



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 7, 2024 – 04:09 am GMT

PDB ID : 6HAW  
Title : Crystal structure of bovine cytochrome bc1 in complex with 2-pyrazolyl quinolone inhibitor WDH2G7  
Authors : Amporndanai, K.; Hong, W.D.; O'Neill, P.M.; Hasnain, S.S.; Antonyuk, S.V.  
Deposited on : 2018-08-08  
Resolution : 3.45 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

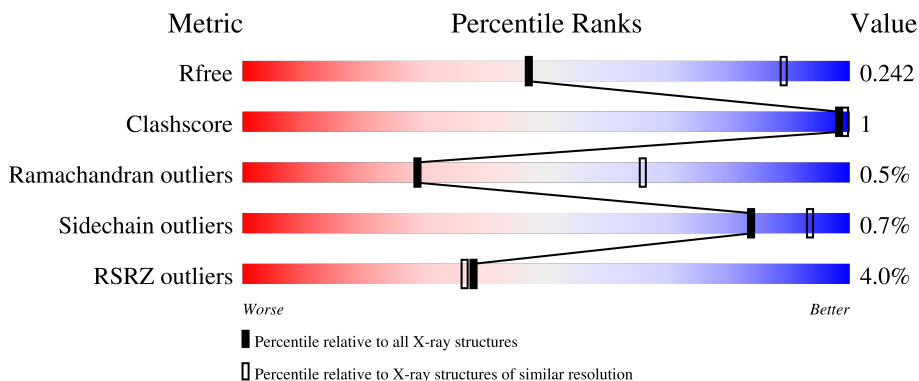
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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.



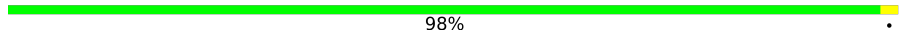
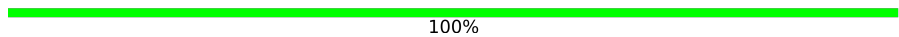
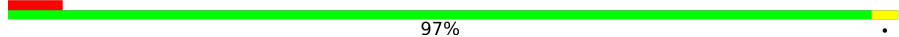

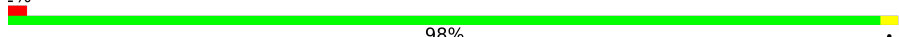
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	
2	B	413	
3	C	378	
4	D	239	
5	E	196	

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Mol	Chain	Length	Quality of chain
6	F	99	 98%
7	G	74	 100%
8	H	64	 97%
9	I	46	 89%
10	J	59	 98%

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
12	PGE	C	407	-	-	-	X
13	PO4	A	503	-	-	-	X
13	PO4	A	504	-	-	-	X
13	PO4	B	501	-	-	-	X
19	PEE	C	405	X	-	-	-
19	PEE	E	204	X	-	-	-
20	FX2	C	406	X	-	-	-

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 16062 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3331	2081	590	640	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P31800
A	?	-	TYR	deletion	UNP P31800
A	?	-	ASP	deletion	UNP P31800
A	?	-	GLU	deletion	UNP P31800
A	?	-	ASP	deletion	UNP P31800
A	?	-	ALA	deletion	UNP P31800

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	413	3073	1931	538	597	7	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P23004
B	?	-	LEU	deletion	UNP P23004
B	?	-	GLY	deletion	UNP P23004
B	?	-	LEU	deletion	UNP P23004
B	?	-	SER	deletion	UNP P23004

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	378	2996	2007	471	500	18	0	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	239	1851	1181	322	333	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1450	907	254	282	7	0	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	99	853	542	153	156	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	74	612	400	113	98	1	0	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	64	490	297	84	104	5	0	0	0

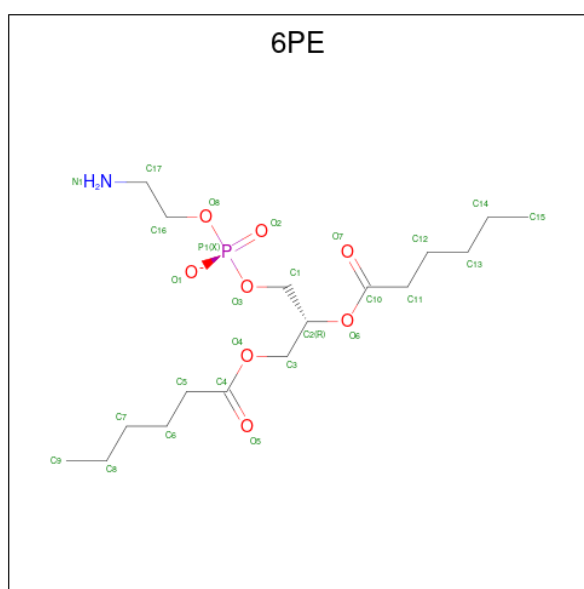
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	46	322	201	63	57	1	0	0	0

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	59	487	320	84	83	0	0	0

- Molecule 11 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula:  $C_{17}H_{33}NO_8P$ ).



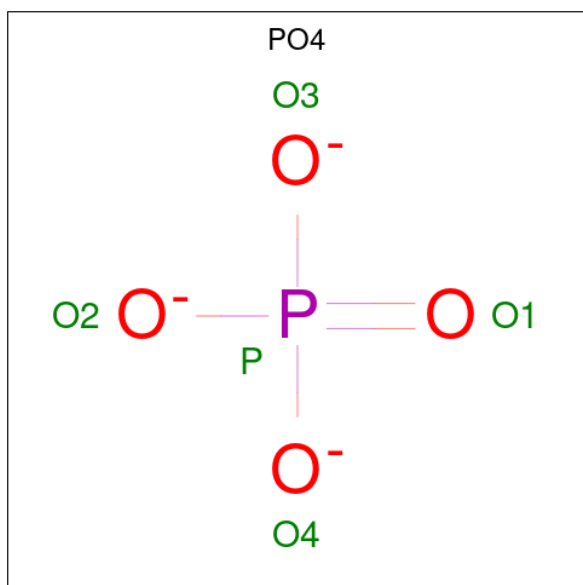
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	A	1	23	13	1	8	1	0	0

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



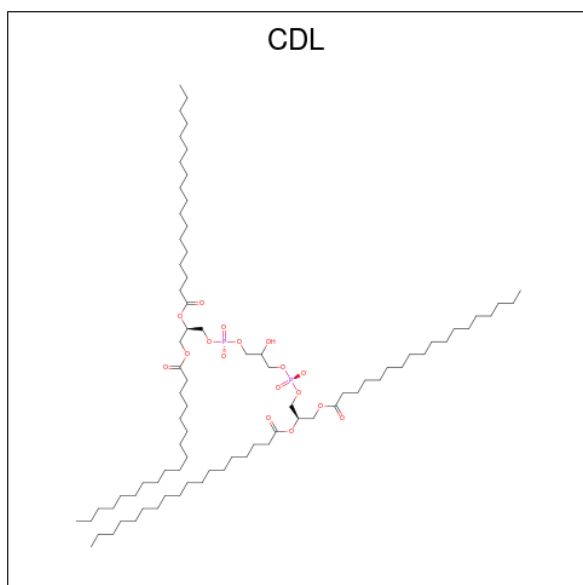
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	P	0	0
			5	4	1		
13	A	1	Total	O	P	0	0
			5	4	1		
13	A	1	Total	O	P	0	0
			5	4	1		
13	B	1	Total	O	P	0	0
			5	4	1		
13	D	1	Total	O	P	0	0
			5	4	1		
13	E	1	Total	O	P	0	0
			5	4	1		
13	F	1	Total	O	P	0	0
			5	4	1		
13	F	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			34	17	15	2		

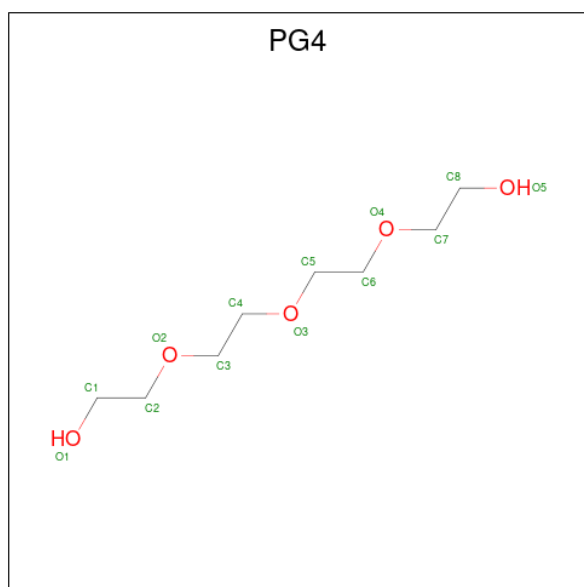
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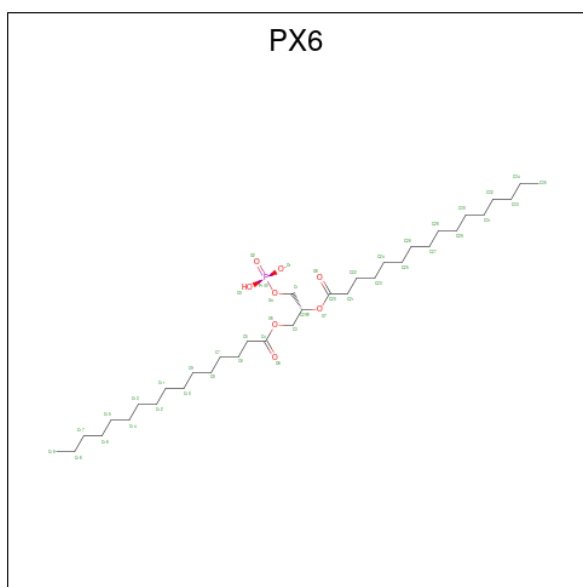
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
14	C	1	38	19	17	2	0	0
14	D	1	27	12	13	2	0	0
14	E	1	28	13	13	2	0	0

- Molecule 15 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



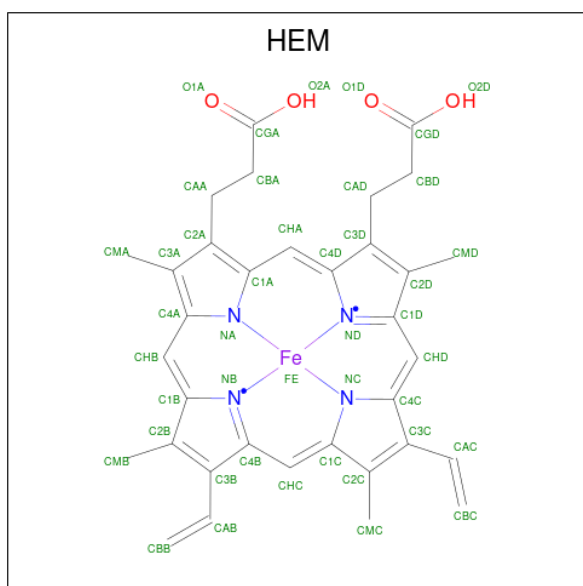
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	B	1	13	8	5	0	0

- Molecule 16 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	C	O	P	0	0
			17	9	7	1		
16	C	1	Total	C	O	P	0	0
			14	6	7	1		

- Molecule 17 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



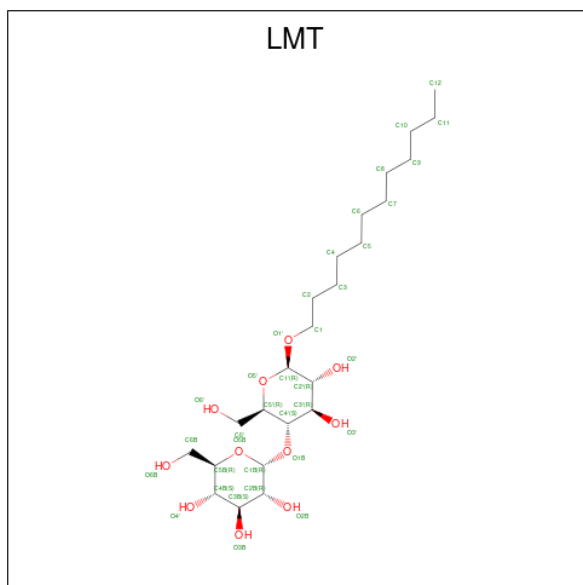
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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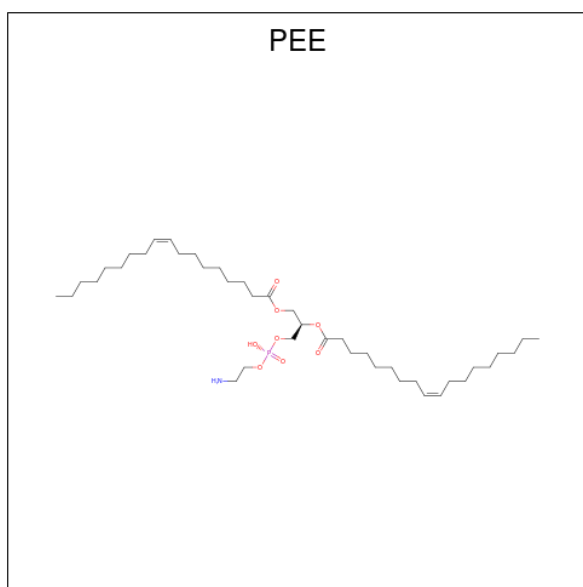
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
17	C	1	43	34	1	4	4	0	0

- Molecule 18 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



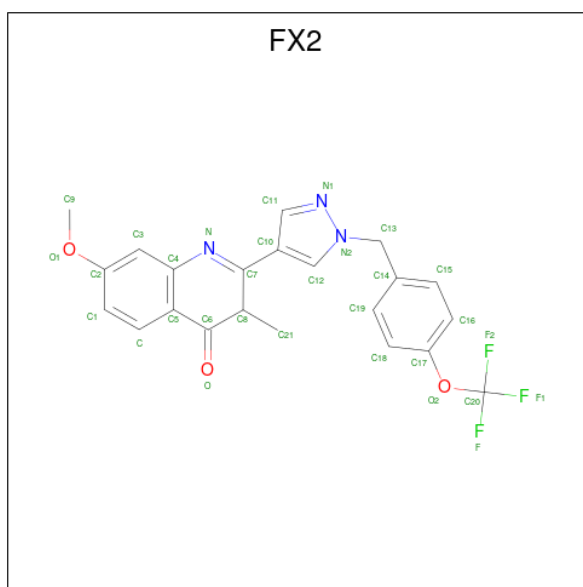
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	C	1	35	24	11	0	0

- Molecule 19 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



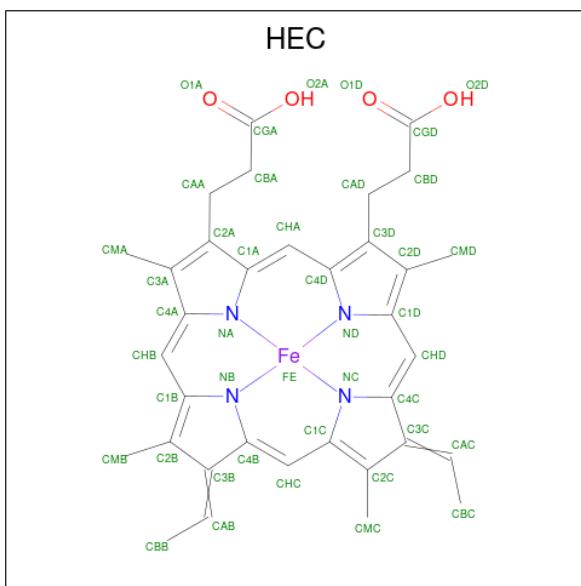
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
19	C	1	34	24	1	8	1	0	0
19	E	1	20	10	1	8	1	0	0

- Molecule 20 is 7-methoxy-3-methyl-2-[1-[[4-(trifluoromethoxy)phenyl]methyl]pyrazol-4-yl]-3 {H}-quinolin-4-one (three-letter code: FX2) (formula: C<sub>22</sub>H<sub>18</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



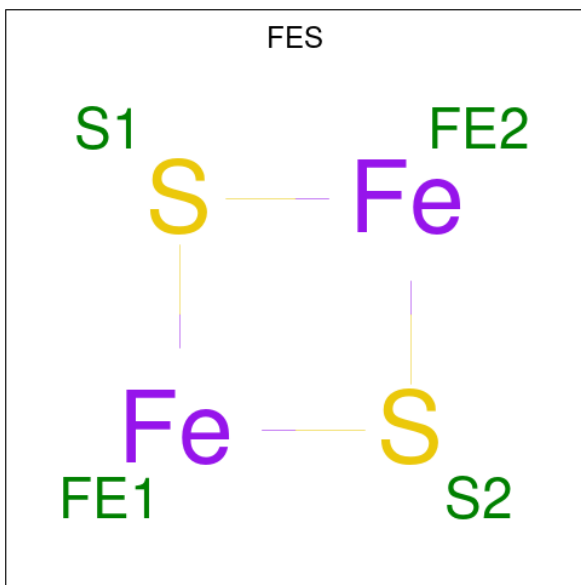
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
20	C	1	31	22	3	3	3	0	0

- Molecule 21 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

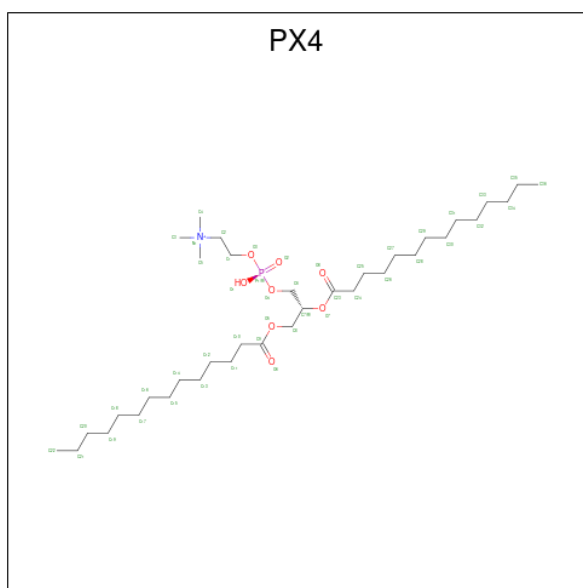
- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

- Molecule 23 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter

code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	E	1	Total	C	N	O	P	0	0
			28	18	1	8	1		

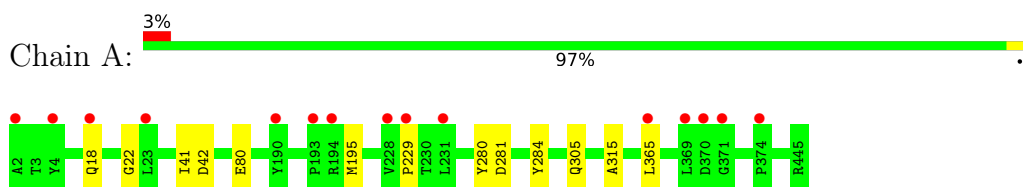
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	10	Total	O	0	0
			10	10		
24	B	4	Total	O	0	0
			4	4		
24	C	8	Total	O	0	0
			8	8		
24	D	4	Total	O	0	0
			4	4		
24	E	2	Total	O	0	0
			2	2		
24	H	1	Total	O	0	0
			1	1		
24	J	1	Total	O	0	0
			1	1		

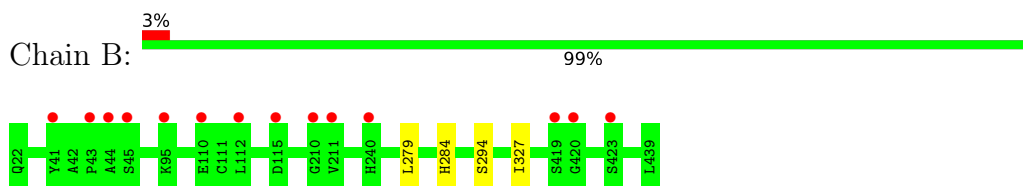
### 3 Residue-property plots [i](#)

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

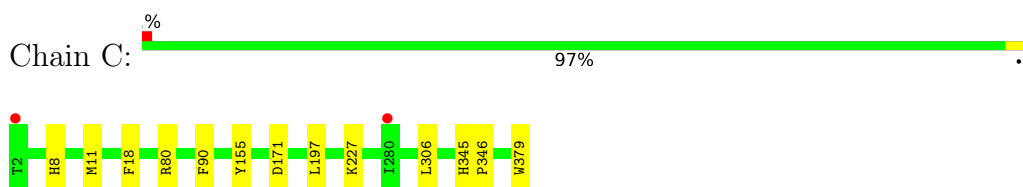
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



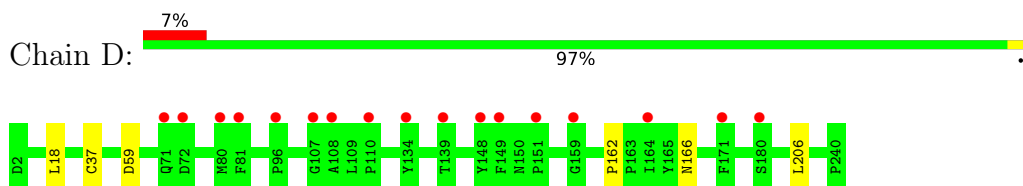
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



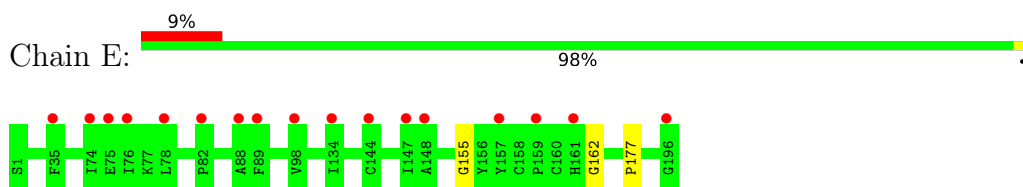
- Molecule 3: Cytochrome b



- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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



- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:  98%



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:  100%


There are no outlier residues recorded for this chain.

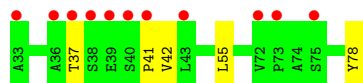
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:  6% 97%



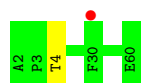
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:  24% 89% 11%



- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:  2% 98%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.69Å 212.69Å 347.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.10 – 3.45 92.10 – 3.45	Depositor EDS
% Data completeness (in resolution range)	89.2 (92.10-3.45) 89.2 (92.10-3.45)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.49Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.210 , 0.242 0.209 , 0.242	Depositor DCC
$R_{free}$ test set	2762 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.3	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	16062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: PG4, LMT, CDL, FX2, FES, HEM, HEC, PO4, PGE, 6PE, PEE, PX4, PX6

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	0/3400	0.64	0/4620
2	B	0.43	0/3128	0.63	0/4248
3	C	0.47	0/3092	0.61	0/4231
4	D	0.43	0/1910	0.61	0/2601
5	E	0.45	0/1482	0.62	0/2014
6	F	0.42	0/872	0.65	0/1174
7	G	0.51	0/633	0.65	0/859
8	H	0.39	0/495	0.66	0/670
9	I	0.53	0/326	0.87	0/445
10	J	0.46	0/500	0.64	0/675
All	All	0.44	0/15838	0.63	0/21537

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

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	3331	0	3189	5	0
2	B	3073	0	3020	3	0
3	C	2996	0	3058	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1851	0	1749	5	0
5	E	1450	0	1357	0	0
6	F	853	0	825	1	0
7	G	612	0	601	0	0
8	H	490	0	433	1	0
9	I	322	0	317	2	0
10	J	487	0	487	0	0
11	A	23	0	19	2	0
12	A	7	0	9	0	0
12	C	30	0	42	0	0
13	A	15	0	0	0	0
13	B	5	0	0	0	0
13	D	5	0	0	0	0
13	E	5	0	0	0	0
13	F	10	0	0	0	0
13	G	15	0	0	0	0
14	A	34	0	24	2	0
14	C	38	0	20	0	0
14	D	27	0	15	0	0
14	E	28	0	17	0	0
15	B	13	0	18	0	0
16	B	17	0	14	0	0
16	C	14	0	8	0	0
17	C	86	0	60	2	0
18	C	35	0	46	0	0
19	C	34	0	42	0	0
19	E	20	0	14	0	0
20	C	31	0	0	0	0
21	D	43	0	32	3	0
22	E	4	0	0	0	0
23	E	28	0	30	0	0
24	A	10	0	0	0	0
24	B	4	0	0	0	0
24	C	8	0	0	0	0
24	D	4	0	0	0	0
24	E	2	0	0	0	0
24	H	1	0	0	0	0
24	J	1	0	0	0	0
All	All	16062	0	15446	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 20 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)
4:D:37:CYS:SG	21:D:501:HEC:CAB	2.88	0.61
1:A:18:GLN:HE21	1:A:22:GLY:HA2	1.68	0.58
4:D:37:CYS:SG	21:D:501:HEC:HBB3	2.44	0.58
17:C:401:HEM:HBC2	17:C:401:HEM:HMC1	1.88	0.56
11:A:501:6PE:H28	14:A:506:CDL:HB31	1.94	0.49

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	434/438 (99%)	420 (97%)	12 (3%)	2 (0%)	29	66
2	B	409/413 (99%)	396 (97%)	13 (3%)	0	100	100
3	C	376/378 (100%)	362 (96%)	13 (4%)	1 (0%)	41	75
4	D	237/239 (99%)	227 (96%)	9 (4%)	1 (0%)	34	70
5	E	194/196 (99%)	184 (95%)	7 (4%)	3 (2%)	10	43
6	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
7	G	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
8	H	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
9	I	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	20
10	J	57/59 (97%)	54 (95%)	2 (4%)	1 (2%)	8	39
All	All	1982/2006 (99%)	1905 (96%)	67 (3%)	10 (0%)	29	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	37	THR

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Mol	Chain	Res	Type
9	I	41	PRO
1	A	315	ALA
3	C	155	TYR
5	E	177	PRO

### 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	347/363 (96%)	344 (99%)	3 (1%)	78	91
2	B	318/324 (98%)	318 (100%)	0	100	100
3	C	325/326 (100%)	318 (98%)	7 (2%)	52	77
4	D	190/204 (93%)	189 (100%)	1 (0%)	88	95
5	E	149/168 (89%)	149 (100%)	0	100	100
6	F	87/91 (96%)	87 (100%)	0	100	100
7	G	63/66 (96%)	63 (100%)	0	100	100
8	H	53/61 (87%)	53 (100%)	0	100	100
9	I	30/38 (79%)	29 (97%)	1 (3%)	38	68
10	J	49/49 (100%)	49 (100%)	0	100	100
All	All	1611/1690 (95%)	1599 (99%)	12 (1%)	84	93

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	227	LYS
3	C	306	LEU
9	I	78	TYR
3	C	379	TRP
3	C	18	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	166	ASN
4	D	225	HIS
5	E	121	GLN
5	E	100	HIS
3	C	322	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

32 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
13	PO4	G	101	-	4,4,4	0.91	0	6,6,6	0.27	0
13	PO4	A	504	-	4,4,4	0.97	0	6,6,6	0.42	0
14	CDL	A	506	-	33,33,99	1.23	2 (6%)	37,43,111	1.20	3 (8%)
12	PGE	A	502	-	6,6,9	0.55	0	5,5,8	0.31	0
12	PGE	C	409	-	9,9,9	0.47	0	8,8,8	0.23	0
13	PO4	F	501	-	4,4,4	0.89	0	6,6,6	0.46	0
14	CDL	E	205	-	27,27,99	1.20	2 (7%)	32,36,111	1.44	6 (18%)
13	PO4	A	505	-	4,4,4	0.98	0	6,6,6	0.43	0
18	LMT	C	403	-	36,36,36	0.66	1 (2%)	47,47,47	0.86	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	PGE	C	408	-	9,9,9	0.44	0	8,8,8	0.29	0
13	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.39	0
16	PX6	B	503	-	16,16,43	1.25	1 (6%)	19,20,48	1.43	2 (10%)
17	HEM	C	401	3	41,50,50	1.35	6 (14%)	45,82,82	1.59	10 (22%)
11	6PE	A	501	-	22,22,26	1.54	2 (9%)	25,27,31	1.35	3 (12%)
13	PO4	B	501	-	4,4,4	0.90	0	6,6,6	0.50	0
14	CDL	C	404	-	37,37,99	1.65	4 (10%)	43,49,111	1.39	4 (9%)
12	PGE	C	407	-	9,9,9	0.50	0	8,8,8	0.36	0
19	PEE	E	204	-	19,19,50	1.42	2 (10%)	22,24,55	1.36	2 (9%)
13	PO4	F	502	-	4,4,4	0.99	0	6,6,6	0.35	0
20	FX2	C	406	-	30,34,34	1.76	5 (16%)	39,50,50	1.16	5 (12%)
23	PX4	E	202	-	27,27,45	1.40	2 (7%)	33,35,53	1.31	4 (12%)
13	PO4	D	502	-	4,4,4	0.92	0	6,6,6	0.34	0
15	PG4	B	502	-	12,12,12	0.50	0	11,11,11	0.18	0
19	PEE	C	405	-	33,33,50	1.38	3 (9%)	36,38,55	1.17	2 (5%)
16	PX6	C	410	-	13,13,43	1.27	1 (7%)	16,17,48	1.26	2 (12%)
17	HEM	C	402	3	41,50,50	1.32	6 (14%)	45,82,82	1.49	7 (15%)
21	HEC	D	501	4	32,50,50	2.47	12 (37%)	24,82,82	2.27	6 (25%)
22	FES	E	201	-	0,4,4	-	-	-	-	-
13	PO4	G	102	-	4,4,4	0.89	0	6,6,6	0.46	0
14	CDL	D	503	-	26,26,99	1.45	2 (7%)	31,35,111	1.31	4 (12%)
13	PO4	G	103	-	4,4,4	0.89	0	6,6,6	0.51	0
13	PO4	E	203	-	4,4,4	0.97	0	6,6,6	0.57	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	A	506	-	-	15/41/41/110	-
12	PGE	A	502	-	-	3/4/4/7	-
12	PGE	C	409	-	-	4/7/7/7	-
14	CDL	E	205	-	-	19/31/31/110	-
18	LMT	C	403	-	-	8/21/61/61	0/2/2/2
12	PGE	C	408	-	-	3/7/7/7	-
16	PX6	B	503	-	-	7/17/17/45	-
17	HEM	C	401	3	-	5/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	6PE	A	501	-	-	11/26/26/30	-
14	CDL	C	404	-	-	19/46/46/110	-
12	PGE	C	407	-	-	5/7/7/7	-
19	PEE	E	204	-	1/1/4/8	13/22/22/54	-
20	FX2	C	406	-	1/1/4/4	2/11/31/31	0/3/4/4
23	PX4	E	202	-	-	17/31/31/49	-
15	PG4	B	502	-	-	7/10/10/10	-
19	PEE	C	405	-	1/1/4/8	14/37/37/54	-
16	PX6	C	410	-	-	9/13/13/45	-
17	HEM	C	402	3	-	2/12/54/54	-
21	HEC	D	501	4	-	2/10/54/54	-
22	FES	E	201	-	-	-	0/1/1/1
14	CDL	D	503	-	-	18/31/31/110	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C3C-C2C	7.55	1.48	1.40
20	C	406	FX2	C5-C4	6.99	1.49	1.40
21	D	501	HEC	C2B-C3B	6.47	1.47	1.40
14	C	404	CDL	OA6-CA5	5.32	1.47	1.35
14	C	404	CDL	OB6-CB5	5.10	1.48	1.34

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	501	HEC	C1D-C2D-C3D	-6.26	102.64	107.00
23	E	202	PX4	O7-C23-C24	5.06	122.40	111.50
21	D	501	HEC	CMC-C2C-C3C	4.74	131.39	125.82
14	C	404	CDL	OA6-CA5-C11	4.71	119.76	111.09
14	A	506	CDL	OB6-CB5-C51	4.57	121.35	111.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	C	405	PEE	C2
19	E	204	PEE	C2
20	C	406	FX2	C8



5 of 183 torsion outliers are listed below:

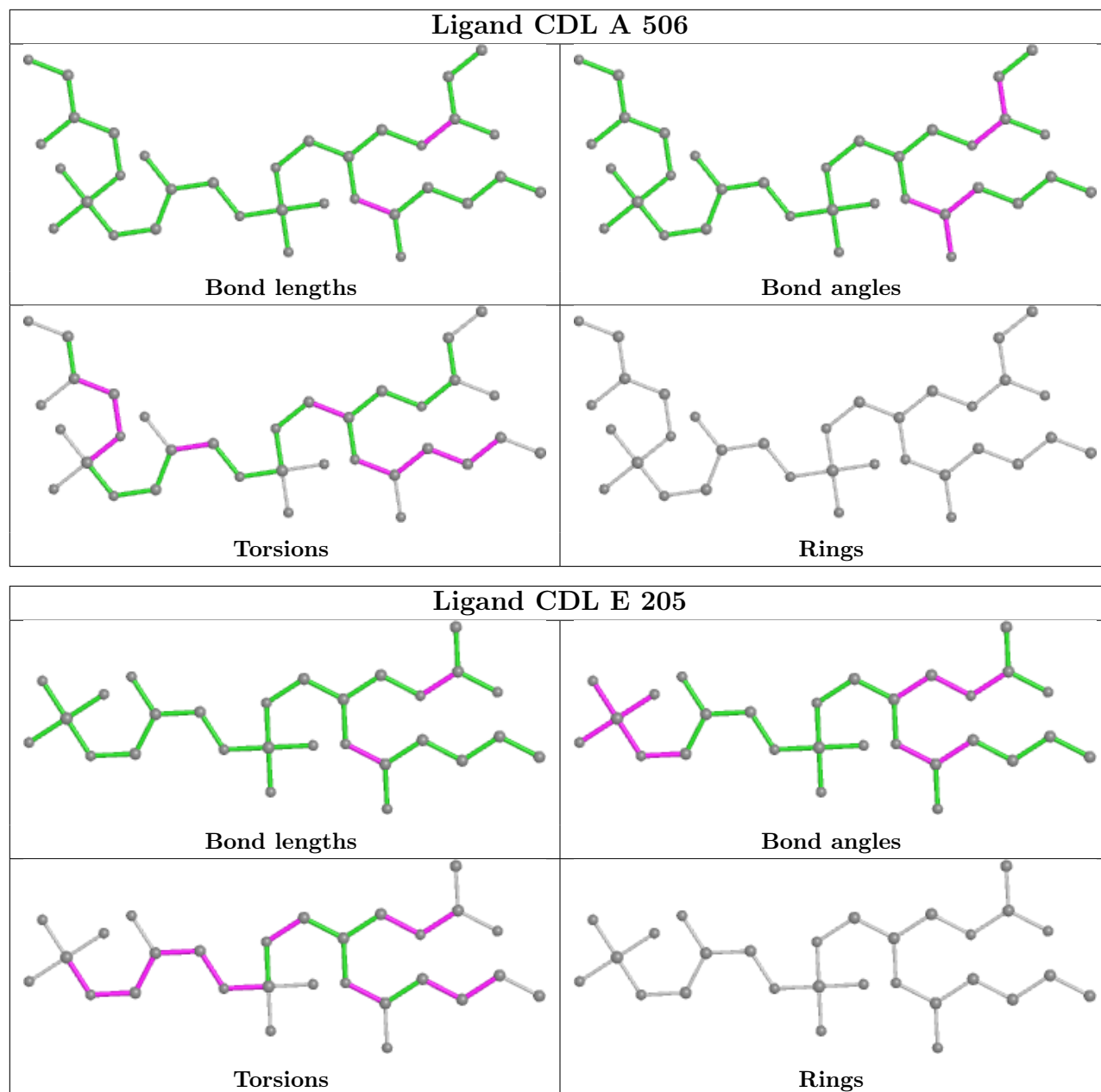
Mol	Chain	Res	Type	Atoms
11	A	501	6PE	C1-O3-P1-O1
11	A	501	6PE	C11-C10-O6-C2
11	A	501	6PE	O8-C16-C17-N1
14	A	506	CDL	C51-CB5-OB6-CB4
14	C	404	CDL	CA3-OA5-PA1-OA4

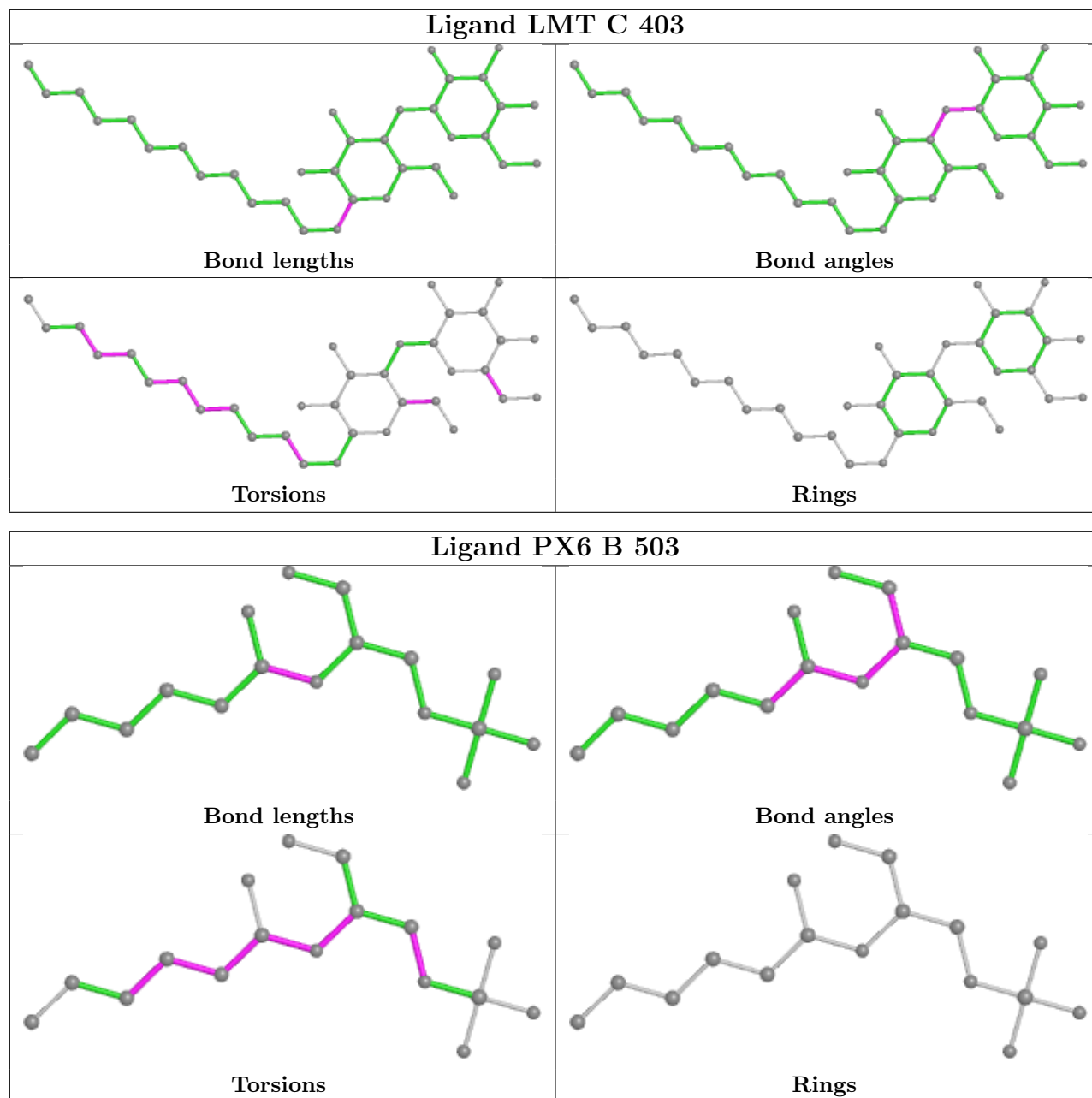
There are no ring outliers.

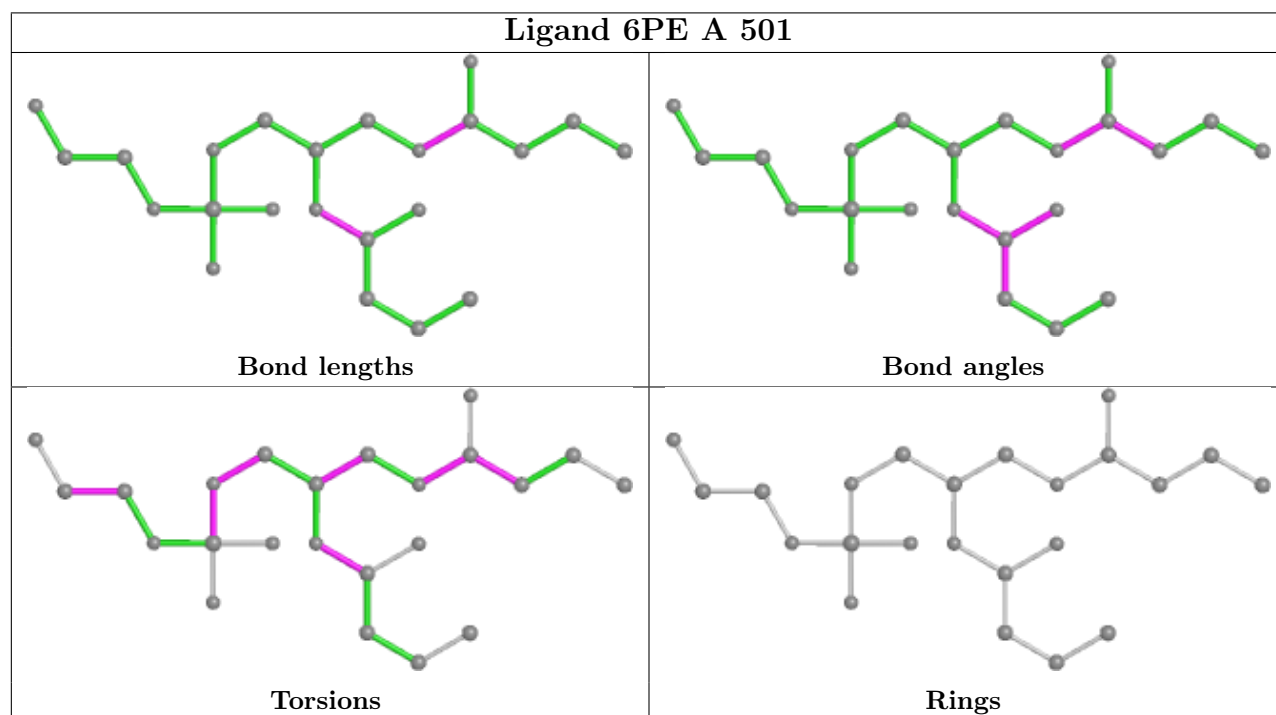
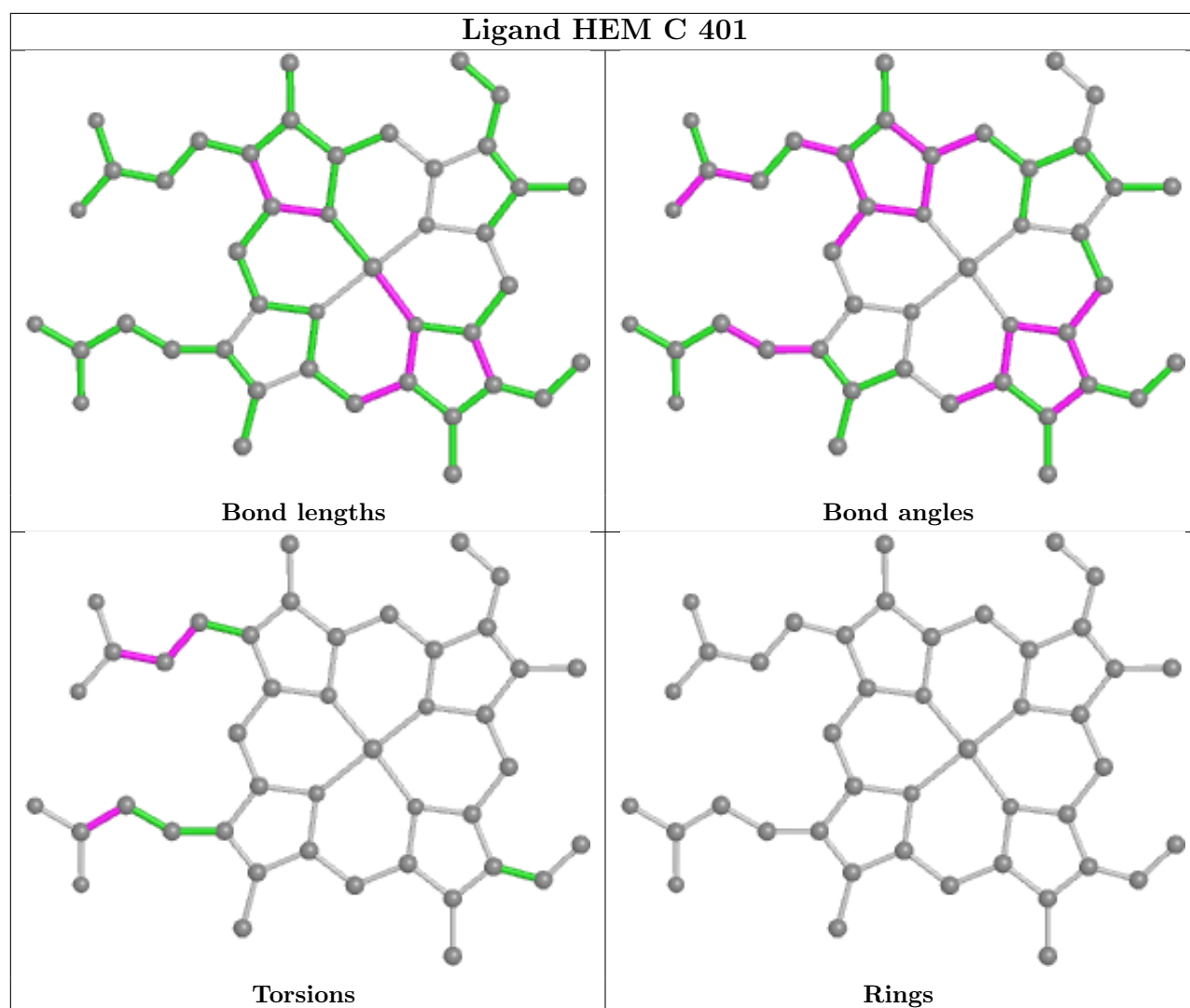
5 monomers are involved in 7 short contacts:

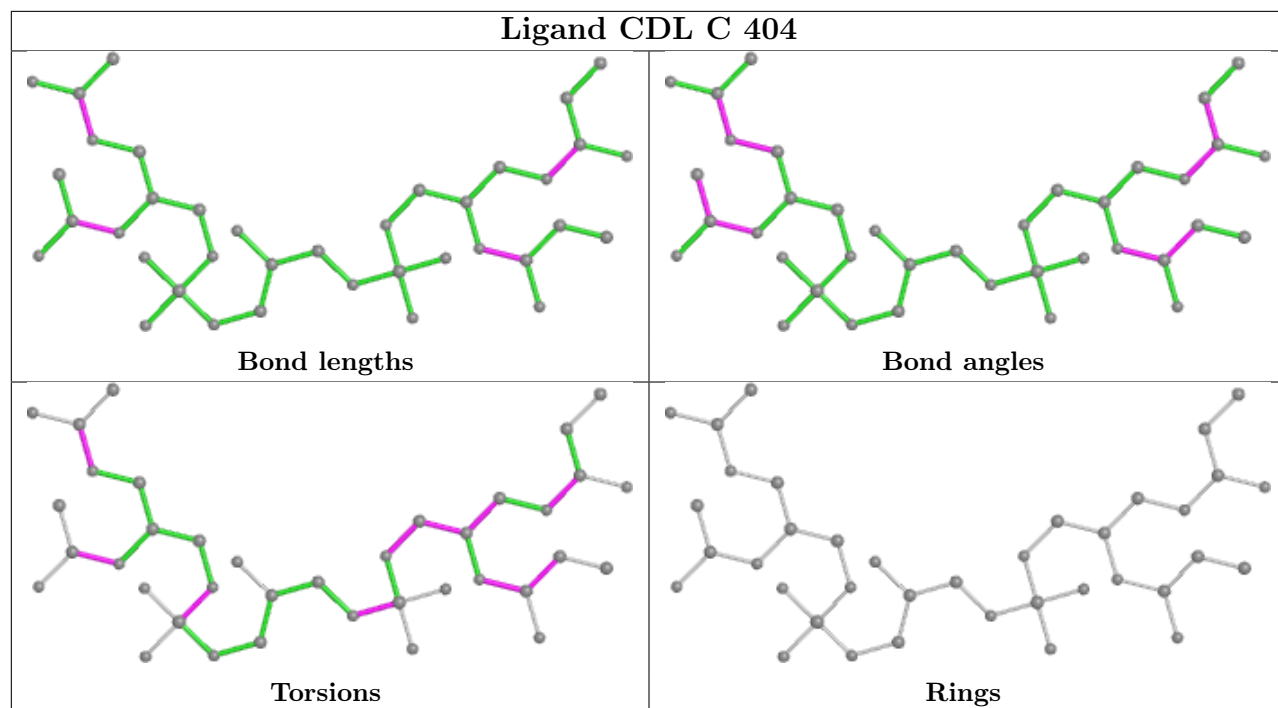
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	506	CDL	2	0
17	C	401	HEM	1	0
11	A	501	6PE	2	0
17	C	402	HEM	1	0
21	D	501	HEC	3	0

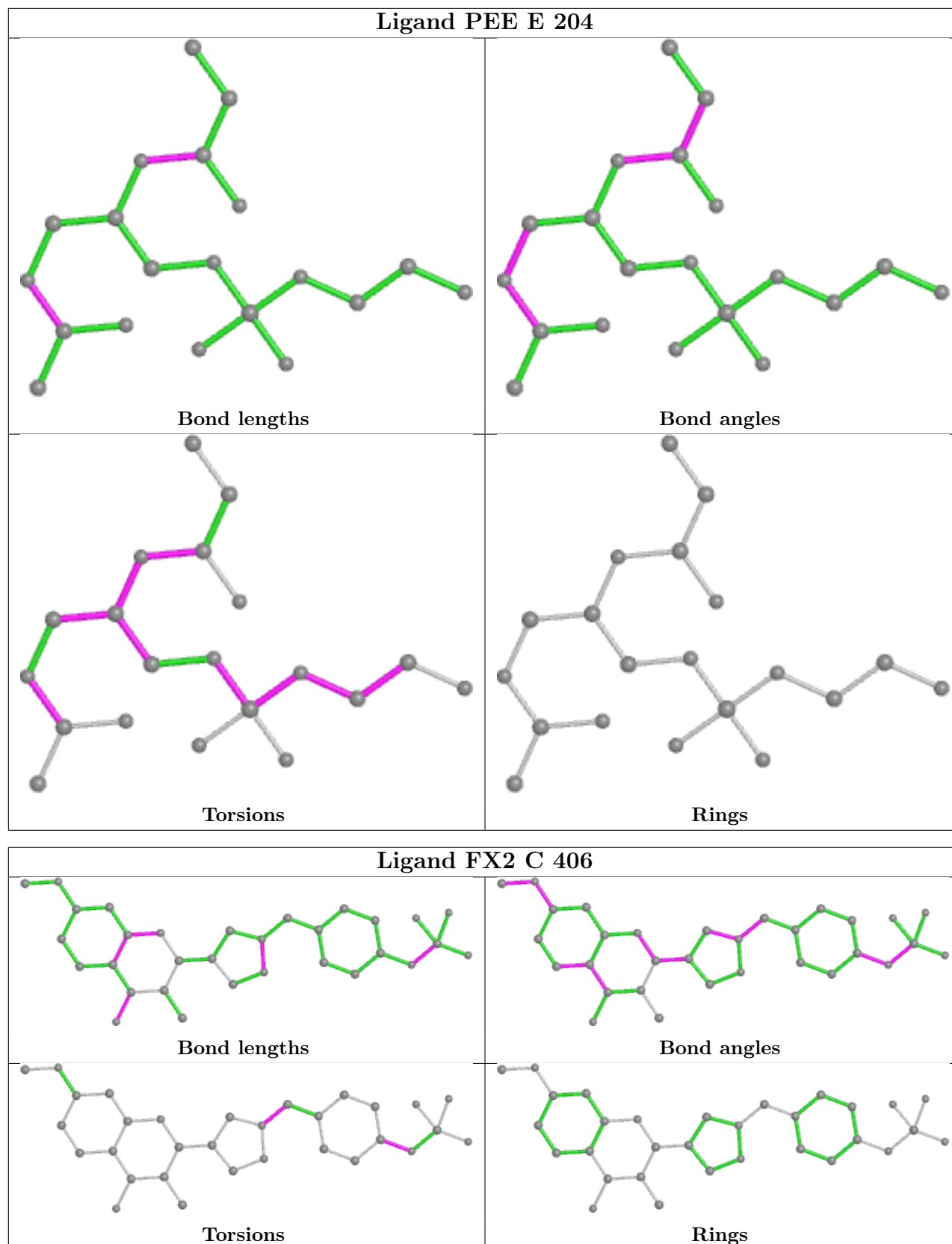
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

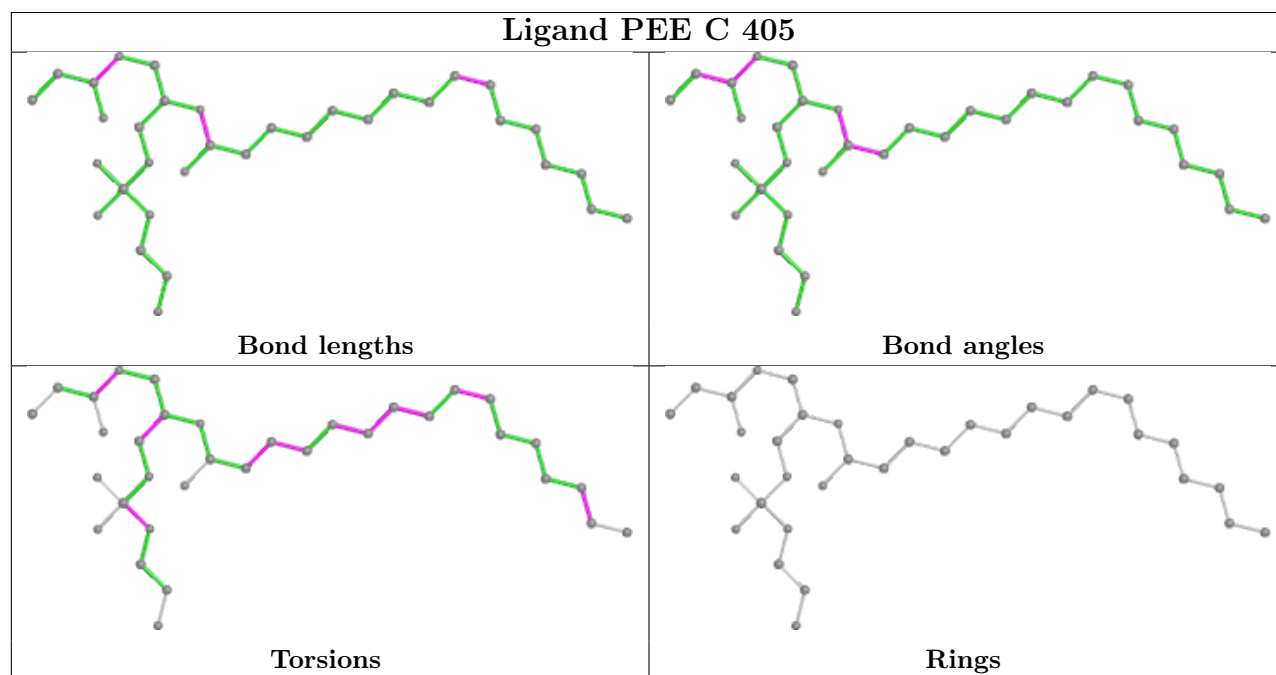
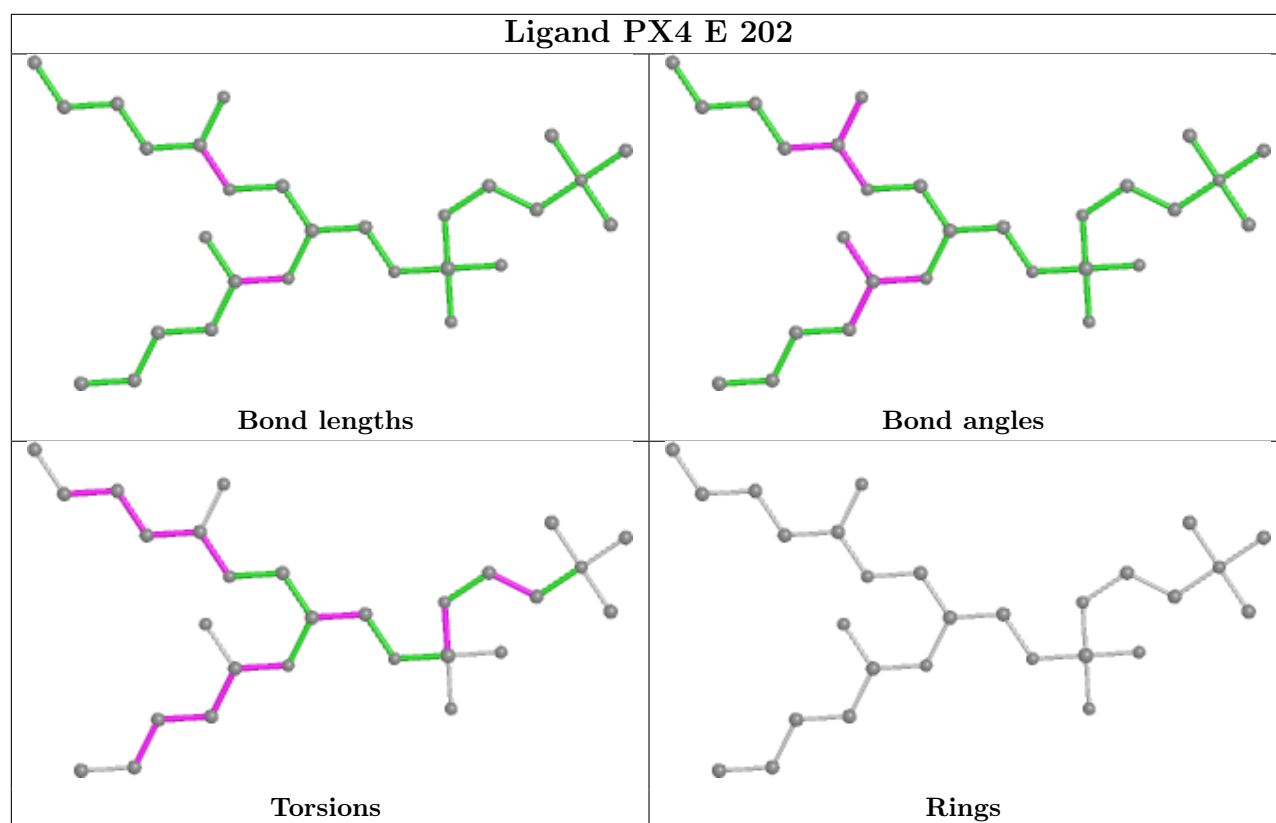


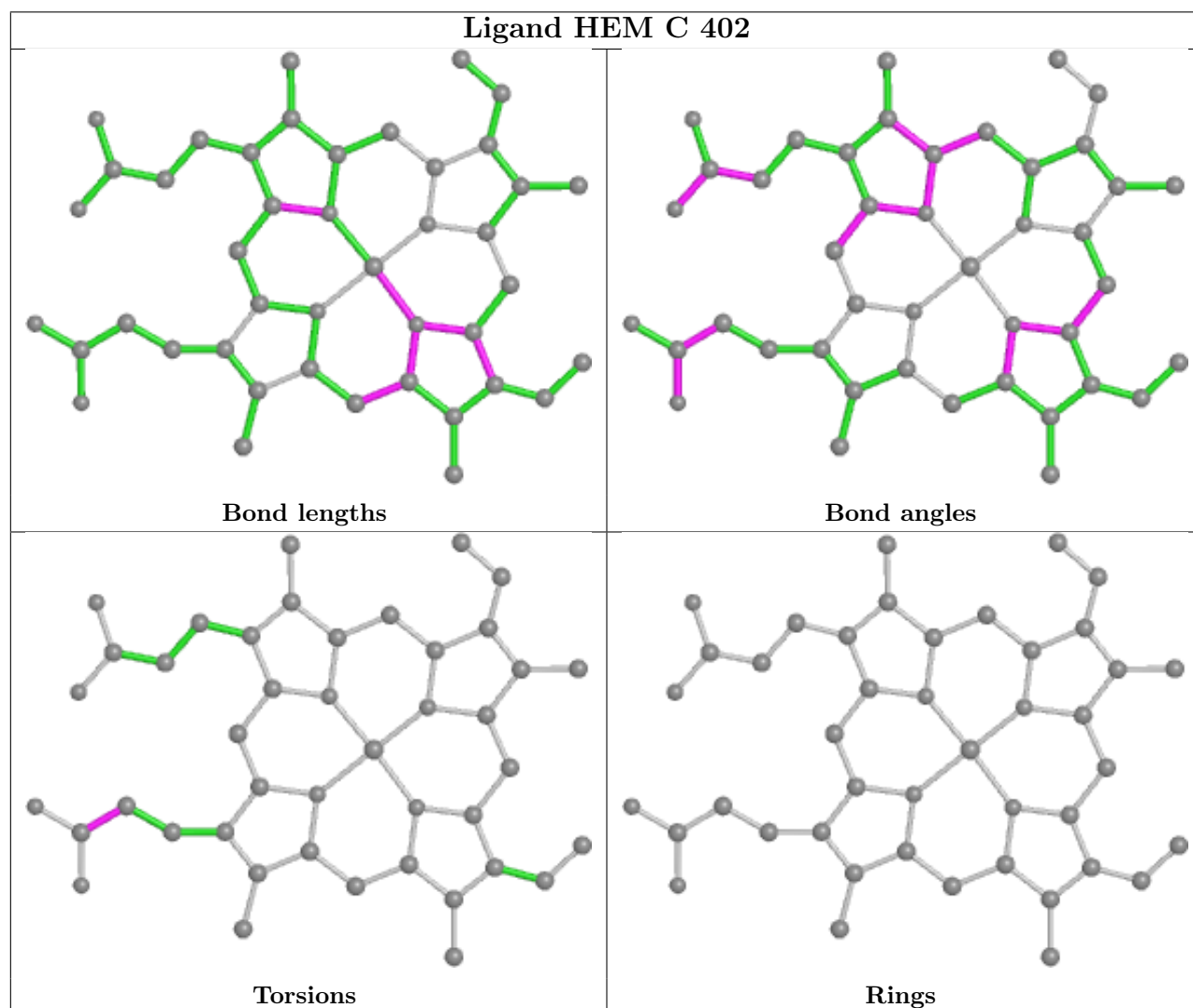
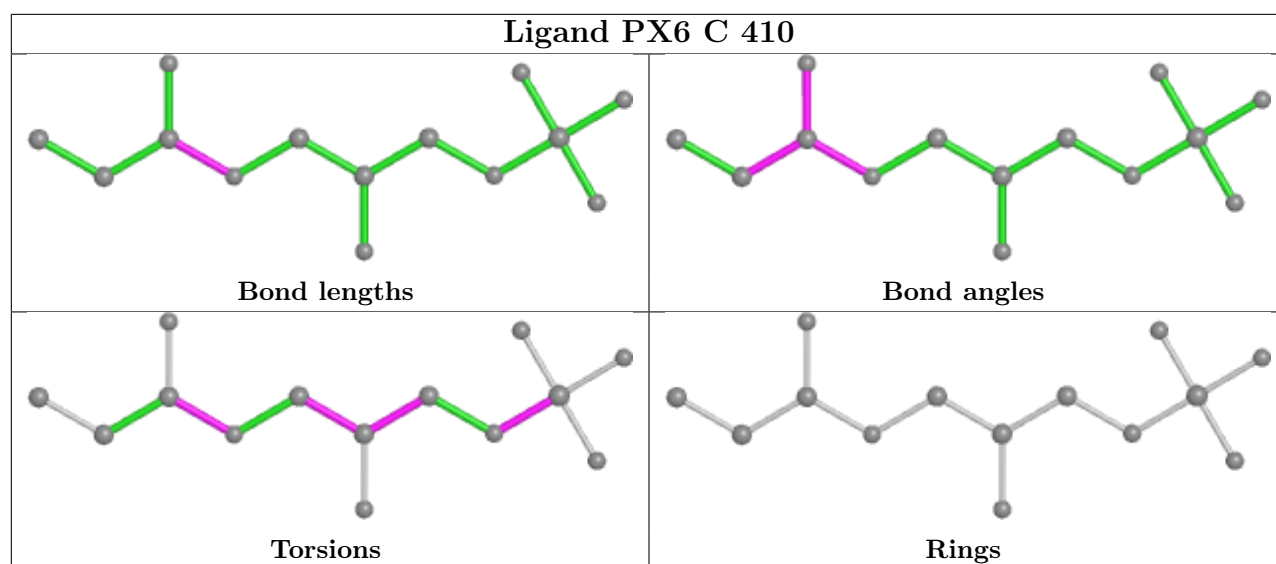




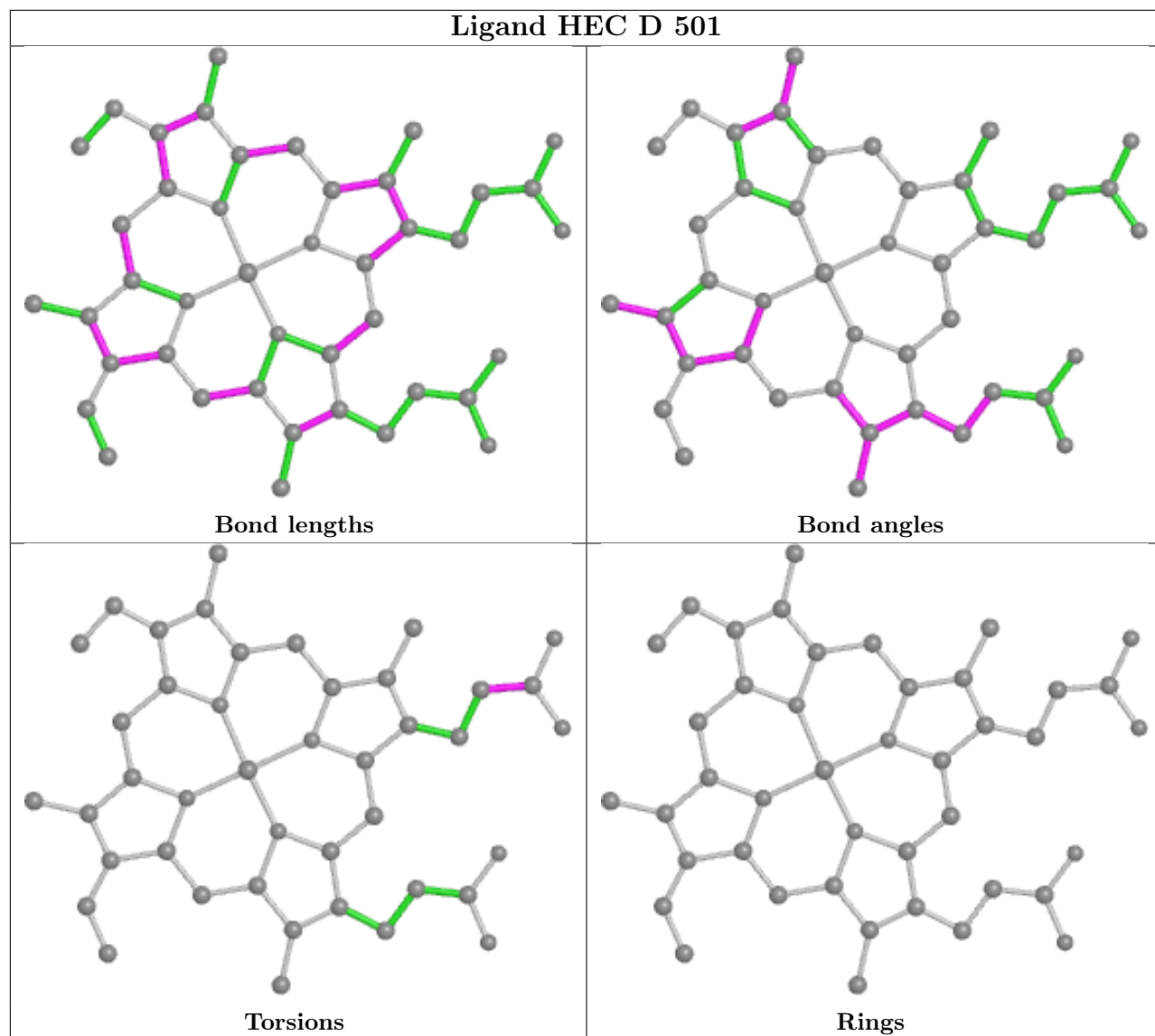


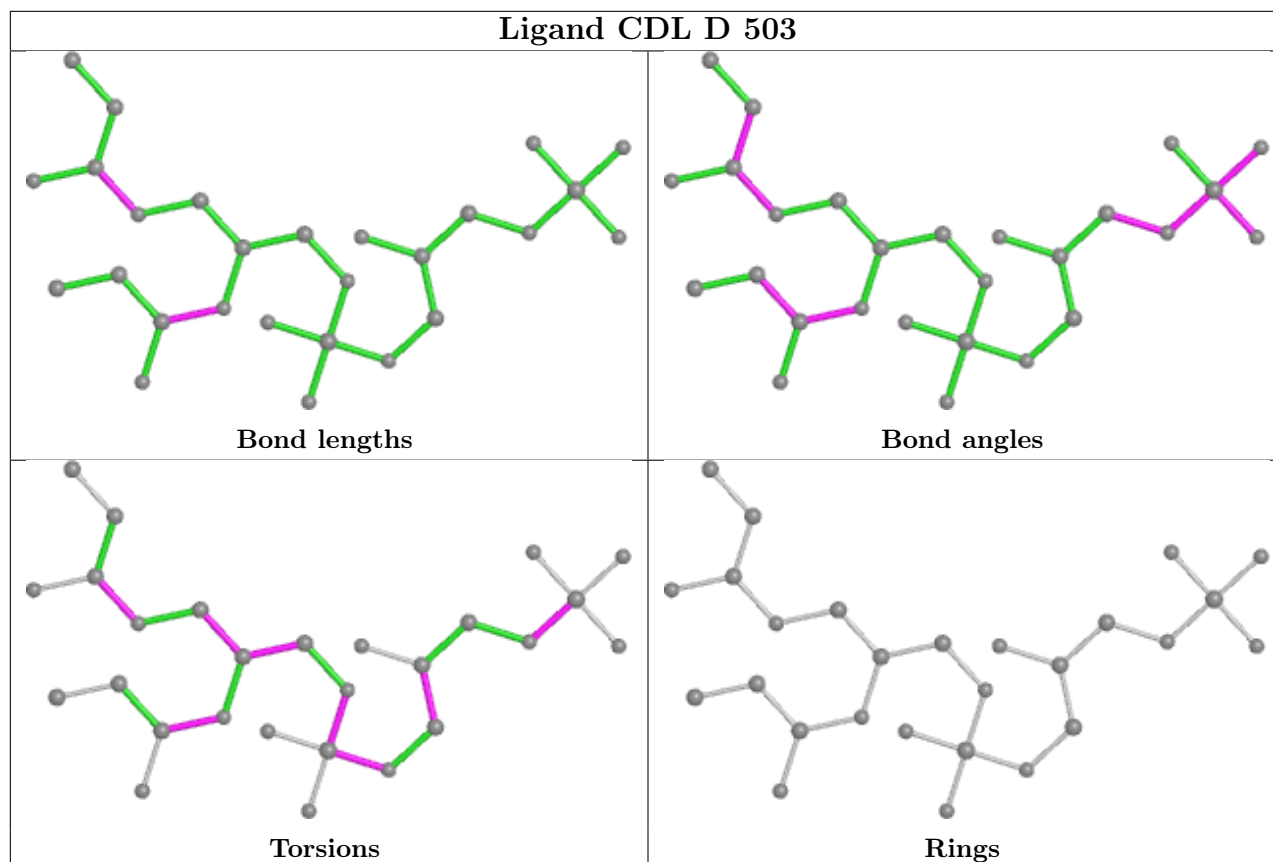












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	229:GLY	C	235:ALA	N	11.37
1	A	221:GLY	C	228:VAL	N	9.55

## 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	438/438 (100%)	0.19	15 (3%) 45 43	60, 93, 119, 131	0
2	B	413/413 (100%)	0.23	14 (3%) 45 43	71, 96, 122, 143	0
3	C	378/378 (100%)	0.01	2 (0%) 91 89	63, 84, 117, 146	0
4	D	239/239 (100%)	0.43	17 (7%) 16 18	73, 116, 143, 153	0
5	E	196/196 (100%)	0.35	17 (8%) 10 13	68, 138, 182, 215	0
6	F	99/99 (100%)	0.02	0 100 100	67, 87, 120, 166	0
7	G	74/74 (100%)	0.09	0 100 100	68, 93, 135, 142	0
8	H	64/64 (100%)	0.44	4 (6%) 20 20	111, 138, 151, 159	0
9	I	46/46 (100%)	1.15	11 (23%) 0 0	116, 128, 149, 154	0
10	J	59/59 (100%)	0.11	1 (1%) 70 67	79, 101, 139, 158	0
All	All	2006/2006 (100%)	0.22	81 (4%) 38 36	60, 98, 149, 215	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	4.8
4	D	108	ALA	4.6
5	E	89	PHE	4.5
5	E	144	CYS	4.1
1	A	228	VAL	3.8

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

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

### 6.3 Carbohydrates [i](#)

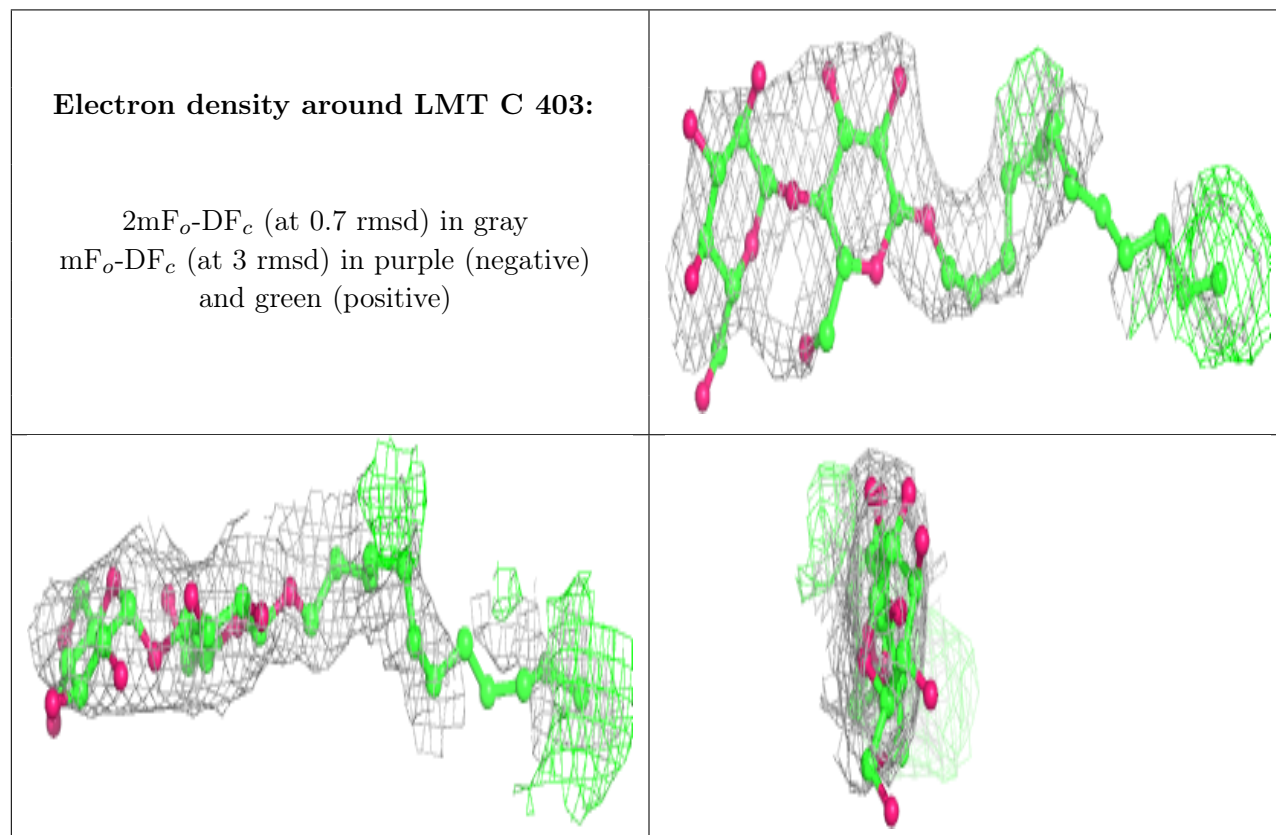
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

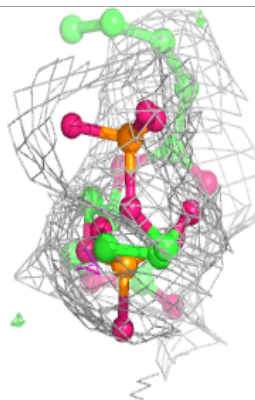
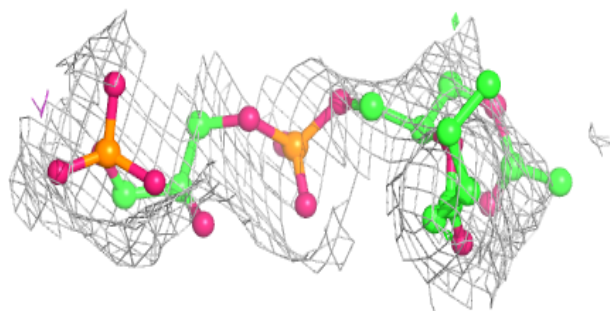
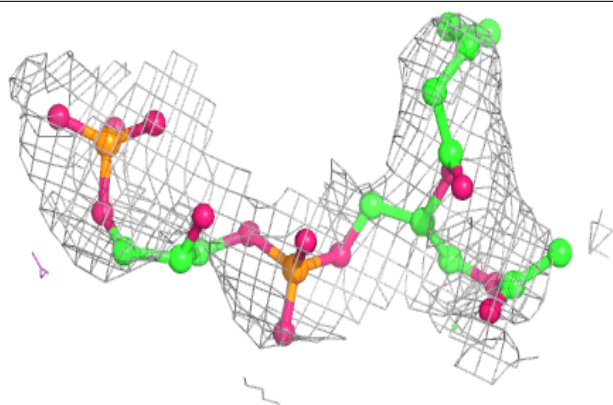
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	PO4	D	502	5/5	0.61	0.24	185,185,186,187	0
18	LMT	C	403	35/35	0.63	0.36	147,181,189,191	0
13	PO4	G	102	5/5	0.65	0.22	169,170,172,179	0
13	PO4	B	501	5/5	0.66	0.58	162,162,164,168	0
14	CDL	E	205	28/100	0.68	0.25	147,195,219,228	0
13	PO4	A	503	5/5	0.71	0.41	144,147,149,150	0
16	PX6	C	410	14/44	0.72	0.34	128,153,171,175	0
12	PGE	A	502	7/10	0.72	0.24	90,91,93,94	0
13	PO4	E	203	5/5	0.73	0.31	164,165,170,170	0
16	PX6	B	503	17/44	0.73	0.27	110,152,160,160	0
13	PO4	A	504	5/5	0.76	0.48	148,149,151,151	0
12	PGE	C	409	10/10	0.78	0.39	87,94,99,99	0
13	PO4	G	103	5/5	0.78	0.17	156,157,158,160	0
13	PO4	F	501	5/5	0.78	0.32	145,150,152,153	0
12	PGE	C	407	10/10	0.79	0.49	105,119,128,128	0
13	PO4	A	505	5/5	0.82	0.37	129,131,132,138	0
14	CDL	A	506	34/100	0.85	0.23	122,151,159,160	0
12	PGE	C	408	10/10	0.85	0.48	69,74,78,78	0
15	PG4	B	502	13/13	0.85	0.29	73,85,87,88	0
13	PO4	F	502	5/5	0.88	0.41	137,140,141,143	0
20	FX2	C	406	31/31	0.88	0.42	120,124,143,147	0
13	PO4	G	101	5/5	0.89	0.20	122,124,128,128	0
19	PEE	E	204	20/51	0.90	0.45	93,103,109,113	0
14	CDL	D	503	27/100	0.91	0.28	96,108,145,147	0
11	6PE	A	501	23/27	0.92	0.21	102,127,141,143	0
23	PX4	E	202	28/46	0.92	0.32	107,122,133,135	0
14	CDL	C	404	38/100	0.93	0.29	84,95,107,110	0
22	FES	E	201	4/4	0.94	0.09	241,242,245,246	0
19	PEE	C	405	34/51	0.94	0.36	75,80,89,92	0
21	HEC	D	501	43/43	0.97	0.40	114,121,128,132	0
17	HEM	C	402	43/43	0.98	0.27	64,67,70,72	0
17	HEM	C	401	43/43	0.98	0.27	71,73,80,82	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.

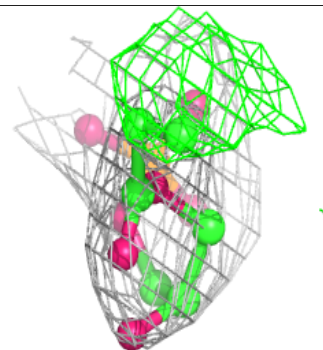
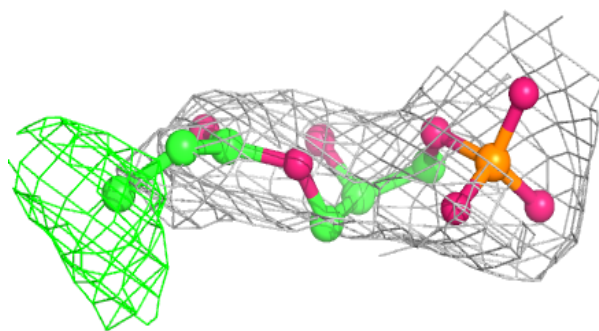
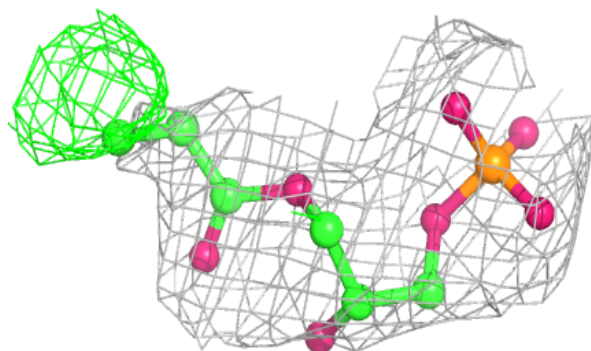


**Electron density around CDL E 205:**

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

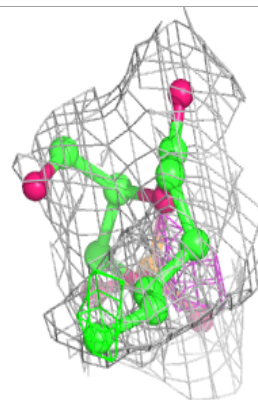
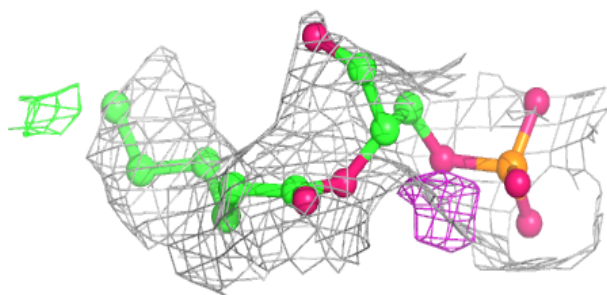
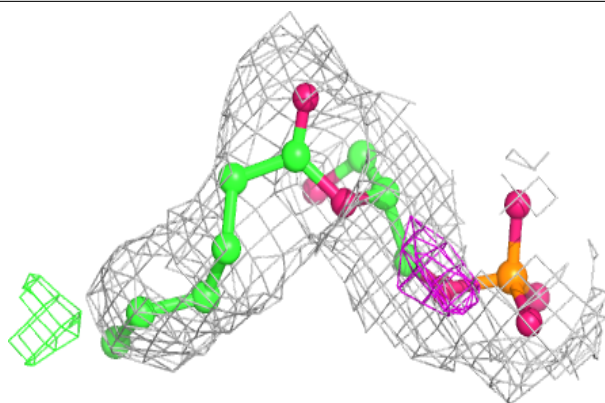
**Electron density around PX6 C 410:**

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

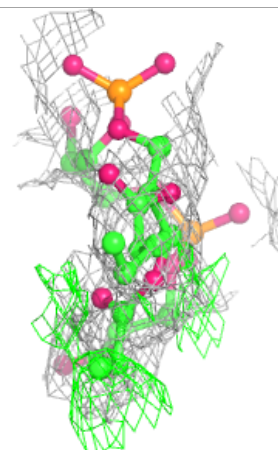
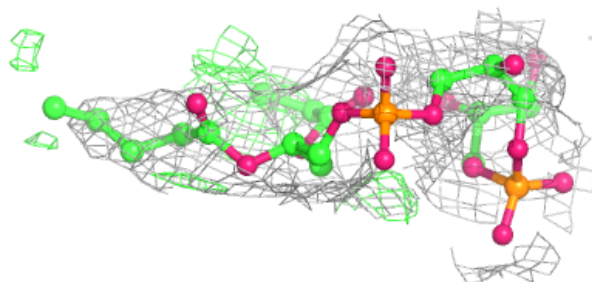
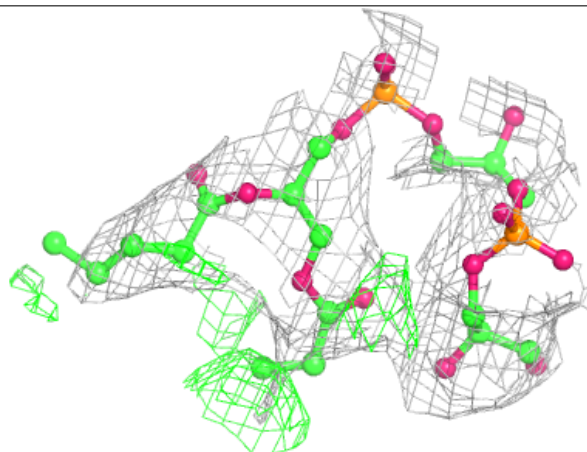


**Electron density around PX6 B 503:**

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

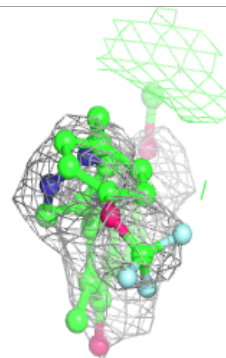
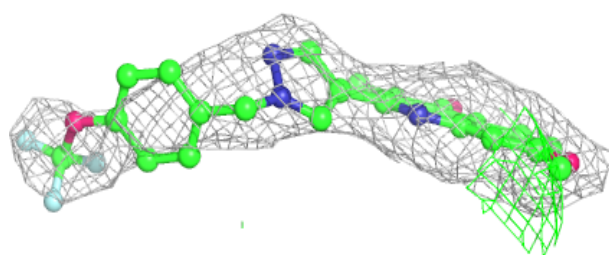
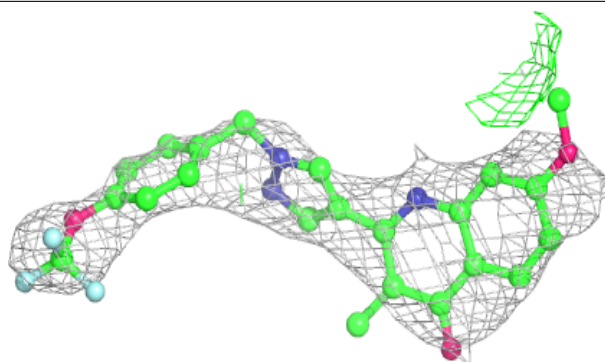
**Electron density around CDL A 506:**

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

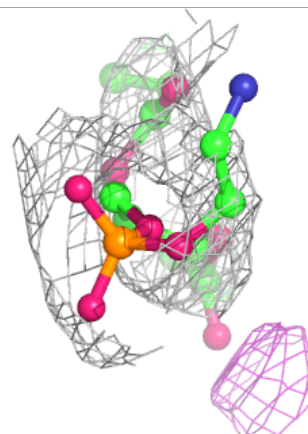
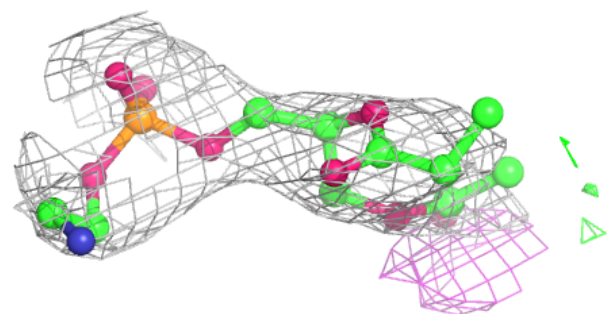
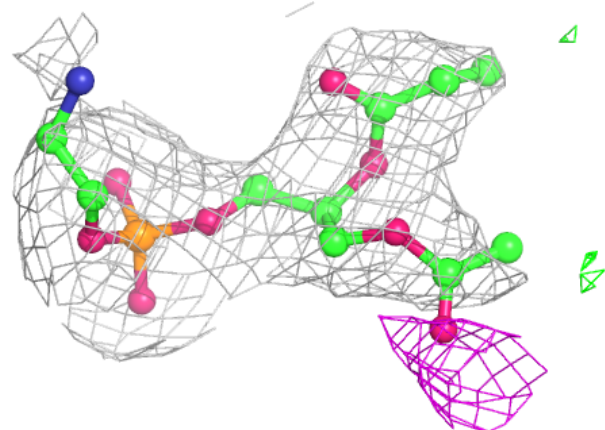


**Electron density around FX2 C 406:**

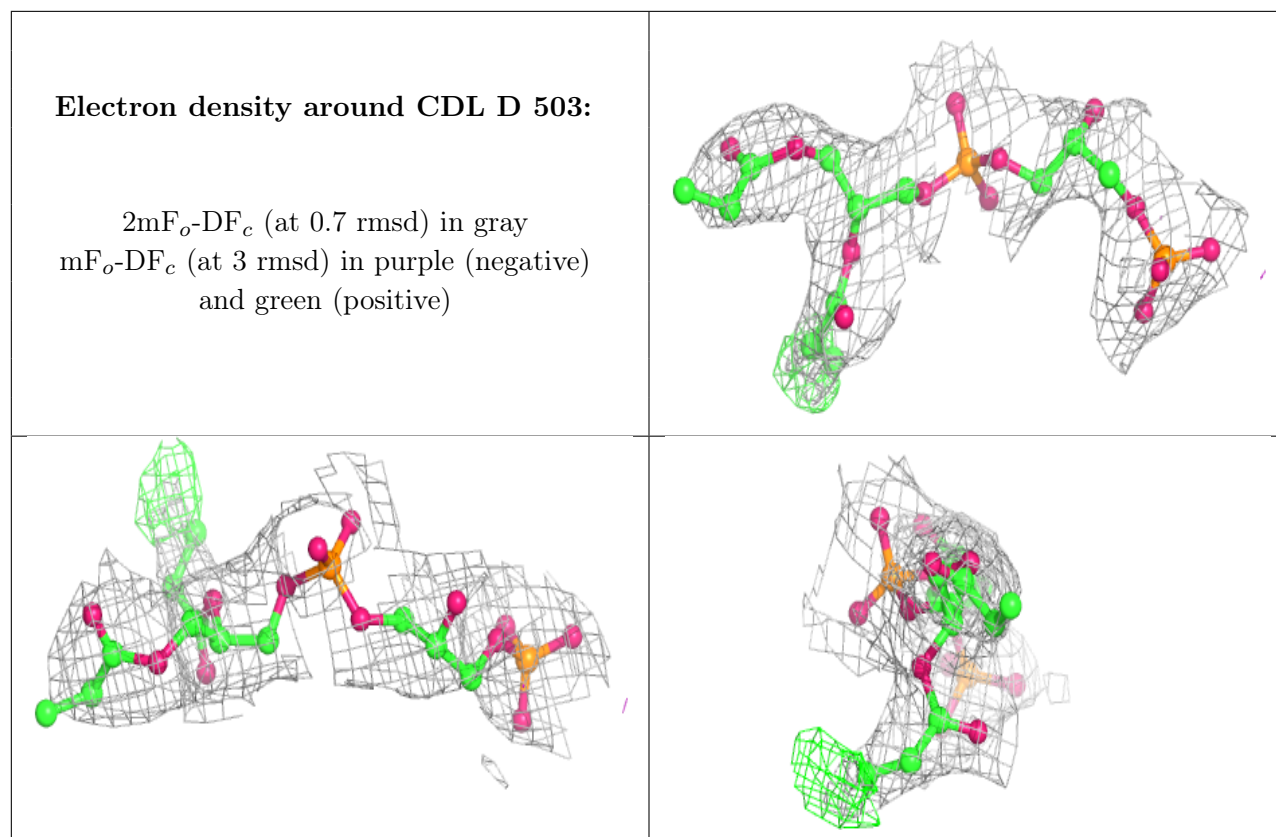
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PEE E 204:**

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

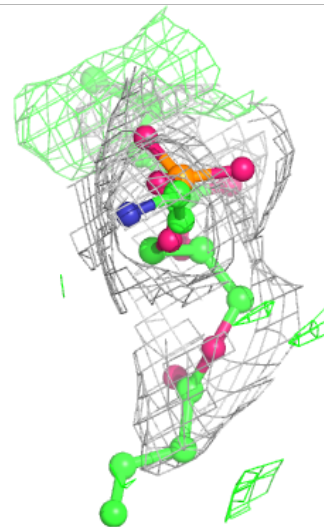
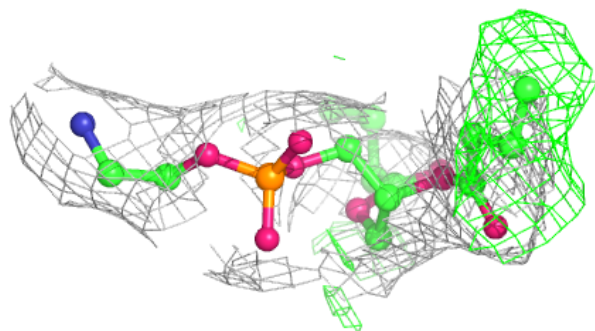
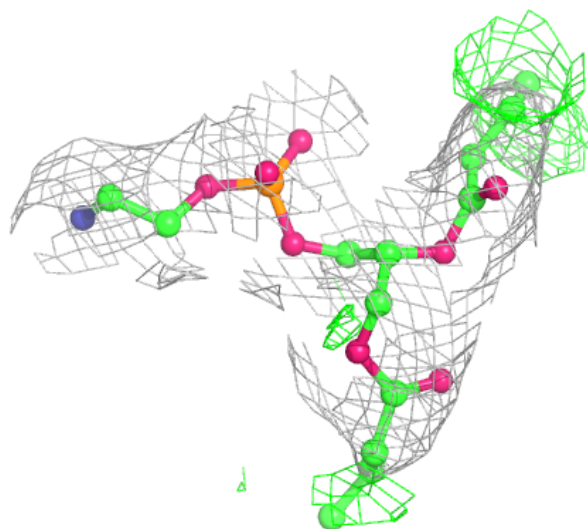






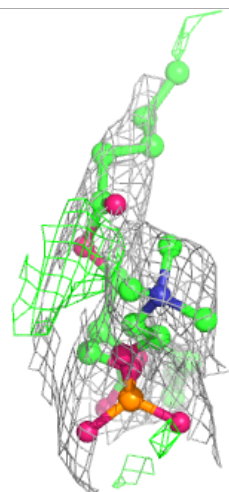
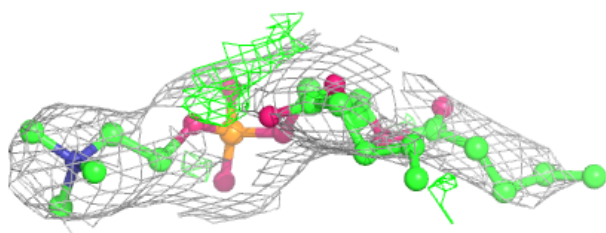
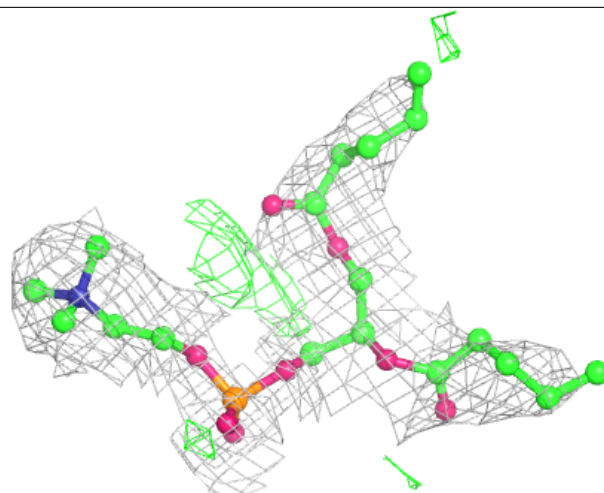
**Electron density around 6PE A 501:**

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



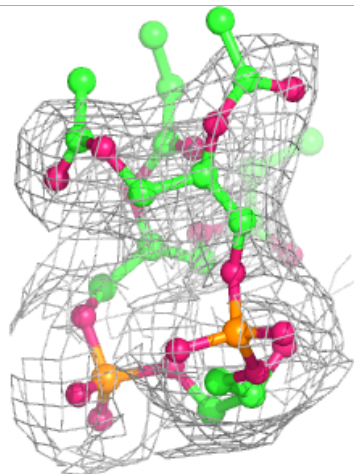
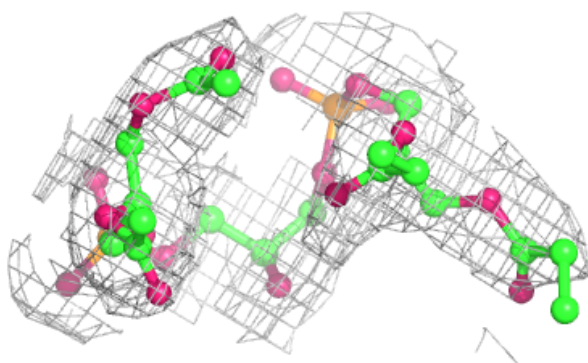
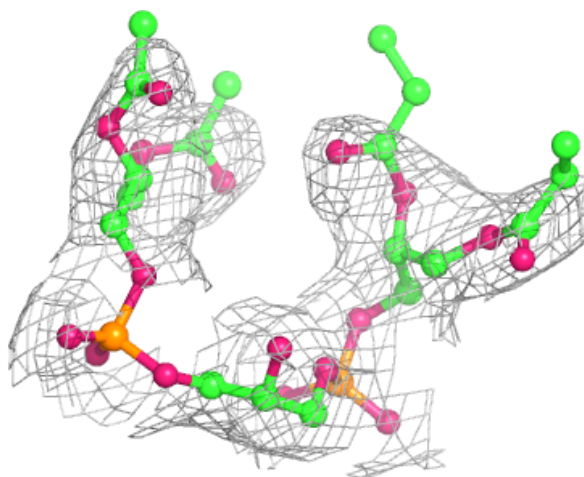
**Electron density around PX4 E 202:**

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



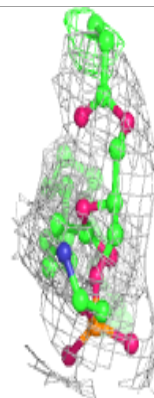
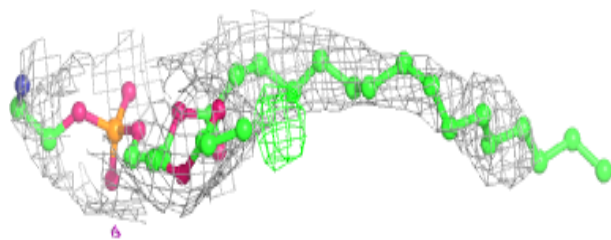
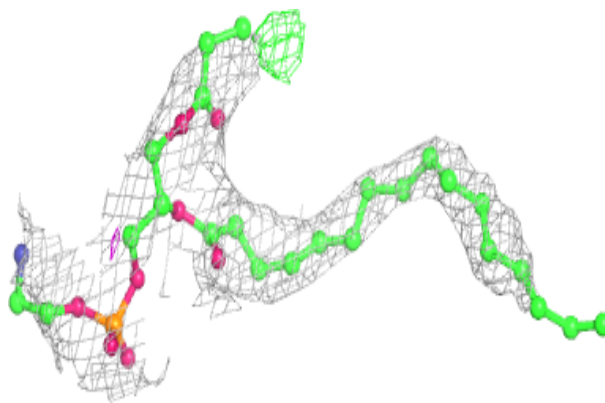
**Electron density around CDL C 404:**

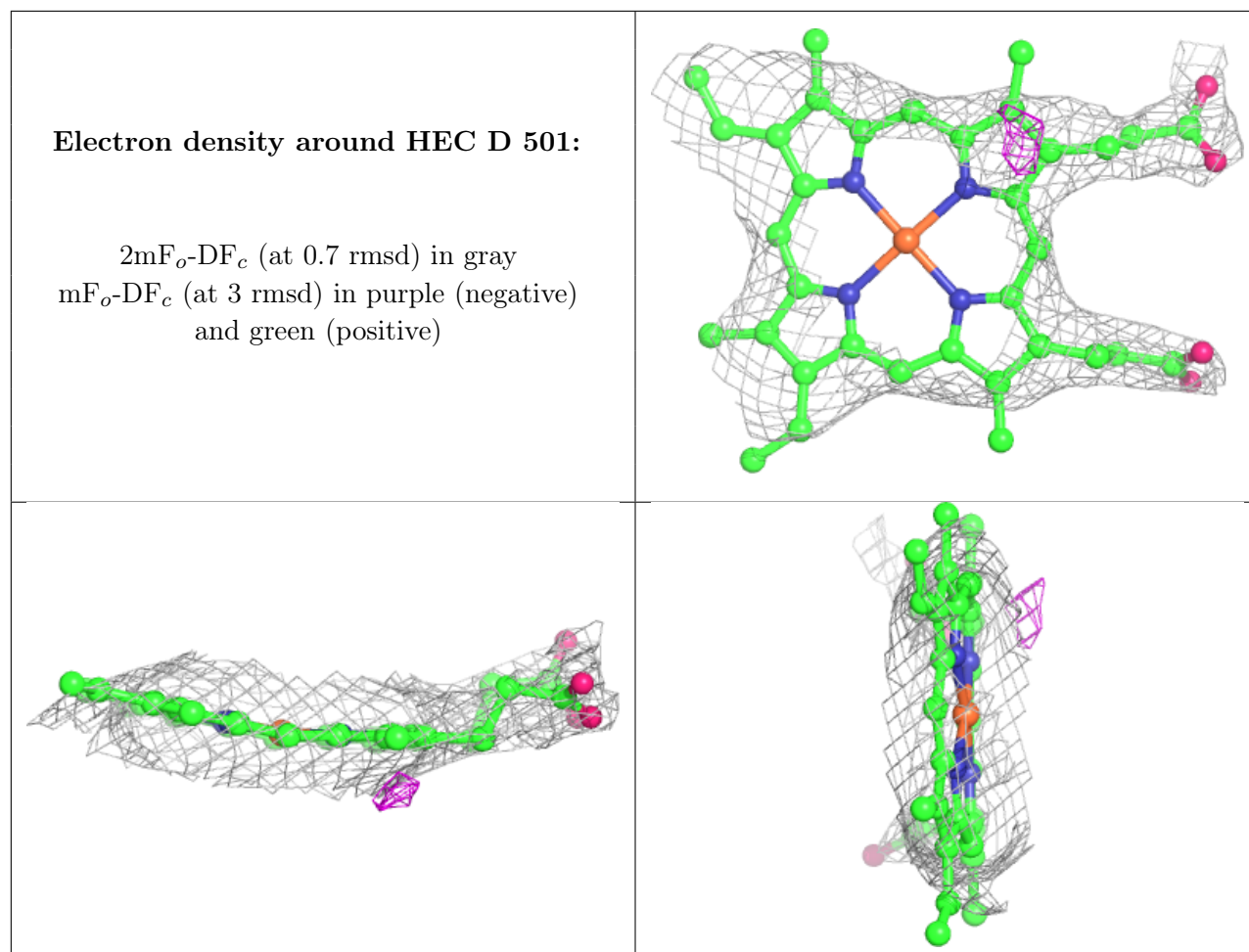
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PEE C 405:**

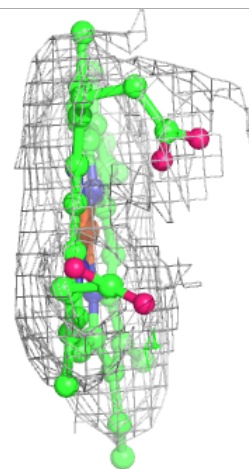
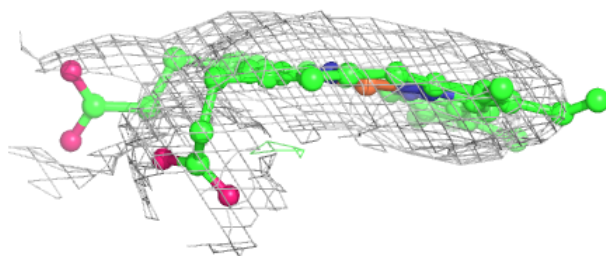
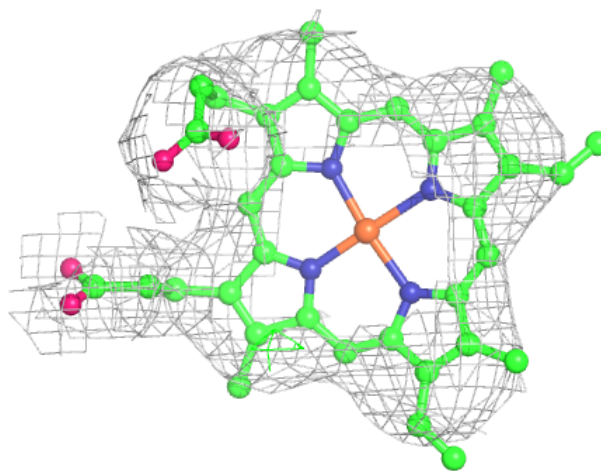
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

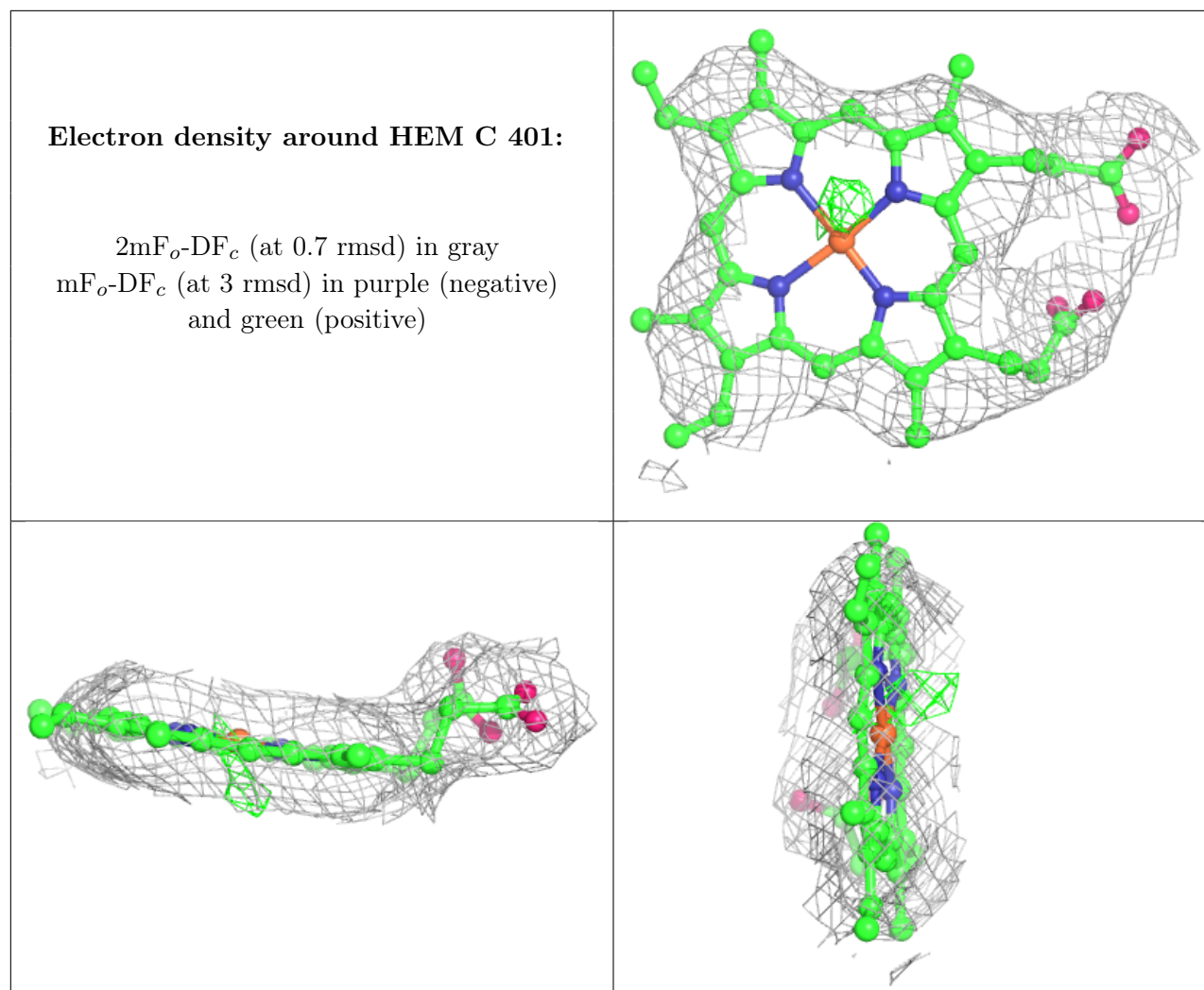




**Electron density around HEM C 402:**

$2mF_o-DF_c$  (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.