



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:30 am BST

PDB ID : 6HAW
Title : Crystal structure of bovine cytochrome bc1 in complex with 2-pyrazolyl quinolone inhibitor WDH2G7
Authors : Ampornpanai, K.; Hong, W.D.; O'Neill, P.M.; Hasnain, S.S.; Antonyuk, S.V.
Deposited on : 2018-08-08
Resolution : 3.45 Å(reported)

This is a 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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

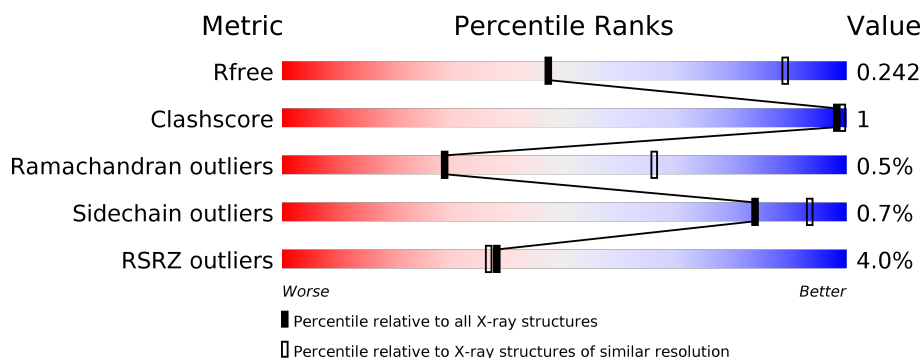
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



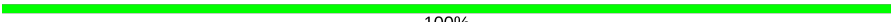
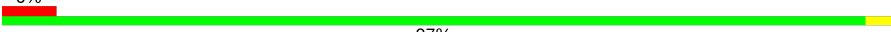


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	438	<div> <div>3%</div> <div>97%</div> </div>
2	B	413	<div> <div>3%</div> <div>99%</div> </div>
3	C	378	<div> <div>%</div> <div>97%</div> </div>
4	D	239	<div> <div>7%</div> <div>97%</div> </div>
5	E	196	<div> <div>9%</div> <div>98%</div> </div>
6	F	99	<div> <div></div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	74	 100%
8	H	64	 6% 97%
9	I	46	 24% 89% 11%
10	J	59	 2% 98%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PGE	C	407	-	-	-	X
13	PO4	A	503	-	-	-	X
13	PO4	A	504	-	-	-	X
13	PO4	B	501	-	-	-	X
19	PEE	C	405	X	-	-	-
19	PEE	E	204	X	-	-	-
20	FX2	C	406	X	-	-	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 16062 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			2996	2007	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
			1851	1181	322	333	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
			1450	907	254	282	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
			853	542	153	156	2			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			612	400	113	98	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
			490	297	84	104	5			

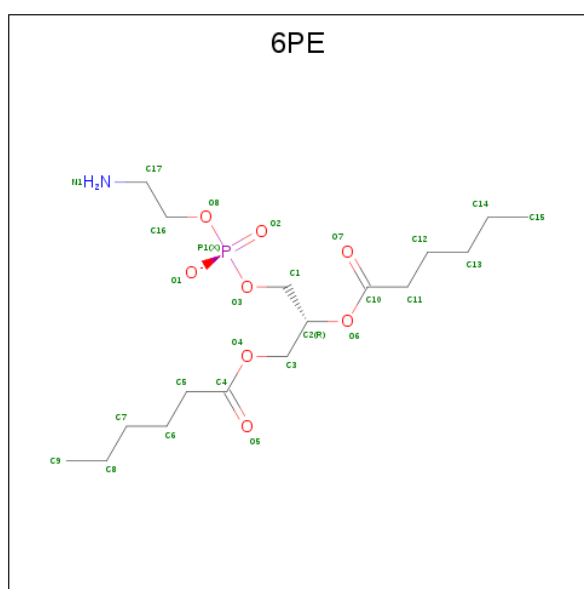
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			322	201	63	57	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
			487	320	84	83				

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



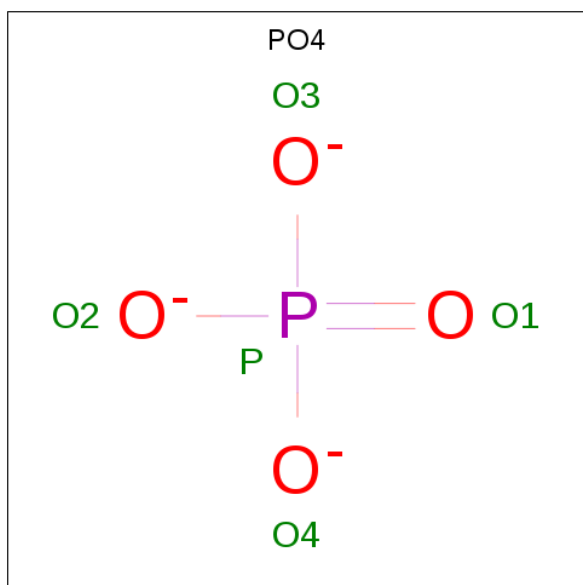
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

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



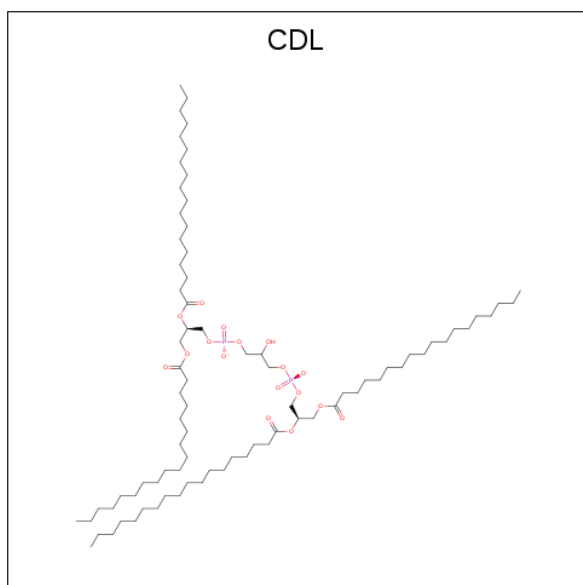
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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



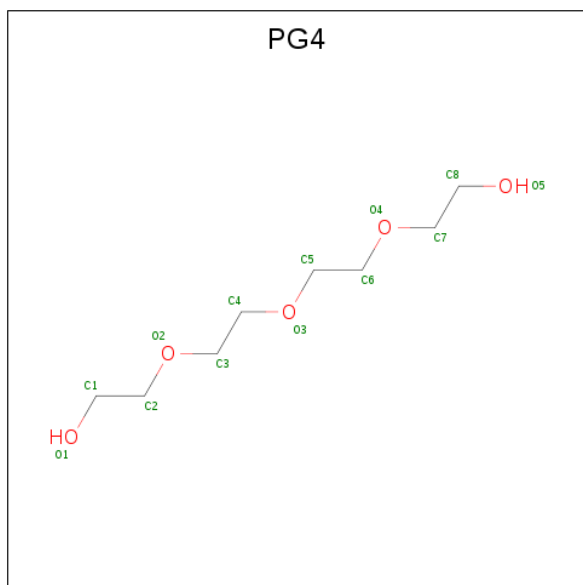
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			34	17	15	2		

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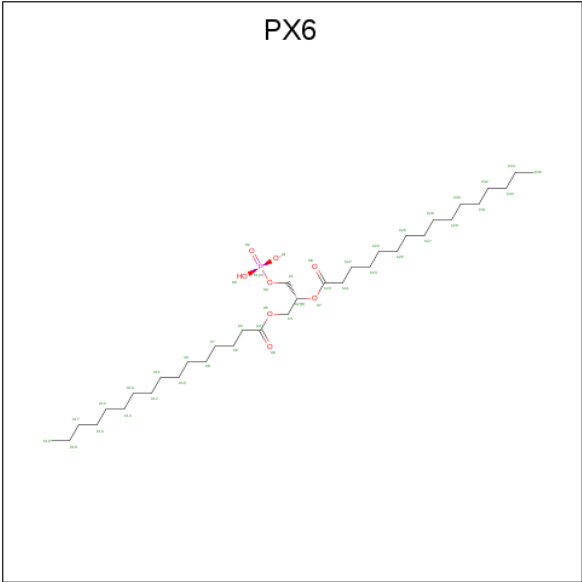
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			38	19	17	2		
14	D	1	Total	C	O	P	0	0
			27	12	13	2		
14	E	1	Total	C	O	P	0	0
			28	13	13	2		

- Molecule 15 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



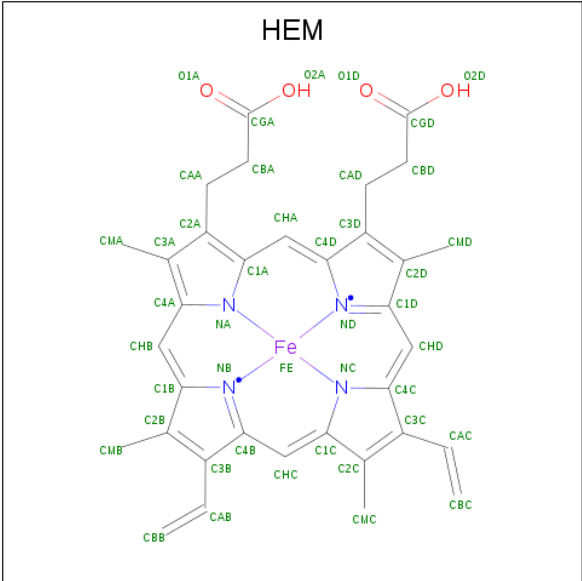
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	O		0	0
			13	8	5			

- Molecule 16 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: $C_{35}H_{68}O_8P$).



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

- Molecule 17 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



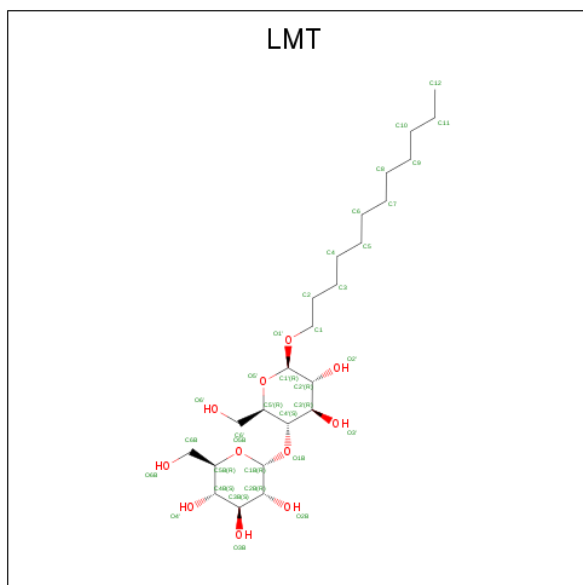
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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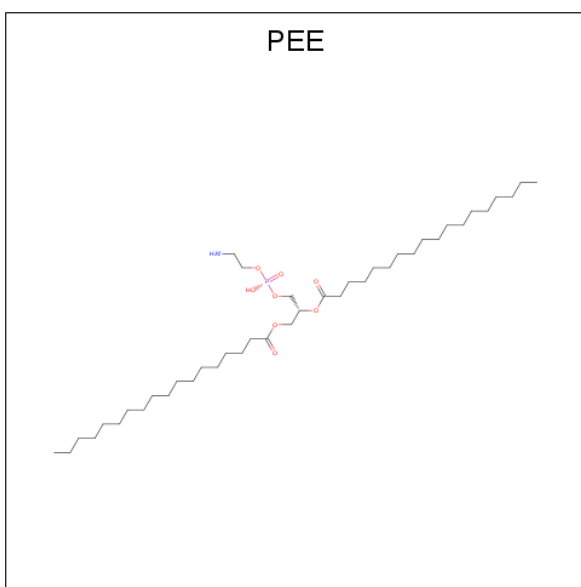
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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



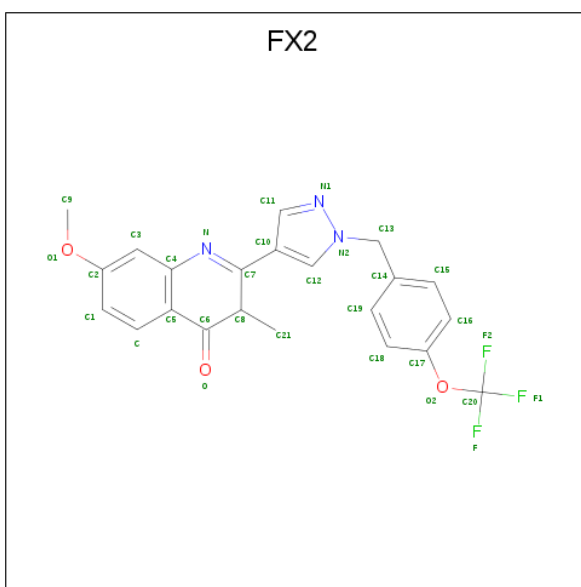
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O		
			35	24	11		
						0	0

- Molecule 19 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



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

- Molecule 20 is 7-methoxy-3-methyl-2-[1-[[4-(trifluoromethoxy)phenyl]methyl]pyrazol-4-yl]-3 {H}-quinolin-4-one (three-letter code: FX2) (formula: C₂₂H₁₈F₃N₃O₃) (labeled as "Ligand of Interest" by author).



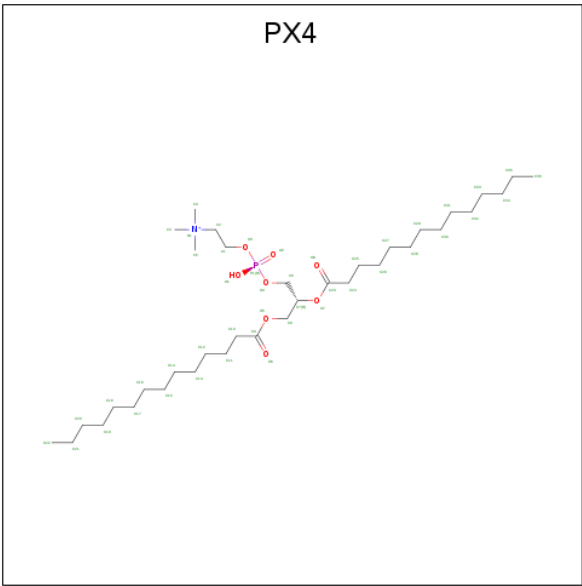
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total	C	F	N	O	0	0
			31	22	3	3	3		

- # HEC

Diagram illustrating the structure of a four-center ferrous sulfide (FES) molecule. The molecule consists of two iron (Fe) atoms and two sulfur (S) atoms arranged in a square. The top-left atom is labeled S1 (green), the top-right is FE2 (green), the bottom-left is FE1 (green), and the bottom-right is S2 (green). The bonds between S1 and FE2, and between FE1 and S2, are colored yellow. The bonds between S1 and FE1, and between FE2 and S2, are colored purple.



code: PX4) (formula: C₃₆H₇₃NO₈P).



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

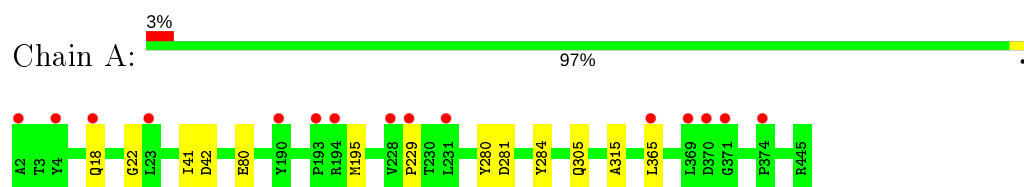
- Molecule 24 is water.

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

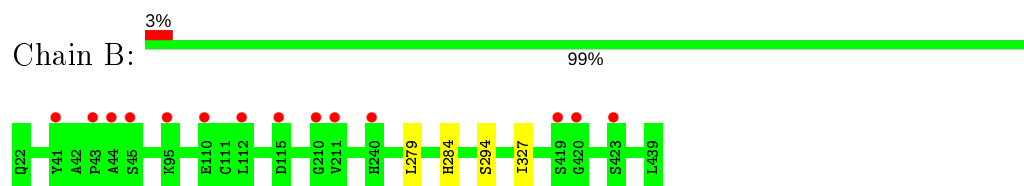
3 Residue-property plots [i](#)

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

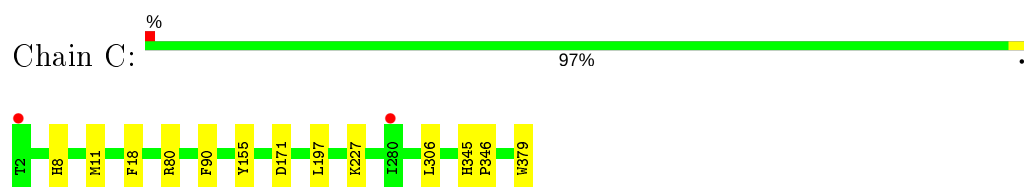
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



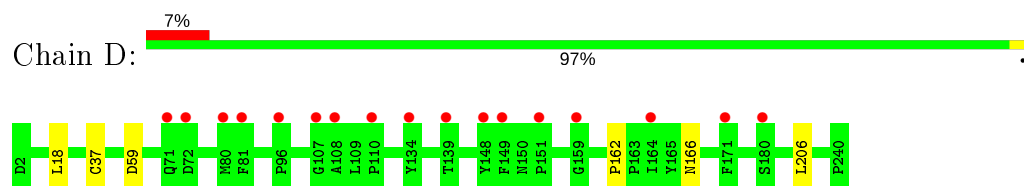
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



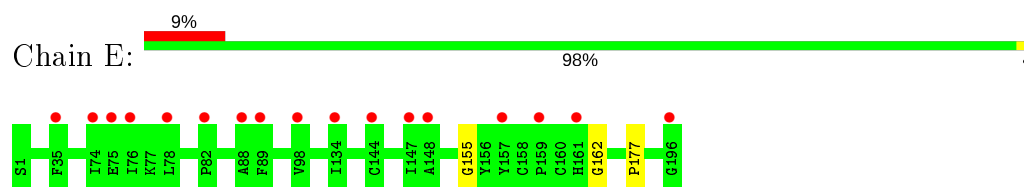
- Molecule 3: Cytochrome b



- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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



- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:  98% .



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:  100%


There are no outlier residues recorded for this chain.

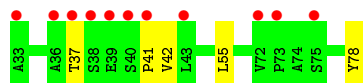
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:  97% .



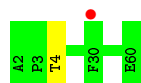
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:  89% 11%



- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:  98% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	212.69Å 212.69Å 347.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.10 – 3.45 92.10 – 3.45	Depositor EDS
% Data completeness (in resolution range)	89.2 (92.10-3.45) 89.2 (92.10-3.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.210 , 0.242 0.209 , 0.242	Depositor DCC
R_{free} test set	2762 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16062	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PGE, CDL, PO4, LMT, PX6, FX2, 6PE, PG4, FES, HEC, PEE, PX4, 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	0.43	0/3400	0.64	0/4620
2	B	0.43	0/3128	0.63	0/4248
3	C	0.47	0/3092	0.61	0/4231
4	D	0.43	0/1910	0.61	0/2601
5	E	0.45	0/1482	0.62	0/2014
6	F	0.42	0/872	0.65	0/1174
7	G	0.51	0/633	0.65	0/859
8	H	0.39	0/495	0.66	0/670
9	I	0.53	0/326	0.87	0/445
10	J	0.46	0/500	0.64	0/675
All	All	0.44	0/15838	0.63	0/21537

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3331	0	3189	5	0
2	B	3073	0	3020	3	0
3	C	2996	0	3058	3	0

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

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

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:CYS:SG	21:D:501:HEC:CAB	2.88	0.61
1:A:18:GLN:HE21	1:A:22:GLY:HA2	1.68	0.58
4:D:37:CYS:SG	21:D:501:HEC:HBB3	2.44	0.58
17:C:401:HEM:HMC1	17:C:401:HEM:HBC2	1.88	0.56
11:A:501:6PE:H28	14:A:506:CDL:HB31	1.94	0.49
3:C:8:HIS:HB3	3:C:11:MET:HB2	1.96	0.47
6:F:71:ARG:HB3	6:F:73:GLN:HG3	1.96	0.47
4:D:37:CYS:SG	21:D:501:HEC:CBB	3.04	0.45
4:D:166:ASN:H	4:D:166:ASN:HD22	1.65	0.44
3:C:197:LEU:HD21	17:C:402:HEM:HMA3	2.00	0.44
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.54	0.43
11:A:501:6PE:H6	14:A:506:CDL:H712	2.00	0.43
3:C:345:HIS:HA	3:C:346:PRO:HA	1.75	0.42
1:A:80:GLU:HG2	2:B:284:HIS:HB2	2.02	0.42
1:A:305:GLN:NE2	9:I:42:VAL:HG12	2.34	0.42
2:B:279:LEU:HA	2:B:294:SER:HB3	2.01	0.42
2:B:327:ILE:HG21	9:I:55:LEU:HD11	2.00	0.41
1:A:41:ILE:HG12	1:A:195:MET:HG2	2.02	0.41
4:D:18:LEU:HD22	4:D:206:LEU:HB2	2.04	0.40
8:H:38:GLU:HA	8:H:41:ASP:HB2	2.04	0.40

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	434/438 (99%)	420 (97%)	12 (3%)	2 (0%)	29	66
2	B	409/413 (99%)	396 (97%)	13 (3%)	0	100	100
3	C	376/378 (100%)	362 (96%)	13 (4%)	1 (0%)	41	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	237/239 (99%)	227 (96%)	9 (4%)	1 (0%)	34	70
5	E	194/196 (99%)	184 (95%)	7 (4%)	3 (2%)	10	43
6	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
7	G	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
8	H	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
9	I	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	20
10	J	57/59 (97%)	54 (95%)	2 (4%)	1 (2%)	8	39
All	All	1982/2006 (99%)	1905 (96%)	67 (3%)	10 (0%)	29	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	37	THR
9	I	41	PRO
1	A	315	ALA
3	C	155	TYR
5	E	177	PRO
4	D	162	PRO
1	A	229	PRO
5	E	155	GLY
5	E	162	GLY
10	J	4	THR

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	347/363 (96%)	344 (99%)	3 (1%)	78	91
2	B	318/324 (98%)	318 (100%)	0	100	100
3	C	325/326 (100%)	318 (98%)	7 (2%)	52	77
4	D	190/204 (93%)	189 (100%)	1 (0%)	88	95
5	E	149/168 (89%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	87/91 (96%)	87 (100%)	0	100	100
7	G	63/66 (96%)	63 (100%)	0	100	100
8	H	53/61 (87%)	53 (100%)	0	100	100
9	I	30/38 (79%)	29 (97%)	1 (3%)	38	68
10	J	49/49 (100%)	49 (100%)	0	100	100
All	All	1611/1690 (95%)	1599 (99%)	12 (1%)	84	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	281	ASP
1	A	365	LEU
3	C	18	PHE
3	C	80	ARG
3	C	90	PHE
3	C	171	ASP
3	C	227	LYS
3	C	306	LEU
3	C	379	TRP
4	D	59	ASP
9	I	78	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
2	B	290	ASN
3	C	322	GLN
4	D	166	ASN
4	D	225	HIS
5	E	100	HIS
5	E	121	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
20	FX2	C	406	-	30,34,34	1.76	5 (16%)	39,50,50	1.16	5 (12%)
23	PX4	E	202	-	27,27,45	1.40	2 (7%)	33,35,53	1.31	4 (12%)
16	PX6	B	503	-	16,16,43	1.25	1 (6%)	19,20,48	1.43	2 (10%)
14	CDL	E	205	-	27,27,99	1.20	2 (7%)	32,36,111	1.44	6 (18%)
11	6PE	A	501	-	22,22,26	1.54	2 (9%)	25,27,31	1.35	3 (12%)
13	PO4	F	501	-	4,4,4	0.89	0	6,6,6	0.46	0
19	PEE	C	405	-	33,33,50	1.21	2 (6%)	36,38,55	1.12	2 (5%)
13	PO4	E	203	-	4,4,4	0.97	0	6,6,6	0.57	0
17	HEM	C	401	3	27,50,50	0.88	2 (7%)	17,82,82	1.22	1 (5%)
13	PO4	G	102	-	4,4,4	0.89	0	6,6,6	0.46	0
14	CDL	C	404	-	37,37,99	1.65	4 (10%)	43,49,111	1.39	4 (9%)
14	CDL	A	506	-	33,33,99	1.23	2 (6%)	37,43,111	1.20	3 (8%)
12	PGE	C	407	-	9,9,9	0.50	0	8,8,8	0.36	0
19	PEE	E	204	-	19,19,50	1.42	2 (10%)	22,24,55	1.36	2 (9%)
21	HEC	D	501	4	26,50,50	2.69	12 (46%)	18,82,82	2.53	7 (38%)
16	PX6	C	410	-	13,13,43	1.27	1 (7%)	16,17,48	1.26	2 (12%)
17	HEM	C	402	3	27,50,50	0.80	1 (3%)	17,82,82	1.13	0
13	PO4	A	505	-	4,4,4	0.98	0	6,6,6	0.43	0
13	PO4	G	103	-	4,4,4	0.89	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PO4	D	502	-	4,4,4	0.92	0	6,6,6	0.34	0
12	PGE	C	409	-	9,9,9	0.47	0	8,8,8	0.23	0
13	PO4	G	101	-	4,4,4	0.91	0	6,6,6	0.27	0
13	PO4	B	501	-	4,4,4	0.90	0	6,6,6	0.50	0
12	PGE	A	502	-	6,6,9	0.55	0	5,5,8	0.31	0
12	PGE	C	408	-	9,9,9	0.44	0	8,8,8	0.29	0
13	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.39	0
15	PG4	B	502	-	12,12,12	0.50	0	11,11,11	0.18	0
18	LMT	C	403	-	36,36,36	0.66	1 (2%)	47,47,47	0.86	1 (2%)
14	CDL	D	503	-	26,26,99	1.45	2 (7%)	31,35,111	1.31	4 (12%)
13	PO4	A	504	-	4,4,4	0.97	0	6,6,6	0.42	0
13	PO4	F	502	-	4,4,4	0.99	0	6,6,6	0.35	0
22	FES	E	201	-	0,4,4	0.00	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FX2	C	406	-	1/1/4/4	2/11/31/31	0/3/4/4
23	PX4	E	202	-	-	17/31/31/49	-
14	CDL	E	205	-	-	19/31/31/110	-
16	PX6	C	410	-	-	9/13/13/45	-
11	6PE	A	501	-	-	11/26/26/30	-
16	PX6	B	503	-	-	7/17/17/45	-
12	PGE	C	408	-	-	3/7/7/7	-
19	PEE	C	405	-	1/1/4/4	16/37/37/54	-
15	PG4	B	502	-	-	7/10/10/10	-
14	CDL	C	404	-	-	19/46/46/110	-
12	PGE	C	407	-	-	5/7/7/7	-
19	PEE	E	204	-	1/1/4/4	13/22/22/54	-
14	CDL	A	506	-	-	15/41/41/110	-
14	CDL	D	503	-	-	18/31/31/110	-
12	PGE	A	502	-	-	3/4/4/7	-
18	LMT	C	403	-	-	8/21/61/61	0/2/2/2
22	FES	E	201	-	-	-	0/1/1/1
17	HEM	C	401	3	-	1/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGE	C	409	-	-	4/7/7/7	-
17	HEM	C	402	3	-	0/6/54/54	-
21	HEC	D	501	4	-	0/6/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C3C-C2C	7.55	1.48	1.40
20	C	406	FX2	C5-C4	6.99	1.49	1.40
21	D	501	HEC	C3B-C2B	6.47	1.47	1.40
14	C	404	CDL	OA6-CA5	5.32	1.47	1.35
14	C	404	CDL	OB6-CB5	5.10	1.48	1.34
14	C	404	CDL	OB8-CB7	5.03	1.48	1.33
19	E	204	PEE	O2-C10	4.94	1.48	1.34
11	A	501	6PE	O6-C10	4.83	1.47	1.34
19	C	405	PEE	O3-C30	4.78	1.47	1.33
11	A	501	6PE	O4-C4	4.68	1.47	1.33
14	D	503	CDL	OA8-CA7	4.66	1.47	1.33
14	D	503	CDL	OA6-CA5	4.64	1.47	1.34
14	A	506	CDL	OB8-CB7	4.57	1.46	1.33
23	E	202	PX4	O7-C23	4.51	1.47	1.34
16	B	503	PX6	O7-C20	4.46	1.46	1.34
14	E	205	CDL	OB6-CB5	4.45	1.46	1.34
23	E	202	PX4	O5-C9	4.43	1.46	1.33
14	A	506	CDL	OB6-CB5	4.39	1.46	1.34
16	C	410	PX6	O5-C4	4.19	1.45	1.33
19	C	405	PEE	O2-C10	4.17	1.46	1.34
21	D	501	HEC	C2A-C3A	3.53	1.48	1.37
21	D	501	HEC	C3D-C2D	3.39	1.47	1.37
20	C	406	FX2	N1-N2	3.36	1.40	1.35
21	D	501	HEC	C3B-C4B	3.33	1.49	1.43
21	D	501	HEC	C4A-C3A	3.18	1.49	1.42
21	D	501	HEC	C1A-C2A	3.08	1.49	1.42
21	D	501	HEC	C3C-C4C	3.00	1.48	1.43
17	C	401	HEM	C4D-C3D	2.73	1.48	1.42
21	D	501	HEC	C1C-CHC	2.72	1.48	1.41
14	C	404	CDL	OA8-CA7	2.71	1.46	1.33
14	E	205	CDL	OB8-CB7	2.68	1.46	1.33
20	C	406	FX2	C4-N	-2.58	1.34	1.39
19	E	204	PEE	O3-C30	2.55	1.46	1.33
20	C	406	FX2	O-C6	2.50	1.25	1.22
17	C	402	HEM	C4D-C3D	2.48	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C4D-CHA	2.43	1.47	1.41
21	D	501	HEC	C1B-CHB	2.31	1.47	1.41
21	D	501	HEC	C1D-CHD	2.30	1.47	1.41
18	C	403	LMT	O1'-C1'	2.23	1.44	1.40
17	C	401	HEM	C3B-C2B	-2.21	1.37	1.40
20	C	406	FX2	O2-C2O	2.14	1.43	1.31

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	501	HEC	C1D-C2D-C3D	-6.26	102.64	107.00
23	E	202	PX4	O7-C23-C24	5.06	122.40	111.50
21	D	501	HEC	CMC-C2C-C3C	4.74	131.39	125.82
14	C	404	CDL	OA6-CA5-C11	4.71	119.76	111.09
14	A	506	CDL	OB6-CB5-C51	4.57	121.35	111.50
11	A	501	6PE	O6-C10-C11	4.37	120.92	111.50
21	D	501	HEC	CMB-C2B-C3B	4.30	130.88	125.82
16	B	503	PX6	O7-C20-C21	4.24	120.64	111.50
19	C	405	PEE	O3-C30-C31	4.17	122.32	111.38
19	E	204	PEE	O2-C10-C11	4.13	122.31	110.80
14	E	205	CDL	OB6-CB5-C51	3.74	119.56	111.50
14	E	205	CDL	CB6-OB8-CB7	3.71	126.42	117.10
14	D	503	CDL	OA6-CA5-C11	3.53	120.65	110.80
14	A	506	CDL	OB8-CB7-C71	3.53	120.63	111.38
14	D	503	CDL	OA8-CA7-C31	3.50	120.56	111.38
14	C	404	CDL	OB8-CB7-C71	3.41	120.32	111.38
16	C	410	PX6	O5-C4-C5	3.32	120.10	111.38
14	C	404	CDL	OB6-CB5-C51	3.28	119.95	110.80
17	C	401	HEM	CBA-CAA-C2A	-3.12	106.74	112.49
20	C	406	FX2	C9-O1-C2	3.06	124.15	117.51
14	E	205	CDL	PA1-OA2-CA2	2.93	126.36	118.30
23	E	202	PX4	O7-C23-O8	-2.89	116.71	123.70
23	E	202	PX4	O5-C9-C10	2.76	120.58	111.91
20	C	406	FX2	C13-N2-C12	2.74	132.69	129.19
19	C	405	PEE	O2-C10-C11	2.68	117.28	111.50
11	A	501	6PE	O4-C4-C5	2.65	120.21	111.91
21	D	501	HEC	CAA-CBA-CGA	-2.56	108.37	112.67
14	E	205	CDL	OA4-PA1-OA3	2.27	119.56	110.68
14	C	404	CDL	CA6-OA8-CA7	2.25	122.75	117.10
21	D	501	HEC	CBD-CAD-C3D	-2.24	108.35	112.49
16	B	503	PX6	O7-C2-C3	2.22	116.34	108.36
14	E	205	CDL	OB8-CB6-CB4	2.20	114.85	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	503	CDL	PB2-OB2-CB2	2.18	124.31	118.30
20	C	406	FX2	C20-O2-C17	2.18	125.21	118.01
11	A	501	6PE	O6-C10-O7	-2.12	118.59	123.70
23	E	202	PX4	O5-C9-O6	-2.08	118.33	123.59
20	C	406	FX2	C10-C7-N	-2.08	115.50	118.13
14	A	506	CDL	OB6-CB5-OB7	-2.08	118.68	123.70
18	C	403	LMT	C1B-O1B-C4'	-2.07	112.83	117.96
19	E	204	PEE	C3-O3-C30	2.06	122.28	117.10
14	D	503	CDL	OB4-PB2-OB3	2.05	118.69	110.68
16	C	410	PX6	O5-C4-O6	-2.04	118.44	123.59
21	D	501	HEC	CMD-C2D-C3D	2.03	128.76	124.94
21	D	501	HEC	C3C-C4C-NC	2.01	114.73	110.94
20	C	406	FX2	C-C5-C6	2.01	122.80	119.80
14	E	205	CDL	OA5-PA1-OA2	-2.01	101.40	106.73

All (3) chirality outliers are listed below:

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

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	C	406	FX2	C14-C13-N2-C12
23	E	202	PX4	C1-O3-P1-O2
23	E	202	PX4	C24-C23-O7-C7
14	E	205	CDL	C1-CA2-OA2-PA1
14	E	205	CDL	CA2-OA2-PA1-OA4
14	E	205	CDL	CA2-OA2-PA1-OA5
14	E	205	CDL	C1-CB2-OB2-PB2
14	E	205	CDL	CB4-CB6-OB8-CB7
11	A	501	6PE	C1-O3-P1-O1
11	A	501	6PE	C11-C10-O6-C2
11	A	501	6PE	O8-C16-C17-N1
19	C	405	PEE	C4-O4P-P-O1P
19	C	405	PEE	C4-O4P-P-O2P
19	C	405	PEE	C4-O4P-P-O3P
14	C	404	CDL	CA3-OA5-PA1-OA4
14	C	404	CDL	C11-CA5-OA6-CA4
14	A	506	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	E	204	PEE	O4P-C4-C5-N
19	E	204	PEE	C4-O4P-P-O1P
16	C	410	PX6	C1-O4-P1-O1
16	C	410	PX6	C1-O4-P1-O3
14	D	503	CDL	CA2-OA2-PA1-OA3
14	D	503	CDL	CA2-OA2-PA1-OA4
14	D	503	CDL	CA3-OA5-PA1-OA3
14	D	503	CDL	CB2-OB2-PB2-OB3
14	D	503	CDL	CB2-OB2-PB2-OB4
14	D	503	CDL	CB2-OB2-PB2-OB5
23	E	202	PX4	O8-C23-O7-C7
11	A	501	6PE	O7-C10-O6-C2
14	A	506	CDL	OB7-CB5-OB6-CB4
14	C	404	CDL	OA7-CA5-OA6-CA4
14	E	205	CDL	C71-CB7-OB8-CB6
19	E	204	PEE	C31-C30-O3-C3
16	C	410	PX6	O4-C1-C2-O7
14	D	503	CDL	O1-C1-CA2-OA2
23	E	202	PX4	C10-C9-O5-C8
23	E	202	PX4	O6-C9-O5-C8
16	B	503	PX6	C21-C20-O7-C2
14	E	205	CDL	C51-CB5-OB6-CB4
14	C	404	CDL	C31-CA7-OA8-CA6
14	D	503	CDL	CB2-C1-CA2-OA2
16	B	503	PX6	O8-C20-O7-C2
19	C	405	PEE	C31-C30-O3-C3
16	C	410	PX6	C5-C4-O5-C3
14	D	503	CDL	C31-CA7-OA8-CA6
12	C	409	PGE	O2-C3-C4-O3
14	E	205	CDL	O1-C1-CB2-OB2
14	A	506	CDL	O1-C1-CB2-OB2
14	E	205	CDL	OB9-CB7-OB8-CB6
19	C	405	PEE	O5-C30-O3-C3
16	C	410	PX6	O6-C4-O5-C3
14	D	503	CDL	OA9-CA7-OA8-CA6
14	C	404	CDL	OA9-CA7-OA8-CA6
19	E	204	PEE	O5-C30-O3-C3
16	B	503	PX6	C20-C21-C22-C23
14	E	205	CDL	OB7-CB5-OB6-CB4
14	A	506	CDL	CB5-C51-C52-C53
14	E	205	CDL	O1-C1-CA2-OA2
14	A	506	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
16	C	410	PX6	O7-C2-C3-O5
23	E	202	PX4	C1-O3-P1-O4
14	E	205	CDL	CB2-OB2-PB2-OB5
11	A	501	6PE	C1-O3-P1-O8
14	C	404	CDL	CA3-OA5-PA1-OA2
14	A	506	CDL	CA3-OA5-PA1-OA2
19	E	204	PEE	C1-O3P-P-O4P
14	D	503	CDL	CA2-OA2-PA1-OA5
14	D	503	CDL	CA3-OA5-PA1-OA2
14	A	506	CDL	OA5-CA3-CA4-CA6
12	C	407	PGE	O3-C5-C6-O4
15	B	502	PG4	O3-C5-C6-O4
19	C	405	PEE	C14-C15-C16-C17
18	C	403	LMT	C11-C10-C9-C8
16	B	503	PX6	C21-C22-C23-C24
19	C	405	PEE	C13-C14-C15-C16
18	C	403	LMT	O1'-C1-C2-C3
14	E	205	CDL	CB2-C1-CA2-OA2
12	A	502	PGE	O1-C1-C2-O2
23	E	202	PX4	C9-C10-C11-C12
18	C	403	LMT	C7-C8-C9-C10
12	C	407	PGE	O2-C3-C4-O3
19	E	204	PEE	O4-C10-O2-C2
19	C	405	PEE	C17-C18-C19-C20
19	C	405	PEE	C11-C12-C13-C14
14	C	404	CDL	C51-CB5-OB6-CB4
19	E	204	PEE	C11-C10-O2-C2
14	C	404	CDL	OB7-CB5-OB6-CB4
19	E	204	PEE	O2-C2-C3-O3
11	A	501	6PE	C2-C1-O3-P1
14	A	506	CDL	OB5-CB3-CB4-CB6
14	A	506	CDL	CA2-C1-CB2-OB2
18	C	403	LMT	C4-C5-C6-C7
19	C	405	PEE	C10-C11-C12-C13
18	C	403	LMT	O5B-C5B-C6B-O6B
16	B	503	PX6	C3-C2-O7-C20
14	E	205	CDL	CA2-OA2-PA1-OA3
16	C	410	PX6	C1-O4-P1-O2
14	E	205	CDL	C51-C52-C53-C54
19	C	405	PEE	C22-C23-C24-C25
14	E	205	CDL	CB5-C51-C52-C53
23	E	202	PX4	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	E	202	PX4	C24-C25-C26-C27
19	C	405	PEE	C15-C16-C17-C18
12	C	409	PGE	O1-C1-C2-O2
14	C	404	CDL	C71-CB7-OB8-CB6
16	B	503	PX6	C2-C1-O4-P1
19	E	204	PEE	C1-C2-C3-O3
19	C	405	PEE	C18-C19-C20-C21
14	A	506	CDL	OB5-CB3-CB4-OB6
14	E	205	CDL	CB4-CB3-OB5-PB2
14	A	506	CDL	CA4-CA3-OA5-PA1
14	A	506	CDL	C51-C52-C53-C54
19	C	405	PEE	O3P-C1-C2-C3
14	C	404	CDL	OB5-CB3-CB4-CB6
15	B	502	PG4	O2-C3-C4-O3
15	B	502	PG4	C6-C5-O3-C4
12	C	408	PGE	C1-C2-O2-C3
18	C	403	LMT	O5'-C5'-C6'-O6'
19	C	405	PEE	O3P-C1-C2-O2
14	E	205	CDL	CA2-C1-CB2-OB2
16	C	410	PX6	O4-C1-C2-C3
14	C	404	CDL	OB9-CB7-OB8-CB6
11	A	501	6PE	O6-C2-C3-O4
15	B	502	PG4	C8-C7-O4-C6
14	C	404	CDL	CB4-CB3-OB5-PB2
23	E	202	PX4	C1-O3-P1-O1
14	E	205	CDL	CB2-OB2-PB2-OB3
14	C	404	CDL	CB2-OB2-PB2-OB3
14	A	506	CDL	CA3-OA5-PA1-OA3
19	E	204	PEE	C1-O3P-P-O2P
14	D	503	CDL	CA3-OA5-PA1-OA4
19	E	204	PEE	O3P-C1-C2-C3
12	A	502	PGE	O2-C3-C4-O3
14	C	404	CDL	OB5-CB3-CB4-OB6
23	E	202	PX4	O3-C1-C2-N1
14	D	503	CDL	CA3-CA4-CA6-OA8
14	C	404	CDL	OB6-CB4-CB6-OB8
14	D	503	CDL	OA6-CA4-CA6-OA8
12	C	407	PGE	C6-C5-O3-C4
12	C	409	PGE	C1-C2-O2-C3
12	C	408	PGE	O2-C3-C4-O3
15	B	502	PG4	C3-C4-O3-C5
19	C	405	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	E	202	PX4	C23-C24-C25-C26
12	C	407	PGE	C3-C4-O3-C5
15	B	502	PG4	C5-C6-O4-C7
14	C	404	CDL	CB2-OB2-PB2-OB5
12	C	407	PGE	C1-C2-O2-C3
15	B	502	PG4	O4-C7-C8-O5
12	C	408	PGE	C3-C4-O3-C5
14	D	503	CDL	OA5-CA3-CA4-OA6
11	A	501	6PE	C5-C4-O4-C3
16	C	410	PX6	C1-C2-C3-O5
19	E	204	PEE	C3-C2-O2-C10
23	E	202	PX4	O4-C6-C7-O7
18	C	403	LMT	C3-C4-C5-C6
11	A	501	6PE	O5-C4-O4-C3
11	A	501	6PE	C1-C2-C3-O4
17	C	401	HEM	C3D-CAD-CBD-CGD
12	A	502	PGE	C4-C3-O2-C2
14	C	404	CDL	C52-C51-CB5-OB6
23	E	202	PX4	C11-C10-C9-O5
14	C	404	CDL	C52-C51-CB5-OB7
14	D	503	CDL	OA7-CA5-OA6-CA4
20	C	406	FX2	C16-C17-O2-C20
12	C	409	PGE	C6-C5-O3-C4
14	D	503	CDL	C11-CA5-OA6-CA4
23	E	202	PX4	C11-C10-C9-O6
14	C	404	CDL	CB3-CB4-CB6-OB8
23	E	202	PX4	O7-C23-C24-C25
19	E	204	PEE	C5-C4-O4P-P
14	A	506	CDL	C52-C51-CB5-OB6
18	C	403	LMT	C5-C6-C7-C8
14	A	506	CDL	C52-C51-CB5-OB7
11	A	501	6PE	O4-C4-C5-C6
23	E	202	PX4	O8-C23-C24-C25
16	B	503	PX6	O7-C20-C21-C22

There are no ring outliers.

5 monomers are involved in 7 short contacts:

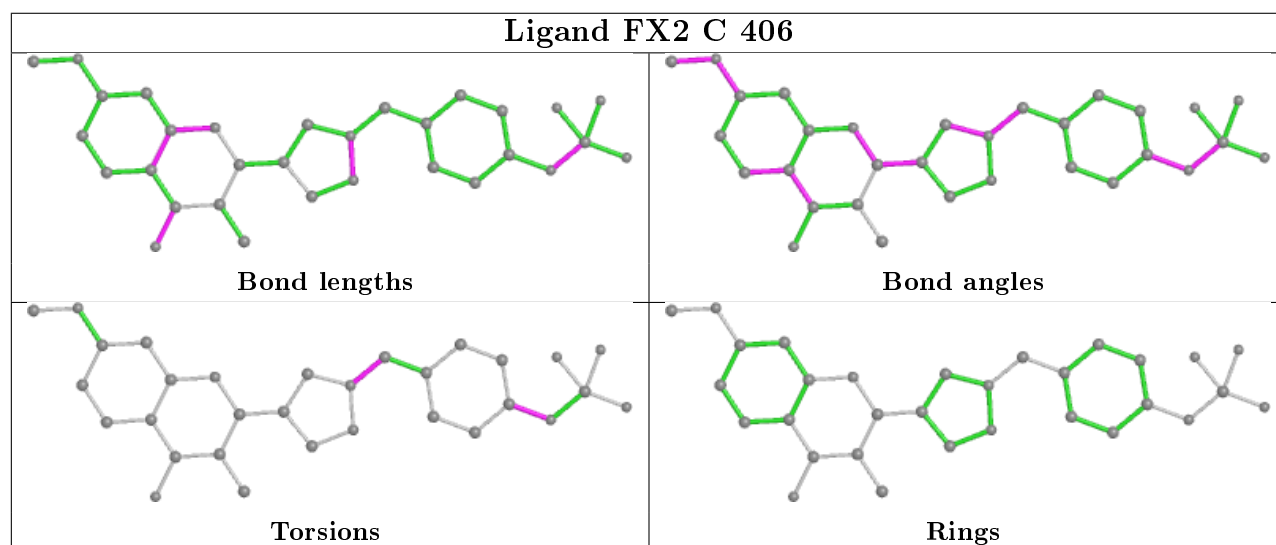
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	501	6PE	2	0
17	C	401	HEM	1	0
14	A	506	CDL	2	0

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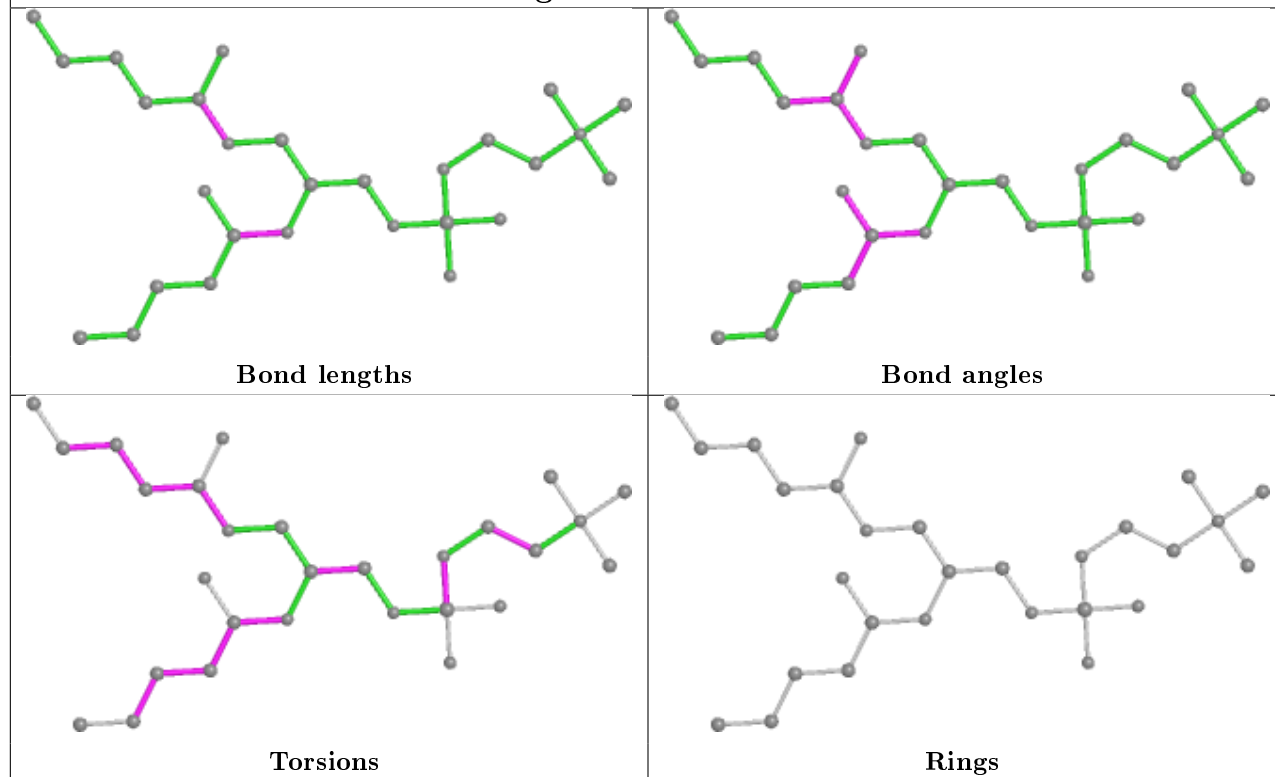
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	D	501	HEC	3	0
17	C	402	HEM	1	0

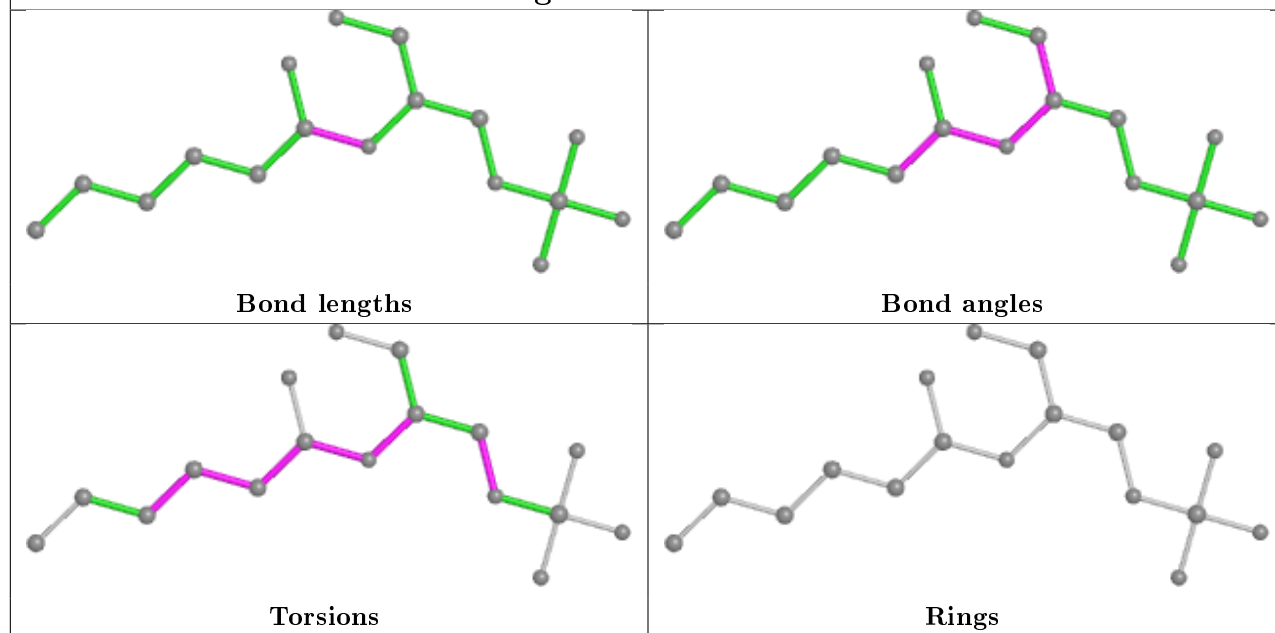
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



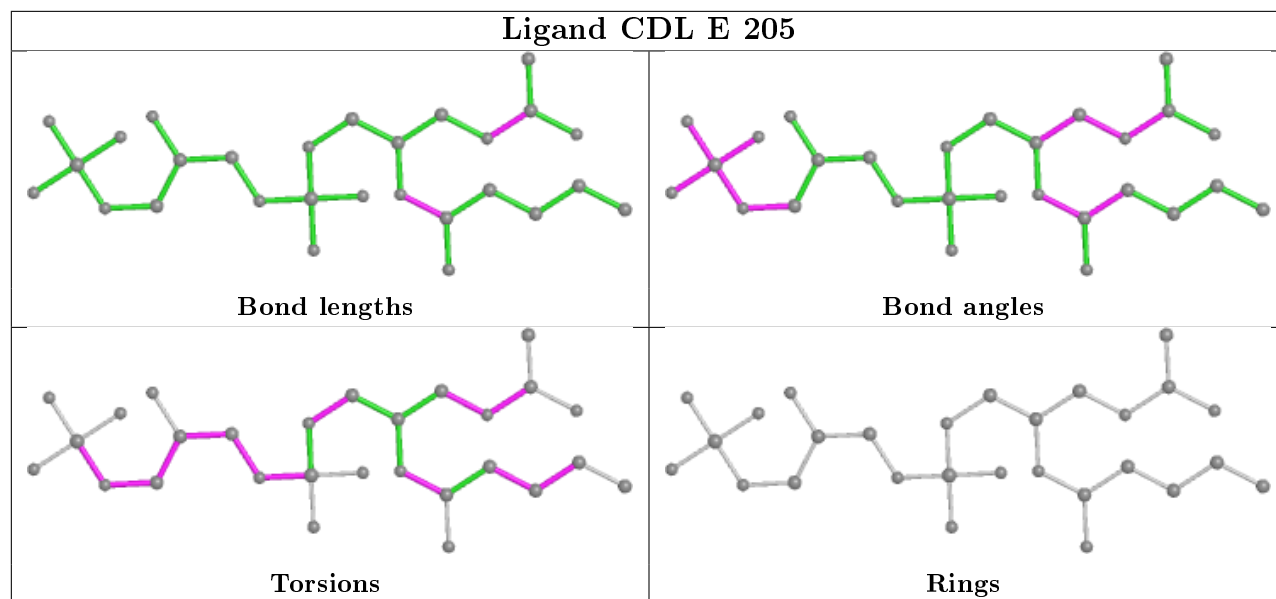
Ligand PX4 E 202



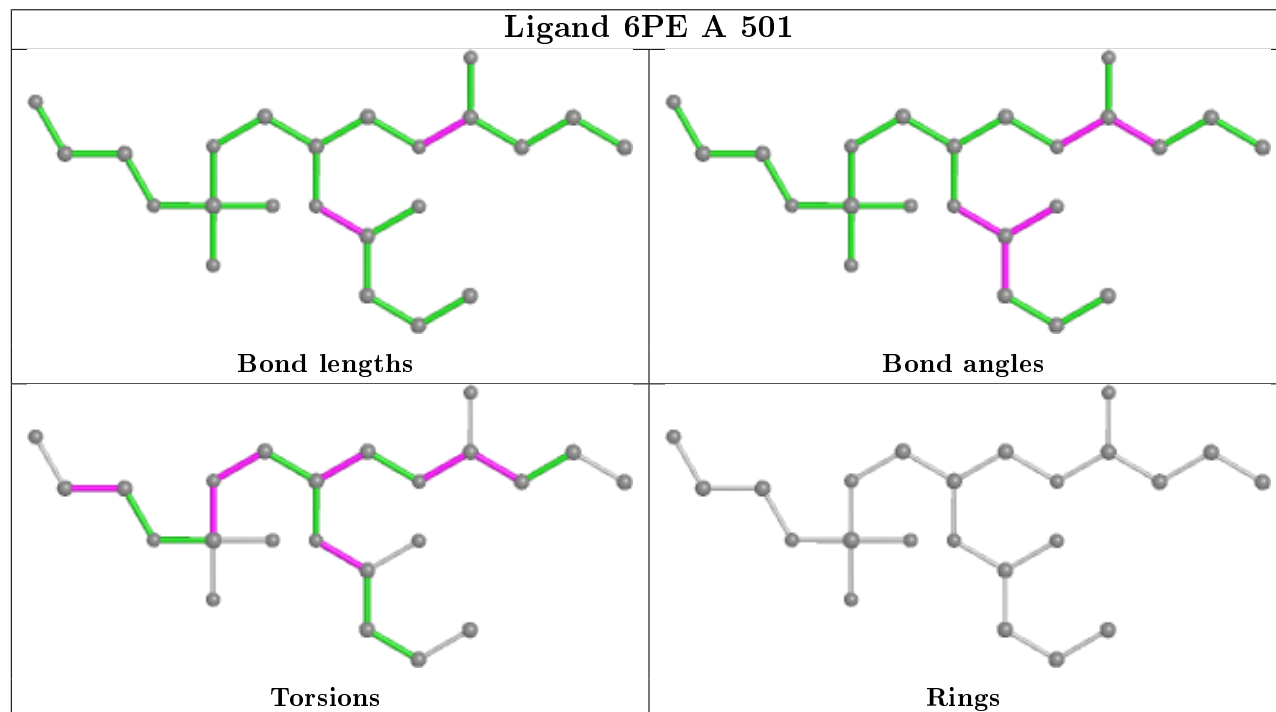
Ligand PX6 B 503



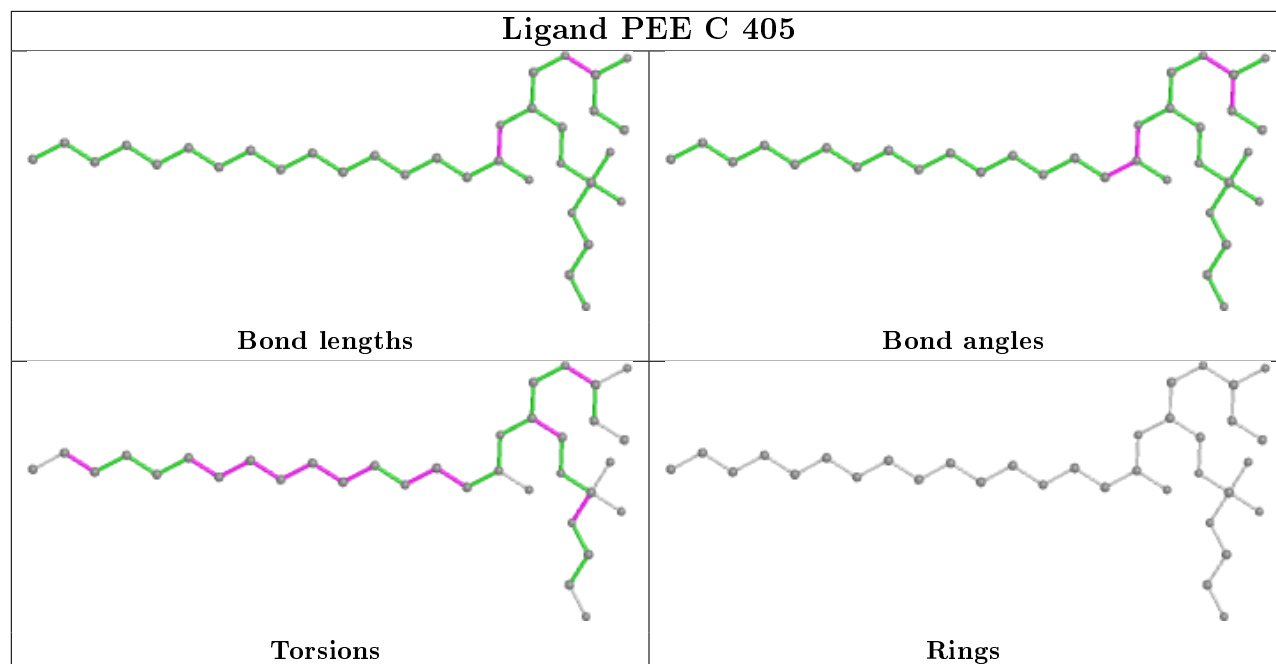
Ligand CDL E 205



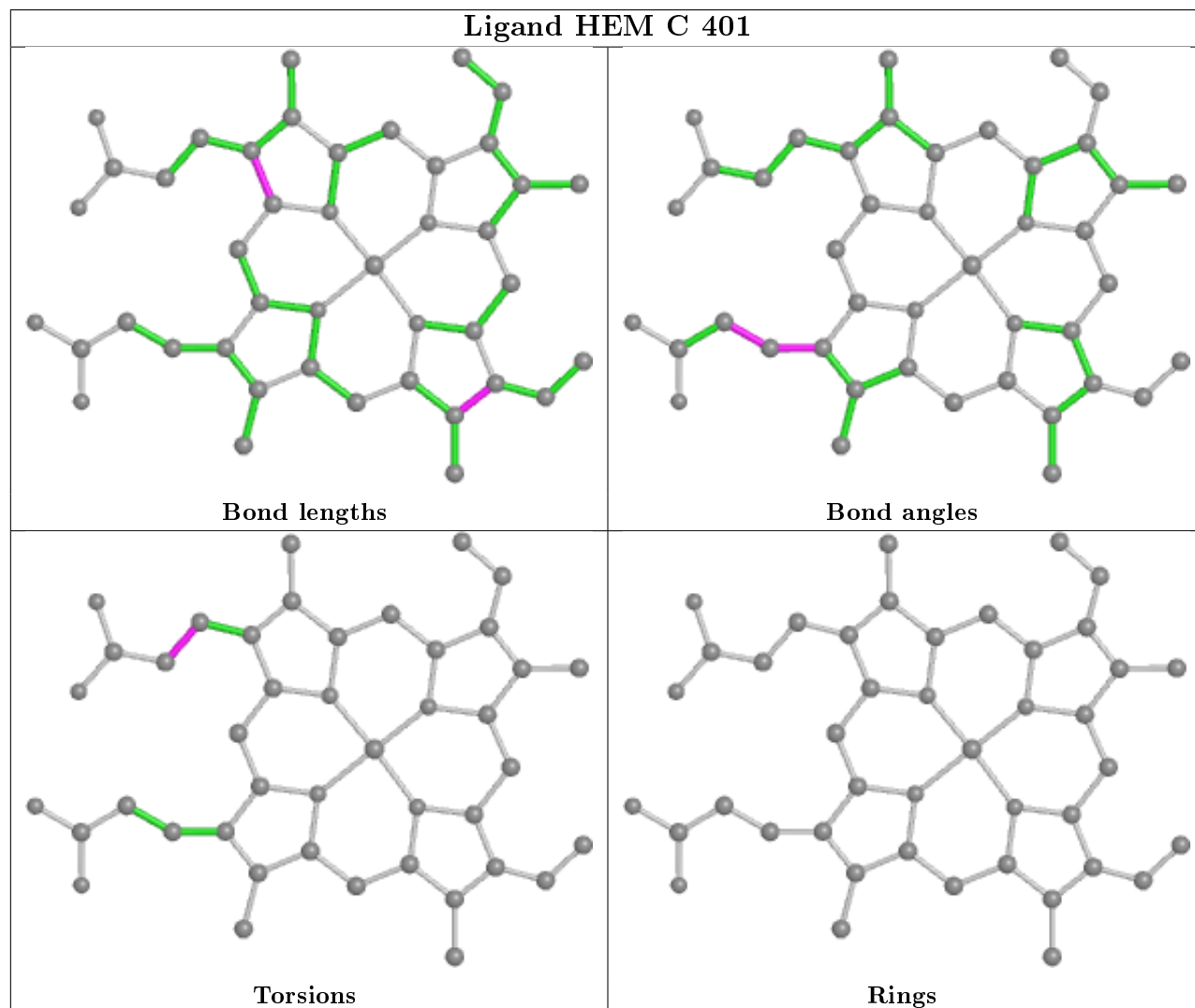
Ligand 6PE A 501

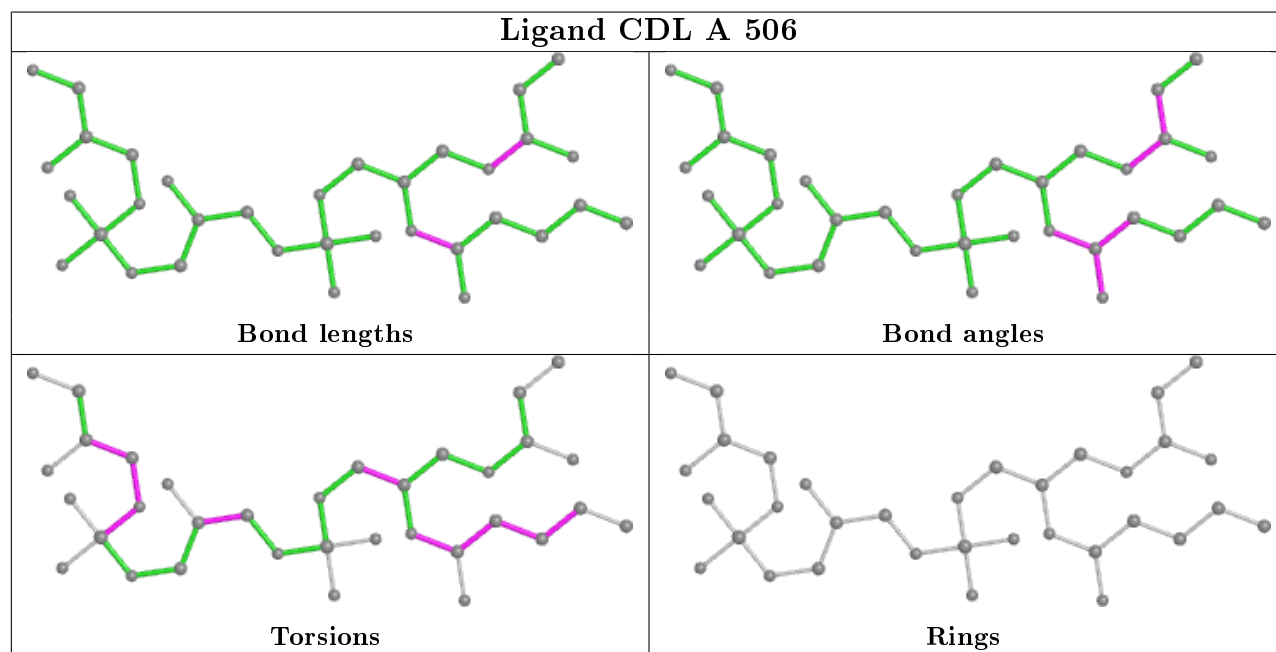
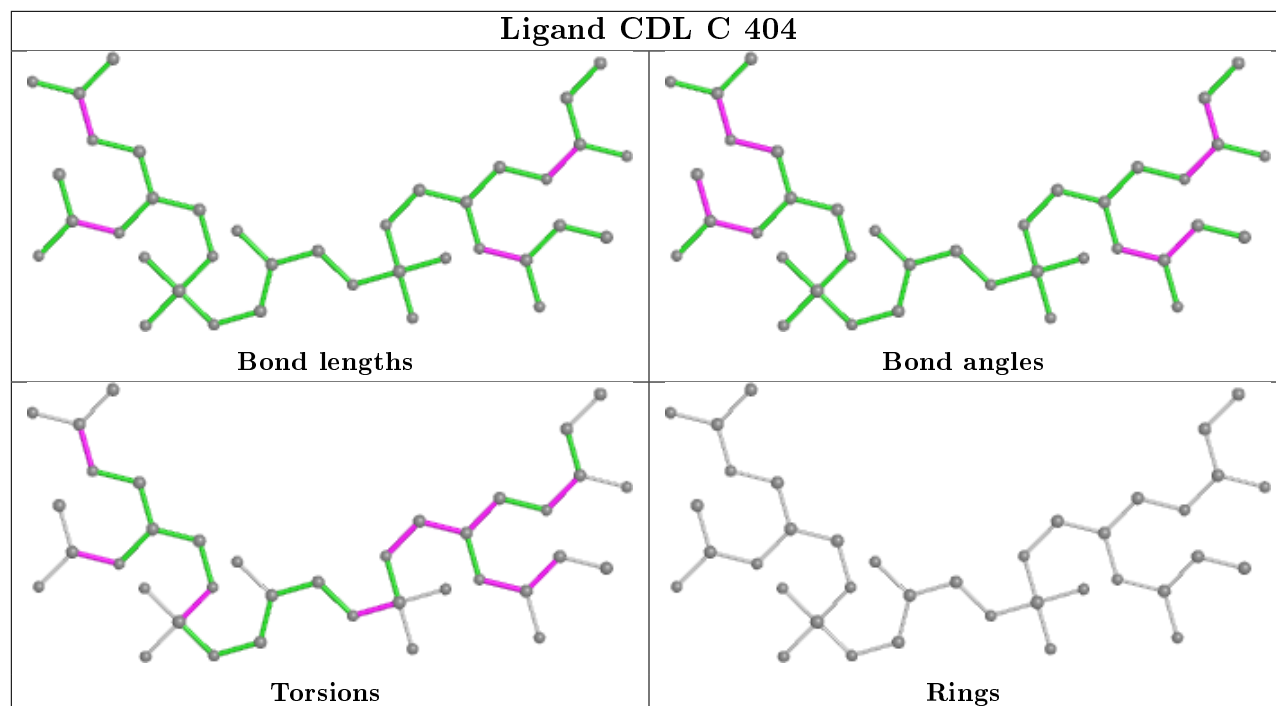


Ligand PEE C 405

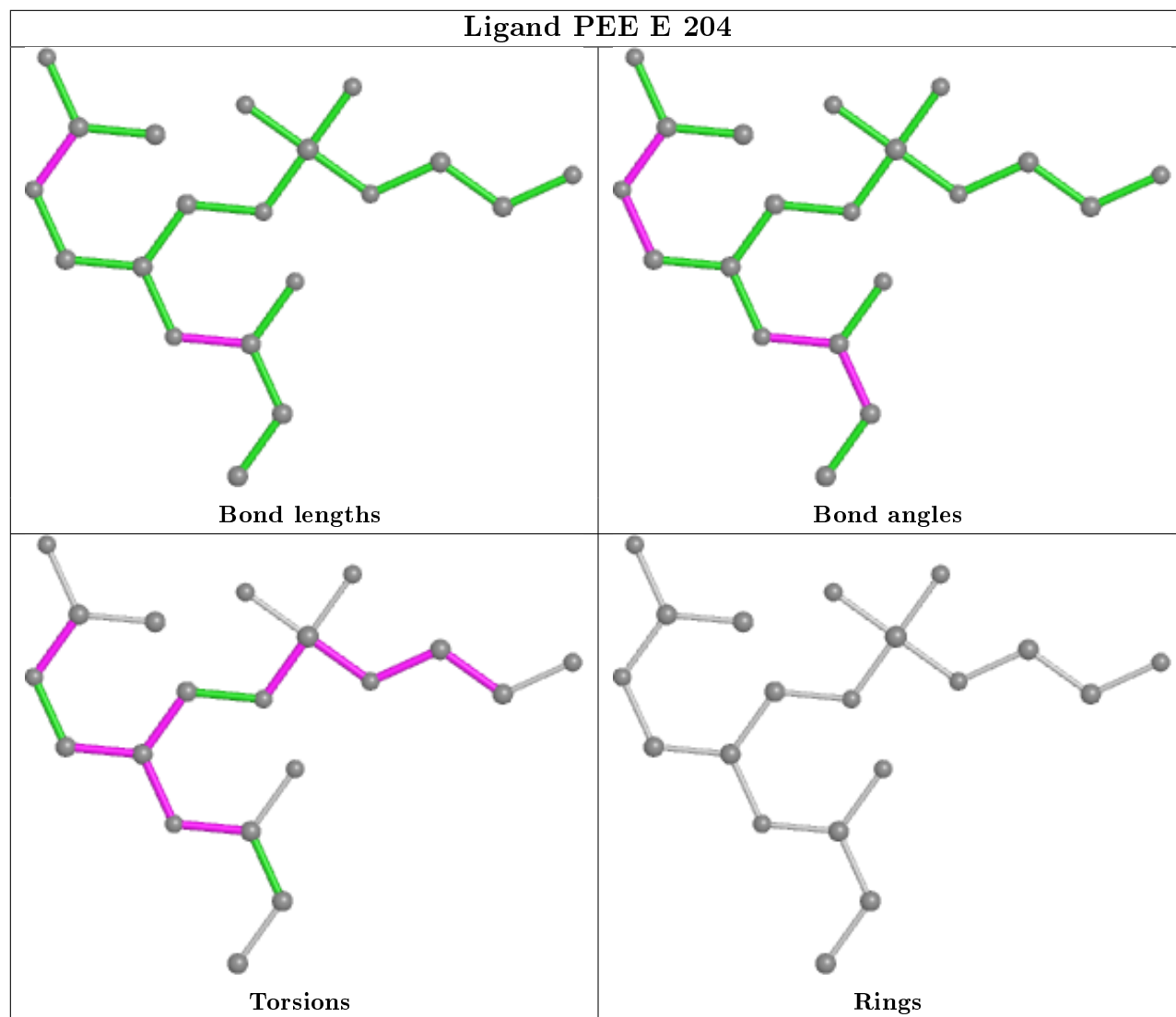


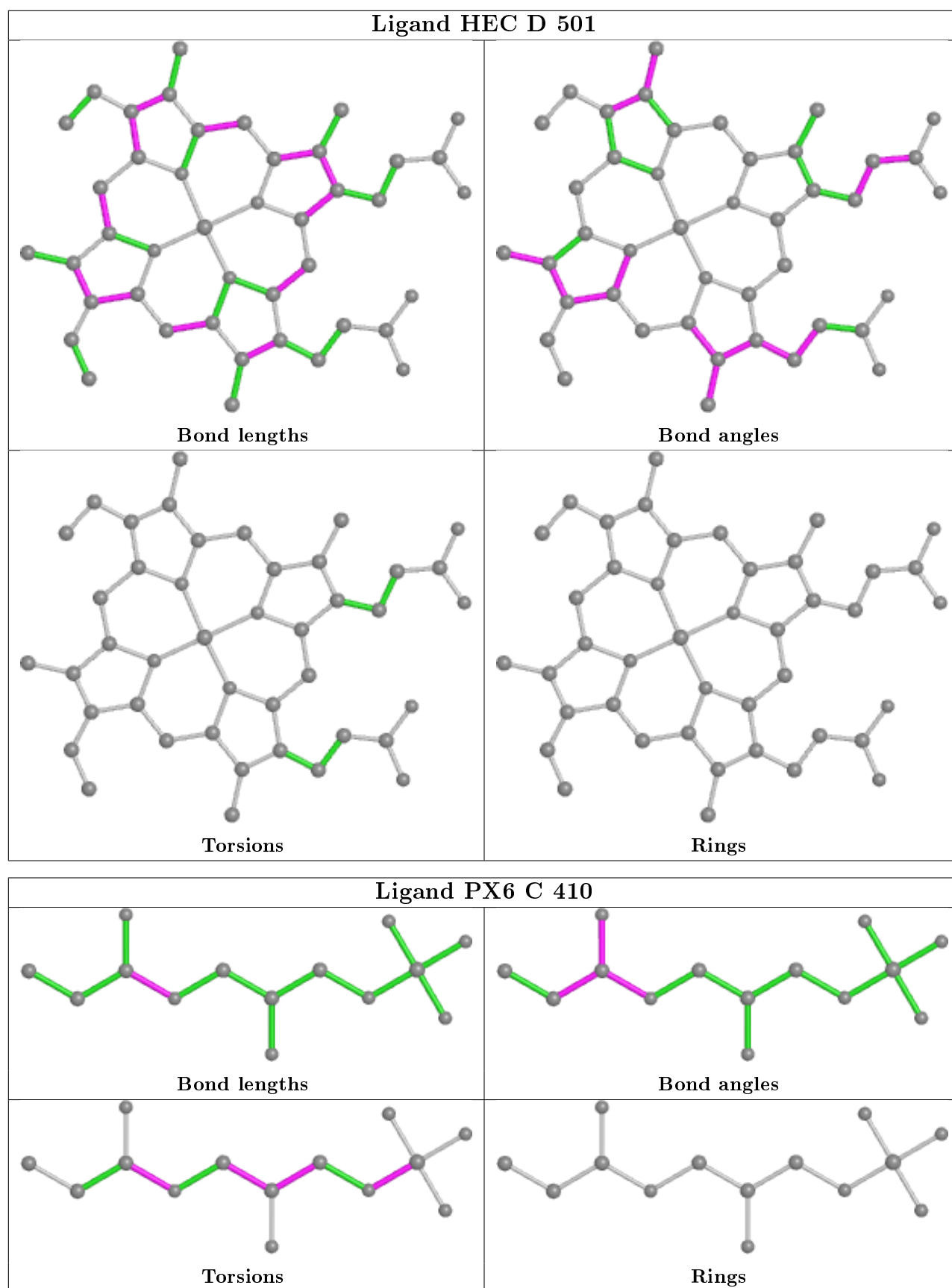
Ligand HEM C 401

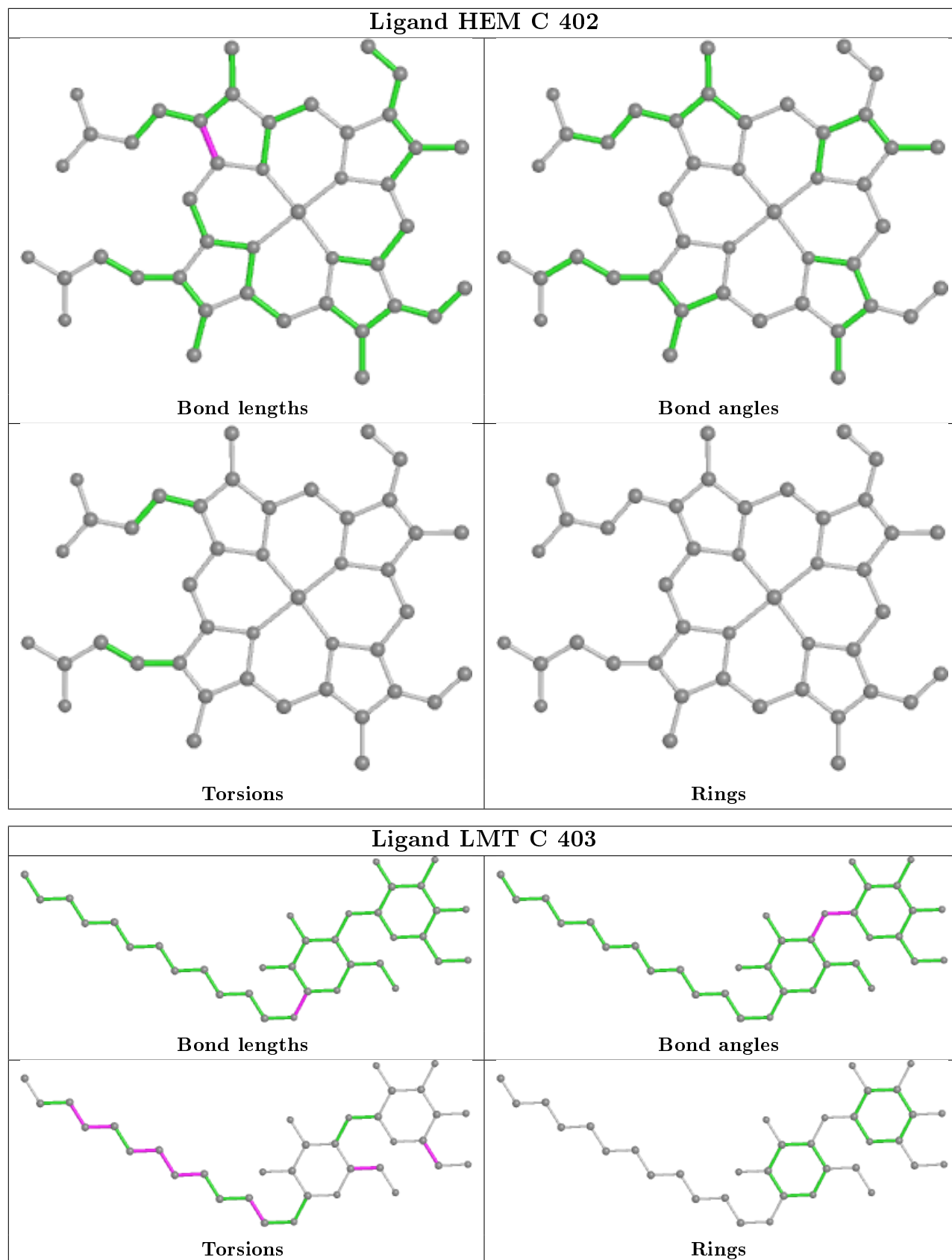


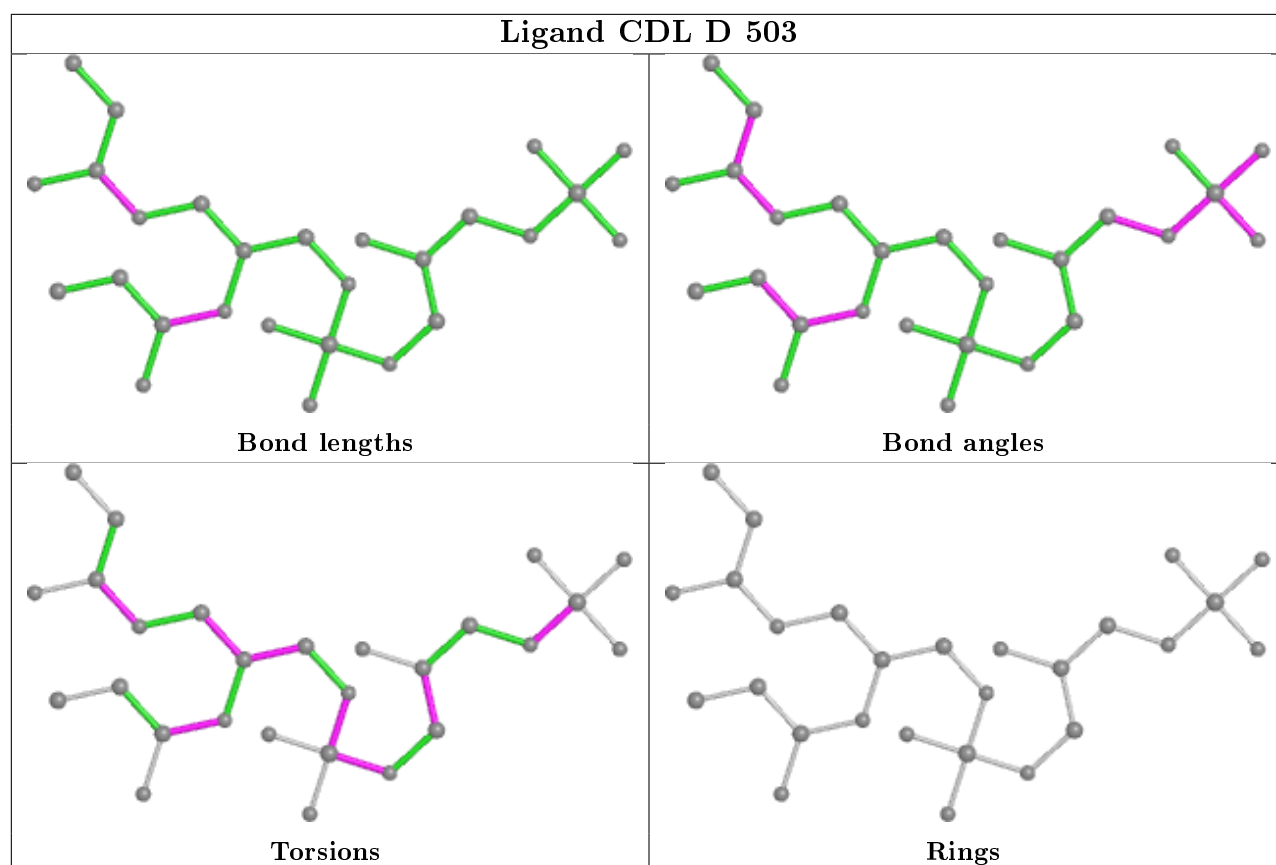


Ligand PEE E 204









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

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

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	4.8
4	D	108	ALA	4.6
5	E	89	PHE	4.5
5	E	144	CYS	4.1
1	A	228	VAL	3.8
1	A	229	PRO	3.5
2	B	44	ALA	3.5
5	E	88	ALA	3.4
4	D	164	ILE	3.4
9	I	43	LEU	3.3
9	I	37	THR	3.3
5	E	159	PRO	3.2
9	I	33	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	43	PRO	3.1
1	A	4	TYR	3.0
1	A	369	LEU	3.0
1	A	371	GLY	3.0
4	D	159	GLY	2.9
5	E	161	HIS	2.9
4	D	134	TYR	2.9
9	I	40	SER	2.9
4	D	139	THR	2.9
2	B	110	GLU	2.8
5	E	98	VAL	2.8
4	D	148	TYR	2.8
1	A	194	ARG	2.8
2	B	41	TYR	2.8
2	B	95	LYS	2.8
9	I	41	PRO	2.8
5	E	147	ILE	2.7
2	B	420	GLY	2.7
9	I	75	SER	2.7
1	A	374	PRO	2.7
4	D	171	PHE	2.7
2	B	423	SER	2.7
9	I	39	GLU	2.7
1	A	23	LEU	2.7
9	I	72	VAL	2.7
2	B	45	SER	2.6
1	A	365	LEU	2.6
2	B	112	LEU	2.6
8	H	24	CYS	2.6
8	H	46	SER	2.6
4	D	80	MET	2.6
9	I	73	PRO	2.6
9	I	38	SER	2.6
10	J	30	PHE	2.5
1	A	370	ASP	2.5
9	I	36	ALA	2.5
4	D	71	GLN	2.5
4	D	107	GLY	2.5
5	E	148	ALA	2.5
2	B	211	VAL	2.5
4	D	72	ASP	2.4
1	A	231	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	2	THR	2.4
8	H	45	SER	2.3
2	B	419	SER	2.3
5	E	157	TYR	2.3
5	E	74	ILE	2.3
4	D	81	PHE	2.3
4	D	151	PRO	2.3
5	E	35	PHE	2.2
1	A	18	GLN	2.2
5	E	82	PRO	2.2
5	E	196	GLY	2.2
5	E	75	GLU	2.2
4	D	110	PRO	2.2
2	B	115	ASP	2.2
1	A	190	TYR	2.2
8	H	14	VAL	2.2
5	E	78	LEU	2.2
4	D	149	PHE	2.1
5	E	76	ILE	2.1
4	D	96	PRO	2.1
4	D	180	SER	2.1
2	B	240	HIS	2.1
3	C	280	ILE	2.0
5	E	134	ILE	2.0
2	B	210	GLY	2.0
1	A	193	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

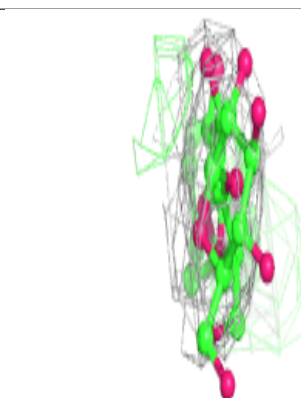
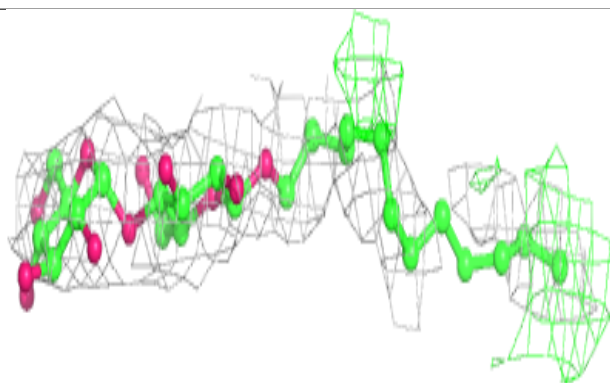
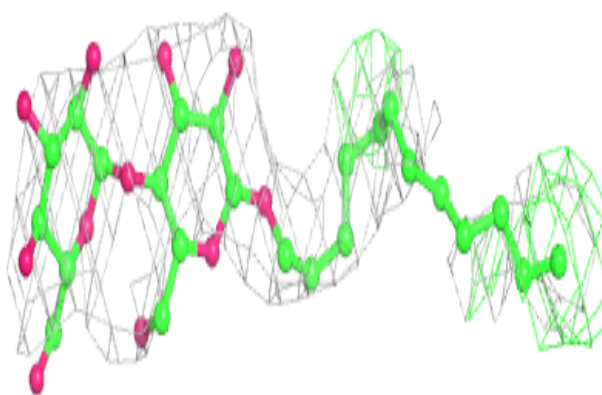
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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

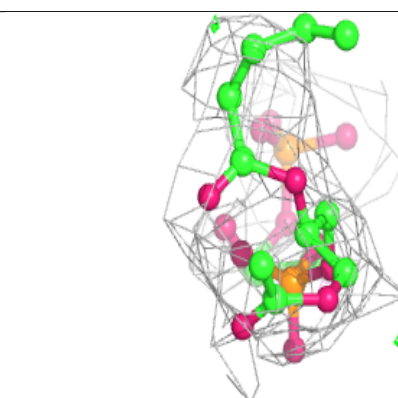
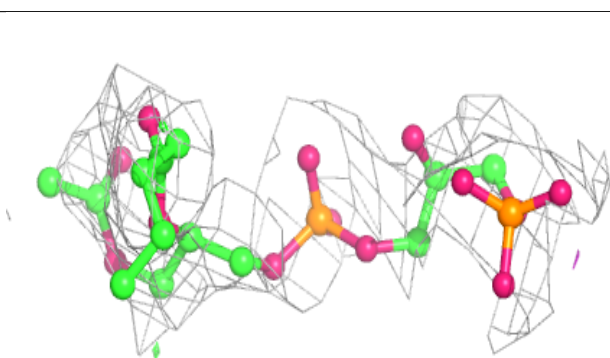
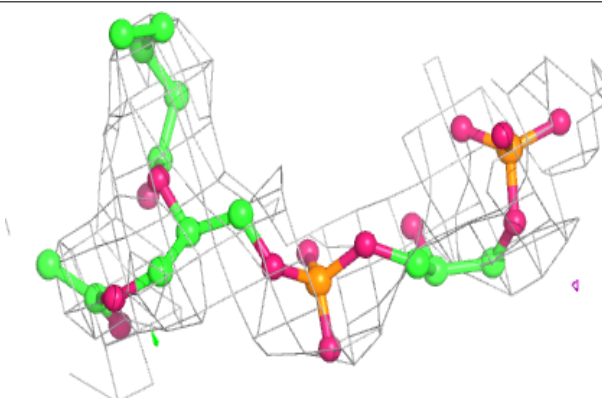
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

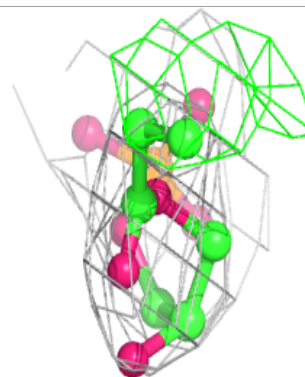
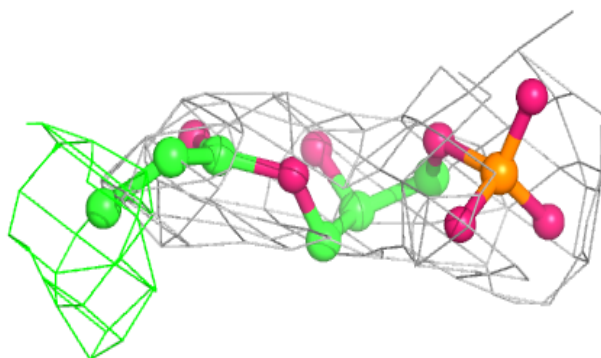
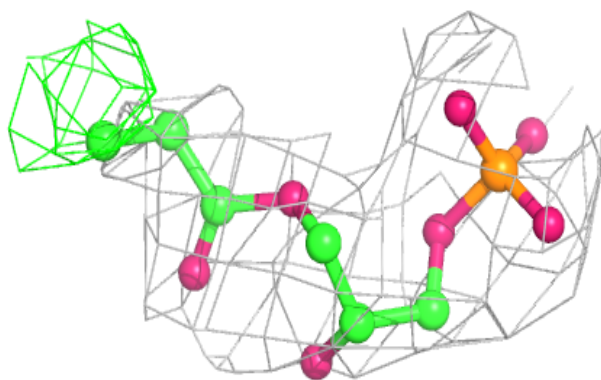
**Electron density around CDL E 205:**

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

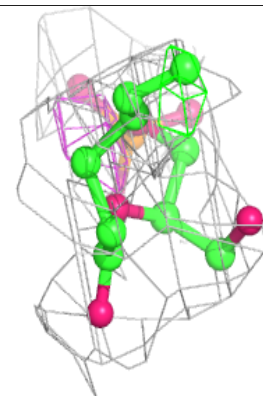
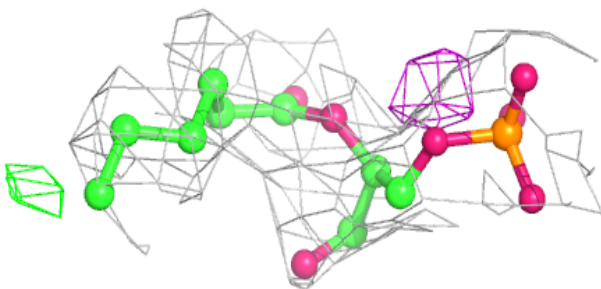
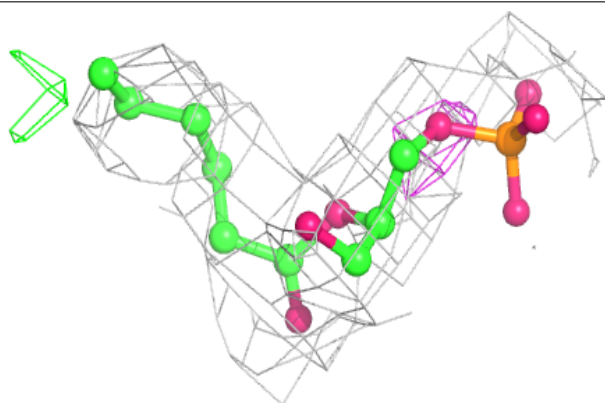


Electron density around PX6 C 410:

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

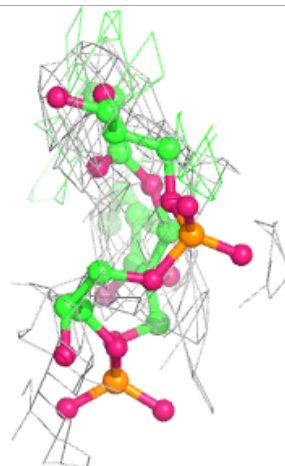
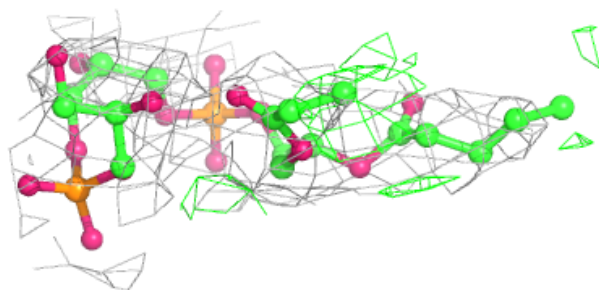
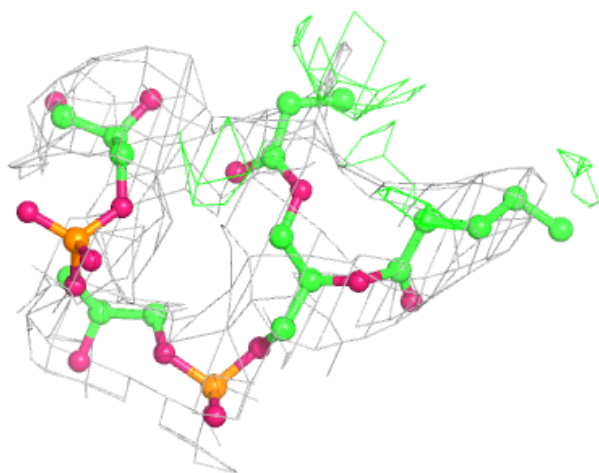
**Electron density around PX6 B 503:**

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



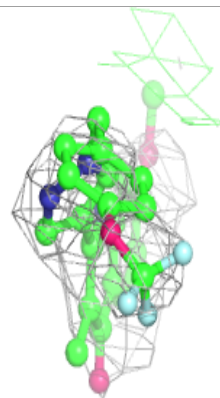
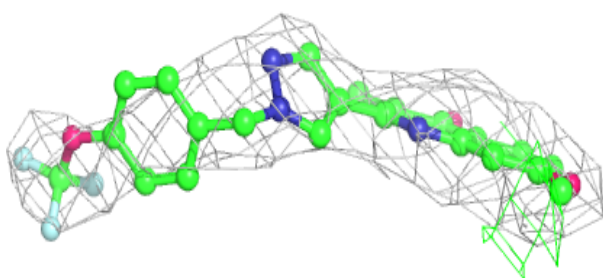
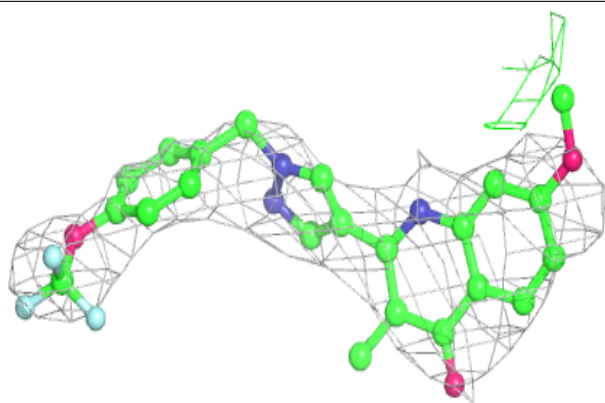
Electron density around CDL A 506:

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

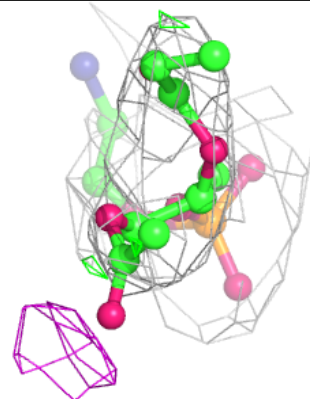
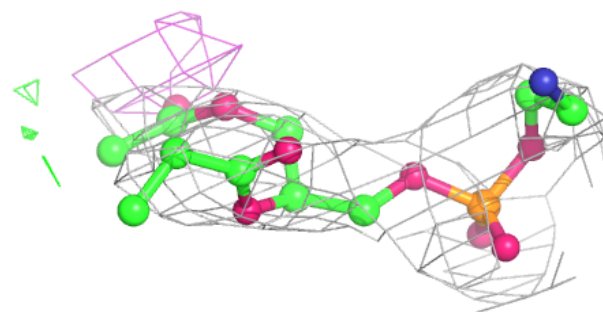
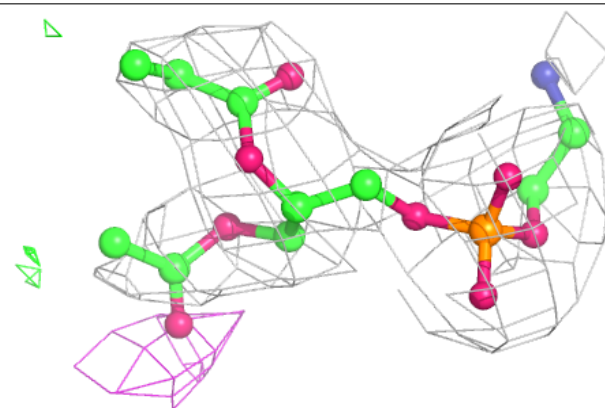


Electron density around FX2 C 406:

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

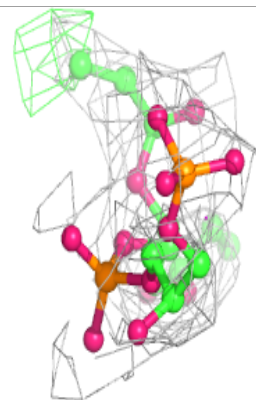
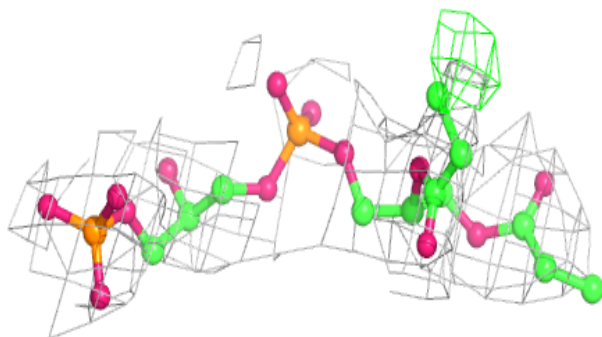
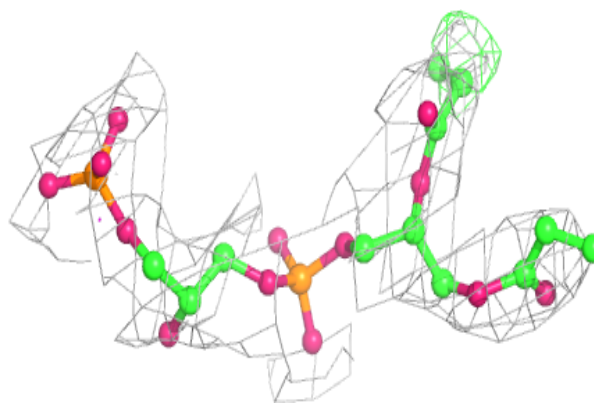
**Electron density around PEE E 204:**

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



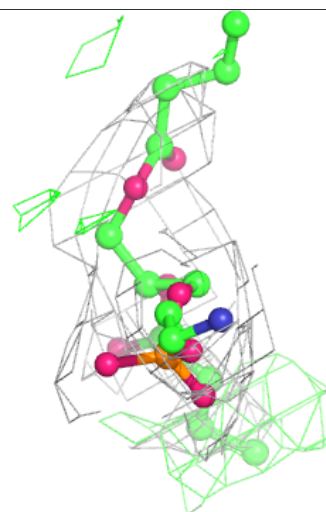
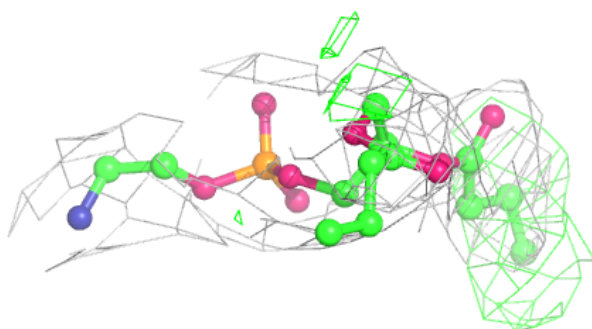
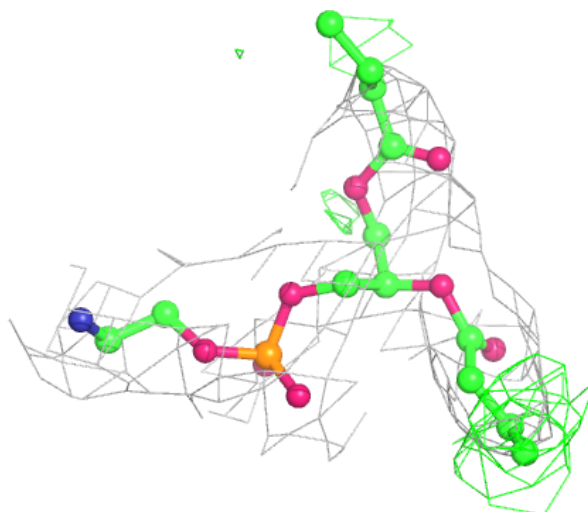
Electron density around CDL D 503:

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



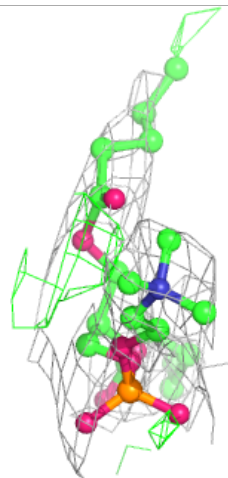
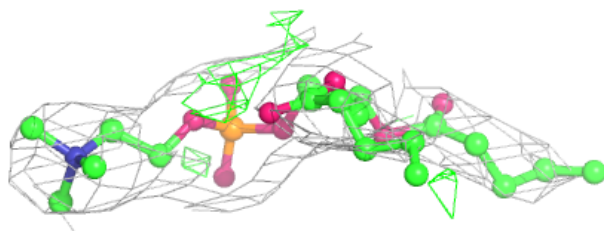
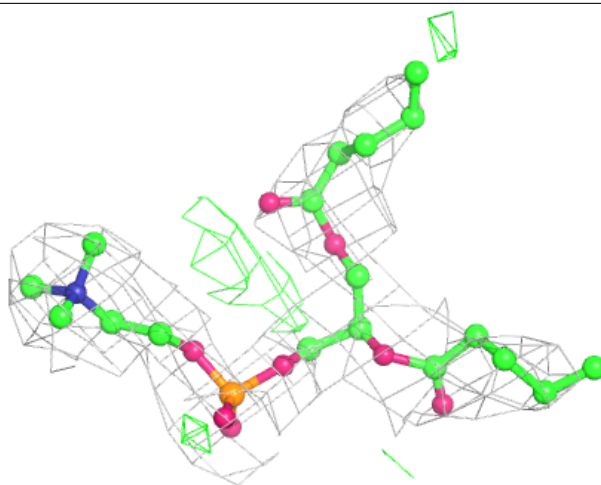
Electron density around 6PE A 501:

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



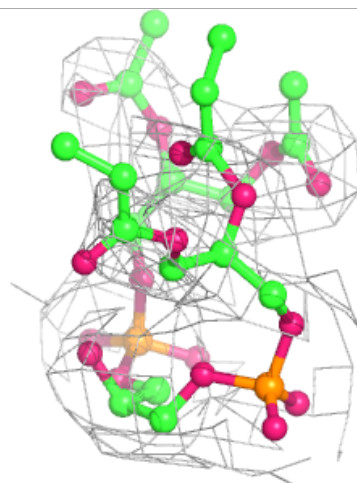
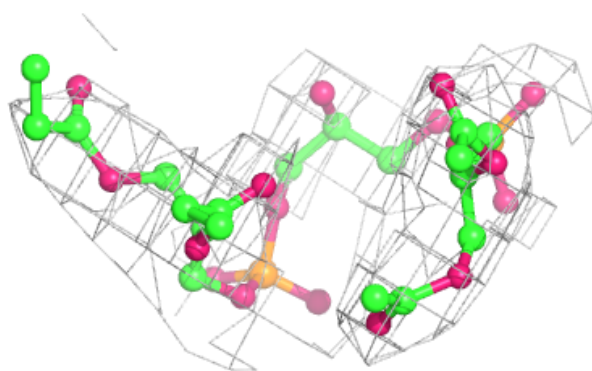
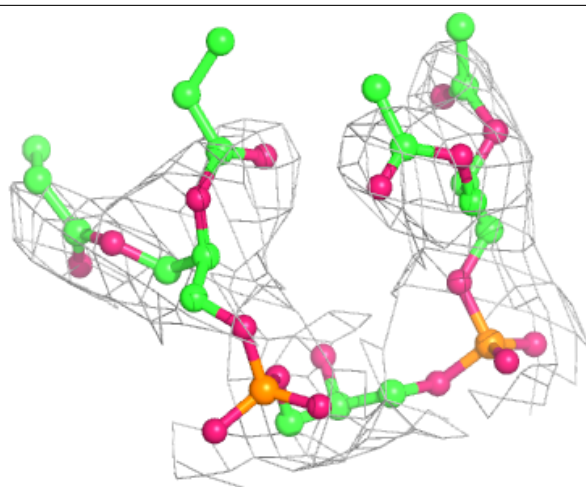
Electron density around PX4 E 202:

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



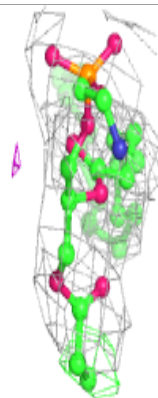
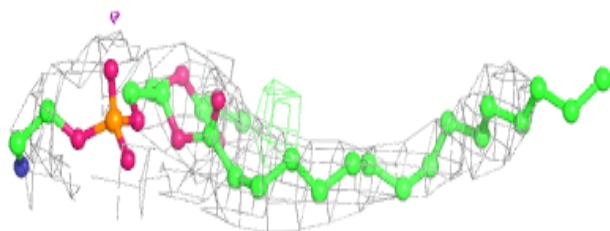
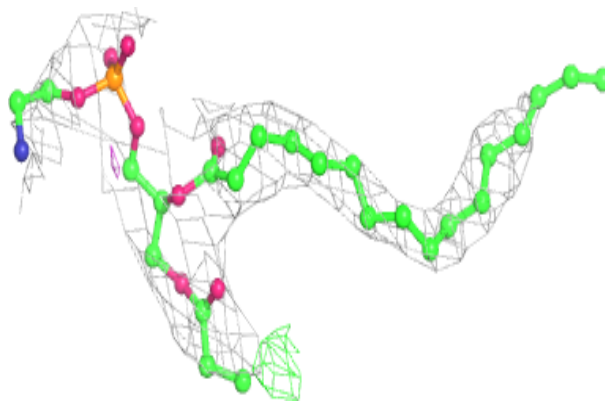
Electron density around CDL C 404:

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



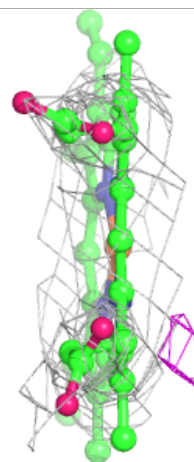
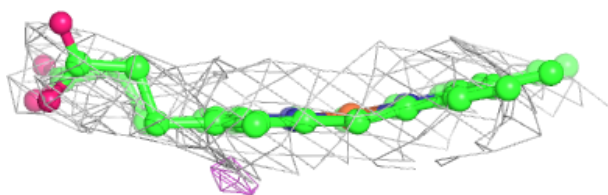
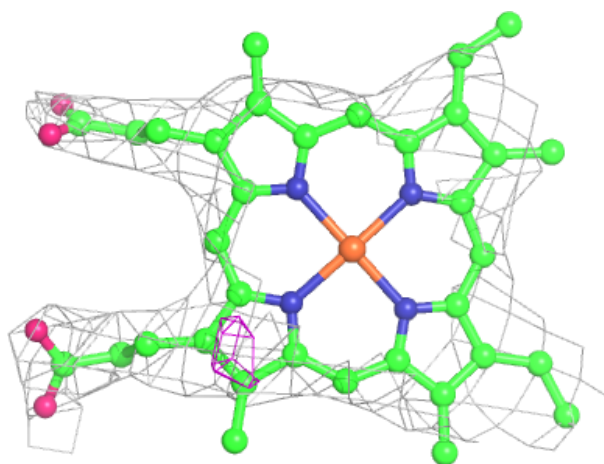
Electron density around PEE C 405:

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



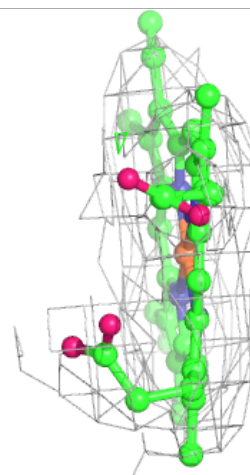
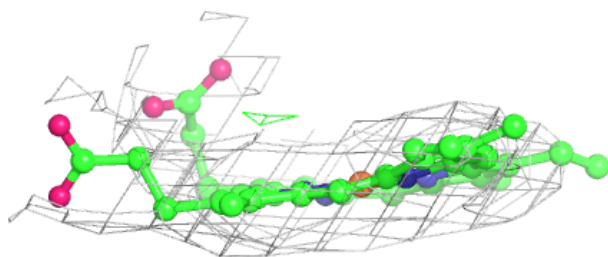
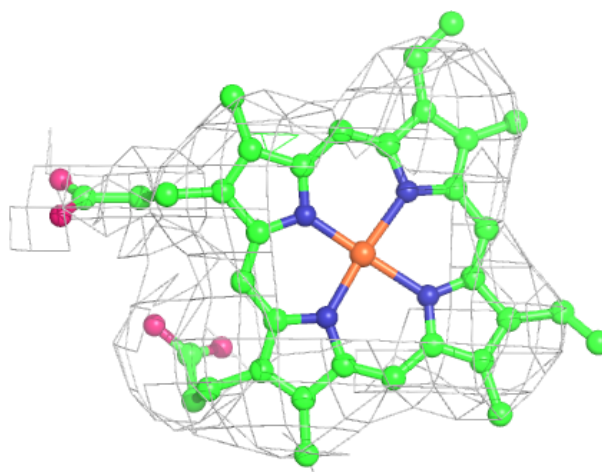
Electron density around HEC D 501:

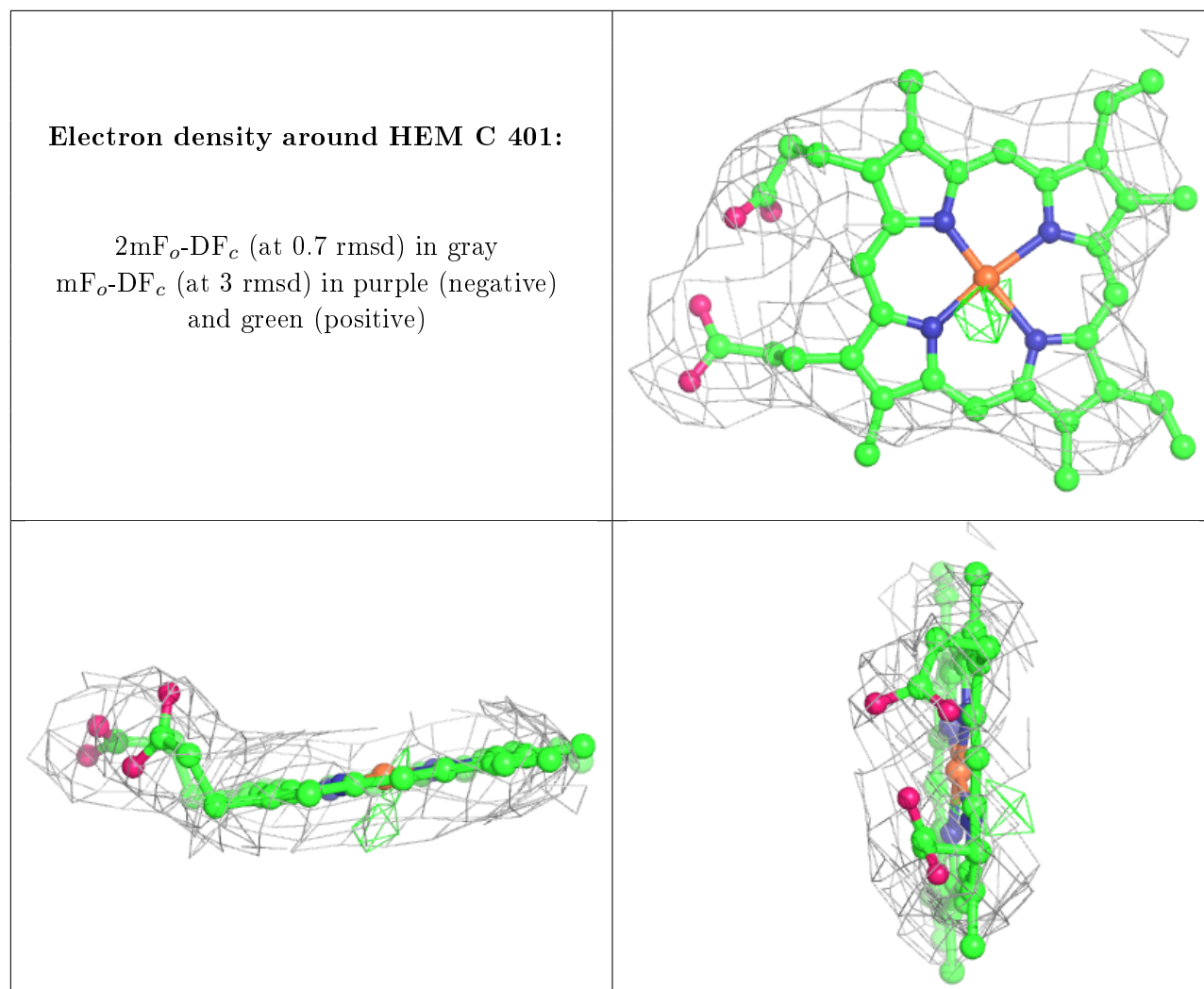
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.