wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 10:34 am BST

PDB ID	:	9GCX / pdb_00009gcx
Title	:	Crystal structure of bovine Cytochrome bc1 in complex with inhibitor F8
Authors	:	Pinthong, N.; Hong, W.; ONeill, P.W.; Antonyuk, S.V.
Deposited on	:	2024-08-03
Resolution	:	3.52 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:

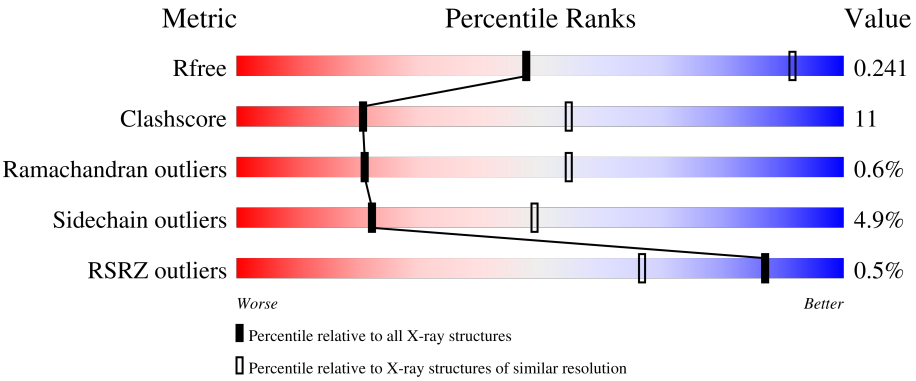
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	68% 21% · 8%
2	B	453	64% 24% · 9%
3	C	379	71% 26% ·
4	D	325	51% 20% · 26%
5	E	274	% 46% 23% · 28%

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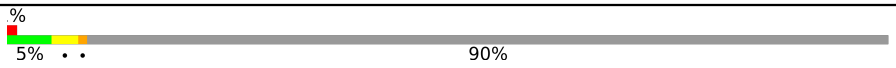
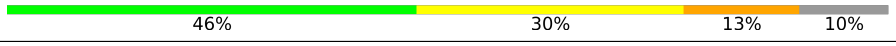
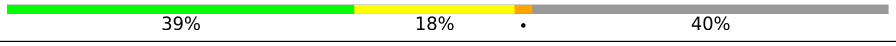
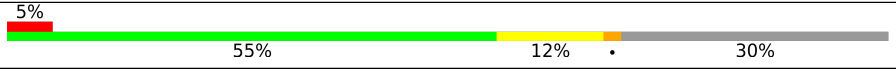
Mol	Chain	Length	Quality of chain
5	I	274	
6	F	111	
7	G	82	
8	H	109	
9	J	64	
10	K	56	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CDL	A	502	-	-	X	-
14	A1IKG	C	505	X	-	-	-
16	HEC	D	501	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 16707 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	440	Total	C	N	O	S	0	0	0
			3402	2129	600	653	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	1	0
			3112	1952	552	601	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	2	0
			3008	2019	470	500	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1901	1213	326	347	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
			1505	946	262	290	7			
5	I	27	Total	C	N	O	S	0	0	0
			191	117	38	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			860	547	155	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	405	116	98	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
			529	321	96	107	5			

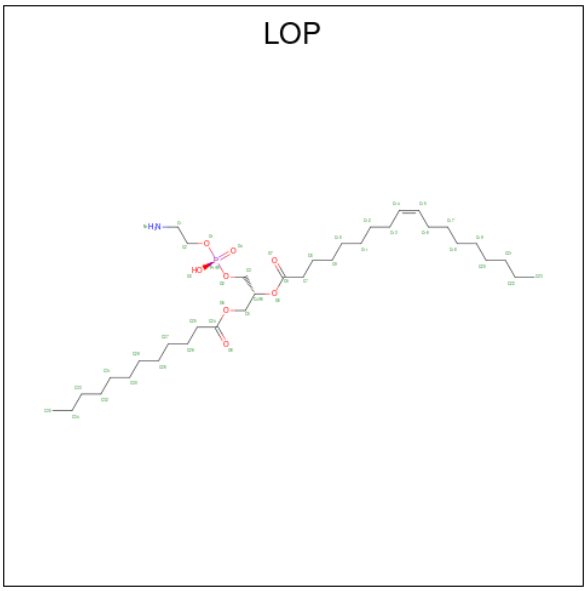
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	56	Total	C	N	O	0	0	0
			466	307	81	78			

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

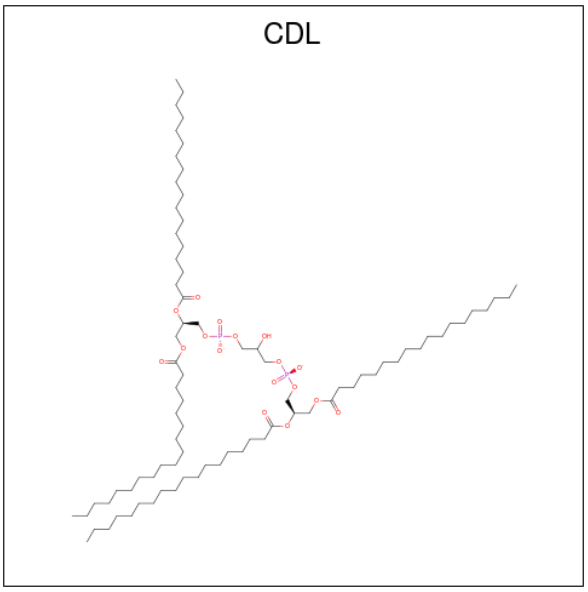
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	39	Total	C	N	O	0	0	0
			290	192	49	49			

- Molecule 11 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: $C_{35}H_{68}NO_8P$).



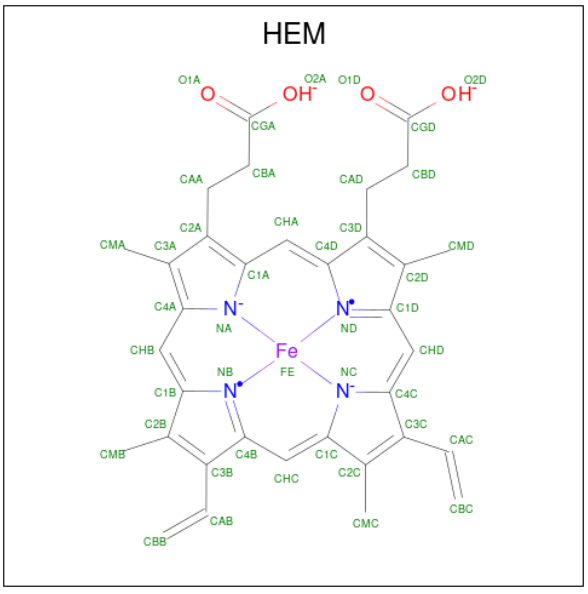
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	E	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



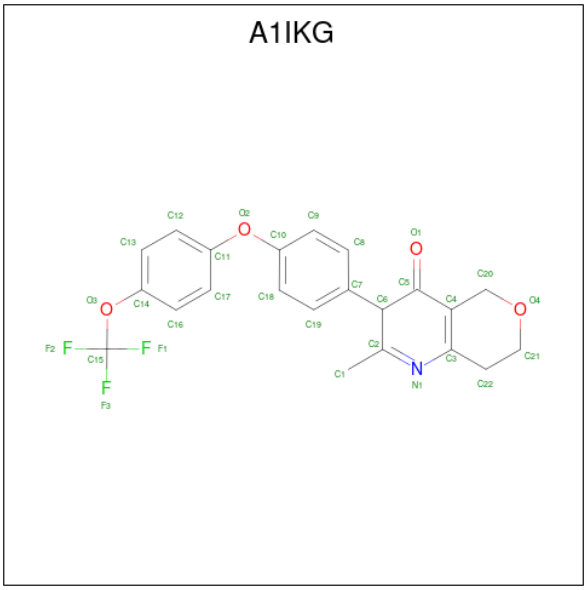
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			84	65	17	2		
12	C	1	Total	C	O	P	0	0
			100	81	17	2		
12	D	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



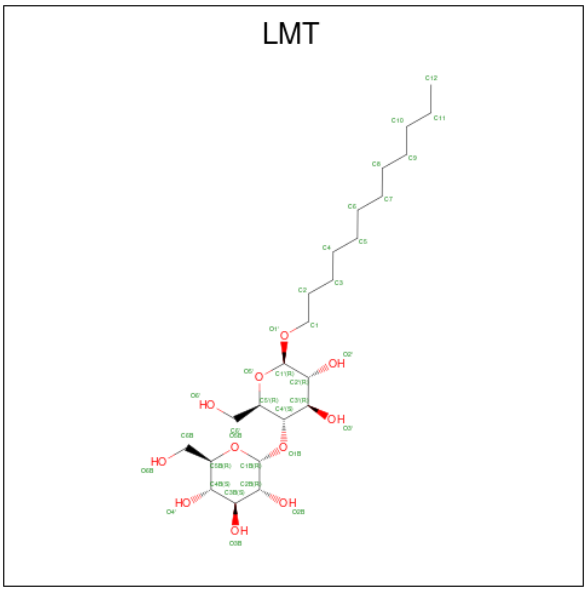
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is 2-methyl-3-(4-(4-(trifluoromethoxy)phenoxy)phenyl)-1,5,7,8-tetrahydro-4H-pyrano[4,3-b]pyridin-4-one (CCD ID: A1IKG) (formula: $C_{22}H_{18}F_3NO_4$).



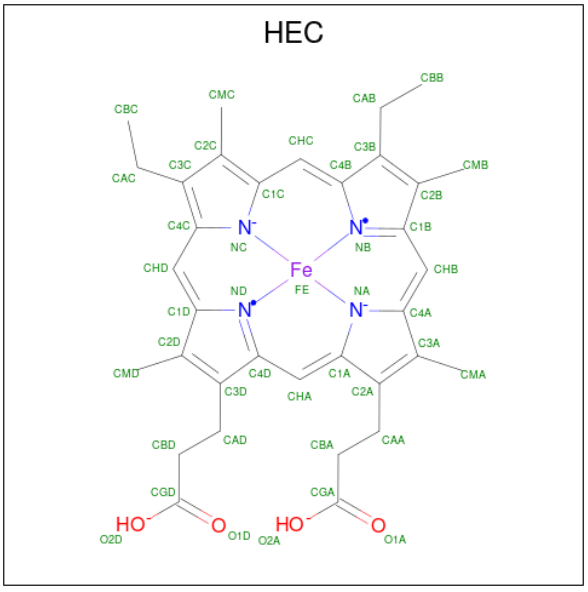
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	F	N	O	0	0
			30	22	3	1	4		

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



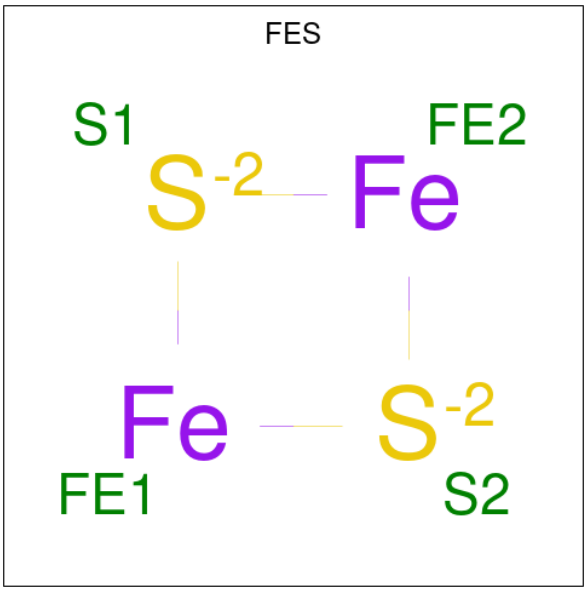
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	C	1	35	24	11	0	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



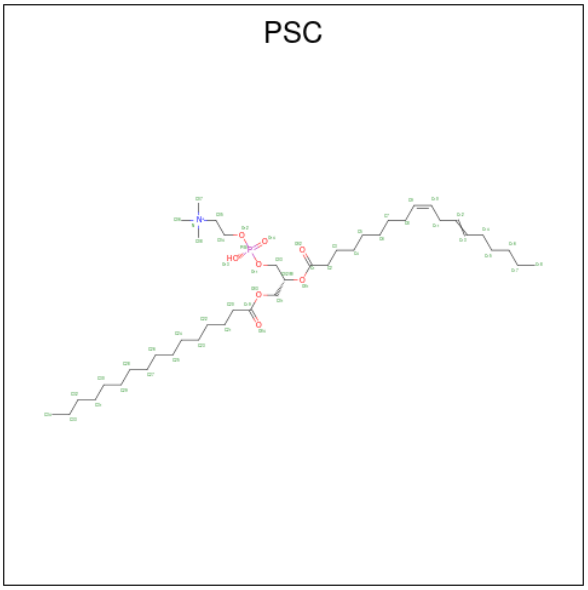
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
16	D	1	43	34	1	4	4	0	0

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



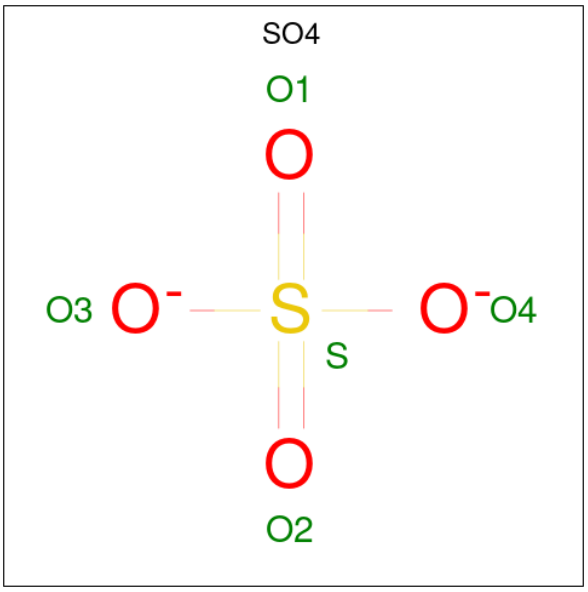
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 18 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	1	Total O S 5 4 1	0	0
19	G	1	Total O S 5 4 1	0	0
19	G	1	Total O S 5 4 1	0	0

- Molecule 20 is water.

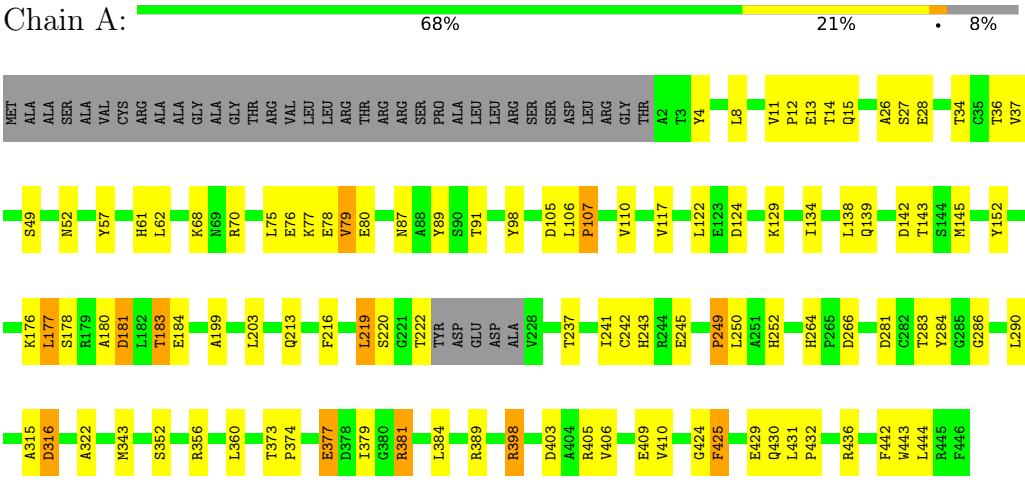
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	3	Total O 3 3	0	0
20	B	1	Total O 1 1	0	0
20	C	4	Total O 4 4	0	0
20	E	1	Total O 1 1	0	0
20	F	1	Total O 1 1	0	0

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.

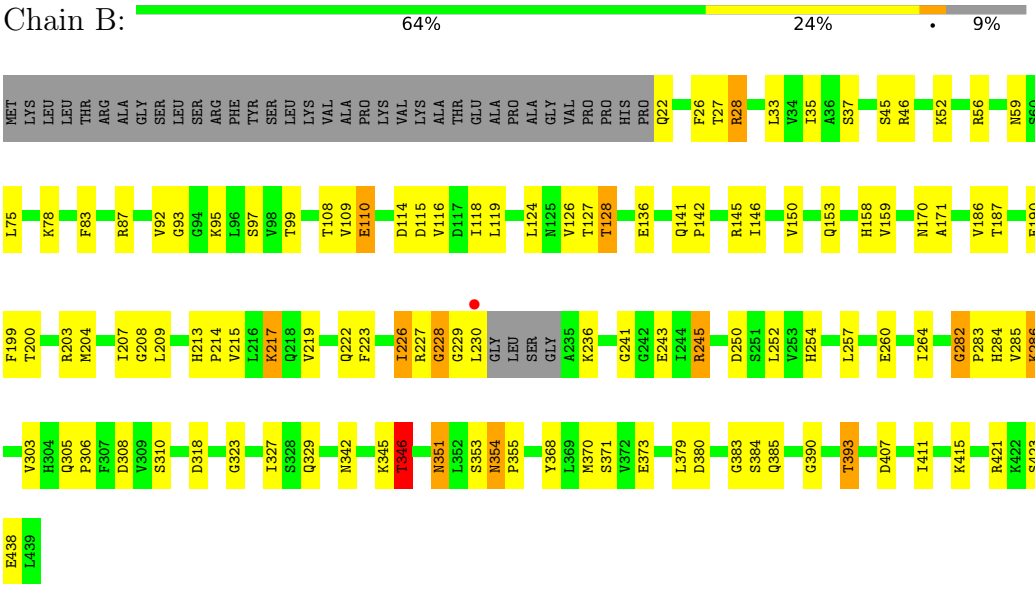
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



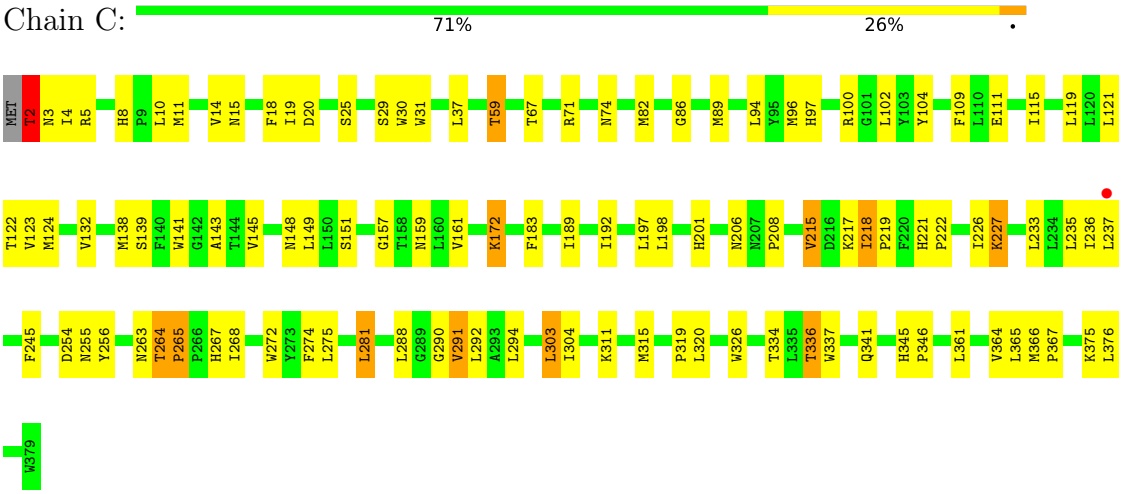
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



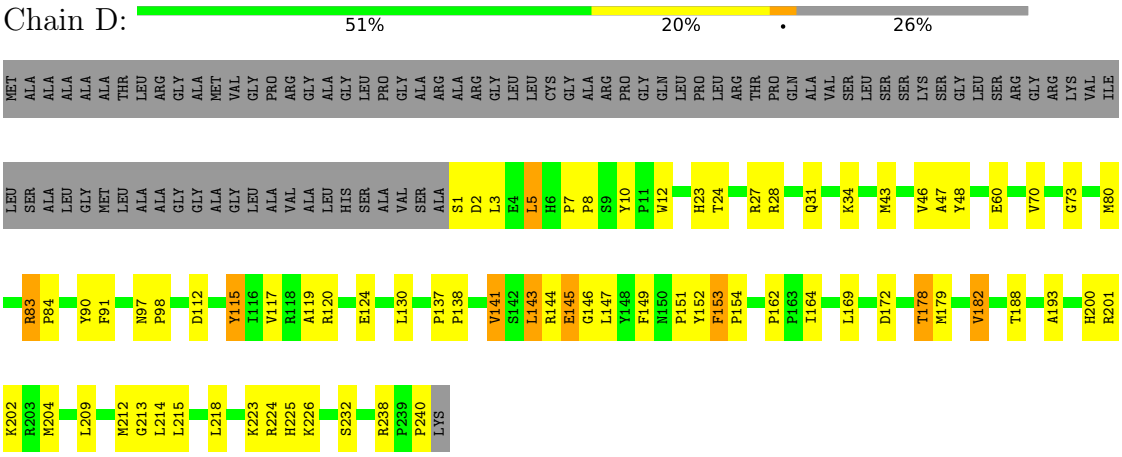
• Molecule 3: Cytochrome b

Chain C:



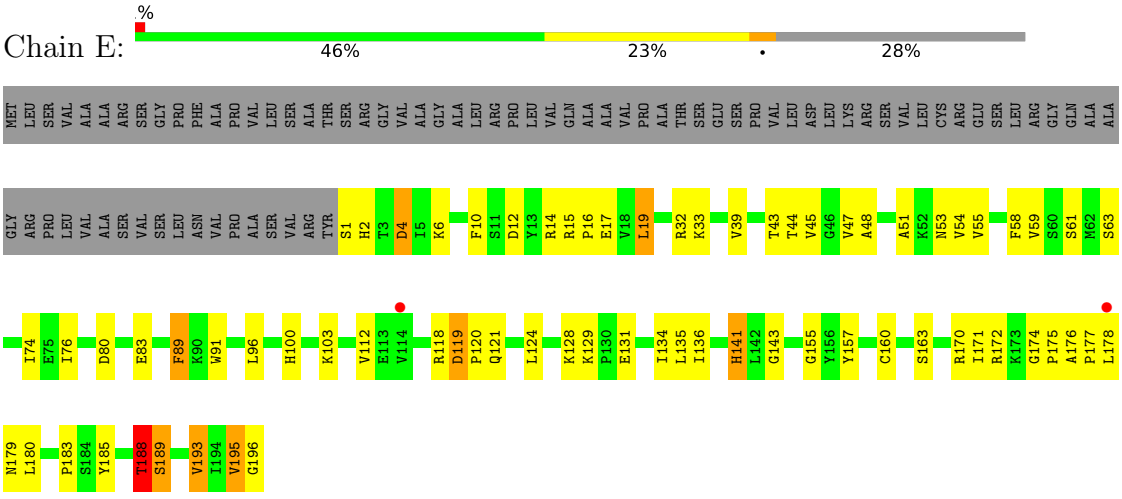
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



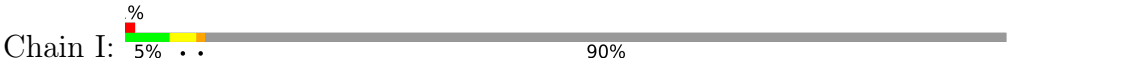
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

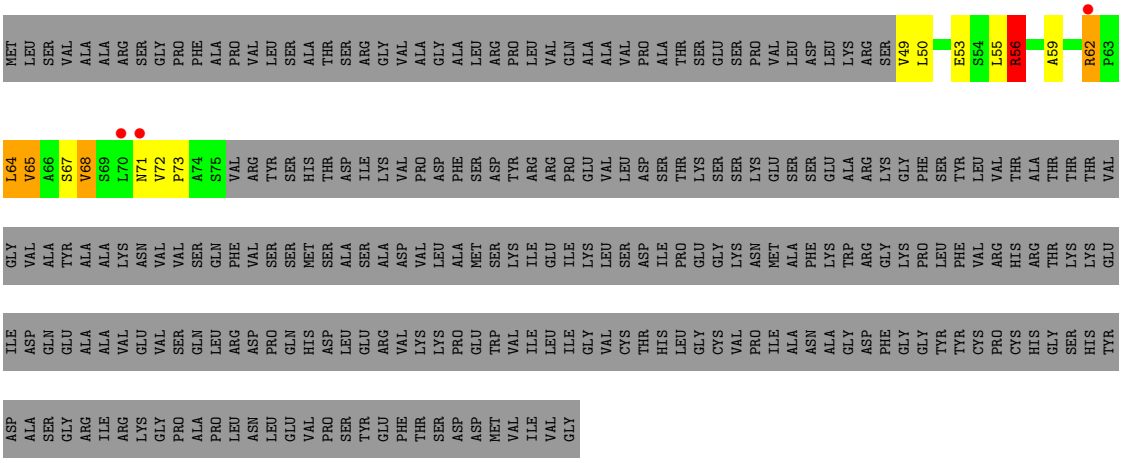
Chain E:



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

Chain I:





• Molecule 6: Cytochrome b-c1 complex subunit 7

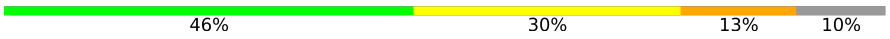
Chain F:

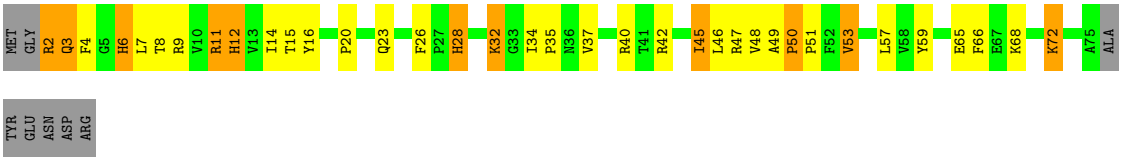




• Molecule 7: Cytochrome b-c1 complex subunit 8

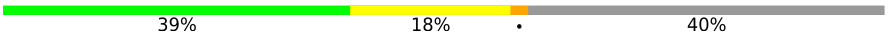
Chain G:

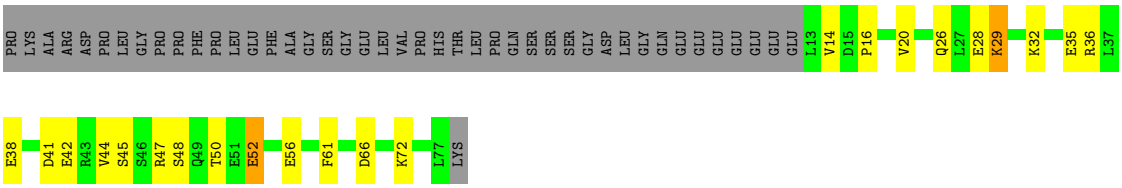




• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:

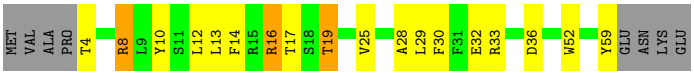




• Molecule 9: Cytochrome b-c1 complex subunit 9

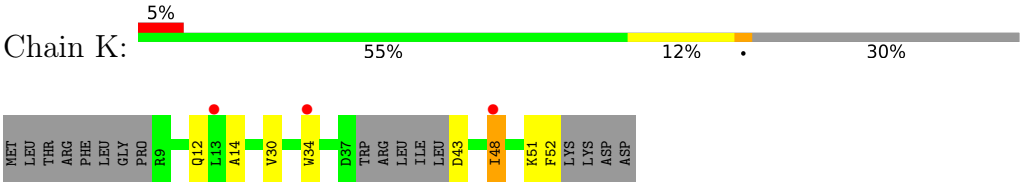
Chain J:





• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain K:


5%
55%
12%
30%
MET
LEU
THR
ARG
PHE
LEU
GLY
PRO
R9
Q12
L13
A14
V30
W34
D37
TRP
ARG
LEU
ILE
LEU
D43
I48
K51
F52
LYS
LYS
ASP
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	210.08Å 210.08Å 344.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.52 30.00 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.52) 98.9 (30.00-3.52)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.188 , 0.241 0.188 , 0.241	Depositor DCC
R_{free} test set	2830 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	117.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16707	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: PSC, FES, LOP, CDL, LMT, HEC, HEM, A1IKG, SO4

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	0.57	0/3473	1.40	29/4713 (0.6%)
2	B	0.57	0/3167	1.40	28/4297 (0.7%)
3	C	0.54	0/3111	1.36	23/4259 (0.5%)
4	D	0.55	0/1960	1.35	13/2665 (0.5%)
5	E	0.57	0/1538	1.35	11/2082 (0.5%)
5	I	0.91	0/192	1.83	5/260 (1.9%)
6	F	0.52	0/879	1.51	13/1180 (1.1%)
7	G	0.61	0/641	1.64	13/869 (1.5%)
8	H	0.52	0/534	1.74	13/718 (1.8%)
9	J	0.57	0/478	1.42	5/644 (0.8%)
10	K	0.67	0/300	1.45	1/414 (0.2%)
All	All	0.57	0/16273	1.42	154/22101 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
4	D	0	2
5	E	0	1
5	I	0	1
6	F	0	2
7	G	0	3
9	J	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	346	THR	CA-CB-OG1	-11.05	93.03	109.60
6	F	77	LYS	CB-CG-CD	9.34	132.78	111.30
1	A	183	THR	CA-CB-OG1	-8.99	96.12	109.60
2	B	209	LEU	N-CA-CB	-8.94	96.53	110.57
7	G	2	ARG	CA-CB-CG	8.74	131.57	114.10

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Sidechain
1	A	398	ARG	Sidechain
2	B	282	GLY	Peptide
2	B	421	ARG	Sidechain
4	D	83	ARG	Sidechain

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	3402	0	3306	64	0
2	B	3112	0	3078	76	1
3	C	3008	0	3074	76	0
4	D	1901	0	1833	49	0
5	E	1505	0	1478	38	1
5	I	191	0	203	12	0
6	F	860	0	851	4	0
7	G	620	0	619	23	0
8	H	529	0	511	8	0
9	J	466	0	469	19	0
10	K	290	0	260	8	0
11	A	45	0	67	11	0
11	C	135	0	201	9	0
11	E	45	0	67	7	0
11	G	45	0	67	4	0
12	A	84	0	121	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	100	0	156	11	0
12	D	94	0	141	12	0
13	C	86	0	60	8	0
14	C	30	0	0	0	0
15	C	35	0	46	3	0
16	D	43	0	30	2	0
17	E	4	0	0	0	0
18	E	52	0	80	5	0
19	F	5	0	0	0	0
19	G	10	0	0	0	0
20	A	3	0	0	0	0
20	B	1	0	0	1	0
20	C	4	0	0	0	0
20	E	1	0	0	0	0
20	F	1	0	0	0	0
All	All	16707	0	16718	371	1

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 11.

The worst 5 of 371 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)
12:A:502:CDL:HA22	12:A:502:CDL:H112	1.50	0.93
12:A:502:CDL:H422	12:A:502:CDL:H341	1.54	0.89
1:A:406:VAL:O	1:A:410:VAL:HG23	1.71	0.89
12:D:502:CDL:H342	12:D:502:CDL:H171	1.52	0.88
12:A:502:CDL:H162	3:C:11:MET:HE1	1.55	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLN:NE2	5:E:112:VAL:O[5_555]	1.67	0.53

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	436/480 (91%)	423 (97%)	13 (3%)	0	100 100
2	B	411/453 (91%)	383 (93%)	26 (6%)	2 (0%)	24 58
3	C	378/379 (100%)	362 (96%)	16 (4%)	0	100 100
4	D	238/325 (73%)	227 (95%)	9 (4%)	2 (1%)	16 50
5	E	194/274 (71%)	174 (90%)	15 (8%)	5 (3%)	4 27
5	I	25/274 (9%)	21 (84%)	4 (16%)	0	100 100
6	F	96/111 (86%)	94 (98%)	2 (2%)	0	100 100
7	G	72/82 (88%)	66 (92%)	5 (7%)	1 (1%)	9 38
8	H	63/109 (58%)	61 (97%)	2 (3%)	0	100 100
9	J	54/64 (84%)	54 (100%)	0	0	100 100
10	K	35/56 (62%)	28 (80%)	5 (14%)	2 (6%)	1 13
All	All	2002/2607 (77%)	1893 (95%)	97 (5%)	12 (1%)	21 55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	228	GLY
5	E	141	HIS
5	E	143	GLY
5	E	155	GLY
10	K	12	GLN

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	364/394 (92%)	356 (98%)	8 (2%)	45	66
2	B	324/355 (91%)	316 (98%)	8 (2%)	42	64
3	C	327/327 (100%)	311 (95%)	16 (5%)	22	49
4	D	203/257 (79%)	193 (95%)	10 (5%)	22	49
5	E	165/228 (72%)	152 (92%)	13 (8%)	11	37
5	I	21/228 (9%)	14 (67%)	7 (33%)	0	2
6	F	90/99 (91%)	83 (92%)	7 (8%)	11	37
7	G	65/72 (90%)	59 (91%)	6 (9%)	8	32
8	H	62/99 (63%)	58 (94%)	4 (6%)	15	42
9	J	47/54 (87%)	44 (94%)	3 (6%)	16	43
10	K	25/46 (54%)	24 (96%)	1 (4%)	28	54
All	All	1693/2159 (78%)	1610 (95%)	83 (5%)	22	49

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	59	VAL
8	H	38	GLU
6	F	84	GLU
7	G	45	ILE
5	I	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	164	HIS
7	G	23	GLN
2	B	277	HIS
2	B	270	ASN
7	G	28	HIS

5.3.3 RNA

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)

19 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	$\#\|Z\| > 2$
12	CDL	A	502	-	83,83,99	0.52	0	89,95,111	0.87	3 (3%)
12	CDL	C	504	-	99,99,99	0.43	0	105,111,111	0.79	2 (1%)
14	A1IKG	C	505	-	32,33,33	1.57	6 (18%)	40,48,48	1.46	7 (17%)
17	FES	E	201	5	0,4,4	-	-	-		
11	LOP	C	507	-	44,44,44	0.56	0	47,49,49	0.76	2 (4%)
13	HEM	C	502	3	50,50,50	1.71	12 (24%)	66,82,82	1.48	13 (19%)
11	LOP	G	101	-	44,44,44	0.44	0	47,49,49	1.25	3 (6%)
15	LMT	C	508	-	36,36,36	0.52	0	47,47,47	0.84	2 (4%)
11	LOP	A	501	-	44,44,44	0.49	0	47,49,49	0.80	0
13	HEM	C	501	3	50,50,50	1.73	11 (22%)	66,82,82	1.90	20 (30%)
11	LOP	C	503	-	44,44,44	0.56	0	47,49,49	0.95	3 (6%)
16	HEC	D	501	4	50,50,50	2.70	26 (52%)	68,82,82	2.87	34 (50%)
12	CDL	D	502	-	93,93,99	0.44	0	99,105,111	0.63	0
19	SO4	G	103	-	4,4,4	0.28	0	6,6,6	0.11	0
18	PSC	E	203	-	51,51,51	0.56	0	57,59,59	1.28	4 (7%)
11	LOP	E	202	-	44,44,44	0.45	0	47,49,49	0.92	2 (4%)
11	LOP	C	506	-	44,44,44	0.62	0	47,49,49	0.90	1 (2%)
19	SO4	F	201	-	4,4,4	0.30	0	6,6,6	0.17	0
19	SO4	G	102	-	4,4,4	0.34	0	6,6,6	0.12	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
12	CDL	A	502	-	-	52/93/93/110	-
13	HEM	C	502	3	-	4/14/54/54	-
18	PSC	E	203	-	-	28/55/55/55	-
12	CDL	C	504	-	-	54/110/110/110	-
11	LOP	G	101	-	-	27/48/48/48	-
13	HEM	C	501	3	-	4/14/54/54	-
11	LOP	C	503	-	-	17/48/48/48	-
11	LOP	E	202	-	-	23/48/48/48	-
15	LMT	C	508	-	-	7/21/61/61	0/2/2/2
16	HEC	D	501	4	1/1/3/7	5/14/54/54	-
11	LOP	C	506	-	-	21/48/48/48	-
14	A1IKG	C	505	-	1/1/6/6	0/13/40/40	0/4/4/4
11	LOP	A	501	-	-	22/48/48/48	-
12	CDL	D	502	-	-	49/104/104/110	-
17	FES	E	201	5	-	-	0/1/1/1
11	LOP	C	507	-	-	33/48/48/48	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	505	A1IKG	C6-C2	-6.04	1.42	1.52
13	C	502	HEM	C1B-NB	-5.33	1.31	1.40
16	D	501	HEC	FE-NB	5.24	2.11	1.94
16	D	501	HEC	C2A-C3A	5.10	1.47	1.36
16	D	501	HEC	C3D-C2D	5.00	1.47	1.36

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	501	HEC	C1C-C2C-C3C	-7.41	98.16	106.83
16	D	501	HEC	C3D-C4D-ND	7.05	117.18	110.36
16	D	501	HEC	C2B-C1B-NB	6.66	117.86	109.88
18	E	203	PSC	O01-C1-C2	6.49	125.50	111.50
11	G	101	LOP	O5-C6-C7	6.29	125.06	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	505	A1IKG	C6
16	D	501	HEC	NA

5 of 346 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	LOP	N1-C1-C2-O1
11	A	501	LOP	C2-O1-P1-O4
11	C	507	LOP	N1-C1-C2-O1
11	C	507	LOP	C2-O1-P1-O2
11	C	507	LOP	C2-O1-P1-O3

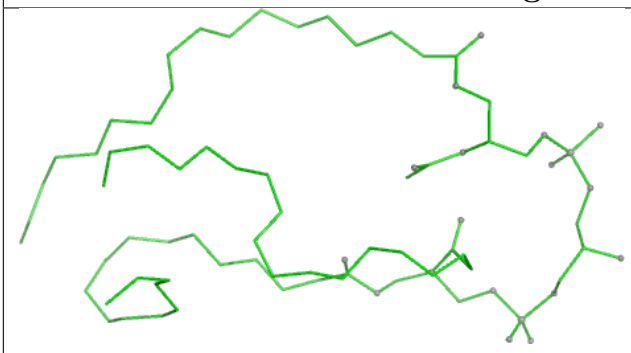
There are no ring outliers.

13 monomers are involved in 84 short contacts:

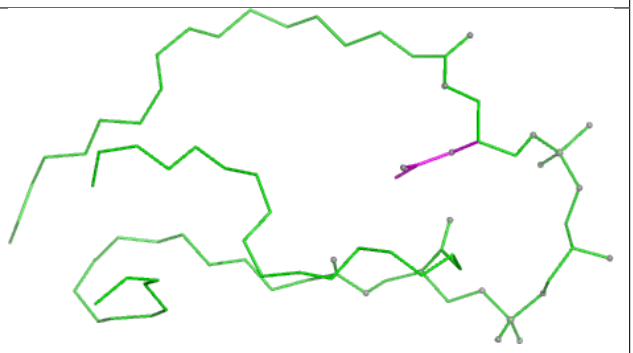
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	502	CDL	21	0
12	C	504	CDL	11	0
13	C	502	HEM	5	0
11	G	101	LOP	4	0
15	C	508	LMT	3	0
11	A	501	LOP	11	0
13	C	501	HEM	3	0
11	C	503	LOP	5	0
16	D	501	HEC	2	0
12	D	502	CDL	12	0
18	E	203	PSC	5	0
11	E	202	LOP	7	0
11	C	506	LOP	4	0

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.

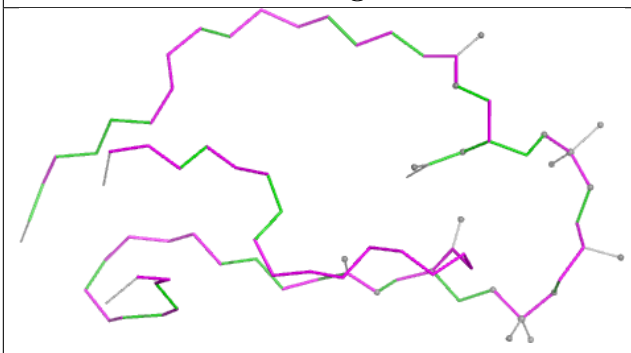
Ligand CDL A 502



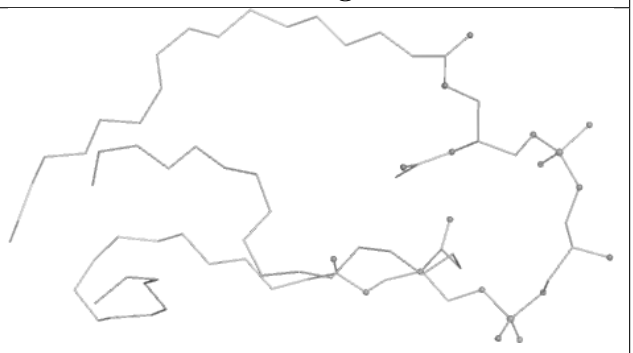
Bond lengths



Bond angles

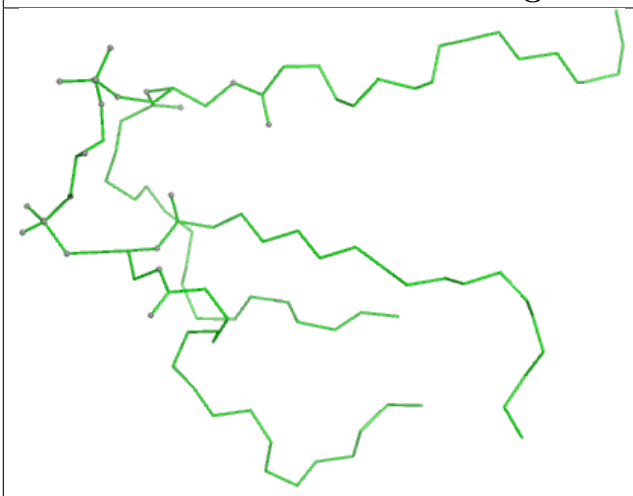


Torsions



Rings

Ligand CDL C 504



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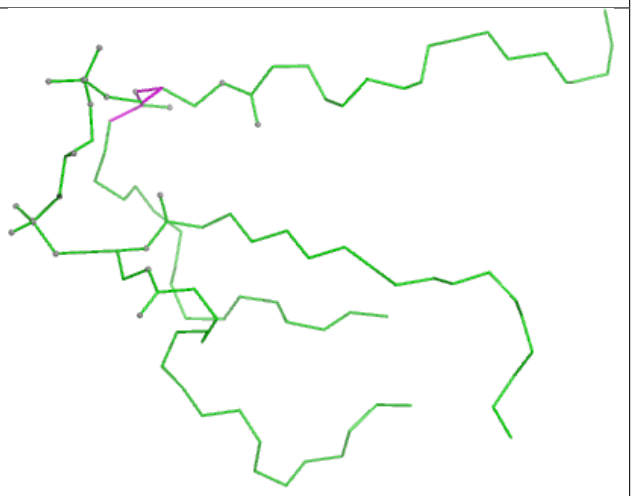

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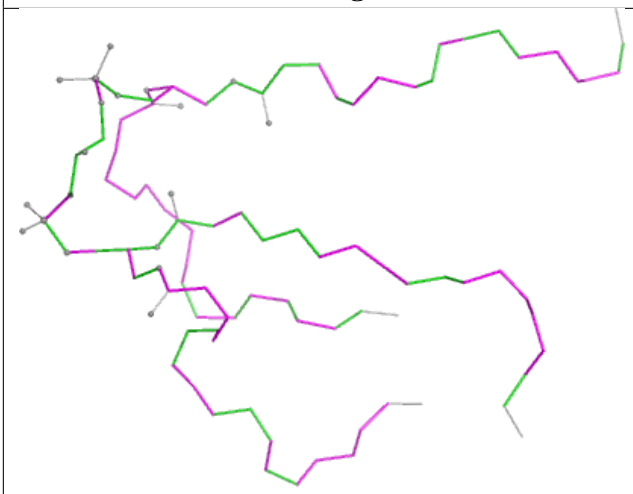
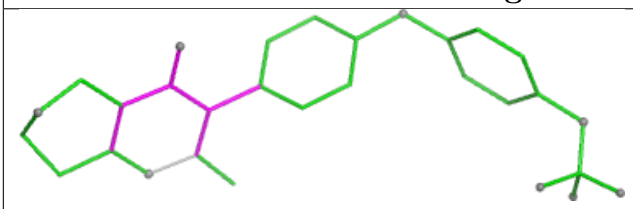


Torsions



Rings

Ligand A1IKG C 505



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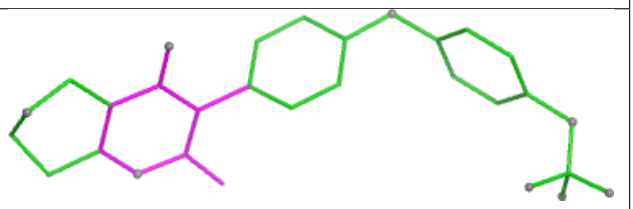

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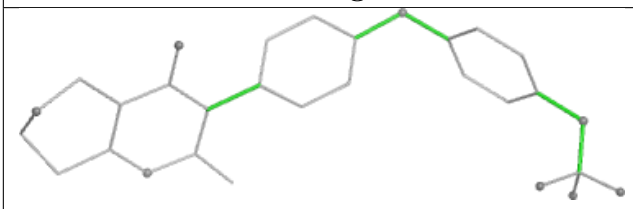

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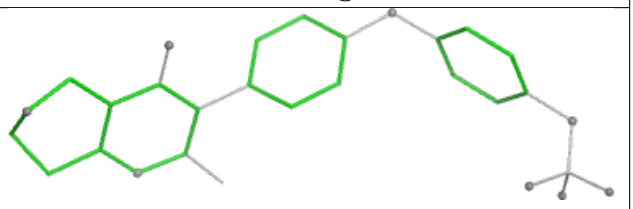
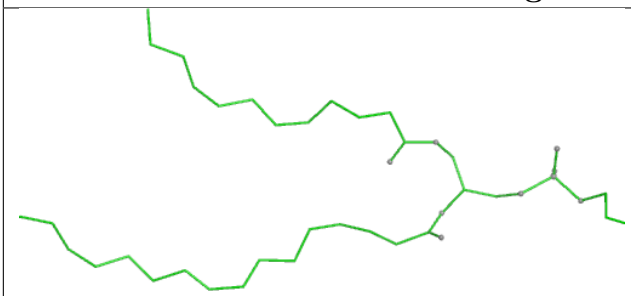
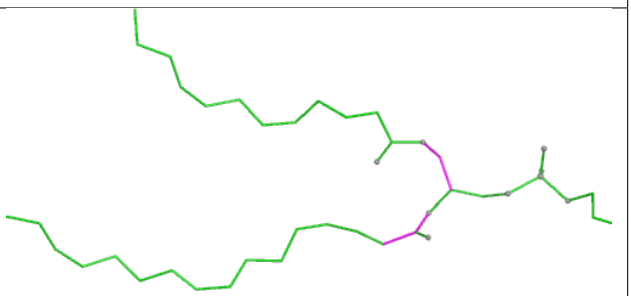


Rings

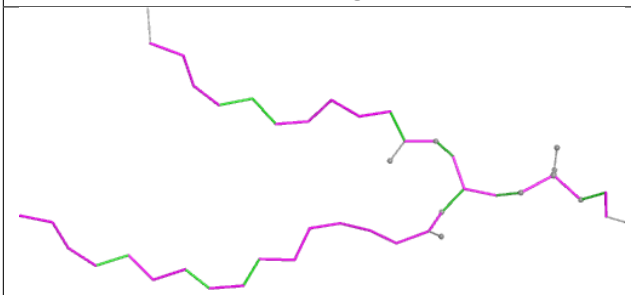
Ligand LOP C 507



Bond lengths



Bond angles

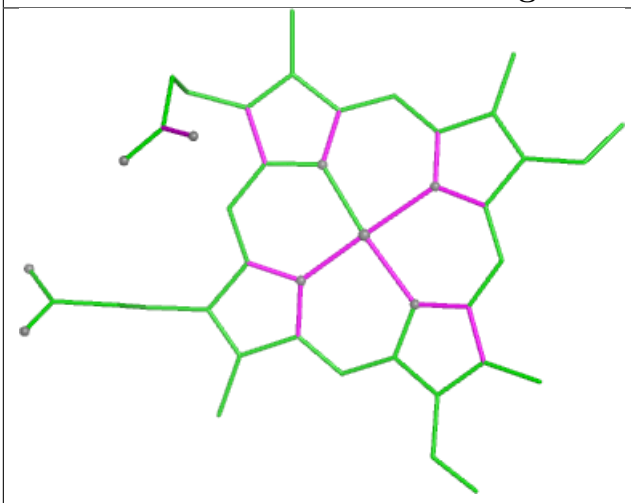


Torsions



Rings

Ligand HEM C 502



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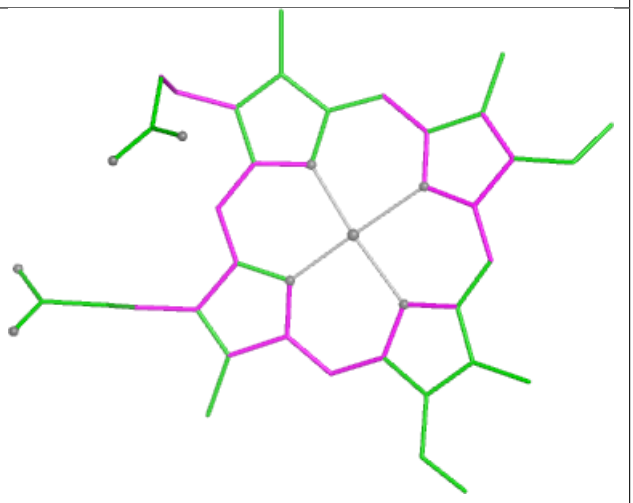
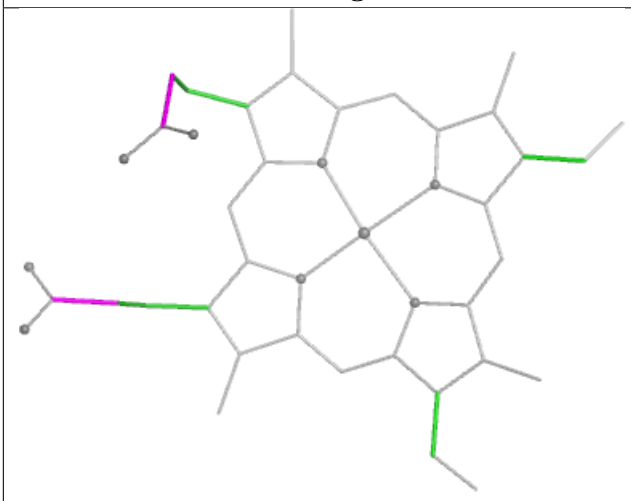


Bond angles



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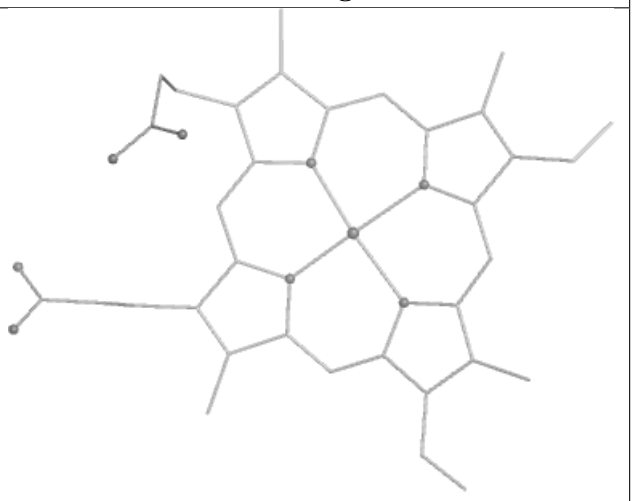
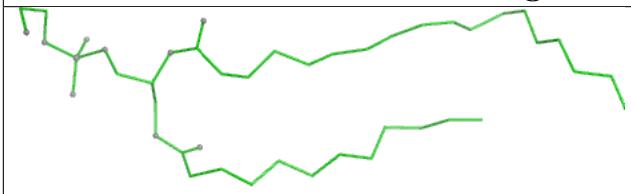
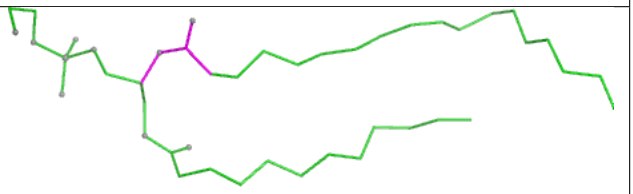


Rings

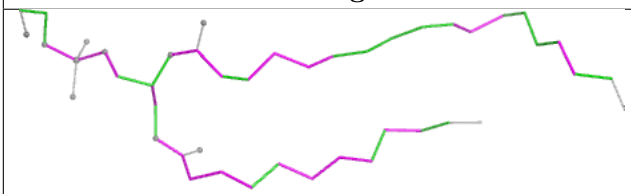
Ligand LOP G 101



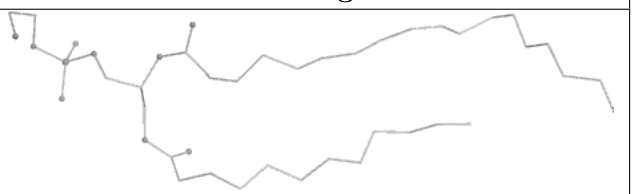
Bond lengths



Bond angles

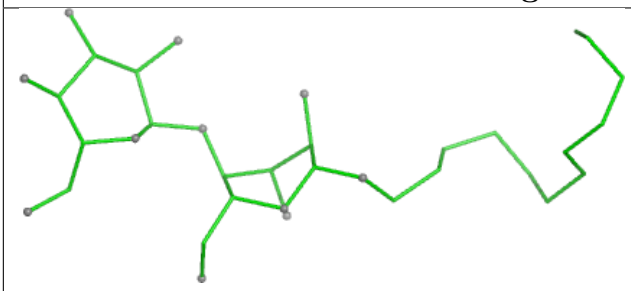


Torsions



Rings

Ligand LMT C 508



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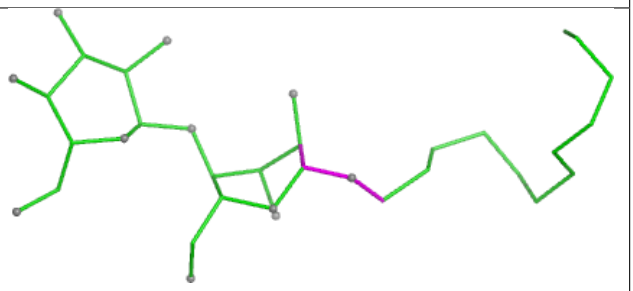
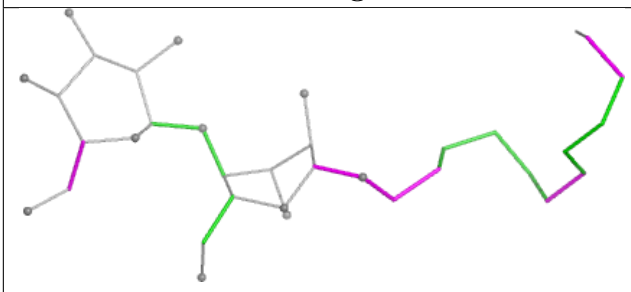
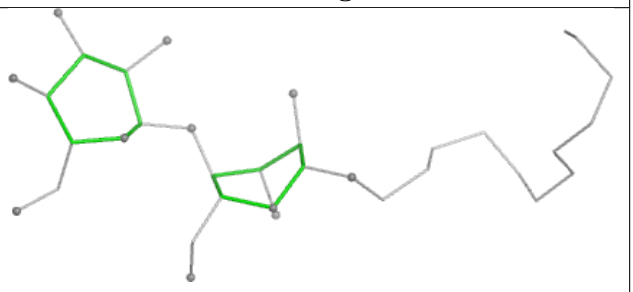


Bond angles

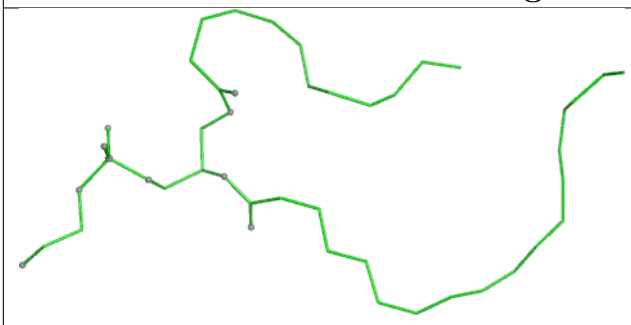


Torsions

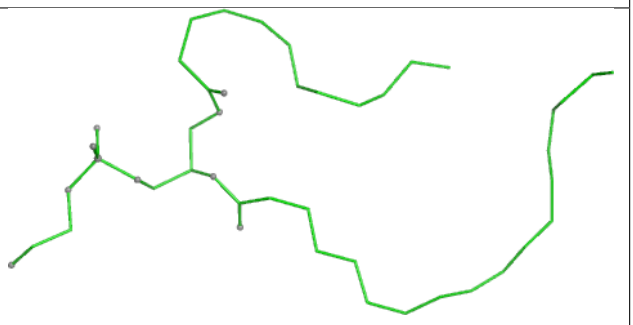


Rings

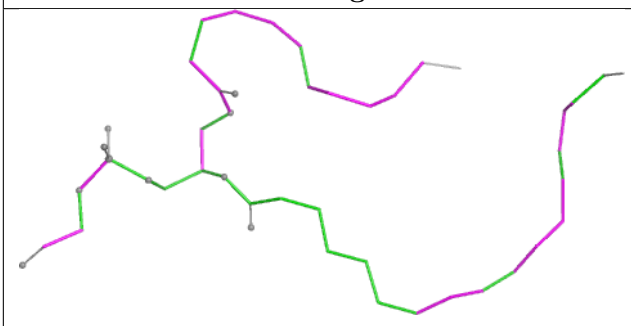
Ligand LOP A 501



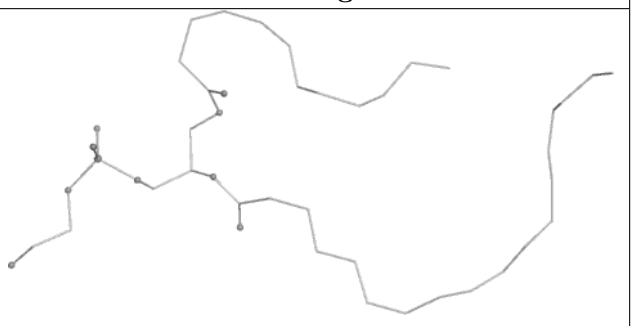
Bond lengths



Bond angles

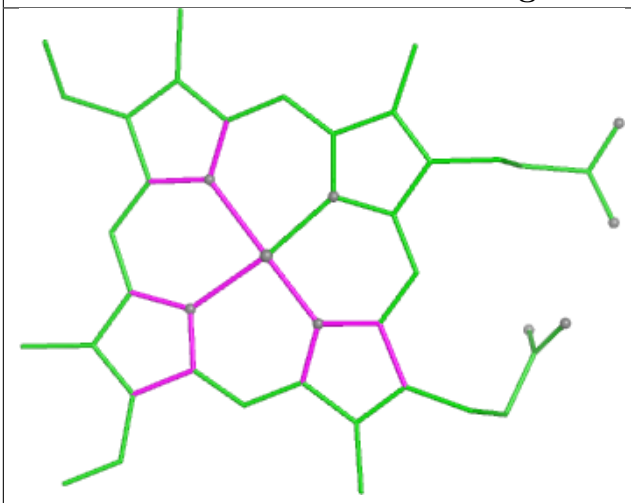


Torsions

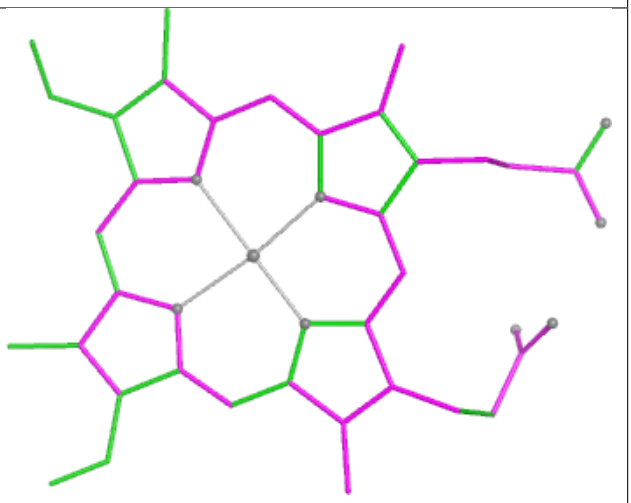


Rings

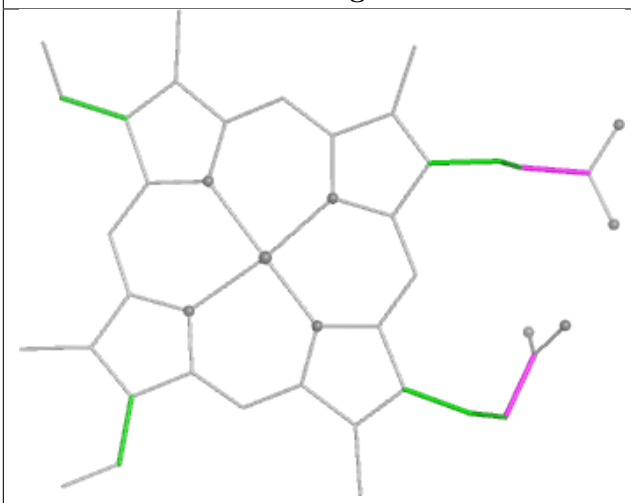
Ligand HEM C 501



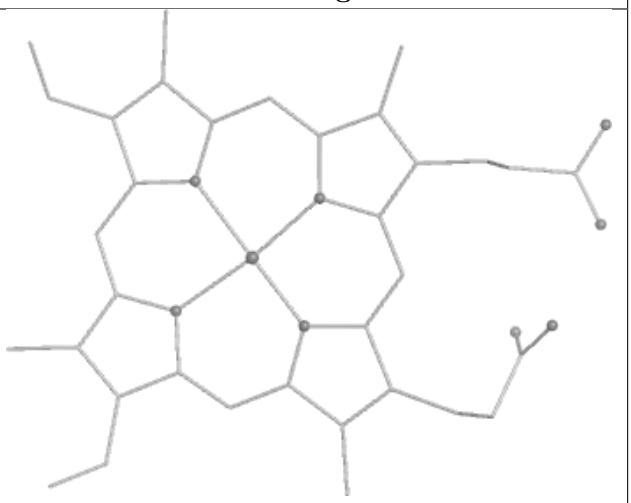
Bond lengths



Bond angles

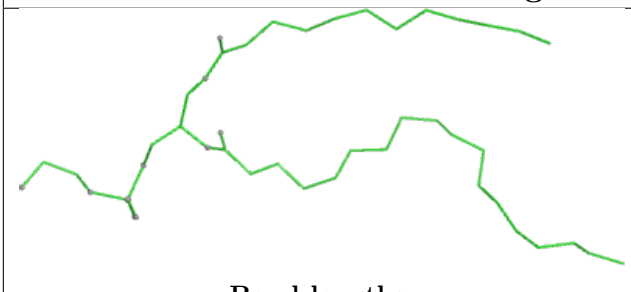


Torsions

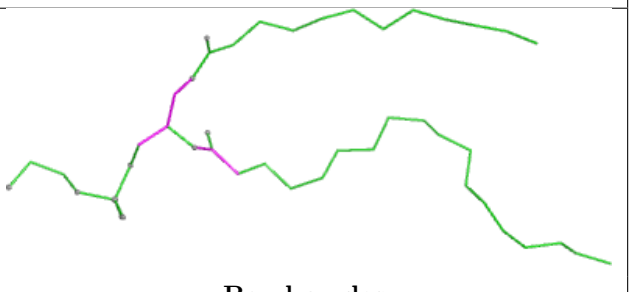


Rings

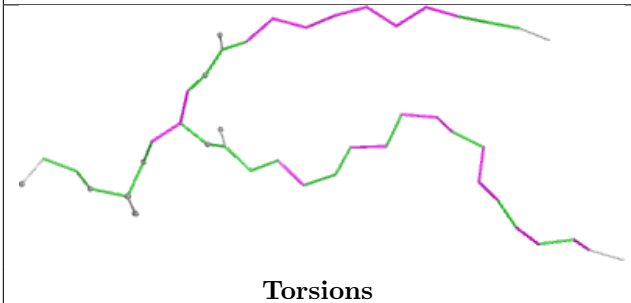
Ligand LOP C 503



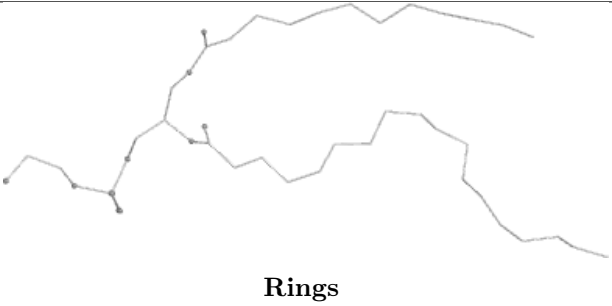
Bond lengths



Bond angles

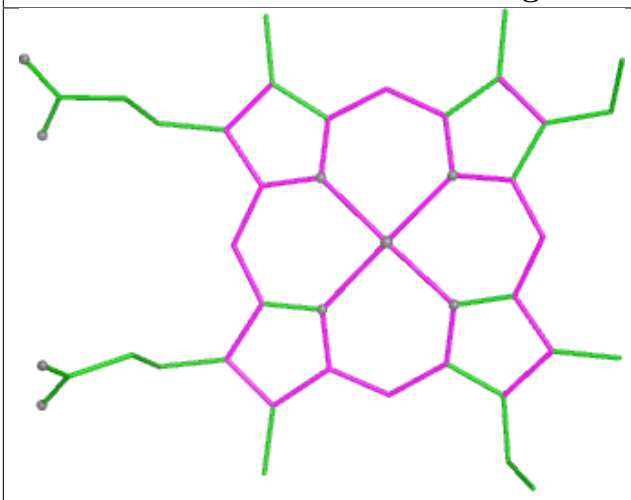


Torsions

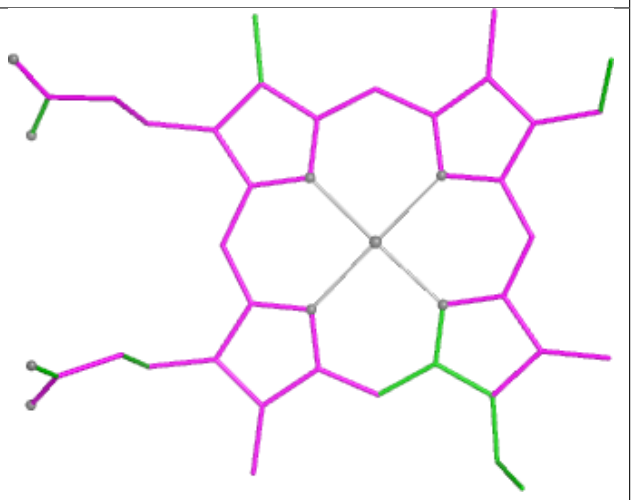


Rings

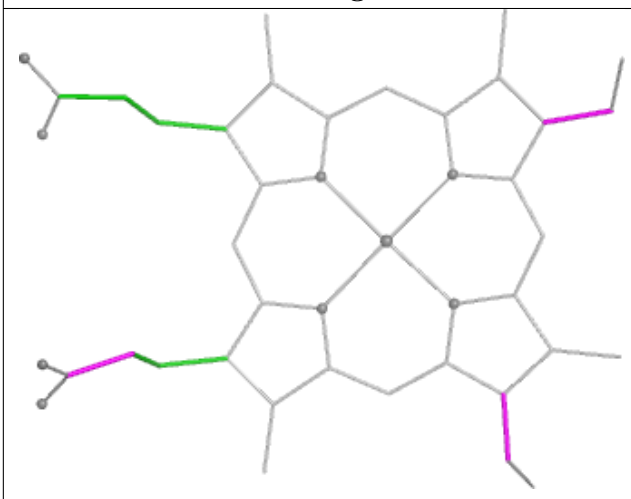
Ligand HEC D 501



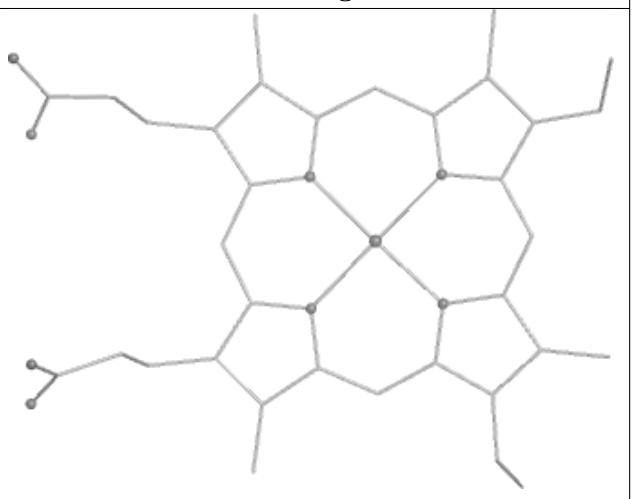
Bond lengths



Bond angles

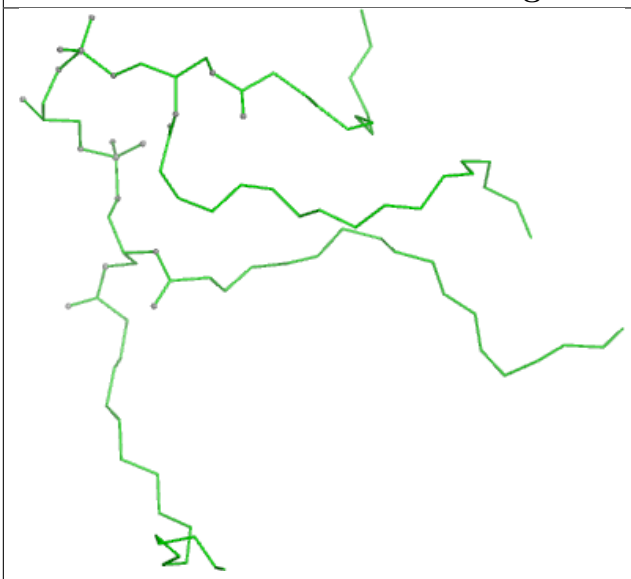


Torsions

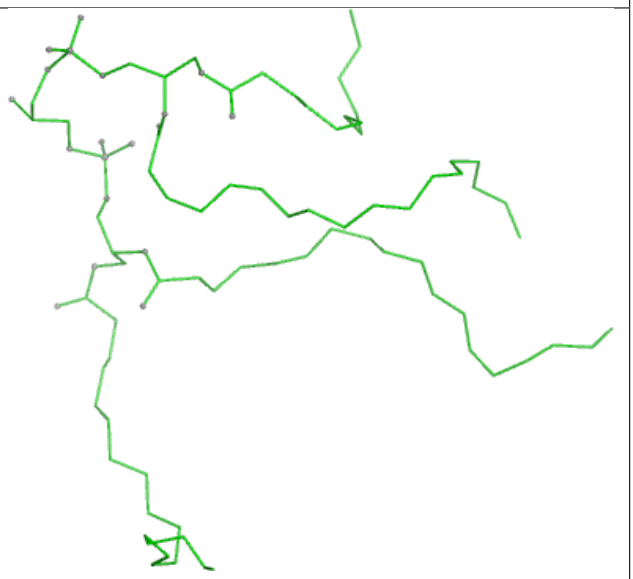


Rings

Ligand CDL D 502



Bond lengths



Bond angles

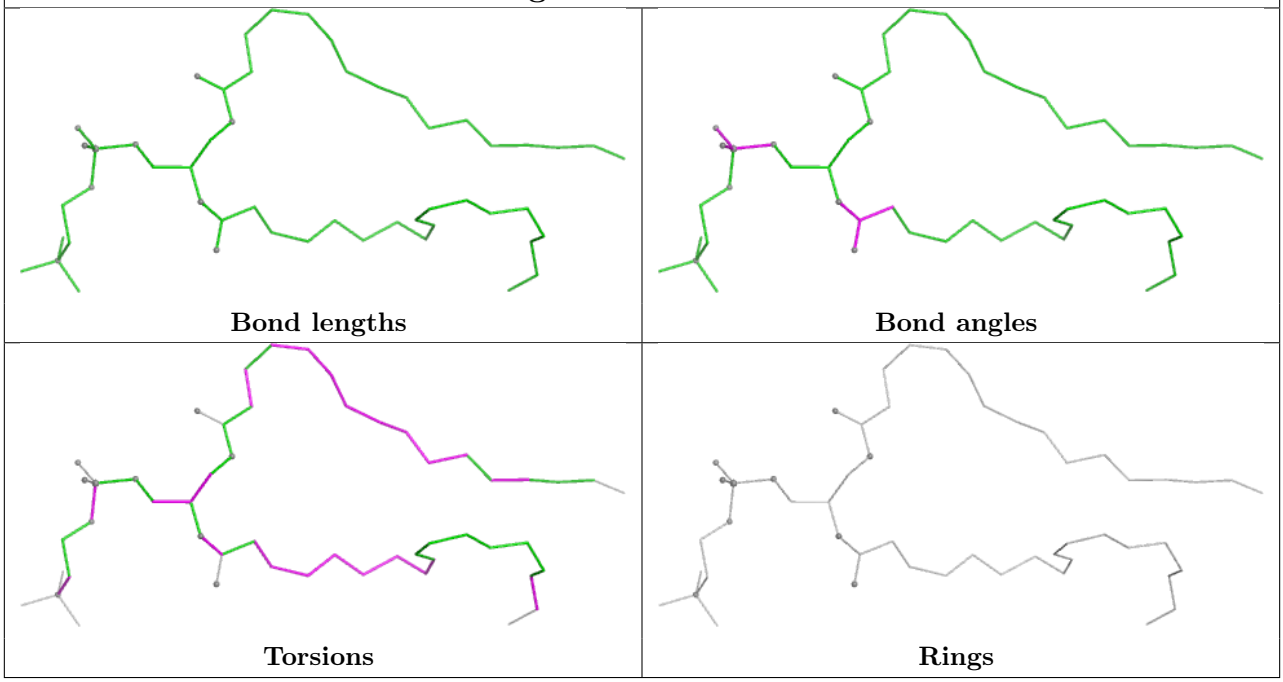


Torsions

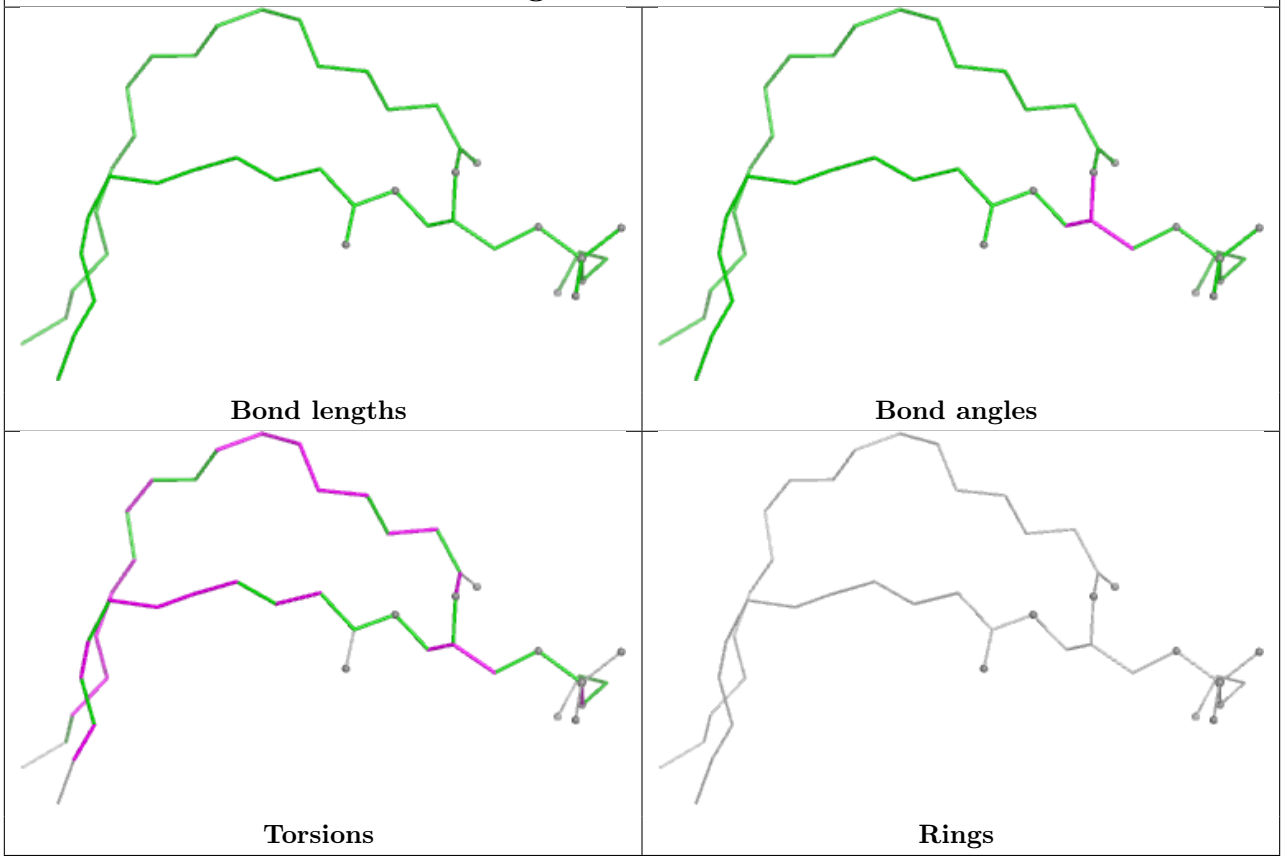


Rings

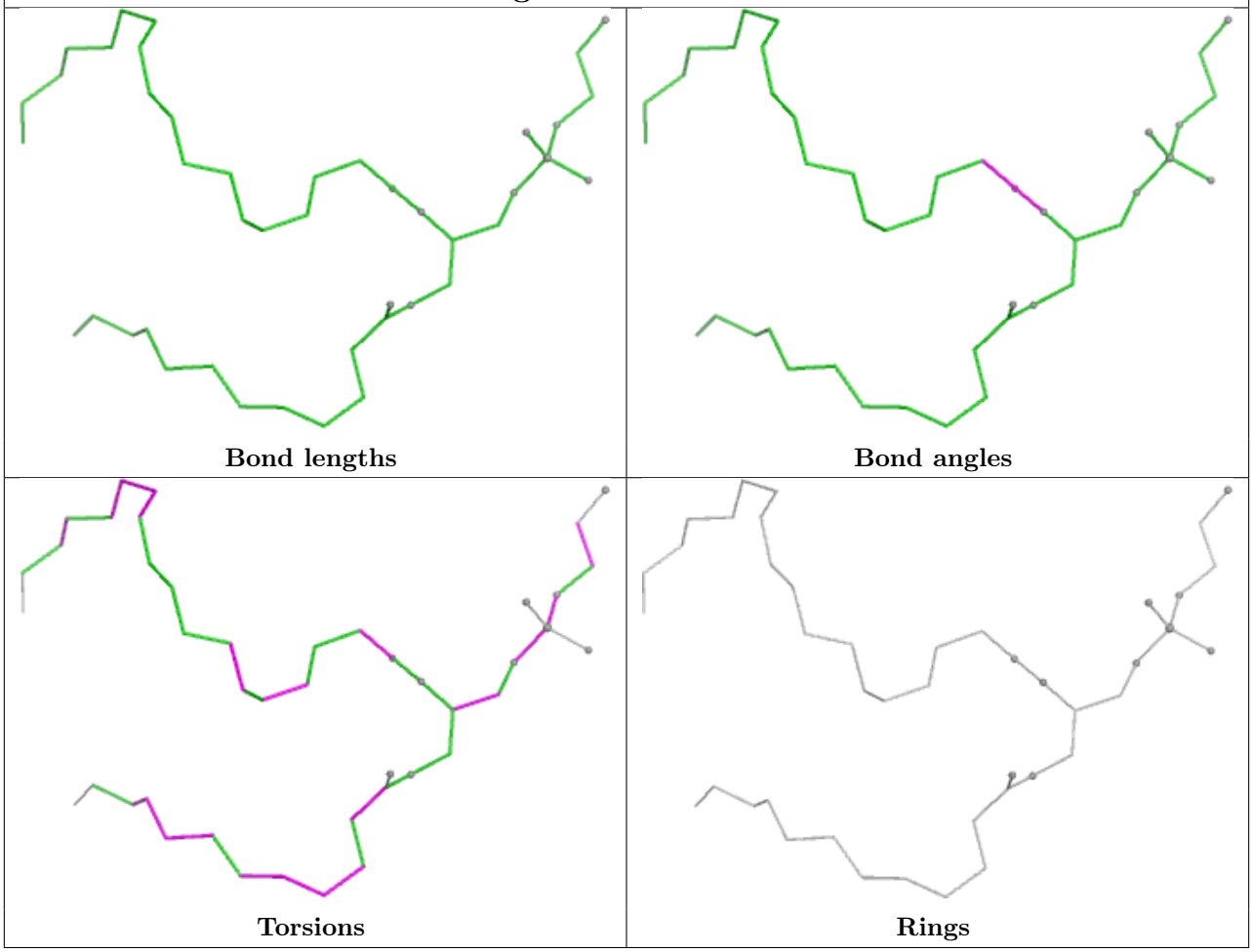
Ligand PSC E 203



Ligand LOP E 202



Ligand LOP C 506



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	440/480 (91%)	-0.77	0 100 100	70, 111, 146, 195	0
2	B	414/453 (91%)	-0.70	1 (0%) 91 81	47, 112, 148, 230	1 (0%)
3	C	378/379 (99%)	-0.63	1 (0%) 90 75	28, 104, 140, 195	3 (0%)
4	D	240/325 (73%)	-0.53	0 100 100	91, 140, 171, 199	0
5	E	196/274 (71%)	-0.31	2 (1%) 79 54	88, 156, 199, 240	0
5	I	27/274 (9%)	0.30	3 (11%) 10 7	101, 143, 177, 188	0
6	F	98/111 (88%)	-0.56	0 100 100	82, 107, 149, 167	0
7	G	74/82 (90%)	-0.61	0 100 100	80, 115, 155, 176	0
8	H	65/109 (59%)	-0.35	0 100 100	126, 164, 182, 200	0
9	J	56/64 (87%)	-0.59	0 100 100	101, 121, 149, 167	0
10	K	39/56 (69%)	0.61	3 (7%) 19 13	152, 185, 233, 265	0
All	All	2027/2607 (77%)	-0.58	10 (0%) 87 67	28, 116, 177, 265	4 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	230	LEU	4.0
5	E	114	VAL	3.1
3	C	237	LEU	2.6
5	E	178	LEU	2.5
10	K	13	LEU	2.5

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

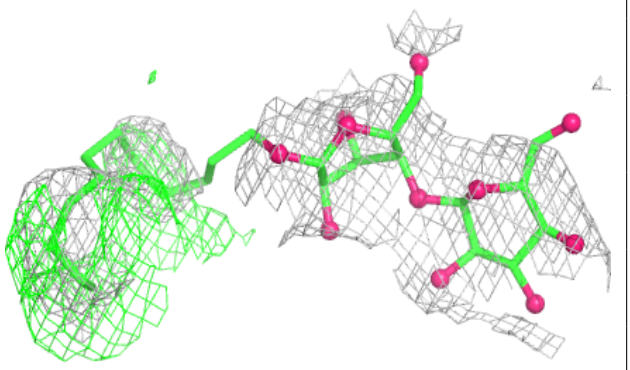
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

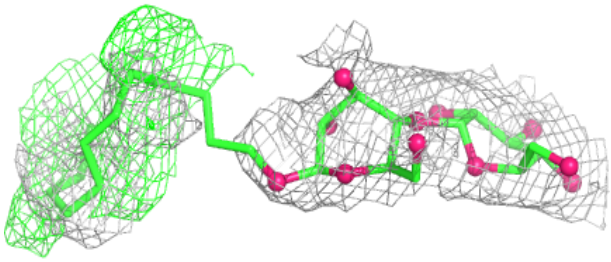
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	LMT	C	508	35/35	0.55	0.15	127,200,240,296	0
11	LOP	C	506	45/45	0.77	0.27	66,143,208,276	0
19	SO4	G	102	5/5	0.77	0.07	160,182,202,241	0
19	SO4	F	201	5/5	0.85	0.16	145,161,171,183	0
11	LOP	G	101	45/45	0.86	0.23	105,180,215,234	0
19	SO4	G	103	5/5	0.88	0.09	139,145,164,170	0
11	LOP	C	507	45/45	0.90	0.20	76,140,205,246	0
11	LOP	A	501	45/45	0.90	0.18	81,186,233,251	0
12	CDL	A	502	84/100	0.91	0.15	109,172,285,348	0
12	CDL	D	502	94/100	0.91	0.16	88,156,187,215	0
18	PSC	E	203	52/52	0.92	0.17	99,147,207,260	0
14	A1IKG	C	505	30/30	0.93	0.12	98,134,186,196	0
12	CDL	C	504	100/100	0.93	0.14	94,149,200,240	0
11	LOP	E	202	45/45	0.96	0.11	93,113,175,262	0
11	LOP	C	503	45/45	0.98	0.09	80,106,125,172	0
17	FES	E	201	4/4	0.98	0.06	220,233,252,274	0
16	HEC	D	501	43/43	0.99	0.07	116,138,150,162	0
13	HEM	C	501	43/43	0.99	0.05	86,94,105,128	0
13	HEM	C	502	43/43	0.99	0.06	62,96,111,124	0

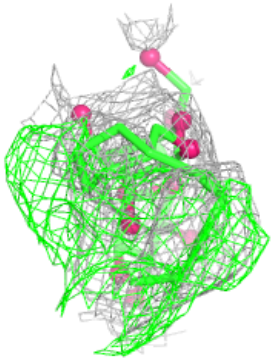
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT C 508:

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

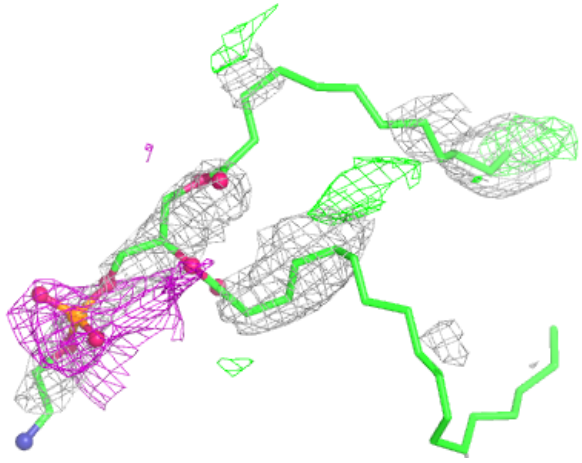


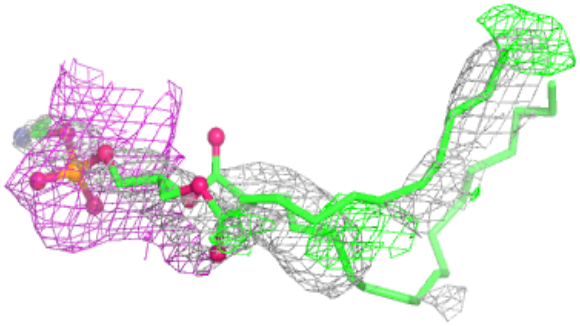


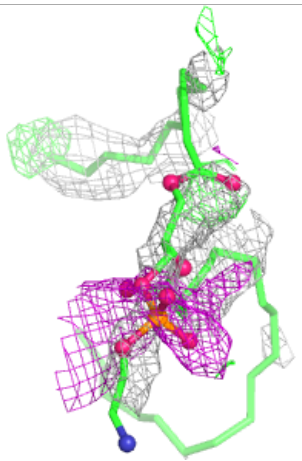


Electron density around LOP C 506:

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

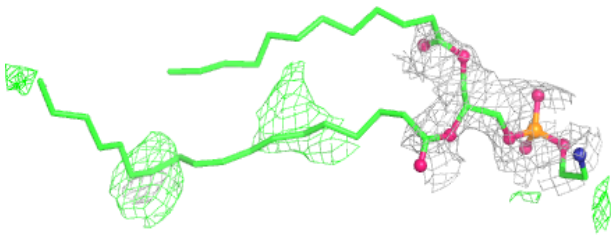


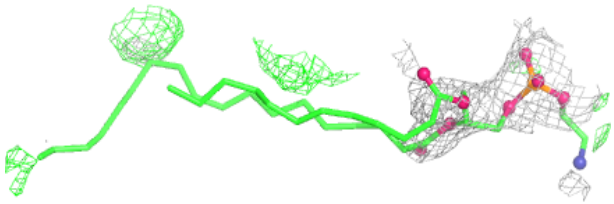


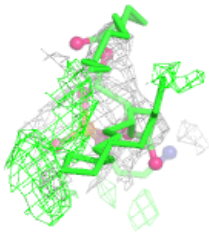


Electron density around LOP G 101:

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

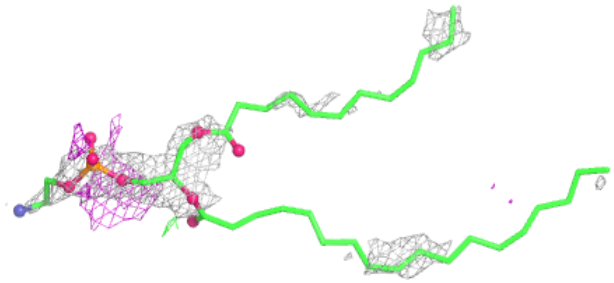


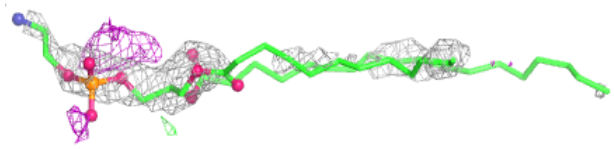


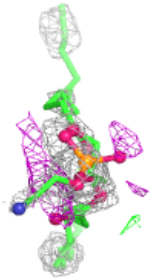


Electron density around LOP C 507:

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

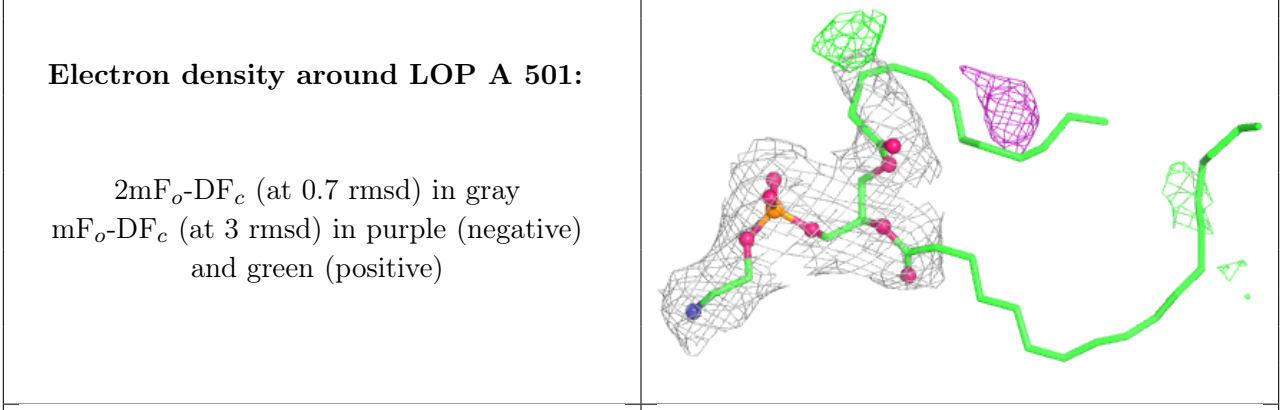


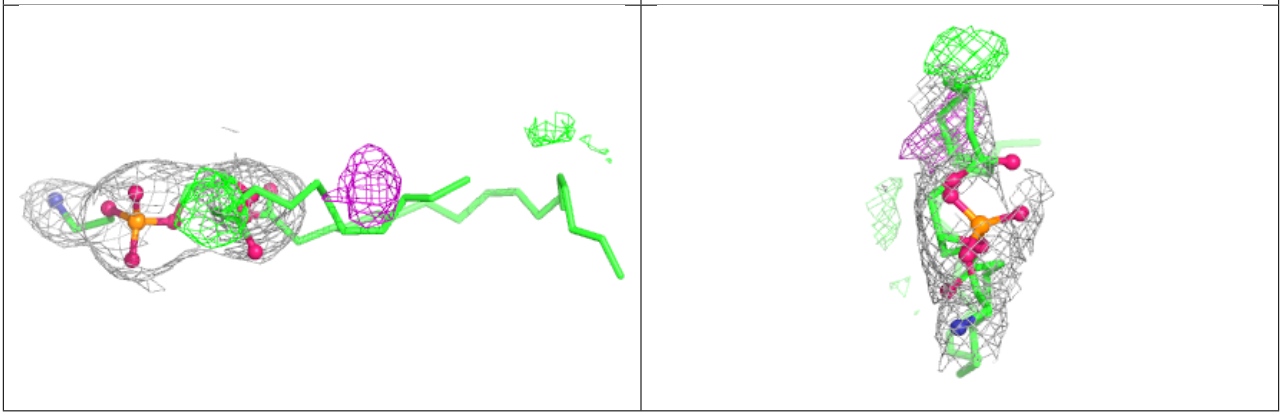




Electron density around LOP A 501:

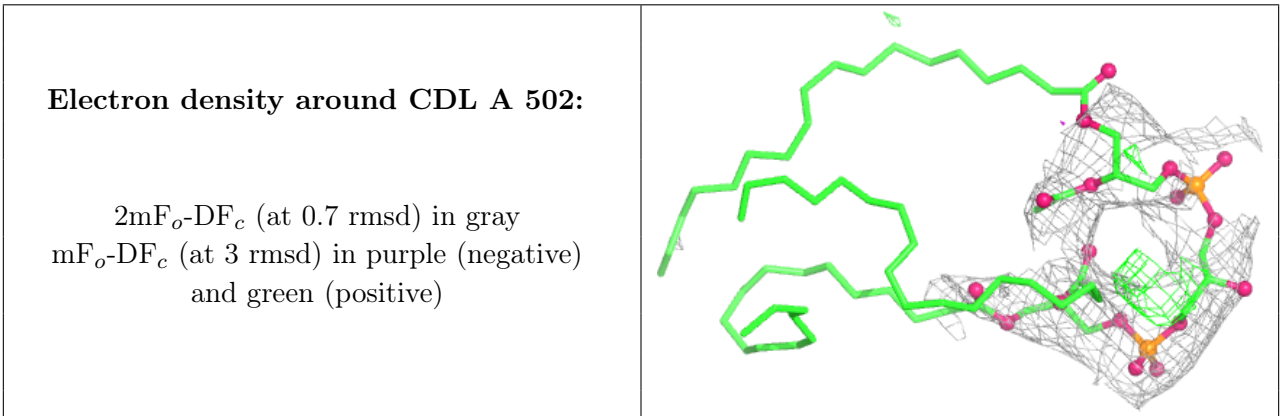
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

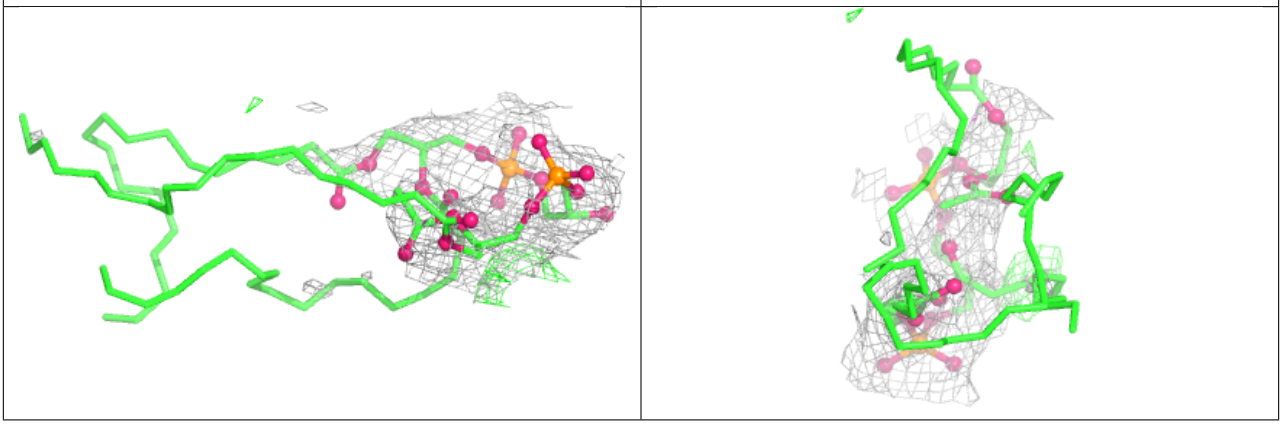




Electron density around CDL A 502:

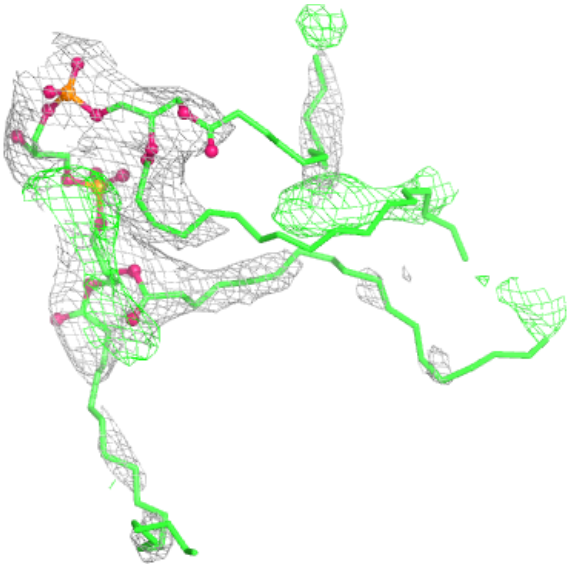
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

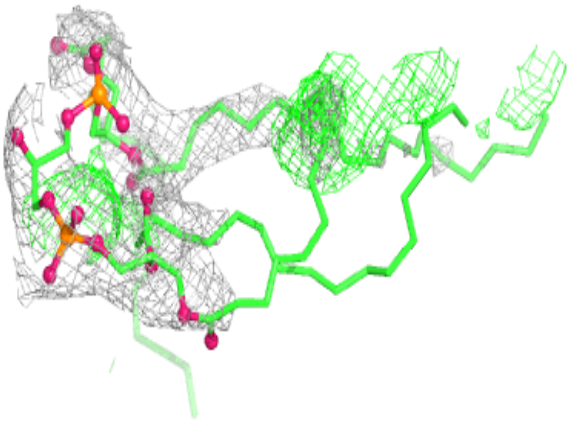


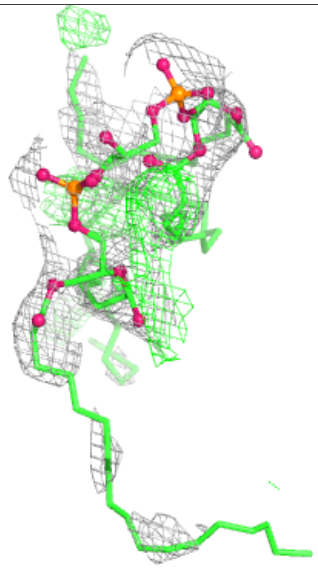


Electron density around CDL D 502:

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

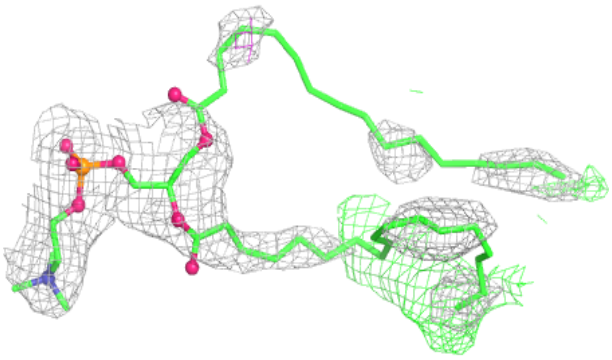


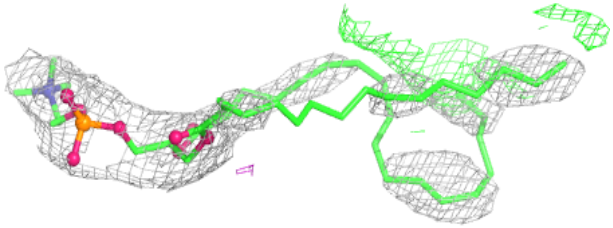


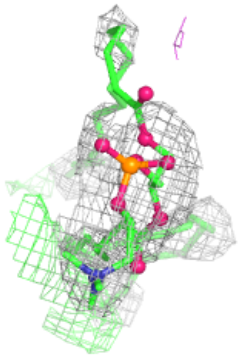


Electron density around PSC E 203:

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

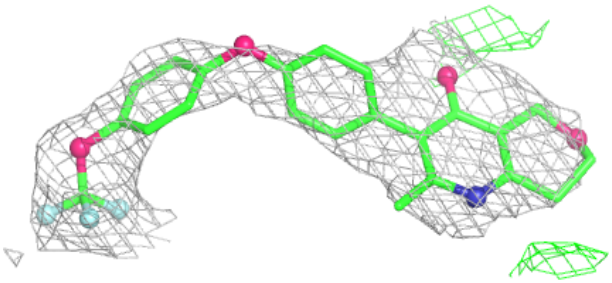


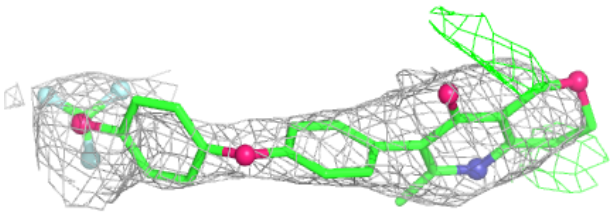


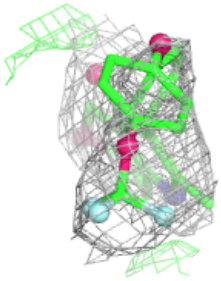


Electron density around A1IKG C 505:

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

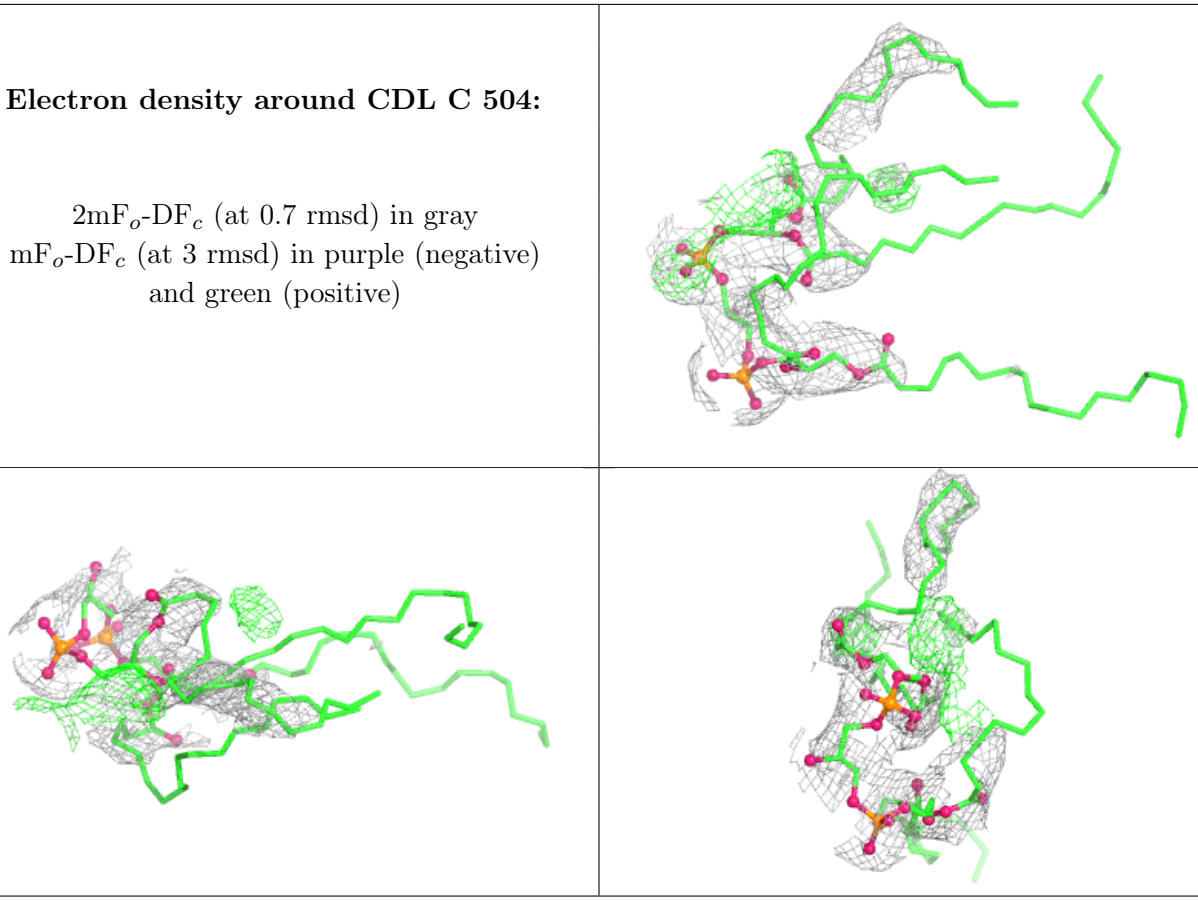






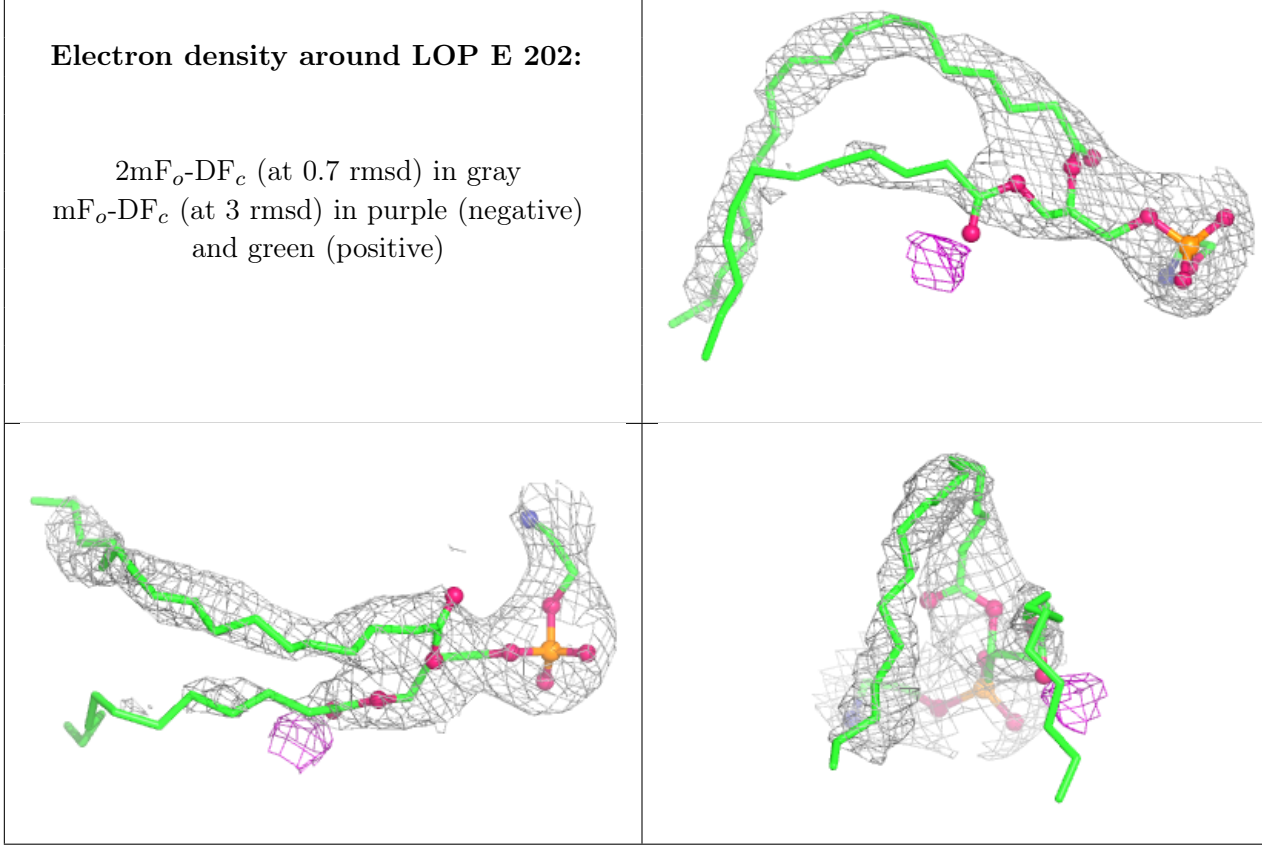
Electron density around CDL C 504:

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



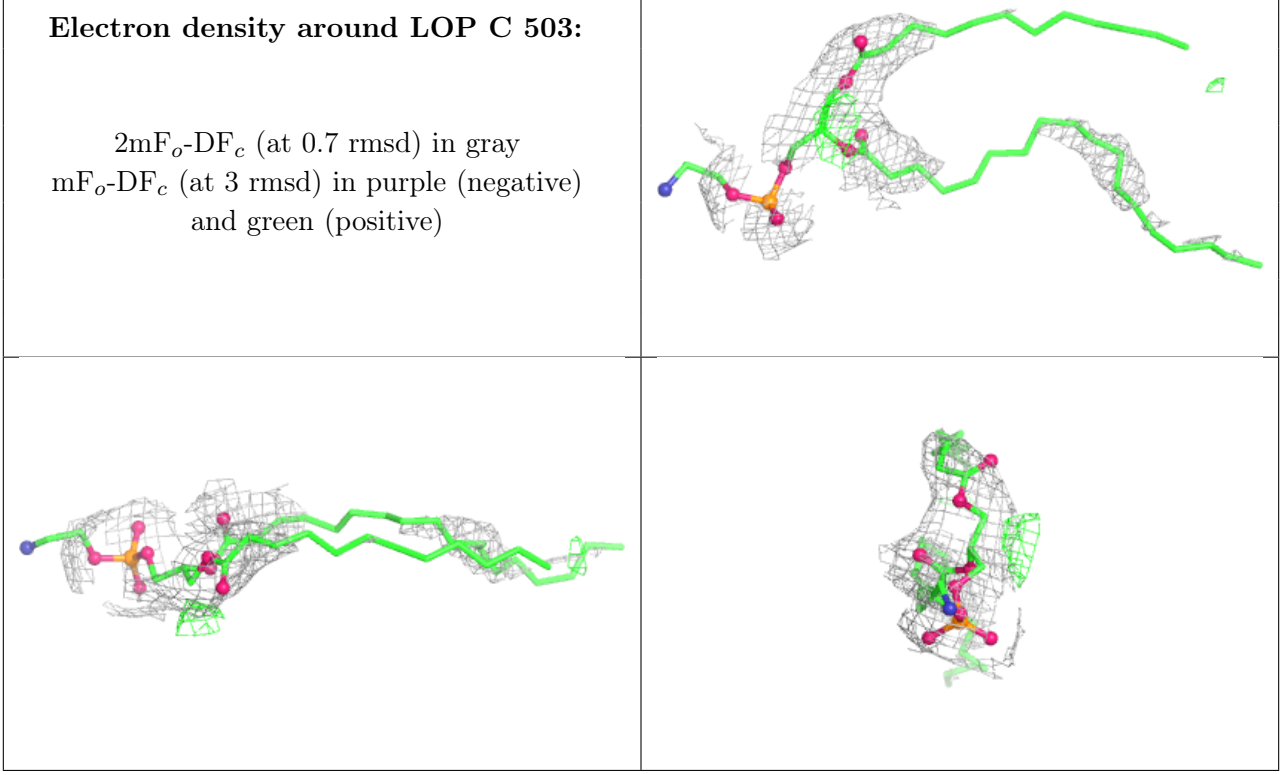
Electron density around LOP E 202:

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



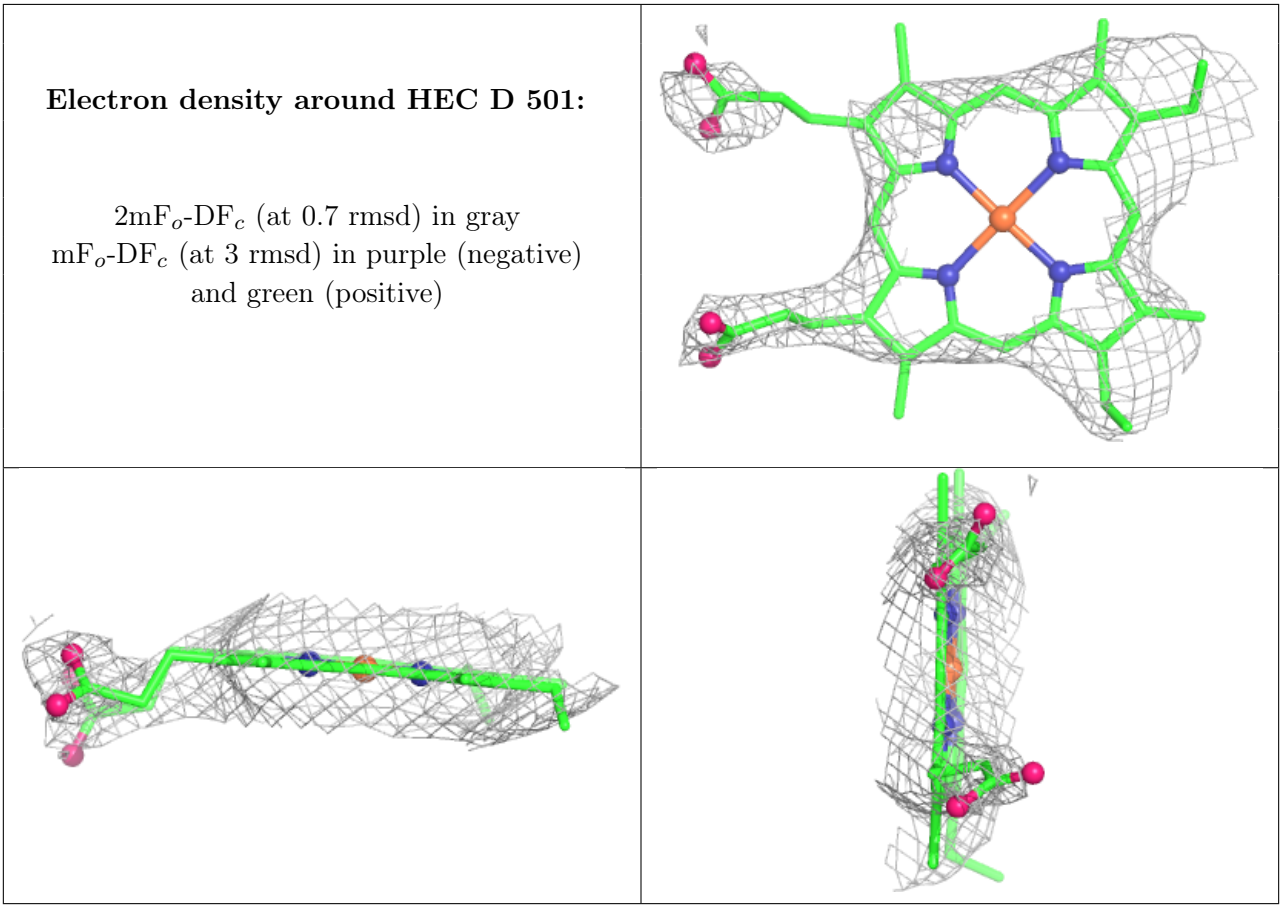
Electron density around LOP C 503:

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



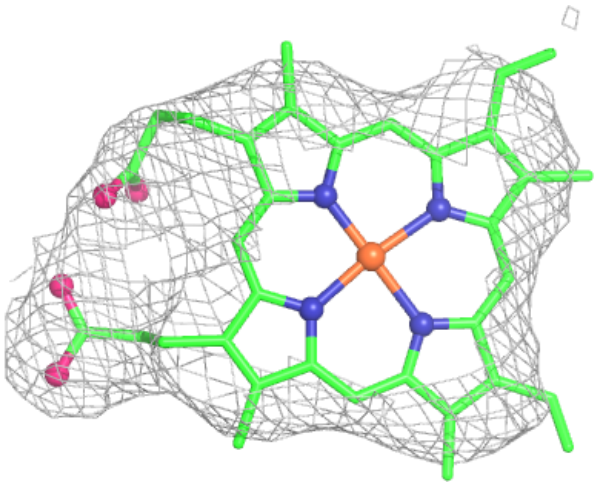
Electron density around HEC D 501:

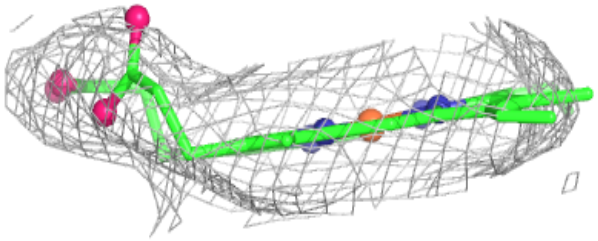
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

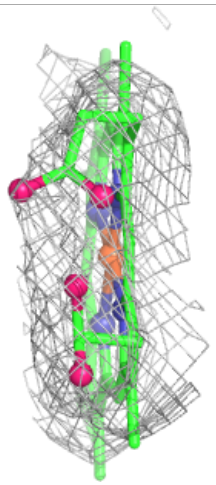


Electron density around HEM C 501:

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

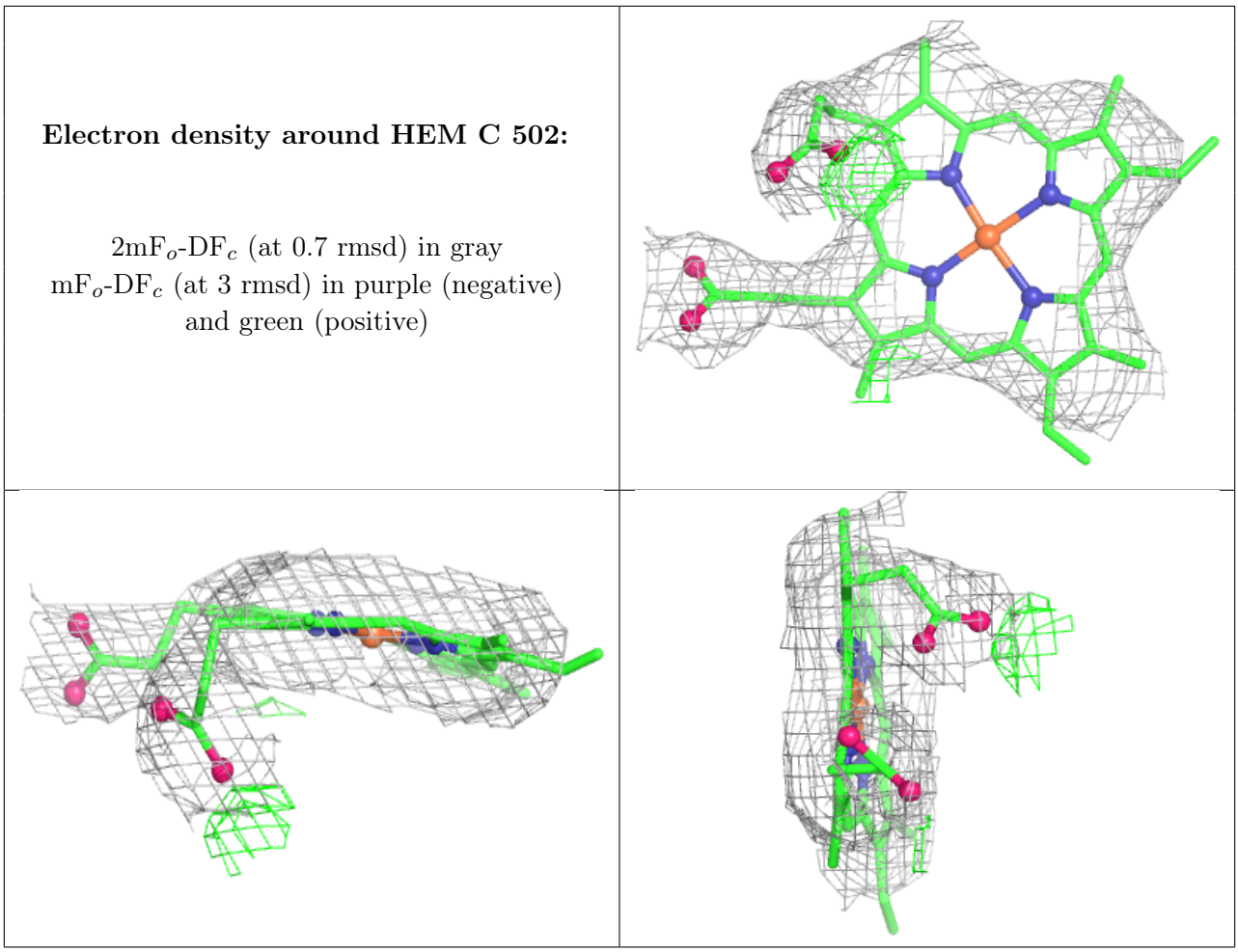






Electron density around HEM C 502:

$2mF_o$-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.