wwPDB X-ray Structure Validation Summary Report (i)

Aug 18, 2026 – 01:46 pm BST

PDB ID	:	5OKD / pdb_00005okd
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

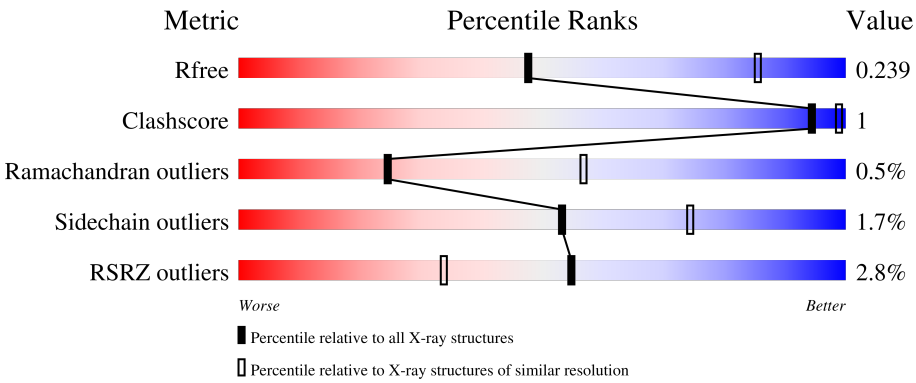
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

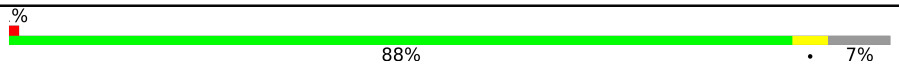
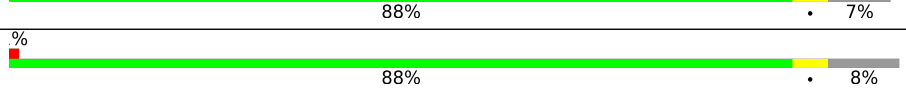
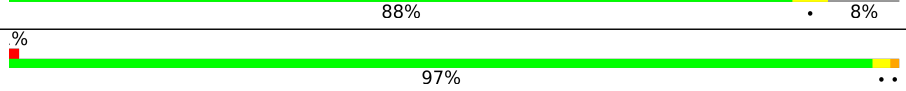
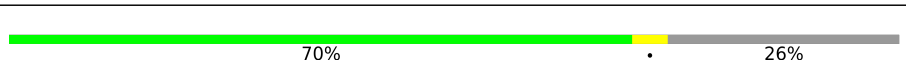
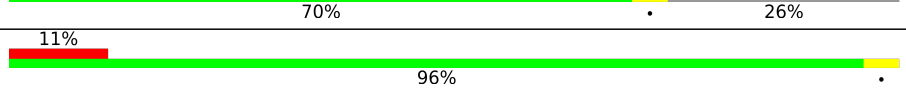
The reported resolution of this entry is 3.10 Å.

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	B	453	
3	C	379	
4	D	325	
5	E	196	

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Mol	Chain	Length	Quality of chain
6	F	111	85% • • 11%
7	G	82	4% 85% 5% 10%
8	H	91	2% 69% • 29%
9	I	47	40% 85% 13% •
10	J	64	2% 84% 8% 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	-	-	-
18	HEC	D	501	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
			Total	C	N	O	S			
1	A	445	3449	2157	608	664	20	0	0	0

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
			Total	C	N	O	S			
2	B	415	3116	1957	553	599	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	378	2996	2007	471	500	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	239	1884	1205	321	343	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1512	951	263	290	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	99	859	545	156	156	2	0	0	0

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
			Total	C	N	O	S			
7	G	74	620	406	116	97	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	65	525	318	95	107	5	0	0	0

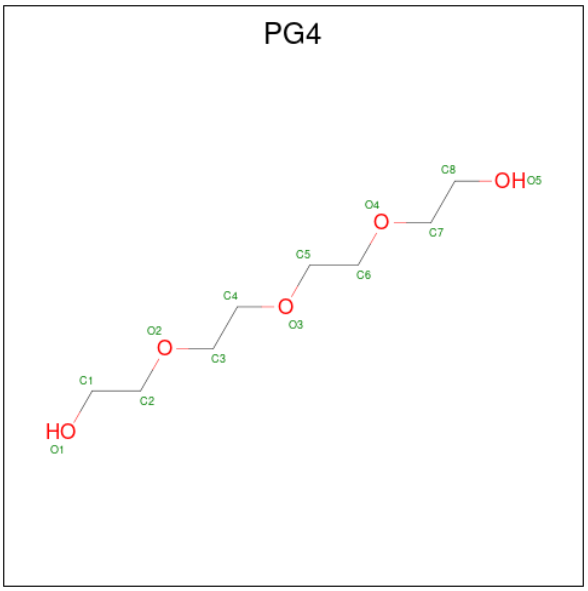
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

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

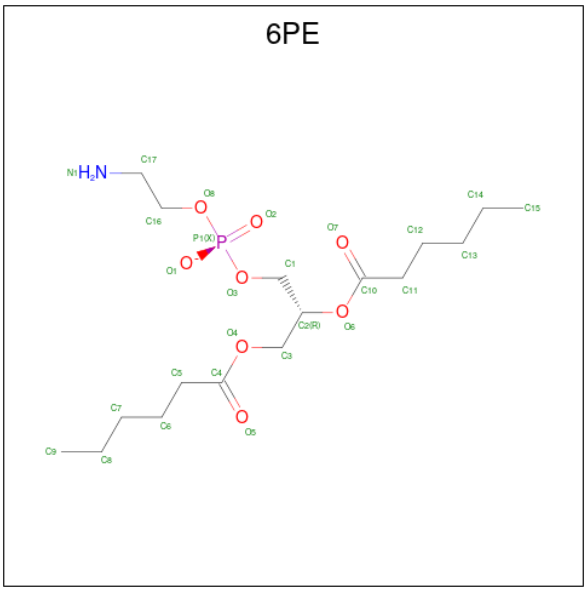
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	59	487	320	84	83	0	0	0

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



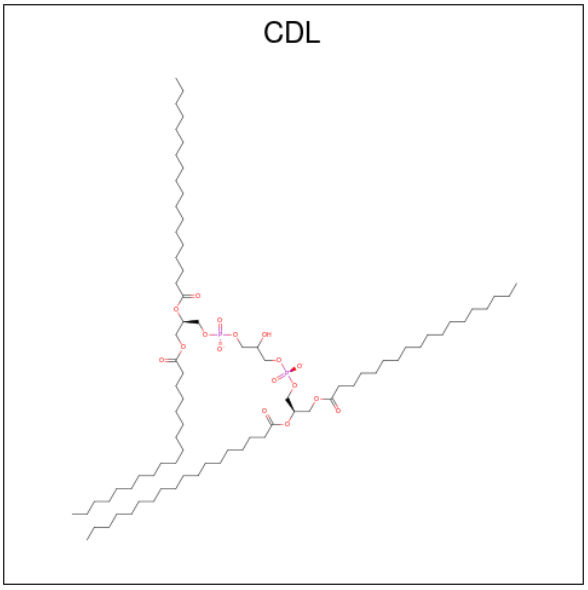
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0

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



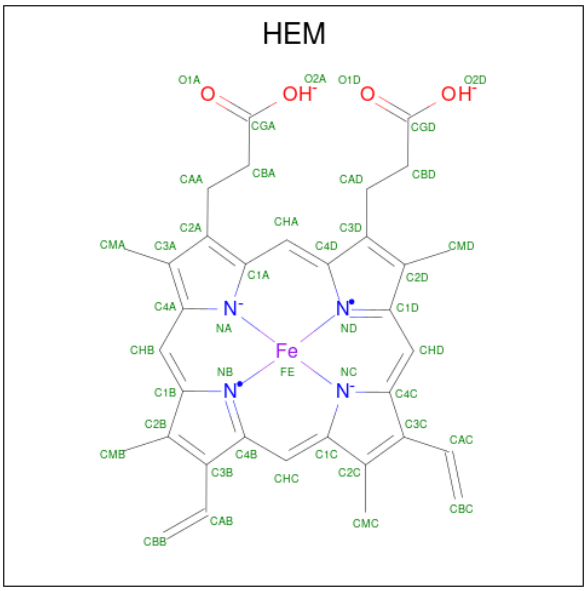
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	A	1	23	13	1	8	1	0	0

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



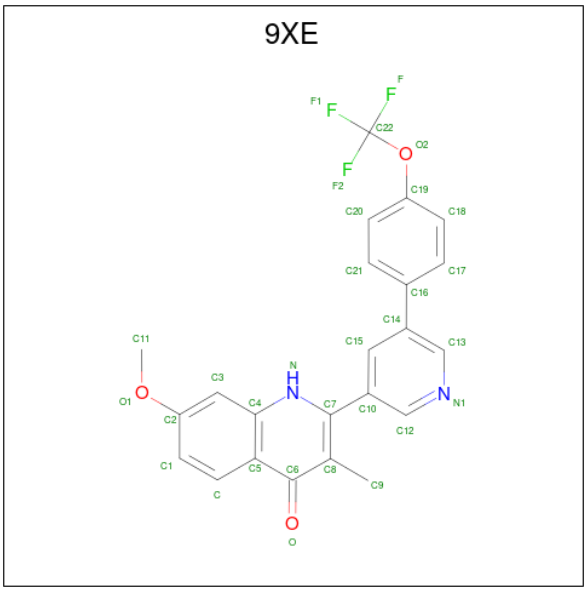
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
13	C	1	34	17	15	2	0	0
			Total	C	O	P		
13	C	1	44	25	17	2	0	0
			Total	C	O	P		
13	D	1	54	35	17	2	0	0
			Total	C	O	P		
13	E	1	60	41	17	2	0	0

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



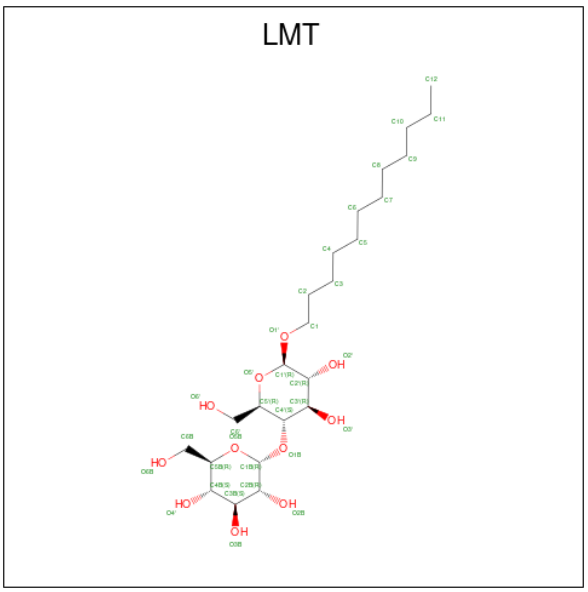
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
14	C	1	43	34	1	4	4	0	0

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



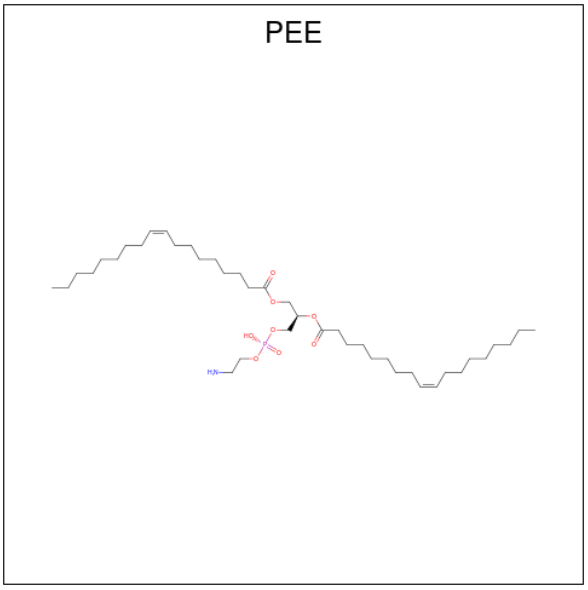
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
15	C	1	31	23	3	2	3	0	0

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



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

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



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

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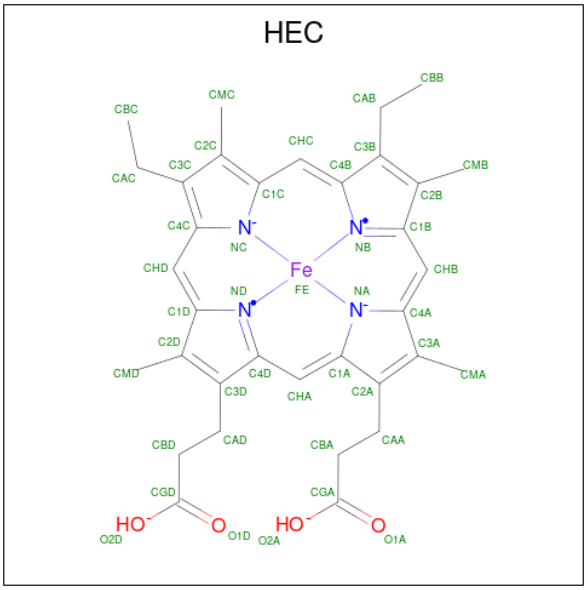
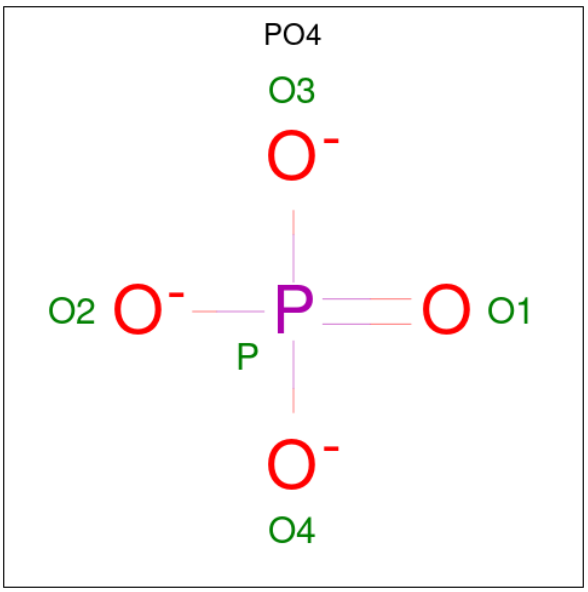
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
17	E	1	41	31	1	8	1	0	0

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



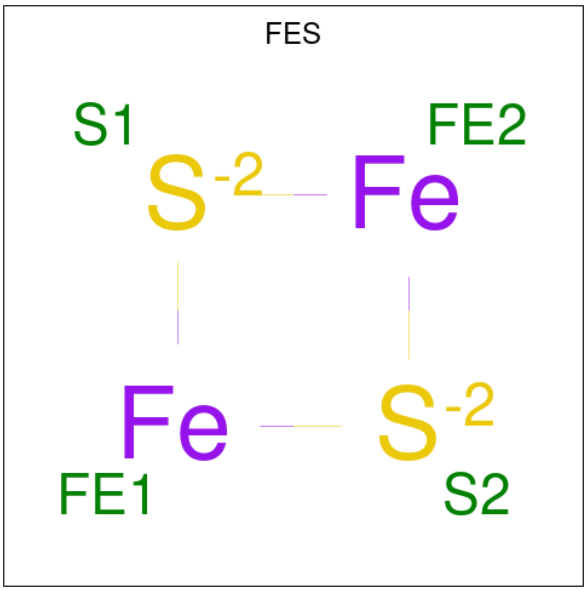
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
18	D	1	43	34	1	4	4	0	0

- Molecule 19 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



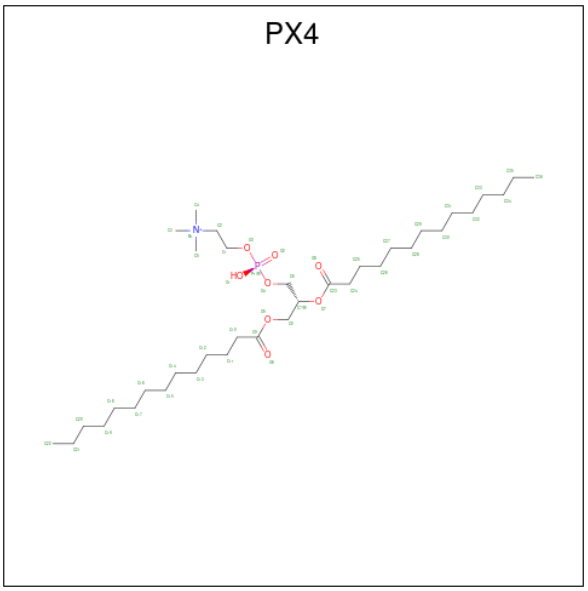
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
19	D	1	5	4	1	0	0
19	E	1	5	4	1	0	0
19	F	1	5	4	1	0	0
19	G	1	5	4	1	0	0
19	G	1	5	4	1	0	0
19	G	1	5	4	1	0	0

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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



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

- Molecule 22 is water.

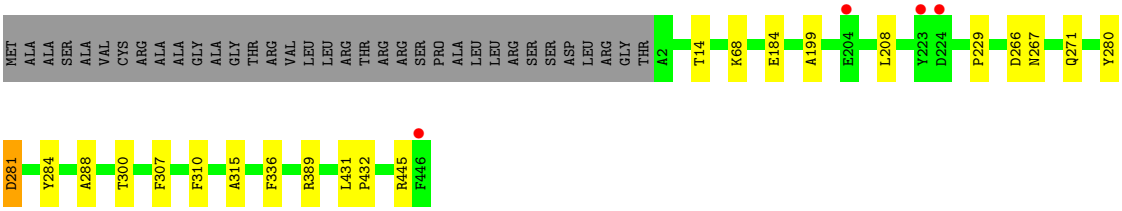
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
22	A	15	15	15	0	0
22	B	12	12	12	0	0
22	C	27	27	27	0	0
22	D	5	5	5	0	0
22	E	6	6	6	0	0
22	F	8	8	8	0	0
22	G	5	5	5	0	0
22	H	1	1	1	0	0
22	J	3	3	3	0	0

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.

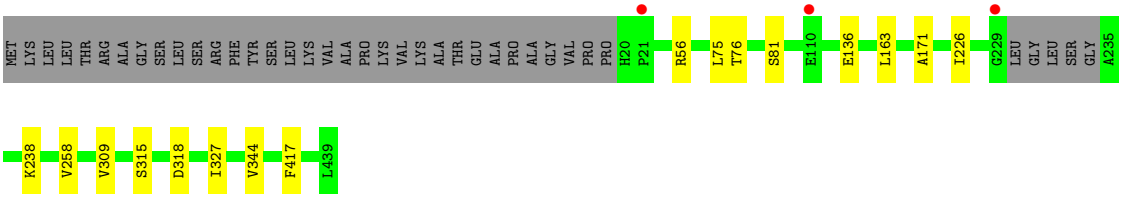
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



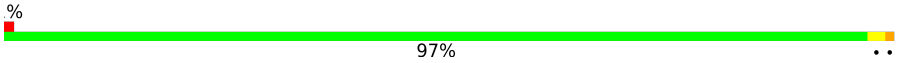
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

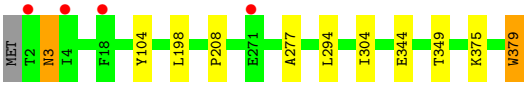
Chain B:



• Molecule 3: Cytochrome b

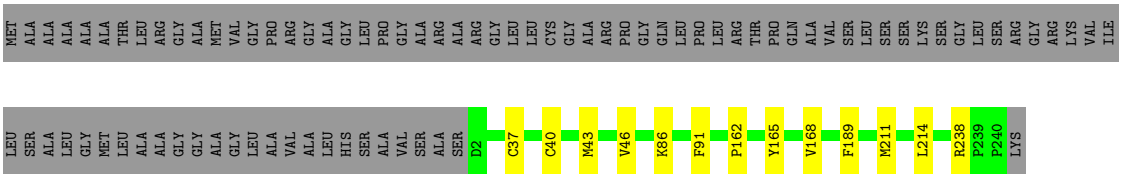
Chain C:





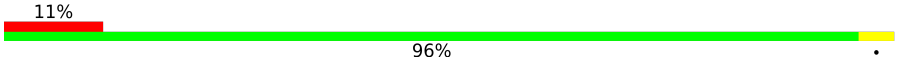
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



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

Chain E:

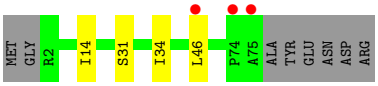


• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:

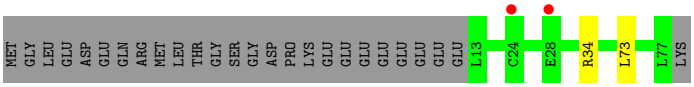
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:



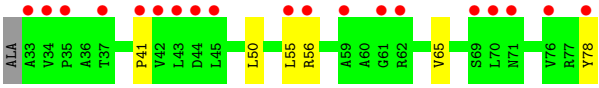
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

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 31.76 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.76-3.10) 99.0 (31.76-3.10)	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 (4.99%)	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)	0.29 , 45.8	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 6PE, HEC, FES, PEE, LMT, 9XE, CDL, HEM, PO4, PX4

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	0.54	0/3522	0.81	1/4781 (0.0%)
2	B	0.54	0/3173	0.84	0/4304
3	C	0.57	1/3092 (0.0%)	0.86	1/4231 (0.0%)
4	D	0.57	0/1943	0.81	0/2642
5	E	0.59	0/1545	0.79	0/2089
6	F	0.52	0/878	0.84	0/1181
7	G	0.59	1/641 (0.2%)	0.84	0/868
8	H	0.59	0/530	0.83	0/714
9	I	0.75	0/342	0.91	0/464
10	J	0.57	0/500	0.86	0/675
All	All	0.56	2/16166 (0.0%)	0.83	2/21949 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	304	ILE	CA-CB	5.15	1.56	1.54
7	G	34	ILE	CA-CB	5.08	1.56	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	304	ILE	CB-CA-C	-5.30	108.66	113.70
1	A	310	PHE	N-CA-C	5.21	121.89	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3449	0	3346	9	0
2	B	3116	0	3089	8	0
3	C	2996	0	3058	6	0
4	D	1884	0	1814	15	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	4	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	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16469	0	16155	41	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.

The worst 5 of 41 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
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
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.89	0.55

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%)	14 44
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%)	30 61
5	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	5 25
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%)	5 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	57/64 (89%)	56 (98%)	1 (2%)	0	100	100
All	All	1994/2228 (90%)	1915 (96%)	69 (4%)	10 (0%)	24	57

5 of 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

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%)	366 (99%)	3 (1%)	73	81
2	B	325/355 (92%)	322 (99%)	3 (1%)	70	80
3	C	325/327 (99%)	320 (98%)	5 (2%)	57	75
4	D	200/257 (78%)	198 (99%)	2 (1%)	68	79
5	E	167/168 (99%)	165 (99%)	2 (1%)	63	78
6	F	88/99 (89%)	84 (96%)	4 (4%)	24	56
7	G	65/72 (90%)	63 (97%)	2 (3%)	35	64
8	H	61/85 (72%)	59 (97%)	2 (3%)	33	63
9	I	38/38 (100%)	35 (92%)	3 (8%)	11	37
10	J	49/54 (91%)	47 (96%)	2 (4%)	27	59
All	All	1687/1850 (91%)	1659 (98%)	28 (2%)	53	74

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	61	SER

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Mol	Chain	Res	Type
10	J	17	THR
6	F	82	LYS
9	I	65	VAL
6	F	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	6	HIS
4	D	225	HIS
4	D	166	ASN
5	E	122	HIS
1	A	271	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	408	-	43,43,99	1.50	4 (9%)	49,55,111	1.30	5 (10%)
15	9XE	C	404	-	34,34,34	1.62	3 (8%)	47,50,50	1.17	5 (10%)
17	PEE	C	409	-	39,39,50	1.19	3 (7%)	42,44,55	0.91	2 (4%)
14	HEM	C	402	3	50,50,50	1.56	6 (12%)	66,82,82	1.55	12 (18%)
19	PO4	F	501	-	4,4,4	0.89	0	6,6,6	0.45	0
19	PO4	E	203	-	4,4,4	0.92	0	6,6,6	0.70	0
12	6PE	A	502	-	22,22,26	1.46	2 (9%)	25,27,31	1.23	2 (8%)
16	LMT	C	405	-	36,36,36	0.65	1 (2%)	47,47,47	1.06	2 (4%)
13	CDL	E	205	-	59,59,99	1.18	4 (6%)	65,71,111	1.06	4 (6%)
19	PO4	G	103	-	4,4,4	0.89	0	6,6,6	0.45	0
19	PO4	G	101	-	4,4,4	0.90	0	6,6,6	0.26	0
20	FES	E	201	-	0,4,4	-	-	-		
11	PG4	C	407	-	12,12,12	0.55	0	11,11,11	0.40	0
11	PG4	C	406	-	12,12,12	0.56	0	11,11,11	0.52	0
21	PX4	E	202	-	36,36,45	1.25	2 (5%)	42,44,53	1.03	2 (4%)
19	PO4	D	502	-	4,4,4	0.86	0	6,6,6	0.50	0
17	PEE	E	204	-	40,40,50	1.20	3 (7%)	43,45,55	1.06	2 (4%)
19	PO4	G	102	-	4,4,4	0.92	0	6,6,6	0.43	0
14	HEM	C	403	3	50,50,50	1.58	8 (16%)	66,82,82	1.42	10 (15%)
11	PG4	A	501	-	12,12,12	0.55	0	11,11,11	0.29	0
13	CDL	D	503	-	53,53,99	1.28	4 (7%)	59,65,111	1.12	4 (6%)
18	HEC	D	501	4	50,50,50	2.93	30 (60%)	68,82,82	2.49	28 (41%)
13	CDL	C	401	-	33,33,99	1.24	2 (6%)	37,43,111	1.28	3 (8%)

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
14	HEM	C	402	3	-	5/14/54/54	-
11	PG4	C	406	-	-	5/10/10/10	-
12	6PE	A	502	-	-	12/26/26/30	-
13	CDL	C	408	-	-	19/52/52/110	-
16	LMT	C	405	-	-	10/21/61/61	0/2/2/2
13	CDL	C	401	-	-	21/41/41/110	-
13	CDL	E	205	-	-	34/69/69/110	-
21	PX4	E	202	-	-	17/40/40/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	9XE	C	404	-	-	5/15/15/15	0/4/4/4
17	PEE	E	204	-	1/1/4/8	27/44/44/54	-
14	HEM	C	403	3	-	2/14/54/54	-
17	PEE	C	409	-	1/1/4/8	17/43/43/54	-
11	PG4	A	501	-	-	5/10/10/10	-
20	FES	E	201	-	-	-	0/1/1/1
11	PG4	C	407	-	-	5/10/10/10	-
13	CDL	D	503	-	-	24/63/63/110	-
18	HEC	D	501	4	1/1/3/7	7/14/54/54	-

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	404	9XE	C7-C8	6.31	1.50	1.37
18	D	501	HEC	FE-NB	5.42	2.11	1.94
13	C	408	CDL	OA6-CA5	5.23	1.47	1.35
15	C	404	9XE	C5-C4	5.23	1.49	1.41
14	C	402	HEM	FE-NB	5.19	2.10	1.94

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	501	HEC	C1B-C2B-C3B	-5.66	101.00	106.96
18	D	501	HEC	C3D-C4D-ND	5.36	115.55	110.36
18	D	501	HEC	C2A-C1A-NA	5.16	115.34	110.32
18	D	501	HEC	C2B-C1B-NB	5.12	116.02	109.88
13	C	401	CDL	OB6-CB5-C51	4.71	121.66	111.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	C	409	PEE	C2
17	E	204	PEE	C2
18	D	501	HEC	NA

5 of 215 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

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Mol	Chain	Res	Type	Atoms
12	A	502	6PE	O8-C16-C17-N1
13	C	401	CDL	CB3-OB5-PB2-OB4
13	C	401	CDL	C51-CB5-OB6-CB4

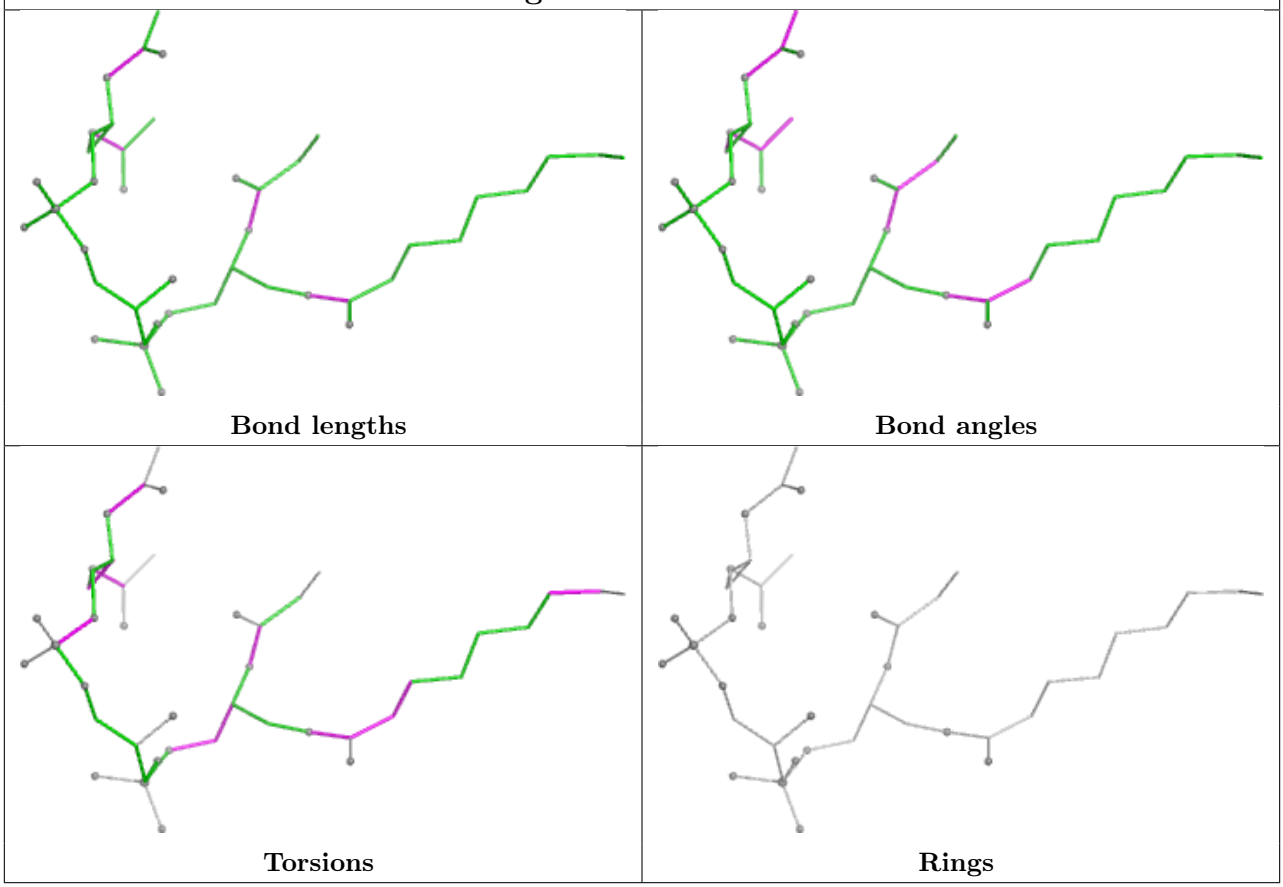
There are no ring outliers.

3 monomers are involved in 8 short contacts:

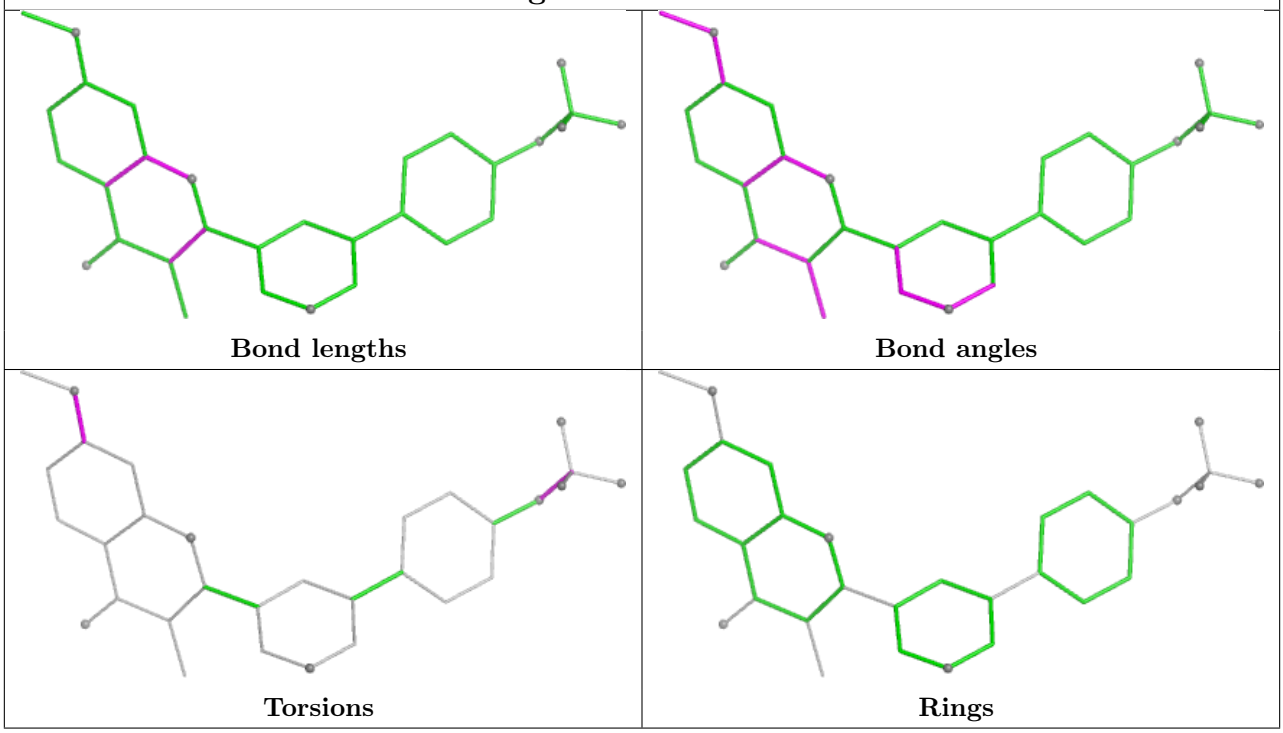
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	402	HEM	2	0
14	C	403	HEM	1	0
18	D	501	HEC	5	0

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.

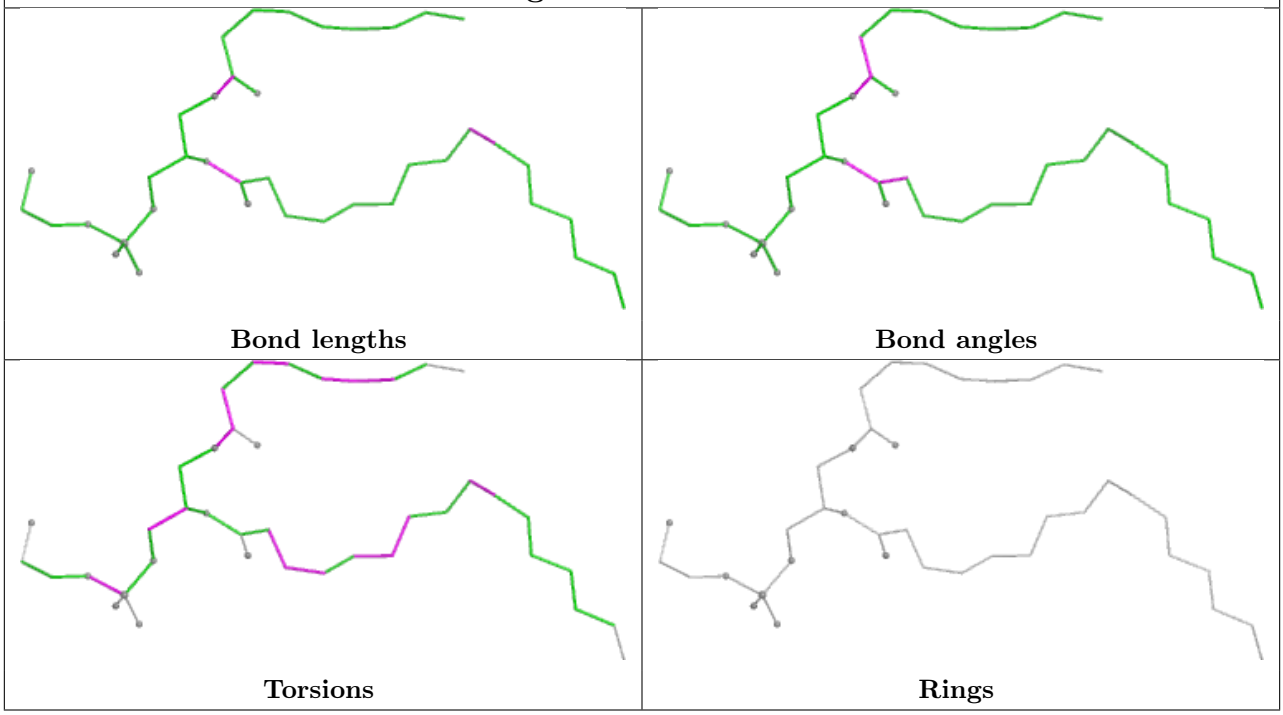
Ligand CDL C 408



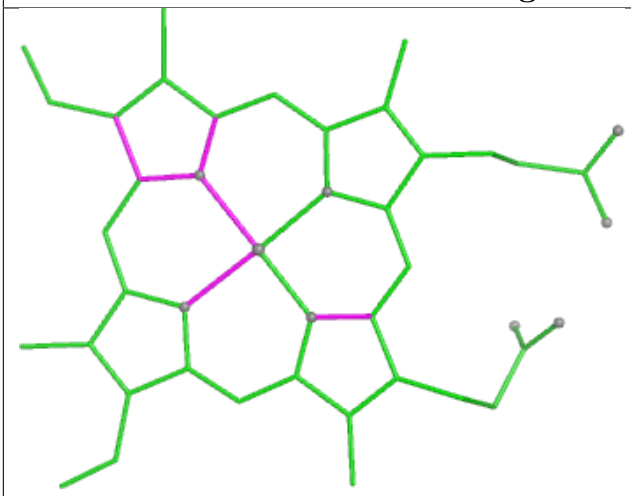
Ligand 9XE C 404



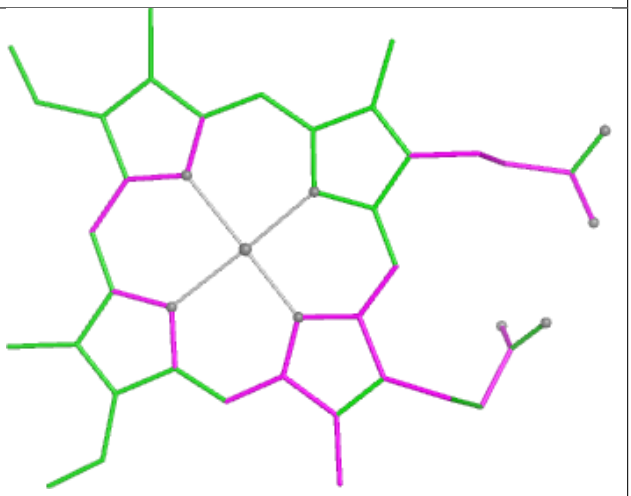
Ligand PEE C 409



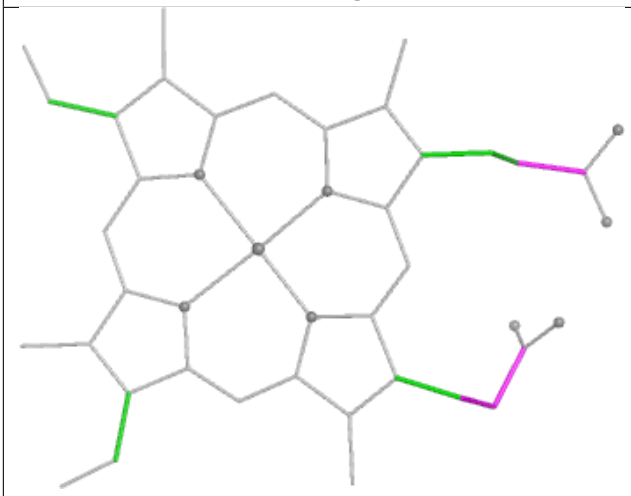
Ligand HEM C 402



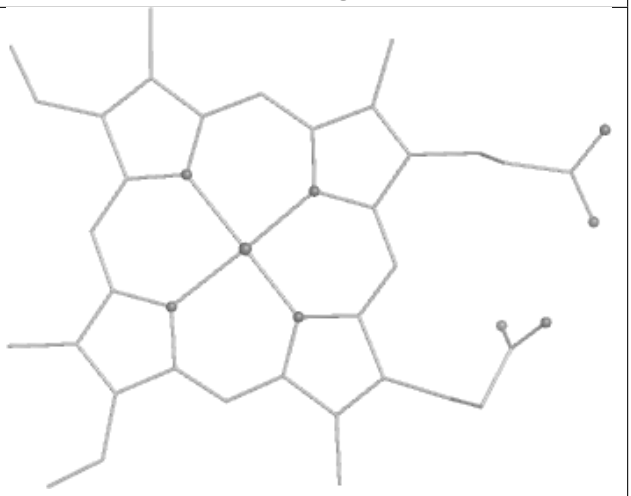
Bond lengths



Bond angles

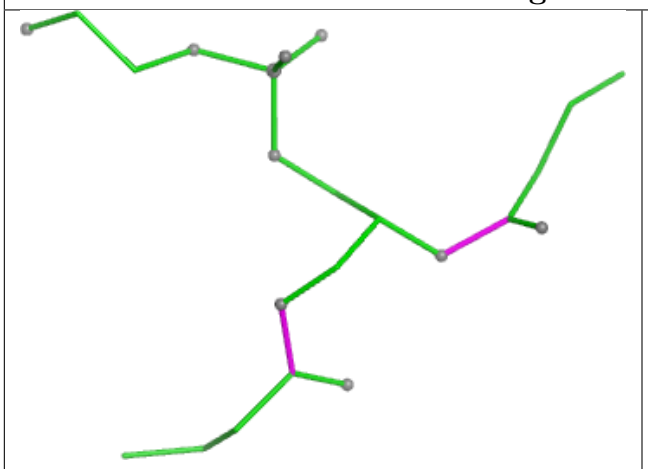


Torsions

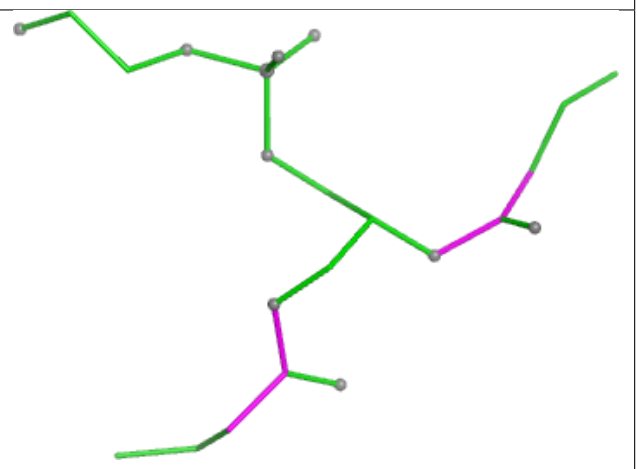


Rings

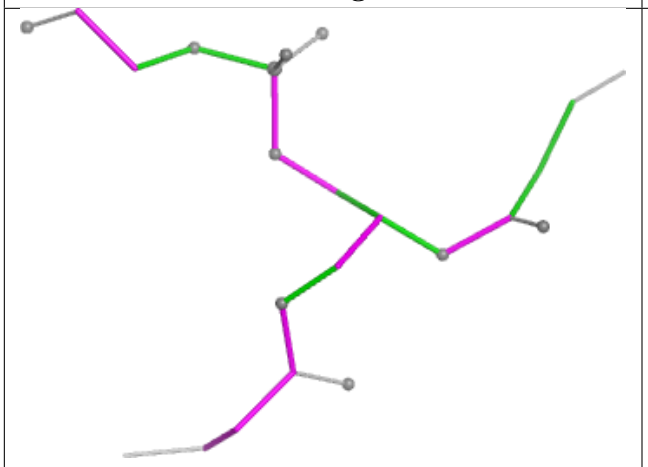
Ligand 6PE A 502



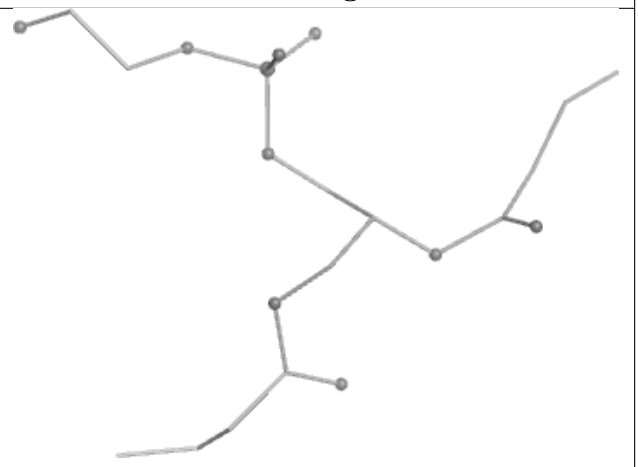
Bond lengths



Bond angles

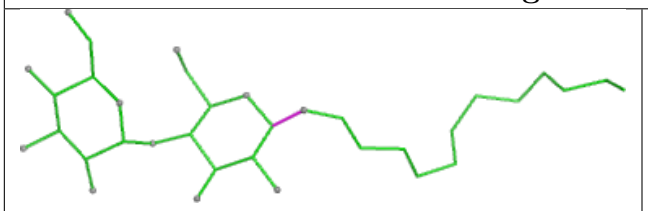


Torsions

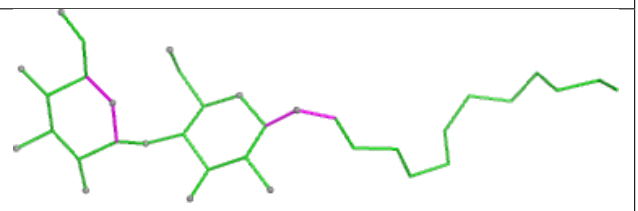


Rings

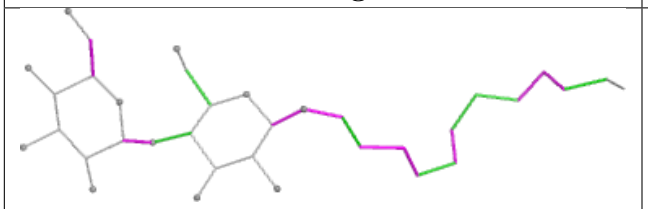
Ligand LMT C 405



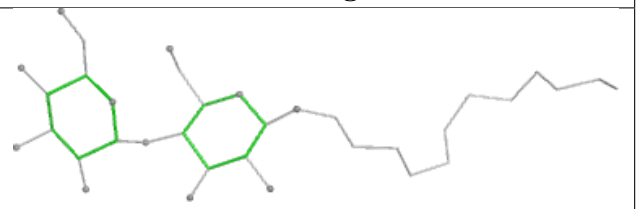
Bond lengths



Bond angles

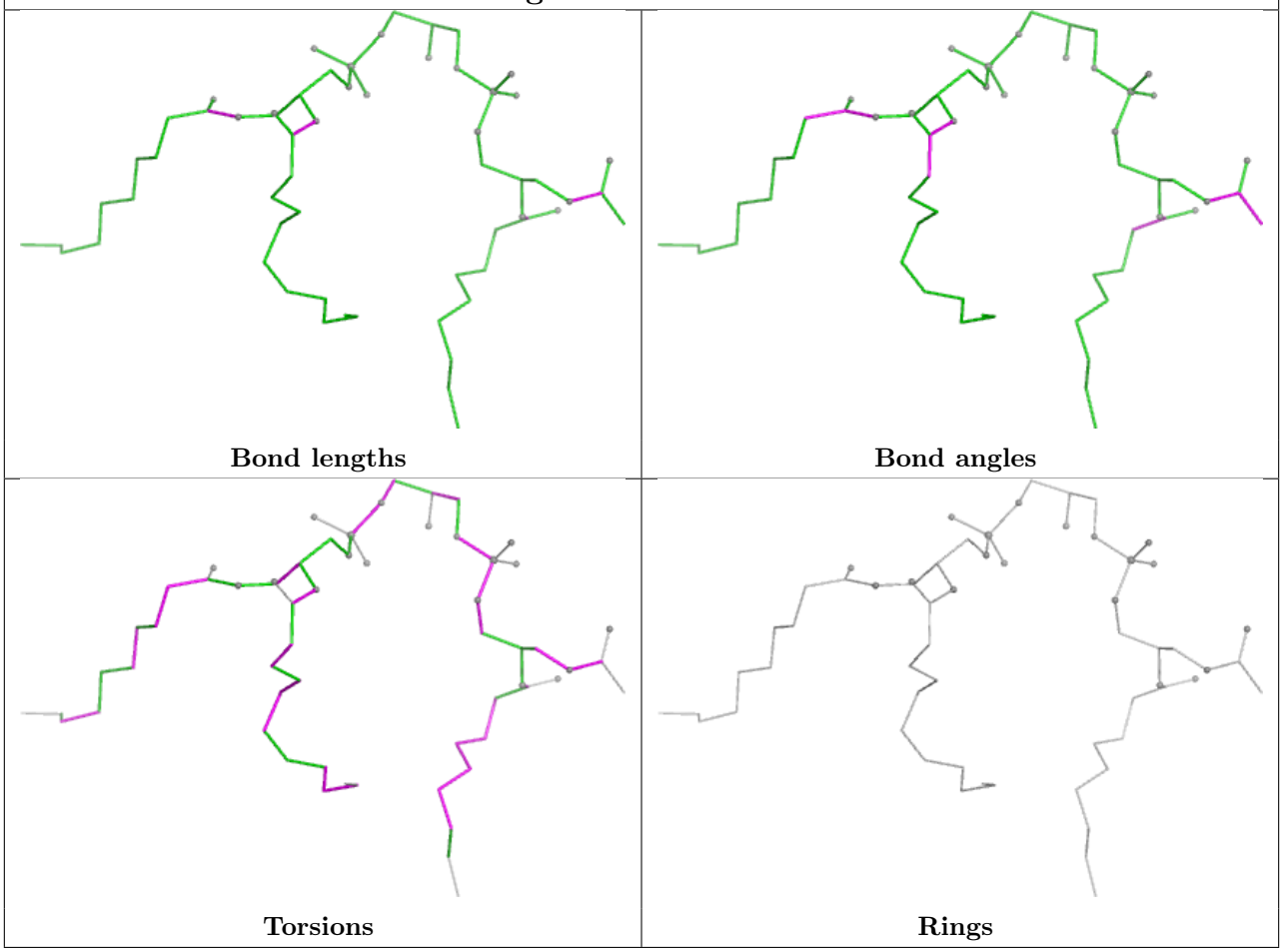


Torsions

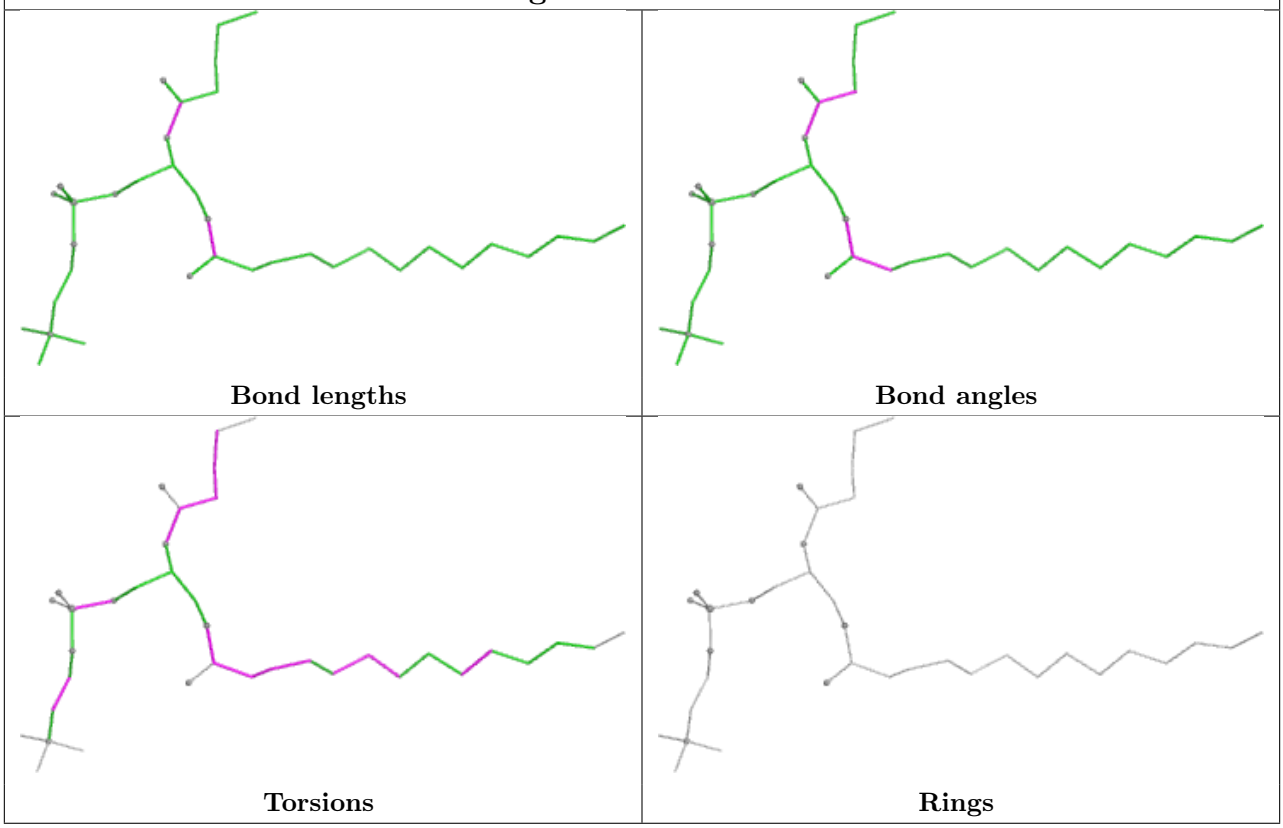


Rings

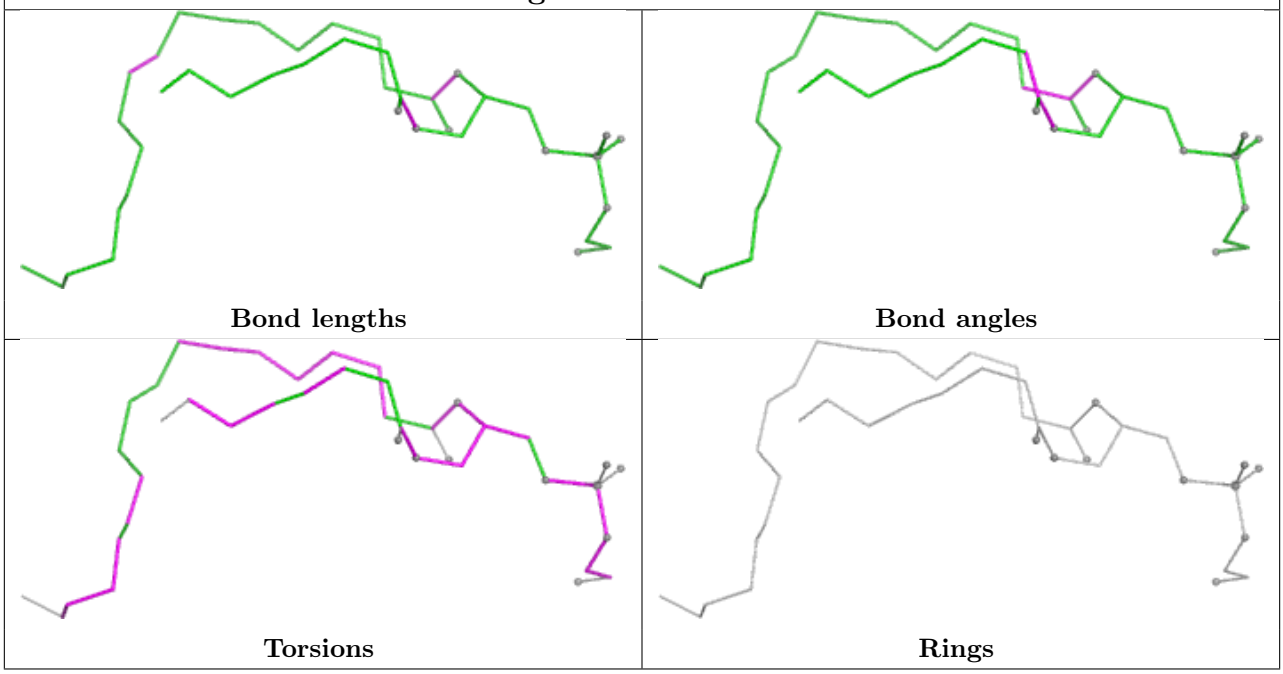
Ligand CDL E 205



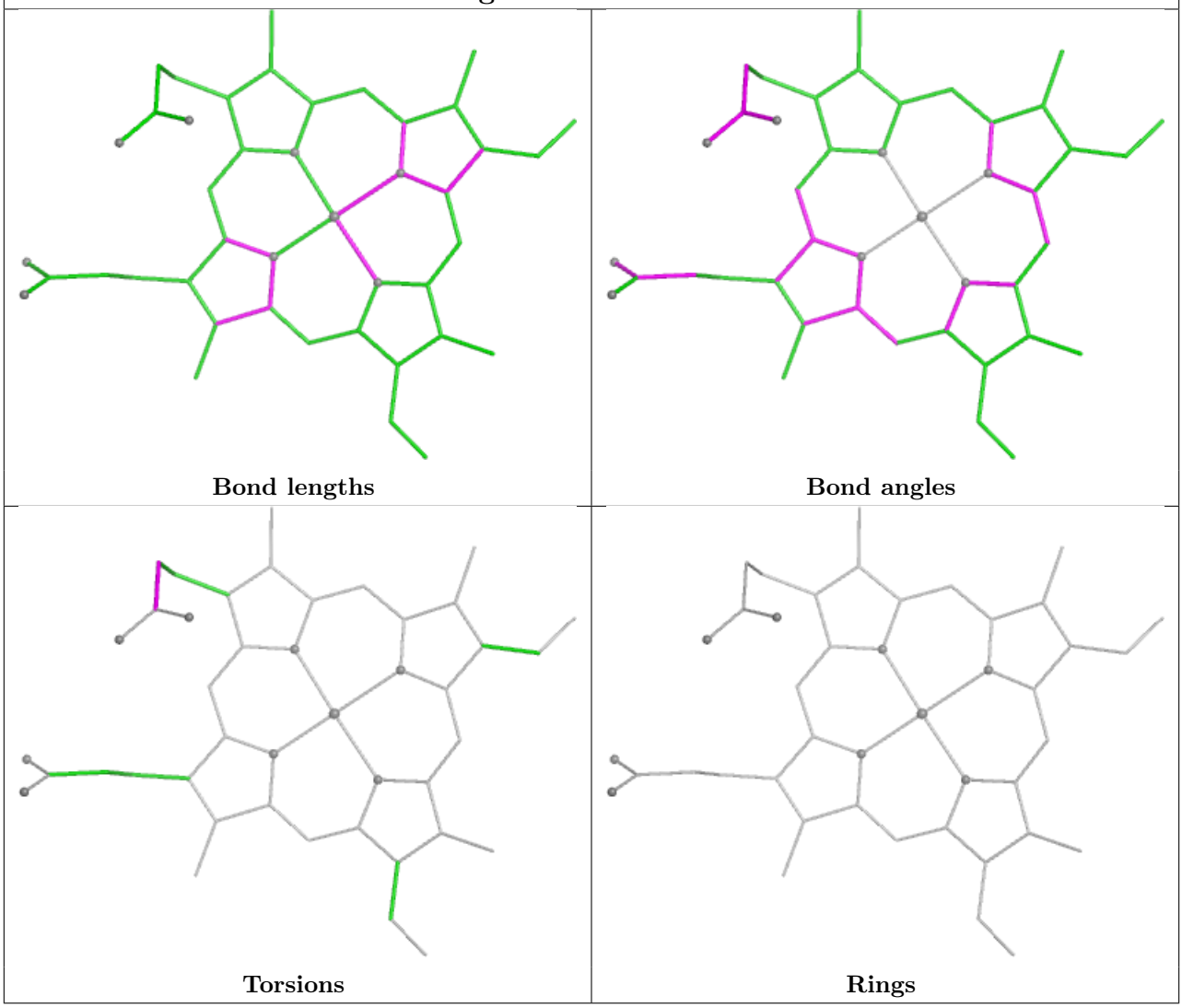
Ligand PX4 E 202



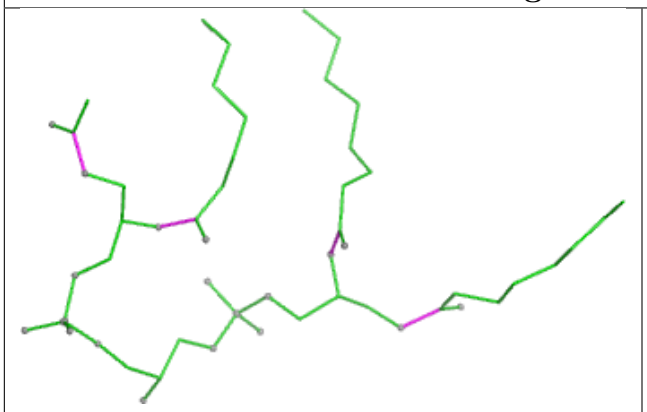
Ligand PEE E 204



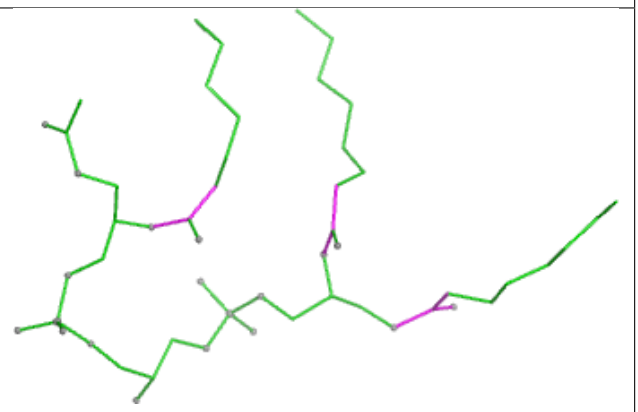
Ligand HEM C 403



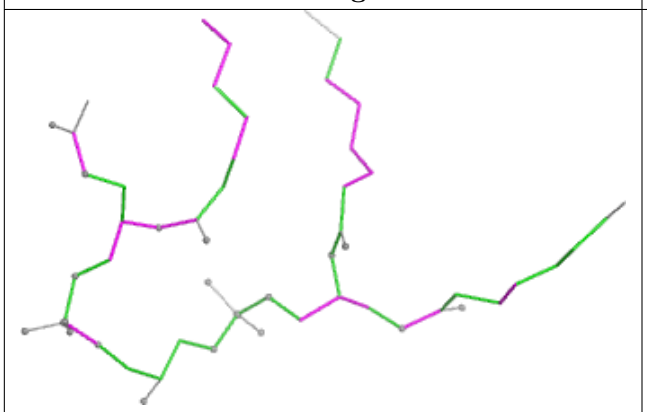
Ligand CDL D 503



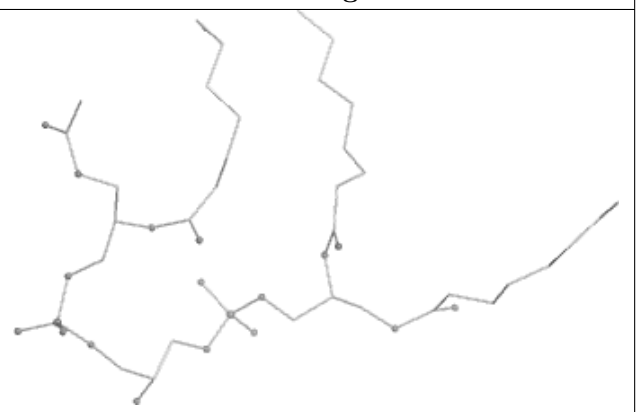
Bond lengths



Bond angles

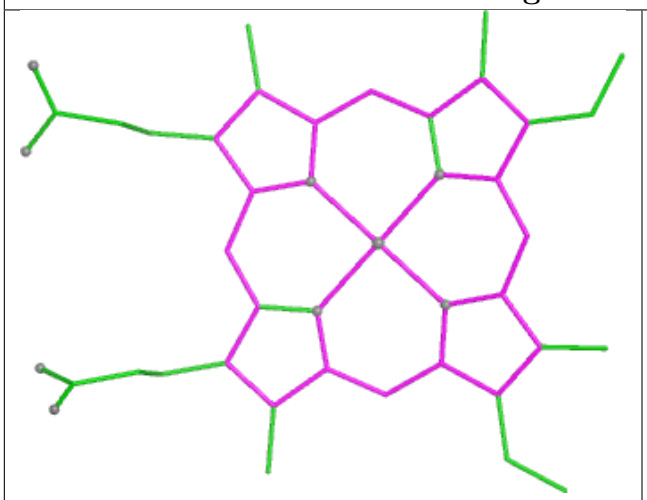


Torsions

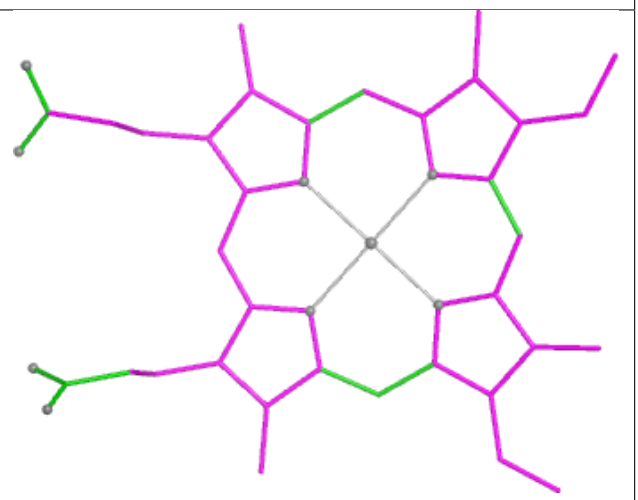


Rings

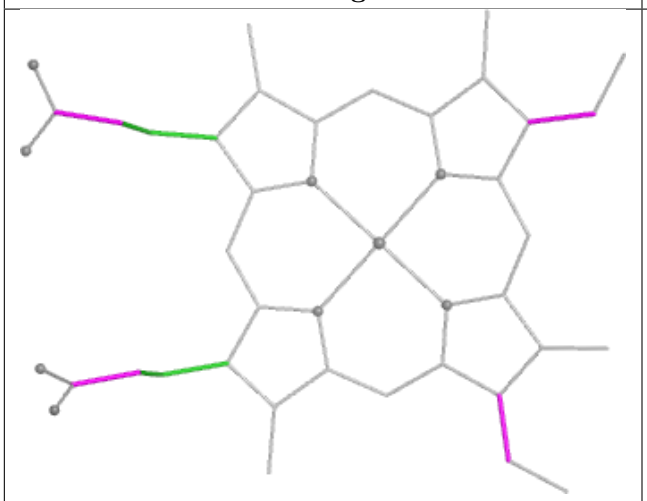
Ligand HEC D 501



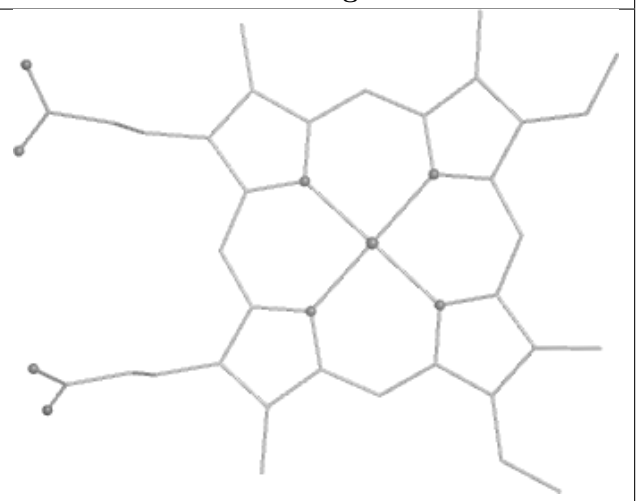
Bond lengths



Bond angles

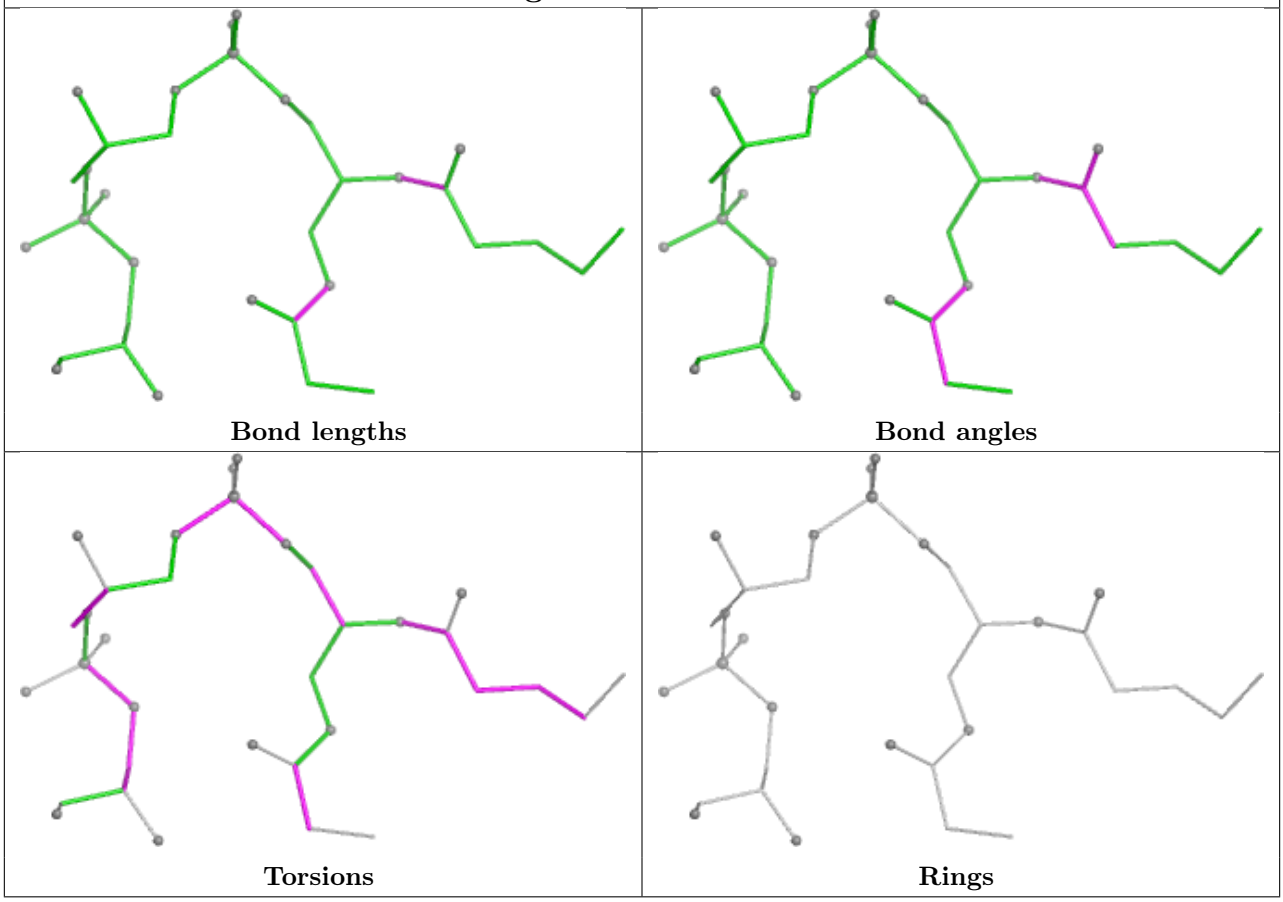


Torsions



Rings

Ligand CDL C 401



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	445/480 (92%)	-0.25	4 (0%)	81	63	62, 92, 126, 188	0
2	B	415/453 (91%)	-0.29	3 (0%)	84	68	68, 95, 122, 179	0
3	C	378/379 (99%)	-0.18	4 (1%)	78	59	63, 84, 123, 152	0
4	D	239/325 (73%)	-0.04	0	100	100	76, 118, 144, 158	0
5	E	196/196 (100%)	0.57	21 (10%)	11	6	77, 141, 182, 194	0
6	F	99/111 (89%)	-0.17	0	100	100	67, 85, 123, 155	0
7	G	74/82 (90%)	-0.13	3 (4%)	41	23	64, 96, 142, 152	0
8	H	65/91 (71%)	0.41	2 (3%)	51	30	124, 143, 161, 168	0
9	I	46/47 (97%)	2.05	19 (41%)	0	0	98, 135, 152, 161	0
10	J	59/64 (92%)	-0.09	1 (1%)	69	48	88, 102, 138, 152	0
All	All	2016/2228 (90%)	-0.06	57 (2%)	55	34	62, 97, 155, 194	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	33	ALA	7.4
9	I	43	LEU	5.9
5	E	178	LEU	5.1
5	E	159	PRO	4.7
5	E	152	ASP	4.4

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

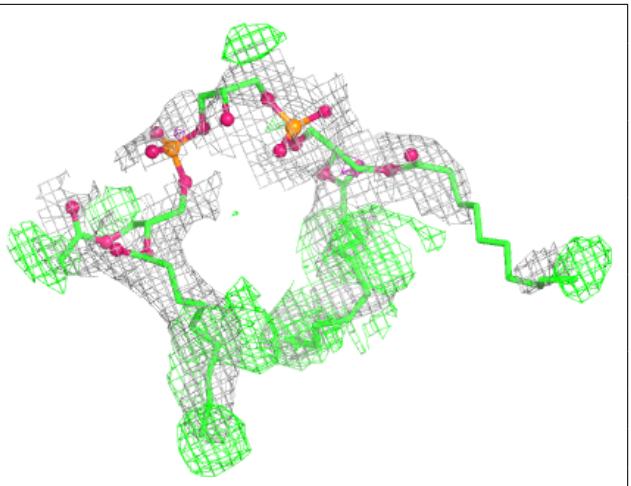
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

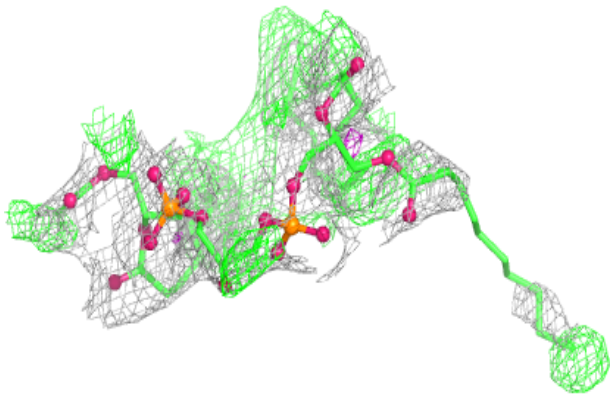
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	CDL	E	205	60/100	0.62	0.25	127,151,185,192	0
16	LMT	C	405	35/35	0.64	0.21	151,166,170,171	0
19	PO4	E	203	5/5	0.69	0.19	156,156,161,161	0
19	PO4	G	102	5/5	0.78	0.12	153,154,156,161	0
19	PO4	D	502	5/5	0.79	0.12	168,169,170,170	0
13	CDL	C	401	34/100	0.83	0.19	144,157,168,169	0
11	PG4	A	501	13/13	0.84	0.15	114,130,142,143	0
19	PO4	G	103	5/5	0.84	0.10	132,134,137,137	0
13	CDL	D	503	54/100	0.88	0.19	94,117,141,142	0
17	PEE	E	204	41/51	0.88	0.21	85,103,111,119	0
11	PG4	C	407	13/13	0.88	0.20	110,116,119,120	0
12	6PE	A	502	23/27	0.90	0.17	96,124,142,145	0
19	PO4	F	501	5/5	0.90	0.18	124,129,132,132	0
21	PX4	E	202	37/46	0.91	0.20	112,129,138,139	0
13	CDL	C	408	44/100	0.92	0.15	84,102,125,127	0
15	9XE	C	404	31/31	0.94	0.10	75,79,90,92	0
17	PEE	C	409	40/51	0.94	0.15	79,91,104,108	0
20	FES	E	201	4/4	0.94	0.06	217,217,217,218	0
19	PO4	G	101	5/5	0.94	0.08	106,107,113,113	0
11	PG4	C	406	13/13	0.95	0.13	98,104,115,115	0
18	HEC	D	501	43/43	0.97	0.11	111,114,120,123	0
14	HEM	C	403	43/43	0.98	0.08	62,65,67,68	0
14	HEM	C	402	43/43	0.98	0.08	68,71,75,79	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:

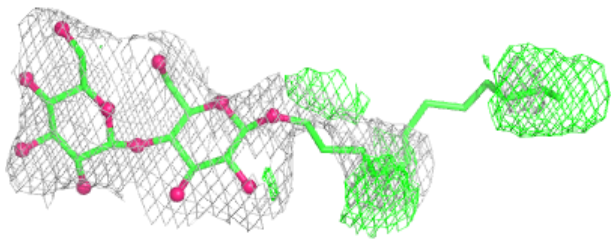
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

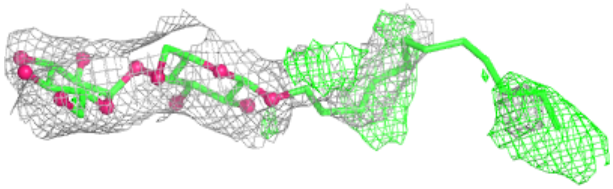


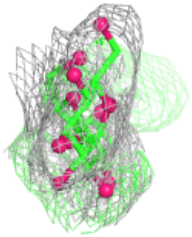


Electron density around LMT C 405:

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

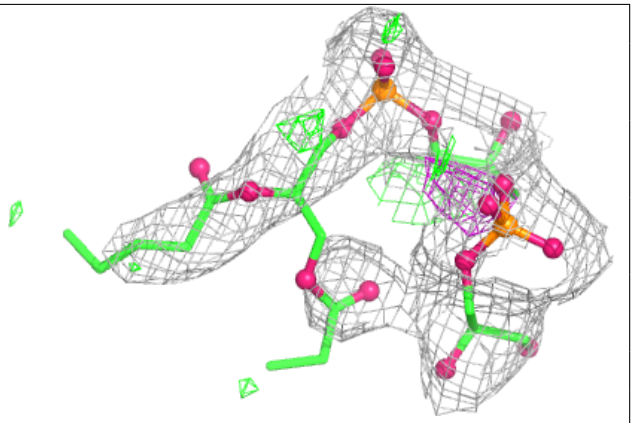


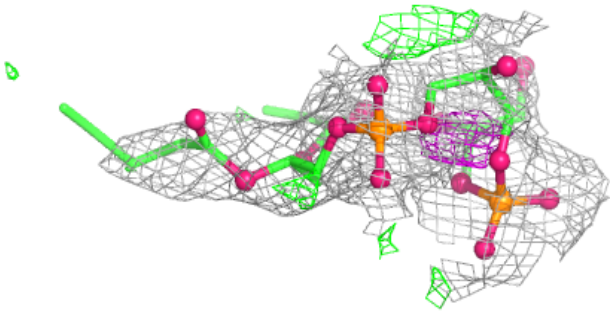


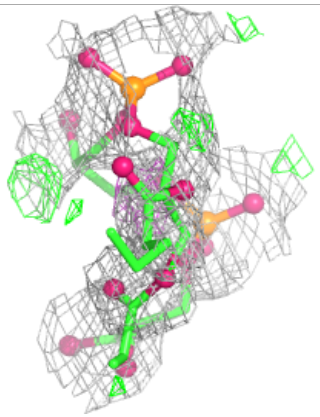


Electron density around CDL C 401:

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







Electron density around CDL D 503:

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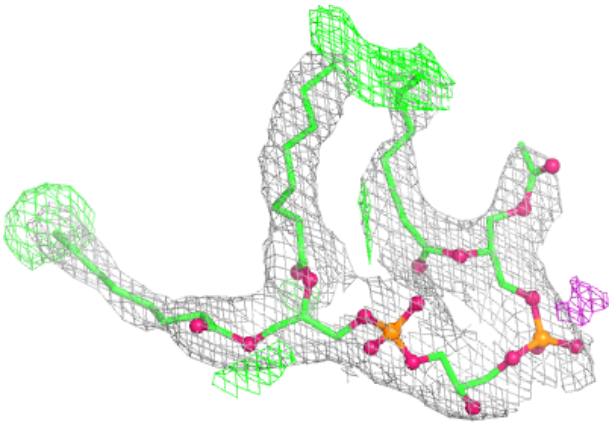
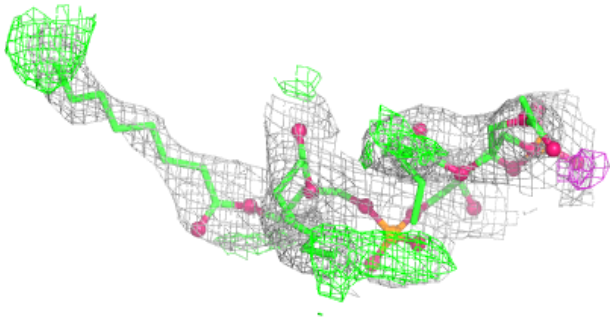
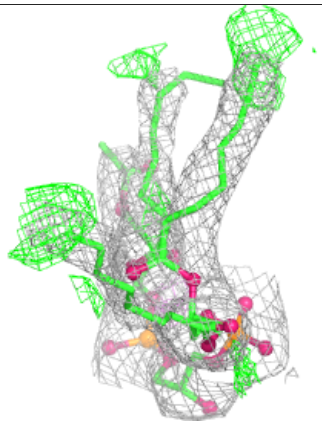
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

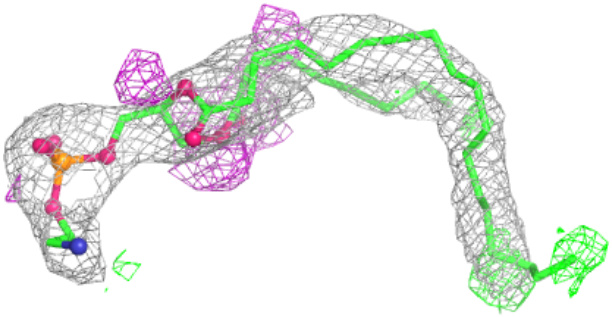


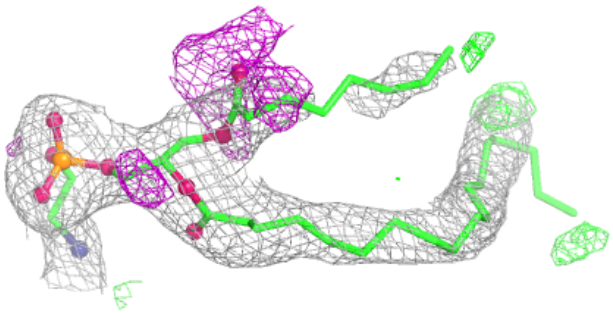


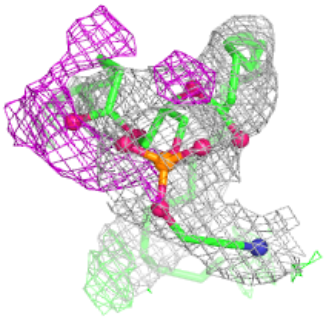


Electron density around PEE E 204:

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

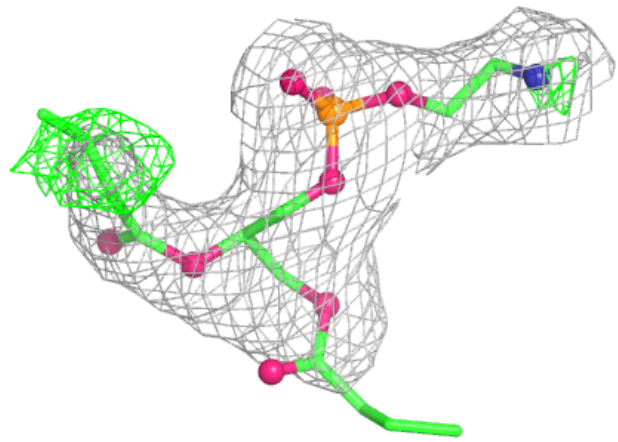


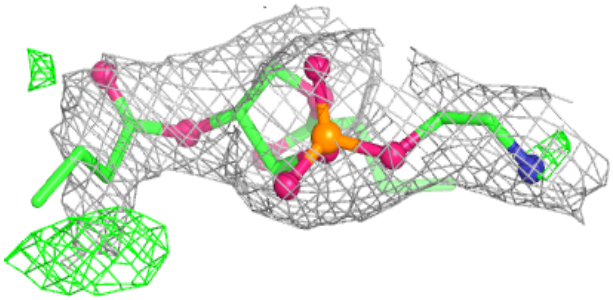


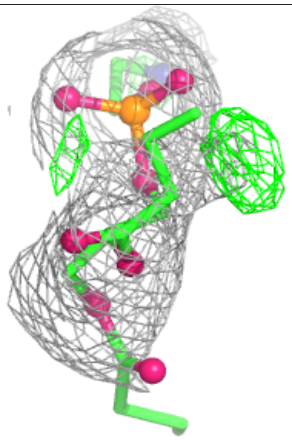


Electron density around 6PE A 502:

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

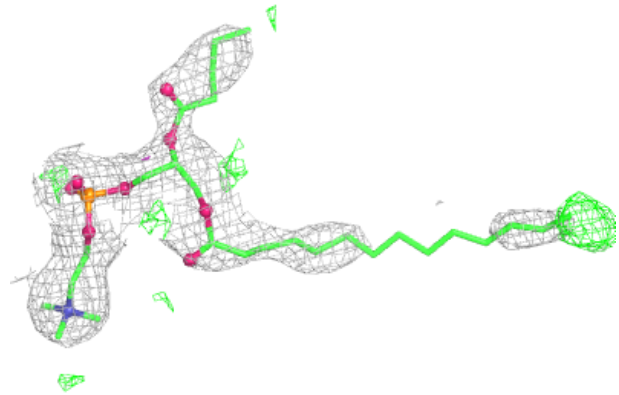


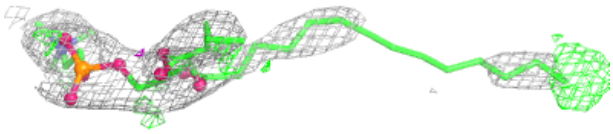


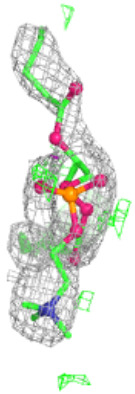


Electron density around PX4 E 202:

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

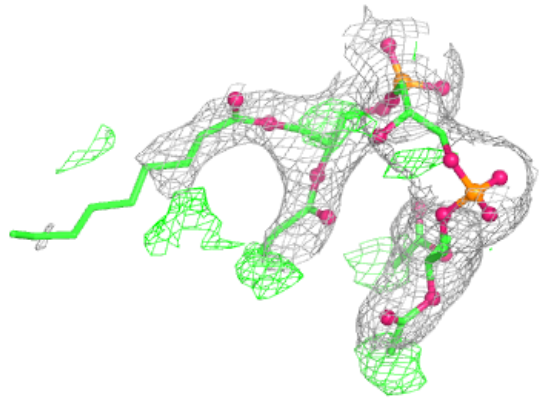


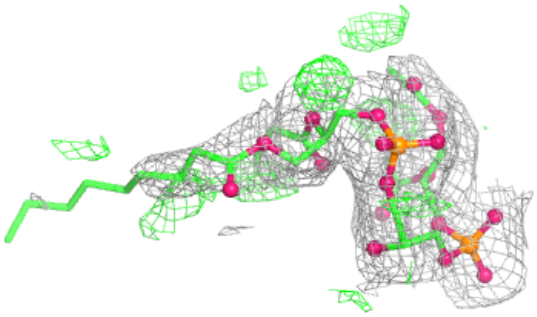


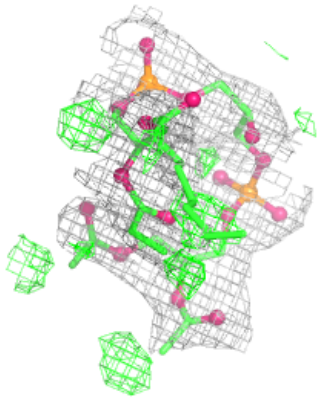


Electron density around CDL C 408:

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

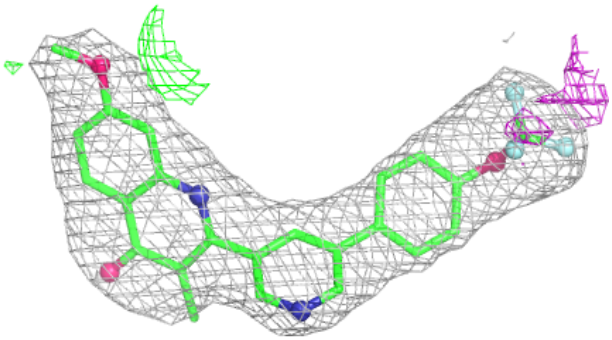


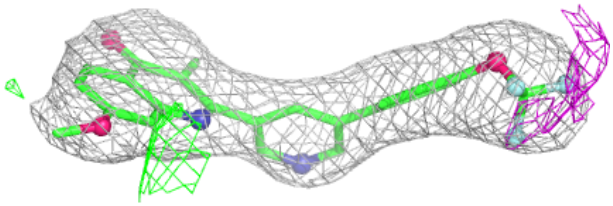


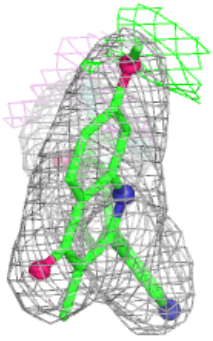


Electron density around 9XE C 404:

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

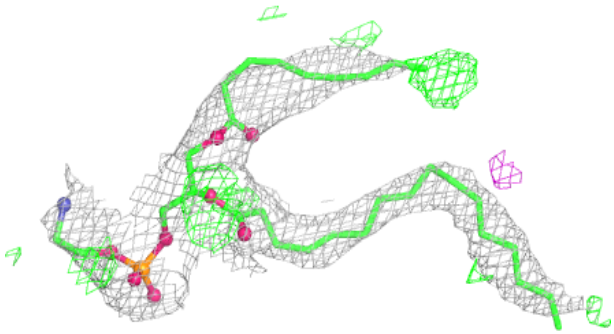


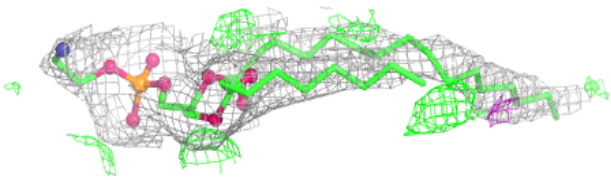


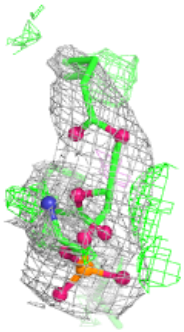


Electron density around PEE C 409:

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

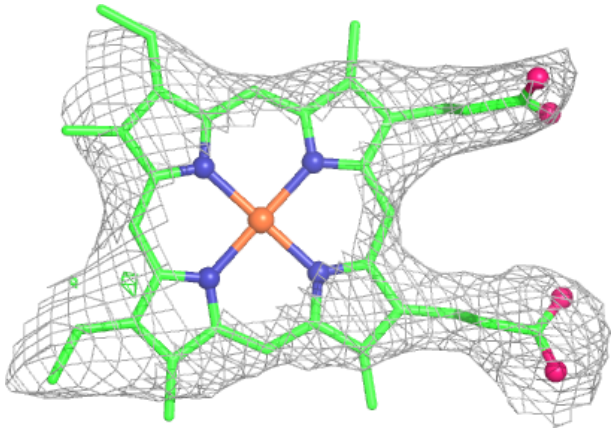


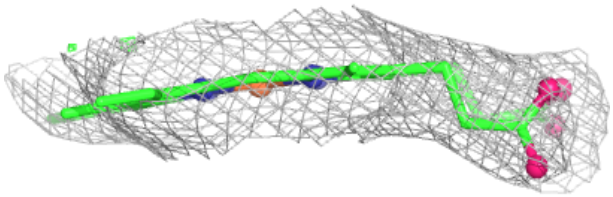


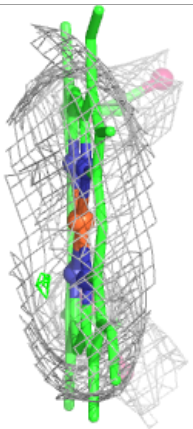


Electron density around HEC D 501:

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

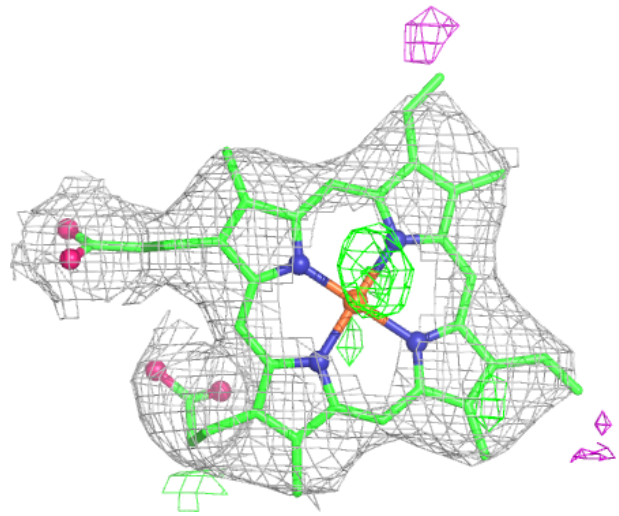


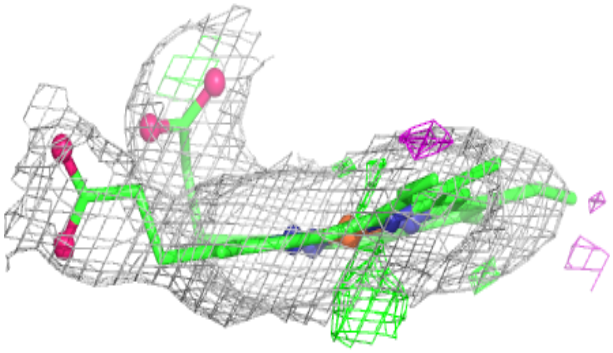


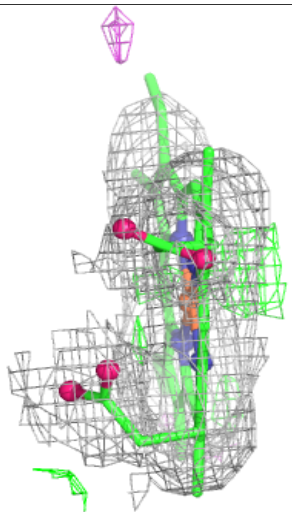


Electron density around HEM C 403:

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

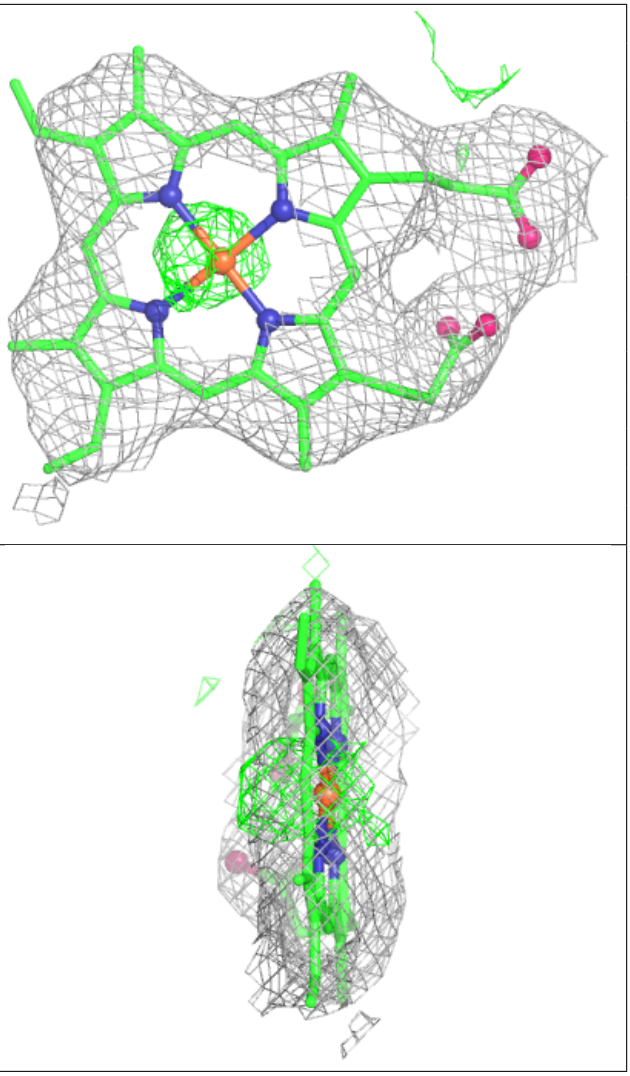






Electron density around HEM C 402:

$2mF_o$-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.