



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 01:50 PM BST

PDB ID : 6XVF
Title : Crystal structure of bovine cytochrome bc1 in complex with tetrahydroquinolone inhibitor JAG021
Authors : Ampornpanai, K.; Hasnain, S.S.; Antonyuk, S.V.
Deposited on : 2020-01-21
Resolution : 3.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

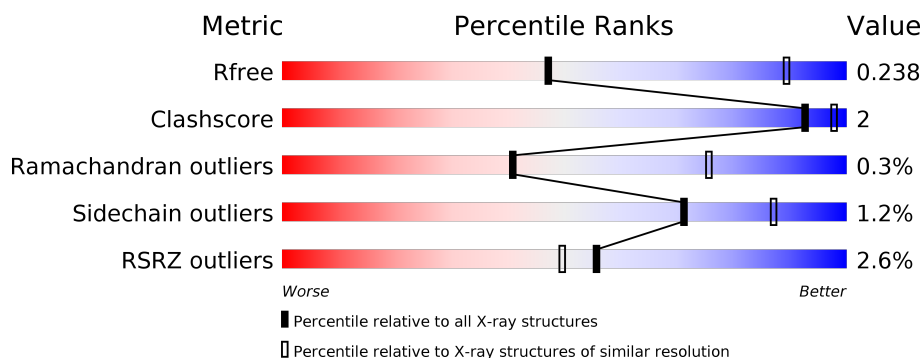
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



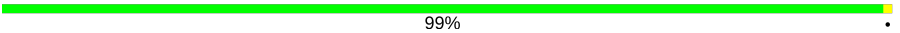
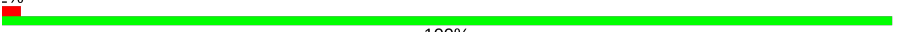

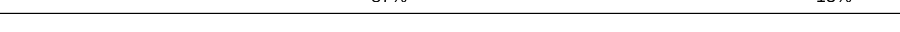
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	445	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>6%</div> <div></div> </div> <div>• •</div> </div>
2	B	418	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div>• •</div> </div>
3	C	378	<div> <div></div> <div> <div></div> <div>94%</div> <div>6%</div> </div> <div>•</div> </div>
4	D	239	<div> <div>8%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>•</div> </div>
5	E	196	<div> <div>3%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>•</div> </div>
6	F	100	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	74	 99%
8	H	64	 2% 100%
9	I	46	 11% 87% 13%
10	J	59	 97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PG4	C	404	-	-	-	X
11	PG4	C	405	-	-	-	X
14	CDL	E	205	-	-	-	X
16	LMT	C	403	-	-	-	X
17	PEE	C	407	X	-	-	-
17	PEE	E	204	X	-	-	-
18	JAG	C	408	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 16121 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
1	A	438	Total	C	N	O	S	0	0	0
			3350	2095	591	644	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3061	1920	541	593	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			2993	2004	471	500	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1859	1187	320	337	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1451	906	254	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			855	542	156	155	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	406	116	97	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			506	307	91	103	5			

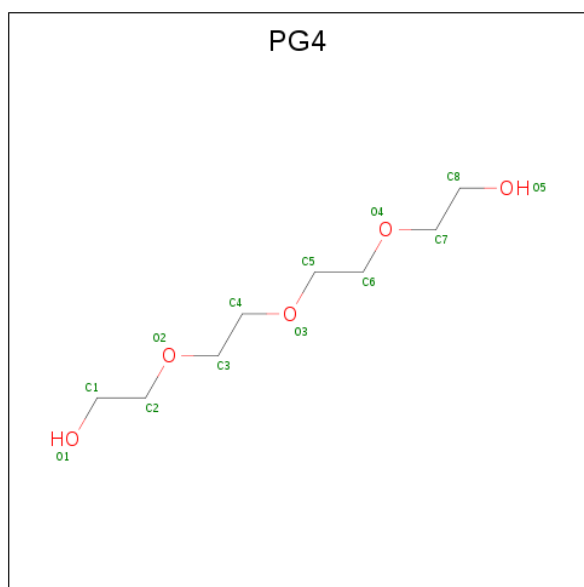
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			329	202	63	63	1			

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

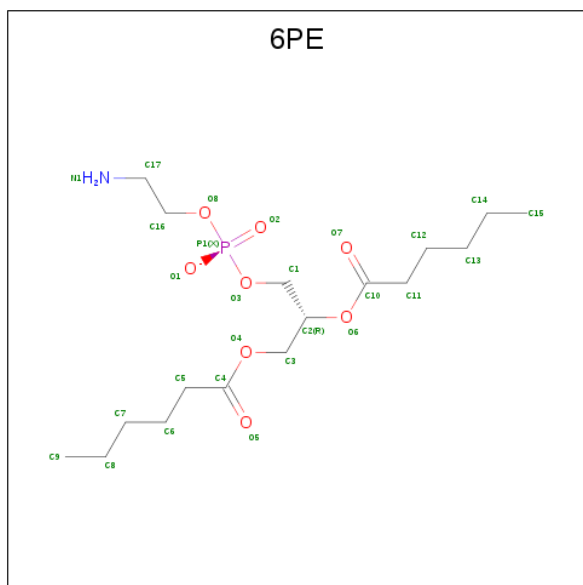
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			481	317	81	83			

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



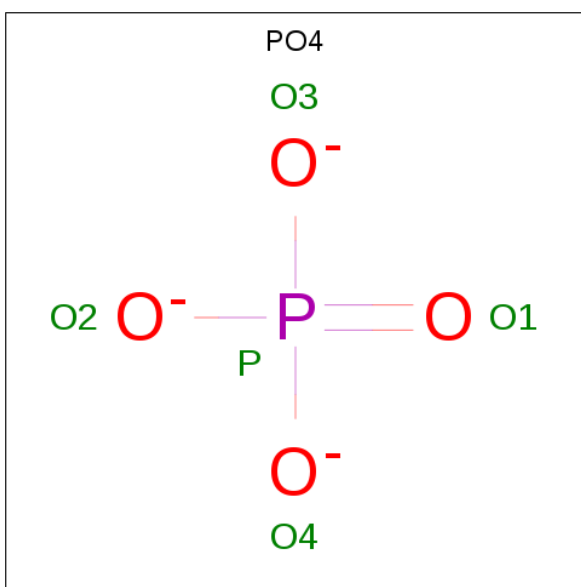
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			13	8	5		
11	C	1	Total	C	O	0	0
			13	8	5		
11	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: $C_{17}H_{33}NO_8P$).



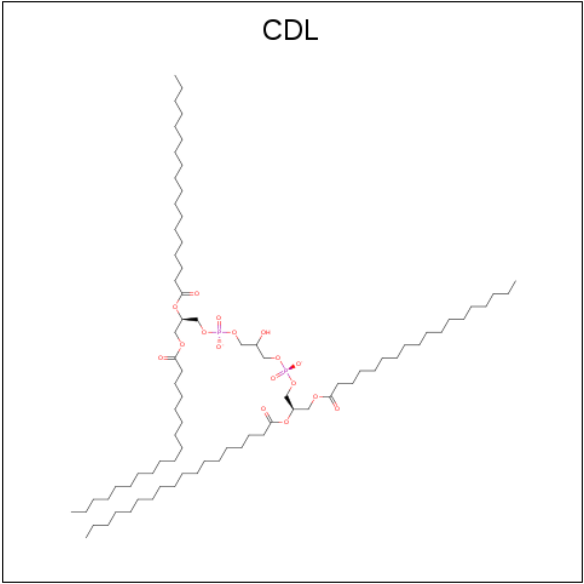
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



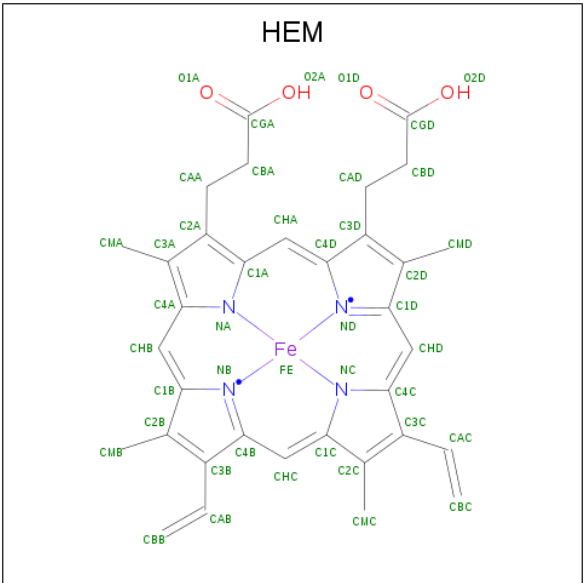
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	P	0	0
			5	4	1		
13	B	1	Total	O	P	0	0
			5	4	1		
13	C	1	Total	O	P	0	0
			5	4	1		
13	D	1	Total	O	P	0	0
			5	4	1		
13	E	1	Total	O	P	0	0
			5	4	1		
13	F	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



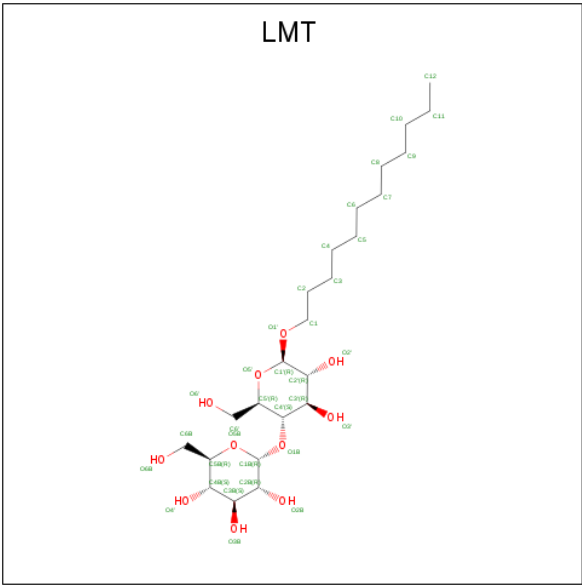
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			34	17	15	2		
14	C	1	Total	C	O	P	0	0
			44	25	17	2		
14	D	1	Total	C	O	P	0	0
			54	35	17	2		
14	E	1	Total	C	O	P	0	0
			60	41	17	2		

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



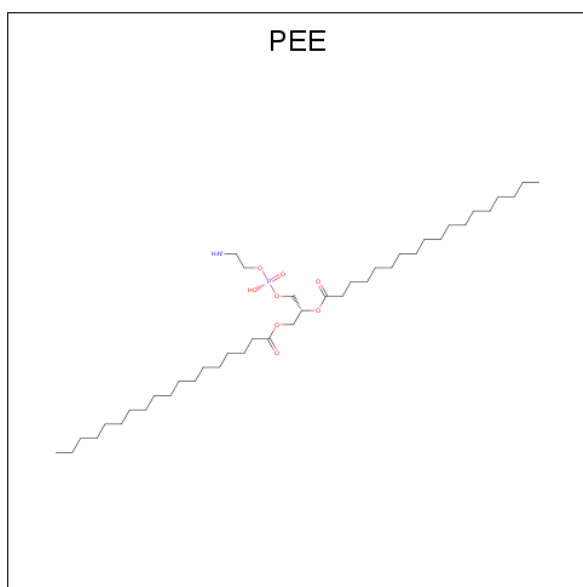
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



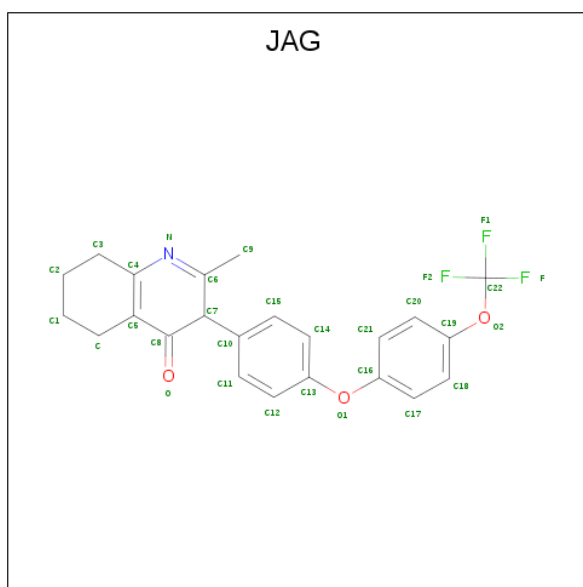
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O		
			35	24	11		

- Molecule 17 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



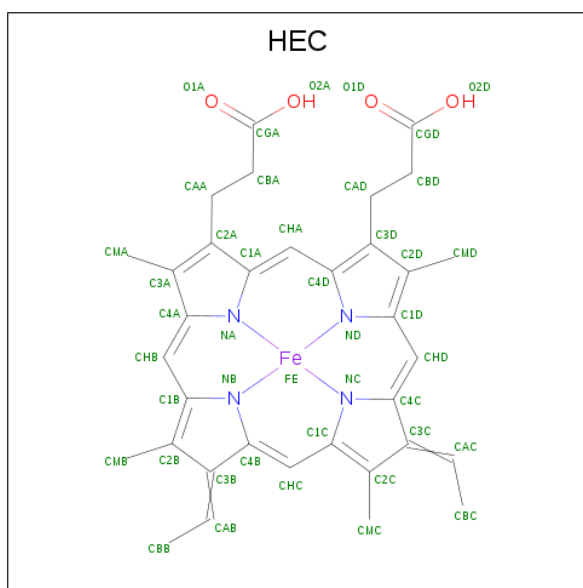
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
17	E	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

- Molecule 18 is 2-methyl-3-[4-[4-(trifluoromethoxy)phenoxy]phenyl]-5,6,7,8-tetrahydro-3 {H}-quinolin-4-one (three-letter code: JAG) (formula: $C_{23}H_{20}F_3NO_3$) (labeled as "Ligand of Interest" by author).



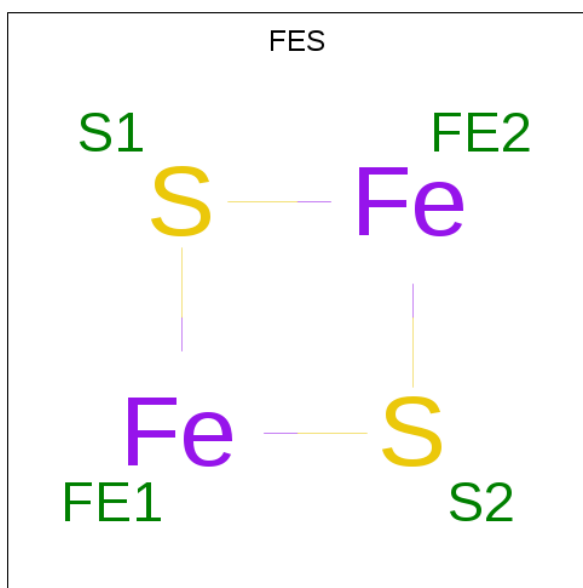
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	F	N	O	0	0
			30	23	3	1	3		

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

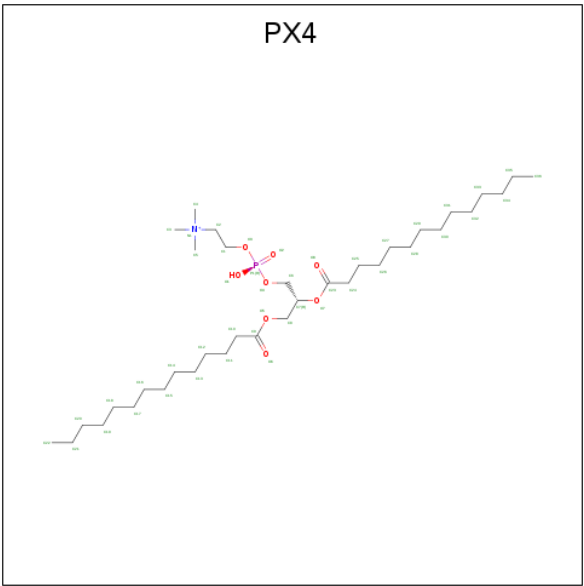
- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter

code: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	E	1	Total	C	N	O	P	0	0
			37	27	1	8	1		

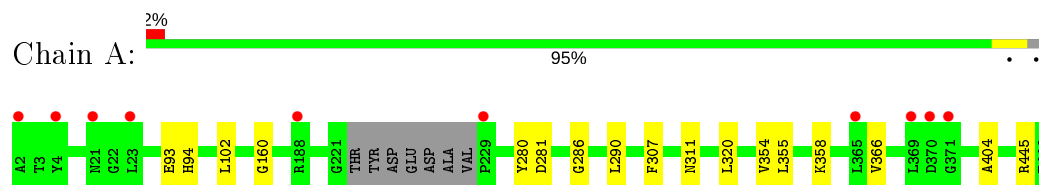
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	6	Total	O	0	0
			6	6		
22	B	2	Total	O	0	0
			2	2		
22	C	4	Total	O	0	0
			4	4		
22	D	2	Total	O	0	0
			2	2		
22	F	1	Total	O	0	0
			1	1		
22	G	1	Total	O	0	0
			1	1		
22	I	2	Total	O	0	0
			2	2		
22	J	1	Total	O	0	0
			1	1		

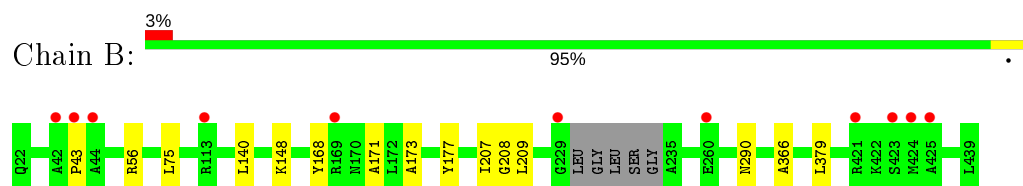
3 Residue-property plots [i](#)

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.

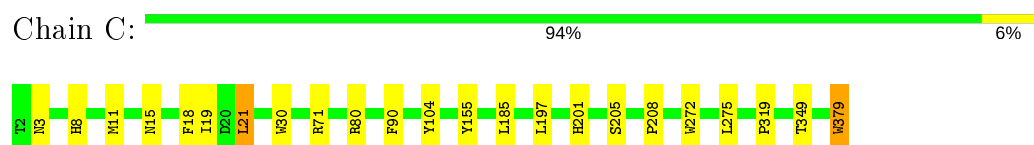
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



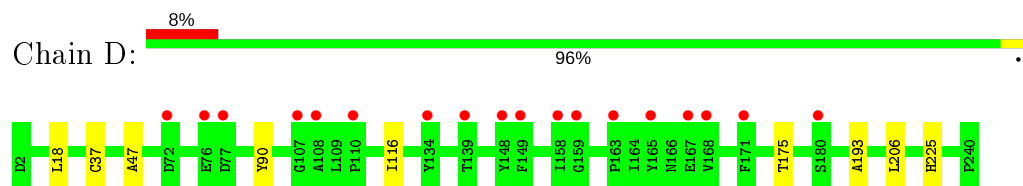
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



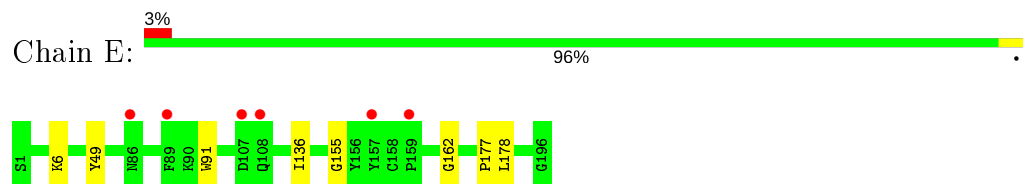
- Molecule 3: Cytochrome b



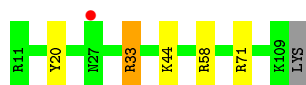
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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



- Molecule 6: Cytochrome b-c1 complex subunit 7



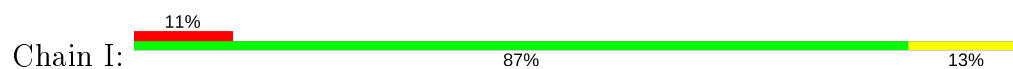
- Molecule 7: Cytochrome b-c1 complex subunit 8



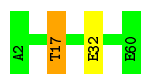
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



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



- Molecule 10: Cytochrome b-c1 complex subunit 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	209.87Å 209.87Å 342.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.88 – 3.50 90.88 – 3.45	Depositor EDS
% Data completeness (in resolution range)	90.4 (90.88-3.50) 90.5 (90.88-3.45)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.217 , 0.232 0.222 , 0.238	Depositor DCC
R_{free} test set	2659 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 113.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16121	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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: JAG, CDL, PO4, LMT, PX4, 6PE, PG4, FES, HEC, PEE, HEM

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	0.42	0/3421	0.66	0/4646
2	B	0.42	0/3115	0.64	0/4230
3	C	0.46	0/3089	0.64	0/4227
4	D	0.42	0/1918	0.65	0/2611
5	E	0.44	0/1484	0.62	0/2015
6	F	0.44	0/874	0.67	0/1177
7	G	0.51	0/641	0.66	0/868
8	H	0.40	0/511	0.69	0/690
9	I	0.51	0/333	0.82	0/453
10	J	0.44	0/494	0.62	0/668
All	All	0.44	0/15880	0.65	0/21585

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	3350	0	3213	10	0
2	B	3061	0	2999	10	0
3	C	2993	0	3049	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1859	0	1764	9	0
5	E	1451	0	1351	4	0
6	F	855	0	827	2	0
7	G	620	0	624	1	0
8	H	506	0	471	0	0
9	I	329	0	328	4	0
10	J	481	0	476	3	0
11	A	13	0	18	0	0
11	C	26	0	36	0	0
12	A	23	0	19	2	0
13	A	5	0	0	0	0
13	B	5	0	0	0	0
13	C	5	0	0	0	0
13	D	5	0	0	0	0
13	E	5	0	0	0	0
13	F	5	0	0	0	0
13	G	15	0	0	0	0
14	A	34	0	24	2	0
14	C	44	0	32	0	0
14	D	54	0	52	0	0
14	E	60	0	64	0	0
15	C	86	0	60	5	0
16	C	35	0	46	0	0
17	C	40	0	54	1	0
17	E	23	0	18	0	0
18	C	30	0	0	0	0
19	D	43	0	32	5	0
20	E	4	0	0	0	0
21	E	37	0	51	1	0
22	A	6	0	0	0	0
22	B	2	0	0	0	0
22	C	4	0	0	0	0
22	D	2	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	0	0
All	All	16121	0	15608	48	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 2.

The worst 5 of 48 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	19:D:501:HEC:CAB	2.66	0.83
2:B:290:ASN:ND2	9:I:56:ARG:HE	1.90	0.68
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.81	0.63
15:C:401:HEM:HMC1	15:C:401:HEM:HBC2	1.80	0.62
4:D:37:CYS:SG	19:D:501:HEC:C3B	2.91	0.59

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	434/445 (98%)	417 (96%)	16 (4%)	1 (0%)	47	81
2	B	409/418 (98%)	395 (97%)	14 (3%)	0	100	100
3	C	376/378 (100%)	362 (96%)	13 (4%)	1 (0%)	41	75
4	D	237/239 (99%)	224 (94%)	13 (6%)	0	100	100
5	E	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	10	45
6	F	97/100 (97%)	97 (100%)	0	0	100	100
7	G	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
8	H	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
9	I	44/46 (96%)	43 (98%)	0	1 (2%)	6	36
10	J	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
All	All	1982/2019 (98%)	1903 (96%)	73 (4%)	6 (0%)	41	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	162	GLY
1	A	445	ARG
3	C	155	TYR

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Mol	Chain	Res	Type
9	I	41	PRO
5	E	177	PRO

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	352/369 (95%)	351 (100%)	1 (0%)	92	97
2	B	314/327 (96%)	314 (100%)	0	100	100
3	C	324/326 (99%)	315 (97%)	9 (3%)	43	72
4	D	193/204 (95%)	192 (100%)	1 (0%)	88	94
5	E	149/168 (89%)	148 (99%)	1 (1%)	84	93
6	F	87/92 (95%)	83 (95%)	4 (5%)	27	61
7	G	65/66 (98%)	65 (100%)	0	100	100
8	H	57/61 (93%)	57 (100%)	0	100	100
9	I	34/38 (90%)	32 (94%)	2 (6%)	19	53
10	J	48/49 (98%)	47 (98%)	1 (2%)	53	79
All	All	1623/1700 (96%)	1604 (99%)	19 (1%)	71	87

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	349	THR
4	D	175	THR
6	F	71	ARG
3	C	205	SER
9	I	49	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS

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Mol	Chain	Res	Type
1	A	165	GLN
2	B	290	ASN
3	C	322	GLN
4	D	225	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

26 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	$\# Z > 2$
14	CDL	C	406	-	43,43,99	1.51	4 (9%)	49,55,111	1.37	6 (12%)
18	JAG	C	408	-	32,33,33	1.65	4 (12%)	42,48,48	1.67	6 (14%)
21	PX4	E	202	-	36,36,45	1.29	2 (5%)	42,44,53	1.18	5 (11%)
14	CDL	A	504	-	33,33,99	1.26	2 (6%)	37,43,111	1.31	3 (8%)
13	PO4	G	102	-	4,4,4	0.93	0	6,6,6	0.44	0
11	PG4	C	404	-	12,12,12	0.53	0	11,11,11	0.36	0
16	LMT	C	403	-	36,36,36	0.78	1 (2%)	47,47,47	1.21	6 (12%)
13	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.48	0
13	PO4	D	502	-	4,4,4	0.96	0	6,6,6	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PO4	B	501	-	4,4,4	0.93	0	6,6,6	0.41	0
14	CDL	E	205	-	59,59,99	1.21	4 (6%)	65,71,111	1.11	7 (10%)
15	HEM	C	402	3	27,50,50	0.86	2 (7%)	17,82,82	1.20	3 (17%)
13	PO4	F	501	-	4,4,4	0.86	0	6,6,6	0.55	0
15	HEM	C	401	3	27,50,50	0.91	2 (7%)	17,82,82	1.59	3 (17%)
13	PO4	C	409	-	4,4,4	0.91	0	6,6,6	0.45	0
13	PO4	E	203	-	4,4,4	0.92	0	6,6,6	0.64	0
13	PO4	G	101	-	4,4,4	0.95	0	6,6,6	0.38	0
17	PEE	C	407	-	39,39,50	1.12	2 (5%)	42,44,55	1.09	3 (7%)
11	PG4	C	405	-	12,12,12	0.49	0	11,11,11	0.34	0
17	PEE	E	204	-	21,21,50	1.51	2 (9%)	24,26,55	1.52	3 (12%)
13	PO4	G	103	-	4,4,4	0.88	0	6,6,6	0.87	0
14	CDL	D	503	-	53,53,99	1.32	4 (7%)	59,65,111	1.11	6 (10%)
19	HEC	D	501	4	26,50,50	2.66	12 (46%)	18,82,82	2.52	6 (33%)
12	6PE	A	502	-	22,22,26	1.53	2 (9%)	25,27,31	1.35	3 (12%)
20	FES	E	201	5	0,4,4	0.00	-	-	-	-
11	PG4	A	501	-	12,12,12	0.50	0	11,11,11	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PEE	E	204	-	1/1/4/4	16/25/25/54	-
16	LMT	C	403	-	-	9/21/61/61	0/2/2/2
20	FES	E	201	5	-	-	0/1/1/1
14	CDL	C	406	-	-	17/52/52/110	-
18	JAG	C	408	-	1/1/6/6	3/13/40/40	0/4/4/4
14	CDL	E	205	-	-	37/69/69/110	-
21	PX4	E	202	-	-	23/40/40/49	-
15	HEM	C	402	3	-	0/6/54/54	-
19	HEC	D	501	4	-	0/6/54/54	-
14	CDL	D	503	-	-	24/63/63/110	-
12	6PE	A	502	-	-	14/26/26/30	-
14	CDL	A	504	-	-	19/41/41/110	-
17	PEE	C	407	-	1/1/4/4	18/43/43/54	-
11	PG4	C	404	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PG4	C	405	-	-	6/10/10/10	-
11	PG4	A	501	-	-	7/10/10/10	-
15	HEM	C	401	3	-	1/6/54/54	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	501	HEC	C3C-C2C	7.78	1.48	1.40
18	C	408	JAG	C5-C4	6.87	1.50	1.37
19	D	501	HEC	C3B-C2B	6.30	1.47	1.40
14	C	406	CDL	OB6-CB5	5.28	1.49	1.34
14	C	406	CDL	OA6-CA5	5.27	1.47	1.35

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	408	JAG	C10-C7-C8	6.35	121.02	111.37
19	D	501	HEC	C1D-C2D-C3D	-5.64	103.07	107.00
19	D	501	HEC	CMB-C2B-C3B	5.07	131.79	125.82
17	E	204	PEE	O2-C10-C11	4.93	122.13	111.50
14	C	406	CDL	OA6-CA5-C11	4.75	119.82	111.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	C	408	JAG	C7
17	C	407	PEE	C2
17	E	204	PEE	C2

5 of 199 torsion outliers are listed below:

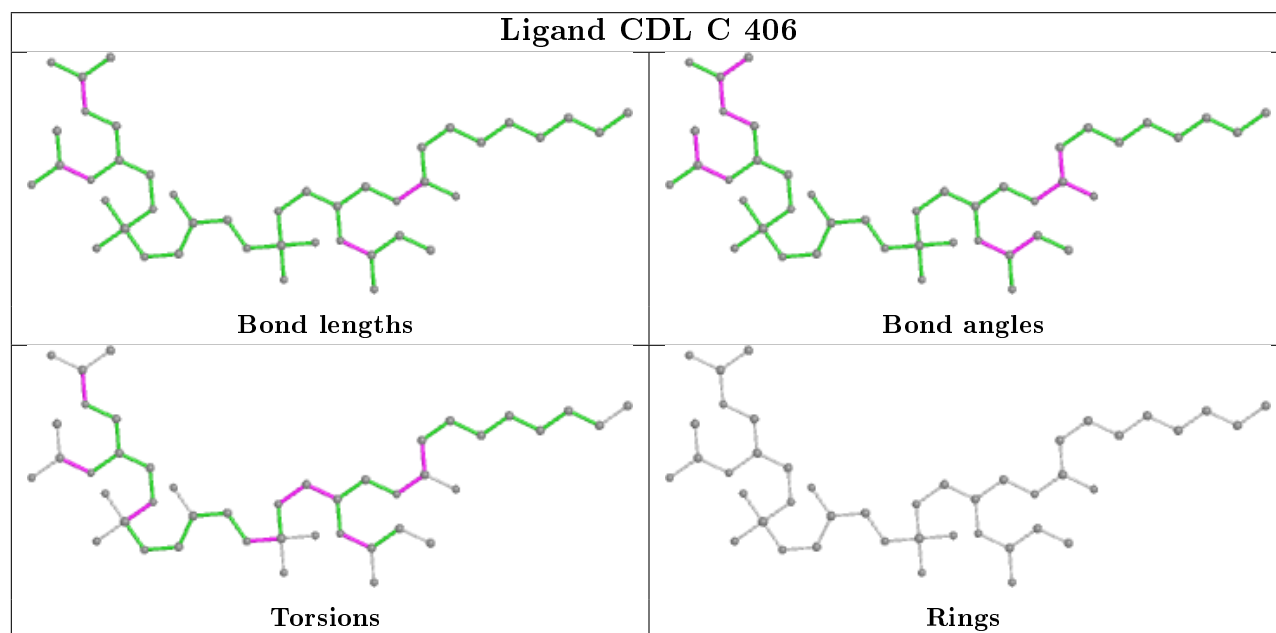
Mol	Chain	Res	Type	Atoms
14	C	406	CDL	CA3-OA5-PA1-OA4
14	C	406	CDL	C11-CA5-OA6-CA4
14	C	406	CDL	CB2-OB2-PB2-OB3
18	C	408	JAG	F2-C22-O2-C19
21	E	202	PX4	C1-O3-P1-O2

There are no ring outliers.

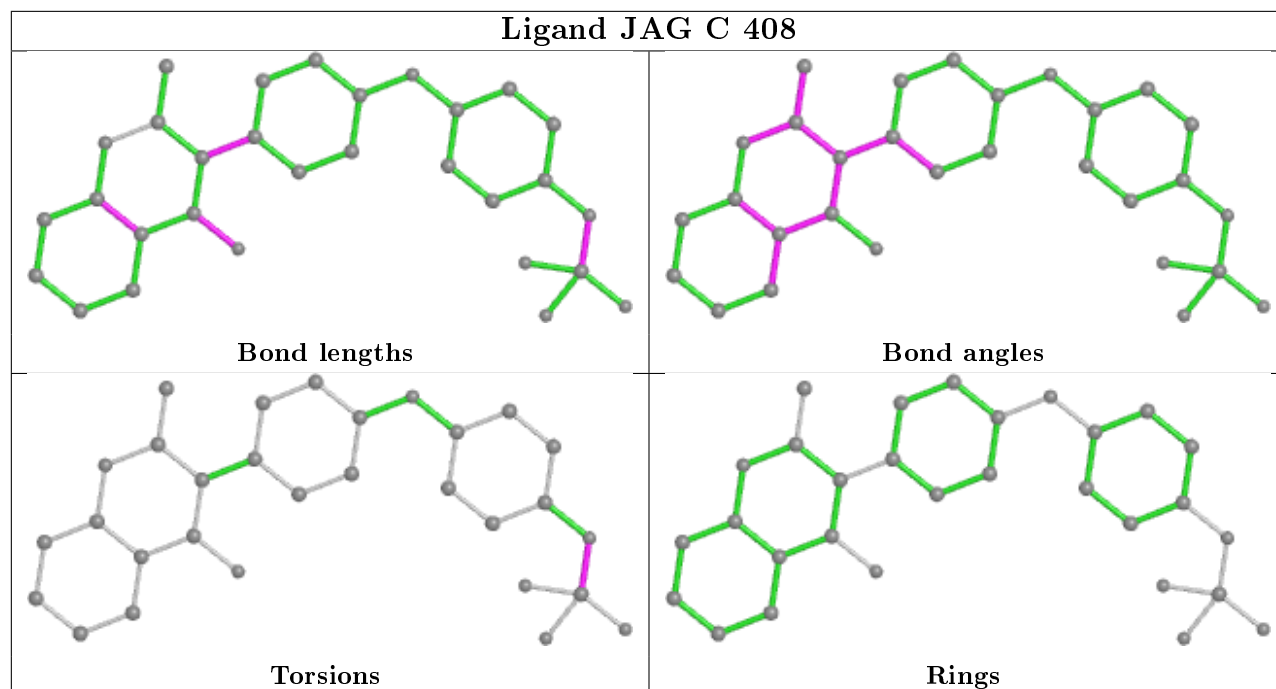
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	202	PX4	1	0
14	A	504	CDL	2	0
15	C	402	HEM	2	0
15	C	401	HEM	3	0
17	C	407	PEE	1	0
19	D	501	HEC	5	0
12	A	502	6PE	2	0

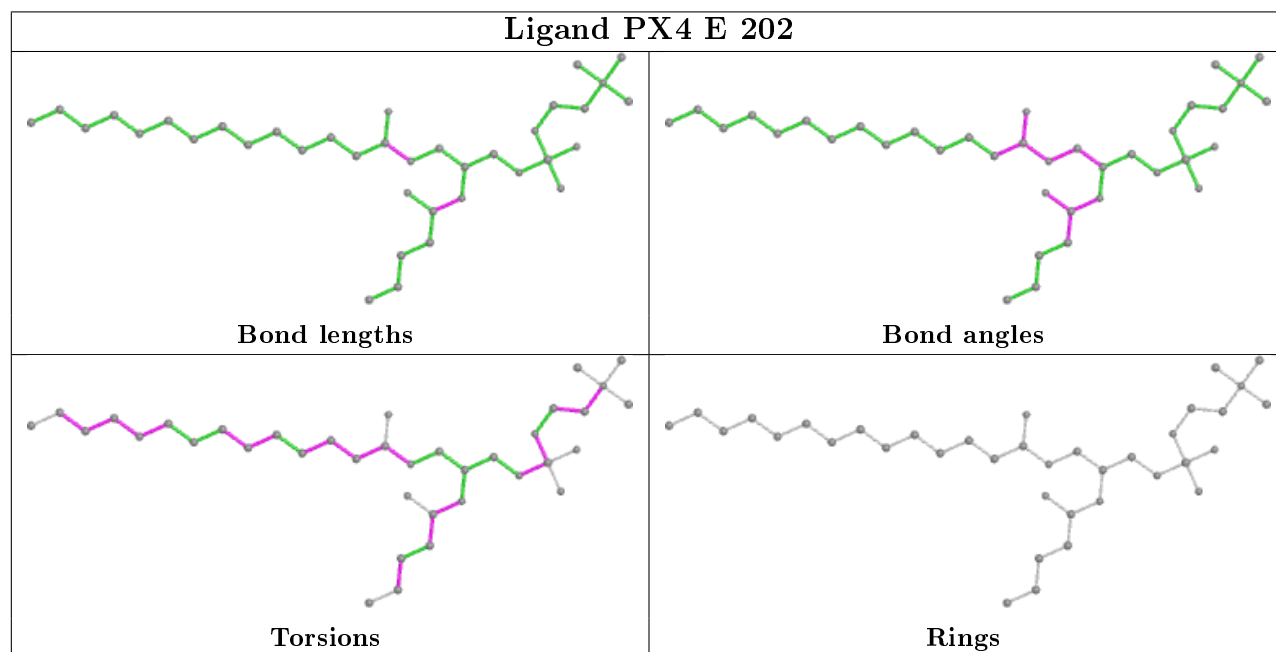
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

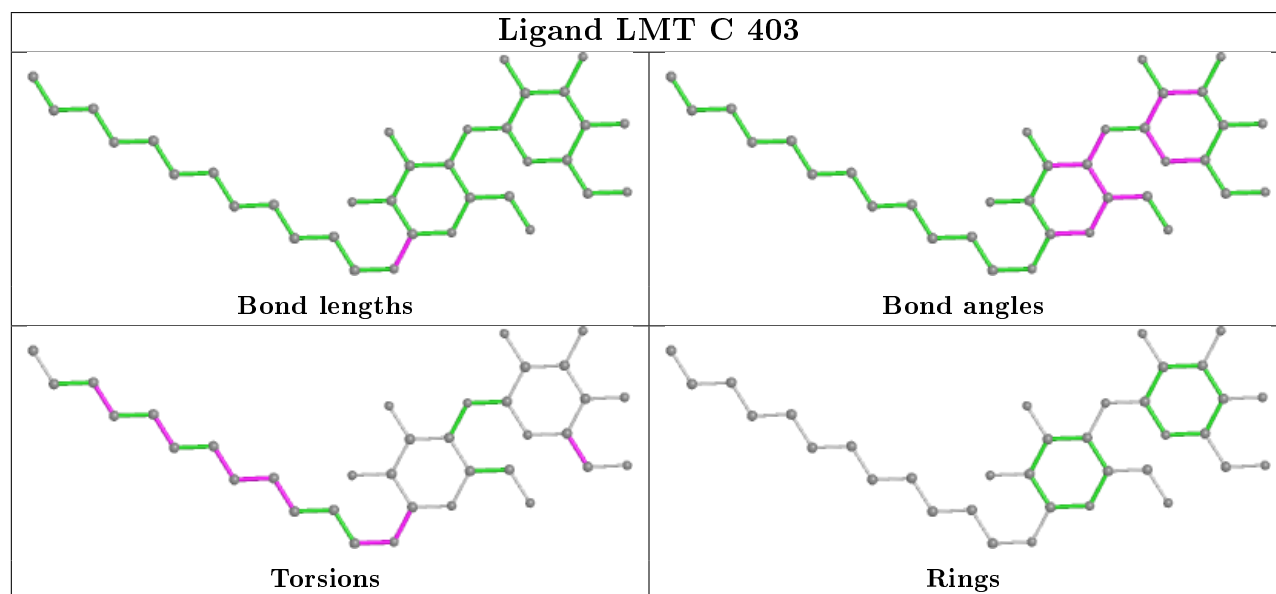
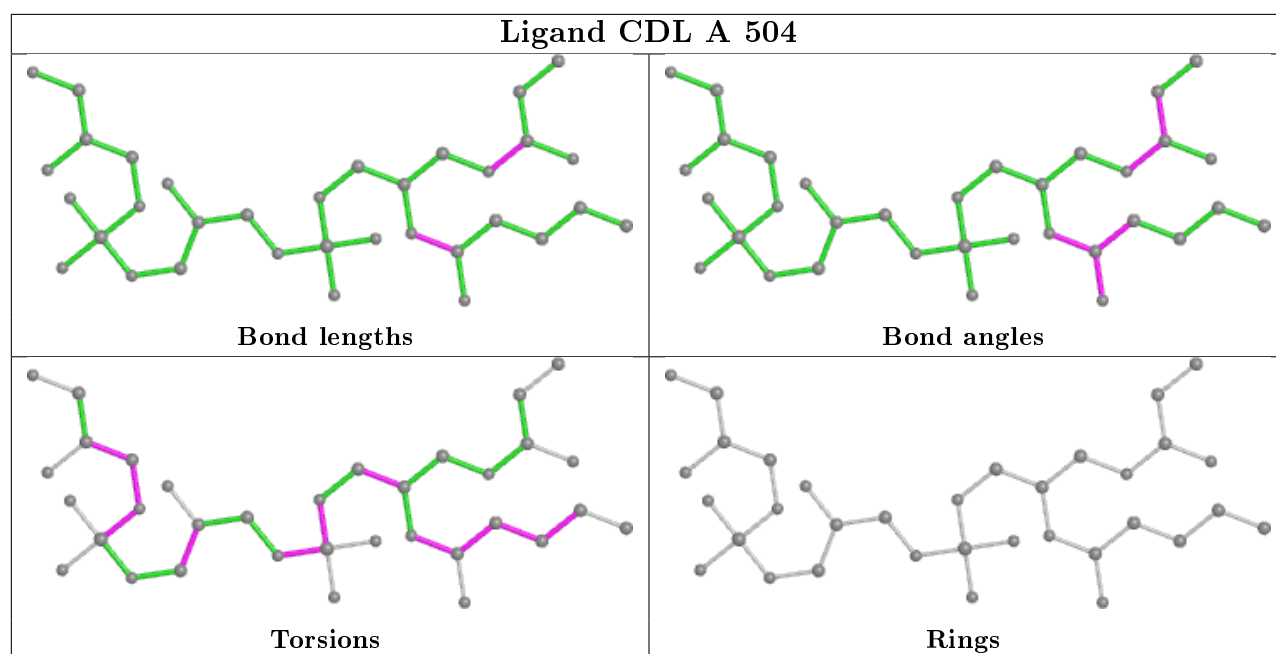


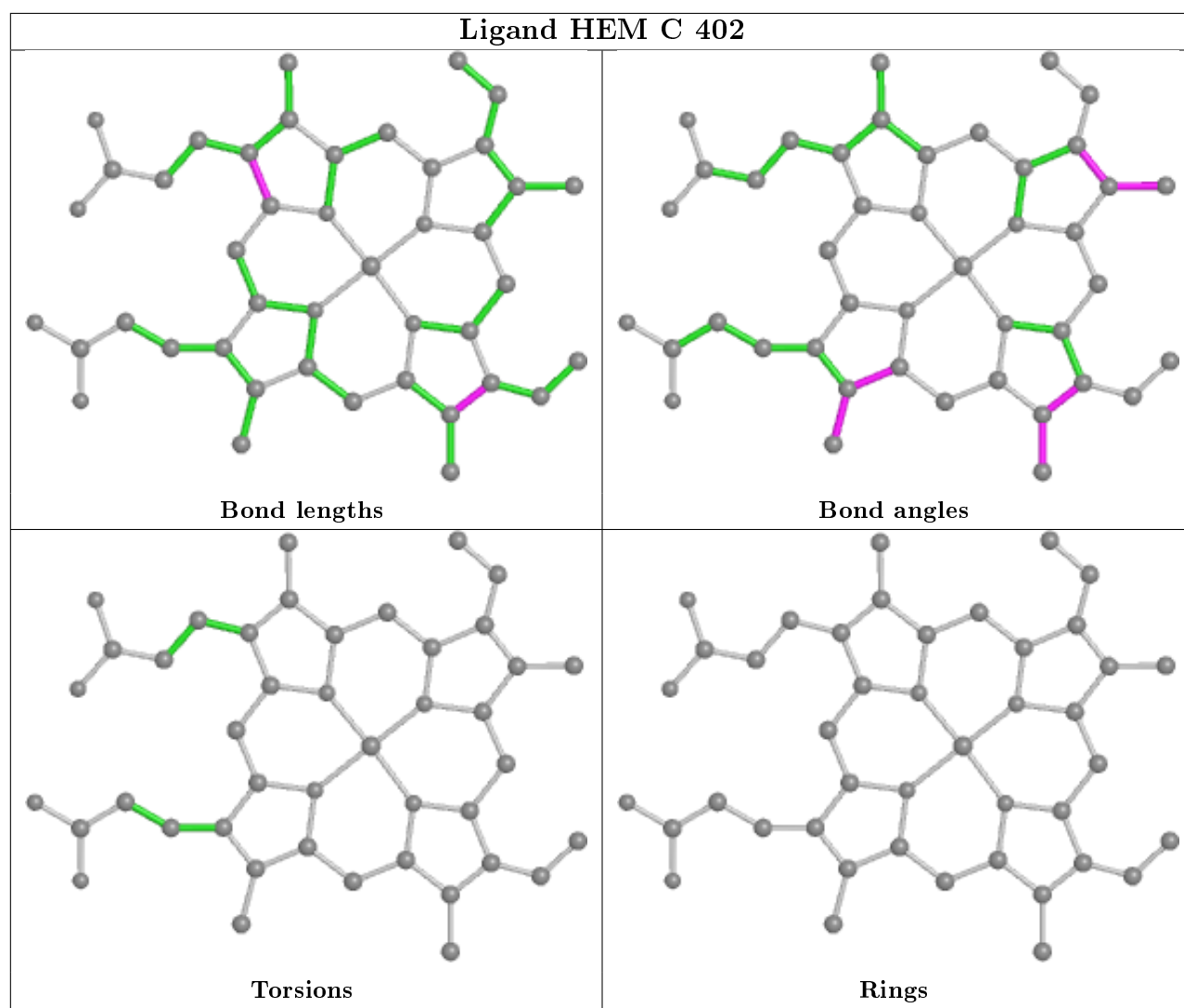
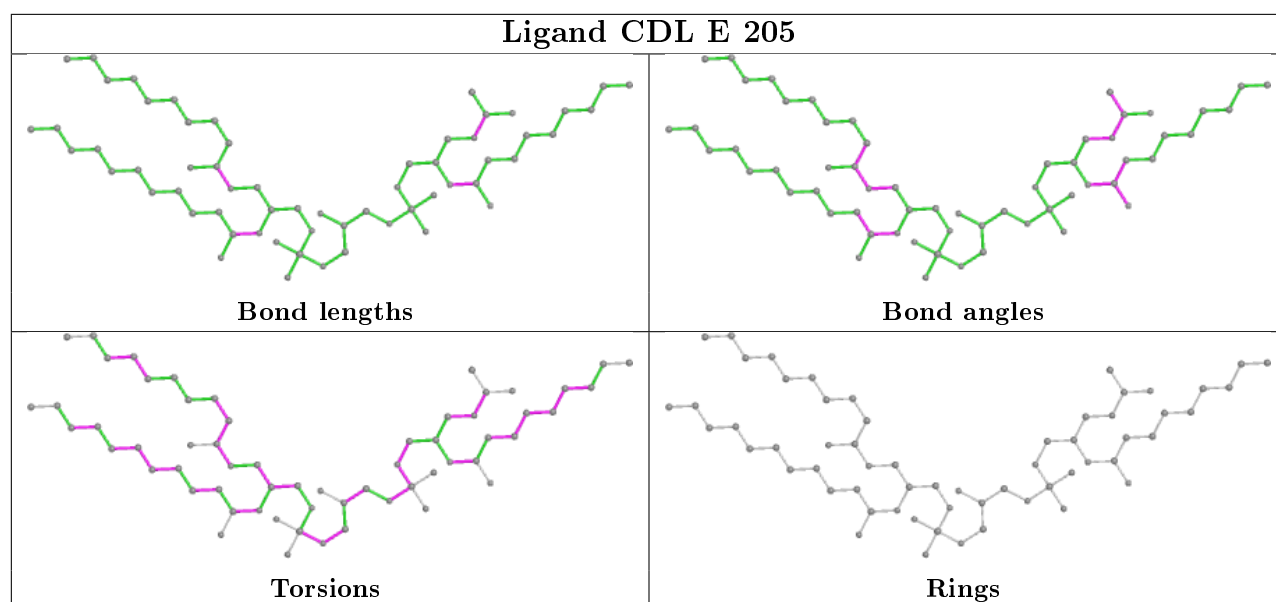
Ligand JAG C 408

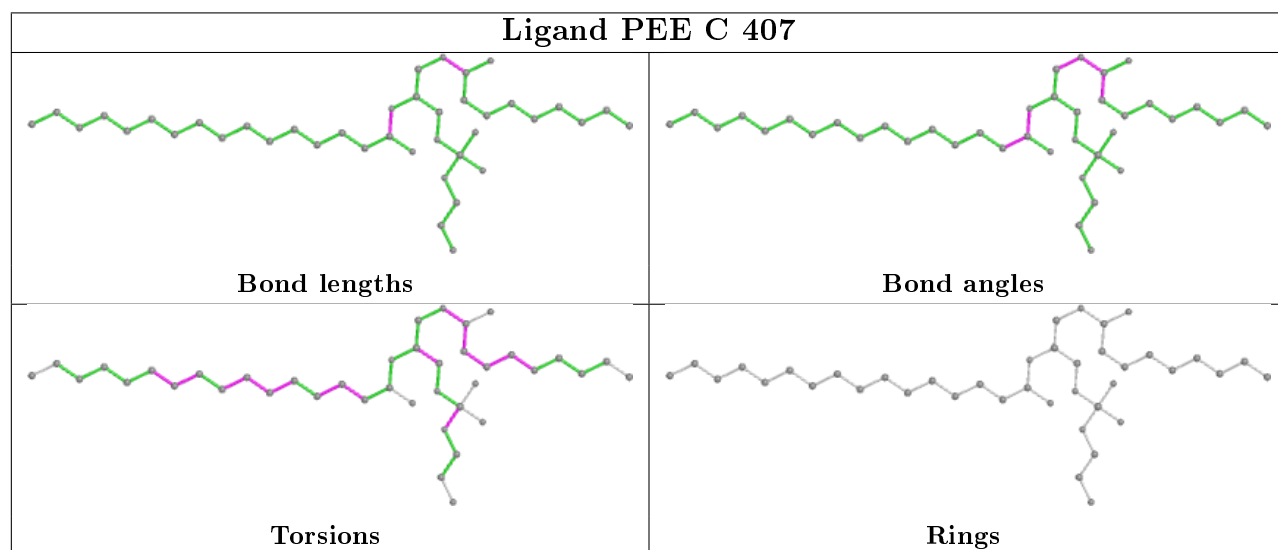
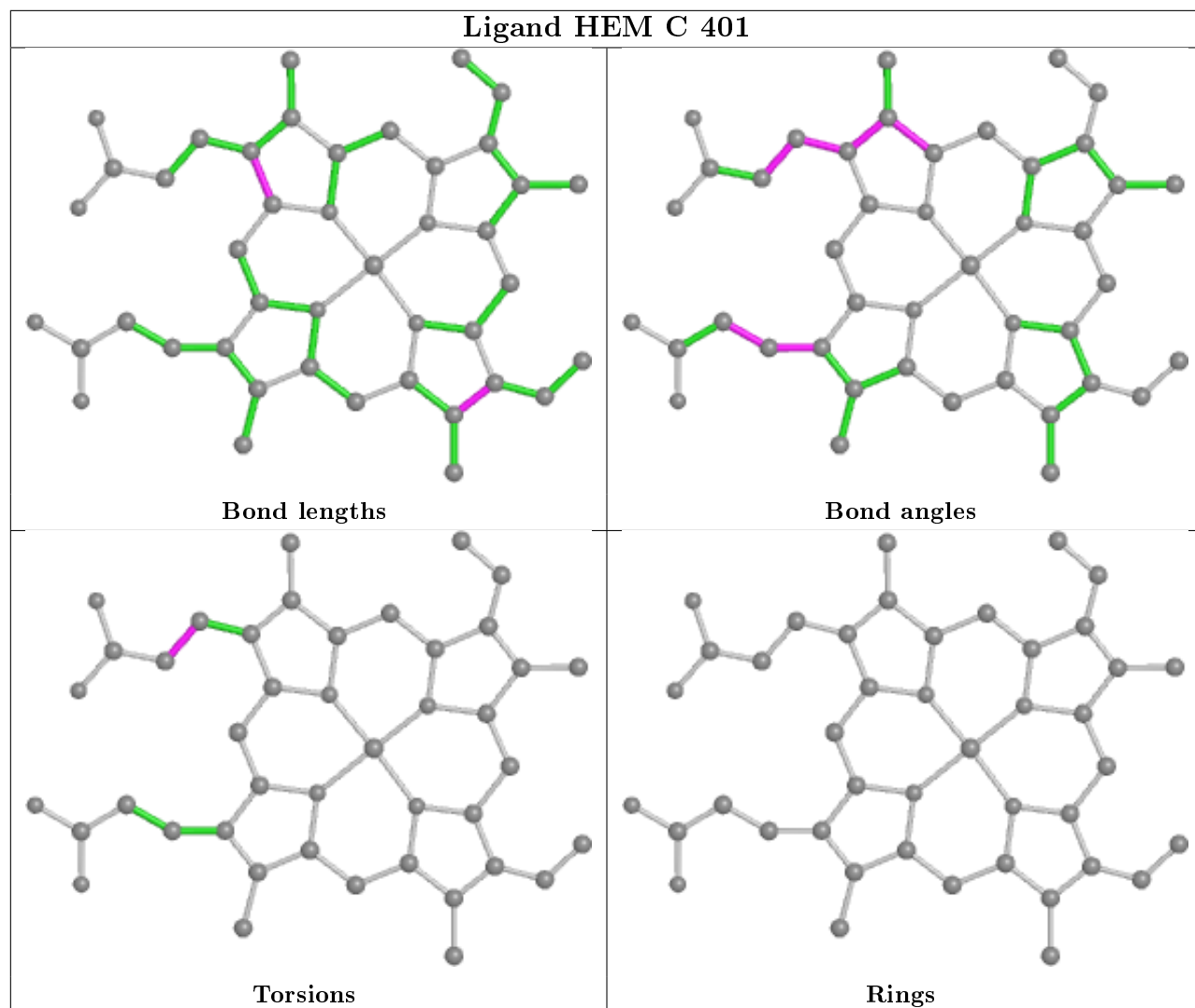


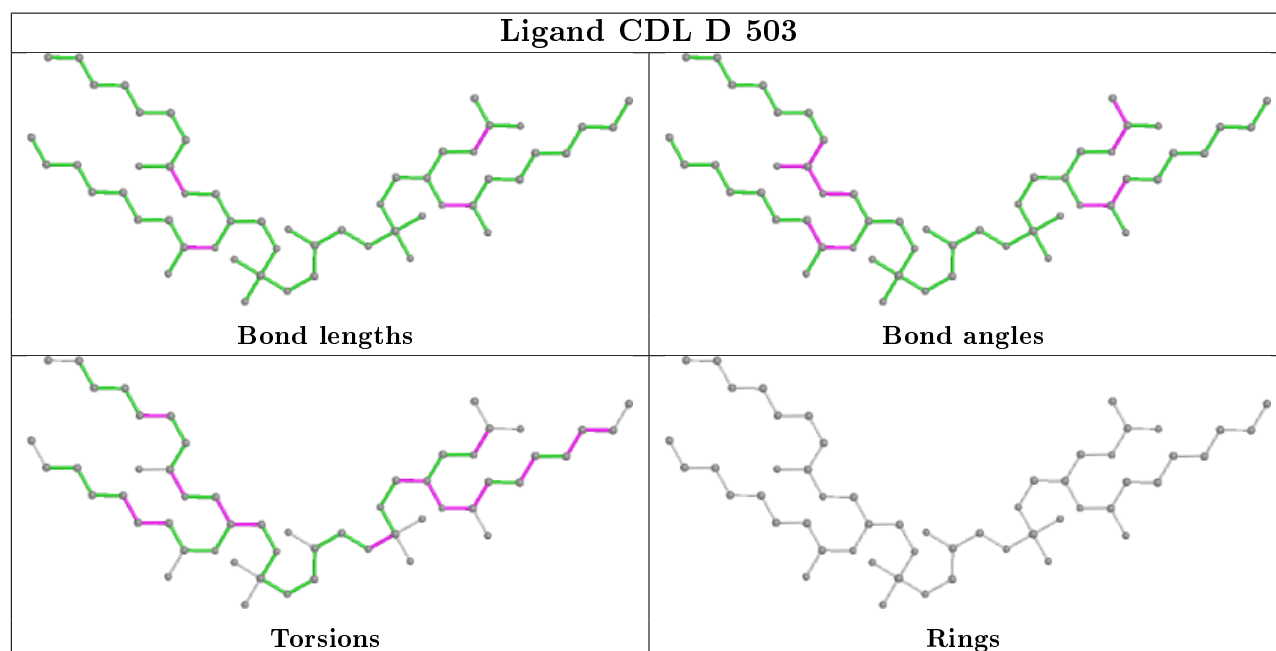
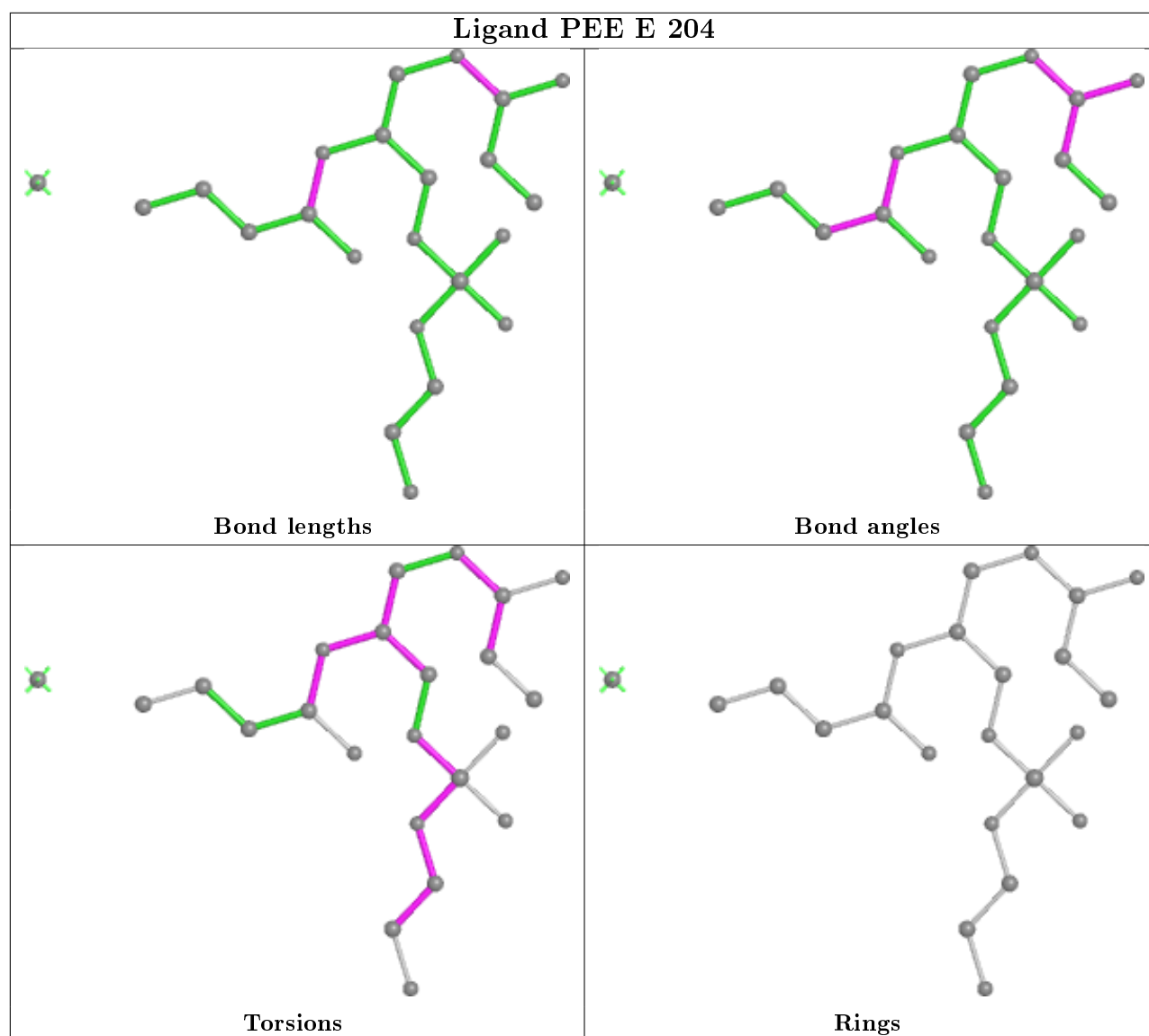
Ligand PX4 E 202

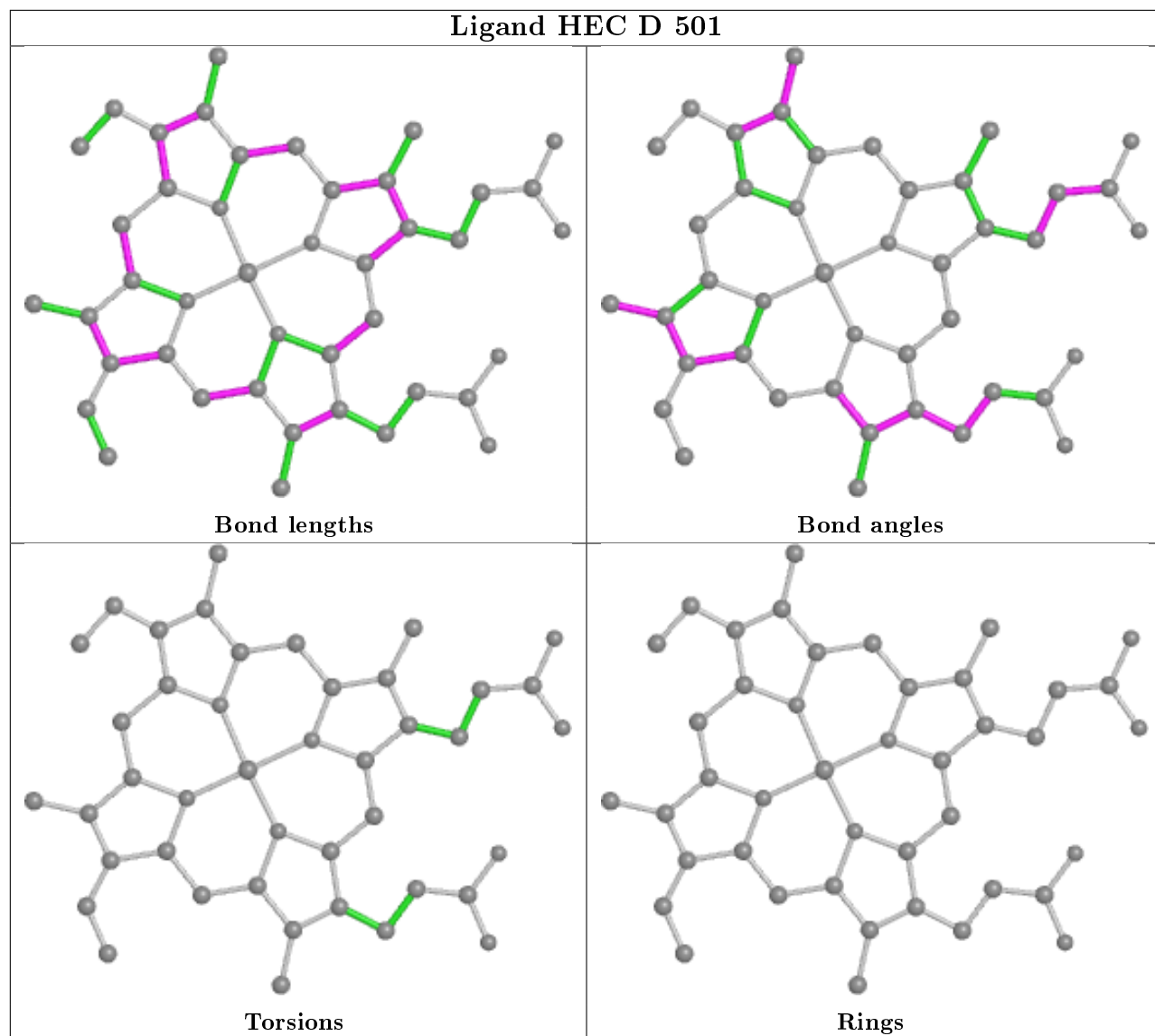


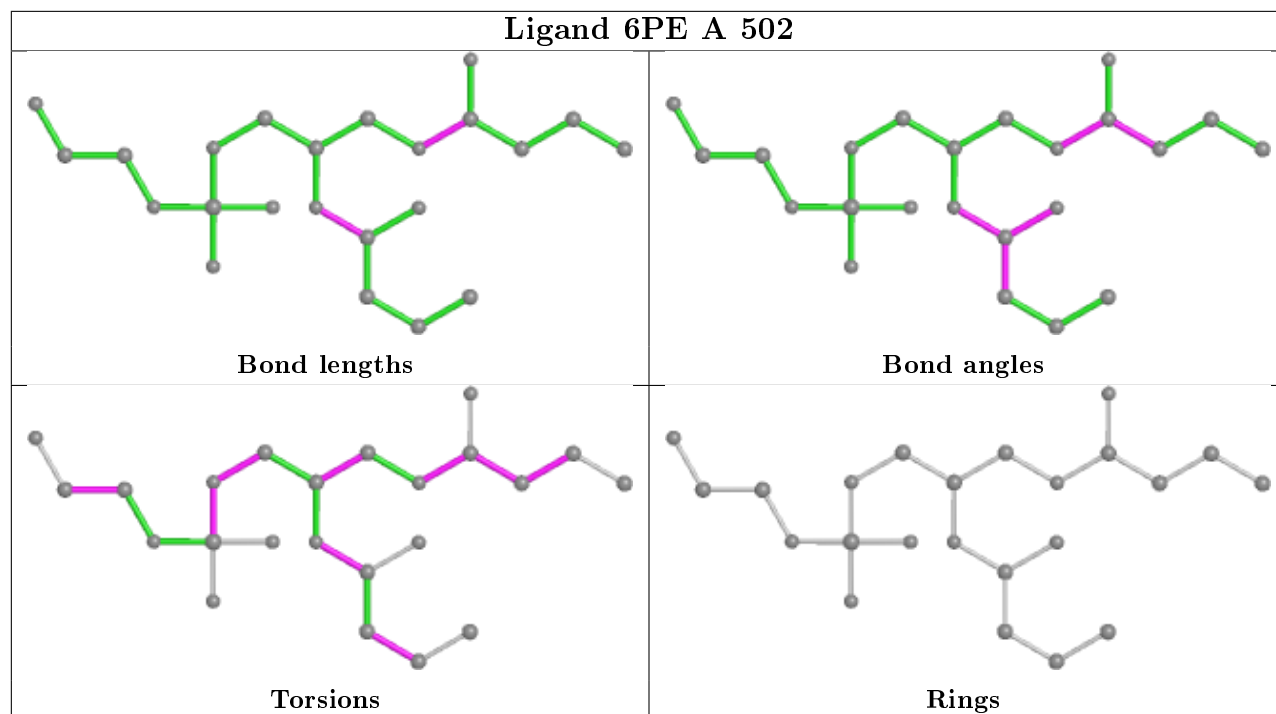












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	438/445 (98%)	0.10	10 (2%) 60 54	114, 154, 190, 222	0
2	B	413/418 (98%)	-0.05	11 (2%) 54 48	120, 154, 188, 209	0
3	C	378/378 (100%)	-0.19	0 100 100	116, 143, 179, 207	0
4	D	239/239 (100%)	0.30	18 (7%) 14 14	143, 187, 215, 236	0
5	E	196/196 (100%)	0.15	6 (3%) 49 43	128, 202, 250, 290	1 (0%)
6	F	99/100 (99%)	-0.19	1 (1%) 82 77	83, 146, 190, 234	0
7	G	74/74 (100%)	-0.15	0 100 100	125, 157, 195, 215	0
8	H	64/64 (100%)	0.26	1 (1%) 72 66	213, 237, 254, 261	0
9	I	46/46 (100%)	0.89	5 (10%) 5 6	162, 186, 217, 227	12 (26%)
10	J	59/59 (100%)	-0.24	0 100 100	151, 177, 216, 261	0
All	All	2006/2019 (99%)	0.03	52 (2%) 56 49	83, 159, 227, 290	13 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	77	ASP	4.9
5	E	86	ASN	4.5
4	D	108	ALA	4.3
1	A	2	ALA	4.1
2	B	43	PRO	3.9

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

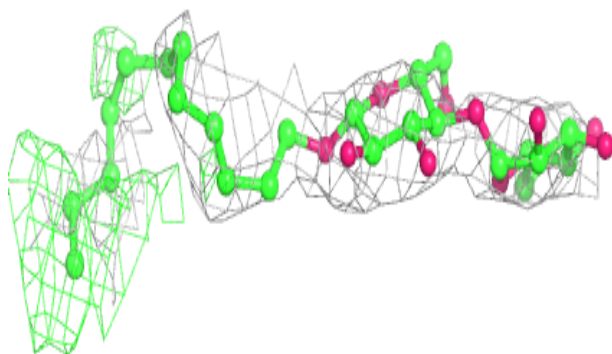
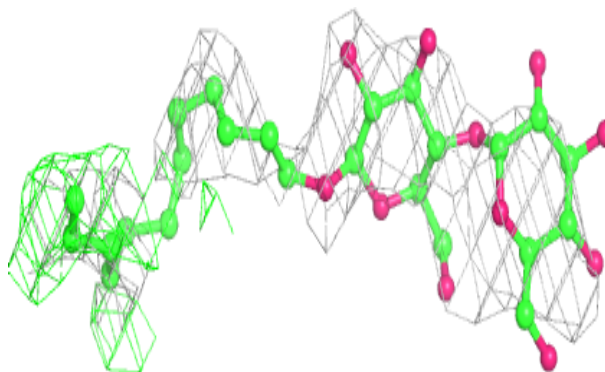
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	LMT	C	403	35/35	0.44	0.44	217,247,256,256	0
13	PO4	D	502	5/5	0.47	0.22	237,240,240,245	0
13	PO4	E	203	5/5	0.49	0.31	248,249,253,256	0
13	PO4	G	102	5/5	0.54	0.24	245,247,249,252	0
14	CDL	E	205	60/100	0.59	0.53	190,215,255,259	0
11	PG4	A	501	13/13	0.64	0.39	184,194,202,202	0
11	PG4	C	404	13/13	0.65	0.76	147,157,168,169	0
13	PO4	B	501	5/5	0.70	0.26	202,206,209,210	0
13	PO4	C	409	5/5	0.70	0.28	210,211,212,213	0
13	PO4	G	101	5/5	0.71	0.19	200,200,204,207	0
13	PO4	G	103	5/5	0.76	0.17	223,223,224,231	0
13	PO4	F	501	5/5	0.78	0.29	209,212,214,215	0
11	PG4	C	405	13/13	0.78	0.49	148,156,159,160	0
14	CDL	A	504	34/100	0.80	0.25	169,204,218,219	0
18	JAG	C	408	30/30	0.81	0.41	113,136,170,175	0
17	PEE	E	204	23/51	0.85	0.54	96,159,165,168	0
14	CDL	D	503	54/100	0.86	0.47	140,180,226,237	0
13	PO4	A	503	5/5	0.87	0.34	155,157,160,162	0
21	PX4	E	202	37/46	0.88	0.42	155,175,183,186	0
12	6PE	A	502	23/27	0.91	0.23	163,189,200,203	0
14	CDL	C	406	44/100	0.92	0.34	149,157,166,168	0
17	PEE	C	407	40/51	0.94	0.41	130,139,146,149	0
20	FES	E	201	4/4	0.96	0.12	286,290,293,295	0
19	HEC	D	501	43/43	0.96	0.44	184,189,199,202	0
15	HEM	C	402	43/43	0.98	0.27	117,118,120,121	0
15	HEM	C	401	43/43	0.98	0.29	129,132,137,140	0

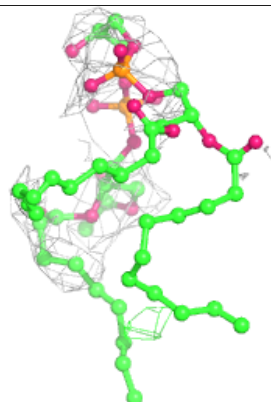
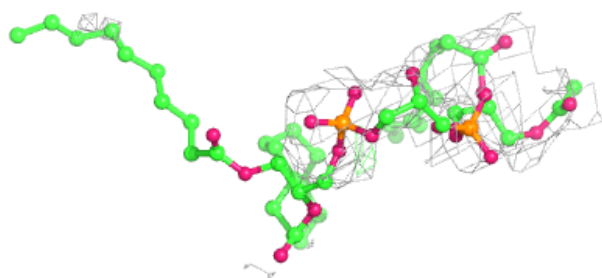
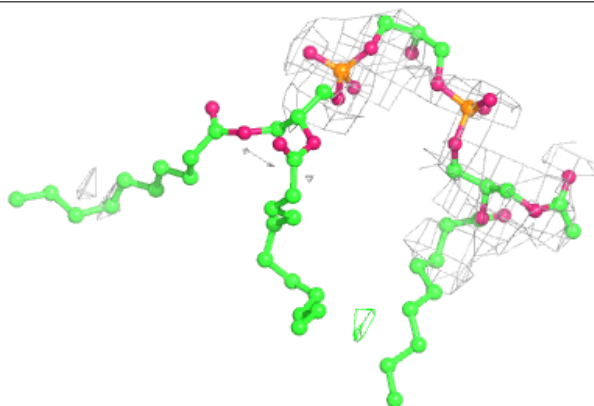
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT C 403:

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

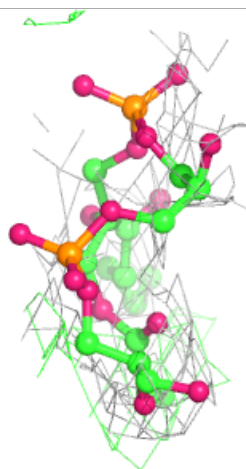
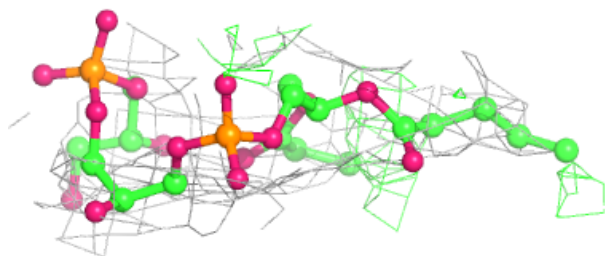
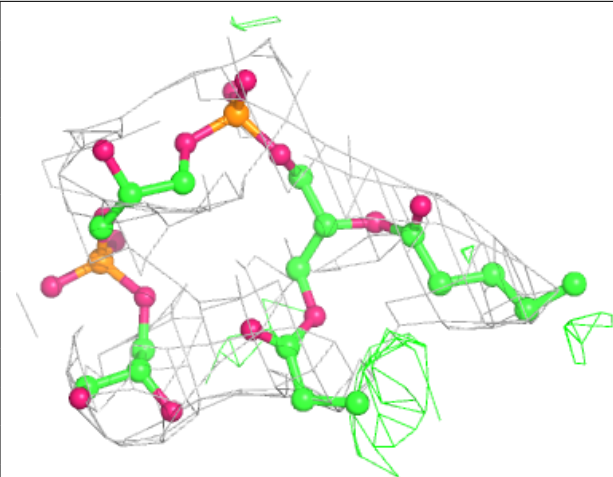
**Electron density around CDL E 205:**

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



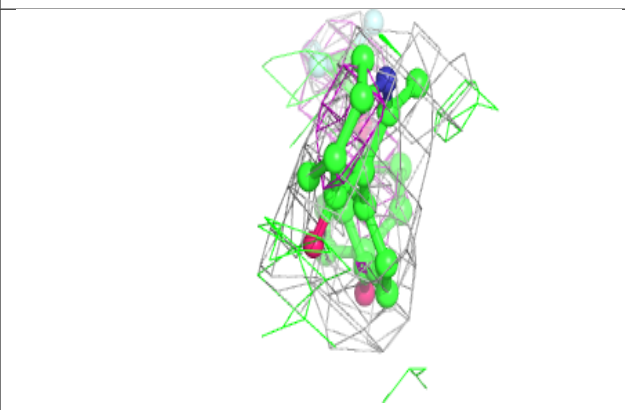
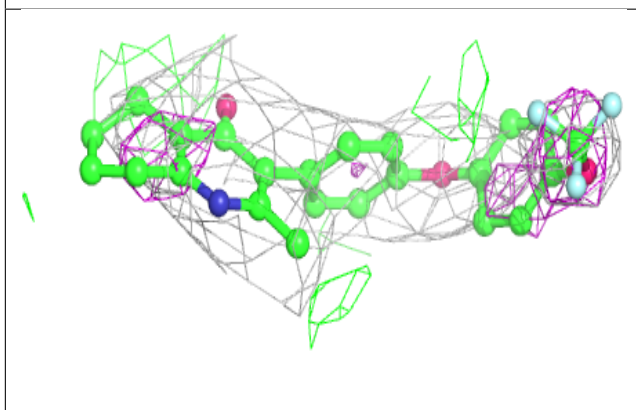
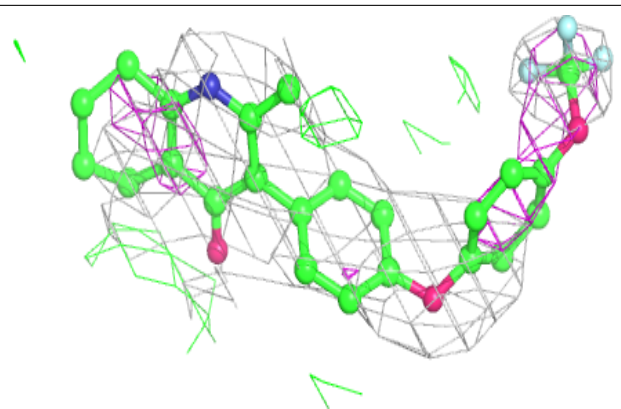
Electron density around CDL A 504:

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

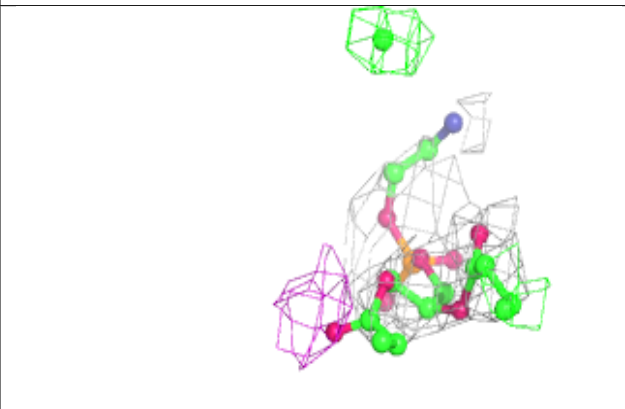
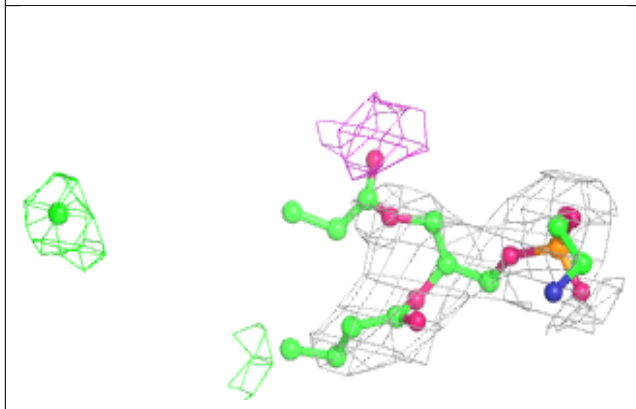
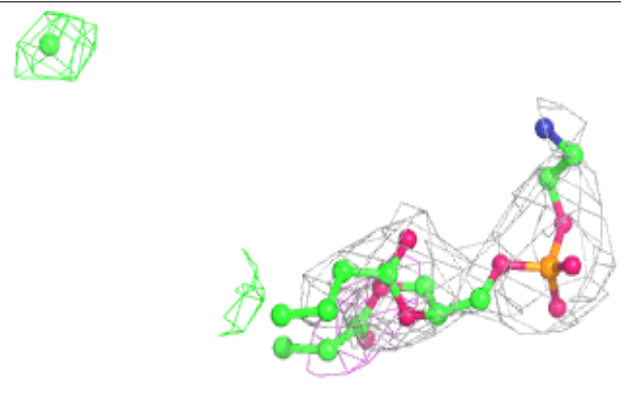


Electron density around JAG C 408:

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

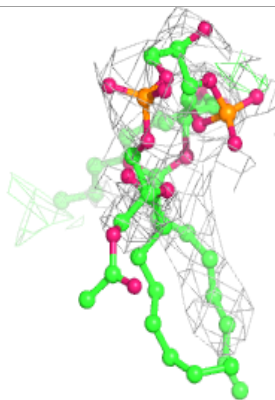
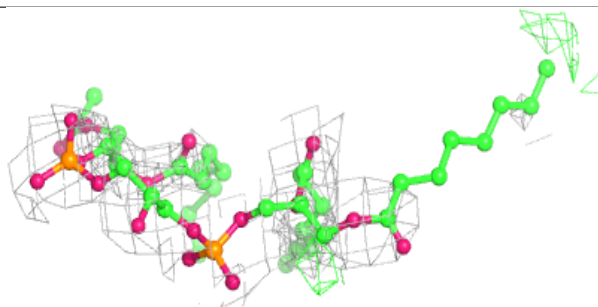
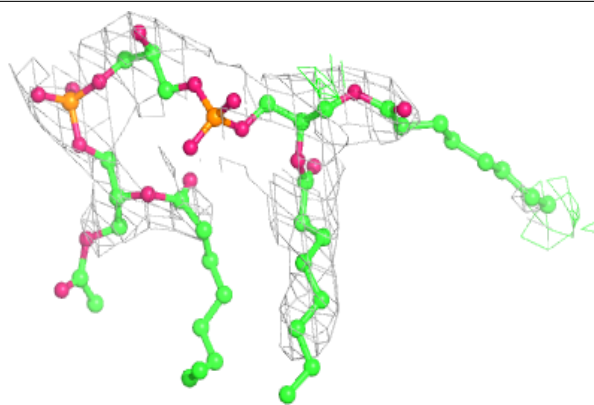
**Electron density around PEE E 204:**

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

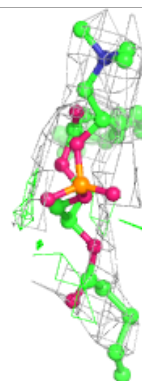
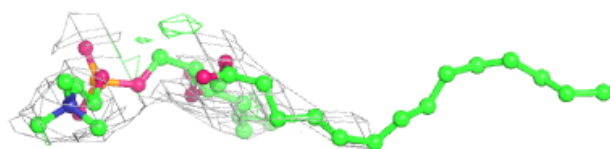
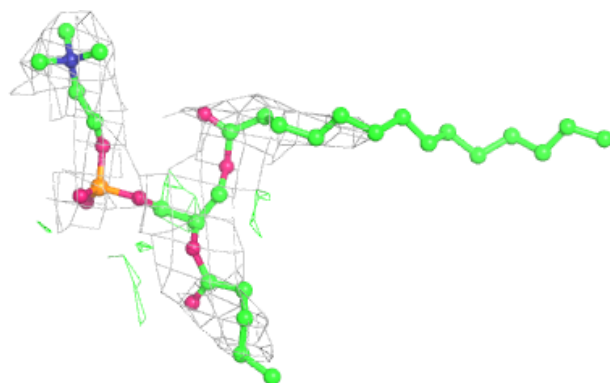


Electron density around CDL D 503:

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

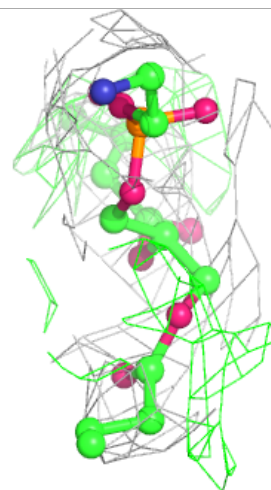
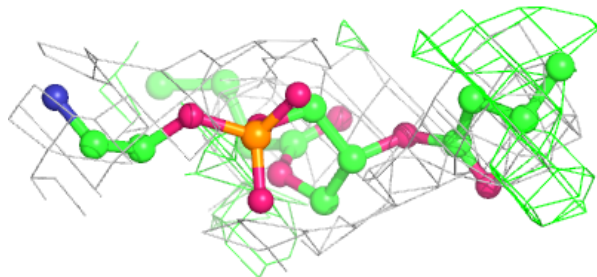
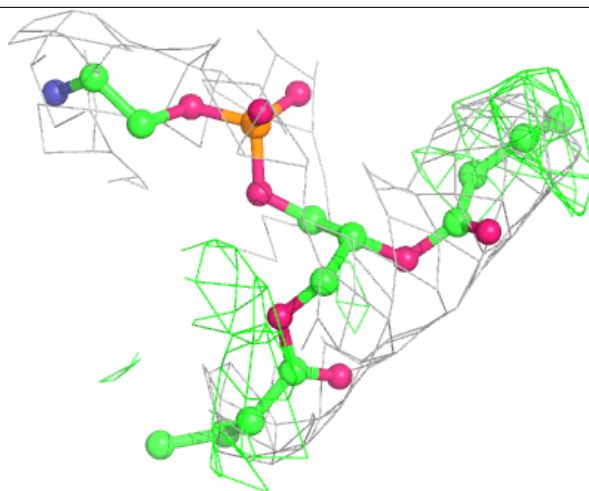
**Electron density around PX4 E 202:**

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



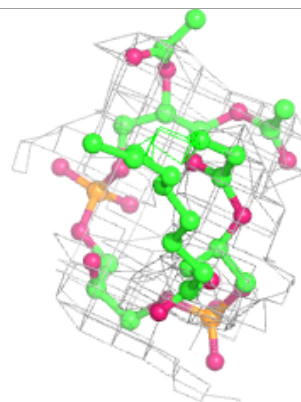
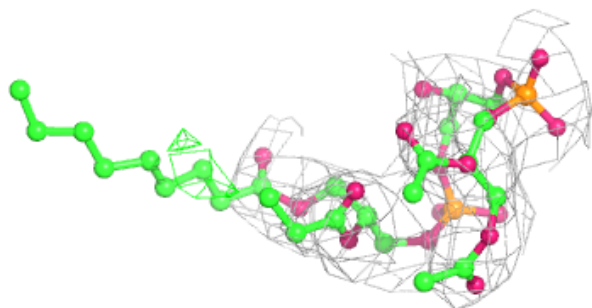
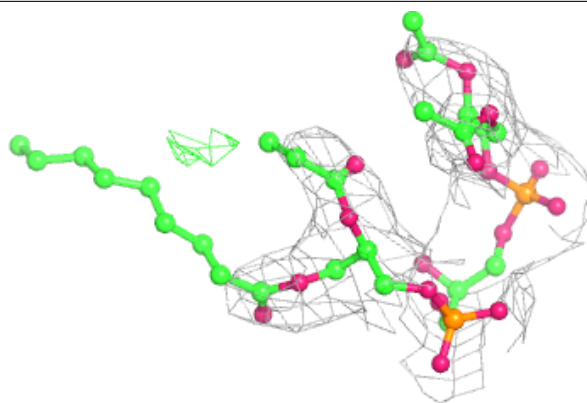
Electron density around 6PE A 502:

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

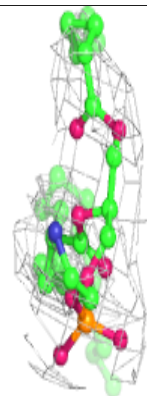
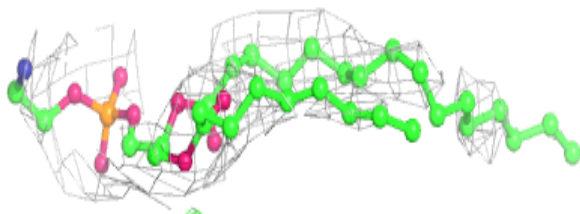


Electron density around CDL C 406:

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

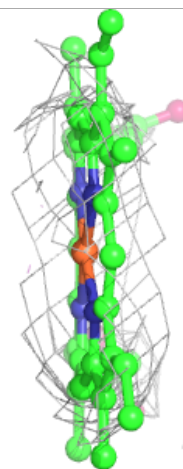
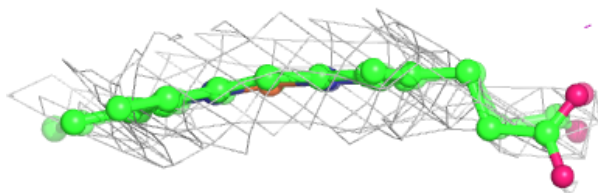
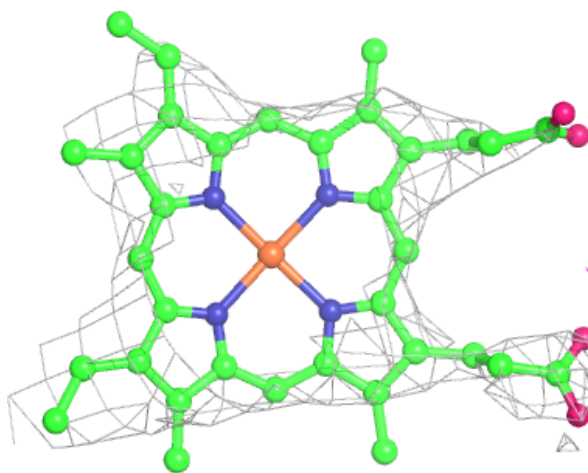
**Electron density around PEE C 407:**

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



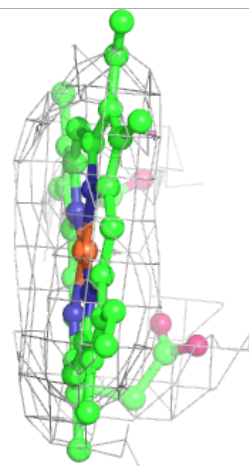
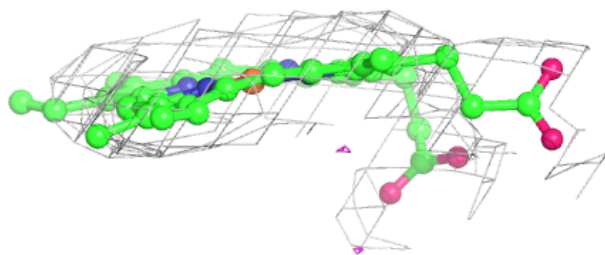
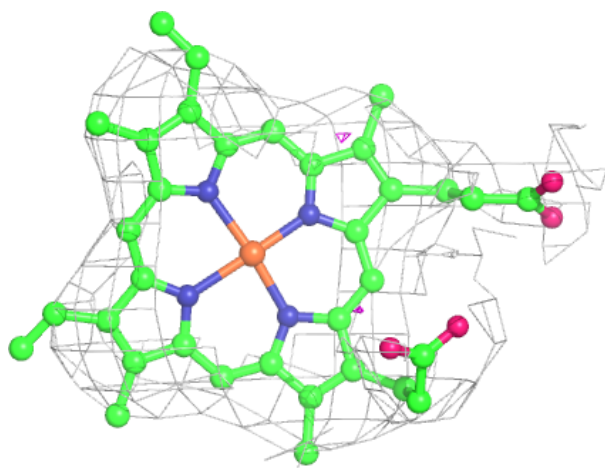
Electron density around HEC D 501:

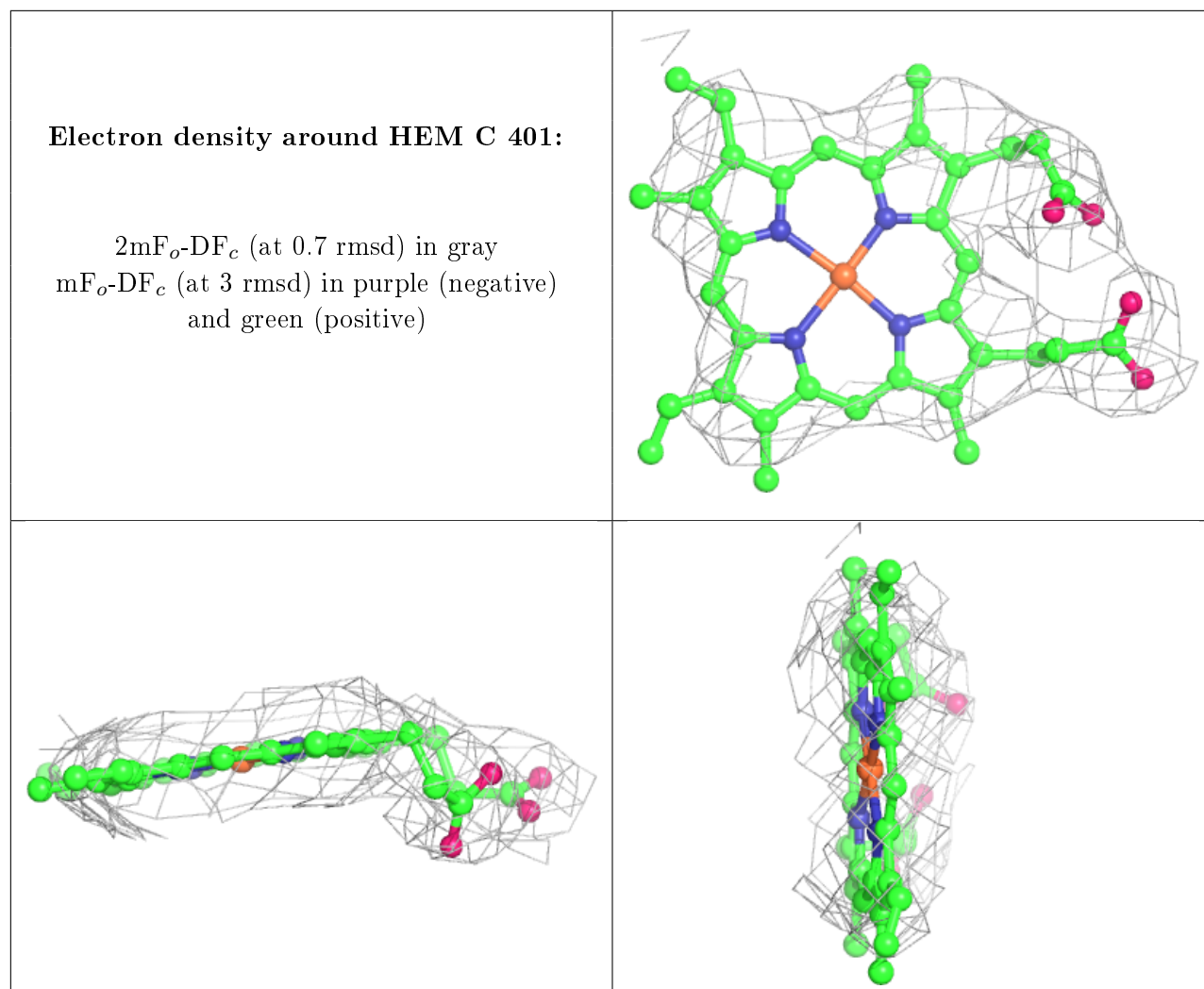
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 ⓘ

There are no such residues in this entry.