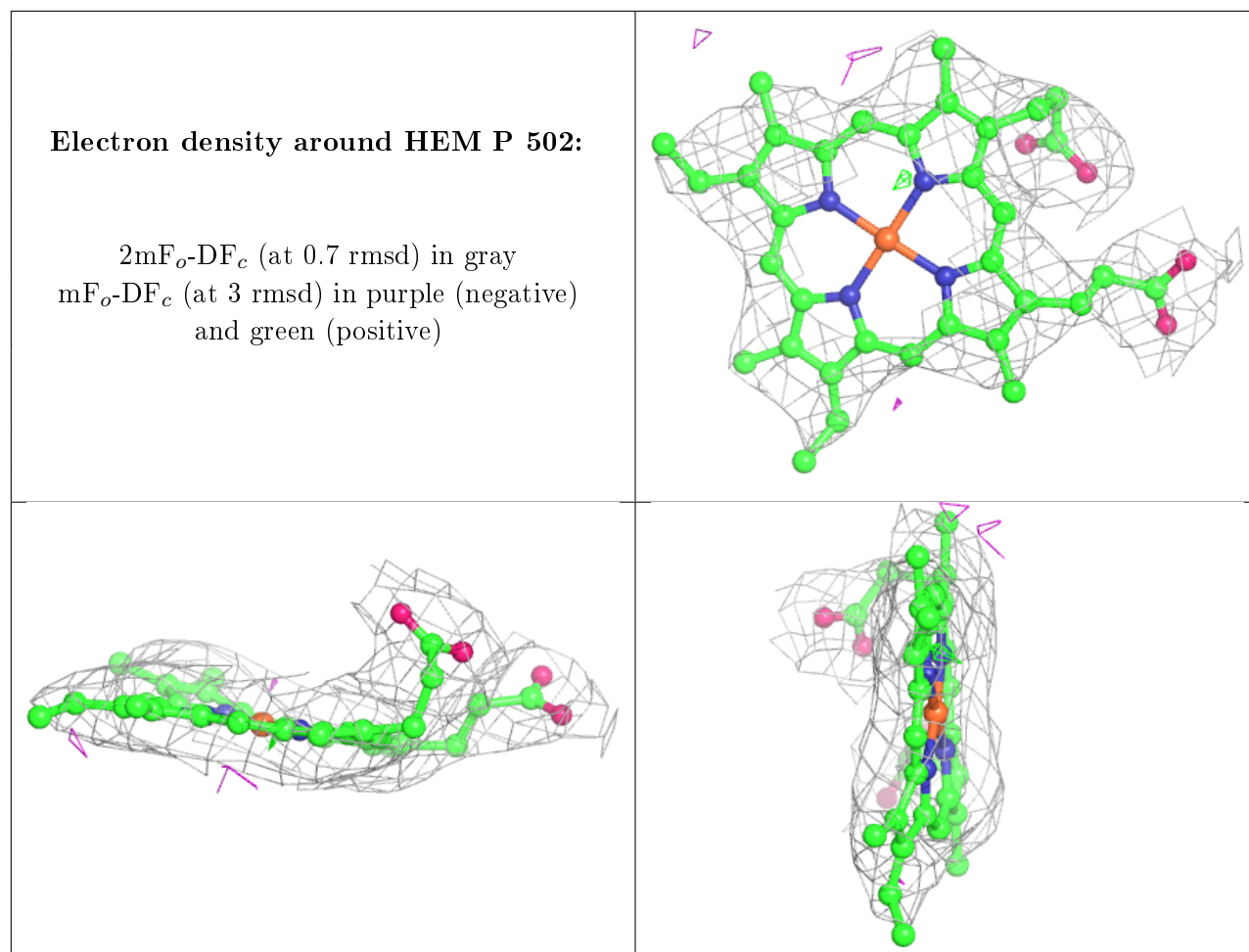


**Electron density around HEM C 502:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.