



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:16 AM UTC

PDB ID : 2D2C / pdb\_00002d2c  
Title : Crystal Structure Of Cytochrome B6F Complex with DBMIB From M. Laminosus  
Authors : Yan, J.; Kurisu, G.; Cramer, W.A.  
Deposited on : 2005-09-07  
Resolution : 3.80 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

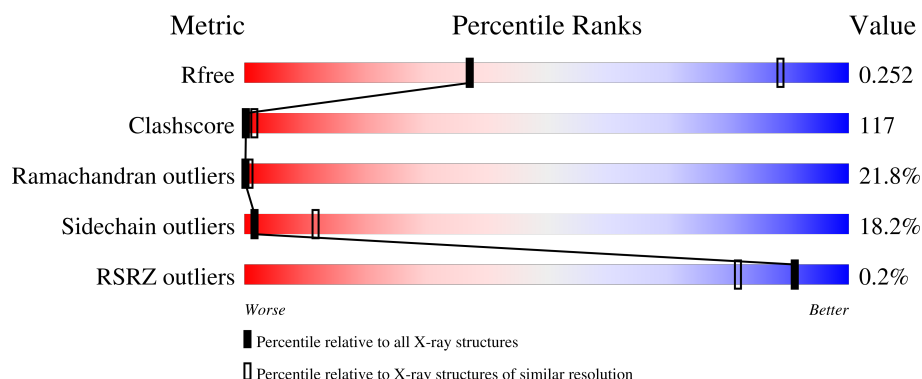
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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.





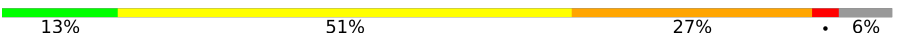


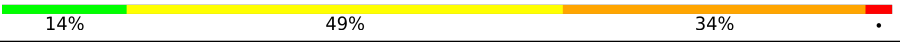
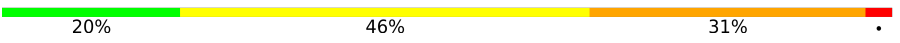
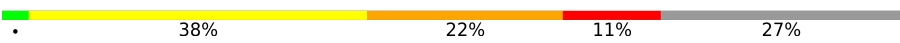
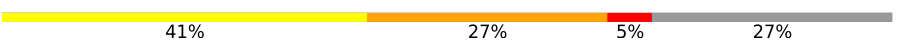

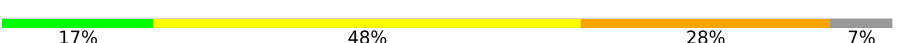
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	215	<div> <div>6%</div> <div>53%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div>
1	N	215	<div> <div>9%</div> <div>49%</div> <div>28%</div> <div>7%</div> <div>6%</div> </div>
2	B	160	<div> <div>9%</div> <div>41%</div> <div>26%</div> <div>9%</div> <div>14%</div> </div>
2	O	160	<div> <div>•</div> <div>39%</div> <div>34%</div> <div>9%</div> <div>14%</div> </div>
3	C	289	<div> <div>13%</div> <div>55%</div> <div>24%</div> <div>6%</div> <div>•</div> </div>

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
3	P	289	
4	D	179	
4	Q	179	
5	E	32	
5	R	32	
6	F	35	
6	S	35	
7	G	37	
7	T	37	
8	H	29	
8	U	29	

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
10	OPC	B	305	-	-	X	-
11	BNT	B	309	-	-	X	-
11	BNT	O	1309	-	-	X	-
12	CLA	B	201	X	-	-	-
12	CLA	O	1201	X	-	-	-
13	FES	D	201	-	-	X	-
13	FES	Q	201	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14984 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			
1	N	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			
2	O	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			
3	P	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			
4	Q	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	138	ARG	LYS	conflict	UNP P83794
Q	138	ARG	LYS	conflict	UNP P83794

- Molecule 5 is a protein called Cytochrome b6-f complex subunit VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			
5	R	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

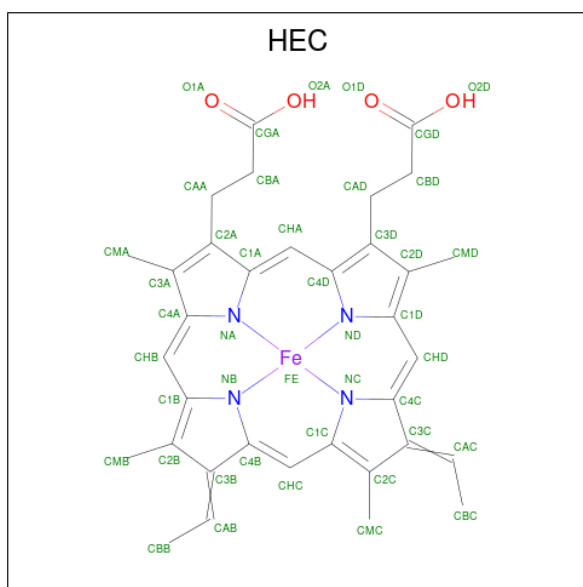
- Molecule 7 is a protein called Cytochrome b6-f complex subunit V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	27	Total	C	N	O	0	0	0
			216	146	34	36			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit VIII.

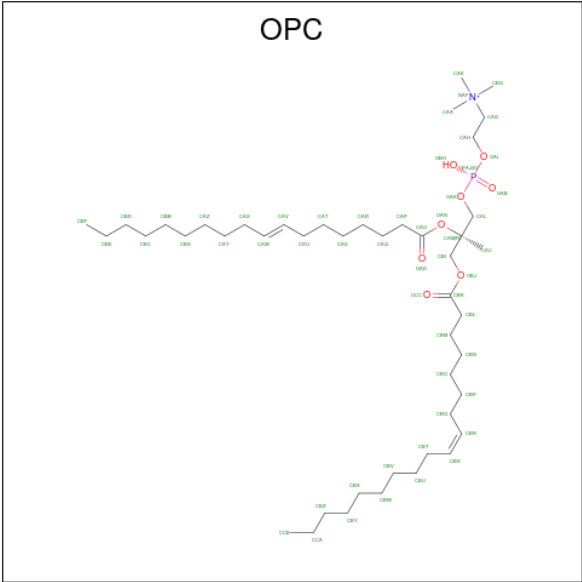
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

- Molecule 9 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



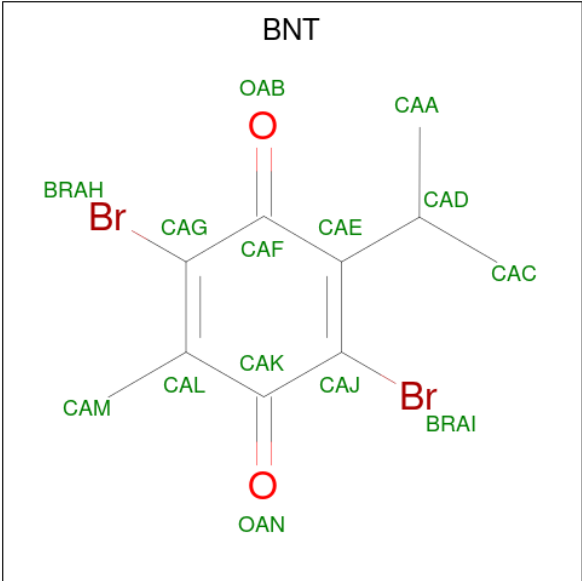
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 10 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



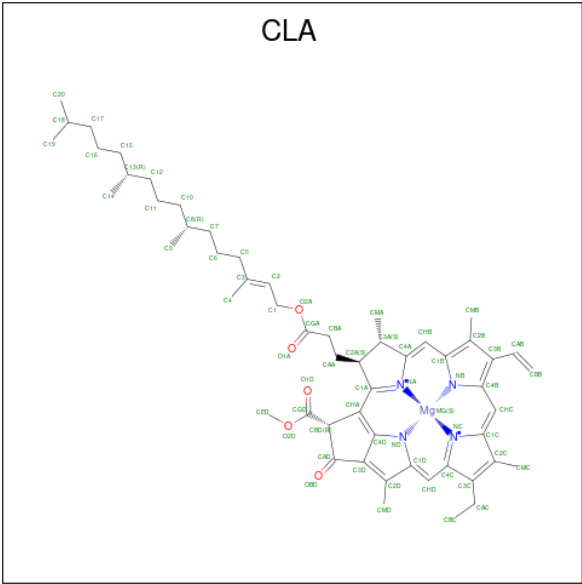
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	N	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	O	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 11 is 2,5-DIBROMO-3-ISOPROPYL-6-METHYLBENZO-1,4-QUINONE (CCD ID: BNT) (formula: C<sub>10</sub>H<sub>10</sub>Br<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	Br	C	O	0	0
			14	2	10	2		
11	O	1	Total	Br	C	O	0	0
			14	2	10	2		

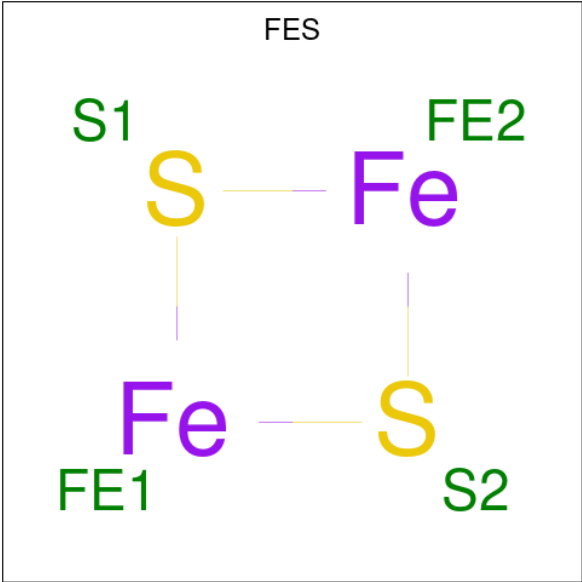
- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
12	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0

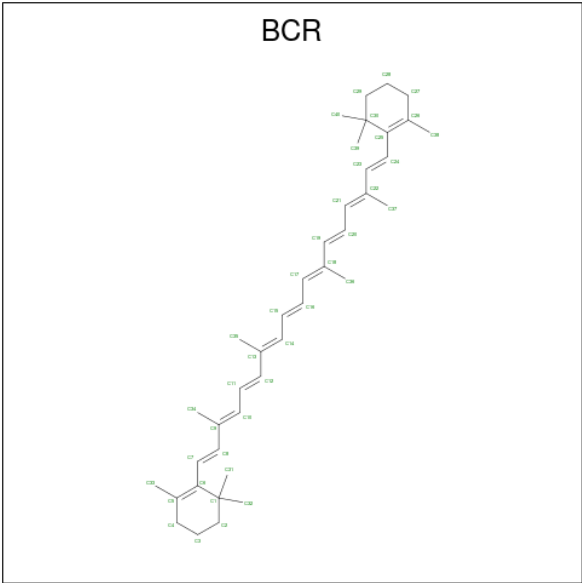
- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	Fe	S	0	0
			4	2	2		
13	Q	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	E	1	Total	C	0	0
			40	40		
14	R	1	Total	C	0	0
			40	40		

- Molecule 15 is water.

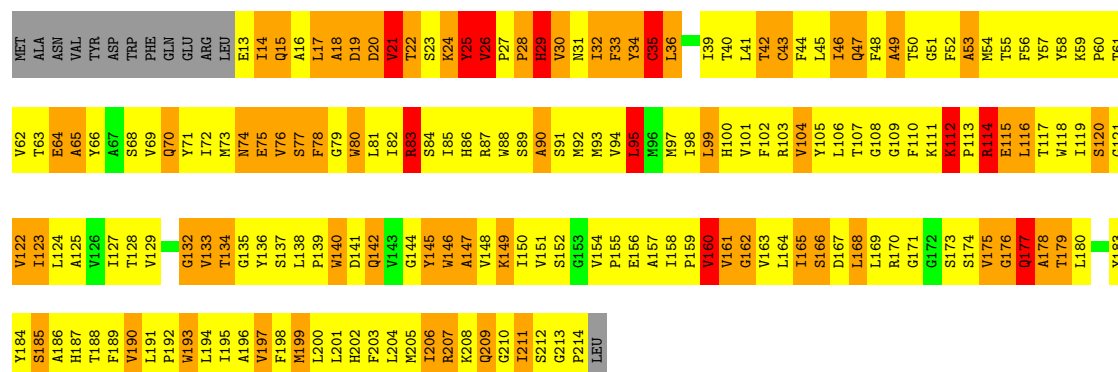
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	O	0	0
			1	1		
15	N	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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

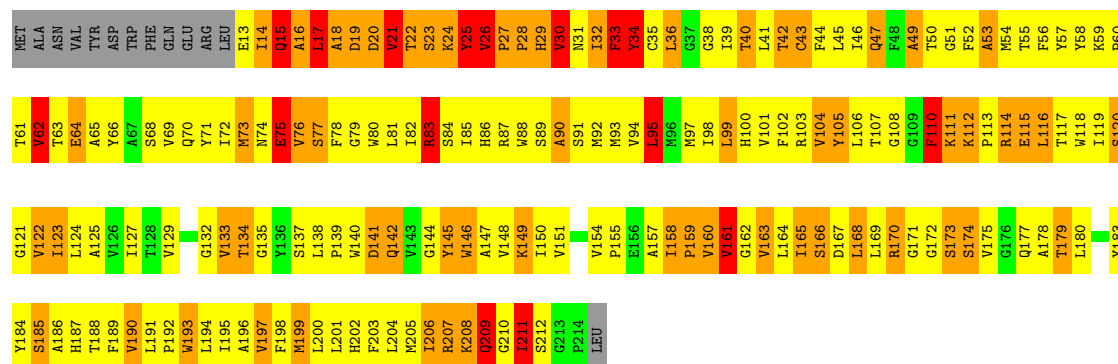
#### • Molecule 1: Cytochrome b6

Chain A: 



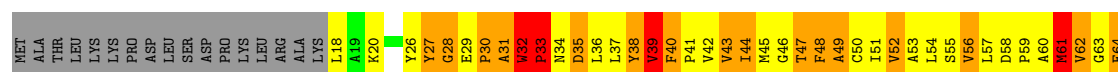
#### • Molecule 1: Cytochrome b6

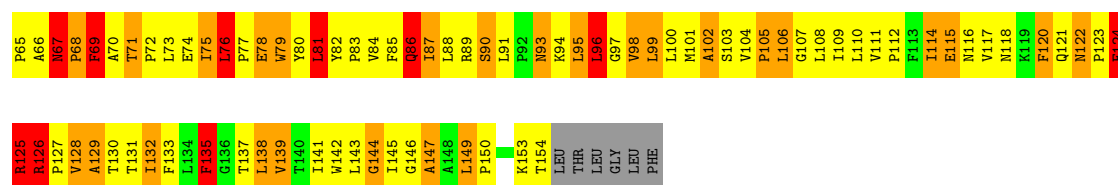
Chain N: 



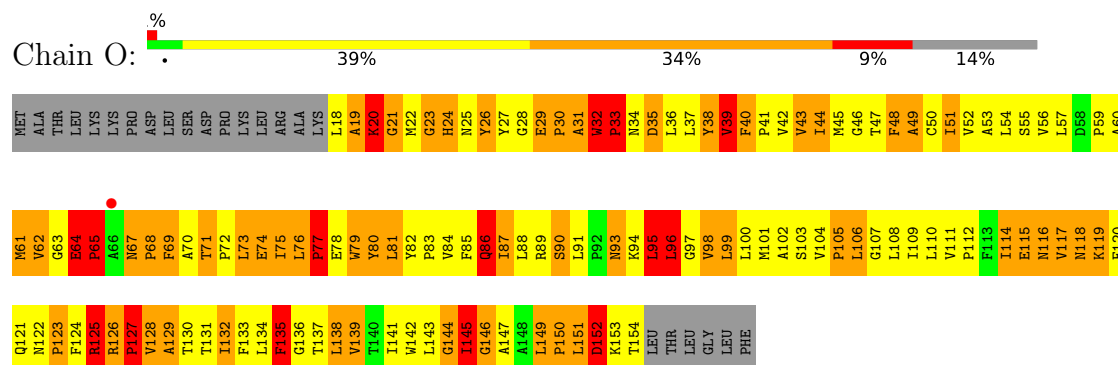
#### • Molecule 2: Cytochrome b6-f complex subunit 4

Chain B: 

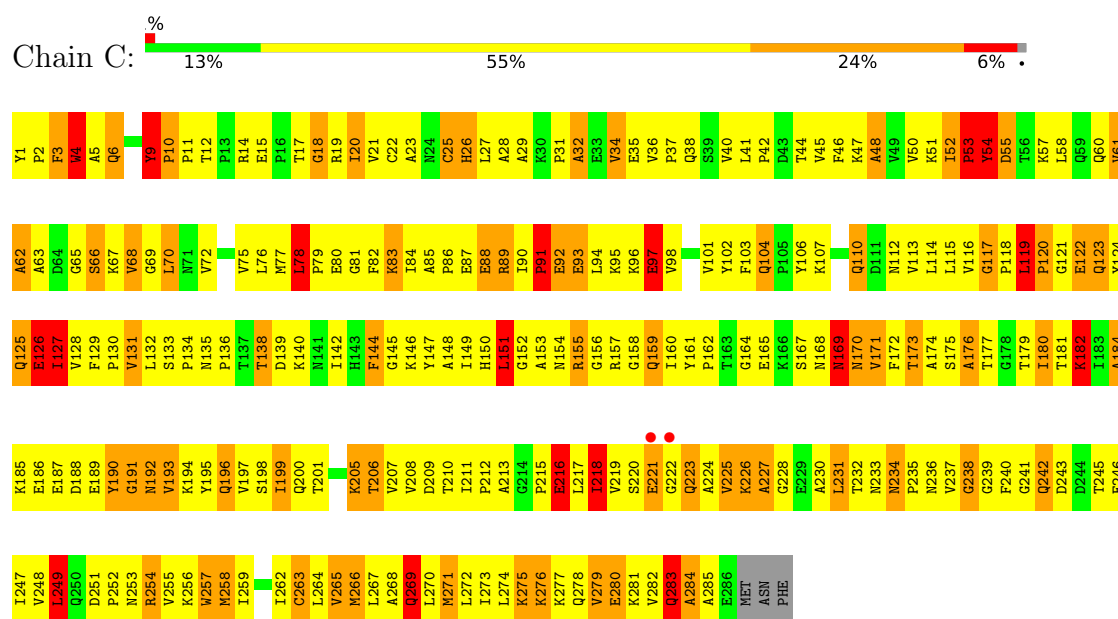




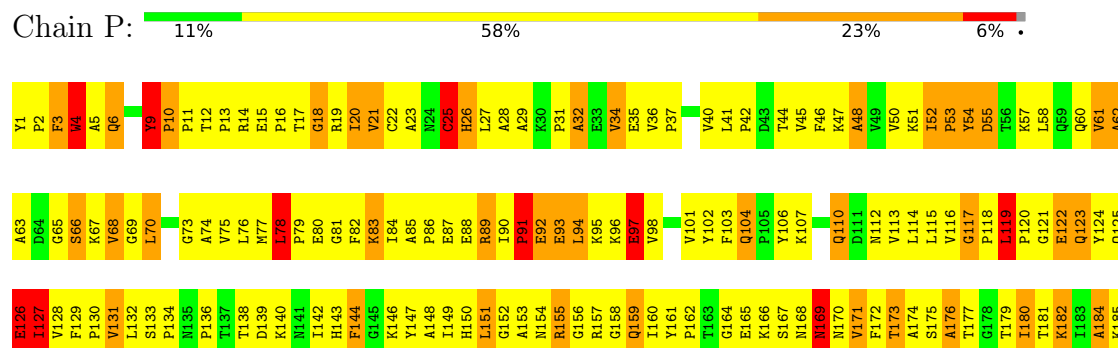
### • Molecule 2: Cytochrome b6-f complex subunit 4

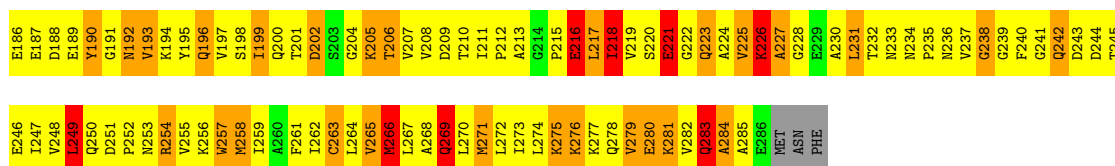


### • Molecule 3: Apocytochrome f

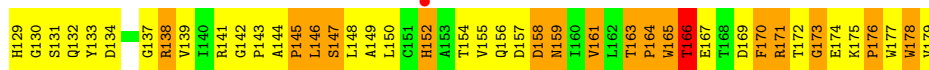
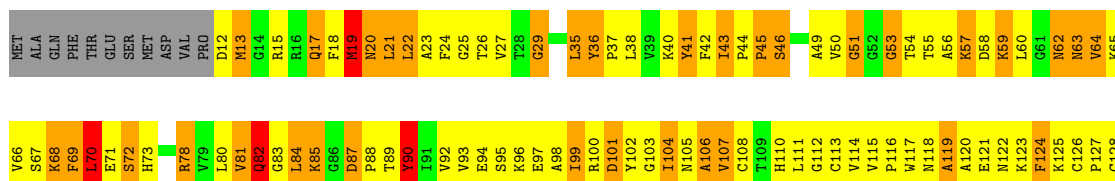
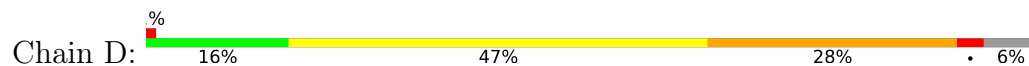


### • Molecule 3: Apocytochrome f

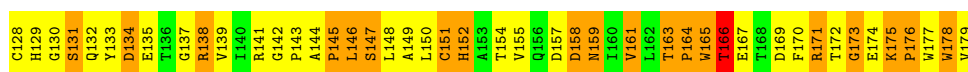
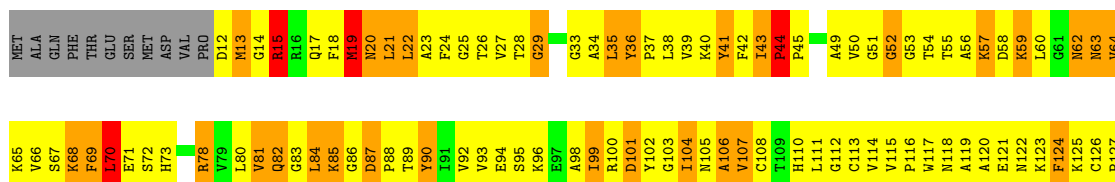
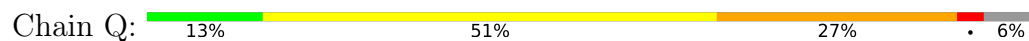




• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



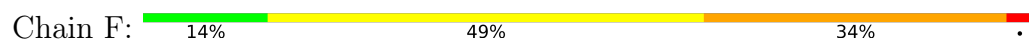
• Molecule 5: Cytochrome b6-f complex subunit VI



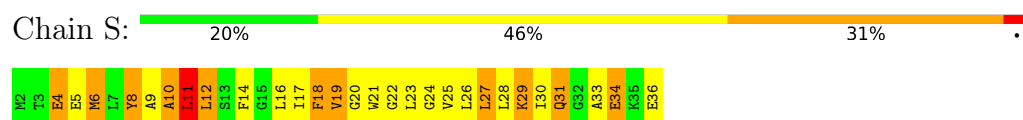
• Molecule 5: Cytochrome b6-f complex subunit VI



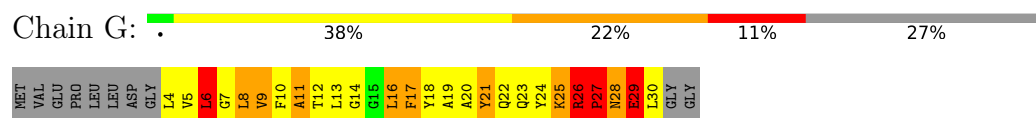
• Molecule 6: Cytochrome b6-f complex subunit VII



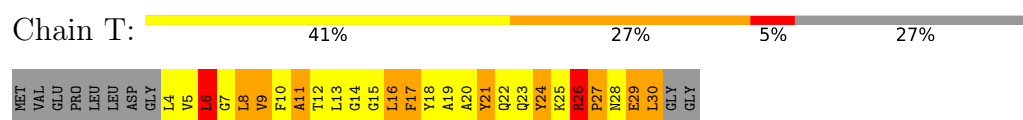
- Molecule 6: Cytochrome b6-f complex subunit VII



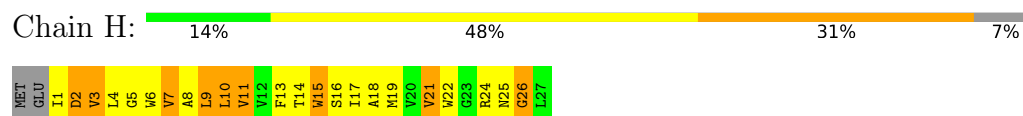
- Molecule 7: Cytochrome b6-f complex subunit V



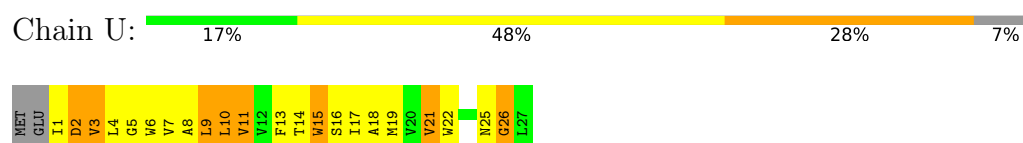
- Molecule 7: Cytochrome b6-f complex subunit V



- Molecule 8: Cytochrome b6-f complex subunit VIII



- Molecule 8: Cytochrome b6-f complex subunit VIII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.59Å 156.59Å 361.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.76 – 3.80 24.76 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.76-3.80) 93.2 (24.76-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.276 , 0.378 0.263 , 0.252	Depositor DCC
$R_{free}$ test set	1490 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 188.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: FES, BNT, CLA, HEC, OPC, BCR

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	0.76	0/1641	1.23	18/2239 (0.8%)
1	N	0.77	1/1641 (0.1%)	1.18	20/2239 (0.9%)
2	B	0.75	0/1102	1.51	24/1515 (1.6%)
2	O	0.82	0/1102	1.62	27/1515 (1.8%)
3	C	0.67	0/2248	1.22	30/3061 (1.0%)
3	P	0.69	0/2248	1.22	29/3061 (0.9%)
4	D	0.81	0/1312	1.29	19/1786 (1.1%)
4	Q	0.78	0/1312	1.29	21/1786 (1.2%)
5	E	0.83	0/253	1.51	9/340 (2.6%)
5	R	0.83	0/253	1.47	11/340 (3.2%)
6	F	0.74	0/274	1.09	3/366 (0.8%)
6	S	0.78	0/274	1.09	3/366 (0.8%)
7	G	0.80	0/221	1.56	8/299 (2.7%)
7	T	0.88	0/221	1.38	5/299 (1.7%)
8	H	0.71	0/220	1.29	5/301 (1.7%)
8	U	0.72	0/220	1.25	4/301 (1.3%)
All	All	0.75	1/14542 (0.0%)	1.30	236/19814 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	O	0	1
All	All	0	2

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	27	PRO	CA-C	5.85	1.57	1.52

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	126	ARG	CA-C-N	-16.80	98.84	119.84
2	O	126	ARG	C-N-CA	-16.80	98.84	119.84
2	O	40	PHE	N-CA-C	-11.98	96.46	112.75
2	B	40	PHE	N-CA-C	-11.61	96.96	112.75
5	E	16	PHE	N-CA-C	-11.20	99.87	113.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	TYR	Sidechain
2	O	80	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	1593	0	1623	473	0
1	N	1593	0	1623	486	0
2	B	1067	0	1106	369	0
2	O	1067	0	1106	399	0
3	C	2200	0	2216	445	0
3	P	2200	0	2216	496	0
4	D	1280	0	1265	234	0
4	Q	1280	0	1265	230	0
5	E	248	0	284	140	0
5	R	248	0	284	124	0
6	F	270	0	282	96	0
6	S	270	0	282	82	0
7	G	216	0	220	90	0
7	T	216	0	220	103	0
8	H	214	0	224	39	0
8	U	214	0	224	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	129	0	97	17	0
9	C	43	0	31	3	0
9	N	129	0	97	18	0
9	P	43	0	31	4	0
10	B	54	0	83	34	0
10	C	54	0	83	20	0
10	N	54	0	83	14	0
10	O	54	0	83	17	0
11	B	14	0	10	10	0
11	O	14	0	10	12	0
12	B	65	0	70	8	0
12	O	65	0	70	9	0
13	D	4	0	0	3	0
13	Q	4	0	0	2	0
14	E	40	0	56	11	0
14	R	40	0	56	8	0
15	A	1	0	0	1	0
15	N	1	0	0	2	0
All	All	14984	0	15300	3534	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 117.

The worst 5 of 3534 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:HA	1:A:103:ARG:HH11	1.06	1.18
1:N:162:GLY:O	1:N:165:ILE:HG22	1.45	1.16
1:A:106:LEU:HG	5:E:18:ILE:HD12	1.22	1.16
3:C:171:VAL:HG13	3:C:234:ASN:HB2	1.22	1.14
3:P:271:MET:HB3	4:Q:23:ALA:HA	1.15	1.14

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	200/215 (93%)	90 (45%)	64 (32%)	46 (23%)	0	0
1	N	200/215 (93%)	92 (46%)	58 (29%)	50 (25%)	0	0
2	B	135/160 (84%)	56 (42%)	45 (33%)	34 (25%)	0	0
2	O	135/160 (84%)	52 (38%)	39 (29%)	44 (33%)	0	0
3	C	284/289 (98%)	153 (54%)	83 (29%)	48 (17%)	0	2
3	P	284/289 (98%)	153 (54%)	81 (28%)	50 (18%)	0	2
4	D	166/179 (93%)	85 (51%)	50 (30%)	31 (19%)	0	1
4	Q	166/179 (93%)	86 (52%)	49 (30%)	31 (19%)	0	1
5	E	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
5	R	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
6	F	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1
6	S	33/35 (94%)	15 (46%)	12 (36%)	6 (18%)	0	2
7	G	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	2
7	T	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	2
8	H	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
8	U	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
All	All	1796/1952 (92%)	869 (48%)	536 (30%)	391 (22%)	0	1

5 of 391 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	20	ASP
1	A	21	VAL
1	A	22	THR
1	A	26	VAL

### 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	172/184 (94%)	146 (85%)	26 (15%)	3	16
1	N	172/184 (94%)	145 (84%)	27 (16%)	2	15
2	B	116/136 (85%)	98 (84%)	18 (16%)	2	15
2	O	116/136 (85%)	90 (78%)	26 (22%)	1	5
3	C	240/243 (99%)	194 (81%)	46 (19%)	1	9
3	P	240/243 (99%)	195 (81%)	45 (19%)	1	10
4	D	136/146 (93%)	111 (82%)	25 (18%)	1	11
4	Q	136/146 (93%)	110 (81%)	26 (19%)	1	9
5	E	25/25 (100%)	19 (76%)	6 (24%)	1	4
5	R	25/25 (100%)	18 (72%)	7 (28%)	0	2
6	F	27/27 (100%)	23 (85%)	4 (15%)	3	16
6	S	27/27 (100%)	22 (82%)	5 (18%)	1	11
7	G	21/28 (75%)	15 (71%)	6 (29%)	0	2
7	T	21/28 (75%)	15 (71%)	6 (29%)	0	2
8	H	22/24 (92%)	20 (91%)	2 (9%)	9	32
8	U	22/24 (92%)	20 (91%)	2 (9%)	9	32
All	All	1518/1626 (93%)	1241 (82%)	277 (18%)	2	12

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	12	ASP
4	Q	63	ASN
5	R	22	ILE
4	D	69	PHE
4	D	41	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	105	ASN
4	Q	122	ASN
4	D	17	GLN
3	C	283	GLN
4	Q	132	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

20 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	FES	Q	201	4	0,4,4	-	-	-		
9	HEC	C	301	3	46,50,50	2.20	11 (23%)	58,82,82	1.43	7 (12%)
9	HEC	P	301	3	46,50,50	2.20	14 (30%)	58,82,82	1.45	7 (12%)
14	BCR	R	1101	-	41,41,41	2.58	13 (31%)	56,56,56	2.42	21 (37%)
14	BCR	E	101	-	41,41,41	2.48	13 (31%)	56,56,56	2.43	20 (35%)
9	HEC	N	303	15,1	46,50,50	1.95	11 (23%)	58,82,82	2.10	10 (17%)
10	OPC	N	1305	-	53,53,54	1.36	8 (15%)	59,61,64	1.17	4 (6%)
10	OPC	C	306	-	53,53,54	1.36	8 (15%)	59,61,64	1.20	4 (6%)
9	HEC	N	301	1	46,50,50	2.24	16 (34%)	58,82,82	1.58	8 (13%)
9	HEC	A	303	15,1	46,50,50	1.95	11 (23%)	58,82,82	1.63	6 (10%)
13	FES	D	201	4	0,4,4	-	-	-		
9	HEC	A	301	1	46,50,50	2.24	14 (30%)	58,82,82	1.50	6 (10%)
11	BNT	O	1309	-	12,14,14	3.33	5 (41%)	13,21,21	1.53	2 (15%)
10	OPC	B	305	-	53,53,54	1.36	8 (15%)	59,61,64	1.09	3 (5%)
9	HEC	A	302	1	46,50,50	2.07	14 (30%)	58,82,82	1.90	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	OPC	O	1306	-	53,53,54	1.36	8 (15%)	59,61,64	1.12	4 (6%)
9	HEC	N	302	1	46,50,50	2.15	14 (30%)	58,82,82	1.98	8 (13%)
11	BNT	B	309	-	12,14,14	3.18	5 (41%)	13,21,21	1.57	2 (15%)
12	CLA	O	1201	-	69,73,73	2.01	17 (24%)	82,113,113	1.86	13 (15%)
12	CLA	B	201	-	69,73,73	2.05	16 (23%)	82,113,113	1.93	15 (18%)

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
13	FES	Q	201	4	-	-	0/1/1/1
9	HEC	C	301	3	-	7/14/54/54	-
9	HEC	P	301	3	-	7/14/54/54	-
14	BCR	R	1101	-	-	7/29/63/63	0/2/2/2
14	BCR	E	101	-	-	7/29/63/63	0/2/2/2
9	HEC	N	303	15,1	-	6/14/54/54	-
10	OPC	N	1305	-	-	17/57/57/60	-
10	OPC	C	306	-	-	11/57/57/60	-
9	HEC	N	301	1	-	6/14/54/54	-
9	HEC	A	303	15,1	-	6/14/54/54	-
13	FES	D	201	4	-	-	0/1/1/1
9	HEC	A	301	1	-	8/14/54/54	-
11	BNT	O	1309	-	-	0/4/28/28	0/1/1/1
10	OPC	B	305	-	-	11/57/57/60	-
9	HEC	A	302	1	-	8/14/54/54	-
10	OPC	O	1306	-	-	16/57/57/60	-
9	HEC	N	302	1	-	7/14/54/54	-
11	BNT	B	309	-	-	0/4/28/28	0/1/1/1
12	CLA	O	1201	-	4/4/15/20	14/39/115/115	-
12	CLA	B	201	-	4/4/15/20	10/39/115/115	-

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	1309	BNT	CAD-CAE	-9.09	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	309	BNT	CAD-CAE	-8.38	1.40	1.52
14	R	1101	BCR	C30-C25	8.24	1.64	1.53
12	O	1201	CLA	C3A-C2A	-7.17	1.35	1.54
9	C	301	HEC	CAC-C3C	6.88	1.57	1.35

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	302	HEC	CBA-CAA-C2A	-8.54	88.92	112.53
9	N	303	HEC	CBC-CAC-C3C	-8.36	110.72	127.43
9	A	302	HEC	CBA-CAA-C2A	-8.03	90.33	112.53
12	B	201	CLA	C4A-NA-C1A	7.37	110.04	106.68
9	A	303	HEC	CBB-CAB-C3B	-7.35	112.74	127.43

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	201	CLA	C2A
12	B	201	CLA	C8
12	B	201	CLA	C3A
12	B	201	CLA	ND
12	O	1201	CLA	C2A

5 of 148 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	HEC	C2C-C3C-CAC-CBC
9	A	301	HEC	C4C-C3C-CAC-CBC
9	A	302	HEC	C2B-C3B-CAB-CBB
9	A	302	HEC	C4B-C3B-CAB-CBB
9	A	303	HEC	C3A-C2A-CAA-CBA

There are no ring outliers.

20 monomers are involved in 177 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Q	201	FES	2	0
9	C	301	HEC	3	0
9	P	301	HEC	4	0
14	R	1101	BCR	8	0
14	E	101	BCR	11	0

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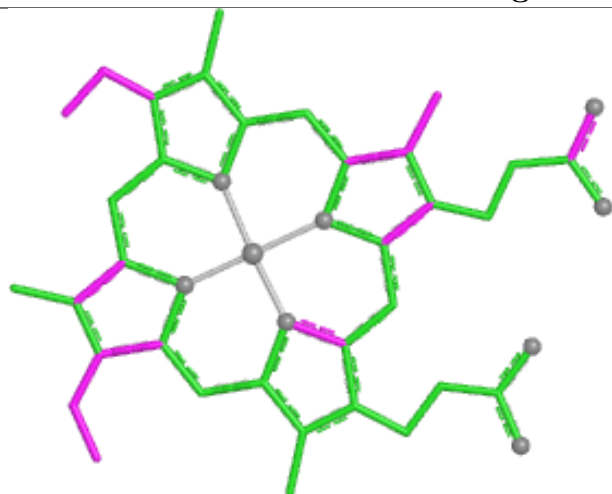
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	303	HEC	8	0
10	N	1305	OPC	14	0
10	C	306	OPC	20	0
9	N	301	HEC	6	0
9	A	303	HEC	3	0
13	D	201	FES	3	0
9	A	301	HEC	3	0
11	O	1309	BNT	12	0
10	B	305	OPC	34	0
9	A	302	HEC	11	0
10	O	1306	OPC	17	0
9	N	302	HEC	5	0
11	B	309	BNT	10	0
12	O	1201	CLA	9	0
12	B	201	CLA	8	0

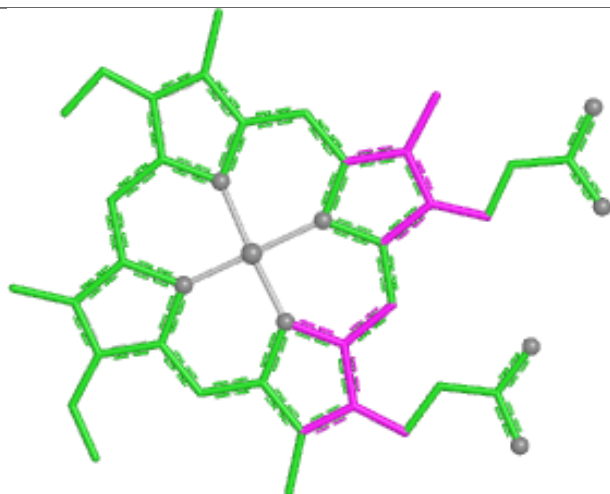
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



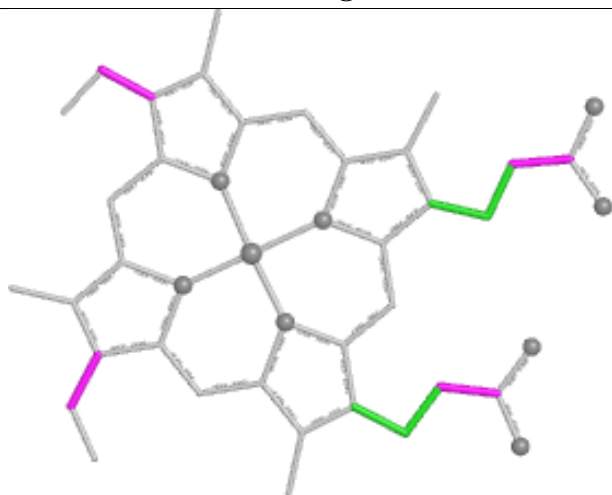
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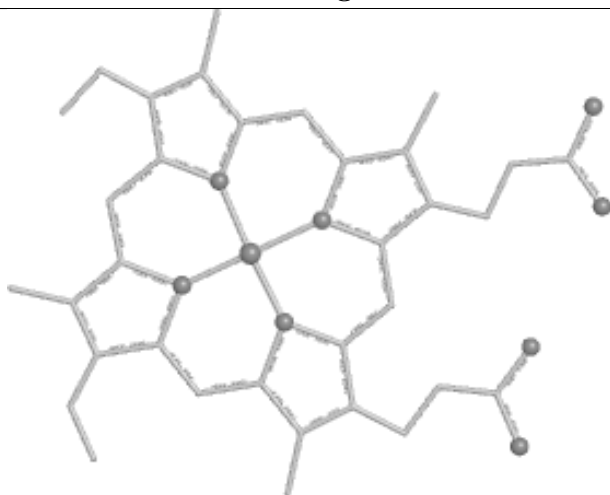
Bond lengths



Bond angles

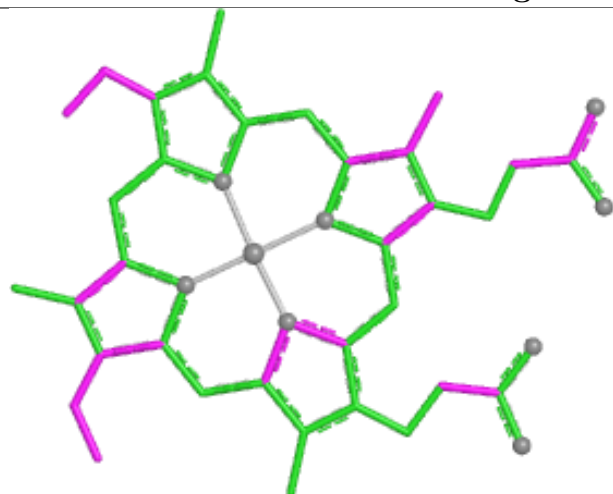


Torsions

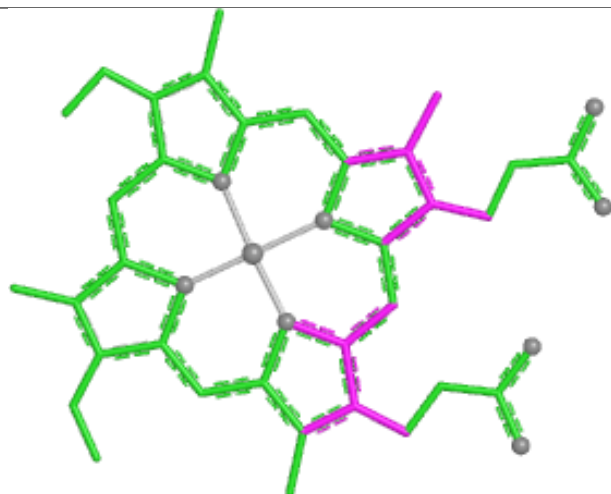


Rings

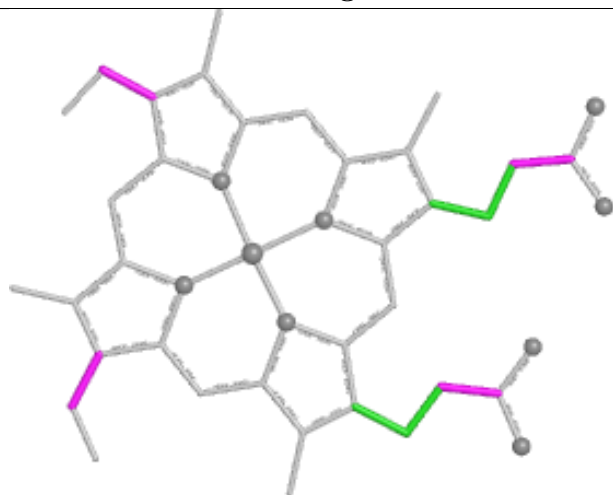
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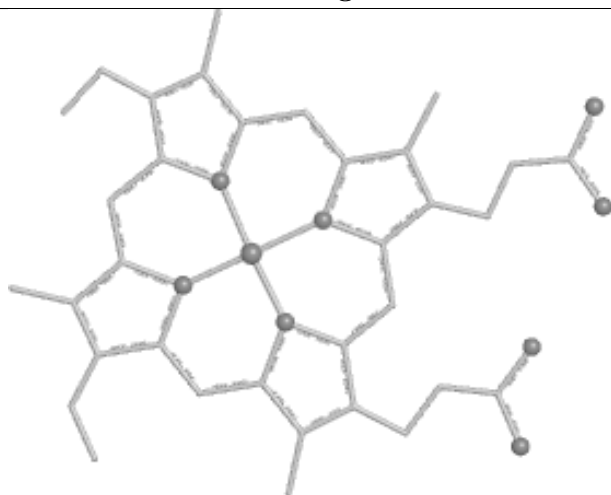
Bond lengths



Bond angles



Torsions

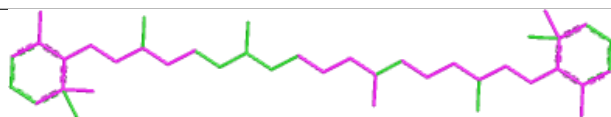


Rings

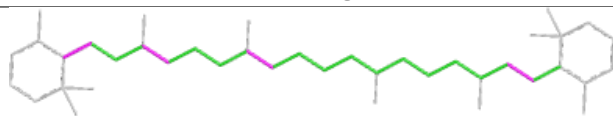
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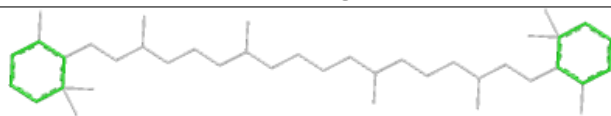
Bond lengths



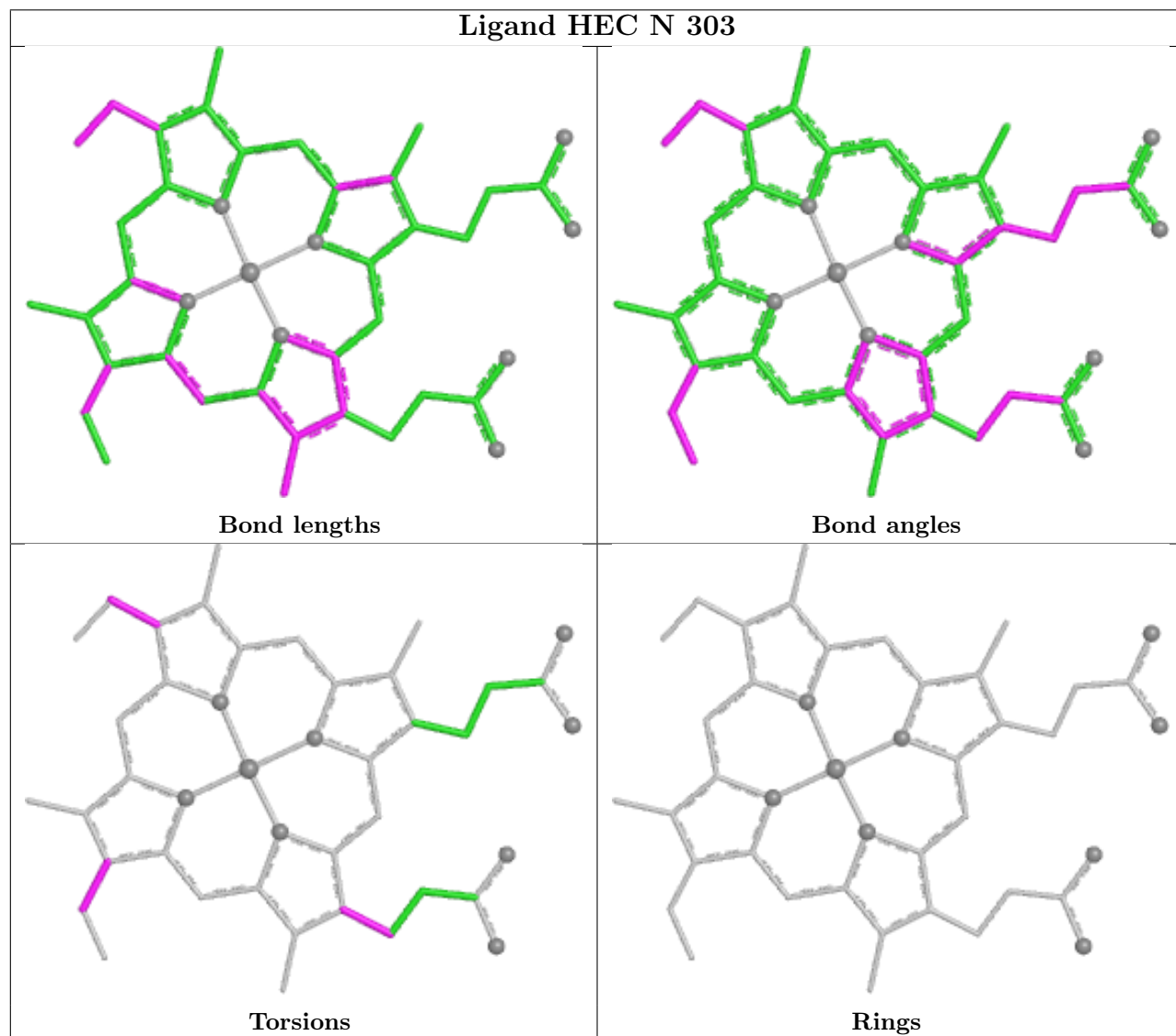
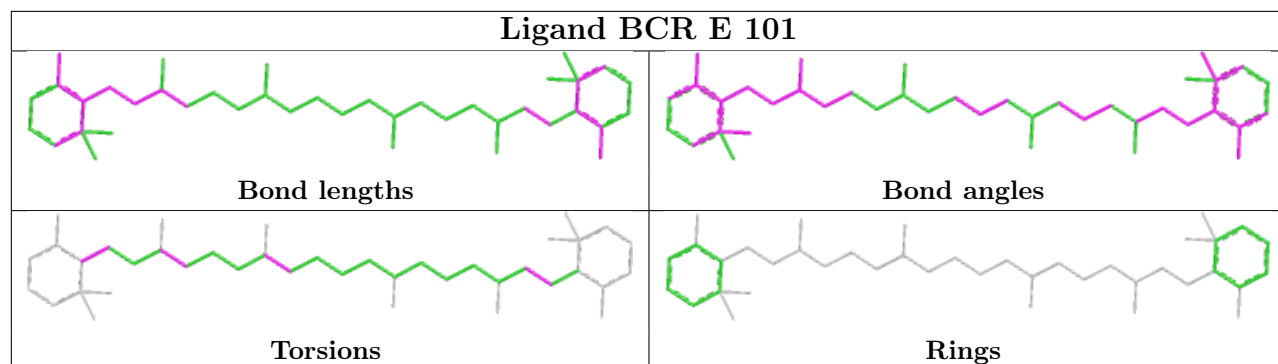
Bond angles

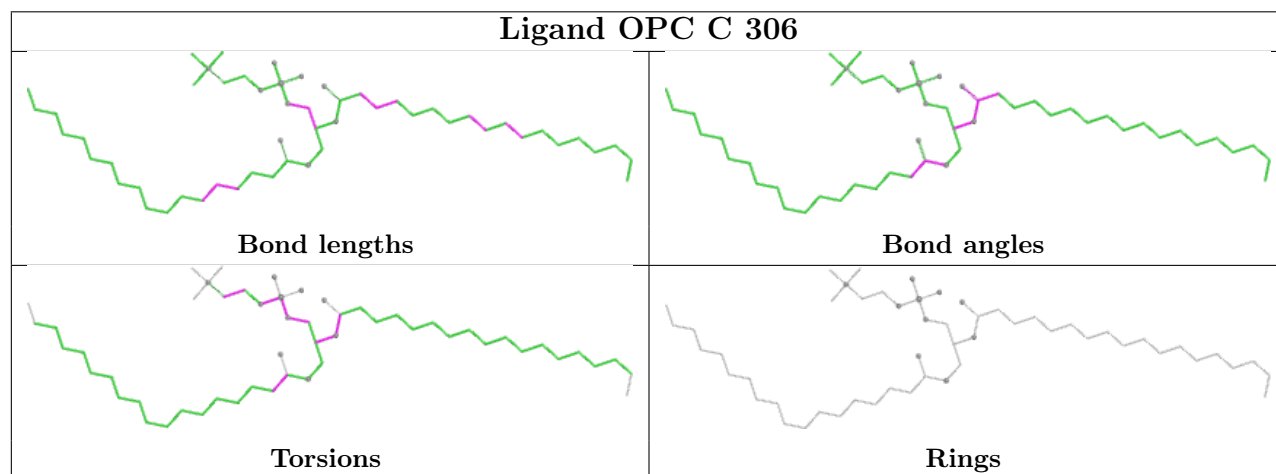
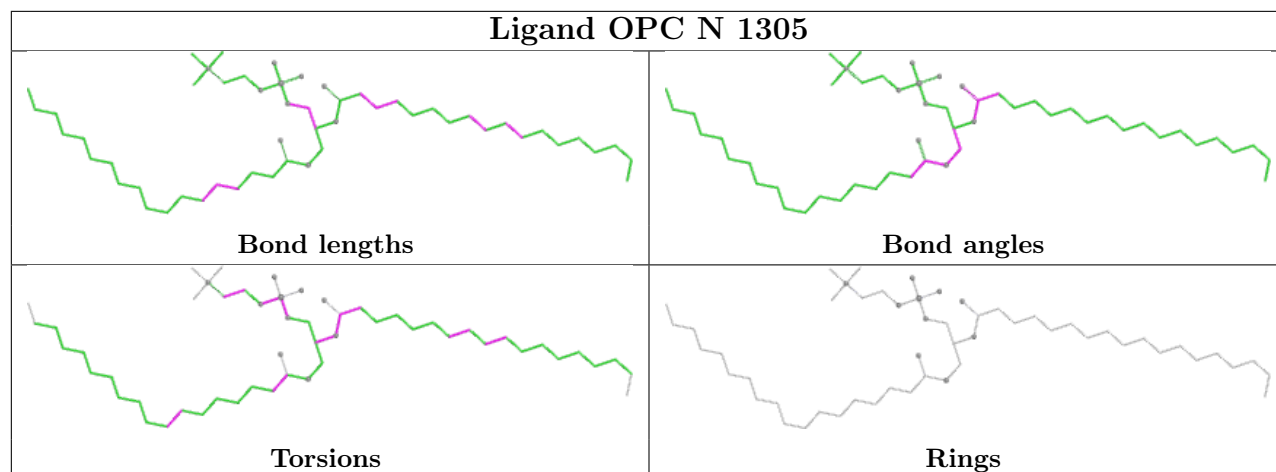


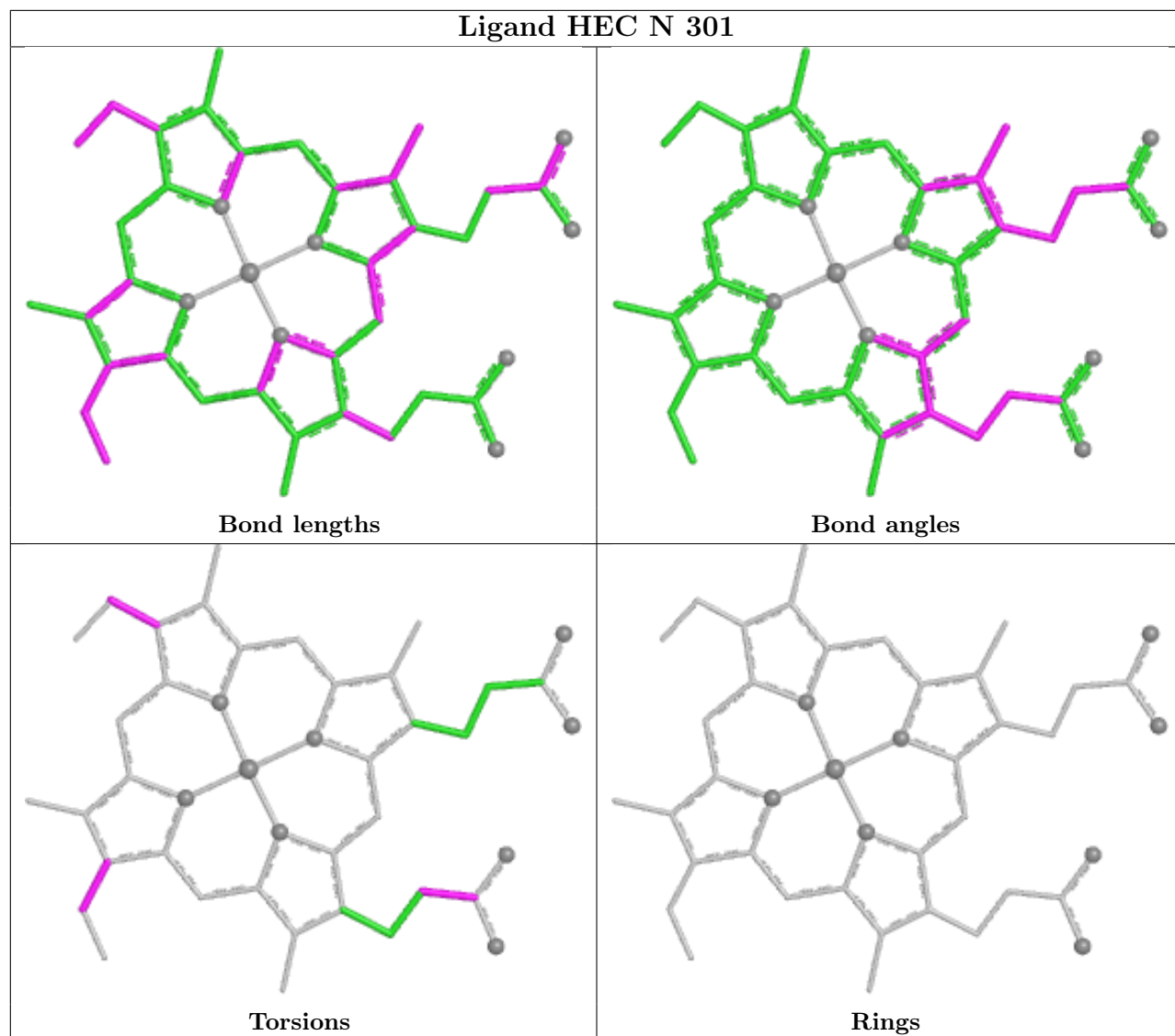
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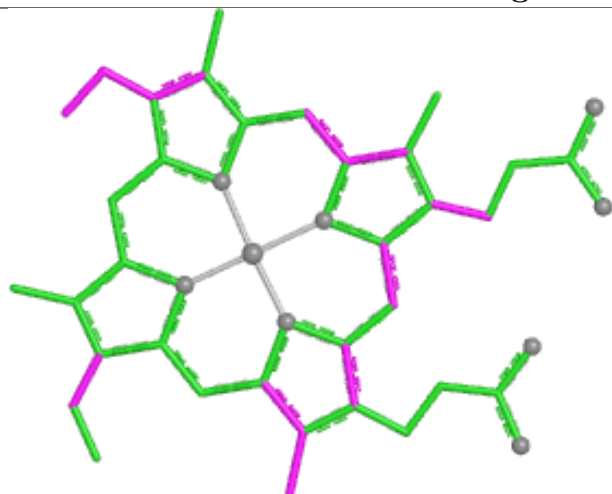
Rings



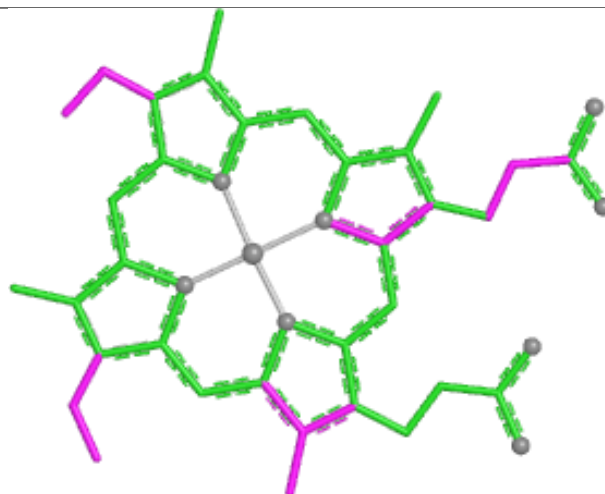




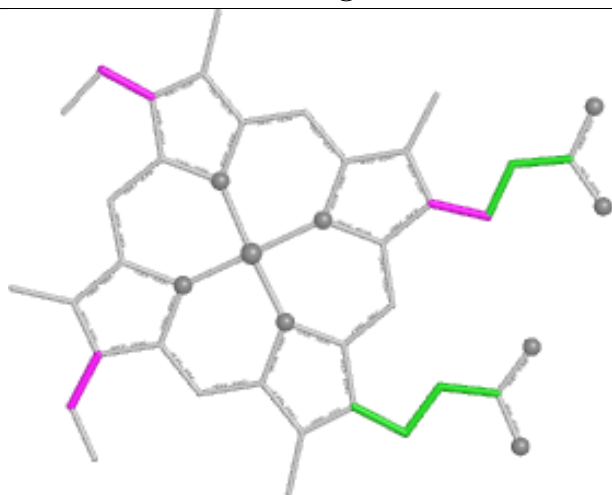
## Ligand HEC A 303



Bond lengths



Bond angles

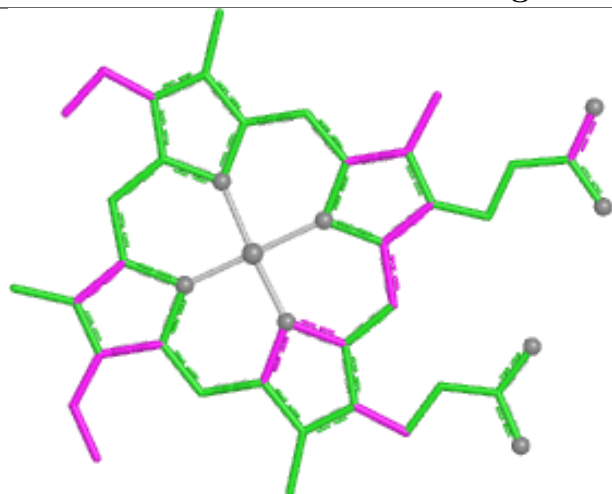


Torsions

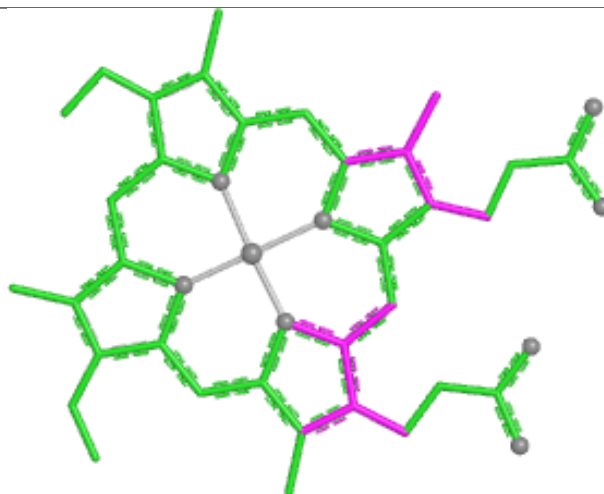


Rings

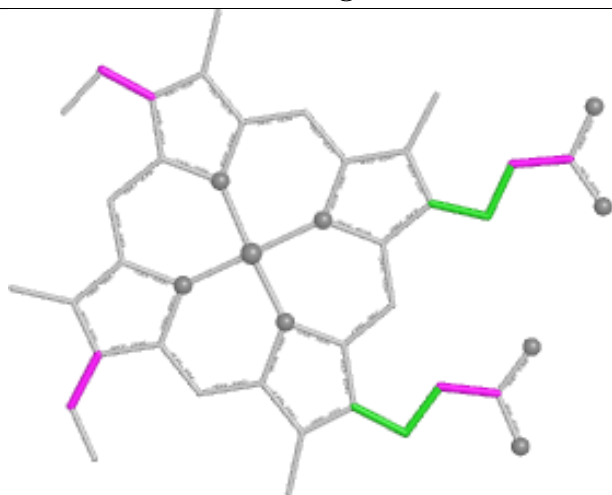
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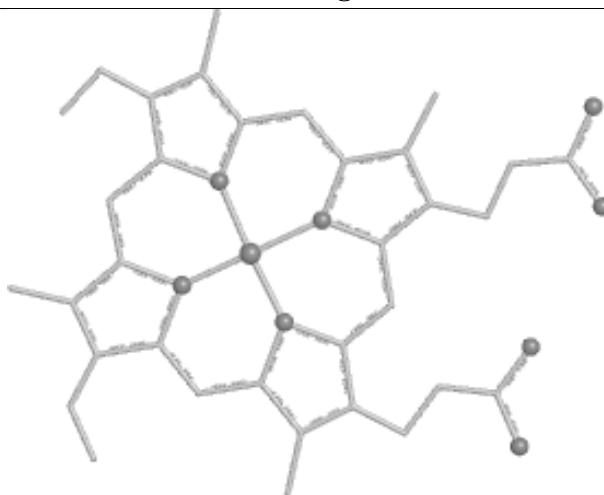
Bond lengths



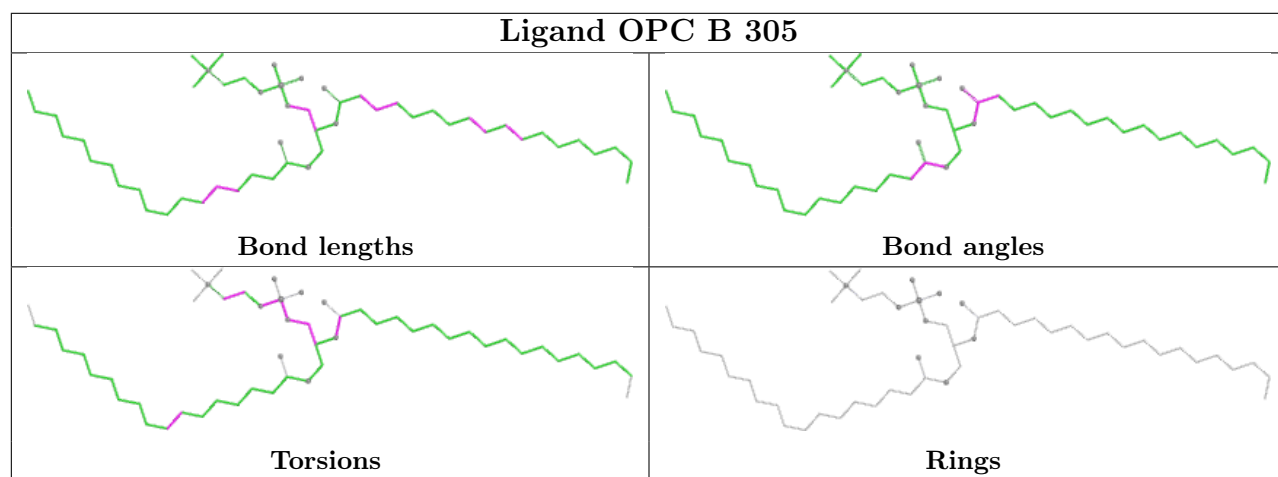
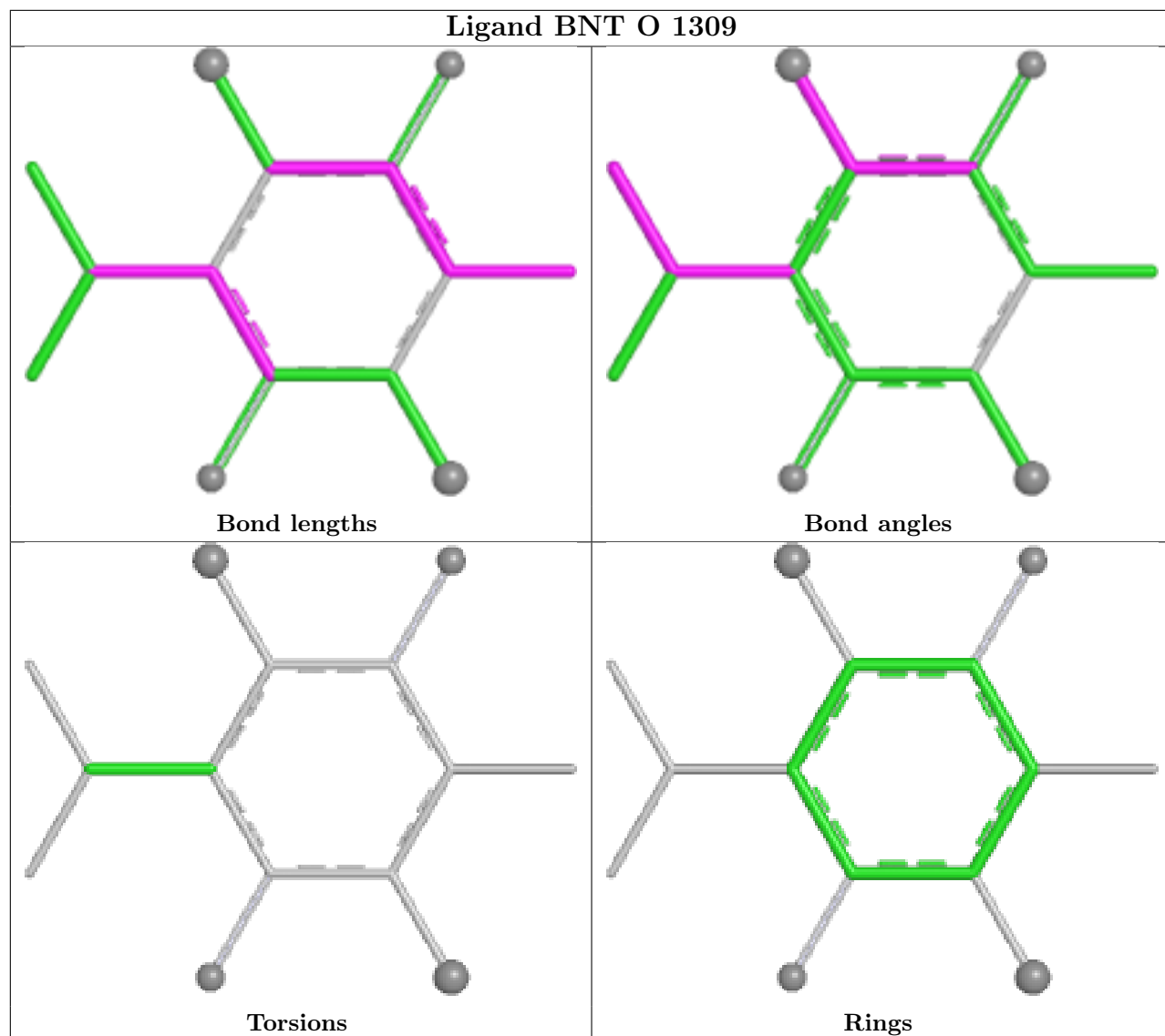
Bond angles



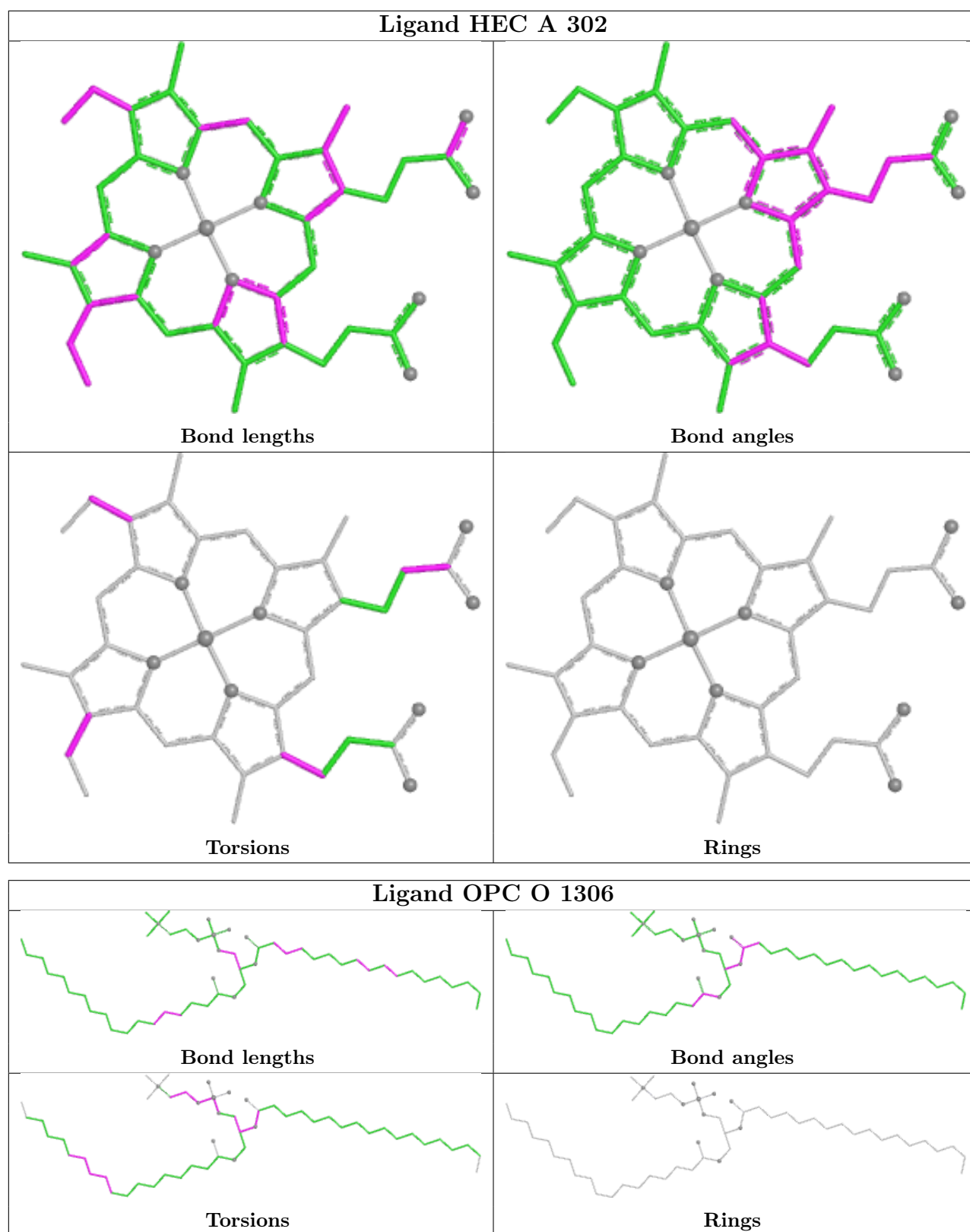
Torsions

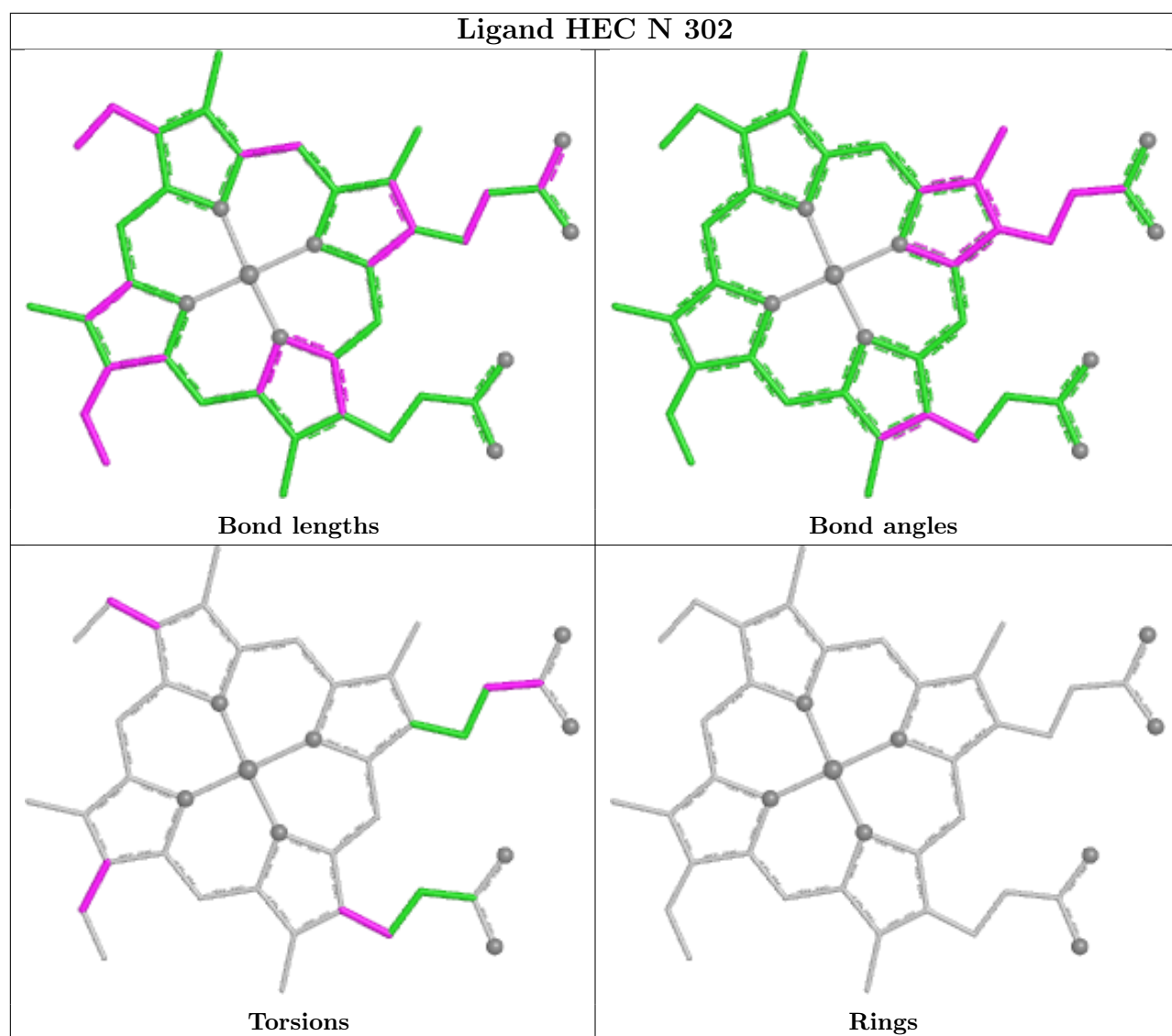


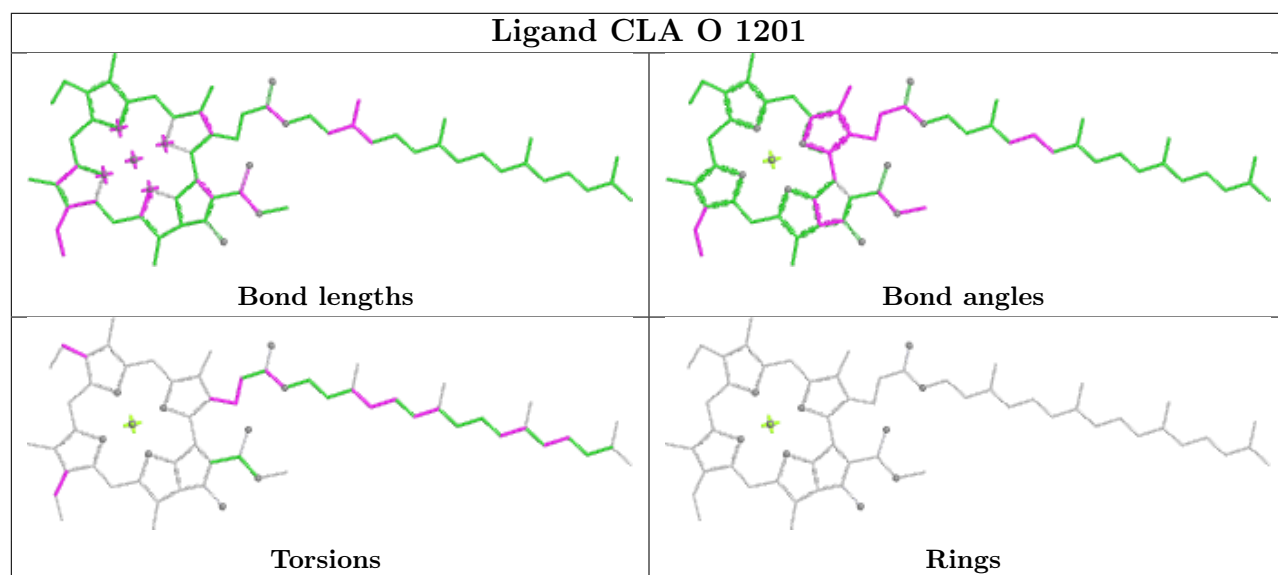
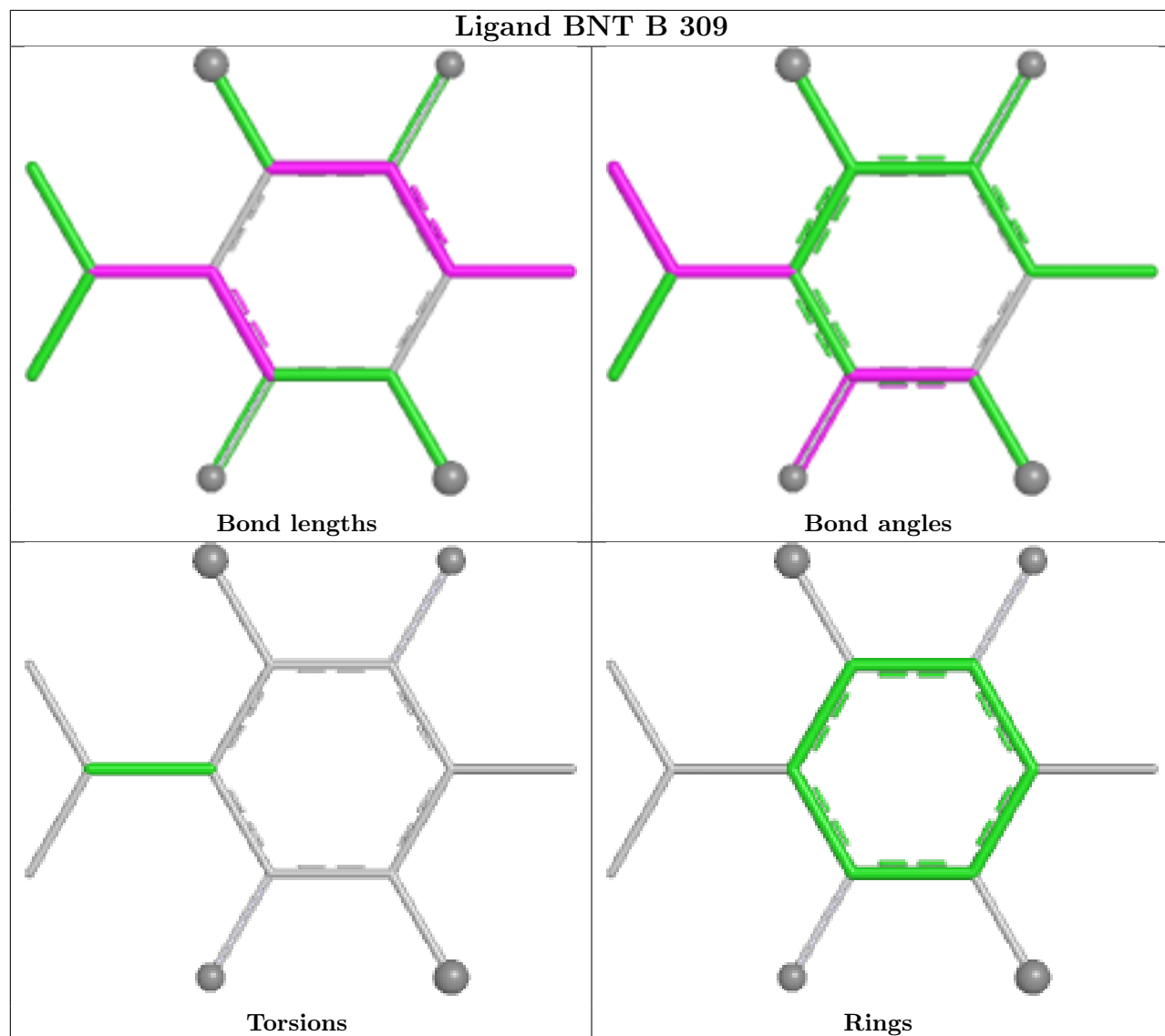
Rings

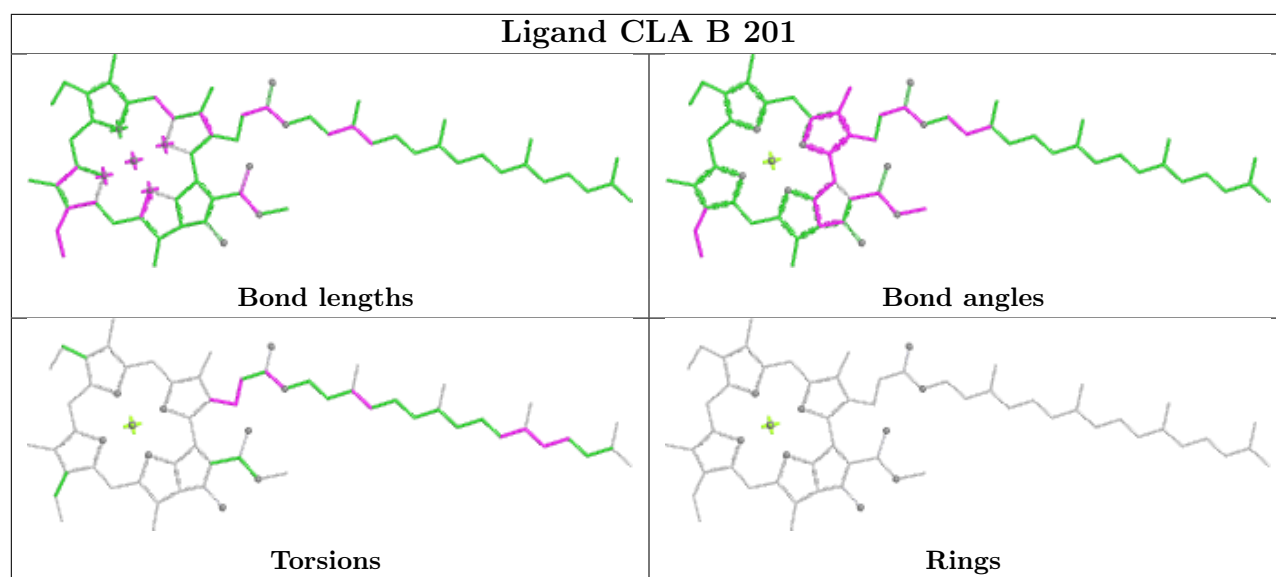












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	202/215 (93%)	-1.34	0	100	100	12, 58, 120, 164	0
1	N	202/215 (93%)	-1.38	0	100	100	11, 53, 104, 158	0
2	B	137/160 (85%)	-1.34	0	100	100	16, 67, 137, 177	0
2	O	137/160 (85%)	-1.23	1 (0%)	84	65	13, 63, 130, 183	0
3	C	286/289 (98%)	-1.12	2 (0%)	84	65	5, 85, 150, 200	1 (0%)
3	P	286/289 (98%)	-1.13	0	100	100	0, 85, 160, 200	1 (0%)
4	D	168/179 (93%)	-0.98	1 (0%)	85	68	18, 93, 169, 200	0
4	Q	168/179 (93%)	-1.03	0	100	100	26, 94, 158, 195	0
5	E	32/32 (100%)	-1.14	0	100	100	20, 67, 163, 195	0
5	R	32/32 (100%)	-1.23	0	100	100	21, 59, 111, 162	0
6	F	35/35 (100%)	-1.21	0	100	100	8, 69, 133, 144	0
6	S	35/35 (100%)	-1.35	0	100	100	16, 71, 113, 153	0
7	G	27/37 (72%)	-1.33	0	100	100	34, 66, 133, 147	0
7	T	27/37 (72%)	-1.32	0	100	100	30, 76, 136, 178	0
8	H	27/29 (93%)	-1.33	0	100	100	25, 68, 119, 156	0
8	U	27/29 (93%)	-1.30	0	100	100	29, 69, 128, 180	0
All	All	1828/1952 (93%)	-1.20	4 (0%)	91	81	0, 73, 149, 200	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	221	GLU	3.9
4	D	152	HIS	3.0
3	C	222	GLY	2.8
2	O	66	ALA	2.2

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

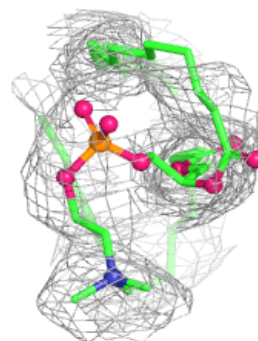
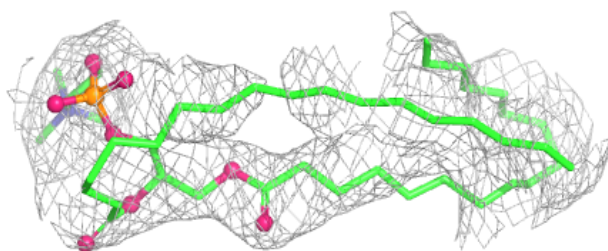
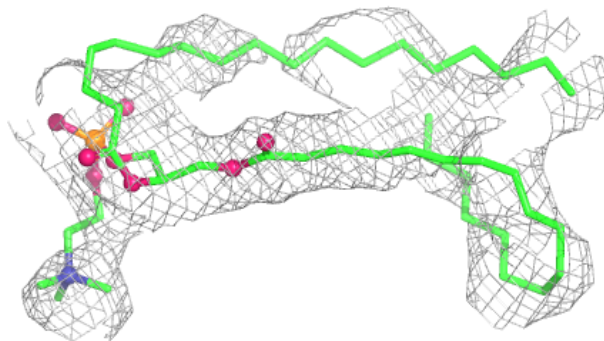
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	OPC	O	1306	54/55	0.98	0.05	73,73,73,73	0
9	HEC	N	303	43/43	0.99	0.05	67,74,74,74	0
10	OPC	B	305	54/55	0.99	0.05	66,66,66,66	0
10	OPC	C	306	54/55	0.99	0.05	84,84,84,84	0
10	OPC	N	1305	54/55	0.99	0.07	107,107,107,107	0
9	HEC	A	303	43/43	0.99	0.06	57,104,104,104	0
11	BNT	B	309	14/14	0.99	0.08	64,64,64,64	0
11	BNT	O	1309	14/14	0.99	0.10	64,64,64,64	0
12	CLA	B	201	65/65	0.99	0.06	20,112,112,112	0
12	CLA	O	1201	65/65	0.99	0.06	29,72,72,72	0
14	BCR	E	101	40/40	0.99	0.07	84,84,84,84	0
14	BCR	R	1101	40/40	0.99	0.09	181,181,181,181	0
9	HEC	A	302	43/43	1.00	0.03	41,58,58,58	0
9	HEC	P	301	43/43	1.00	0.03	54,76,76,76	0
9	HEC	A	301	43/43	1.00	0.02	31,48,48,48	0
9	HEC	C	301	43/43	1.00	0.02	36,59,59,59	0
13	FES	D	201	4/4	1.00	0.01	70,70,97,97	0
13	FES	Q	201	4/4	1.00	0.01	28,28,53,53	0
9	HEC	N	301	43/43	1.00	0.03	26,64,64,64	0
9	HEC	N	302	43/43	1.00	0.03	30,61,61,61	0

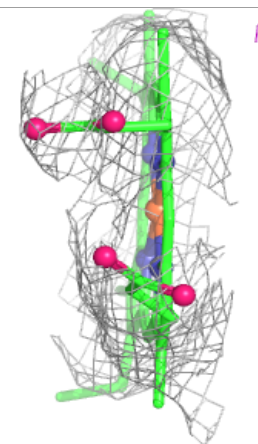
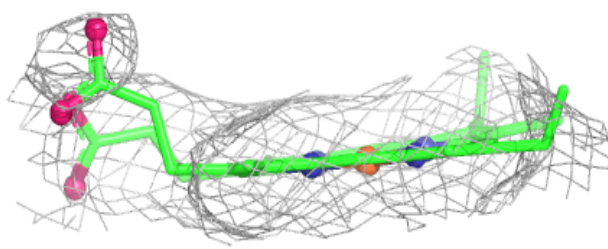
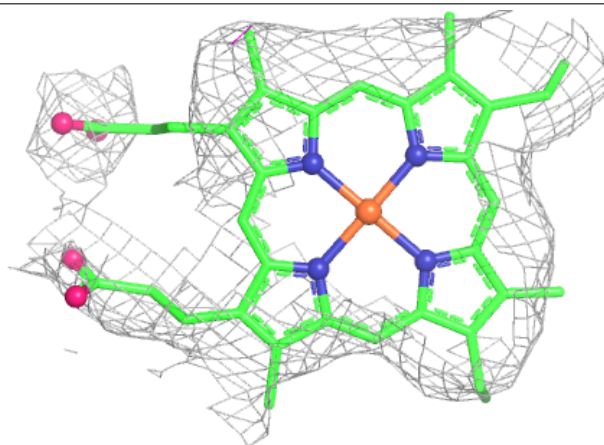
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OPC O 1306:**

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

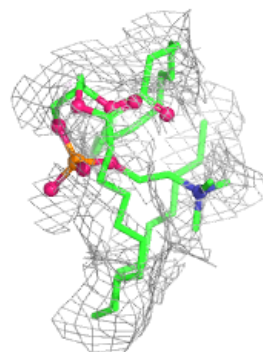
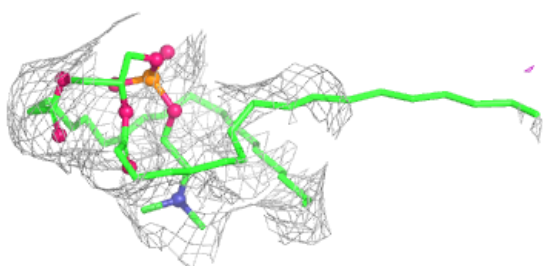
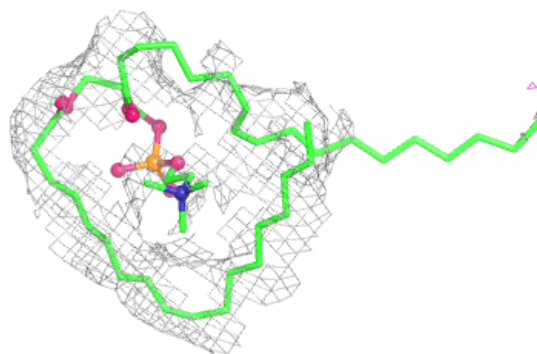
**Electron density around HEC N 303:**

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

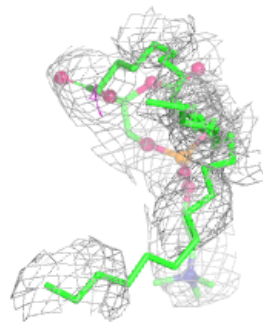
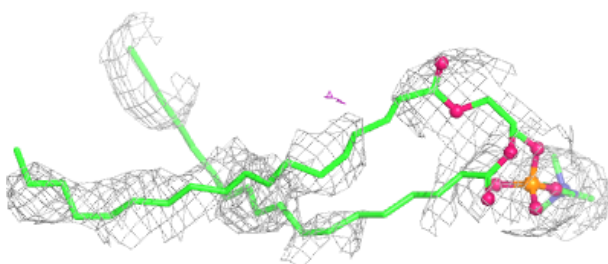
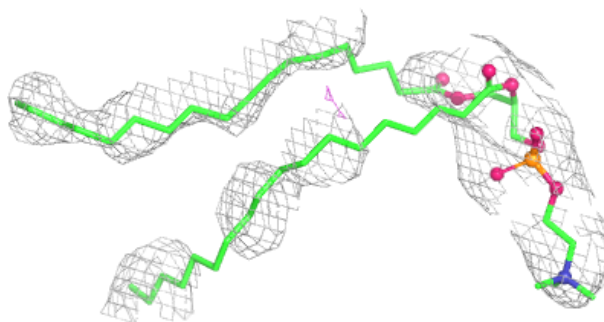


**Electron density around OPC B 305:**

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

**Electron density around OPC C 306:**

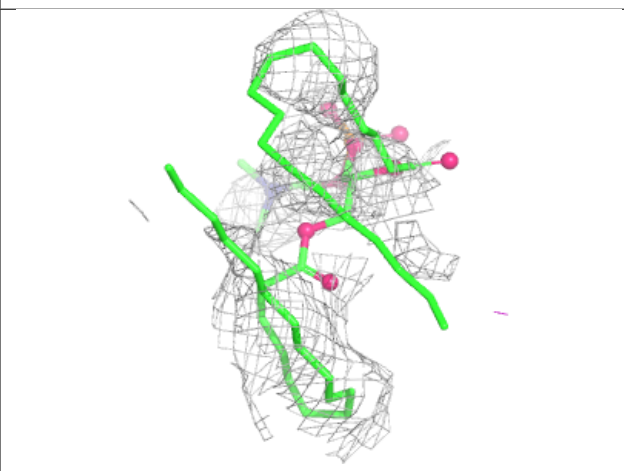
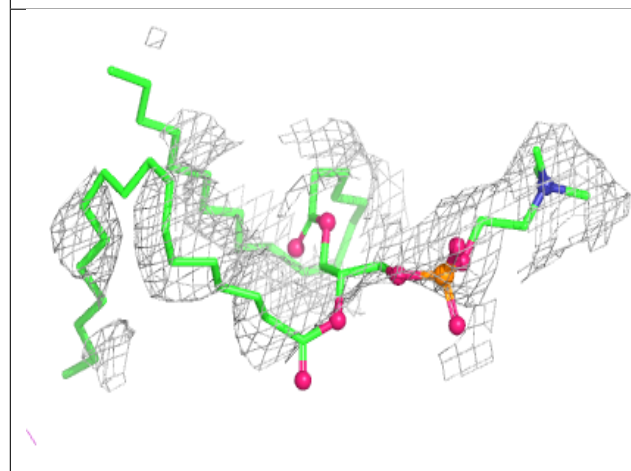
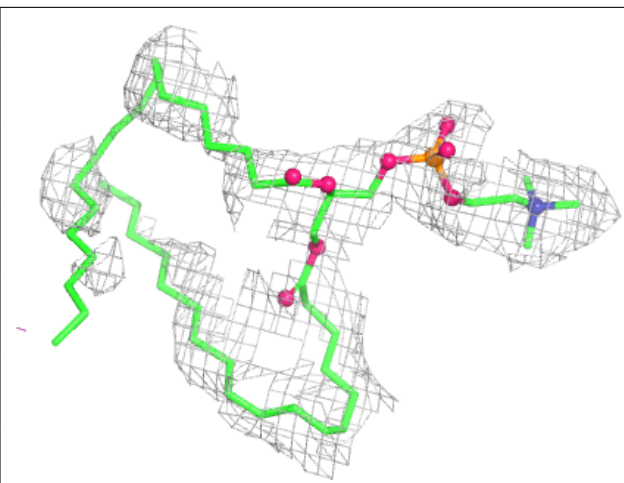
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





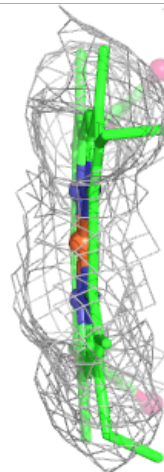
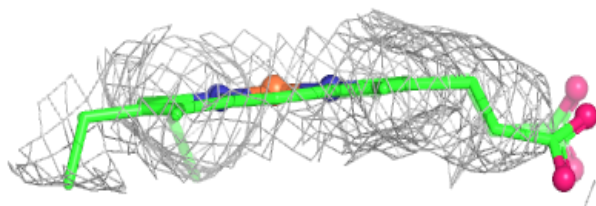
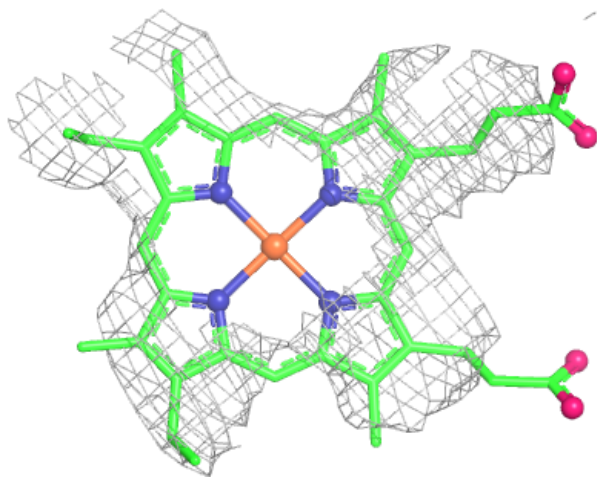
**Electron density around OPC N 1305:**

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



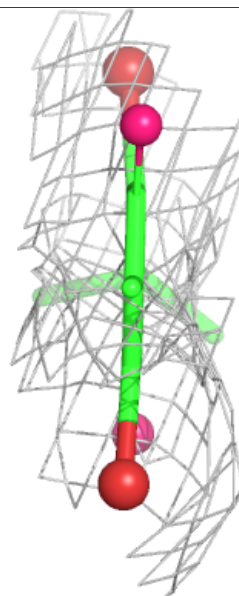
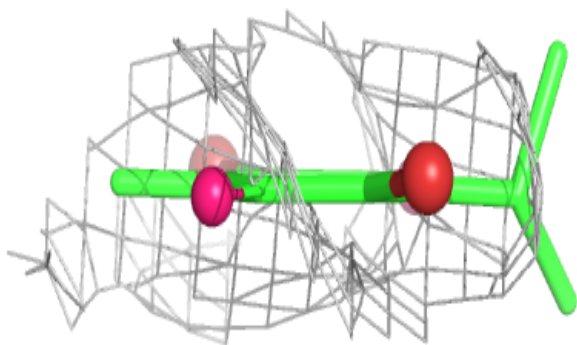
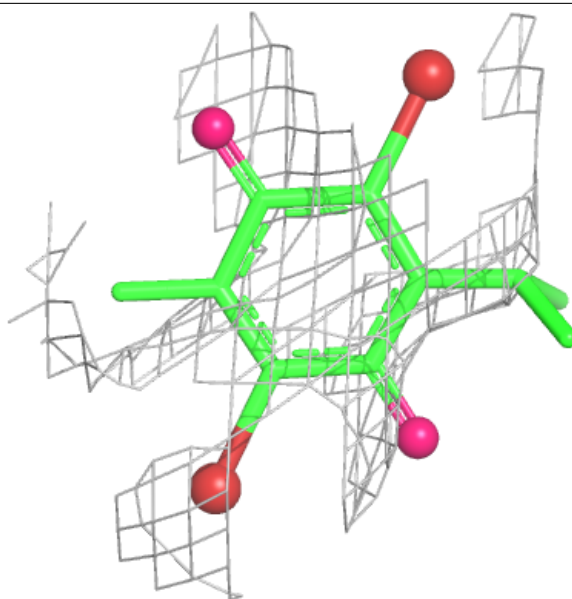
**Electron density around HEC A 303:**

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



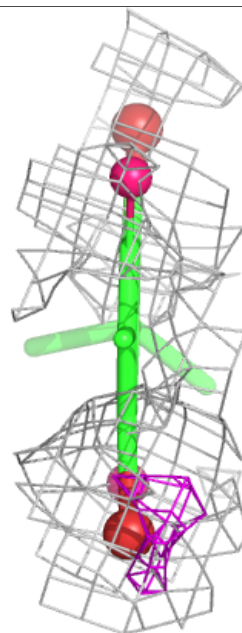
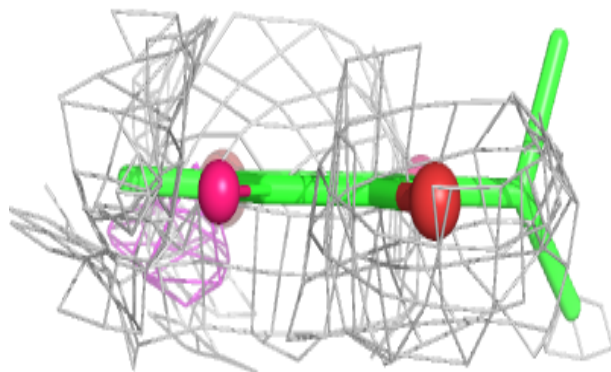
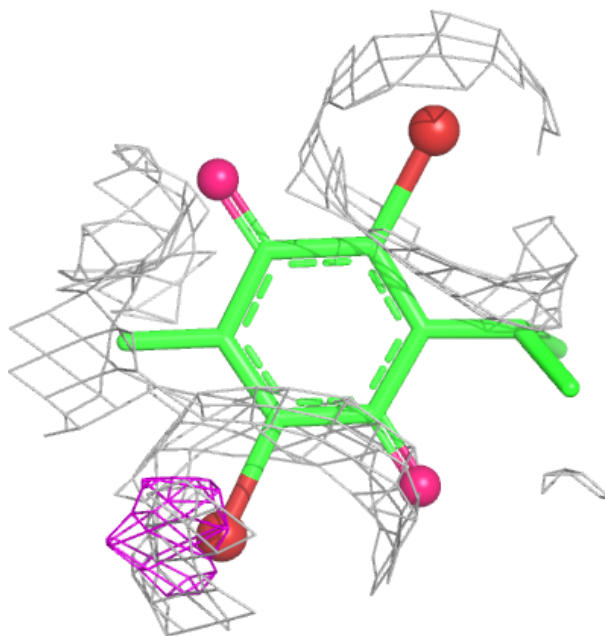
**Electron density around BNT B 309:**

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



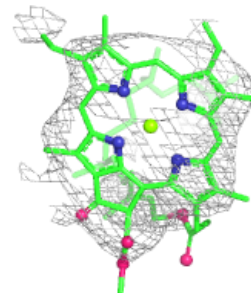
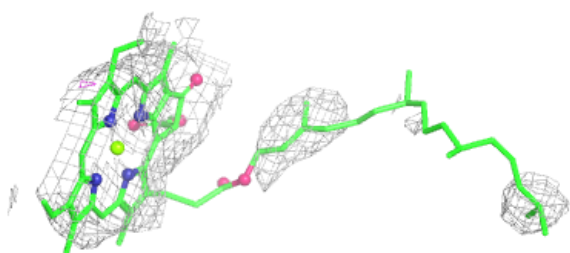
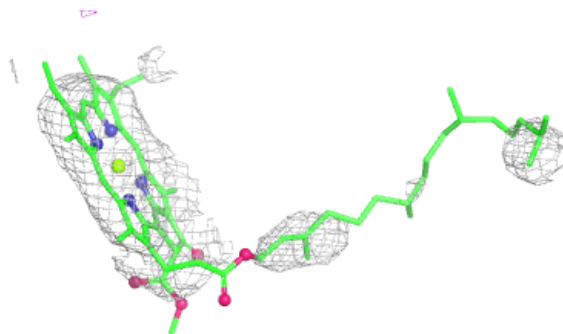
**Electron density around BNT O 1309:**

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and green (positive)

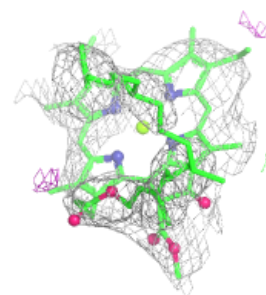
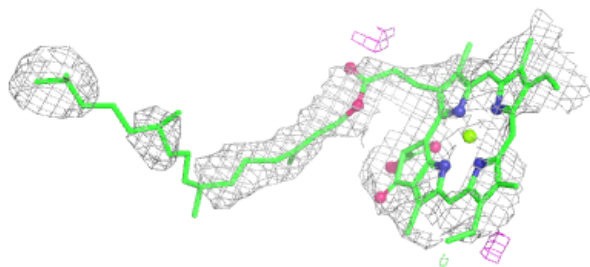
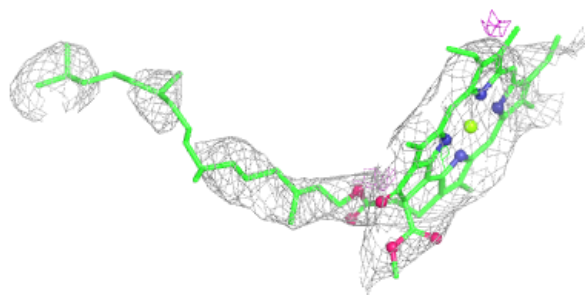


**Electron density around CLA B 201:**

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

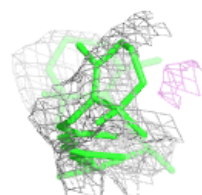
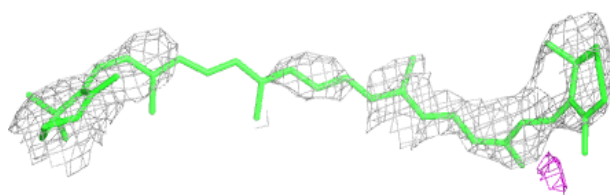
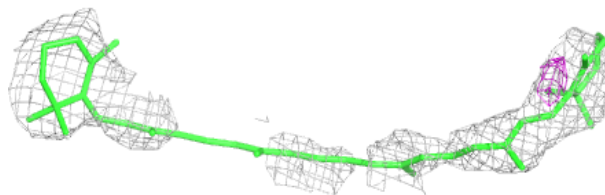
**Electron density around CLA O 1201:**

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

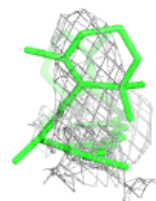
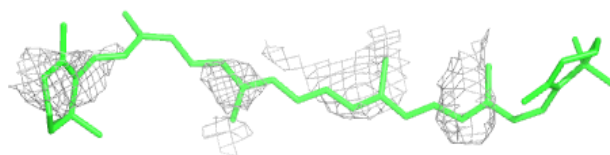
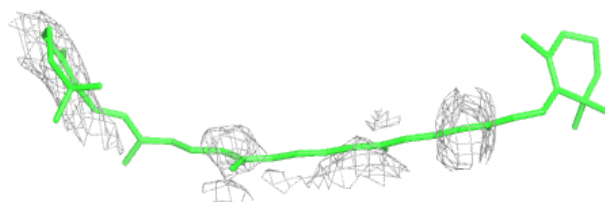


**Electron density around BCR E 101:**

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

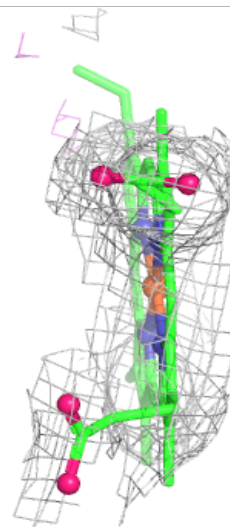
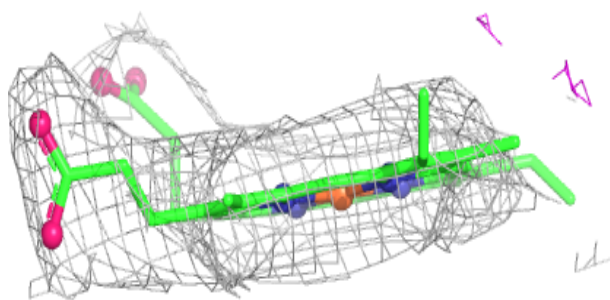
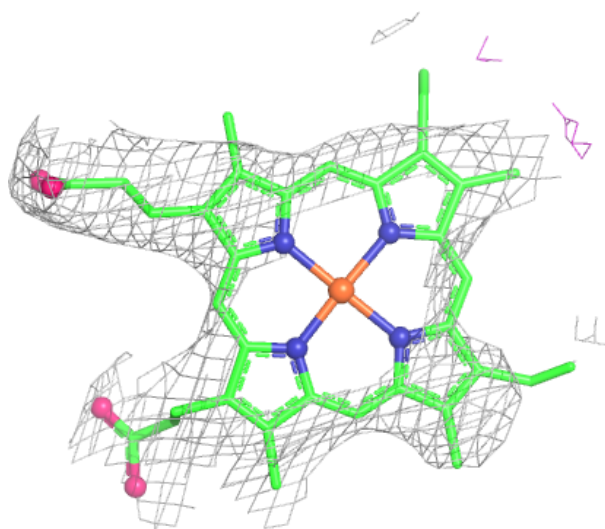
**Electron density around BCR R 1101:**

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



**Electron density around HEC A 302:**

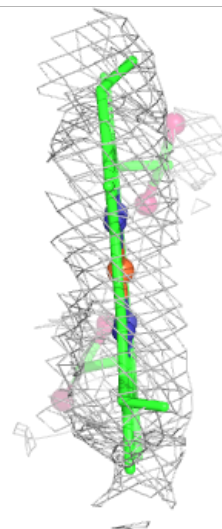
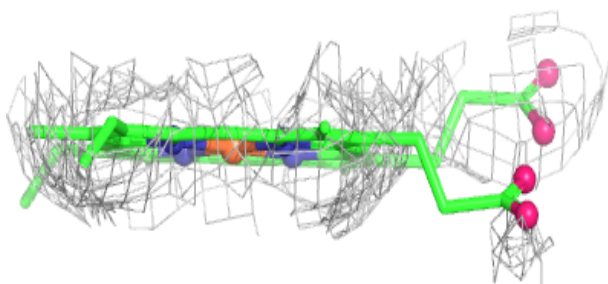
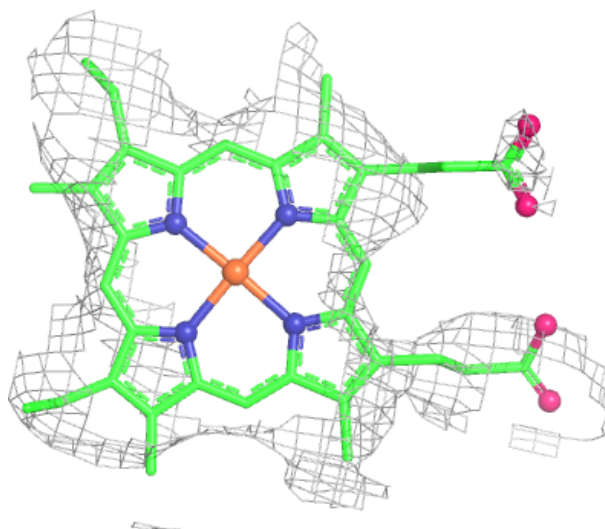
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC P 301:**

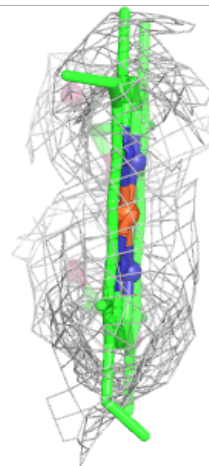
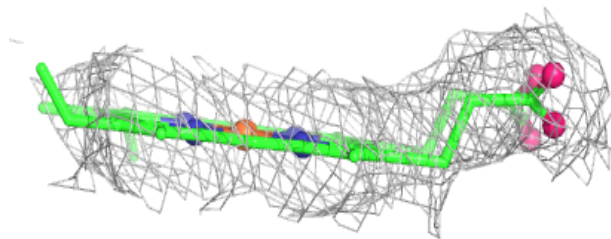
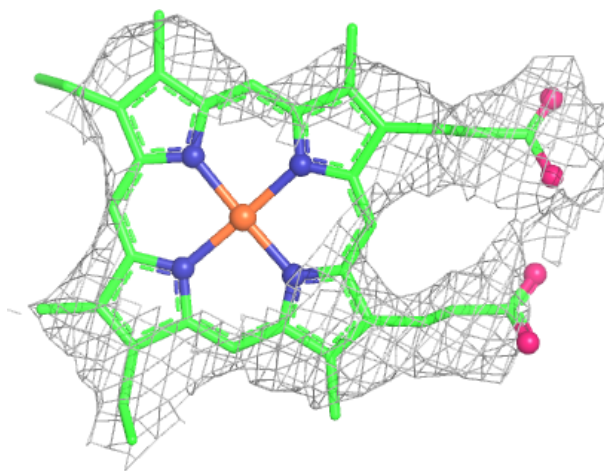
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





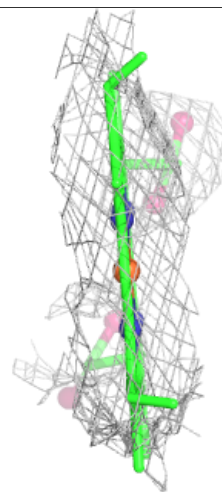
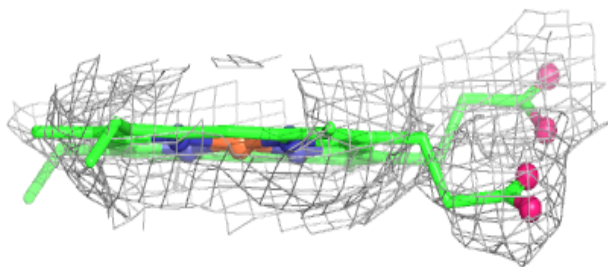
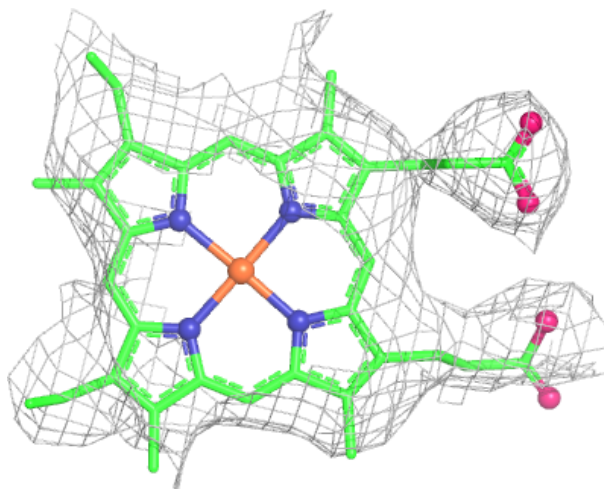
**Electron density around HEC A 301:**

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



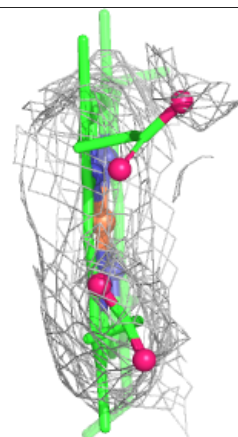
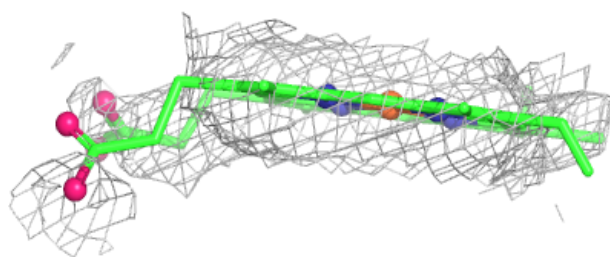
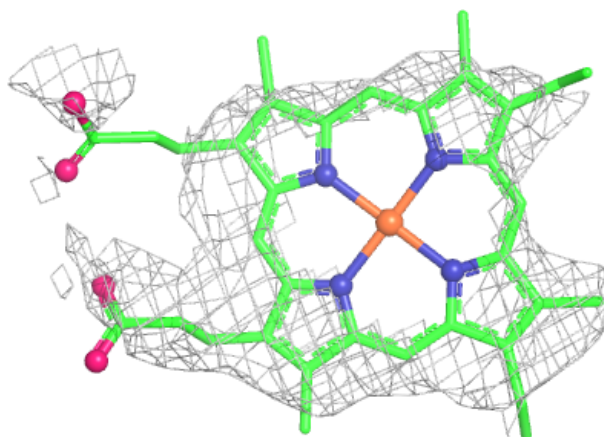
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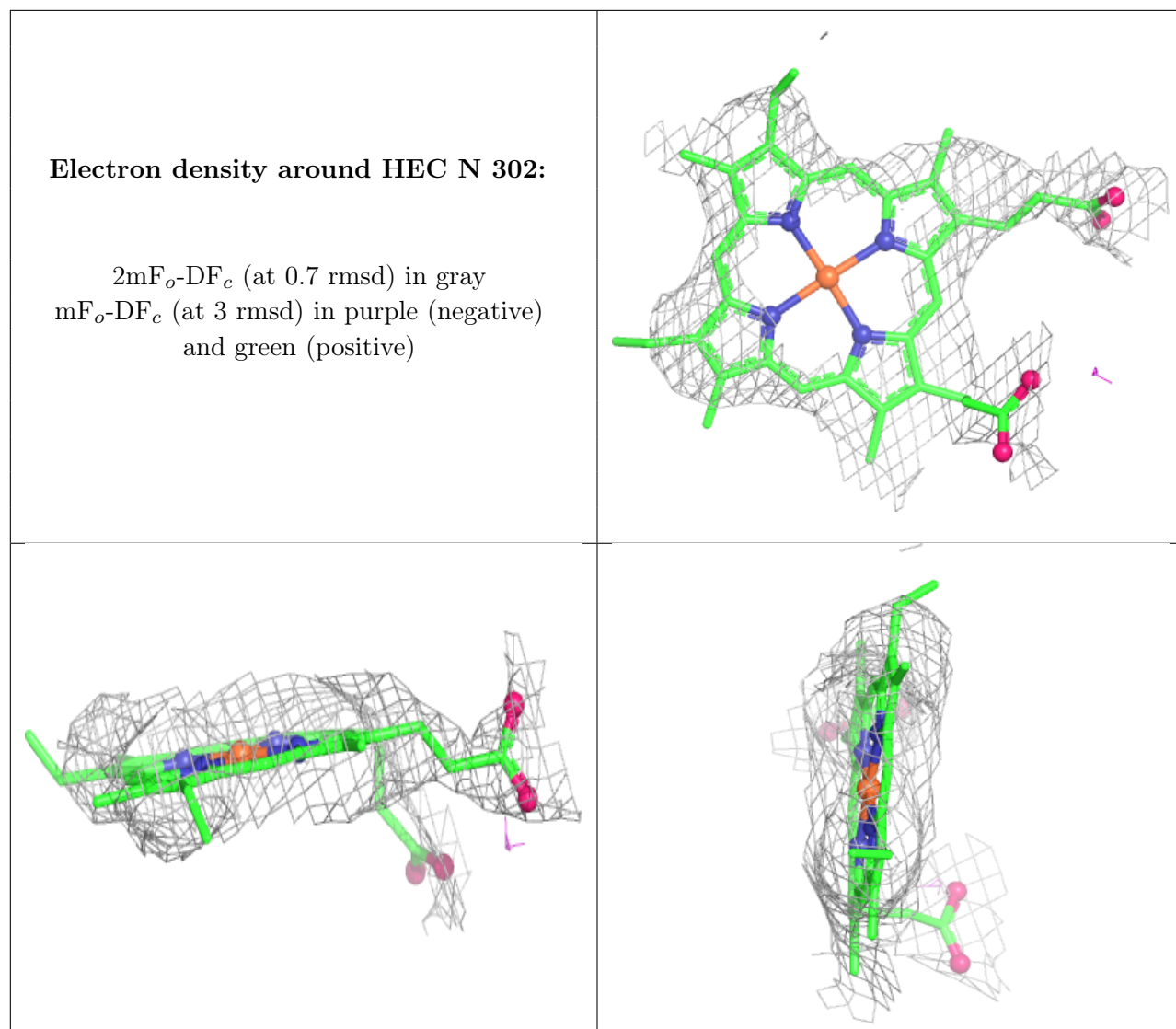
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC N 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.