



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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

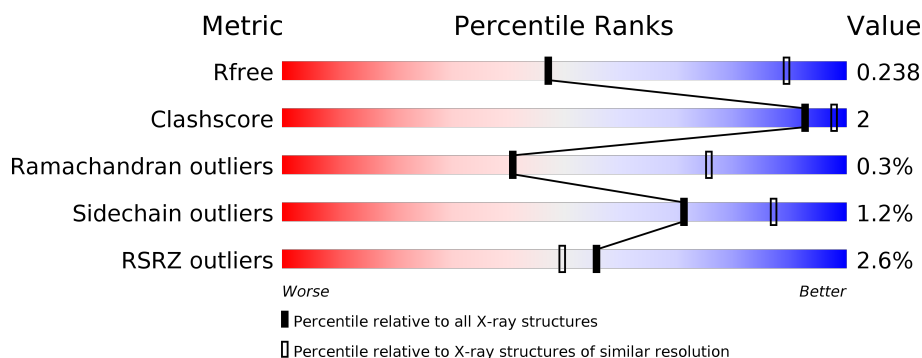
1 Overall quality at a glance

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.



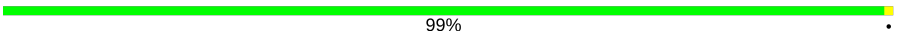

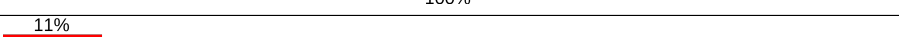

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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></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			

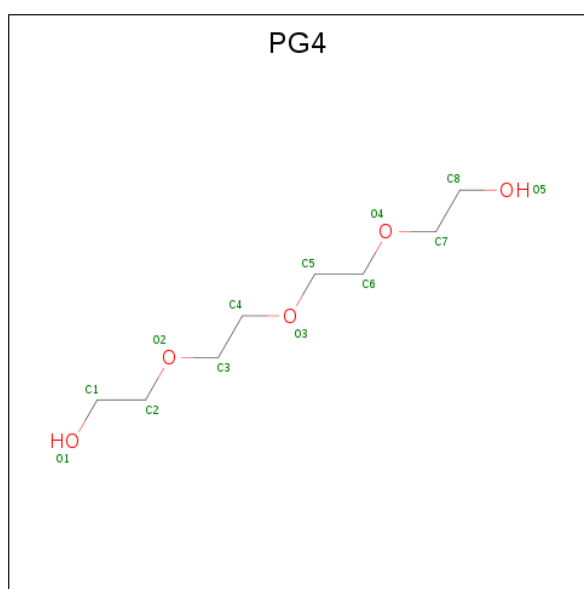
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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.

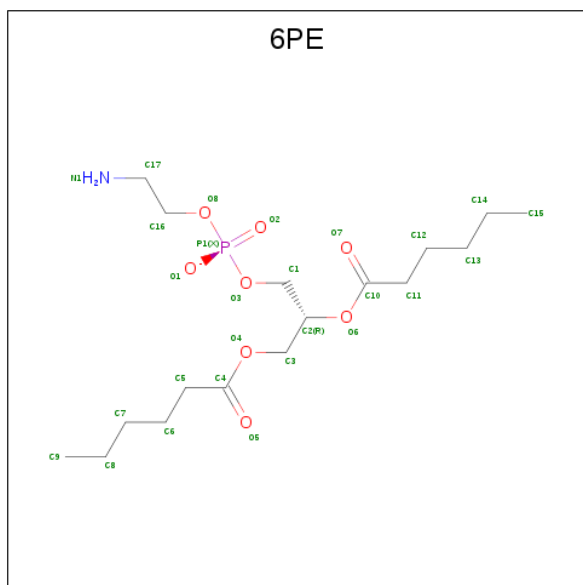
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			481	317	81	83			

- 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: $C_{17}H_{33}NO_8P$).



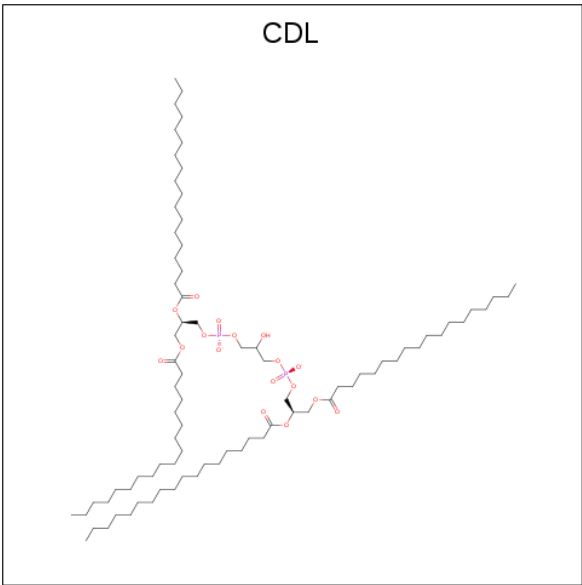
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

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



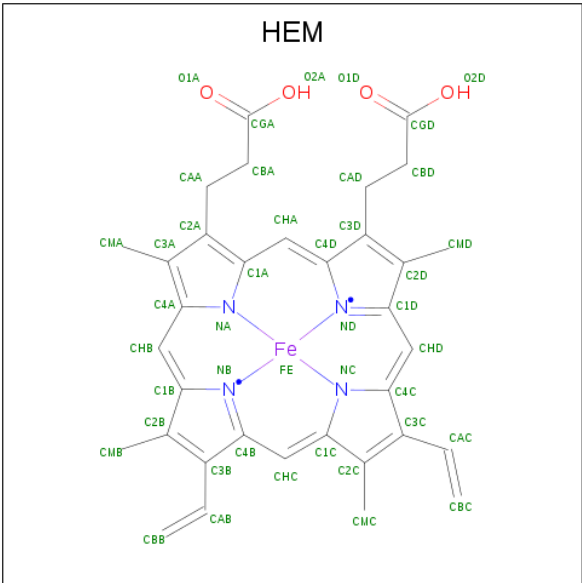
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	P	0	0
			5	4	1		
13	B	1	Total	O	P	0	0
			5	4	1		
13	C	1	Total	O	P	0	0
			5	4	1		
13	D	1	Total	O	P	0	0
			5	4	1		
13	E	1	Total	O	P	0	0
			5	4	1		
13	F	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		
13	G	1	Total	O	P	0	0
			5	4	1		

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



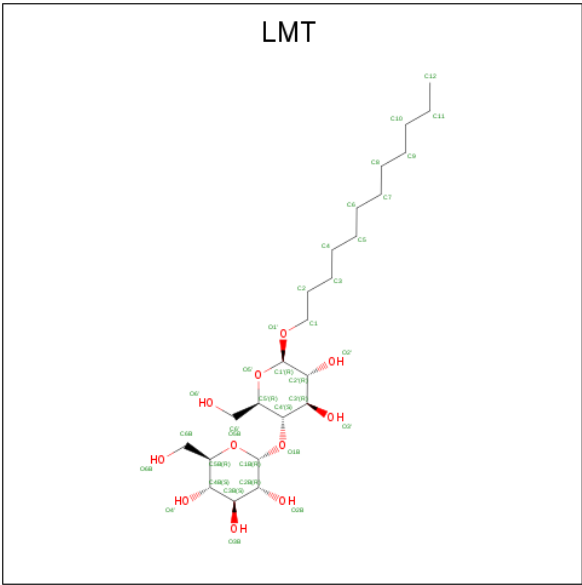
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			34	17	15	2		
14	C	1	Total	C	O	P	0	0
			44	25	17	2		
14	D	1	Total	C	O	P	0	0
			54	35	17	2		
14	E	1	Total	C	O	P	0	0
			60	41	17	2		

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



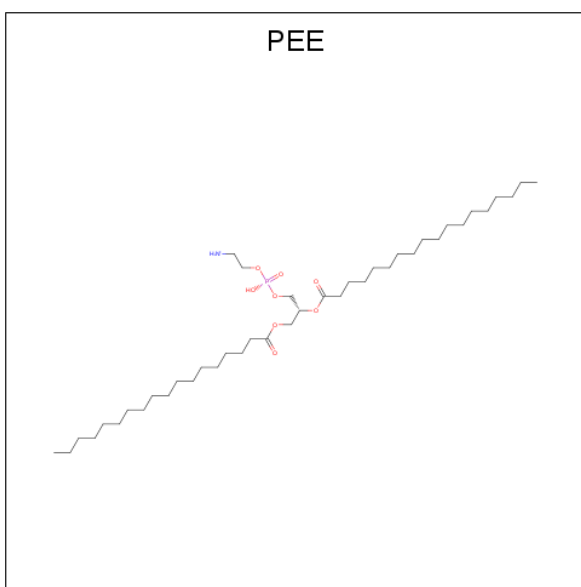
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



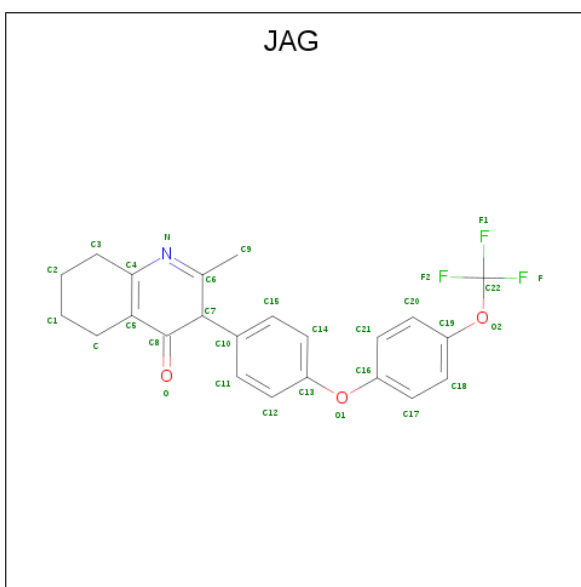
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O		
			35	24	11		

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



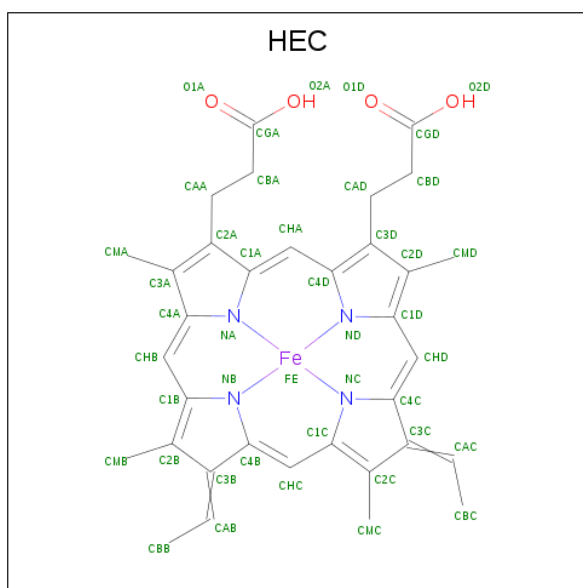
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
17	E	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

- 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).



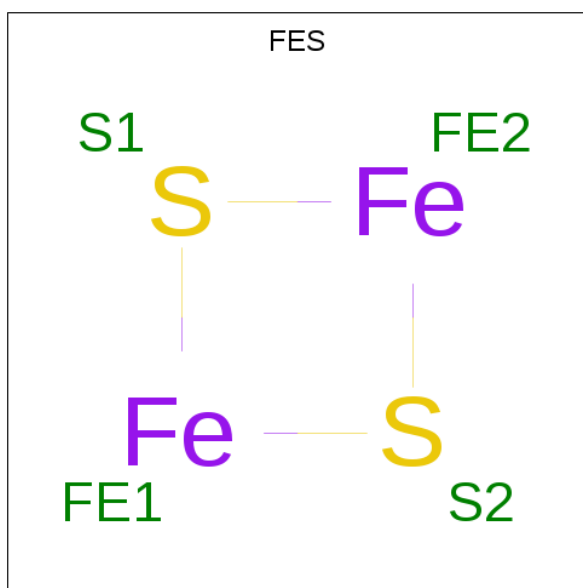
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	F	N	O	0	0
			30	23	3	1	3		

- 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		

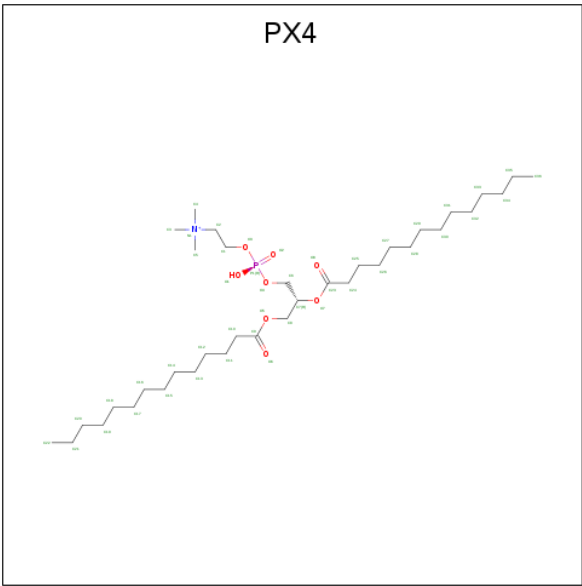
- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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		

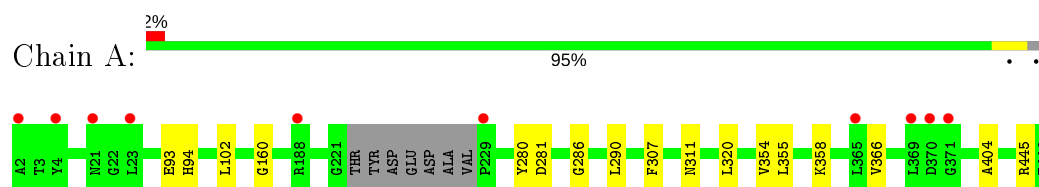
- Molecule 22 is water.

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		

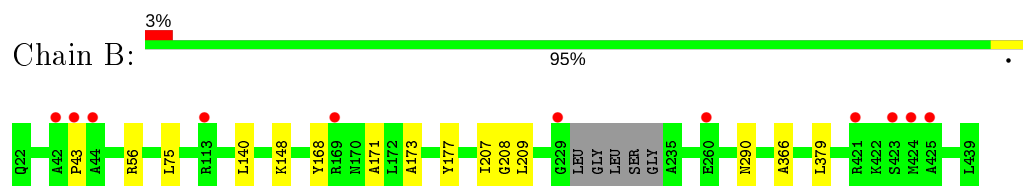
3 Residue-property plots [i](#)

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.

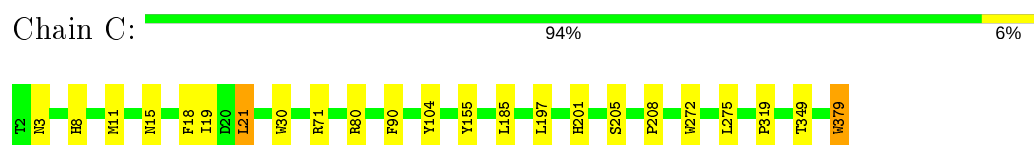
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



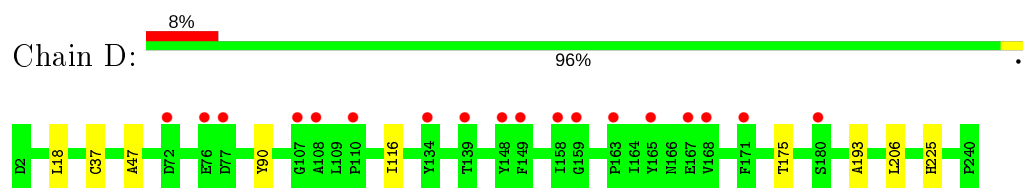
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



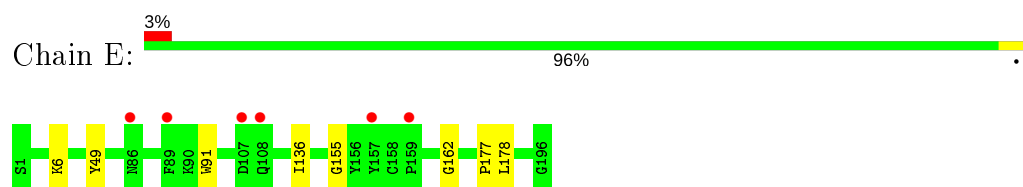
- Molecule 3: Cytochrome b



- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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



- Molecule 6: Cytochrome b-c1 complex subunit 7



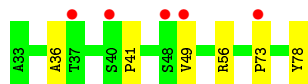
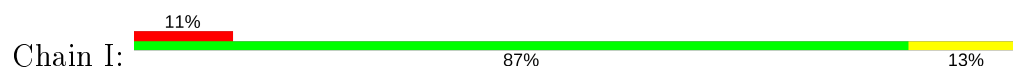
- Molecule 7: Cytochrome b-c1 complex subunit 8



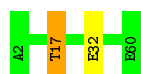
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



- 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.

All (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
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.35	0.57
4:D:37:CYS:SG	19:D:501:HEC:HBB3	2.46	0.56
3:C:71:ARG:NH2	4:D:193:ALA:O	2.41	0.54
4:D:37:CYS:SG	19:D:501:HEC:CBB	2.97	0.53
2:B:290:ASN:HD21	9:I:56:ARG:HE	1.53	0.53
1:A:93:GLU:O	1:A:94:HIS:HD2	1.94	0.50
1:A:93:GLU:O	1:A:94:HIS:CD2	2.66	0.48
3:C:197:LEU:HD21	15:C:402:HEM:HMA3	1.95	0.48
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.50	0.47
1:A:286:GLY:HA3	1:A:290:LEU:HG	1.96	0.47
2:B:75:LEU:HD11	2:B:140:LEU:HD22	1.96	0.47
5:E:49:TYR:HD1	10:J:32:GLU:HG3	1.80	0.46
12:A:502:6PE:H28	14:A:504:CDL:HB31	1.97	0.45
4:D:47:ALA:HA	4:D:90:TYR:HA	1.97	0.45
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.51	0.45
5:E:49:TYR:CD1	10:J:32:GLU:HG3	2.52	0.45
15:C:401:HEM:CMB	15:C:401:HEM:HBB2	2.47	0.45
1:A:160:GLY:H	5:E:6:LYS:NZ	2.16	0.44
3:C:272:TRP:HA	3:C:275:LEU:HG	1.98	0.43
15:C:402:HEM:HMB1	15:C:402:HEM:HBB2	1.99	0.43
2:B:56:ARG:HB2	2:B:171:ALA:HB1	2.00	0.43
1:A:311:ASN:HB2	1:A:320:LEU:HD12	2.00	0.43
3:C:8:HIS:HB3	3:C:11:MET:HB2	2.00	0.43
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.01	0.42
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.54	0.42
3:C:15:ASN:HA	3:C:19:ILE:HD12	2.01	0.42
3:C:30:TRP:NE1	17:C:407:PEE:H14	2.35	0.42
15:C:401:HEM:HMB1	15:C:401:HEM:HBB2	2.01	0.42
1:A:366:VAL:HG21	2:B:43:PRO:HB2	2.02	0.41
3:C:379:TRP:CZ2	6:F:33:ARG:HD3	2.54	0.41
12:A:502:6PE:H6	14:A:504:CDL:H712	2.01	0.41
3:C:319:PRO:HD2	6:F:20:TYR:CE2	2.54	0.41
4:D:116:ILE:HG12	19:D:501:HEC:HMA3	2.01	0.41
1:A:355:LEU:HA	1:A:358:LYS:HD3	2.01	0.41
2:B:208:GLY:C	2:B:209:LEU:HD12	2.40	0.41
21:E:202:PX4:H12	10:J:17:THR:HG23	2.02	0.41
4:D:18:LEU:HD22	4:D:206:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:TRP:HZ3	5:E:136:ILE:CD1	2.33	0.41
3:C:21:LEU:HD22	3:C:201:HIS:NE2	2.35	0.41
1:A:102:LEU:HD21	2:B:366:ALA:HA	2.03	0.40
1:A:354:VAL:HG21	1:A:404:ALA:HA	2.02	0.40
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.03	0.40
2:B:207:ILE:HG22	2:B:379:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/445 (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

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	162	GLY

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Mol	Chain	Res	Type
1	A	445	ARG
3	C	155	TYR
9	I	41	PRO
5	E	177	PRO
5	E	155	GLY

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

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ASP
3	C	3	ASN
3	C	18	PHE
3	C	21	LEU
3	C	80	ARG
3	C	90	PHE
3	C	185	LEU
3	C	205	SER

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Mol	Chain	Res	Type
3	C	349	THR
3	C	379	TRP
4	D	175	THR
5	E	178	LEU
6	F	33	ARG
6	F	44	LYS
6	F	58	ARG
6	F	71	ARG
9	I	49	VAL
9	I	78	TYR
10	J	17	THR

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
1	A	165	GLN
2	B	290	ASN
3	C	322	GLN
4	D	225	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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
14	D	503	CDL	OA8-CA7	5.11	1.48	1.33
17	C	407	PEE	O3-C30	4.88	1.47	1.33
14	D	503	CDL	OB6-CB5	4.88	1.48	1.34
14	E	205	CDL	OA6-CA5	4.83	1.47	1.34
12	A	502	6PE	O6-C10	4.78	1.47	1.34
21	E	202	PX4	O5-C9	4.75	1.47	1.33
14	A	504	CDL	OB8-CB7	4.74	1.47	1.33
17	E	204	PEE	O2-C10	4.63	1.47	1.34
12	A	502	6PE	O4-C4	4.58	1.46	1.33
21	E	202	PX4	O7-C23	4.58	1.47	1.34
14	C	406	CDL	OB8-CB7	4.52	1.46	1.33
14	E	205	CDL	OA8-CA7	4.46	1.46	1.33
17	E	204	PEE	O3-C30	4.43	1.46	1.33
14	E	205	CDL	OB6-CB5	4.33	1.46	1.34
14	D	503	CDL	OA6-CA5	4.32	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	504	CDL	OB6-CB5	4.30	1.46	1.34
17	C	407	PEE	O2-C10	4.03	1.45	1.34
19	D	501	HEC	C2A-C3A	3.37	1.47	1.37
19	D	501	HEC	C3D-C2D	3.31	1.47	1.37
19	D	501	HEC	C3B-C4B	3.23	1.48	1.43
19	D	501	HEC	C4A-C3A	3.07	1.49	1.42
19	D	501	HEC	C1A-C2A	2.99	1.49	1.42
19	D	501	HEC	C3C-C4C	2.89	1.48	1.43
15	C	401	HEM	C4D-C3D	2.83	1.49	1.42
19	D	501	HEC	C1C-CHC	2.78	1.48	1.41
14	C	406	CDL	OA8-CA7	2.76	1.47	1.33
15	C	402	HEM	C4D-C3D	2.75	1.48	1.42
14	E	205	CDL	OB8-CB7	2.66	1.46	1.33
16	C	403	LMT	O1'-C1'	2.65	1.44	1.40
18	C	408	JAG	C10-C7	-2.58	1.50	1.53
14	D	503	CDL	OB8-CB7	2.55	1.46	1.33
18	C	408	JAG	O2-C22	2.34	1.44	1.31
15	C	401	HEM	C3B-C2B	-2.33	1.37	1.40
19	D	501	HEC	C4D-CHA	2.32	1.47	1.41
19	D	501	HEC	C1D-CHD	2.30	1.47	1.41
19	D	501	HEC	C1B-CHB	2.27	1.47	1.41
18	C	408	JAG	O-C8	2.10	1.26	1.22
15	C	402	HEM	C3B-C2B	-2.09	1.37	1.40

All (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
19	D	501	HEC	CMC-C2C-C3C	4.72	131.37	125.82
21	E	202	PX4	O7-C23-C24	4.52	121.25	111.50
14	A	504	CDL	OB6-CB5-C51	4.47	121.14	111.50
12	A	502	6PE	O6-C10-C11	4.42	121.02	111.50
15	C	401	HEM	CBA-CAA-C2A	-4.34	104.48	112.49
18	C	408	JAG	C10-C7-C6	4.31	121.04	111.45
14	E	205	CDL	OA6-CA5-C11	3.95	120.02	111.50
14	A	504	CDL	OB8-CB7-C71	3.84	121.45	111.38
14	E	205	CDL	OB6-CB5-C51	3.80	119.68	111.50
14	D	503	CDL	OB6-CB5-C51	3.79	119.66	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	407	PEE	O3-C30-C31	3.58	123.16	111.91
16	C	403	LMT	C1B-O5B-C5B	3.50	120.55	113.69
14	C	406	CDL	OB6-CB5-C51	3.44	120.38	110.80
14	D	503	CDL	OA8-CA7-C31	3.31	122.29	111.91
14	C	406	CDL	OB8-CB7-C71	3.05	121.49	111.91
17	E	204	PEE	O3-C30-C31	3.04	119.36	111.38
21	E	202	PX4	O5-C9-C10	3.02	121.39	111.91
16	C	403	LMT	O1B-C4'-C3'	2.97	115.18	107.28
16	C	403	LMT	C1'-O5'-C5'	2.93	119.44	113.69
18	C	408	JAG	C8-C5-C4	-2.86	118.31	120.65
14	C	406	CDL	CA6-OA8-CA7	2.80	124.14	117.10
14	D	503	CDL	OA8-CA7-OA9	-2.80	116.52	123.59
17	C	407	PEE	O2-C10-C11	2.78	117.50	111.50
18	C	408	JAG	C11-C10-C7	-2.78	117.43	120.95
12	A	502	6PE	O4-C4-C5	2.74	120.52	111.91
14	E	205	CDL	OA8-CA7-C31	2.69	120.36	111.91
21	E	202	PX4	O7-C23-O8	-2.68	117.22	123.70
19	D	501	HEC	CAA-CBA-CGA	-2.67	108.20	112.67
15	C	402	HEM	CMB-C2B-C3B	2.52	129.40	124.68
18	C	408	JAG	C9-C6-N	-2.47	116.17	119.71
15	C	401	HEM	C1D-C2D-C3D	-2.46	105.29	107.00
14	D	503	CDL	OA6-CA5-C11	2.43	116.74	111.50
14	E	205	CDL	CB6-OB8-CB7	2.37	123.06	117.10
14	D	503	CDL	OB8-CB7-C71	2.32	122.49	112.38
18	C	408	JAG	C-C5-C8	2.31	121.89	118.27
12	A	502	6PE	O6-C10-O7	-2.30	118.15	123.70
14	C	406	CDL	OA8-CA7-C31	2.28	122.30	112.38
14	A	504	CDL	OB6-CB5-OB7	-2.23	118.30	123.70
21	E	202	PX4	O5-C8-C7	2.23	114.92	108.43
15	C	402	HEM	CMC-C2C-C3C	2.20	128.80	124.68
14	E	205	CDL	CA6-OA8-CA7	2.17	125.16	117.12
14	C	406	CDL	OB8-CB7-OB9	-2.16	118.15	123.59
14	D	503	CDL	CA6-OA8-CA7	2.15	125.09	117.12
21	E	202	PX4	O5-C9-O6	-2.15	118.16	123.59
19	D	501	HEC	C4C-C3C-C2C	-2.14	104.04	106.35
17	E	204	PEE	O3-C30-O5	-2.12	118.23	123.59
15	C	401	HEM	CBD-CAD-C3D	-2.12	108.58	112.48
16	C	403	LMT	O5'-C5'-C6'	2.08	111.60	106.44
19	D	501	HEC	CBD-CAD-C3D	-2.06	108.69	112.49
14	E	205	CDL	OB8-CB7-C71	2.06	121.36	112.38
17	C	407	PEE	C3-O3-C30	2.06	124.73	117.12
16	C	403	LMT	C3'-C4'-C5'	-2.03	106.27	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	403	LMT	C1B-C2B-C3B	2.02	114.20	110.00
15	C	402	HEM	CMA-C3A-C4A	-2.01	125.37	128.46
14	E	205	CDL	OB6-CB5-OB7	-2.00	118.87	123.70

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

All (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
21	E	202	PX4	C6-O4-P1-O1
21	E	202	PX4	C24-C23-O7-C7
14	A	504	CDL	CB2-OB2-PB2-OB3
14	A	504	CDL	CB3-OB5-PB2-OB4
14	A	504	CDL	C51-CB5-OB6-CB4
16	C	403	LMT	C2'-C1'-O1'-C1
16	C	403	LMT	O5'-C1'-O1'-C1
16	C	403	LMT	C2-C1-O1'-C1'
14	E	205	CDL	CB3-OB5-PB2-OB3
14	E	205	CDL	C51-CB5-OB6-CB4
17	C	407	PEE	C4-O4P-P-O1P
17	C	407	PEE	C4-O4P-P-O2P
17	E	204	PEE	O4P-C4-C5-N
17	E	204	PEE	C4-O4P-P-O1P
14	D	503	CDL	CB2-OB2-PB2-OB3
12	A	502	6PE	C1-O3-P1-O1
12	A	502	6PE	C11-C10-O6-C2
12	A	502	6PE	O8-C16-C17-N1
14	A	504	CDL	OB7-CB5-OB6-CB4
14	E	205	CDL	OB7-CB5-OB6-CB4
14	D	503	CDL	OB7-CB5-OB6-CB4
12	A	502	6PE	O7-C10-O6-C2
14	D	503	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
14	C	406	CDL	OA7-CA5-OA6-CA4
14	C	406	CDL	C31-CA7-OA8-CA6
18	C	408	JAG	F-C22-O2-C19
14	D	503	CDL	OB9-CB7-OB8-CB6
21	E	202	PX4	C10-C9-O5-C8
17	C	407	PEE	C31-C30-O3-C3
14	D	503	CDL	C71-CB7-OB8-CB6
21	E	202	PX4	O8-C23-O7-C7
17	C	407	PEE	O5-C30-O3-C3
14	D	503	CDL	OA9-CA7-OA8-CA6
14	E	205	CDL	CB4-CB6-OB8-CB7
21	E	202	PX4	O6-C9-O5-C8
14	D	503	CDL	C51-CB5-OB6-CB4
14	E	205	CDL	CB4-CB3-OB5-PB2
11	C	405	PG4	O2-C3-C4-O3
17	E	204	PEE	C31-C30-O3-C3
11	C	404	PG4	O2-C3-C4-O3
14	E	205	CDL	C71-CB7-OB8-CB6
14	D	503	CDL	OA5-CA3-CA4-OA6
14	E	205	CDL	O1-C1-CB2-OB2
14	C	406	CDL	OA9-CA7-OA8-CA6
17	E	204	PEE	O5-C30-O3-C3
14	E	205	CDL	C31-CA7-OA8-CA6
21	E	202	PX4	C9-C10-C11-C12
14	D	503	CDL	CA5-C11-C12-C13
14	E	205	CDL	OA9-CA7-OA8-CA6
14	A	504	CDL	OA5-CA3-CA4-OA6
18	C	408	JAG	F1-C22-O2-C19
14	C	406	CDL	CA3-OA5-PA1-OA2
21	E	202	PX4	C1-O3-P1-O4
14	A	504	CDL	CA3-OA5-PA1-OA2
14	E	205	CDL	CB3-OB5-PB2-OB2
17	C	407	PEE	C4-O4P-P-O3P
14	D	503	CDL	CB2-OB2-PB2-OB5
12	A	502	6PE	C1-O3-P1-O8
14	A	504	CDL	CB5-C51-C52-C53
14	A	504	CDL	OA5-CA3-CA4-CA6
11	C	404	PG4	O3-C5-C6-O4
11	A	501	PG4	O1-C1-C2-O2
14	C	406	CDL	C71-CB7-OB8-CB6
14	E	205	CDL	C11-CA5-OA6-CA4
16	C	403	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	C	407	PEE	C31-C32-C33-C34
14	E	205	CDL	OA7-CA5-OA6-CA4
14	E	205	CDL	CA7-C31-C32-C33
16	C	403	LMT	C11-C10-C9-C8
17	C	407	PEE	C13-C14-C15-C16
14	D	503	CDL	C51-C52-C53-C54
14	C	406	CDL	OB9-CB7-OB8-CB6
21	E	202	PX4	C10-C11-C12-C13
17	C	407	PEE	C14-C15-C16-C17
14	E	205	CDL	C51-C52-C53-C54
14	D	503	CDL	C11-C12-C13-C14
21	E	202	PX4	C12-C13-C14-C15
14	E	205	CDL	C34-C35-C36-C37
21	E	202	PX4	C16-C17-C18-C19
14	D	503	CDL	C53-C54-C55-C56
12	A	502	6PE	C4-C5-C6-C7
12	A	502	6PE	C10-C11-C12-C13
17	C	407	PEE	C18-C19-C20-C21
11	C	404	PG4	O1-C1-C2-O2
17	E	204	PEE	C11-C10-O2-C2
14	E	205	CDL	OB9-CB7-OB8-CB6
14	C	406	CDL	OB7-CB5-OB6-CB4
17	E	204	PEE	O4-C10-O2-C2
14	E	205	CDL	CA5-C11-C12-C13
17	C	407	PEE	C10-C11-C12-C13
14	C	406	CDL	C51-CB5-OB6-CB4
17	C	407	PEE	C11-C12-C13-C14
21	E	202	PX4	C17-C18-C19-C20
14	A	504	CDL	CB3-OB5-PB2-OB2
14	A	504	CDL	OB5-CB3-CB4-CB6
14	E	205	CDL	CA2-C1-CB2-OB2
17	C	407	PEE	C32-C33-C34-C35
11	A	501	PG4	O4-C7-C8-O5
14	E	205	CDL	CA3-CA4-CA6-OA8
21	E	202	PX4	C24-C25-C26-C27
14	E	205	CDL	C54-C55-C56-C57
16	C	403	LMT	O5B-C5B-C6B-O6B
14	D	503	CDL	CB6-CB4-OB6-CB5
14	D	503	CDL	C54-C55-C56-C57
14	E	205	CDL	C12-C13-C14-C15
14	D	503	CDL	C31-C32-C33-C34
17	E	204	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
16	C	403	LMT	C3-C4-C5-C6
21	E	202	PX4	C18-C19-C20-C21
14	C	406	CDL	OB5-CB3-CB4-CB6
17	C	407	PEE	O3P-C1-C2-C3
17	E	204	PEE	O3P-C1-C2-C3
12	A	502	6PE	C5-C4-O4-C3
12	A	502	6PE	C2-C1-O3-P1
14	D	503	CDL	CA3-CA4-CA6-OA8
14	A	504	CDL	CB2-OB2-PB2-OB5
16	C	403	LMT	C6-C7-C8-C9
11	A	501	PG4	O2-C3-C4-O3
17	C	407	PEE	O3P-C1-C2-O2
17	E	204	PEE	O3P-C1-C2-O2
17	C	407	PEE	C15-C16-C17-C18
14	E	205	CDL	C16-C17-C18-C19
14	D	503	CDL	OA6-CA4-CA6-OA8
17	C	407	PEE	C17-C18-C19-C20
14	C	406	CDL	CB4-CB3-OB5-PB2
14	D	503	CDL	OA5-CA3-CA4-CA6
14	D	503	CDL	OB5-CB3-CB4-CB6
14	E	205	CDL	C53-C54-C55-C56
21	E	202	PX4	C13-C14-C15-C16
12	A	502	6PE	C1-C2-C3-O4
12	A	502	6PE	O5-C4-O4-C3
11	C	404	PG4	C3-C4-O3-C5
14	C	406	CDL	OB5-CB3-CB4-OB6
11	C	404	PG4	C4-C3-O2-C2
11	C	405	PG4	C1-C2-O2-C3
11	C	405	PG4	C3-C4-O3-C5
11	C	405	PG4	C6-C5-O3-C4
14	E	205	CDL	OA6-CA4-CA6-OA8
16	C	403	LMT	C2-C3-C4-C5
14	E	205	CDL	C1-CA2-OA2-PA1
21	E	202	PX4	C1-O3-P1-O1
14	A	504	CDL	CA3-OA5-PA1-OA3
14	E	205	CDL	CB3-OB5-PB2-OB4
14	D	503	CDL	CB2-OB2-PB2-OB4
14	E	205	CDL	C14-C15-C16-C17
14	E	205	CDL	C35-C36-C37-C38
11	C	405	PG4	C4-C3-O2-C2
14	A	504	CDL	C51-C52-C53-C54
17	C	407	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	A	504	CDL	OB5-CB3-CB4-OB6
14	D	503	CDL	OB5-CB3-CB4-OB6
11	A	501	PG4	C1-C2-O2-C3
14	E	205	CDL	CB5-C51-C52-C53
21	E	202	PX4	O3-C1-C2-N1
12	A	502	6PE	O6-C2-C3-O4
11	A	501	PG4	C5-C6-O4-C7
11	A	501	PG4	C3-C4-O3-C5
11	A	501	PG4	C8-C7-O4-C6
17	E	204	PEE	C3-C2-O2-C10
14	A	504	CDL	CA4-CA3-OA5-PA1
14	E	205	CDL	OA5-CA3-CA4-OA6
14	C	406	CDL	CB2-OB2-PB2-OB5
14	E	205	CDL	CA2-OA2-PA1-OA5
14	E	205	CDL	CB2-OB2-PB2-OB5
17	E	204	PEE	C1-O3P-P-O4P
21	E	202	PX4	C19-C20-C21-C22
14	E	205	CDL	C52-C53-C54-C55
17	E	204	PEE	O3-C30-C31-C32
17	E	204	PEE	C4-O4P-P-O3P
17	E	204	PEE	O5-C30-C31-C32
14	E	205	CDL	C13-C14-C15-C16
21	E	202	PX4	C1-C2-N1-C4
21	E	202	PX4	C11-C10-C9-O5
17	E	204	PEE	C1-C2-C3-O3
14	A	504	CDL	C52-C51-CB5-OB6
15	C	401	HEM	C3D-CAD-CBD-CGD
21	E	202	PX4	C6-O4-P1-O2
14	A	504	CDL	CB3-OB5-PB2-OB3
14	E	205	CDL	CA2-OA2-PA1-OA3
14	E	205	CDL	CB2-OB2-PB2-OB3
11	C	405	PG4	O1-C1-C2-O2
17	E	204	PEE	C5-C4-O4P-P
14	C	406	CDL	C72-C71-CB7-OB8
21	E	202	PX4	O7-C23-C24-C25
14	E	205	CDL	C32-C31-CA7-OA8
14	D	503	CDL	C52-C51-CB5-OB6
14	A	504	CDL	C52-C51-CB5-OB7
17	C	407	PEE	O3-C30-C31-C32
12	A	502	6PE	O4-C4-C5-C6
14	C	406	CDL	C72-C71-CB7-OB9
12	A	502	6PE	O5-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	504	CDL	O1-C1-CA2-OA2
21	E	202	PX4	C1-C2-N1-C5
14	D	503	CDL	C52-C51-CB5-OB7

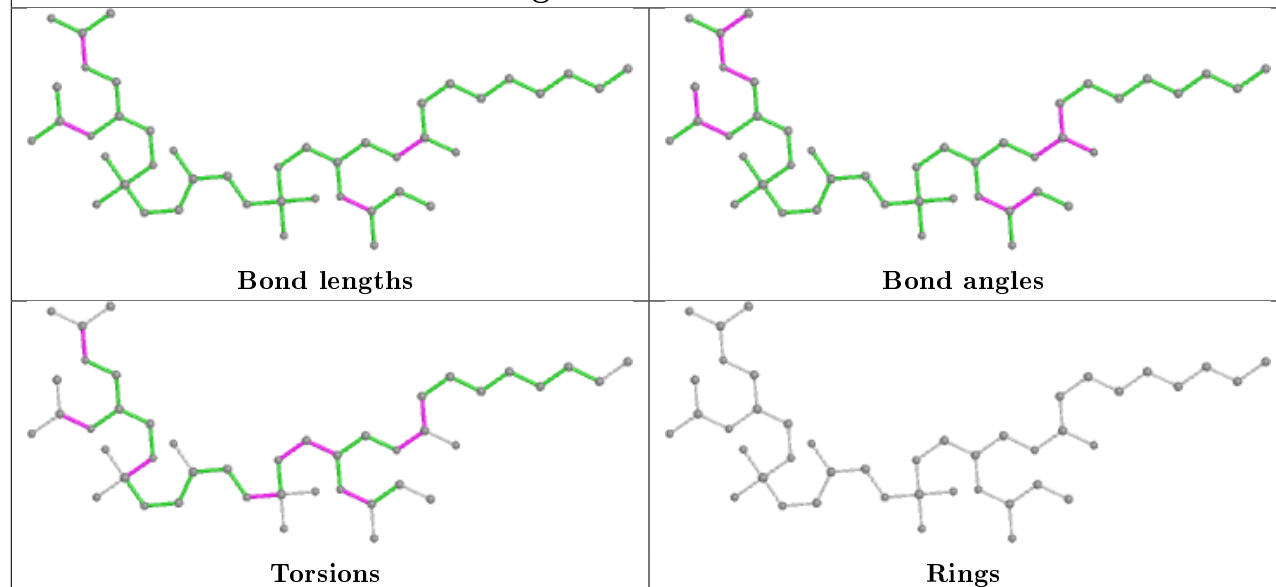
There are no ring outliers.

7 monomers are involved in 14 short contacts:

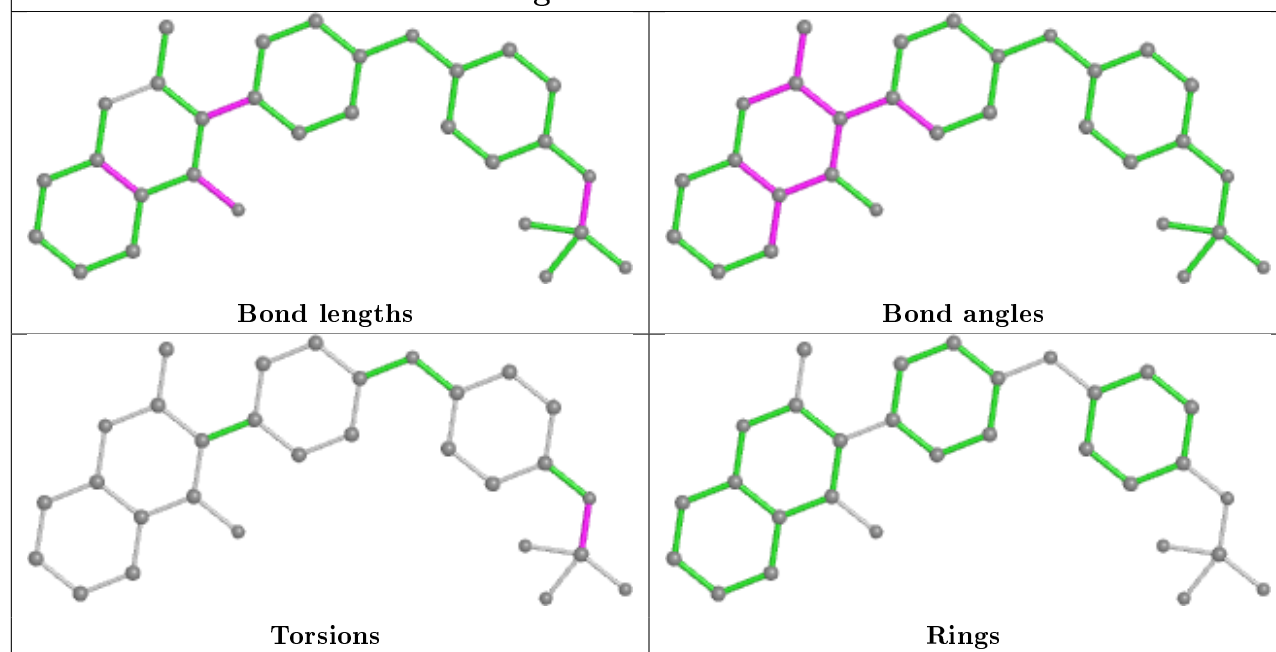
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	202	PX4	1	0
14	A	504	CDL	2	0
15	C	402	HEM	2	0
15	C	401	HEM	3	0
17	C	407	PEE	1	0
19	D	501	HEC	5	0
12	A	502	6PE	2	0

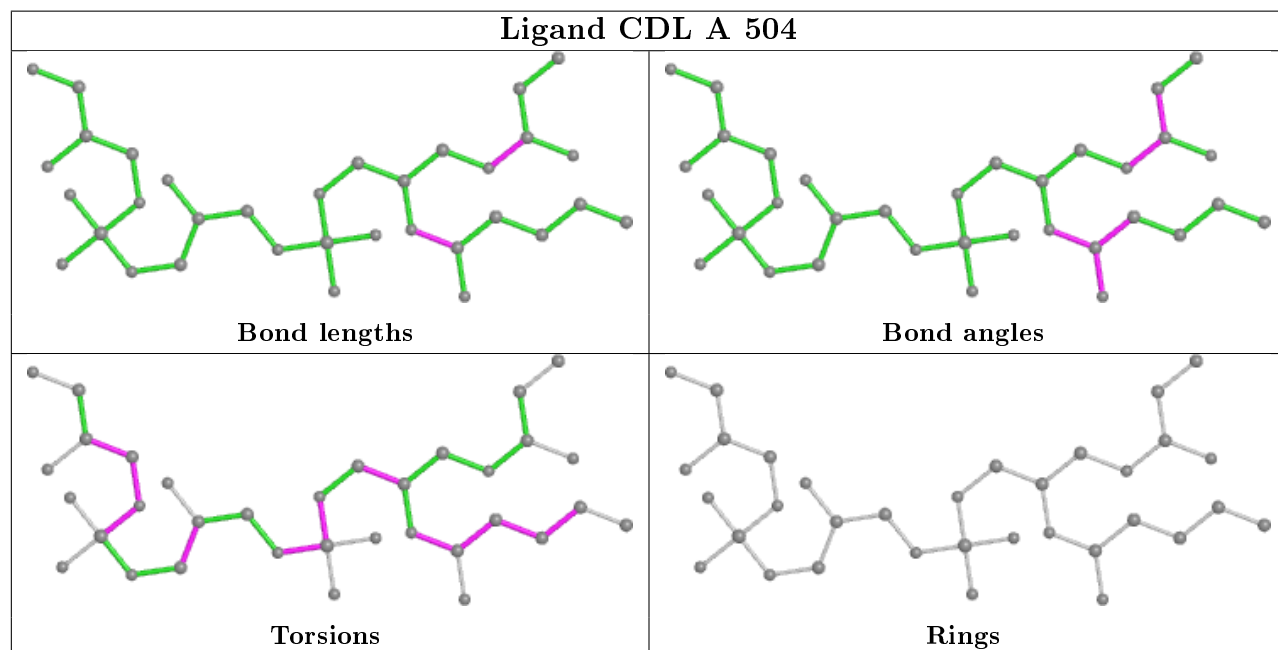
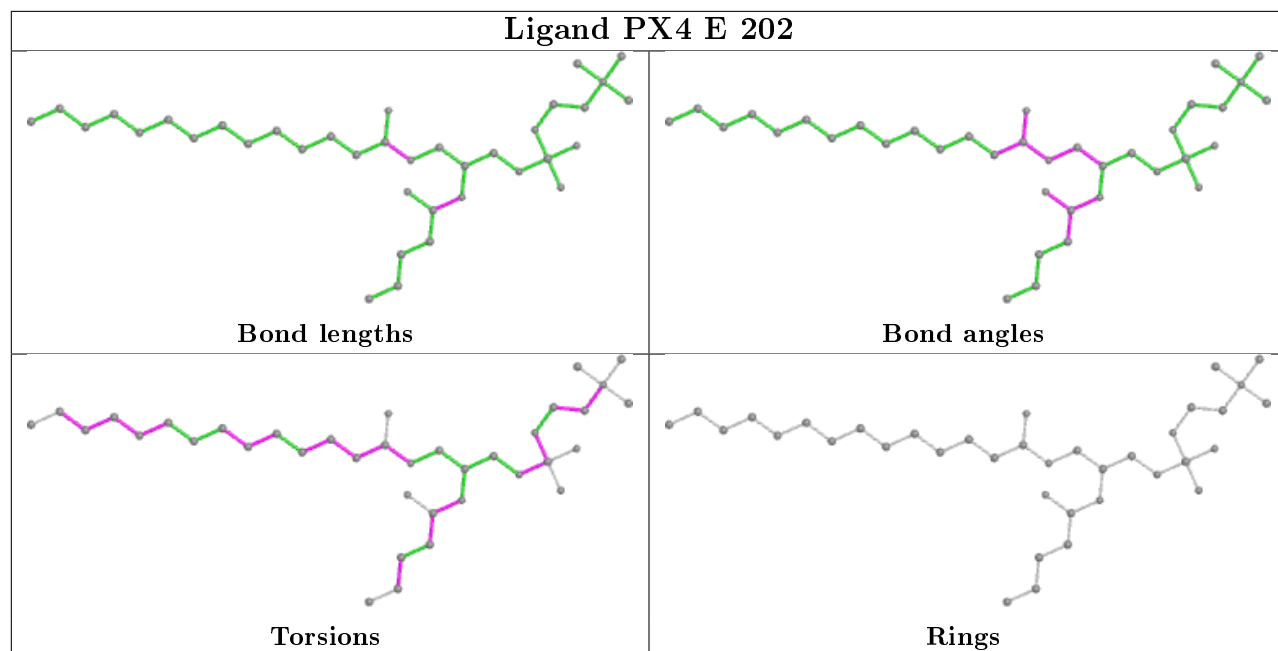
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

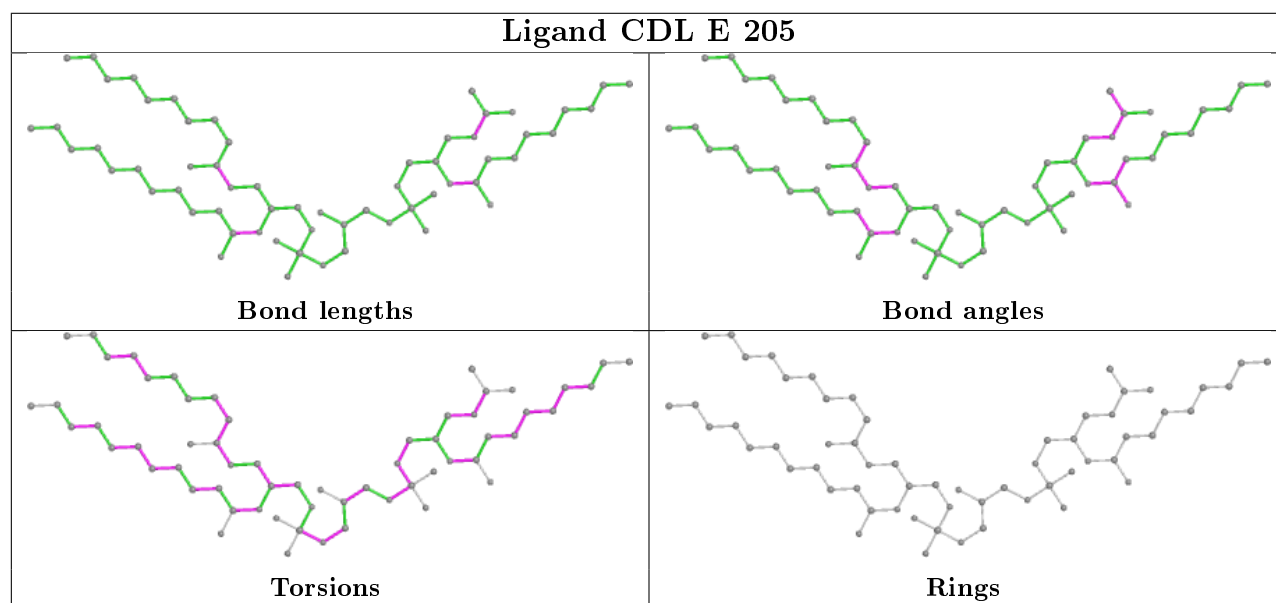
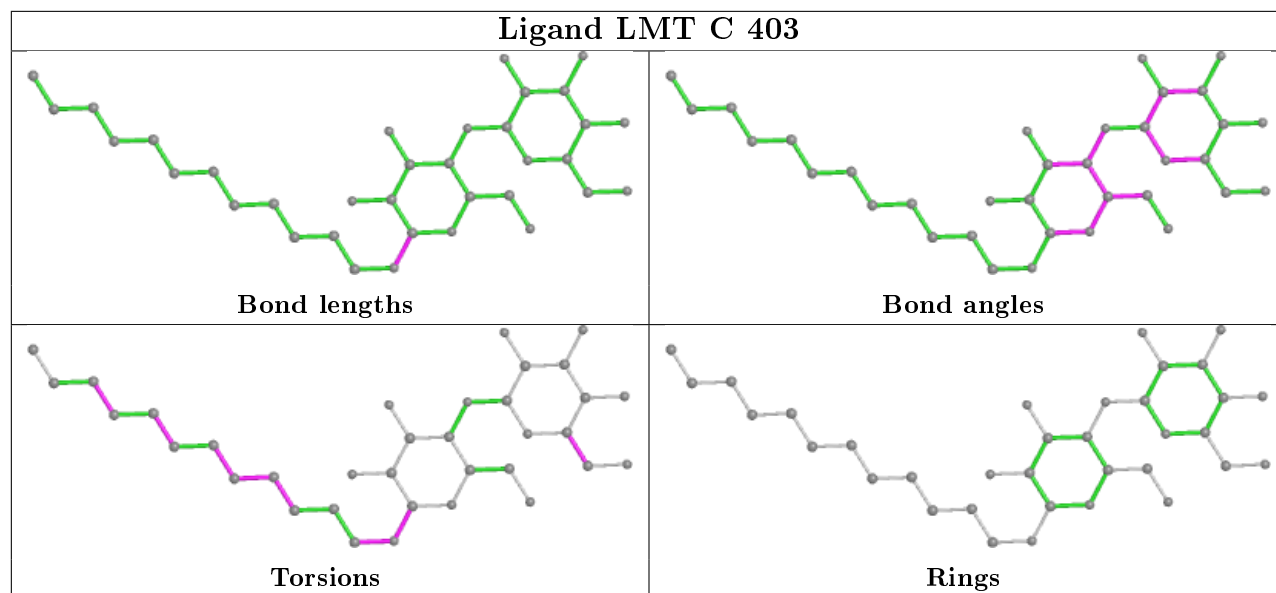
Ligand CDL C 406

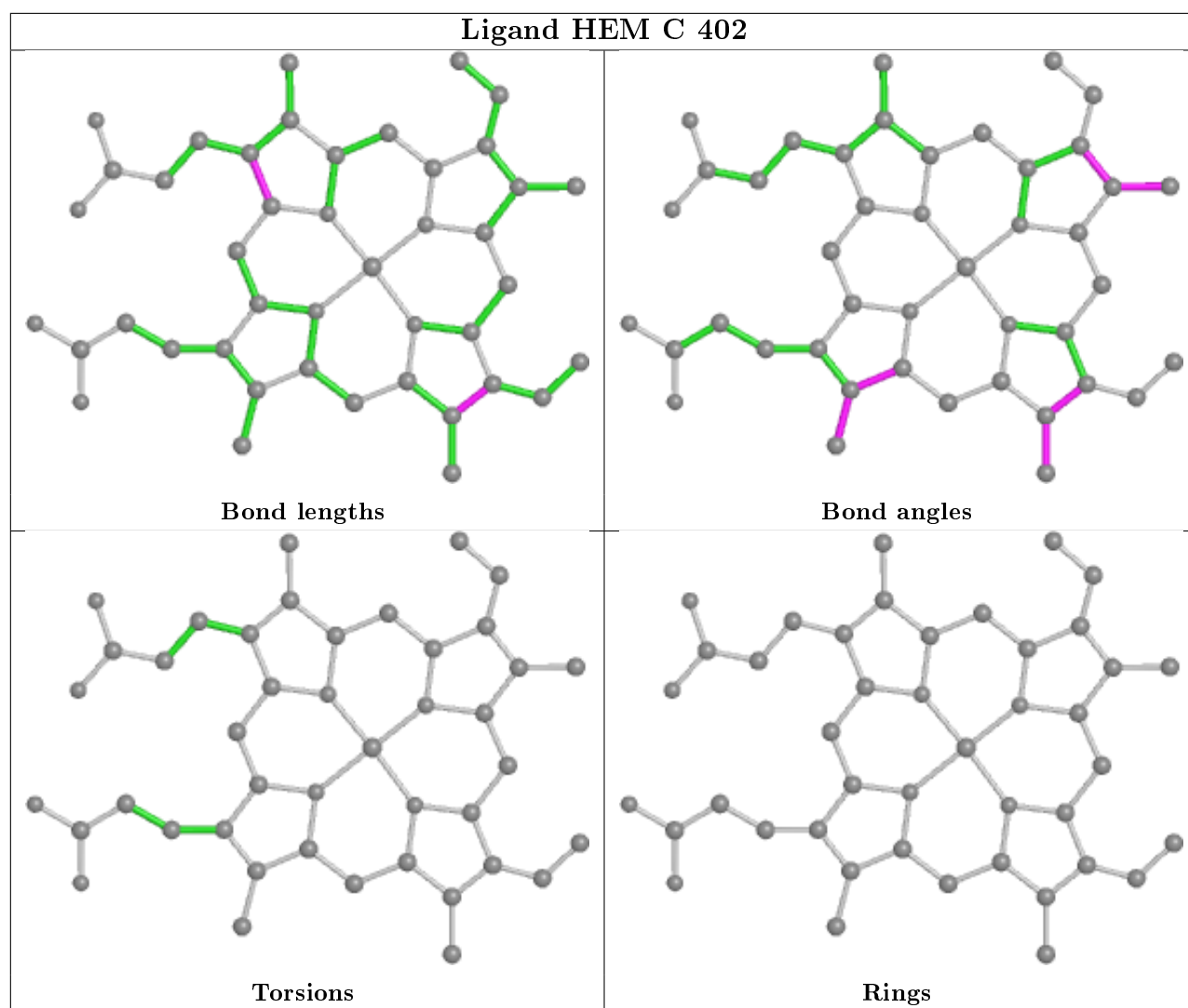


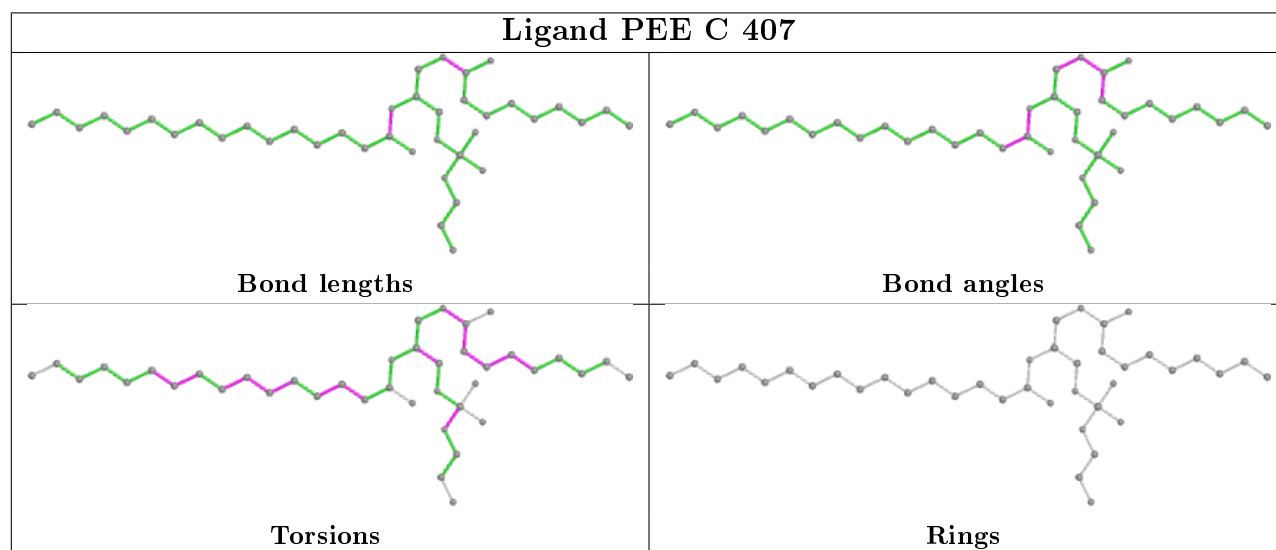
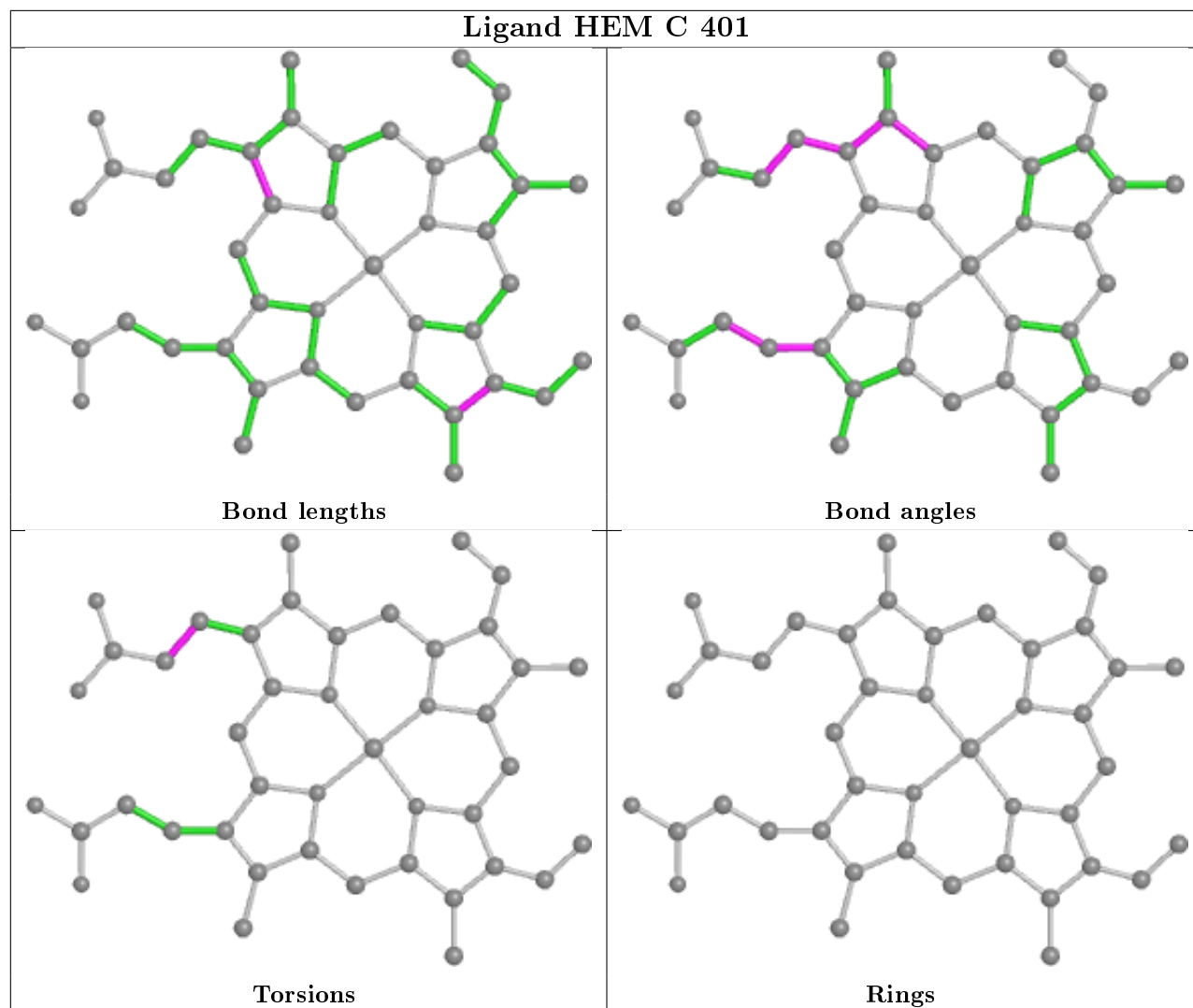
Ligand JAG C 408

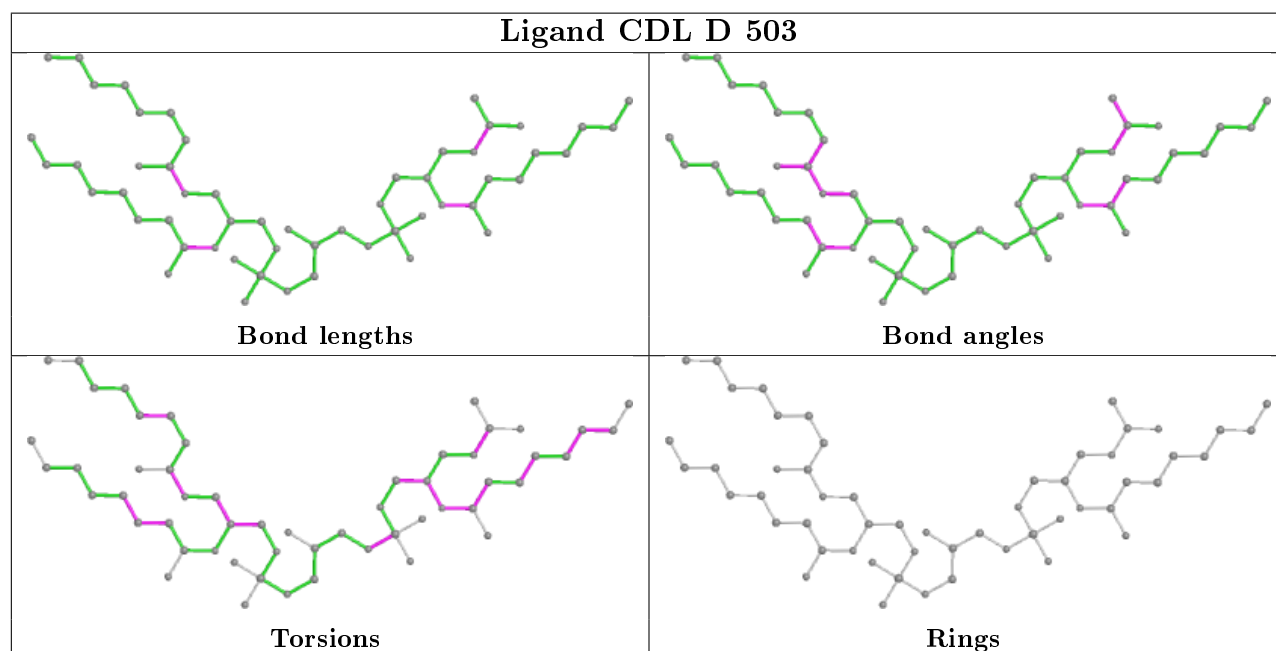
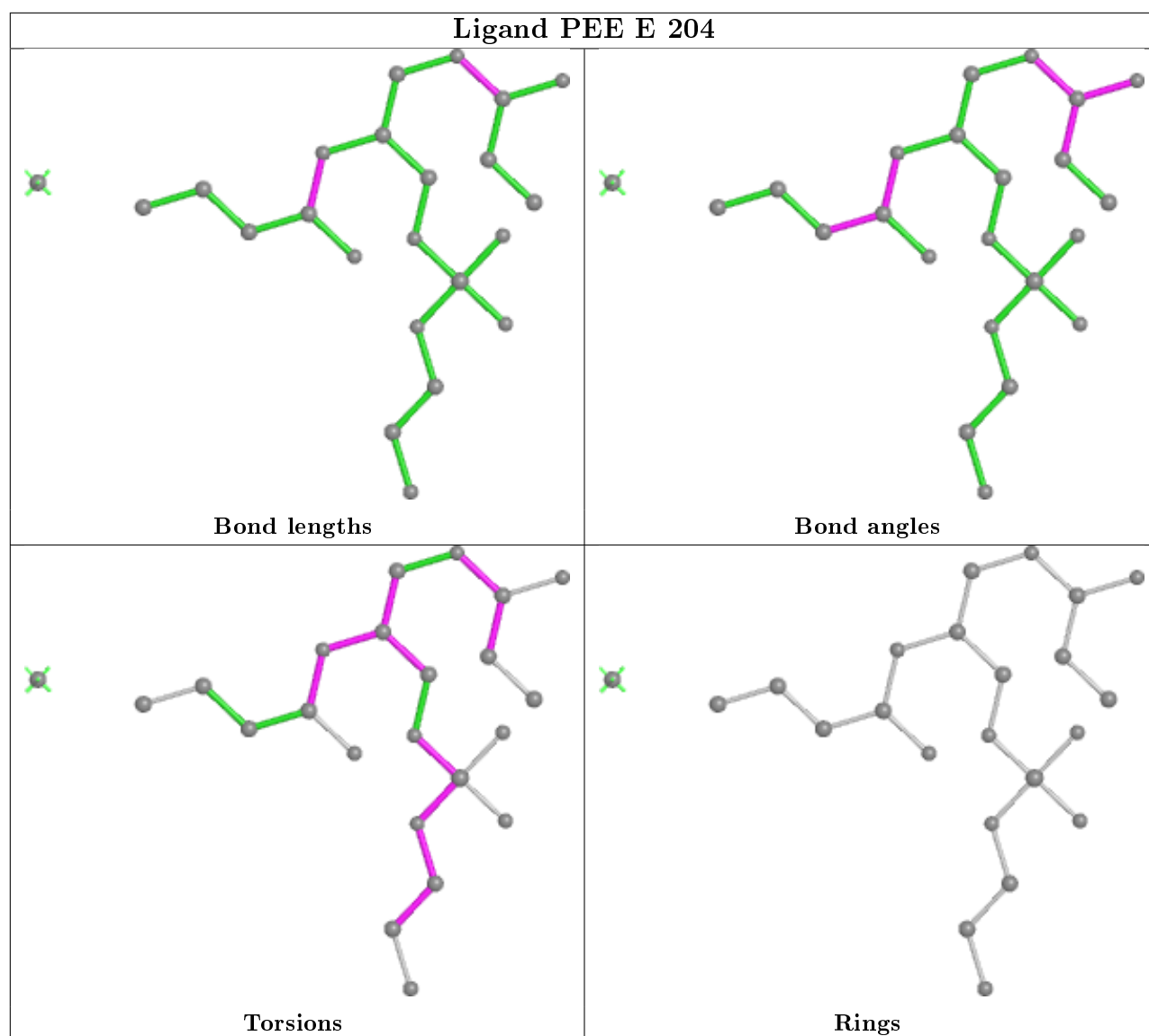


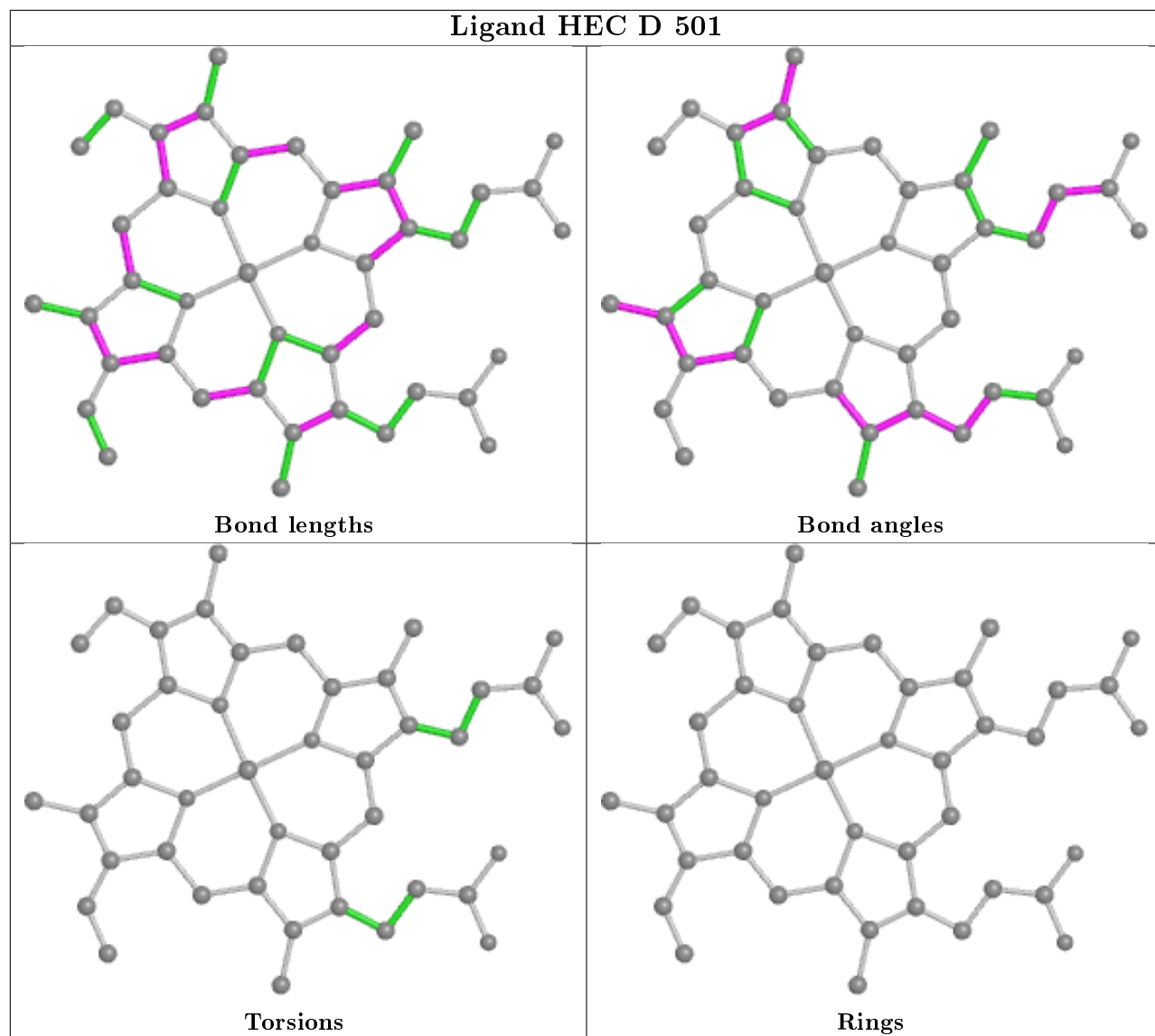


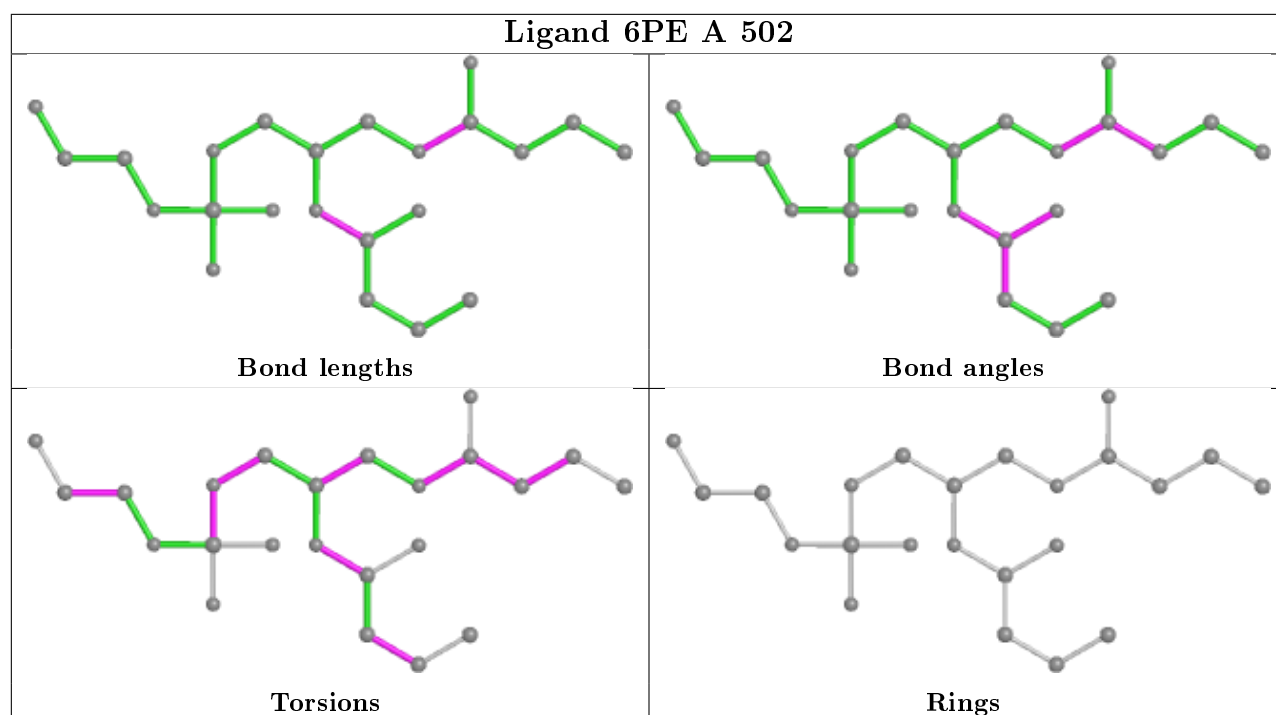












5.7 Other polymers [i](#)

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%)

All (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
4	D	159	GLY	3.7
4	D	171	PHE	3.6
2	B	44	ALA	3.4
9	I	37	THR	3.4
4	D	180	SER	3.2
4	D	107	GLY	3.1
1	A	371	GLY	3.1
1	A	370	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	76	GLU	2.9
4	D	165	TYR	2.9
1	A	369	LEU	2.7
9	I	48	SER	2.7
5	E	157	TYR	2.7
9	I	73	PRO	2.6
5	E	159	PRO	2.6
2	B	169	ARG	2.6
1	A	229	PRO	2.6
2	B	229	GLY	2.5
1	A	23	LEU	2.4
4	D	148	TYR	2.4
9	I	49	VAL	2.4
1	A	21	ASN	2.3
4	D	139	THR	2.3
2	B	260	GLU	2.3
8	H	14	VAL	2.3
5	E	107	ASP	2.3
4	D	134	TYR	2.3
2	B	425	ALA	2.3
4	D	163	PRO	2.2
4	D	110	PRO	2.2
1	A	365	LEU	2.2
2	B	421	ARG	2.2
1	A	4	TYR	2.2
4	D	158	ILE	2.2
9	I	40	SER	2.2
4	D	72	ASP	2.1
5	E	89	PHE	2.1
6	F	27	ASN	2.1
2	B	423	SER	2.1
2	B	424	MET	2.1
2	B	113	ARG	2.1
4	D	167	GLU	2.1
1	A	188	ARG	2.1
4	D	168	VAL	2.1
5	E	108	GLN	2.1
2	B	42	ALA	2.0
4	D	149	PHE	2.0

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 ⓘ

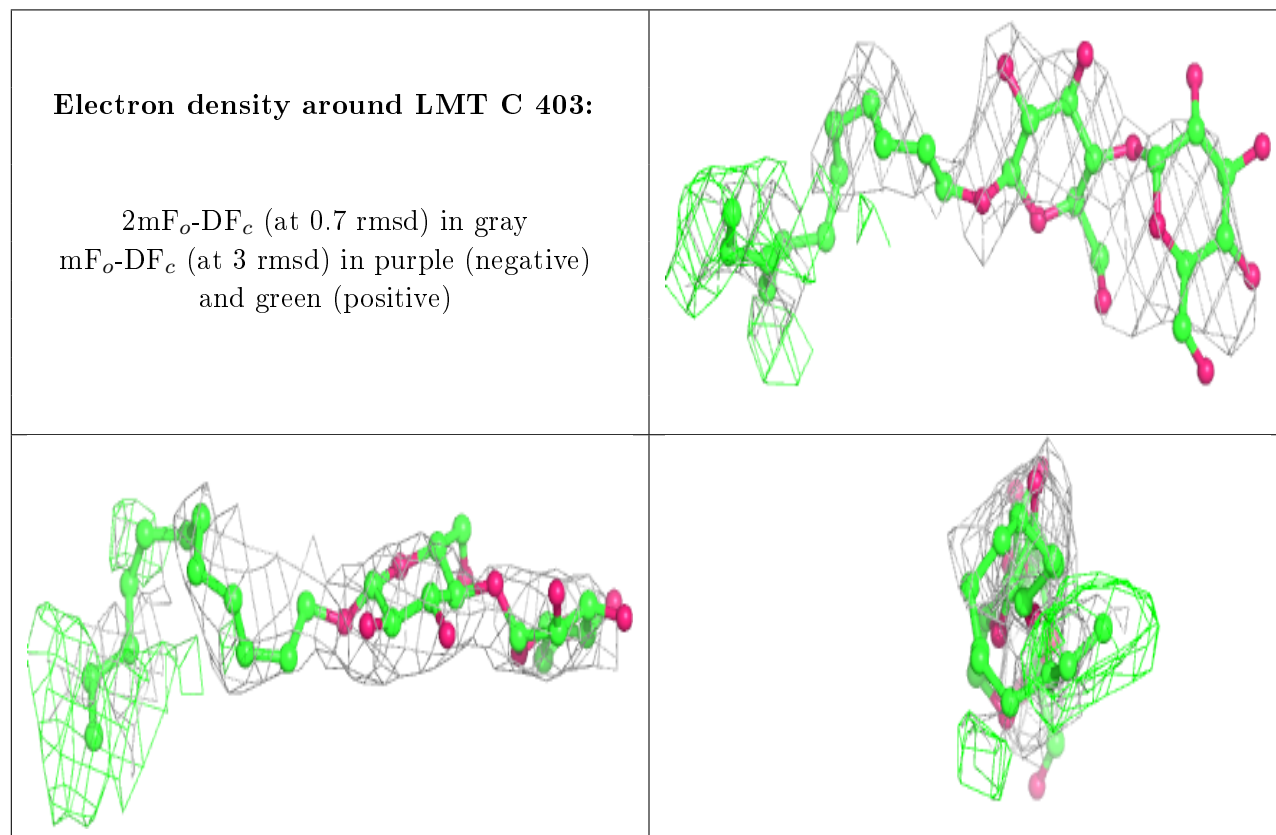
There are no monosaccharides in this entry.

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.

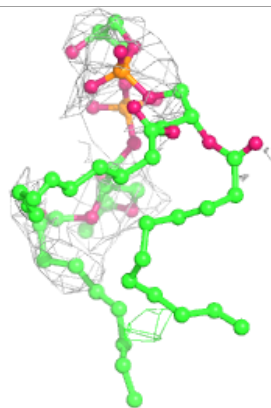
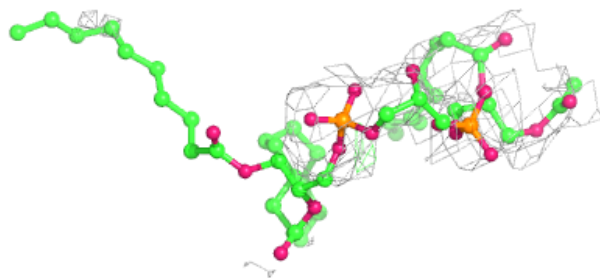
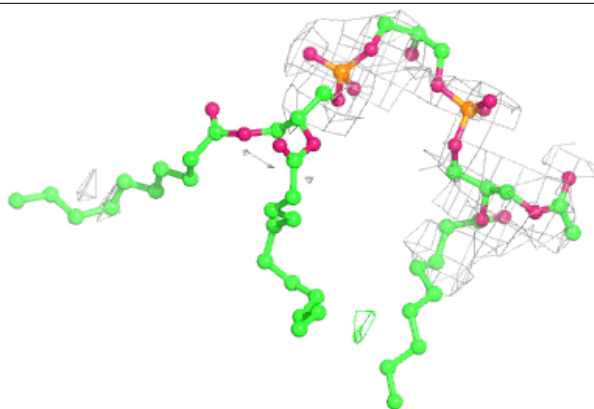
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	LMT	C	403	35/35	0.44	0.44	217,247,256,256	0
13	PO4	D	502	5/5	0.47	0.22	237,240,240,245	0
13	PO4	E	203	5/5	0.49	0.31	248,249,253,256	0
13	PO4	G	102	5/5	0.54	0.24	245,247,249,252	0
14	CDL	E	205	60/100	0.59	0.53	190,215,255,259	0
11	PG4	A	501	13/13	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.



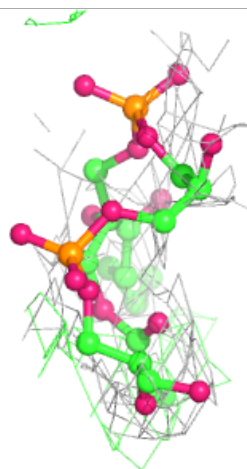
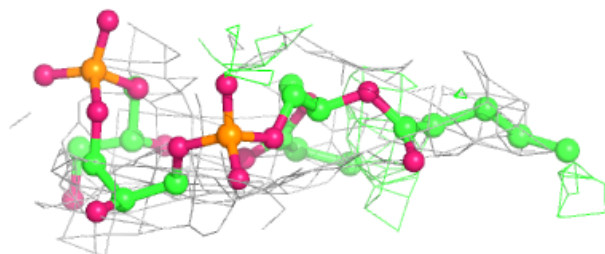
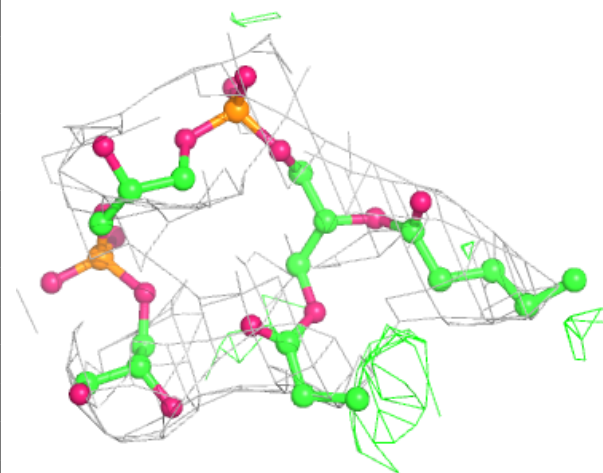
Electron density around CDL E 205:

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



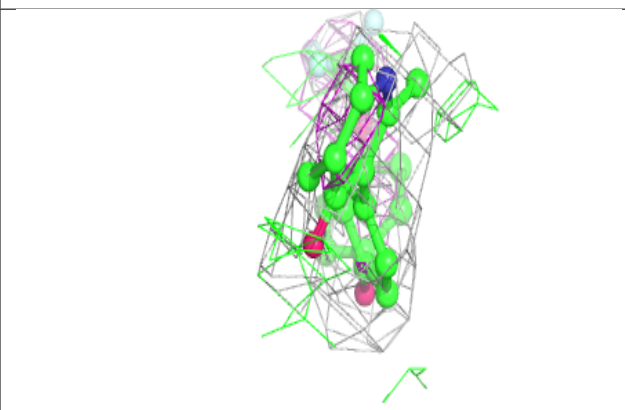
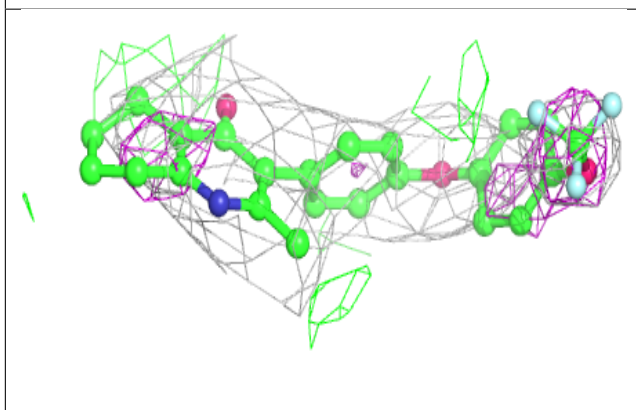
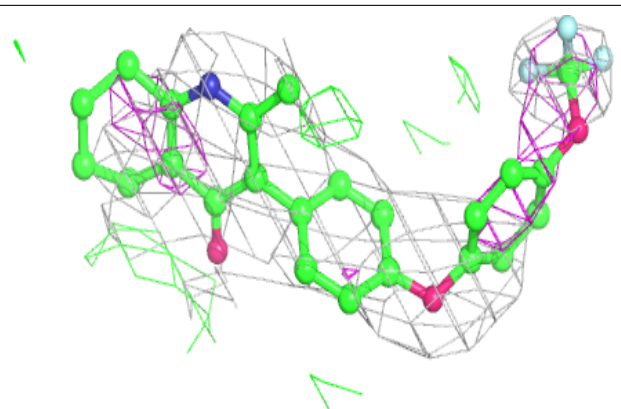
Electron density around CDL A 504:

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

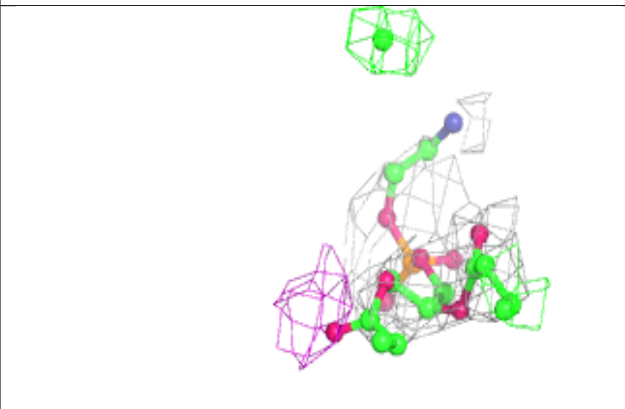
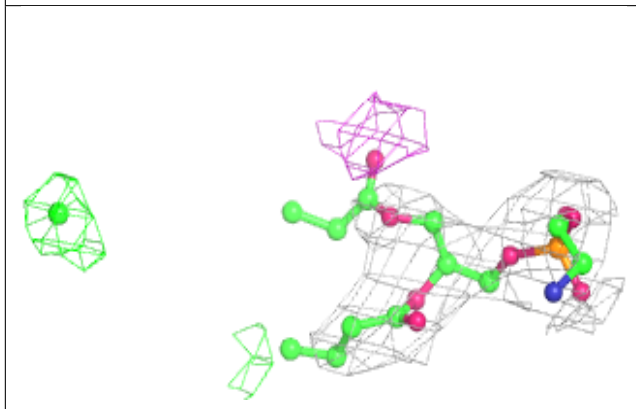
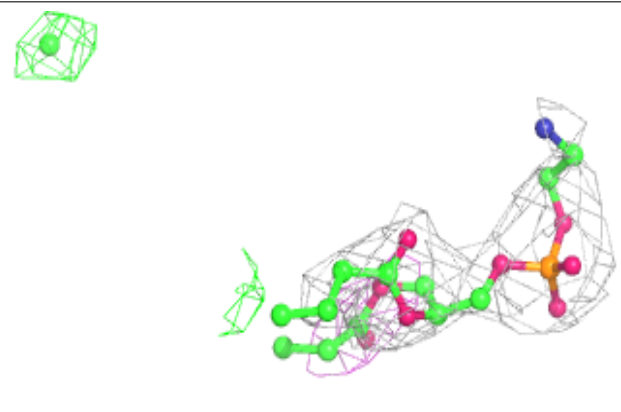


Electron density around JAG C 408:

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

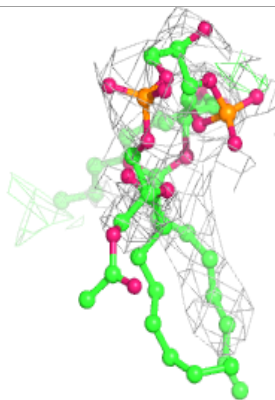
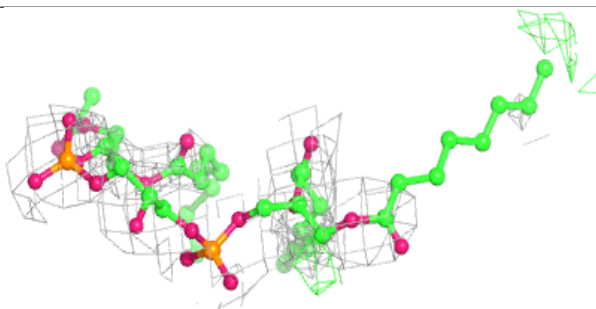
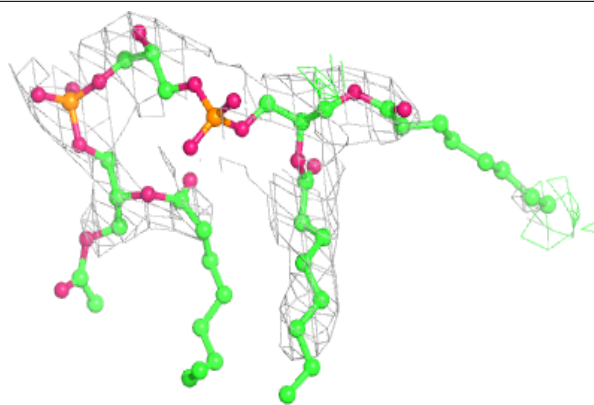
**Electron density around PEE E 204:**

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

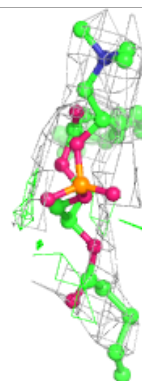
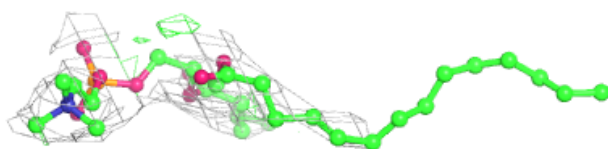
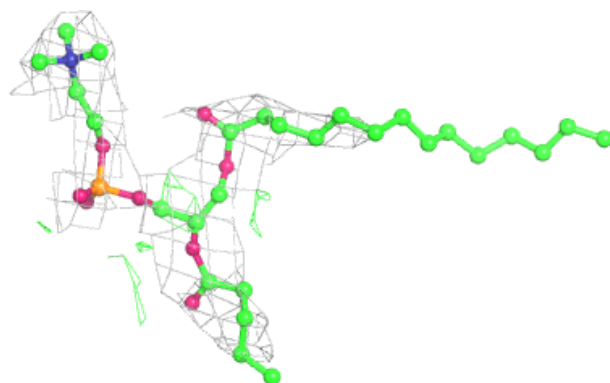


Electron density around CDL D 503:

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

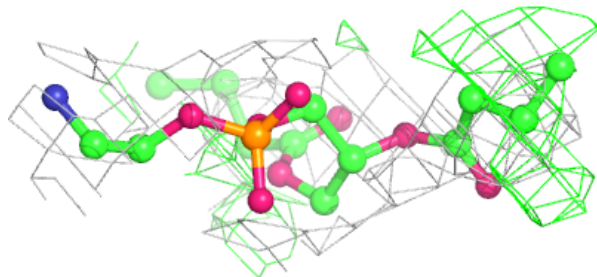
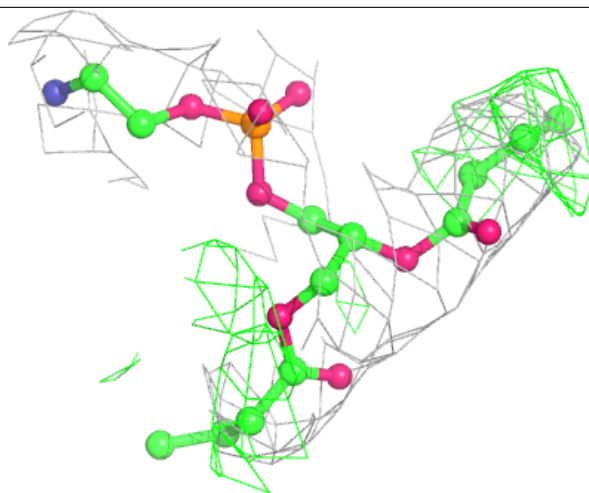
**Electron density around PX4 E 202:**

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



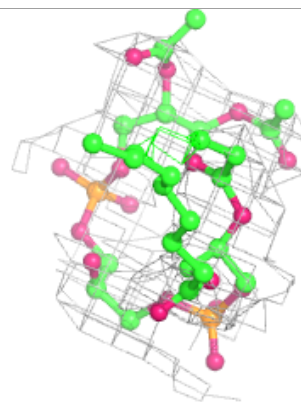
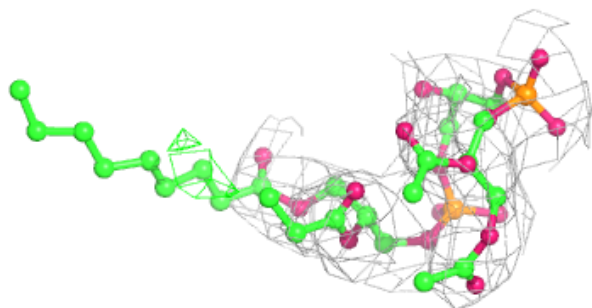
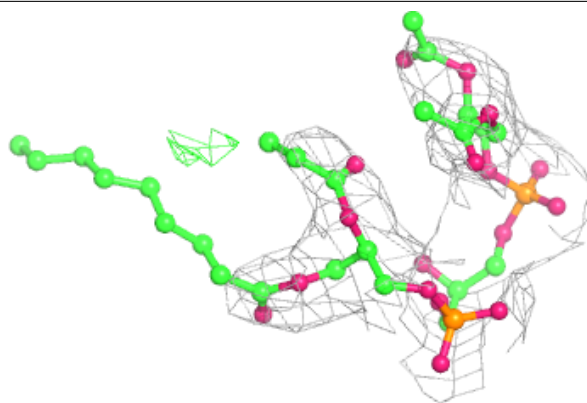
Electron density around 6PE A 502:

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

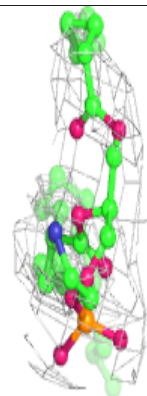
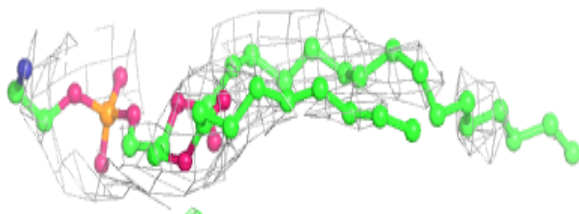


Electron density around CDL C 406:

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

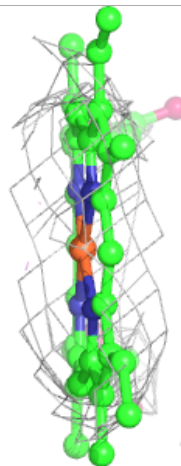
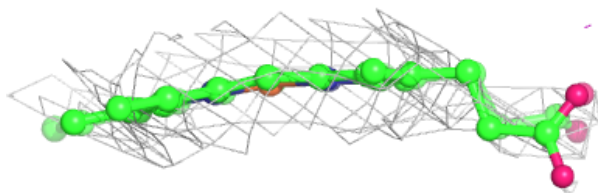
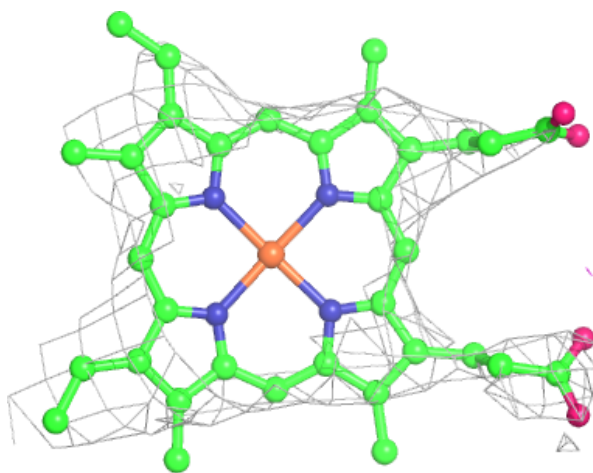
**Electron density around PEE C 407:**

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



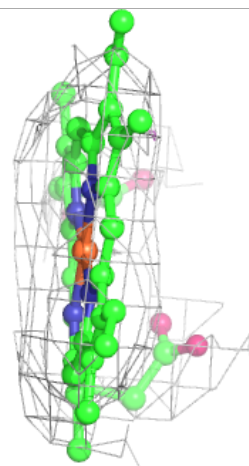
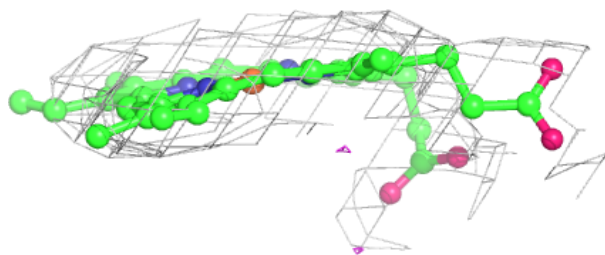
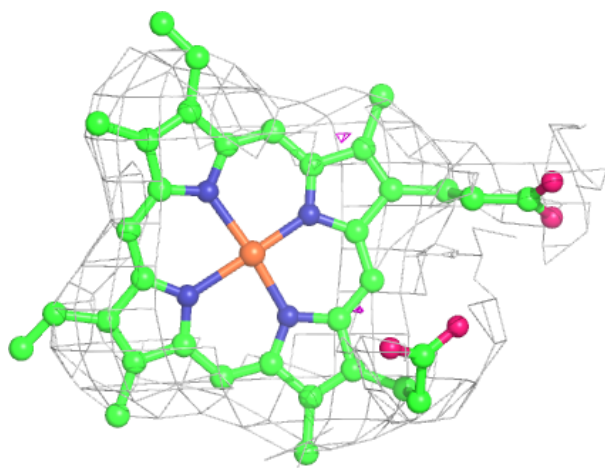
Electron density around HEC D 501:

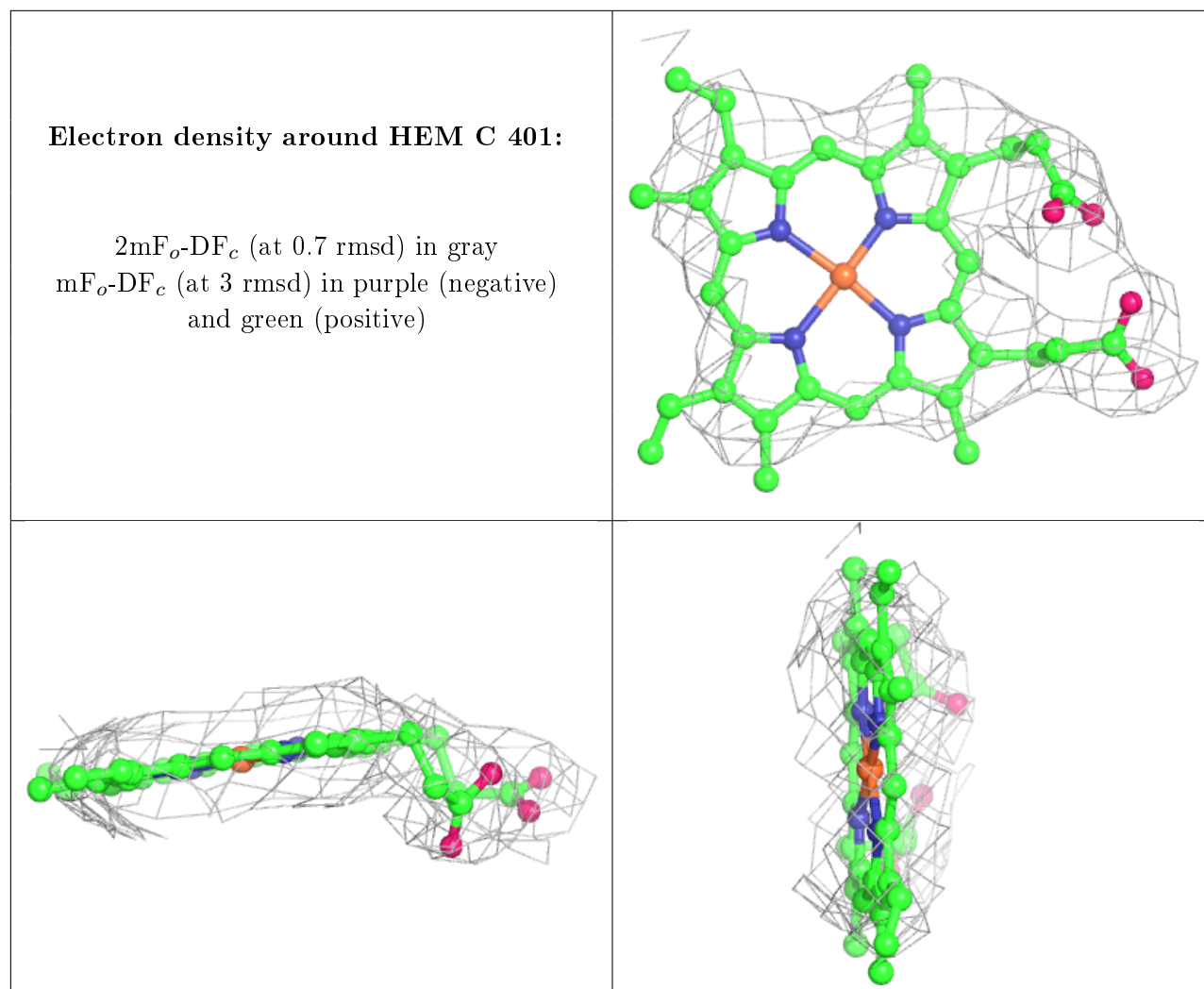
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.