Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:21 pm GMT

PDB ID	:	5OKD
Title	:	Crystal structure of bovine Cytochrome bc1 in complex with inhibitor SCR0911.
Authors	:	Amporndanai, K.; O'Neill, P.M.; Hasnain, S.S.; Antonyuk, S.V.
Deposited on	:	2017-07-25
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

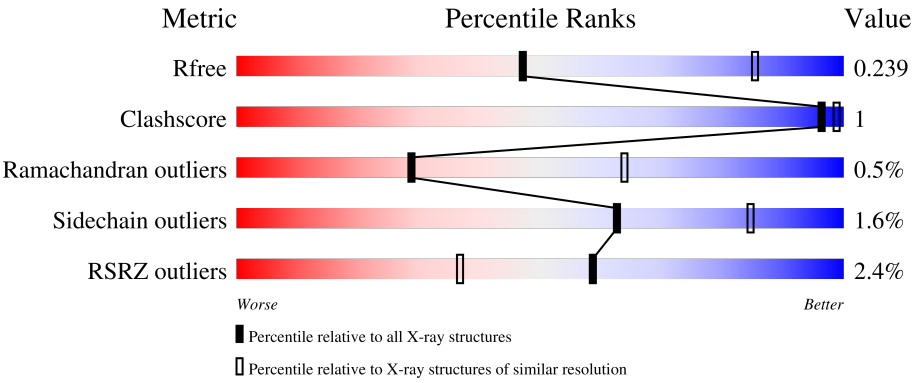
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	480	2% 88% 7%
2	B	453	88% 8%
3	C	379	% 97%
4	D	325	71% 26%
5	E	196	6% 96%

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Mol	Chain	Length	Quality of chain
6	F	111	2% 85% 11%
7	G	82	6% 87% 10%
8	H	91	7% 69% 29%
9	I	47	15% 87% 11%
10	J	64	3% 91% 8%

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
17	PEE	C	409	X	-	-	-
17	PEE	E	204	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 16469 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	445	Total	C	N	O	S	0	0	0
			3449	2157	608	664	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLU	ASP	conflict	UNP P31800
A	227	THR	ALA	conflict	UNP P31800

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3116	1957	553	599	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
			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
			1884	1205	321	343	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
			1512	951	263	290	8			

- 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
			859	545	156	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
			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	65	Total	C	N	O	S	0	0	0
			525	318	95	107	5			

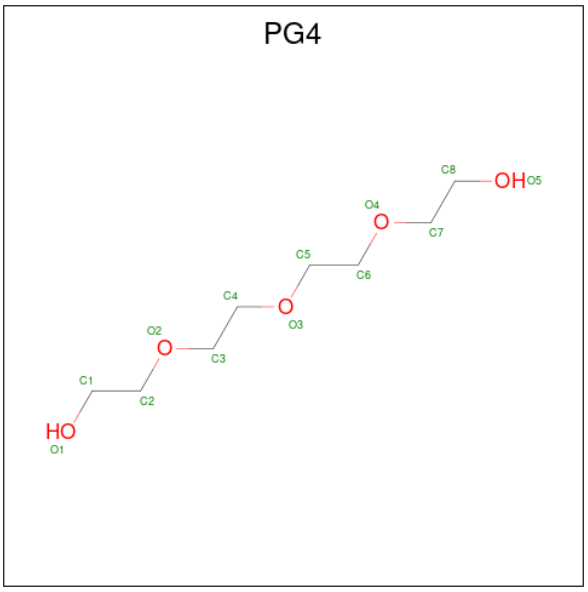
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			338	209	64	64	1			

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

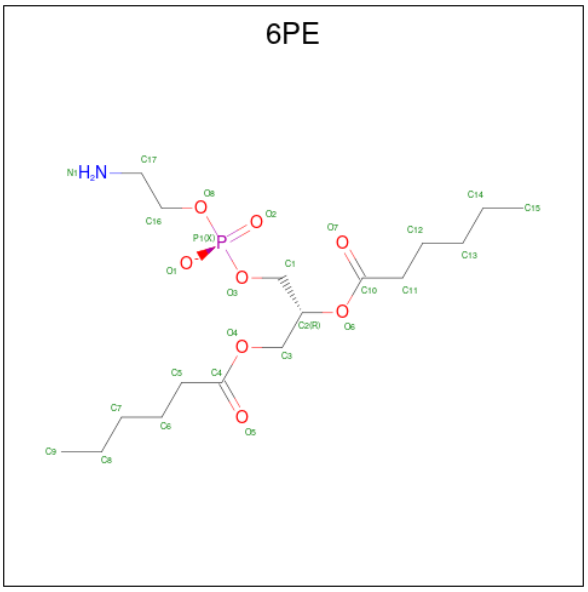
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



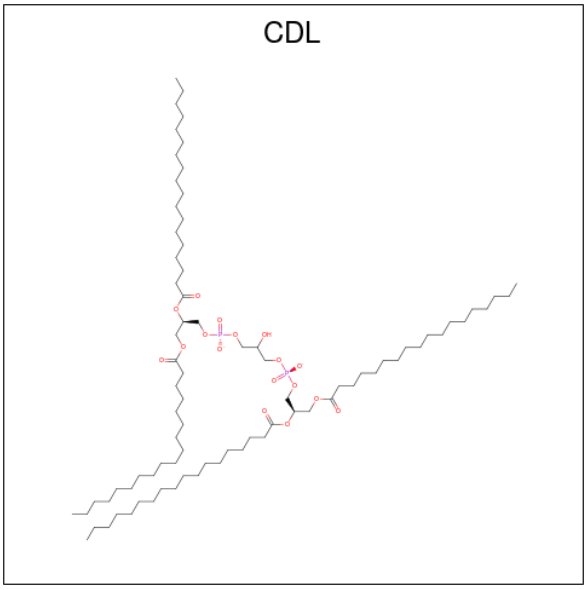
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0

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



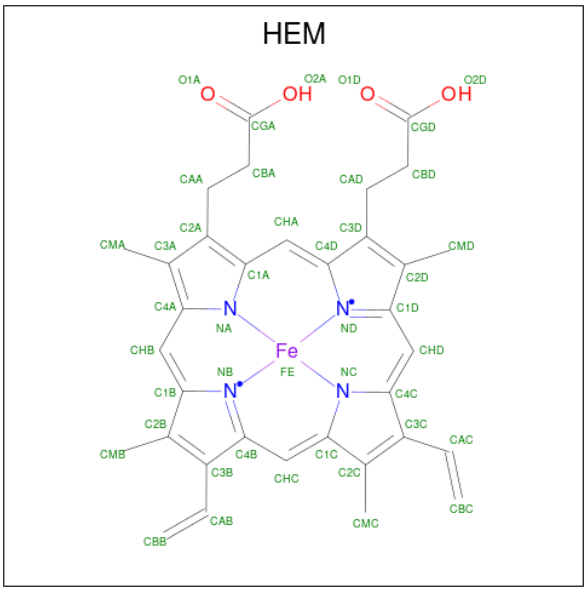
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



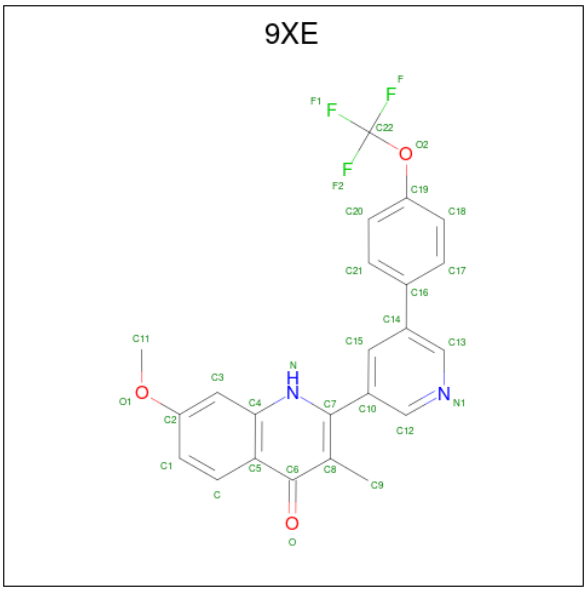
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	O	P		0	0
			34	17	15	2			
13	C	1	Total	C	O	P		0	0
			44	25	17	2			
13	D	1	Total	C	O	P		0	0
			54	35	17	2			
13	E	1	Total	C	O	P		0	0
			60	41	17	2			

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



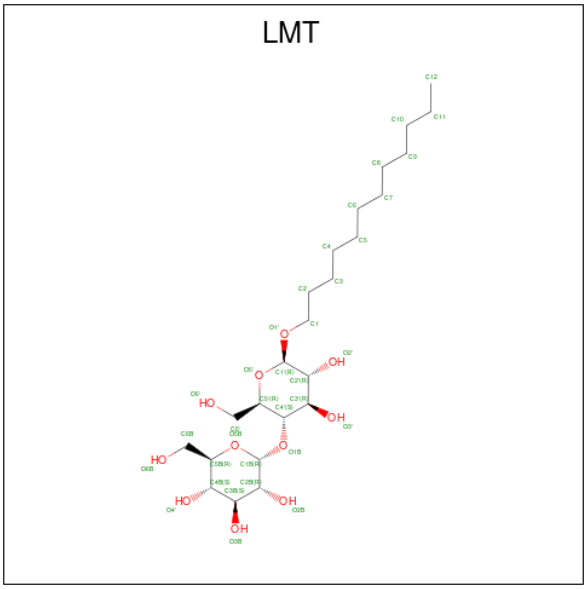
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is 7-methoxy-3-methyl-2-[5-[4-(trifluoromethyloxy)phenyl]pyridin-3-yl]-1 {H}-quinolin-4-one (three-letter code: 9XE) (formula: $C_{23}H_{17}F_3N_2O_3$).



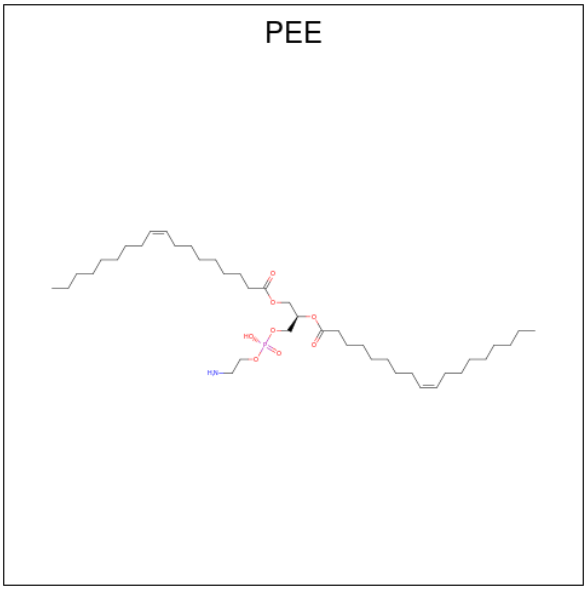
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	F	N	O	0	0
			31	23	3	2	3		

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



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

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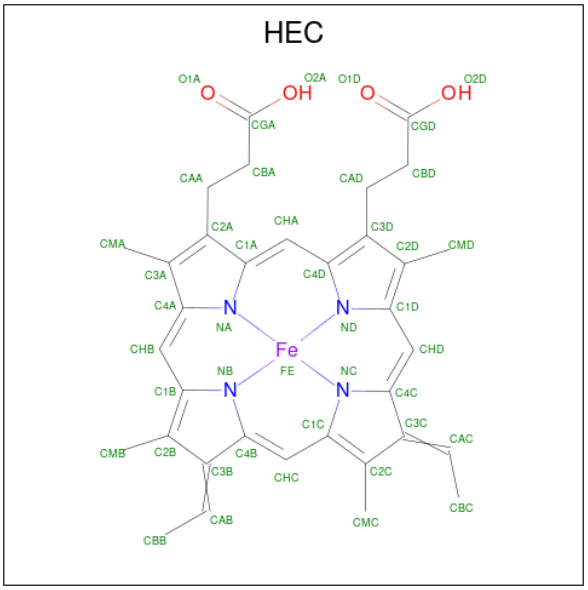
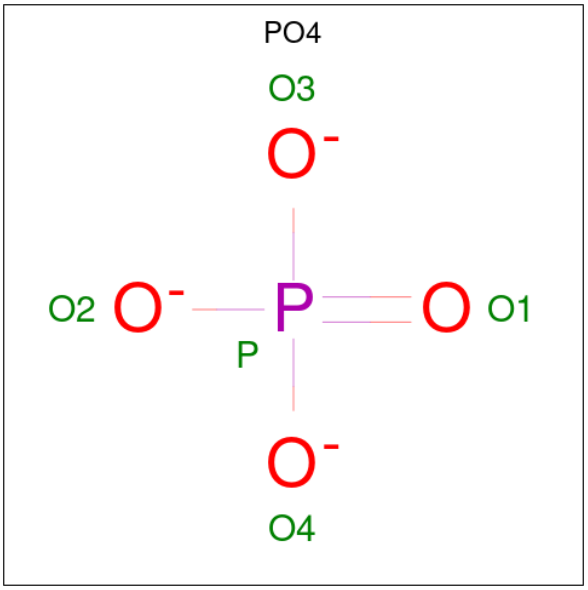
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	E	1	Total	C	N	O	P	0	0
			41	31	1	8	1		

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



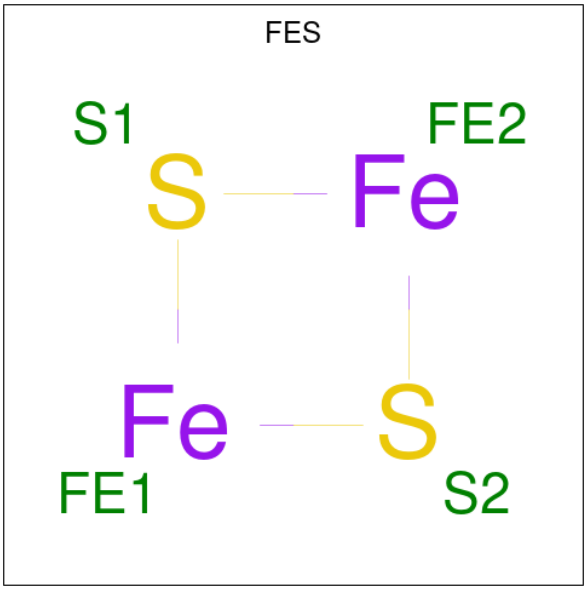
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 19 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



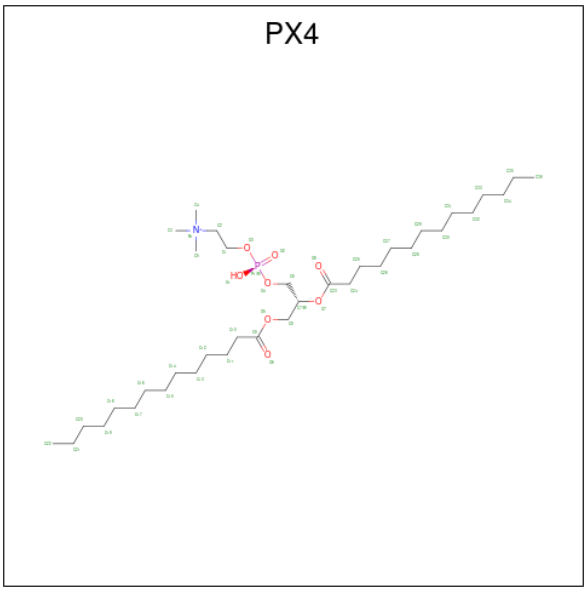
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total O P 5 4 1	0	0
19	E	1	Total O P 5 4 1	0	0
19	F	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0

- 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 4 2 2	0	0

- Molecule 21 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



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.

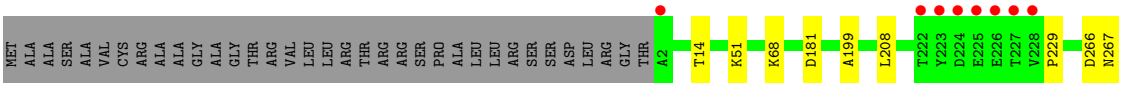
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	15	Total	O	0	0
			15	15		
22	B	12	Total	O	0	0
			12	12		
22	C	27	Total	O	0	0
			27	27		
22	D	5	Total	O	0	0
			5	5		
22	E	6	Total	O	0	0
			6	6		
22	F	8	Total	O	0	0
			8	8		
22	G	5	Total	O	0	0
			5	5		
22	H	1	Total	O	0	0
			1	1		
22	J	3	Total	O	0	0
			3	3		

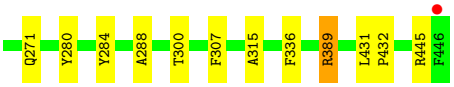
3 Residue-property plots (i)

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

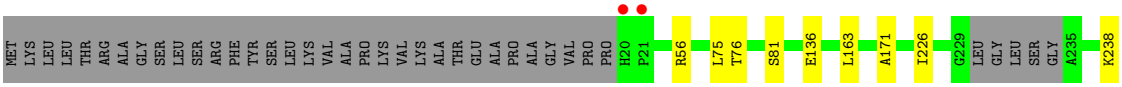
Chain A:

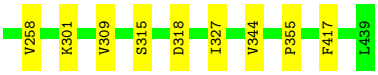




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

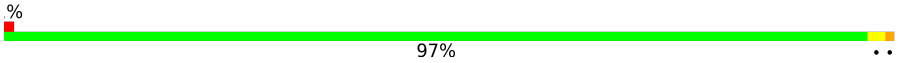
Chain B:





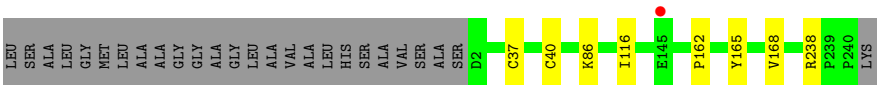
• Molecule 3: Cytochrome b

Chain C:



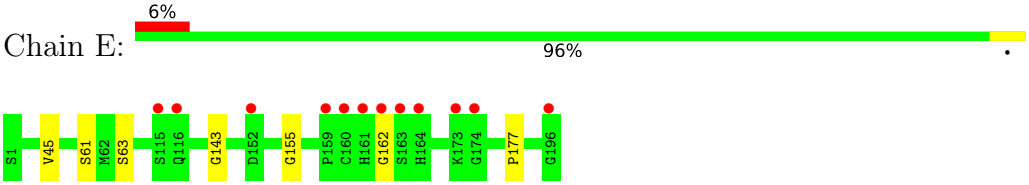
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



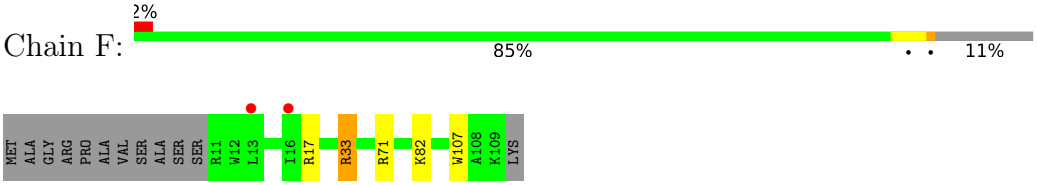
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



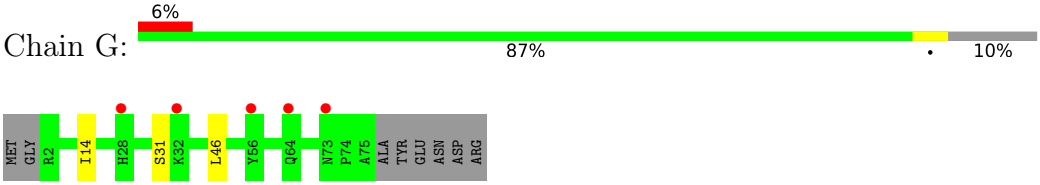
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



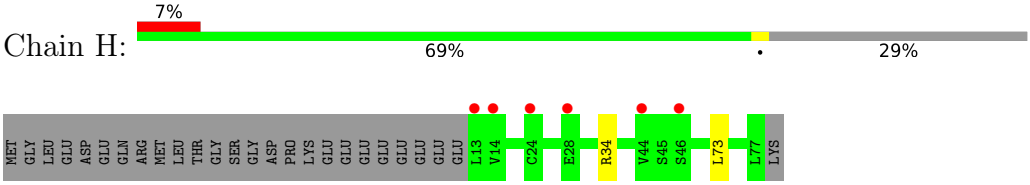
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:



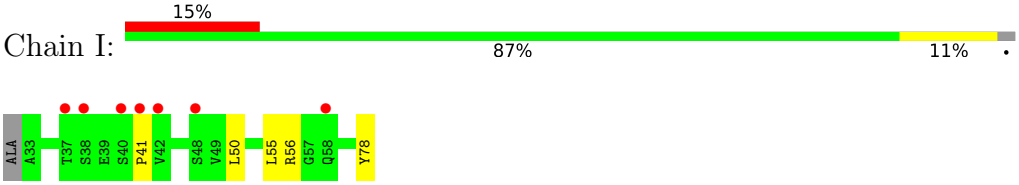
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



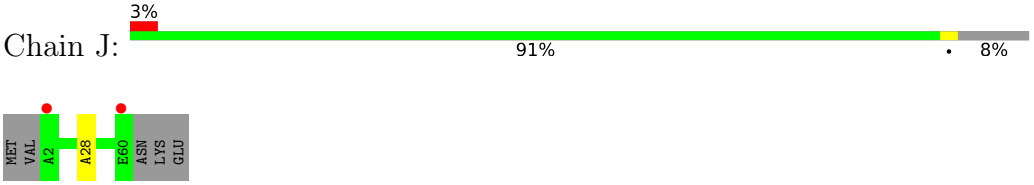
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



• Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	209.87Å 209.87Å 342.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.76 – 3.10 31.72 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.76-3.10) 99.2 (31.72-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.205 , 0.240 0.207 , 0.239	Depositor DCC
R_{free} test set	4037 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	91.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16469	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CDL, PX4, 6PE, PG4, HEM, LMT, PO4, FES, 9XE, HEC, PEE

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	0.37	0/3522	0.61	0/4781
2	B	0.37	0/3173	0.61	0/4304
3	C	0.38	0/3092	0.56	0/4231
4	D	0.37	0/1943	0.56	0/2642
5	E	0.39	0/1545	0.60	0/2089
6	F	0.39	0/878	0.64	0/1181
7	G	0.40	0/641	0.63	0/868
8	H	0.39	0/530	0.59	0/714
9	I	0.46	0/342	0.76	0/464
10	J	0.41	0/500	0.56	0/675
All	All	0.38	0/16166	0.60	0/21949

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	3449	0	3346	8	0
2	B	3116	0	3089	8	0
3	C	2996	0	3058	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1884	0	1814	8	0
5	E	1512	0	1498	1	0
6	F	859	0	836	2	0
7	G	620	0	624	1	0
8	H	525	0	500	0	0
9	I	338	0	356	2	0
10	J	487	0	487	1	0
11	A	13	0	18	0	0
11	C	26	0	36	0	0
12	A	23	0	19	0	0
13	C	78	0	56	0	0
13	D	54	0	52	0	0
13	E	60	0	64	0	0
14	C	86	0	60	3	0
15	C	31	0	0	0	0
16	C	35	0	46	0	0
17	C	40	0	54	0	0
17	E	41	0	59	0	0
18	D	43	0	32	6	0
19	D	5	0	0	0	0
19	E	5	0	0	0	0
19	F	5	0	0	0	0
19	G	15	0	0	0	0
20	E	4	0	0	0	0
21	E	37	0	51	0	0
22	A	15	0	0	0	0
22	B	12	0	0	0	0
22	C	27	0	0	0	0
22	D	5	0	0	0	0
22	E	6	0	0	0	0
22	F	8	0	0	0	0
22	G	5	0	0	0	0
22	H	1	0	0	0	0
22	J	3	0	0	0	0
All	All	16469	0	16155	33	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 (33) 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	18:D:501:HEC:CAB	2.70	0.79
4:D:116:ILE:HG12	18:D:501:HEC:HMA3	1.82	0.61
14:C:402:HEM:HMC1	14:C:402:HEM:HBC2	1.85	0.58
14:C:403:HEM:HMC2	14:C:403:HEM:HBC2	1.87	0.57
4:D:37:CYS:SG	18:D:501:HEC:C3B	2.94	0.56
2:B:163:LEU:HD11	2:B:258:VAL:HG22	1.89	0.54
3:C:375:LYS:O	6:F:17:ARG:NH1	2.44	0.51
14:C:402:HEM:HMB1	14:C:402:HEM:HBB2	1.94	0.50
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.94	0.49
4:D:37:CYS:SG	18:D:501:HEC:HBB3	2.53	0.48
4:D:40:CYS:SG	18:D:501:HEC:HBC3	2.54	0.47
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.50	0.47
2:B:309:VAL:O	9:I:56:ARG:NH1	2.47	0.47
4:D:37:CYS:SG	18:D:501:HEC:CBB	3.03	0.46
4:D:238:ARG:HG3	7:G:14:ILE:HD12	1.97	0.46
1:A:199:ALA:HB3	1:A:208:LEU:HD22	1.98	0.45
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.97	0.45
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.52	0.45
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.52	0.45
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.47	0.43
1:A:288:ALA:HB2	1:A:300:THR:HG22	2.01	0.43
1:A:267:ASN:O	1:A:271:GLN:HG2	2.20	0.42
3:C:277:ALA:HB1	3:C:294:LEU:HD12	2.02	0.42
4:D:165:TYR:CZ	4:D:168:VAL:HG23	2.54	0.42
2:B:76:THR:HG23	2:B:81:SER:HA	2.00	0.42
2:B:56:ARG:HB2	2:B:171:ALA:HB1	2.01	0.41
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.55	0.41
5:E:45:VAL:HG13	10:J:28:ALA:HA	2.03	0.41
1:A:431:LEU:HD12	1:A:432:PRO:HD2	2.03	0.41
1:A:14:THR:OG1	1:A:389:ARG:NH1	2.54	0.41
1:A:336:PHE:CZ	3:C:3:ASN:HB3	2.57	0.40
2:B:56:ARG:NH1	2:B:318:ASP:OD1	2.54	0.40
3:C:379:TRP:CZ2	6:F:33:ARG:HD3	2.56	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	443/480 (92%)	422 (95%)	17 (4%)	4 (1%)	17 52
2	B	411/453 (91%)	398 (97%)	13 (3%)	0	100 100
3	C	376/379 (99%)	362 (96%)	14 (4%)	0	100 100
4	D	237/325 (73%)	228 (96%)	8 (3%)	1 (0%)	34 69
5	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	7 30
6	F	97/111 (87%)	95 (98%)	2 (2%)	0	100 100
7	G	72/82 (88%)	70 (97%)	2 (3%)	0	100 100
8	H	63/91 (69%)	58 (92%)	5 (8%)	0	100 100
9	I	44/47 (94%)	43 (98%)	0	1 (2%)	6 28
10	J	57/64 (89%)	56 (98%)	1 (2%)	0	100 100
All	All	1994/2228 (90%)	1915 (96%)	69 (4%)	10 (0%)	29 64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
5	E	162	GLY
5	E	177	PRO
9	I	41	PRO
1	A	315	ALA
1	A	445	ARG
4	D	162	PRO
5	E	143	GLY
5	E	155	GLY
1	A	229	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/395 (93%)	365 (99%)	4 (1%)	73	89
2	B	325/355 (92%)	320 (98%)	5 (2%)	65	85
3	C	325/327 (99%)	320 (98%)	5 (2%)	65	85
4	D	200/257 (78%)	199 (100%)	1 (0%)	88	94
5	E	167/168 (99%)	165 (99%)	2 (1%)	71	88
6	F	88/99 (89%)	84 (96%)	4 (4%)	27	60
7	G	65/72 (90%)	63 (97%)	2 (3%)	40	70
8	H	61/85 (72%)	59 (97%)	2 (3%)	38	69
9	I	38/38 (100%)	36 (95%)	2 (5%)	22	54
10	J	49/54 (91%)	49 (100%)	0	100	100
All	All	1687/1850 (91%)	1660 (98%)	27 (2%)	62	84

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	68	LYS
1	A	181	ASP
1	A	389	ARG
2	B	226	ILE
2	B	238	LYS
2	B	301	LYS
2	B	315	SER
2	B	355	PRO
3	C	3	ASN
3	C	80	ARG
3	C	90	PHE
3	C	349	THR
3	C	379	TRP
4	D	86	LYS
5	E	61	SER
5	E	63	SER
6	F	33	ARG
6	F	71	ARG
6	F	82	LYS
6	F	107	TRP
7	G	31	SER
7	G	46	LEU
8	H	34	ARG

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Mol	Chain	Res	Type
8	H	73	LEU
9	I	50	LEU
9	I	78	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	165	GLN
1	A	189	HIS
2	B	400	GLN
3	C	15	ASN
8	H	23	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 monosaccharides in this entry.

5.6 Ligand geometry

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CDL	C	401	-	33,33,99	1.24	2 (6%)	37,43,111	1.28	3 (8%)
21	PX4	E	202	-	36,36,45	1.25	2 (5%)	42,44,53	1.03	2 (4%)
19	PO4	F	501	-	4,4,4	0.89	0	6,6,6	0.45	0
18	HEC	D	501	4	32,50,50	2.40	12 (37%)	24,82,82	2.25	5 (20%)
12	6PE	A	502	-	22,22,26	1.46	2 (9%)	25,27,31	1.23	2 (8%)
19	PO4	G	101	-	4,4,4	0.90	0	6,6,6	0.26	0
19	PO4	G	102	-	4,4,4	0.92	0	6,6,6	0.43	0
13	CDL	C	408	-	43,43,99	1.50	4 (9%)	49,55,111	1.30	5 (10%)
11	PG4	C	407	-	12,12,12	0.55	0	11,11,11	0.40	0
19	PO4	D	502	-	4,4,4	0.86	0	6,6,6	0.50	0
14	HEM	C	402	3	41,50,50	1.34	6 (14%)	45,82,82	1.80	12 (26%)
13	CDL	D	503	-	53,53,99	1.28	4 (7%)	59,65,111	1.12	4 (6%)
15	9XE	C	404	-	34,34,34	1.62	3 (8%)	47,50,50	1.17	5 (10%)
16	LMT	C	405	-	36,36,36	0.65	1 (2%)	47,47,47	1.06	2 (4%)
17	PEE	E	204	-	40,40,50	1.20	3 (7%)	43,45,55	1.06	2 (4%)
13	CDL	E	205	-	59,59,99	1.18	4 (6%)	65,71,111	1.06	4 (6%)
19	PO4	E	203	-	4,4,4	0.92	0	6,6,6	0.70	0
20	FES	E	201	-	0,4,4	-	-	-		
11	PG4	C	406	-	12,12,12	0.56	0	11,11,11	0.52	0
14	HEM	C	403	3	41,50,50	1.36	8 (19%)	45,82,82	1.61	10 (22%)
17	PEE	C	409	-	39,39,50	1.19	3 (7%)	42,44,55	0.91	2 (4%)
19	PO4	G	103	-	4,4,4	0.89	0	6,6,6	0.45	0
11	PG4	A	501	-	12,12,12	0.55	0	11,11,11	0.29	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
13	CDL	E	205	-	-	34/69/69/110	-
13	CDL	C	401	-	-	21/41/41/110	-
13	CDL	C	408	-	-	19/52/52/110	-
11	PG4	C	407	-	-	5/10/10/10	-
11	PG4	C	406	-	-	5/10/10/10	-
14	HEM	C	402	3	-	5/12/54/54	-
17	PEE	C	409	-	1/1/4/8	17/43/43/54	-
14	HEM	C	403	3	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PX4	E	202	-	-	17/40/40/49	-
20	FES	E	201	-	-	-	0/1/1/1
13	CDL	D	503	-	-	24/63/63/110	-
18	HEC	D	501	4	-	3/10/54/54	-
15	9XE	C	404	-	-	5/15/15/15	0/4/4/4
16	LMT	C	405	-	-	10/21/61/61	0/2/2/2
17	PEE	E	204	-	1/1/4/8	27/44/44/54	-
11	PG4	A	501	-	-	5/10/10/10	-
12	6PE	A	502	-	-	12/26/26/30	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	501	HEC	C3C-C2C	7.09	1.48	1.40
15	C	404	9XE	C7-C8	6.31	1.50	1.37
18	D	501	HEC	C2B-C3B	6.20	1.47	1.40
13	C	408	CDL	OA6-CA5	5.23	1.47	1.35
15	C	404	9XE	C5-C4	5.23	1.49	1.41
13	C	408	CDL	OB6-CB5	4.98	1.48	1.34
21	E	202	PX4	O7-C23	4.72	1.47	1.34
13	D	503	CDL	OA8-CA7	4.70	1.47	1.33
13	C	408	CDL	OB8-CB7	4.67	1.47	1.33
21	E	202	PX4	O5-C9	4.64	1.46	1.33
13	D	503	CDL	OA6-CA5	4.62	1.47	1.34
13	C	401	CDL	OB8-CB7	4.62	1.46	1.33
13	E	205	CDL	OA8-CA7	4.61	1.46	1.33
13	D	503	CDL	OB6-CB5	4.54	1.47	1.34
12	A	502	6PE	O6-C10	4.52	1.47	1.34
13	E	205	CDL	OA6-CA5	4.52	1.47	1.34
12	A	502	6PE	O4-C4	4.38	1.46	1.33
13	C	401	CDL	OB6-CB5	4.31	1.46	1.34
17	C	409	PEE	O3-C30	4.30	1.45	1.33
17	E	204	PEE	O2-C10	4.29	1.46	1.34
13	E	205	CDL	OB6-CB5	4.27	1.46	1.34
17	E	204	PEE	O3-C30	4.13	1.45	1.33
17	C	409	PEE	O2-C10	4.05	1.45	1.34
14	C	403	HEM	C1B-NB	-3.85	1.33	1.40
17	C	409	PEE	C18-C19	3.69	1.53	1.31
17	E	204	PEE	C18-C19	3.67	1.53	1.31
18	D	501	HEC	C3C-C4C	3.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	402	HEM	C1B-NB	-3.45	1.34	1.40
18	D	501	HEC	C2A-C3A	3.38	1.47	1.37
18	D	501	HEC	C3D-C2D	3.15	1.47	1.37
18	D	501	HEC	C4B-C3B	3.12	1.48	1.43
18	D	501	HEC	C3A-C4A	3.09	1.49	1.42
18	D	501	HEC	C2A-C1A	3.07	1.49	1.42
14	C	403	HEM	C4D-ND	-2.88	1.35	1.40
14	C	402	HEM	C4D-ND	-2.86	1.35	1.40
14	C	402	HEM	FE-NB	2.85	2.10	1.96
15	C	404	9XE	C4-N	-2.78	1.35	1.39
13	C	408	CDL	OA8-CA7	2.78	1.47	1.33
14	C	403	HEM	FE-NB	2.67	2.10	1.96
13	E	205	CDL	OB8-CB7	2.60	1.46	1.33
16	C	405	LMT	O1'-C1'	2.58	1.44	1.40
14	C	403	HEM	C4B-NB	-2.58	1.33	1.38
13	D	503	CDL	OB8-CB7	2.53	1.45	1.33
18	D	501	HEC	C1B-CHB	2.47	1.47	1.41
14	C	402	HEM	C3B-C4B	2.46	1.49	1.44
18	D	501	HEC	C1C-CHC	2.45	1.47	1.41
18	D	501	HEC	C1D-CHD	2.42	1.47	1.41
14	C	402	HEM	CHB-C1B	2.41	1.41	1.35
14	C	402	HEM	C4B-NB	-2.37	1.33	1.38
18	D	501	HEC	C4D-CHA	2.35	1.47	1.41
14	C	403	HEM	C3B-C4B	2.18	1.49	1.44
14	C	403	HEM	C1D-ND	-2.13	1.34	1.38
14	C	403	HEM	CHB-C1B	2.11	1.40	1.35
14	C	403	HEM	C1D-C2D	2.03	1.48	1.44

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	501	HEC	C1D-C2D-C3D	-6.13	102.73	107.00
18	D	501	HEC	CMC-C2C-C3C	4.90	131.58	125.82
13	C	401	CDL	OB6-CB5-C51	4.71	121.66	111.50
14	C	402	HEM	C1B-NB-C4B	4.69	109.92	105.07
13	C	408	CDL	OA6-CA5-C11	4.46	119.29	111.09
21	E	202	PX4	O7-C23-C24	4.28	120.72	111.50
14	C	403	HEM	C1B-NB-C4B	4.20	109.41	105.07
13	E	205	CDL	OB6-CB5-C51	4.08	120.29	111.50
17	E	204	PEE	O2-C10-C11	4.03	120.19	111.50
13	D	503	CDL	OA6-CA5-C11	4.02	120.16	111.50
13	D	503	CDL	OB6-CB5-C51	4.01	120.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	401	CDL	OB8-CB7-C71	3.97	121.79	111.38
12	A	502	6PE	O6-C10-C11	3.94	119.99	111.50
13	E	205	CDL	OA6-CA5-C11	3.87	119.83	111.50
16	C	405	LMT	C1B-O5B-C5B	3.76	121.06	113.69
18	D	501	HEC	CMB-C2B-C3B	3.68	130.15	125.82
14	C	402	HEM	CHC-C4B-NB	3.55	128.28	124.43
14	C	403	HEM	CHC-C4B-NB	3.51	128.25	124.43
14	C	402	HEM	CBA-CAA-C2A	-3.46	106.72	112.62
15	C	404	9XE	C13-N1-C12	3.45	122.19	117.48
14	C	402	HEM	CHD-C1D-ND	3.45	128.18	124.43
18	D	501	HEC	CBD-CAD-C3D	-3.36	106.89	112.62
13	C	408	CDL	OB6-CB5-C51	3.28	119.95	110.80
13	D	503	CDL	OA8-CA7-C31	3.14	121.76	111.91
14	C	402	HEM	CHD-C1D-C2D	-3.14	120.08	124.98
13	C	408	CDL	OB8-CB7-C71	3.09	121.62	111.91
16	C	405	LMT	C1-O1'-C1'	3.05	118.89	113.84
14	C	403	HEM	CHD-C1D-ND	2.96	127.65	124.43
17	C	409	PEE	O3-C30-C31	2.76	120.57	111.91
14	C	402	HEM	CAD-C3D-C4D	2.72	129.41	124.66
21	E	202	PX4	O5-C9-C10	2.71	120.41	111.91
14	C	402	HEM	CMD-C2D-C1D	2.69	129.13	125.04
14	C	403	HEM	C4B-CHC-C1C	2.62	126.02	122.56
14	C	403	HEM	CHA-C4D-ND	2.59	127.58	124.38
17	C	409	PEE	O2-C10-C11	2.56	117.02	111.50
13	E	205	CDL	OA8-CA7-C31	2.55	119.90	111.91
14	C	403	HEM	CHA-C4D-C3D	-2.54	120.57	125.33
14	C	402	HEM	CHA-C4D-ND	2.52	127.49	124.38
14	C	402	HEM	C4B-CHC-C1C	2.48	125.83	122.56
17	E	204	PEE	O3-C30-C31	2.46	119.64	111.91
12	A	502	6PE	O4-C4-C5	2.46	119.62	111.91
14	C	402	HEM	O2D-CGD-CBD	2.42	121.82	114.03
14	C	403	HEM	CHD-C1D-C2D	-2.42	121.20	124.98
15	C	404	9XE	C9-C8-C6	2.38	120.21	116.27
13	D	503	CDL	OA8-CA7-OA9	-2.36	117.64	123.59
14	C	403	HEM	O2A-CGA-CBA	2.32	121.49	114.03
13	C	408	CDL	CA6-OA8-CA7	2.28	122.83	117.10
15	C	404	9XE	C11-O1-C2	2.27	122.44	117.51
14	C	402	HEM	CHA-C4D-C3D	-2.21	121.17	125.33
13	C	401	CDL	OB6-CB5-OB7	-2.20	118.38	123.70
15	C	404	9XE	C5-C4-N	2.20	121.22	119.49
18	D	501	HEC	C4C-C3C-C2C	-2.17	104.01	106.35
15	C	404	9XE	C10-C12-N1	-2.14	120.33	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	408	CDL	OA8-CA7-C31	2.14	121.69	112.38
14	C	403	HEM	O2A-CGA-O1A	-2.12	118.01	123.30
14	C	403	HEM	O2D-CGD-CBD	2.10	120.79	114.03
14	C	402	HEM	O2A-CGA-CBA	2.01	120.50	114.03
13	E	205	CDL	OB8-CB7-C71	2.01	121.14	112.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	C	409	PEE	C2
17	E	204	PEE	C2

All (211) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	502	6PE	C1-O3-P1-O1
12	A	502	6PE	C11-C10-O6-C2
12	A	502	6PE	O8-C16-C17-N1
13	C	401	CDL	CB3-OB5-PB2-OB4
13	C	401	CDL	C51-CB5-OB6-CB4
13	C	408	CDL	CA3-OA5-PA1-OA4
13	D	503	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	OB7-CB5-OB6-CB4
13	D	503	CDL	C51-CB5-OB6-CB4
13	E	205	CDL	CB3-OB5-PB2-OB3
13	E	205	CDL	C51-CB5-OB6-CB4
15	C	404	9XE	F-C22-O2-C19
16	C	405	LMT	C2'-C1'-O1'-C1
16	C	405	LMT	O5'-C1'-O1'-C1
17	C	409	PEE	C4-O4P-P-O3P
17	C	409	PEE	C4-O4P-P-O2P
17	C	409	PEE	C4-O4P-P-O1P
17	E	204	PEE	C4-O4P-P-O1P
17	E	204	PEE	O4P-C4-C5-N
21	E	202	PX4	C6-O4-P1-O1
21	E	202	PX4	C24-C23-O7-C7
13	C	408	CDL	C11-CA5-OA6-CA4
17	C	409	PEE	O5-C30-O3-C3
13	D	503	CDL	OB9-CB7-OB8-CB6
12	A	502	6PE	O7-C10-O6-C2
13	C	401	CDL	OB7-CB5-OB6-CB4
13	E	205	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
21	E	202	PX4	O8-C23-O7-C7
13	D	503	CDL	C31-CA7-OA8-CA6
17	C	409	PEE	C31-C30-O3-C3
17	E	204	PEE	C31-C30-O3-C3
21	E	202	PX4	C10-C9-O5-C8
13	D	503	CDL	C71-CB7-OB8-CB6
17	C	409	PEE	C17-C18-C19-C20
13	D	503	CDL	OA9-CA7-OA8-CA6
17	E	204	PEE	O5-C30-O3-C3
13	C	408	CDL	OA7-CA5-OA6-CA4
13	E	205	CDL	CB4-CB6-OB8-CB7
13	C	401	CDL	OA5-CA3-CA4-OA6
13	E	205	CDL	O1-C1-CB2-OB2
11	C	406	PG4	O2-C3-C4-O3
13	E	205	CDL	CB4-CB3-OB5-PB2
21	E	202	PX4	O6-C9-O5-C8
13	C	408	CDL	C31-CA7-OA8-CA6
11	C	407	PG4	O2-C3-C4-O3
15	C	404	9XE	F2-C22-O2-C19
13	E	205	CDL	C71-CB7-OB8-CB6
13	C	401	CDL	CB5-C51-C52-C53
13	D	503	CDL	CA5-C11-C12-C13
11	A	501	PG4	O1-C1-C2-O2
13	C	408	CDL	OA9-CA7-OA8-CA6
12	A	502	6PE	C1-O3-P1-O8
13	C	401	CDL	CA3-OA5-PA1-OA2
13	C	408	CDL	CA3-OA5-PA1-OA2
13	D	503	CDL	CB2-OB2-PB2-OB5
13	E	205	CDL	CB3-OB5-PB2-OB2
21	E	202	PX4	C9-C10-C11-C12
13	C	401	CDL	OA5-CA3-CA4-CA6
15	C	404	9XE	F1-C22-O2-C19
11	C	406	PG4	O3-C5-C6-O4
17	C	409	PEE	C31-C32-C33-C34
17	E	204	PEE	C33-C34-C35-C36
17	C	409	PEE	C13-C14-C15-C16
13	C	408	CDL	C71-CB7-OB8-CB6
17	C	409	PEE	C14-C15-C16-C17
13	E	205	CDL	C51-C52-C53-C54
13	E	205	CDL	OA7-CA5-OA6-CA4
13	E	205	CDL	C11-CA5-OA6-CA4
16	C	405	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	E	205	CDL	C13-C14-C15-C16
13	D	503	CDL	C11-C12-C13-C14
16	C	405	LMT	C2-C1-O1'-C1'
17	C	409	PEE	C10-C11-C12-C13
13	D	503	CDL	C51-C52-C53-C54
21	E	202	PX4	C12-C13-C14-C15
13	E	205	CDL	CA3-CA4-CA6-OA8
17	E	204	PEE	C11-C10-O2-C2
16	C	405	LMT	C7-C8-C9-C10
12	A	502	6PE	C4-C5-C6-C7
13	C	408	CDL	OB9-CB7-OB8-CB6
17	E	204	PEE	O4-C10-O2-C2
11	A	501	PG4	O4-C7-C8-O5
12	A	502	6PE	C5-C4-O4-C3
16	C	405	LMT	C11-C10-C9-C8
13	D	503	CDL	C53-C54-C55-C56
13	C	408	CDL	C51-CB5-OB6-CB4
13	D	503	CDL	OA5-CA3-CA4-OA6
13	C	408	CDL	OB7-CB5-OB6-CB4
13	E	205	CDL	OB9-CB7-OB8-CB6
17	E	204	PEE	C20-C21-C22-C23
13	E	205	CDL	CA5-C11-C12-C13
13	C	408	CDL	CB4-CB3-OB5-PB2
13	C	401	CDL	OB5-CB3-CB4-CB6
13	C	408	CDL	OB5-CB3-CB4-CB6
13	E	205	CDL	CA2-C1-CB2-OB2
13	D	503	CDL	C31-C32-C33-C34
12	A	502	6PE	O5-C4-O4-C3
11	C	406	PG4	O1-C1-C2-O2
13	D	503	CDL	CA3-CA4-CA6-OA8
17	E	204	PEE	C34-C35-C36-C37
17	E	204	PEE	C31-C32-C33-C34
16	C	405	LMT	O5B-C5B-C6B-O6B
13	C	401	CDL	C51-C52-C53-C54
13	E	205	CDL	C35-C36-C37-C38
13	D	503	CDL	CB6-CB4-OB6-CB5
13	E	205	CDL	CA7-C31-C32-C33
17	E	204	PEE	C23-C24-C25-C26
13	D	503	CDL	OA5-CA3-CA4-CA6
17	C	409	PEE	O3P-C1-C2-C3
13	C	408	CDL	C75-C76-C77-C78
15	C	404	9XE	C3-C2-O1-C11

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Mol	Chain	Res	Type	Atoms
17	E	204	PEE	C12-C13-C14-C15
21	E	202	PX4	C23-C24-C25-C26
17	E	204	PEE	C24-C25-C26-C27
15	C	404	9XE	C1-C2-O1-C11
13	C	408	CDL	OB5-CB3-CB4-OB6
17	C	409	PEE	O3P-C1-C2-O2
12	A	502	6PE	C2-C1-O3-P1
13	E	205	CDL	C1-CA2-OA2-PA1
21	E	202	PX4	C24-C25-C26-C27
21	E	202	PX4	C16-C17-C18-C19
17	C	409	PEE	C11-C12-C13-C14
13	D	503	CDL	OB5-CB3-CB4-CB6
11	A	501	PG4	O2-C3-C4-O3
13	E	205	CDL	C53-C54-C55-C56
21	E	202	PX4	C10-C11-C12-C13
11	C	406	PG4	C3-C4-O3-C5
12	A	502	6PE	C1-C2-C3-O4
17	E	204	PEE	O3P-C1-C2-O2
13	E	205	CDL	OA6-CA4-CA6-OA8
13	C	408	CDL	CB7-C71-C72-C73
17	E	204	PEE	C13-C14-C15-C16
11	C	407	PG4	C1-C2-O2-C3
13	E	205	CDL	C17-C18-C19-C20
17	E	204	PEE	C4-O4P-P-O3P
21	E	202	PX4	C6-O4-P1-O3
13	C	401	CDL	CA3-OA5-PA1-OA3
13	D	503	CDL	CB2-OB2-PB2-OB4
13	E	205	CDL	CB3-OB5-PB2-OB4
21	E	202	PX4	C6-O4-P1-O2
17	E	204	PEE	O3P-C1-C2-C3
14	C	402	HEM	C3D-CAD-CBD-CGD
11	A	501	PG4	C3-C4-O3-C5
11	C	407	PG4	C6-C5-O3-C4
21	E	202	PX4	C13-C14-C15-C16
13	C	401	CDL	OB5-CB3-CB4-OB6
13	D	503	CDL	OB5-CB3-CB4-OB6
21	E	202	PX4	O3-C1-C2-N1
12	A	502	6PE	O6-C2-C3-O4
13	D	503	CDL	OA6-CA4-CA6-OA8
11	A	501	PG4	C5-C6-O4-C7
16	C	405	LMT	C1-C2-C3-C4
13	E	205	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
17	E	204	PEE	C10-C11-C12-C13
17	E	204	PEE	C3-C2-O2-C10
11	C	406	PG4	C4-C3-O2-C2
13	C	401	CDL	CA4-CA3-OA5-PA1
11	C	407	PG4	O1-C1-C2-O2
17	E	204	PEE	O2-C2-C3-O3
13	C	408	CDL	CB2-OB2-PB2-OB5
13	E	205	CDL	CA2-OA2-PA1-OA5
13	E	205	CDL	CB2-OB2-PB2-OB5
17	E	204	PEE	C1-O3P-P-O4P
16	C	405	LMT	C2-C3-C4-C5
13	E	205	CDL	C52-C53-C54-C55
14	C	403	HEM	CAA-CBA-CGA-O1A
14	C	403	HEM	CAA-CBA-CGA-O2A
13	E	205	CDL	C54-C55-C56-C57
13	C	401	CDL	CB3-OB5-PB2-OB2
17	E	204	PEE	C2-C3-O3-C30
13	C	408	CDL	OA6-CA4-CA6-OA8
13	D	503	CDL	C54-C55-C56-C57
17	E	204	PEE	C14-C15-C16-C17
13	E	205	CDL	C12-C13-C14-C15
14	C	402	HEM	CAD-CBD-CGD-O2D
11	C	407	PG4	C3-C4-O3-C5
14	C	402	HEM	CAA-CBA-CGA-O2A
16	C	405	LMT	O5B-C1B-O1B-C4'
13	E	205	CDL	C32-C31-CA7-OA8
17	E	204	PEE	C15-C16-C17-C18
14	C	402	HEM	CAA-CBA-CGA-O1A
17	C	409	PEE	C34-C35-C36-C37
18	D	501	HEC	CAA-CBA-CGA-O2A
14	C	402	HEM	CAD-CBD-CGD-O1D
18	D	501	HEC	CAA-CBA-CGA-O1A
17	E	204	PEE	C11-C12-C13-C14
17	C	409	PEE	O3-C30-C31-C32
17	C	409	PEE	C33-C34-C35-C36
13	E	205	CDL	C16-C17-C18-C19
21	E	202	PX4	C11-C10-C9-O5
13	D	503	CDL	C13-C14-C15-C16
13	E	205	CDL	C32-C31-CA7-OA9
13	C	401	CDL	CB2-C1-CA2-OA2
13	E	205	CDL	C32-C33-C34-C35
13	C	401	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
13	C	401	CDL	CA3-OA5-PA1-OA4
13	C	401	CDL	CB2-OB2-PB2-OB3
13	C	401	CDL	CB3-OB5-PB2-OB3
13	C	408	CDL	CB2-OB2-PB2-OB3
13	E	205	CDL	CA2-OA2-PA1-OA3
17	E	204	PEE	C22-C23-C24-C25
13	C	408	CDL	C72-C71-CB7-OB8
12	A	502	6PE	O4-C4-C5-C6
17	C	409	PEE	O5-C30-C31-C32
17	E	204	PEE	C5-C4-O4P-P
13	C	401	CDL	O1-C1-CA2-OA2
21	E	202	PX4	O7-C23-C24-C25
13	C	401	CDL	C72-C71-CB7-OB8
13	C	401	CDL	C52-C51-CB5-OB7
18	D	501	HEC	CAD-CBD-CGD-O1D
13	D	503	CDL	C12-C13-C14-C15

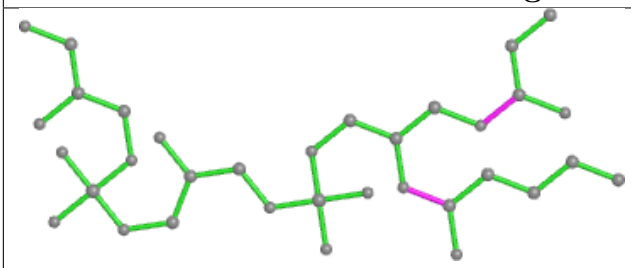
There are no ring outliers.

3 monomers are involved in 9 short contacts:

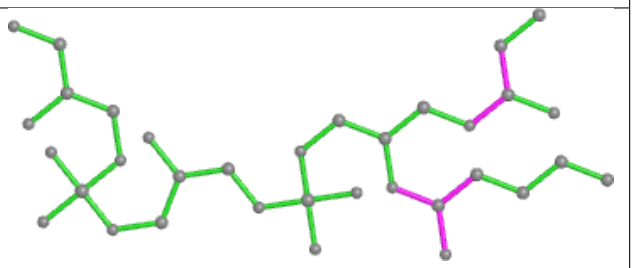
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	501	HEC	6	0
14	C	402	HEM	2	0
14	C	403	HEM	1	0

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 then 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.

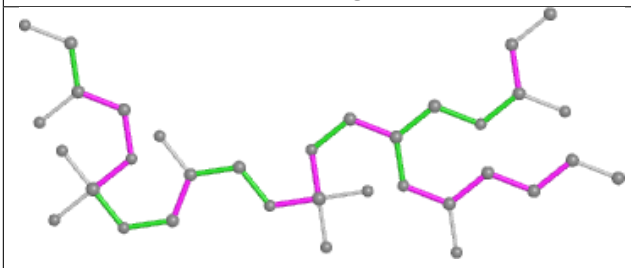
Ligand CDL C 401



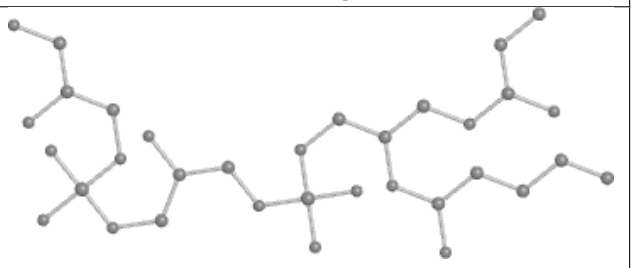
Bond lengths



Bond angles

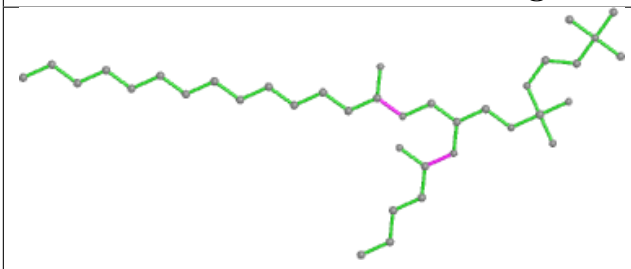


Torsions

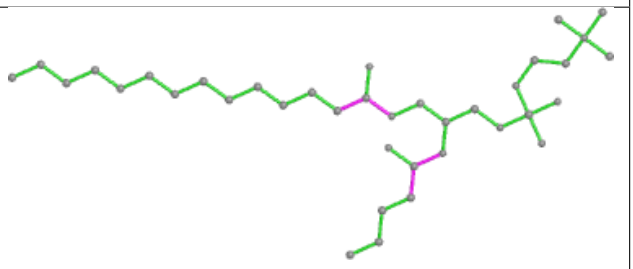


Rings

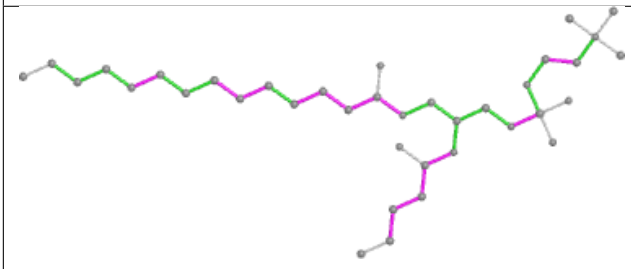
Ligand PX4 E 202



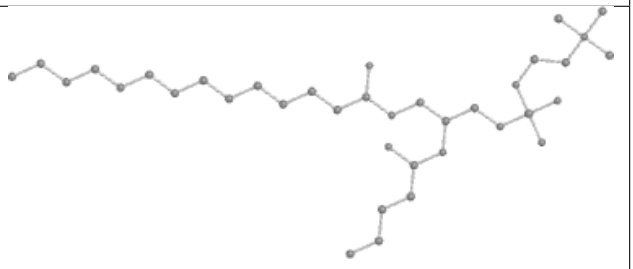
Bond lengths



Bond angles

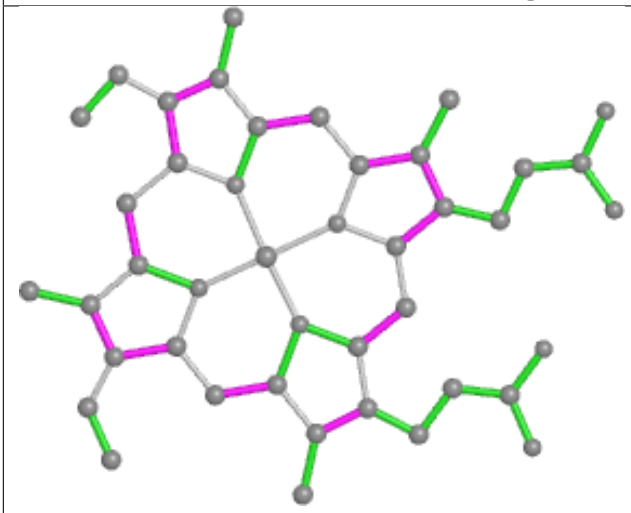


Torsions

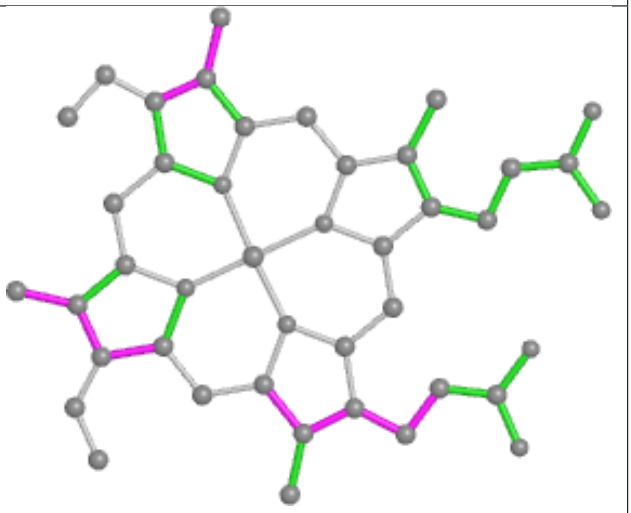


Rings

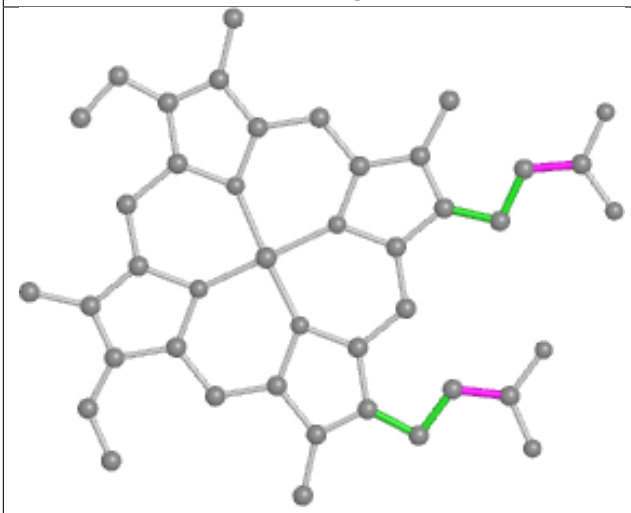
Ligand HEC D 501



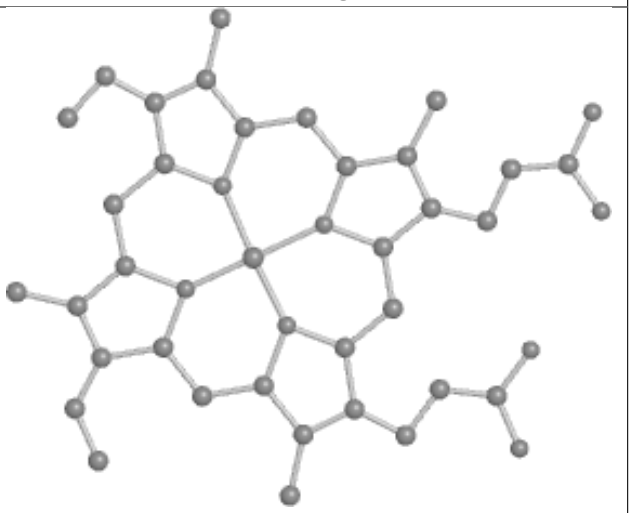
Bond lengths



Bond angles

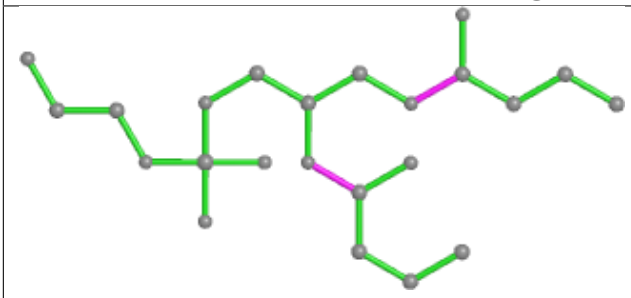


Torsions

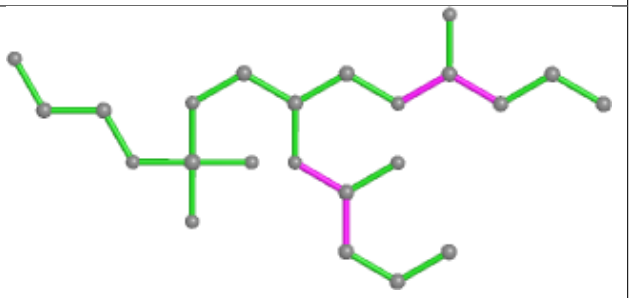


Rings

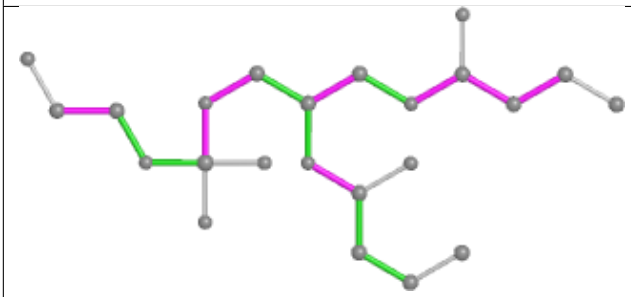
Ligand 6PE A 502



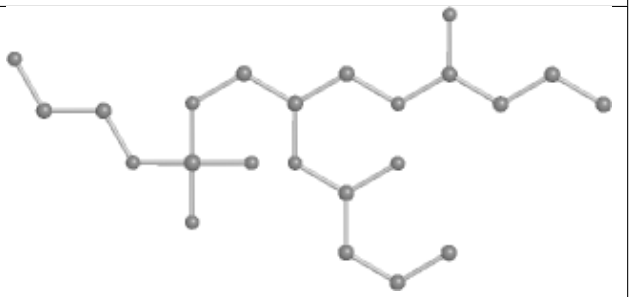
Bond lengths



Bond angles

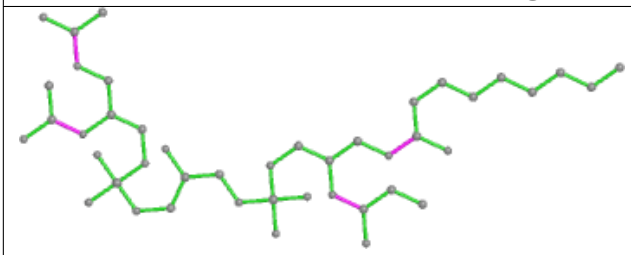


Torsions

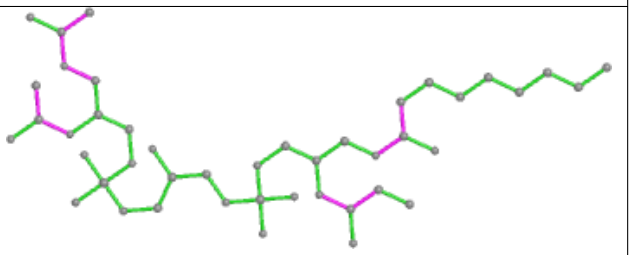


Rings

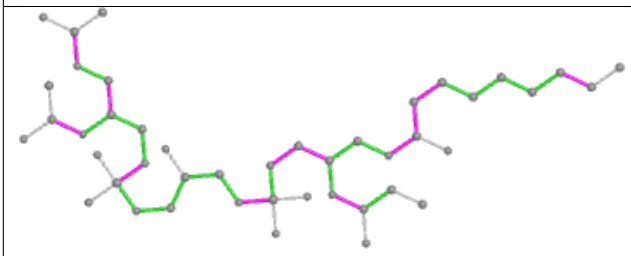
Ligand CDL C 408



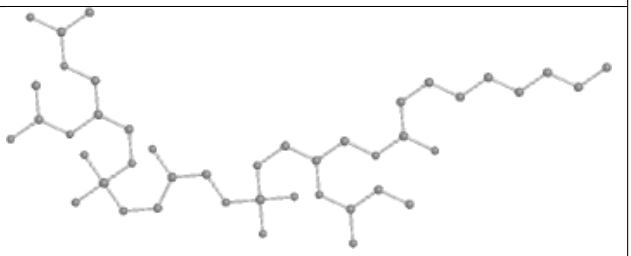
Bond lengths



Bond angles

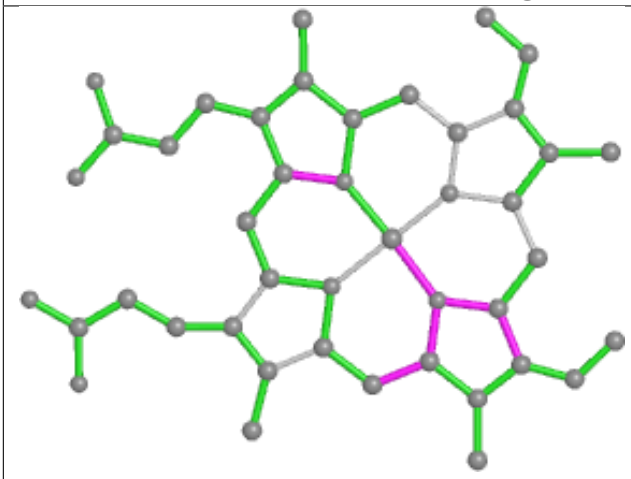


Torsions

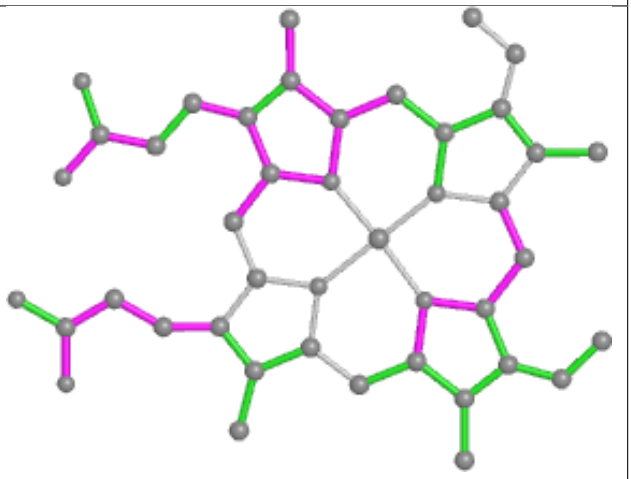


Rings

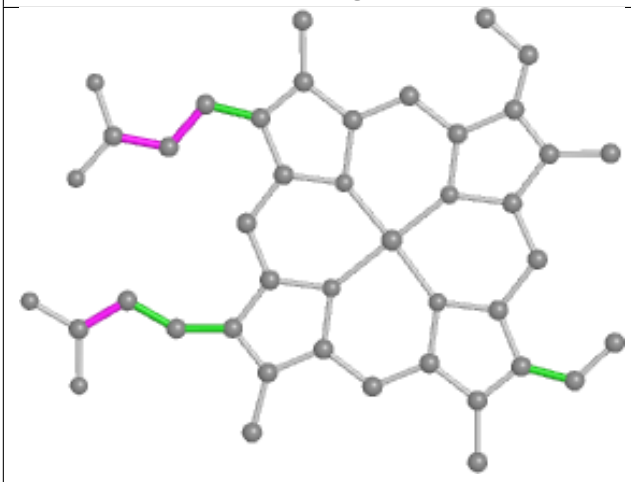
Ligand HEM C 402



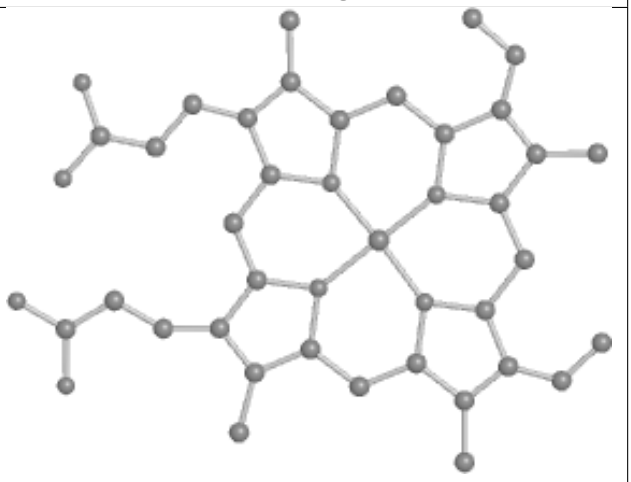
Bond lengths



Bond angles

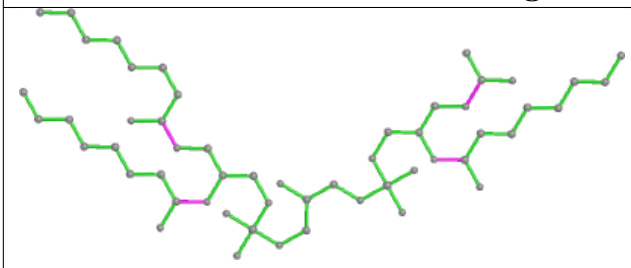


Torsions

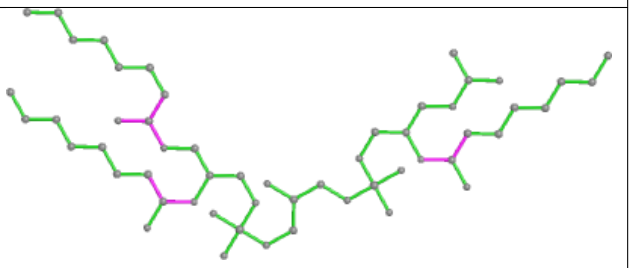


Rings

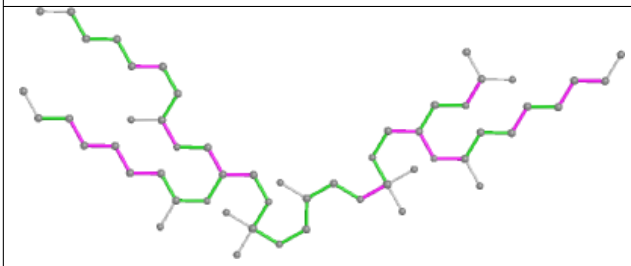
Ligand CDL D 503



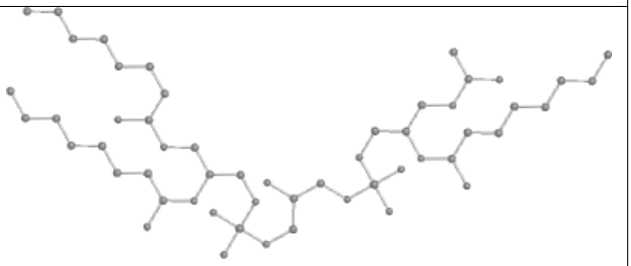
Bond lengths



Bond angles

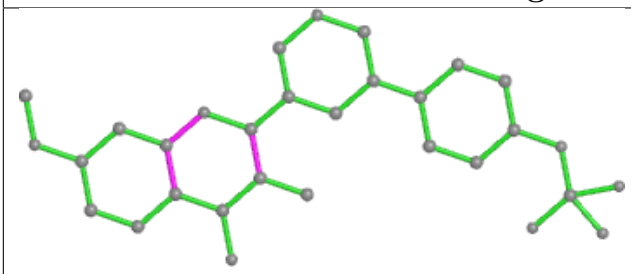


Torsions

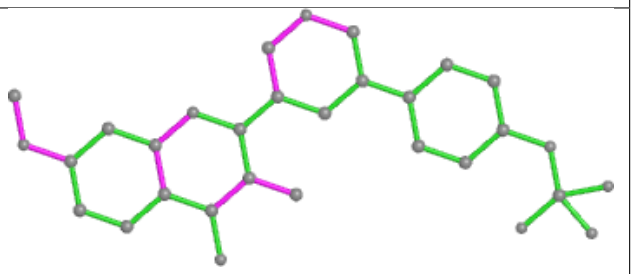


Rings

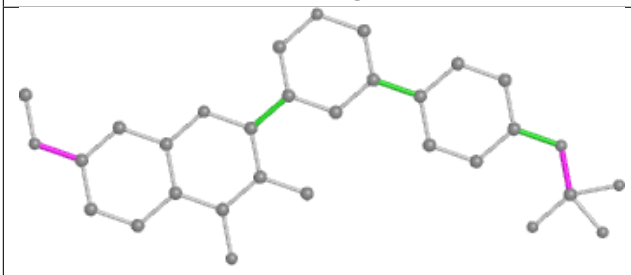
Ligand 9XE C 404



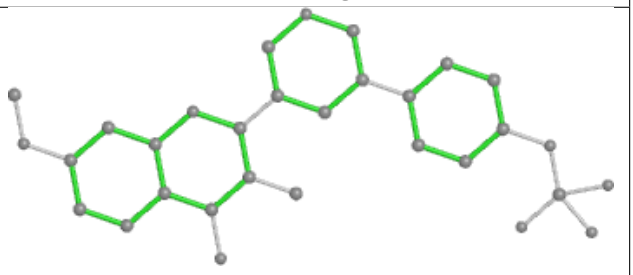
Bond lengths



Bond angles

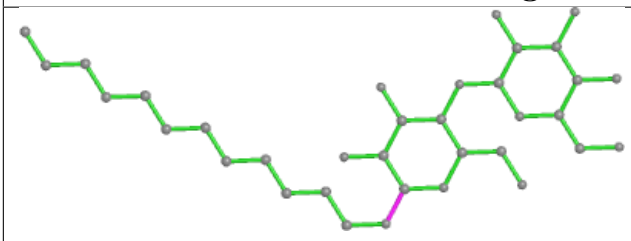


Torsions

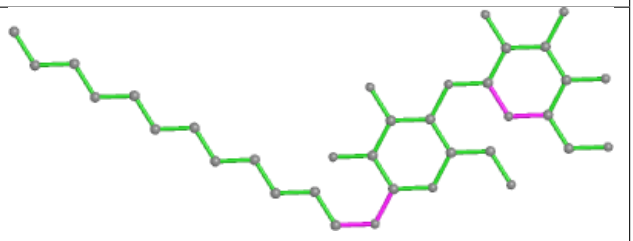


Rings

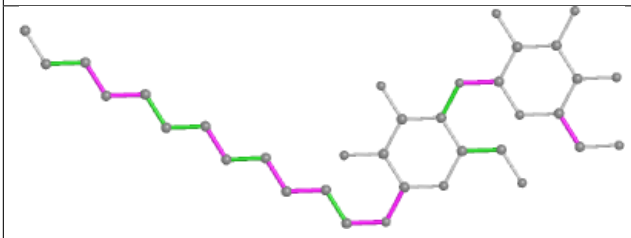
Ligand LMT C 405



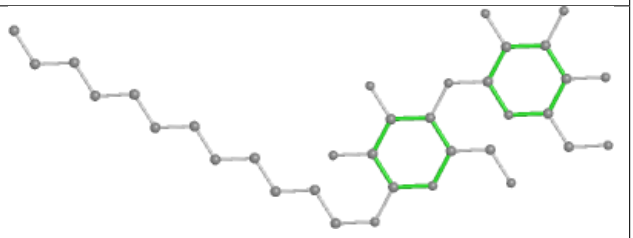
Bond lengths



Bond angles



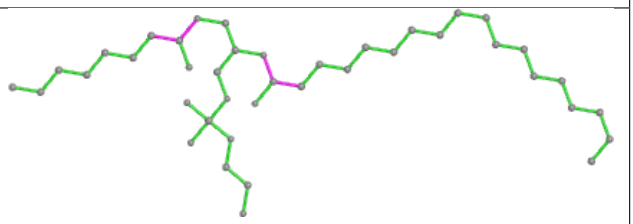
Torsions



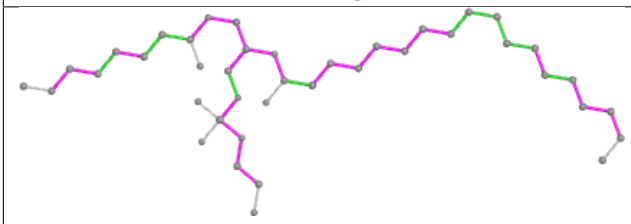
Rings

Ligand PEE E 204

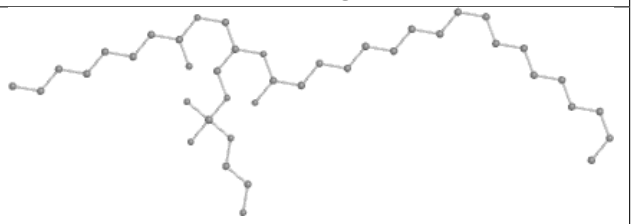
Bond lengths



Bond angles

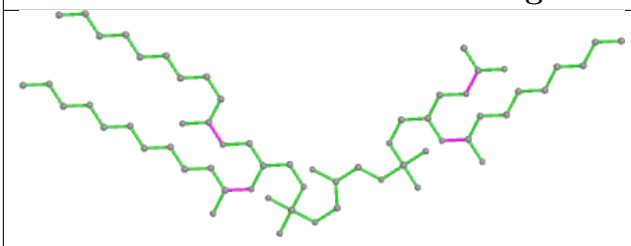


Torsions

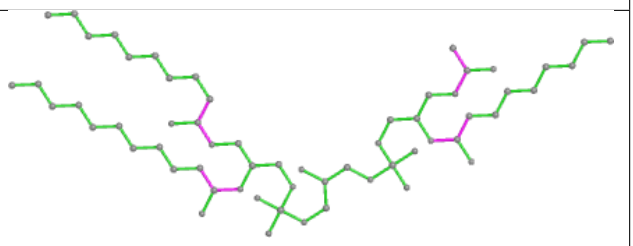


Rings

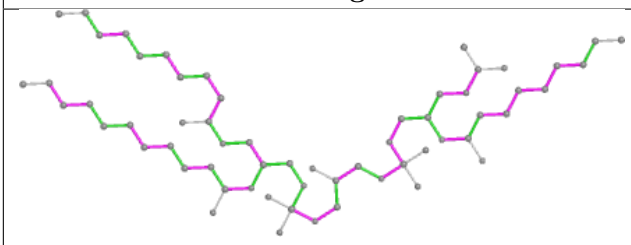
Ligand CDL E 205



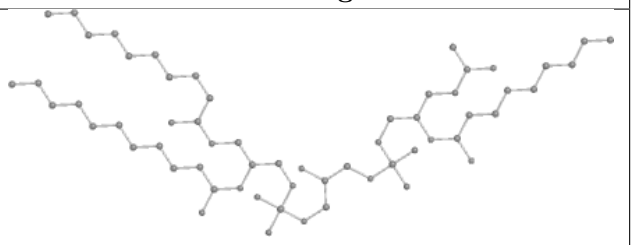
Bond lengths



Bond angles

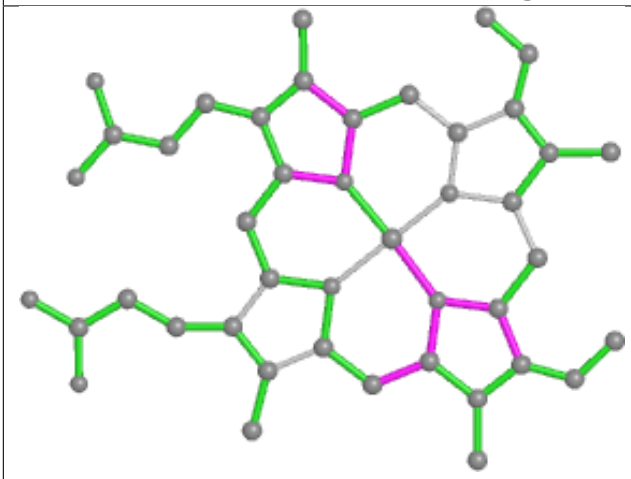


Torsions

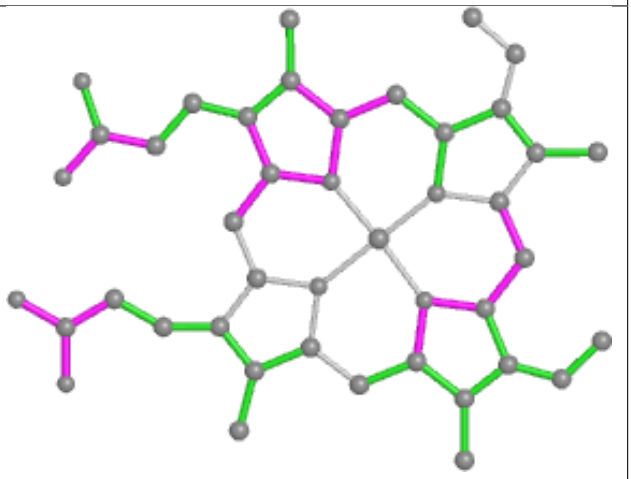


Rings

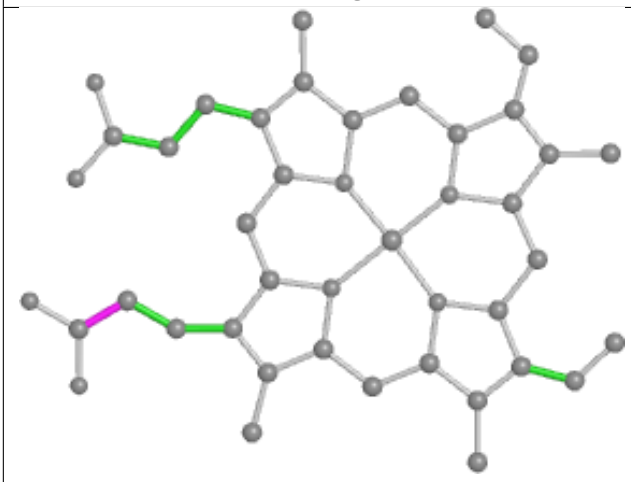
Ligand HEM C 403



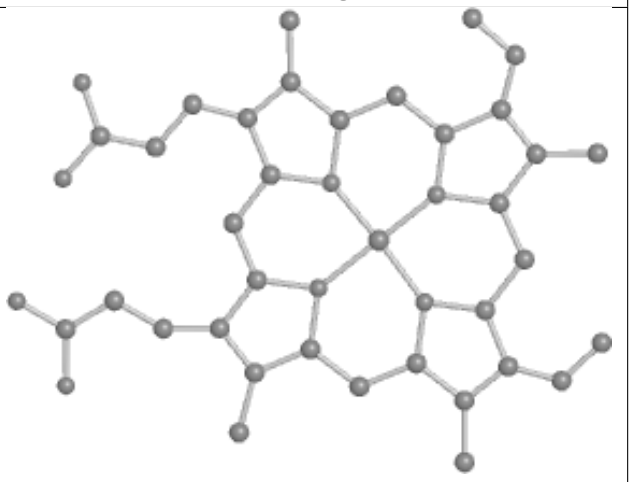
Bond lengths



Bond angles

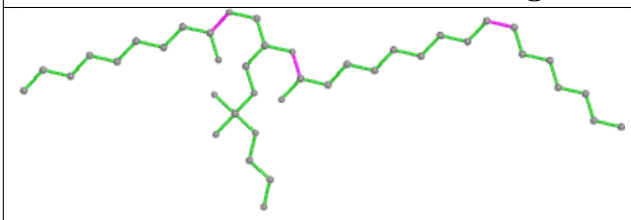


Torsions

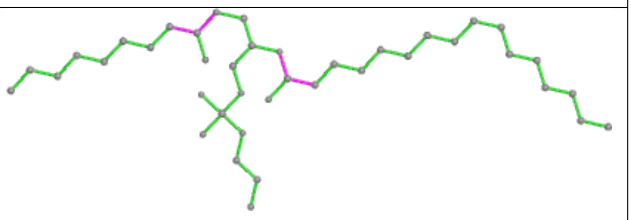


Rings

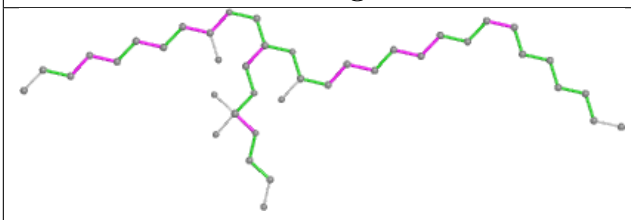
Ligand PEE C 409



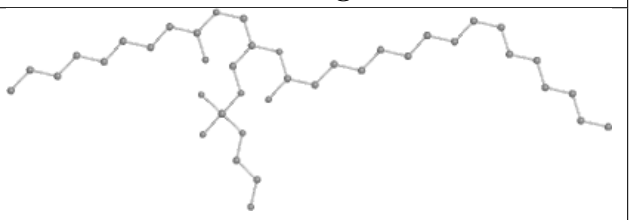
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	445/480 (92%)	-0.29	9 (2%) 65 44	62, 92, 126, 188	0
2	B	415/453 (91%)	-0.45	2 (0%) 91 81	68, 95, 122, 179	0
3	C	378/379 (99%)	-0.35	3 (0%) 86 72	63, 84, 123, 152	0
4	D	239/325 (73%)	-0.15	1 (0%) 92 84	76, 118, 144, 158	0
5	E	196/196 (100%)	0.16	12 (6%) 21 9	77, 141, 182, 194	0
6	F	99/111 (89%)	-0.19	2 (2%) 65 44	67, 85, 123, 155	0
7	G	74/82 (90%)	0.12	5 (6%) 17 7	64, 96, 142, 152	0
8	H	65/91 (71%)	0.26	6 (9%) 9 3	124, 143, 161, 168	0
9	I	46/47 (97%)	1.08	7 (15%) 2 1	98, 135, 152, 161	0
10	J	59/64 (92%)	-0.11	2 (3%) 45 24	88, 102, 138, 152	0
All	All	2016/2228 (90%)	-0.20	49 (2%) 59 37	62, 97, 155, 194	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	41	PRO	5.9
1	A	223	TYR	5.3
1	A	224	ASP	4.7
1	A	446	PHE	4.5
1	A	225	GLU	4.4
1	A	227	THR	4.0
1	A	222	THR	4.0
1	A	226	GLU	3.9
5	E	152	ASP	3.9
5	E	162	GLY	3.9
5	E	161	HIS	3.9
3	C	3	ASN	3.5
2	B	20	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
9	I	42	VAL	3.4
9	I	37	THR	3.4
6	F	13	LEU	3.3
5	E	115	SER	3.3
2	B	21	PRO	3.3
8	H	46	SER	3.3
5	E	159	PRO	3.2
5	E	164	HIS	3.2
9	I	40	SER	3.2
1	A	2	ALA	3.1
10	J	2	ALA	2.8
5	E	163	SER	2.8
5	E	173	LYS	2.7
1	A	228	VAL	2.6
6	F	16	ILE	2.6
9	I	48	SER	2.5
8	H	28	GLU	2.5
5	E	196	GLY	2.5
4	D	145	GLU	2.5
5	E	160	CYS	2.4
3	C	2	THR	2.4
8	H	13	LEU	2.4
7	G	28	HIS	2.4
5	E	116	GLN	2.4
5	E	174	GLY	2.4
9	I	38	SER	2.3
8	H	24	CYS	2.3
7	G	32	LYS	2.3
8	H	14	VAL	2.2
7	G	56	TYR	2.2
7	G	73	ASN	2.2
7	G	64	GLN	2.1
10	J	60	GLU	2.1
9	I	58	GLN	2.1
8	H	44	VAL	2.0
3	C	156	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

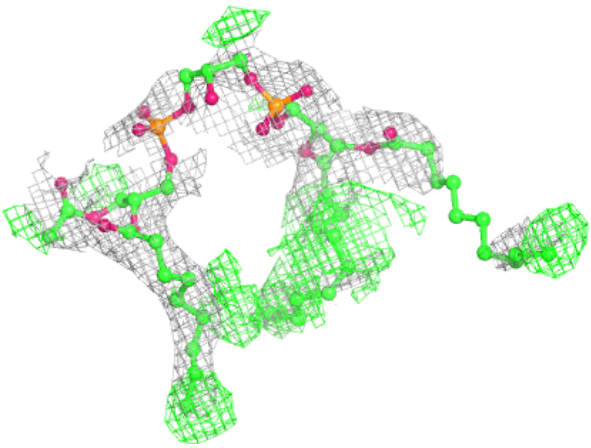
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

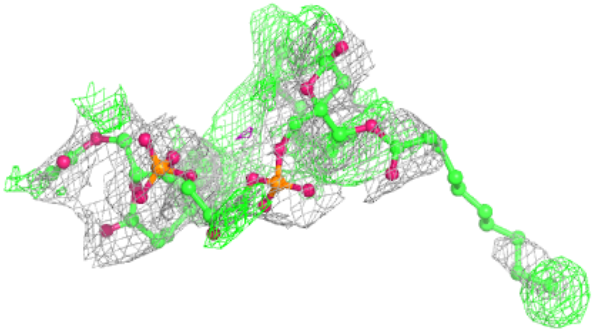
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	PO4	D	502	5/5	0.59	0.35	168,169,170,170	0
11	PG4	A	501	13/13	0.62	0.29	114,130,142,143	0
19	PO4	E	203	5/5	0.67	0.28	156,156,161,161	0
13	CDL	E	205	60/100	0.69	0.36	127,151,185,192	0
13	CDL	C	401	34/100	0.75	0.37	144,157,168,169	0
21	PX4	E	202	37/46	0.75	0.38	112,129,138,139	0
19	PO4	G	102	5/5	0.76	0.29	153,154,156,161	0
11	PG4	C	407	13/13	0.77	0.32	110,116,119,120	0
19	PO4	G	103	5/5	0.80	0.21	132,134,137,137	0
16	LMT	C	405	35/35	0.83	0.36	151,166,170,171	0
13	CDL	D	503	54/100	0.84	0.26	94,117,141,142	0
12	6PE	A	502	23/27	0.85	0.28	96,124,142,145	0
11	PG4	C	406	13/13	0.85	0.28	98,104,115,115	0
19	PO4	F	501	5/5	0.89	0.26	124,129,132,132	0
17	PEE	E	204	41/51	0.89	0.31	85,103,111,119	0
20	FES	E	201	4/4	0.90	0.08	217,217,217,218	0
13	CDL	C	408	44/100	0.92	0.23	84,102,125,127	0
19	PO4	G	101	5/5	0.92	0.12	106,107,113,113	0
17	PEE	C	409	40/51	0.93	0.27	79,91,104,108	0
18	HEC	D	501	43/43	0.95	0.23	111,114,120,123	0
15	9XE	C	404	31/31	0.97	0.16	75,79,90,92	0
14	HEM	C	402	43/43	0.98	0.20	68,71,75,79	0
14	HEM	C	403	43/43	0.99	0.18	62,65,67,68	0

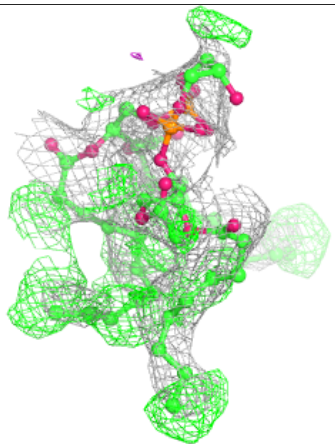
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

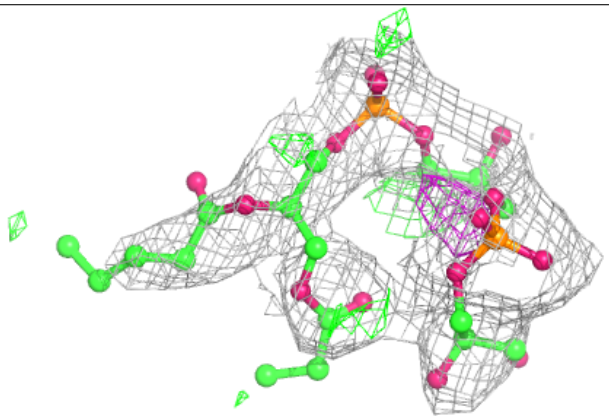


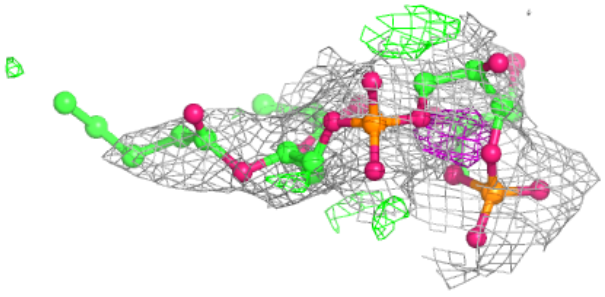


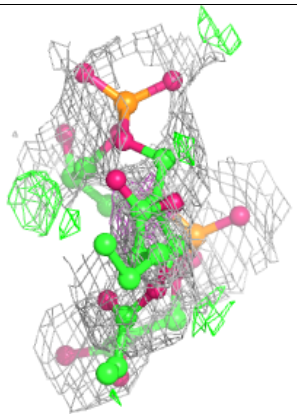


Electron density around CDL C 401:

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

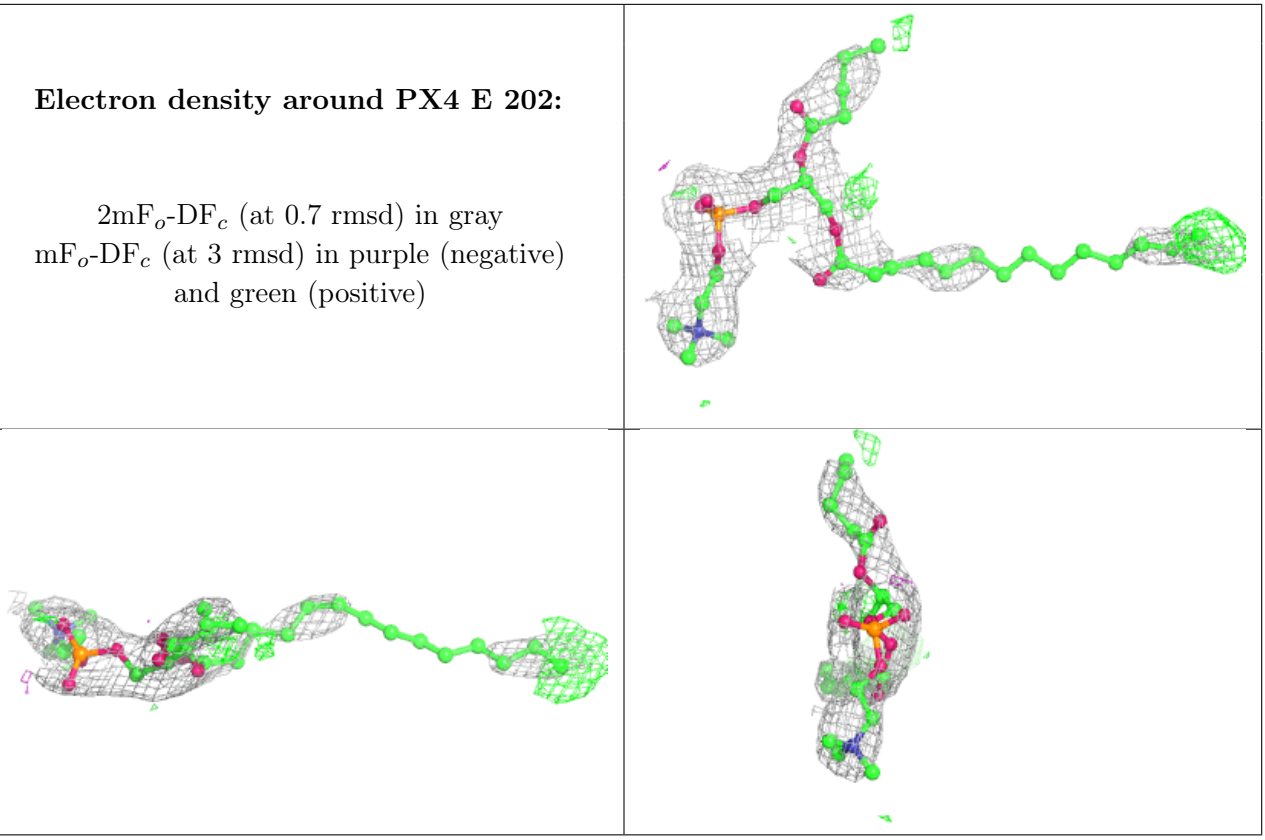






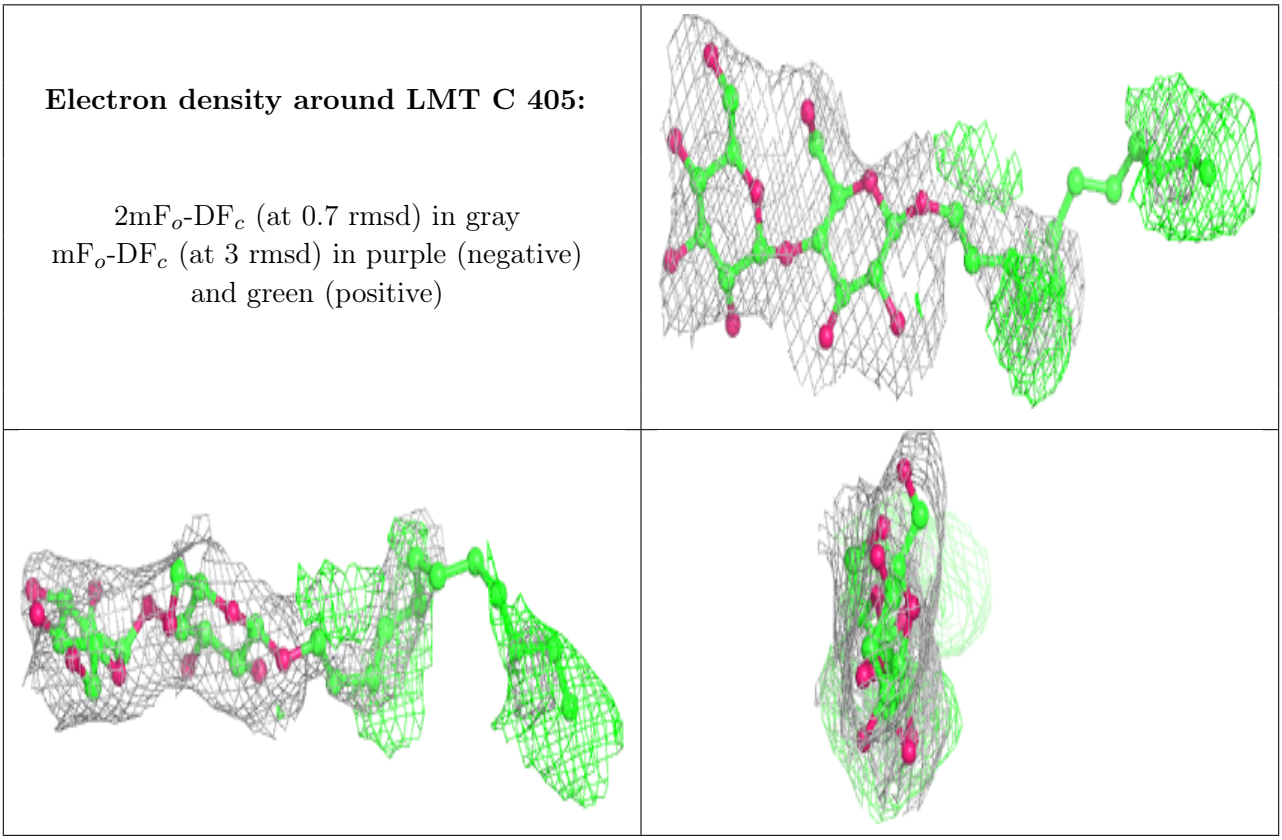
Electron density around PX4 E 202:

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



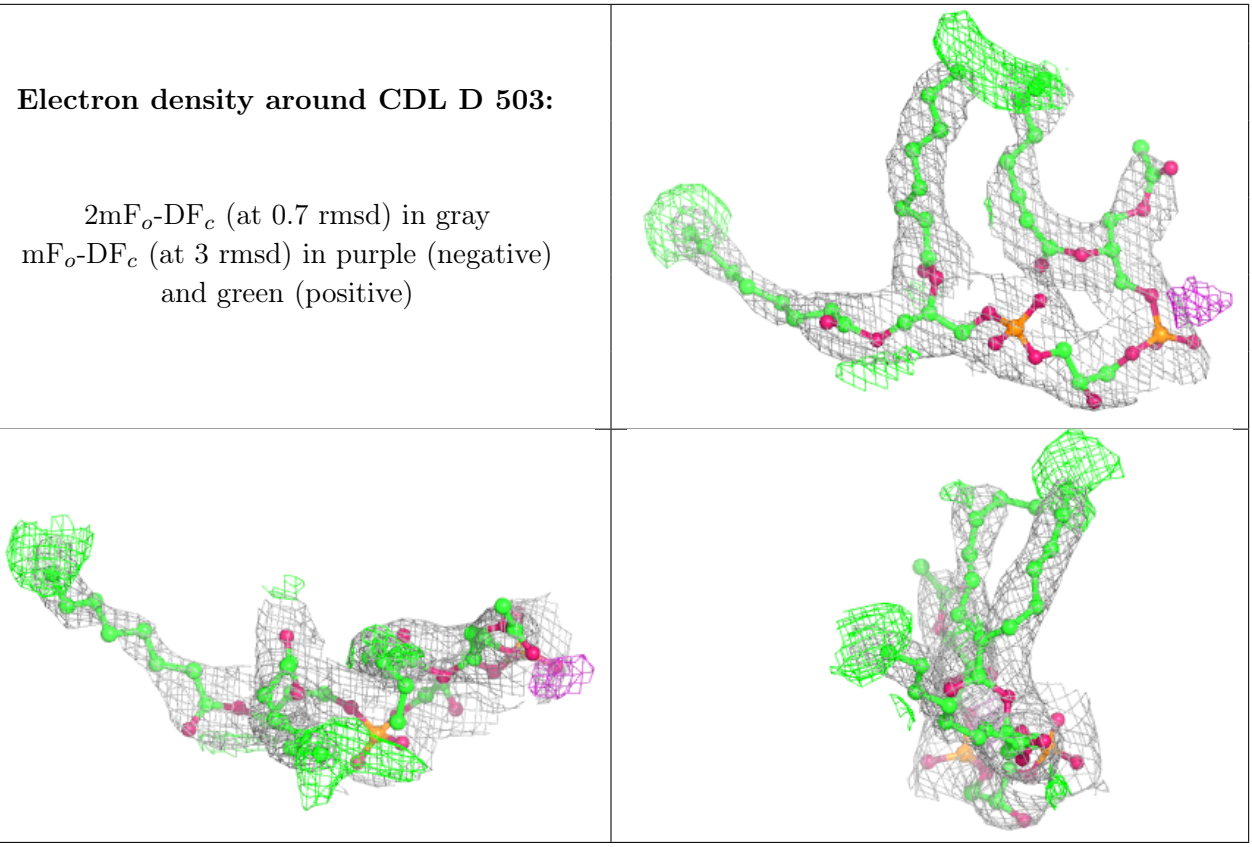
Electron density around LMT C 405:

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



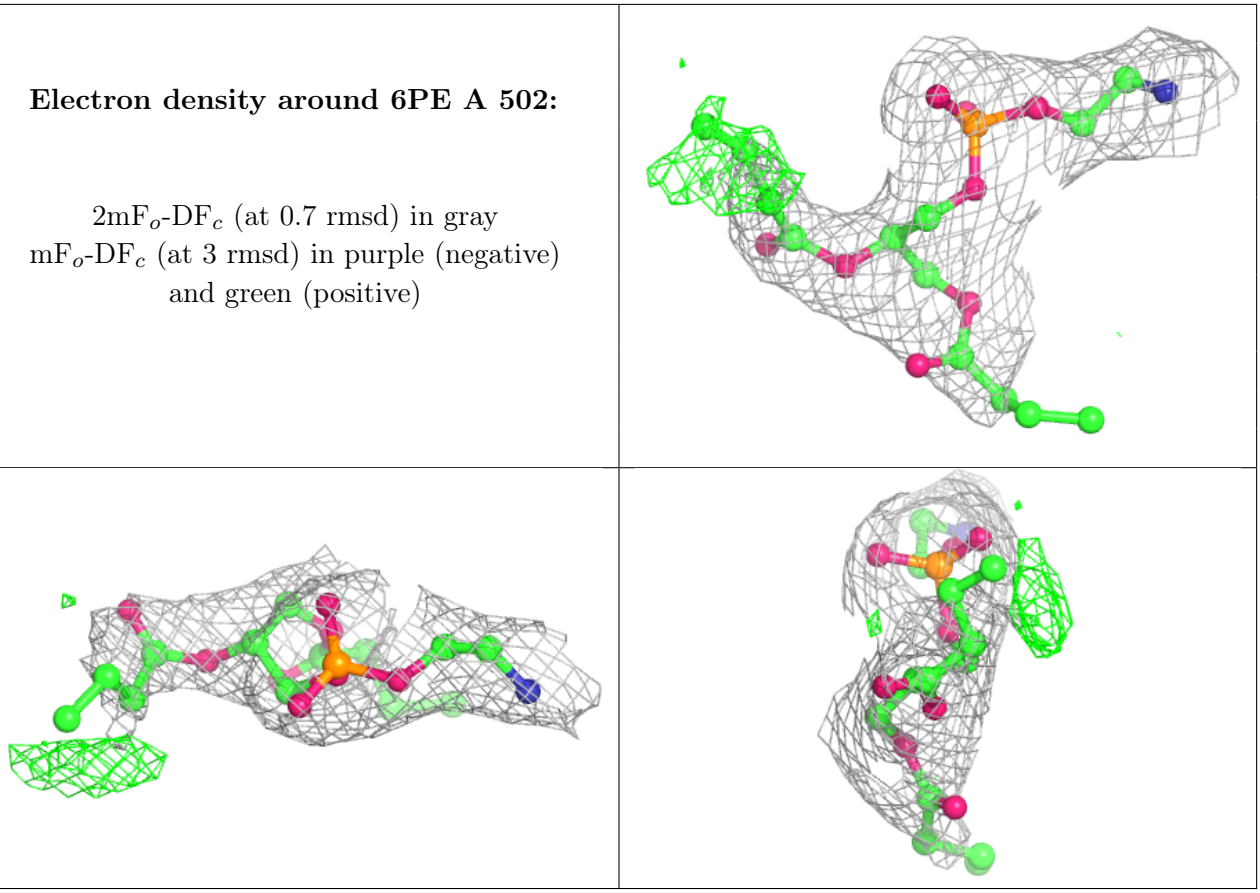
Electron density around CDL D 503:

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



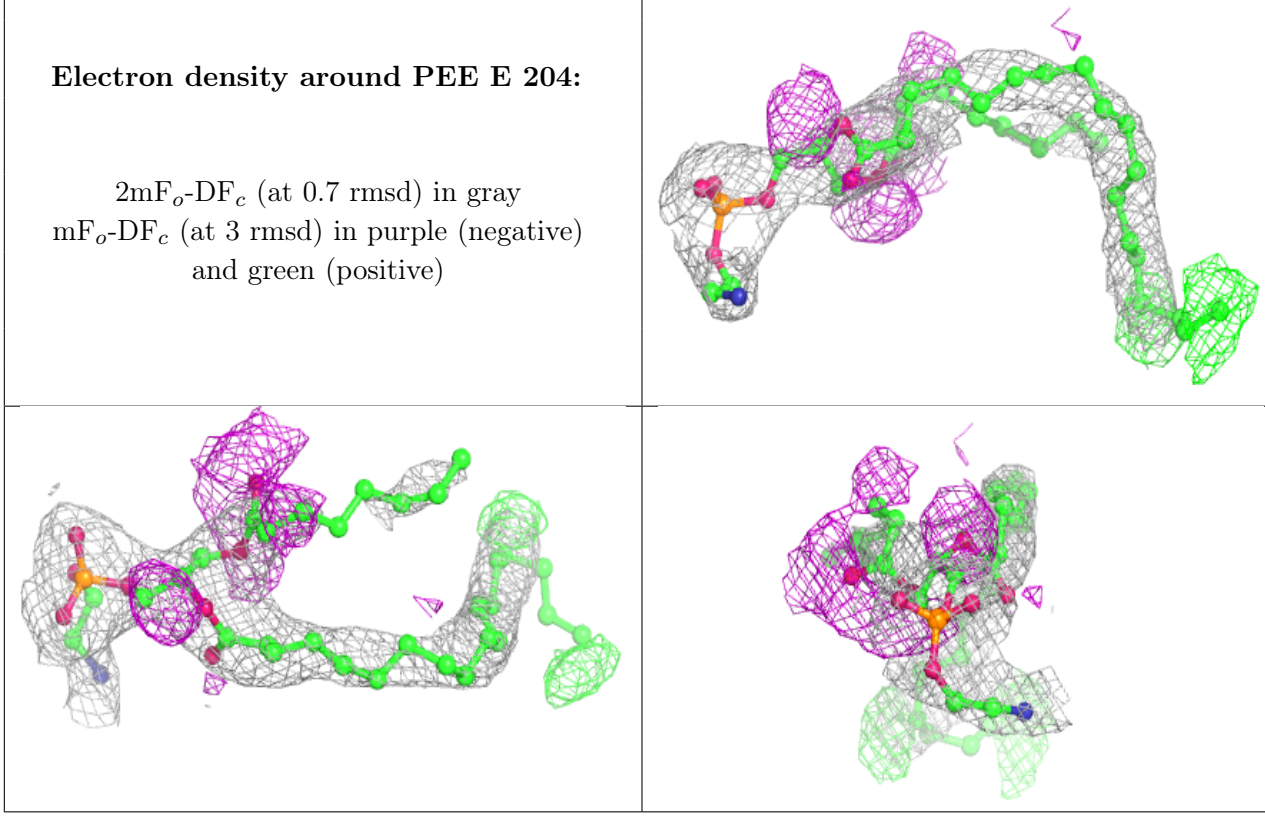
Electron density around 6PE A 502:

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



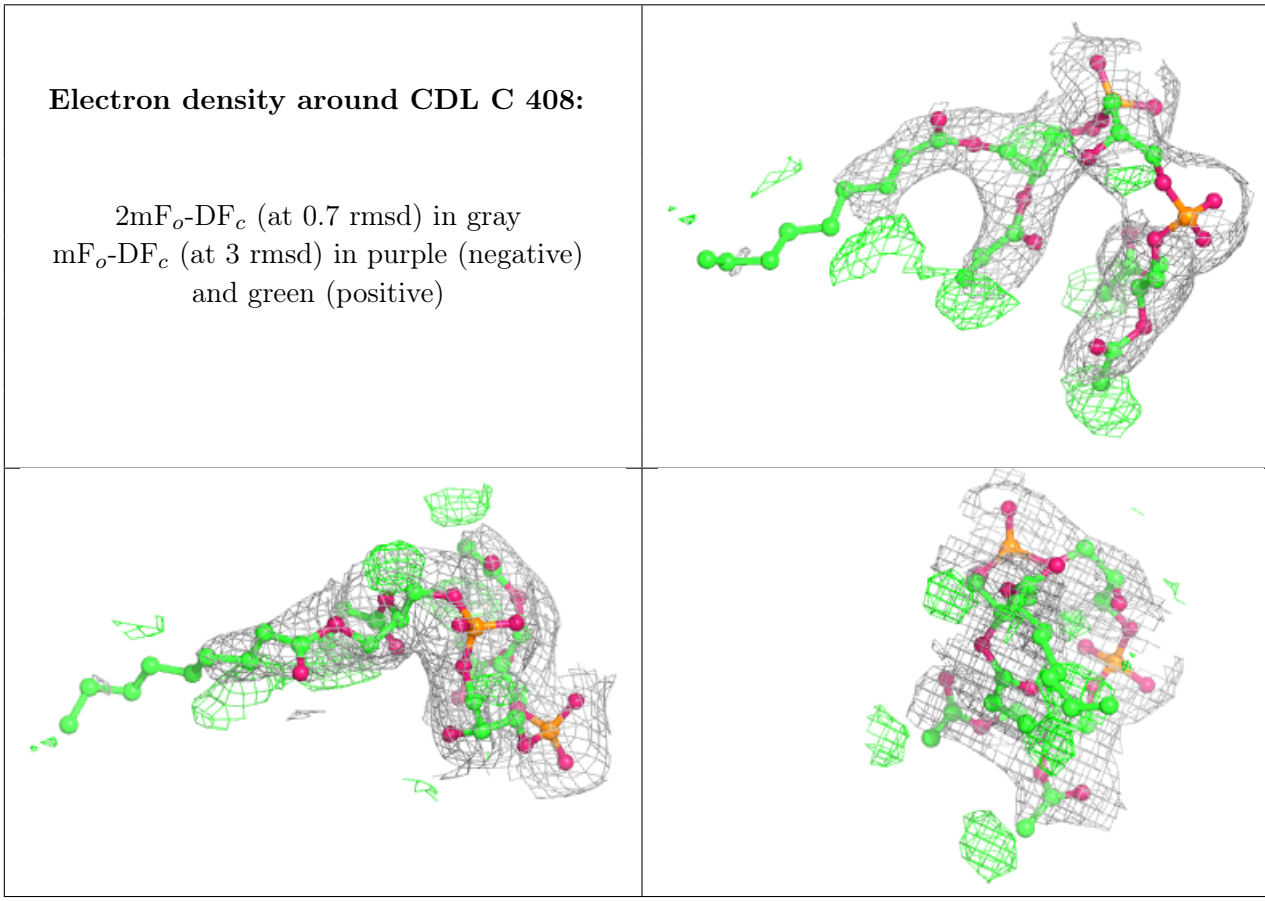
Electron density around PEE E 204:

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



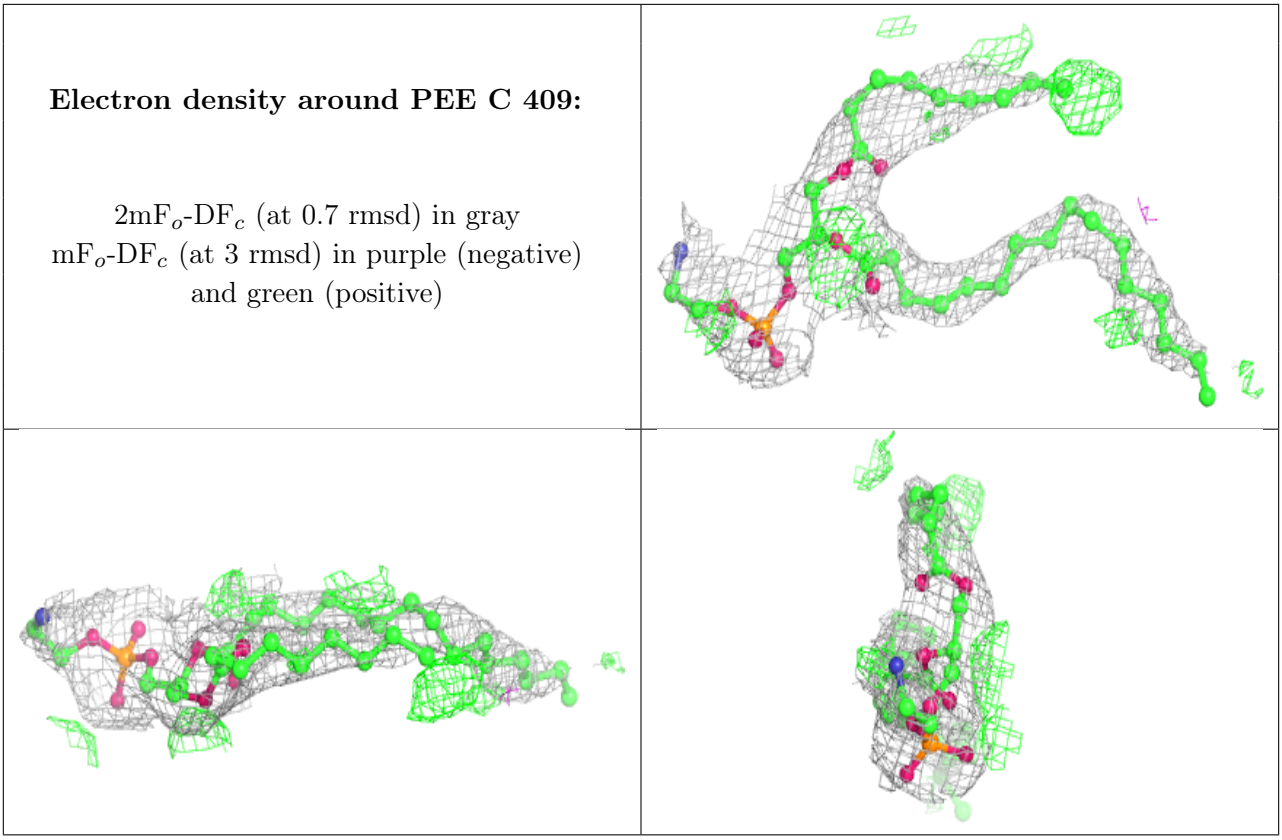
Electron density around CDL C 408:

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



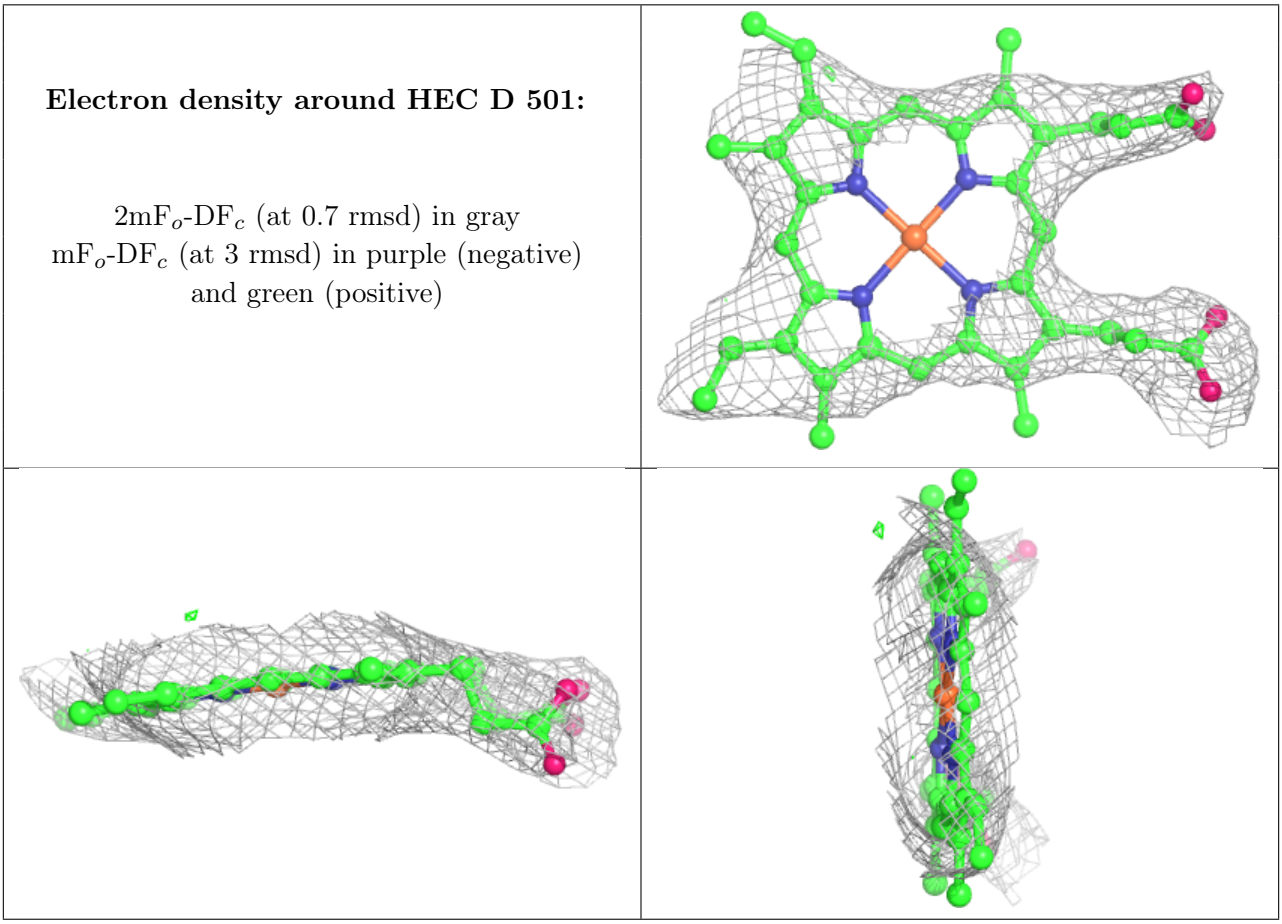
Electron density around PEE C 409:

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



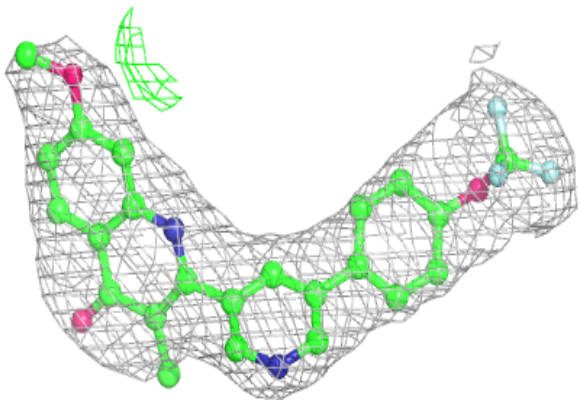
Electron density around HEC D 501:

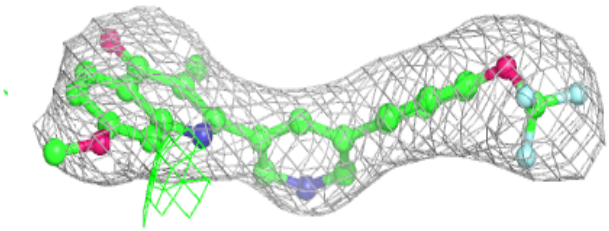
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

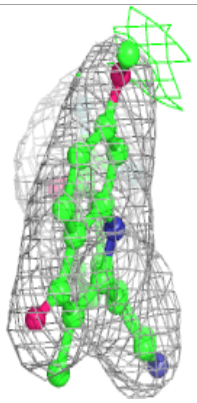


Electron density around 9XE C 404:

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

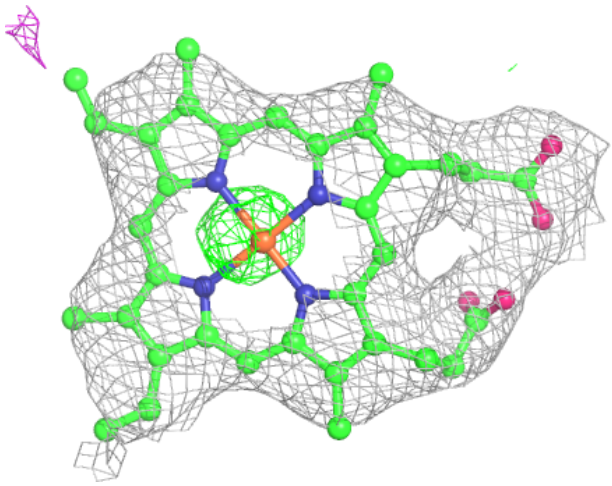


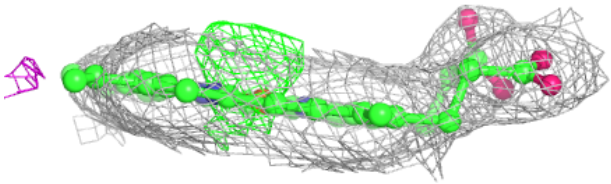


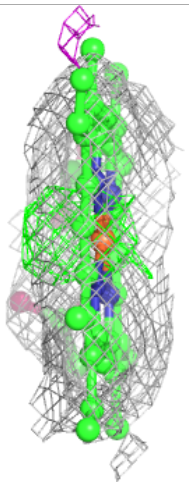


Electron density around HEM C 402:

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

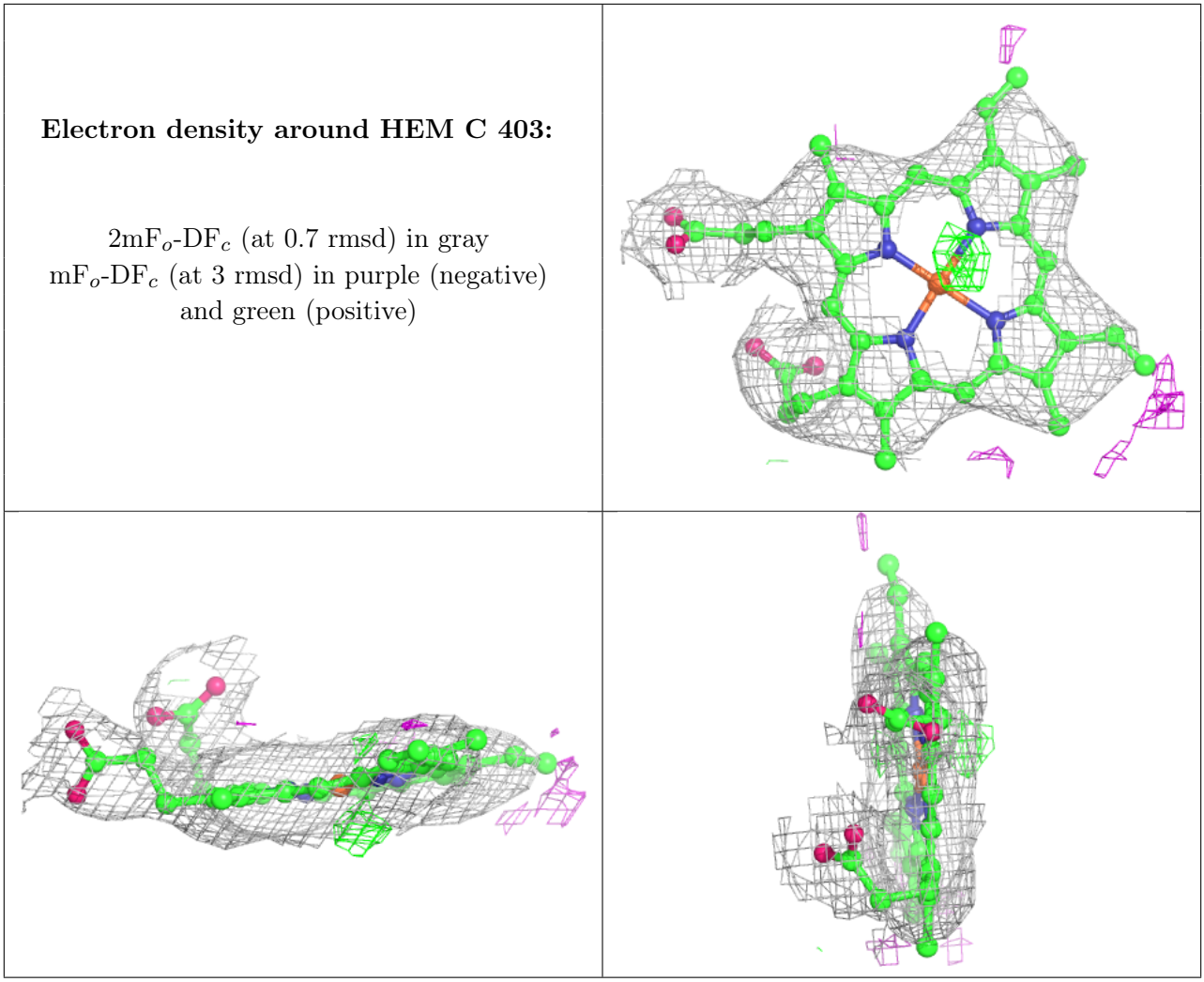






Electron density around HEM C 403:

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



6.5 Other polymers

There are no such residues in this entry.