wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 04:15 AM EDT

PDB ID	:	6NHG
Title	:	Rhodobacter sphaeroides Mitochondrial respiratory chain complex
Authors	:	Xia, D.; Zhou, F.; Esser, L.
Deposited on	:	2018-12-21
Resolution	:	2.80 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:

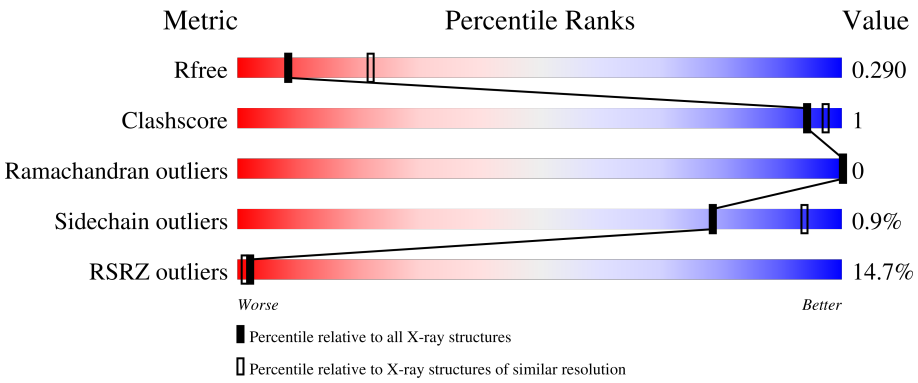
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	446	5%, 97%, .
2	B	439	4%, 95%, . .
3	C	379	3%, 93%, 7%
4	D	241	21%, 98%, .
5	E	196	58%, 94%, 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	110	7% 93% • 5%
7	G	80	10% 85% 8% • 6%
8	H	78	32% 81% 5% 14%
9	I	78	17% 44% 56%
10	J	63	24% 90% 6% •
11	K	55	31% 84% 11% 5%

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	6PE	K	101	-	-	-	X

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 33542 atoms, of which 16676 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	H	N	O	S			
1	A	446	6799	2161	3341	609	668	20	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	425	6328	1998	3147	564	612	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	378	6056	2013	3053	471	501	18	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	241	3778	1225	1859	330	349	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	H	N	O	S			
5	E	196	3015	957	1497	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	H	N	O	S			
6	F	105	1816	576	905	166	167	2	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
7	G	75	1261	410	633	118	99	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	H	N	O	S			
8	H	67	1075	332	527	99	112	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	H	N	O	S			
9	I	34	509	149	265	51	43	1	0	0	0

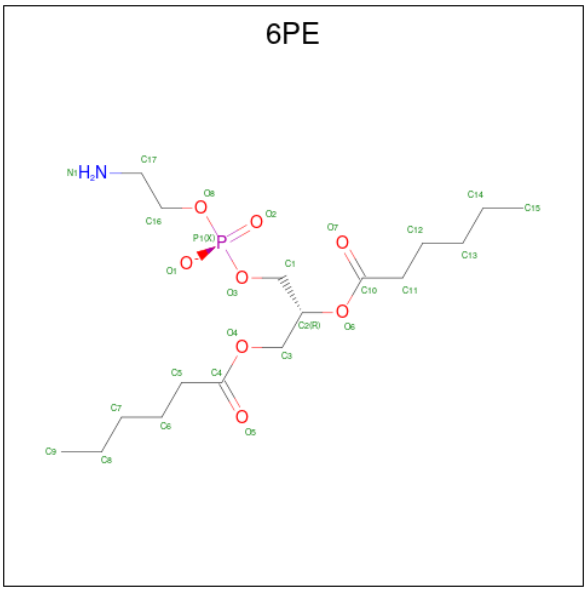
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
10	J	61	1004	329	502	87	86	0	0	0

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

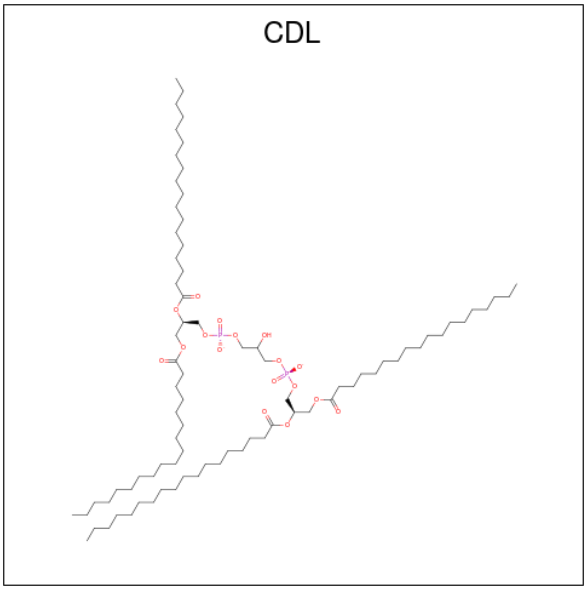
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
11	K	52	865	288	435	77	65	0	0	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
12	A	1	60	17	33	1	8	1	0	0
			Total	C	H	N	O	P		
12	K	1	60	17	33	1	8	1	0	0

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



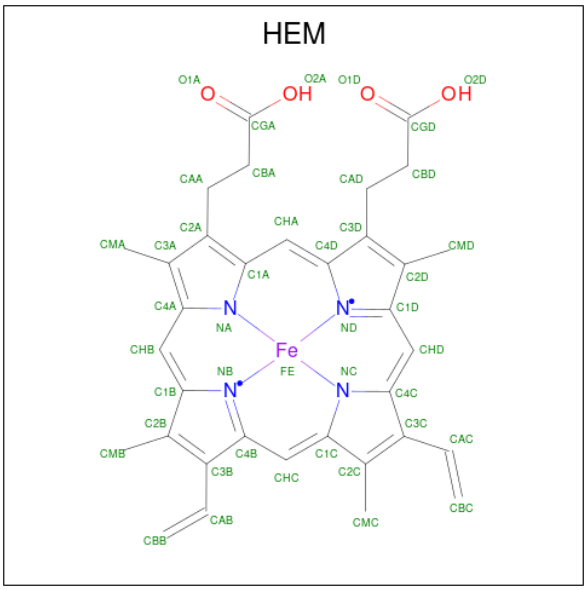
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
13	A	1	124	41	64	17	2	0	0
			Total	C	H	O	P		
13	D	1	124	41	64	17	2	0	0

Continued on next page...

Continued from previous page...

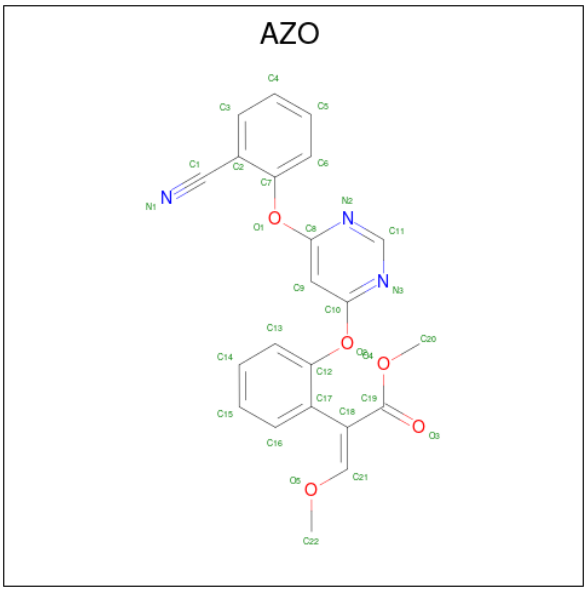
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
13	G	1	124	41	64	17	2	0	0

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



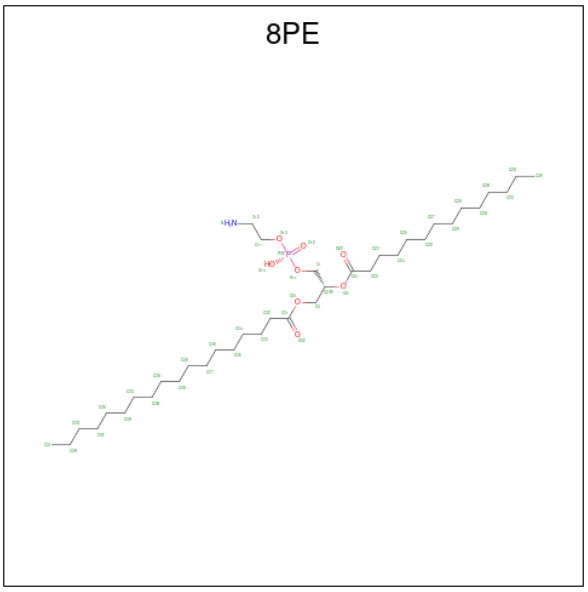
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
14	C	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
14	C	1	73	34	1	30	4	4	0	0

- Molecule 15 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: $C_{22}H_{17}N_3O_5$).



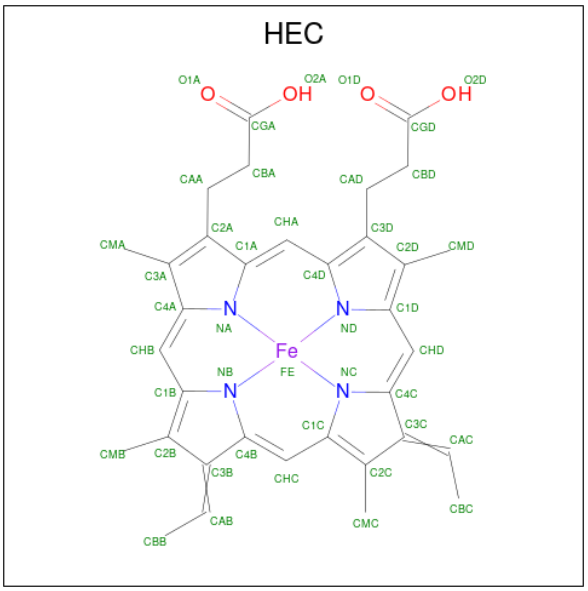
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
15	C	1	47	22	17	3	5	0	0

- Molecule 16 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: $C_{37}H_{74}NO_8P$).



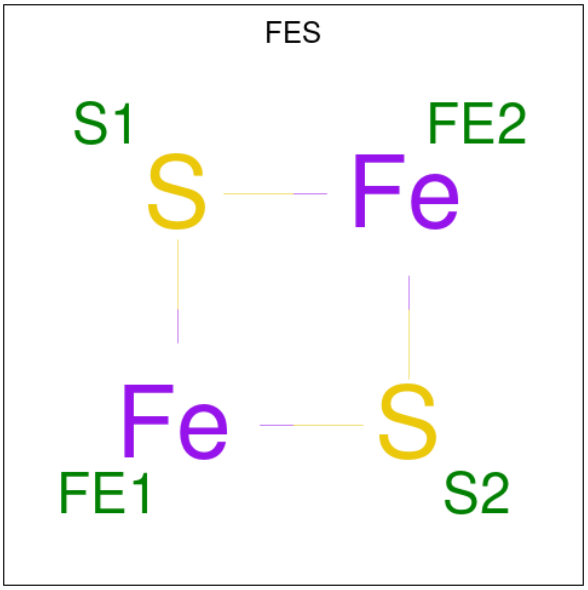
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
16	C	1	120	37	73	1	8	1	0	0

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



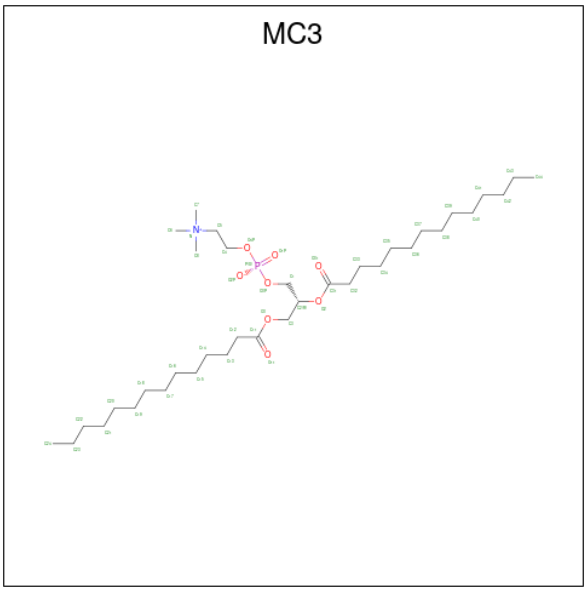
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
17	D	1	75	34	1	32	4	4	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 19 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: $C_{36}H_{72}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
19	J	1	118	36	72	1	8	1	0	0

- Molecule 20 is water.

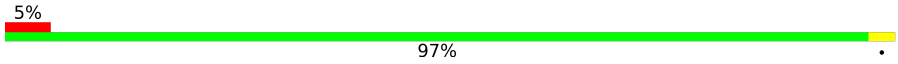
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	A	1	1	1	0	0
20	B	23	23	23	0	0
20	C	1	1	1	0	0
20	F	6	6	6	0	0
20	G	2	2	2	0	0
20	I	1	1	1	0	0

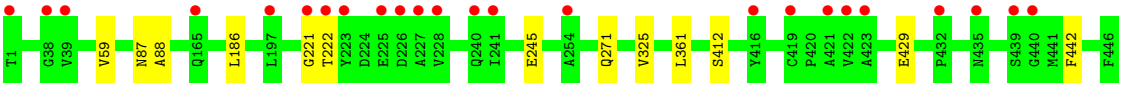
3 Residue-property plots (i)

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

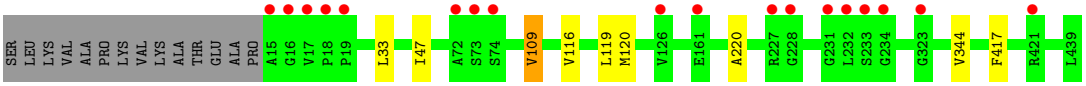
Chain A:





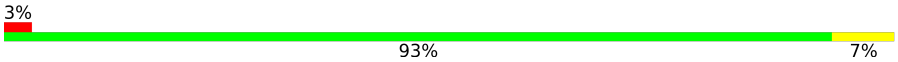
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

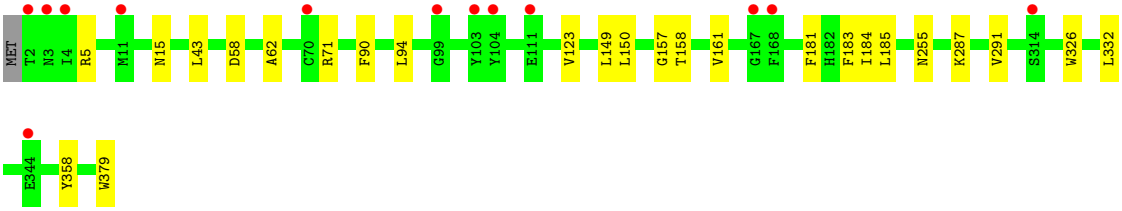
Chain B:



• Molecule 3: Cytochrome b

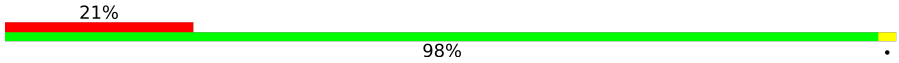
Chain C:

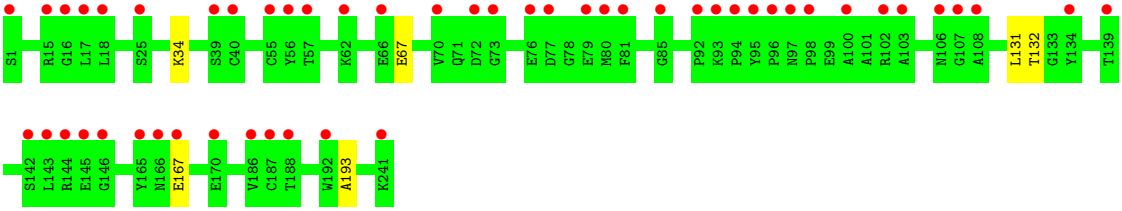




• Molecule 4: Cytochrome c1, heme protein, mitochondrial

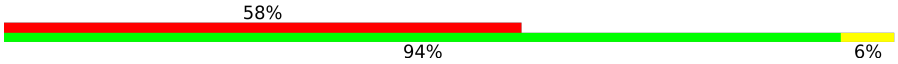
Chain D:

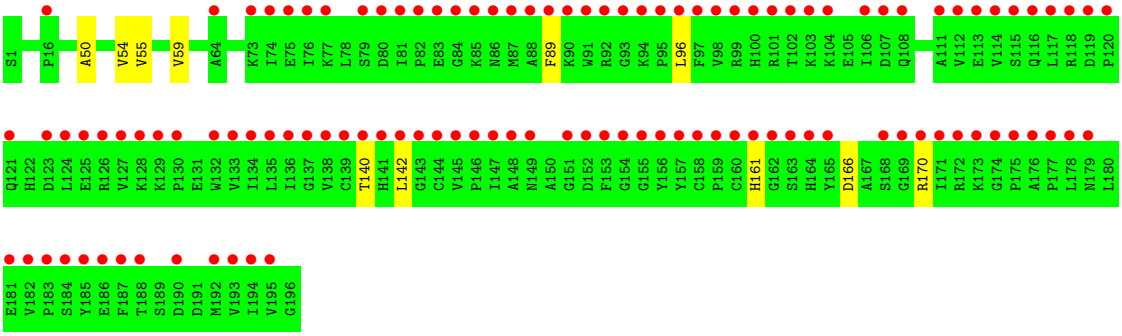




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

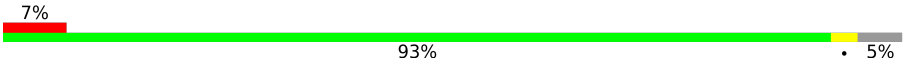
Chain E:

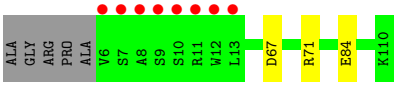




- Molecule 6: Cytochrome b-c1 complex subunit 7

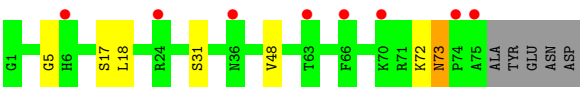
Chain F:





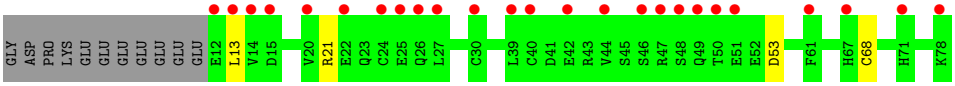
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:



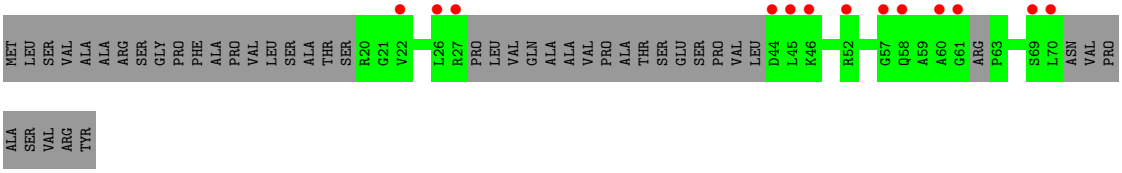
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



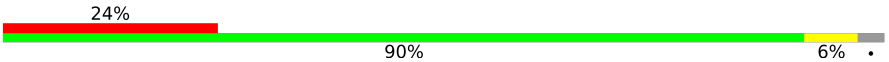
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

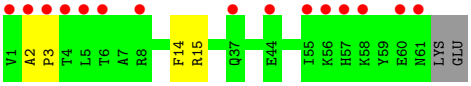
Chain I:



- Molecule 10: Cytochrome b-c1 complex subunit 9

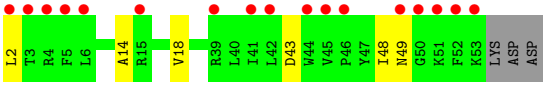
Chain J:





• Molecule 11: Cytochrome b-c1 complex subunit 10

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.18Å 154.18Å 598.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.80 29.87 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.87-2.80) 84.6 (29.87-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.289 0.252 , 0.290	Depositor DCC
R_{free} test set	1999 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	33542	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: MC3, FES, AZO, CDL, 6PE, HEM, 8PE, HEC

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	0.25	0/3531	0.48	0/4792
2	B	0.26	0/3241	0.49	0/4398
3	C	0.25	0/3100	0.45	0/4242
4	D	0.28	0/1978	0.53	0/2684
5	E	0.25	0/1552	0.45	0/2100
6	F	0.25	0/930	0.46	0/1246
7	G	0.27	0/649	0.47	0/878
8	H	0.25	0/553	0.47	0/741
9	I	0.26	0/242	0.66	0/319
10	J	0.25	0/515	0.42	0/696
11	K	0.25	0/446	0.47	0/611
All	All	0.26	0/16737	0.48	0/22707

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	3458	3341	3356	7	0
2	B	3181	3147	3160	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3003	3053	3065	11	0
4	D	1919	1859	1868	5	0
5	E	1518	1497	1503	6	0
6	F	911	905	906	2	0
7	G	628	633	636	4	0
8	H	548	527	530	3	0
9	I	244	265	265	0	0
10	J	502	502	505	3	0
11	K	430	435	435	3	0
12	A	27	33	33	1	0
12	K	27	33	33	0	0
13	A	60	64	64	0	0
13	D	60	64	64	0	0
13	G	60	64	64	0	0
14	C	86	60	60	1	0
15	C	30	17	17	0	0
16	C	47	73	73	0	0
17	D	43	32	30	3	0
18	E	4	0	0	0	0
19	J	46	72	72	1	0
20	A	1	0	0	0	0
20	B	23	0	0	0	0
20	C	1	0	0	0	0
20	F	6	0	0	0	0
20	G	2	0	0	0	0
20	I	1	0	0	0	0
All	All	16866	16676	16739	44	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 44 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)
17:D:1001:HEC:HBC3	17:D:1001:HEC:HMC1	1.67	0.77
3:C:287:LYS:NZ	5:E:140:THR:O	2.25	0.64
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.35	0.58
5:E:166:ASP:OD1	5:E:170:ARG:N	2.36	0.58
10:J:14:PHE:O	19:J:101:MC3:H71	2.04	0.58

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	444/446 (100%)	434 (98%)	10 (2%)	0	100	100
2	B	423/439 (96%)	413 (98%)	10 (2%)	0	100	100
3	C	376/379 (99%)	367 (98%)	9 (2%)	0	100	100
4	D	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
6	F	103/110 (94%)	103 (100%)	0	0	100	100
7	G	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
8	H	65/78 (83%)	64 (98%)	1 (2%)	0	100	100
9	I	28/78 (36%)	25 (89%)	3 (11%)	0	100	100
10	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
11	K	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
All	All	2054/2165 (95%)	2000 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	370/370 (100%)	368 (100%)	2 (0%)	88	96
2	B	332/343 (97%)	331 (100%)	1 (0%)	92	98
3	C	326/327 (100%)	319 (98%)	7 (2%)	53	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	206 (100%)	0	100	100
5	E	168/168 (100%)	168 (100%)	0	100	100
6	F	96/98 (98%)	96 (100%)	0	100	100
7	G	66/70 (94%)	62 (94%)	4 (6%)	18	48
8	H	64/74 (86%)	63 (98%)	1 (2%)	62	88
9	I	25/60 (42%)	25 (100%)	0	100	100
10	J	51/53 (96%)	51 (100%)	0	100	100
11	K	42/45 (93%)	41 (98%)	1 (2%)	49	81
All	All	1746/1814 (96%)	1730 (99%)	16 (1%)	78	94

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	68	CYS
7	G	73	ASN
3	C	255	ASN
7	G	31	SER
3	C	185	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	D	1002	-	59,59,99	1.26	5 (8%)	65,71,111	1.18	5 (7%)
14	HEM	C	1001	3	41,50,50	1.49	6 (14%)	45,82,82	1.43	6 (13%)
18	FES	E	1001	5	0,4,4	-	-	-		
19	MC3	J	101	-	45,45,45	1.37	3 (6%)	51,53,53	0.97	5 (9%)
13	CDL	G	101	-	59,59,99	1.28	6 (10%)	65,71,111	1.00	4 (6%)
12	6PE	K	101	-	26,26,26	1.77	8 (30%)	29,31,31	1.14	2 (6%)
15	AZO	C	1003	-	32,32,32	0.66	0	42,42,42	1.63	8 (19%)
16	8PE	C	1004	-	46,46,46	1.62	6 (13%)	49,51,51	1.07	4 (8%)
14	HEM	C	1002	3	41,50,50	1.46	5 (12%)	45,82,82	1.39	6 (13%)
17	HEC	D	1001	4	32,50,50	2.15	4 (12%)	24,82,82	1.36	1 (4%)
12	6PE	A	501	-	26,26,26	1.74	8 (30%)	29,31,31	1.11	2 (6%)
13	CDL	A	502	-	59,59,99	1.26	7 (11%)	65,71,111	1.09	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	D	1002	-	-	32/70/70/110	-
14	HEM	C	1001	3	-	4/12/54/54	-
19	MC3	J	101	-	-	24/49/49/49	-
18	FES	E	1001	5	-	-	0/1/1/1
13	CDL	G	101	-	-	17/70/70/110	-
12	6PE	K	101	-	-	12/30/30/30	-
15	AZO	C	1003	-	-	2/23/23/23	0/3/3/3
16	8PE	C	1004	-	-	22/50/50/50	-
14	HEM	C	1002	3	-	3/12/54/54	-
17	HEC	D	1001	4	-	3/10/54/54	-
12	6PE	A	501	-	-	13/30/30/30	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	A	502	-	-	25/70/70/110	-

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	1001	HEC	C2B-C3B	-6.35	1.34	1.40
17	D	1001	HEC	C3D-C2D	5.43	1.53	1.37
17	D	1001	HEC	C3C-C2C	-5.37	1.35	1.40
19	J	101	MC3	P-O4P	4.87	1.79	1.59
16	C	1004	8PE	P-O11	4.81	1.78	1.59

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	1003	AZO	C11-N3-C10	5.83	118.86	114.48
13	D	1002	CDL	OA6-CA5-C11	4.55	121.32	111.50
13	A	502	CDL	OB6-CB5-C51	4.14	120.42	111.50
13	G	101	CDL	OB6-CB5-C51	3.88	119.87	111.50
16	C	1004	8PE	O21-C21-C22	3.82	119.72	111.50

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	501	6PE	C1-O3-P1-O2
12	A	501	6PE	C1-O3-P1-O8
12	A	501	6PE	C11-C10-O6-C2
12	K	101	6PE	C16-O8-P1-O1
12	K	101	6PE	C16-O8-P1-O2

There are no ring outliers.

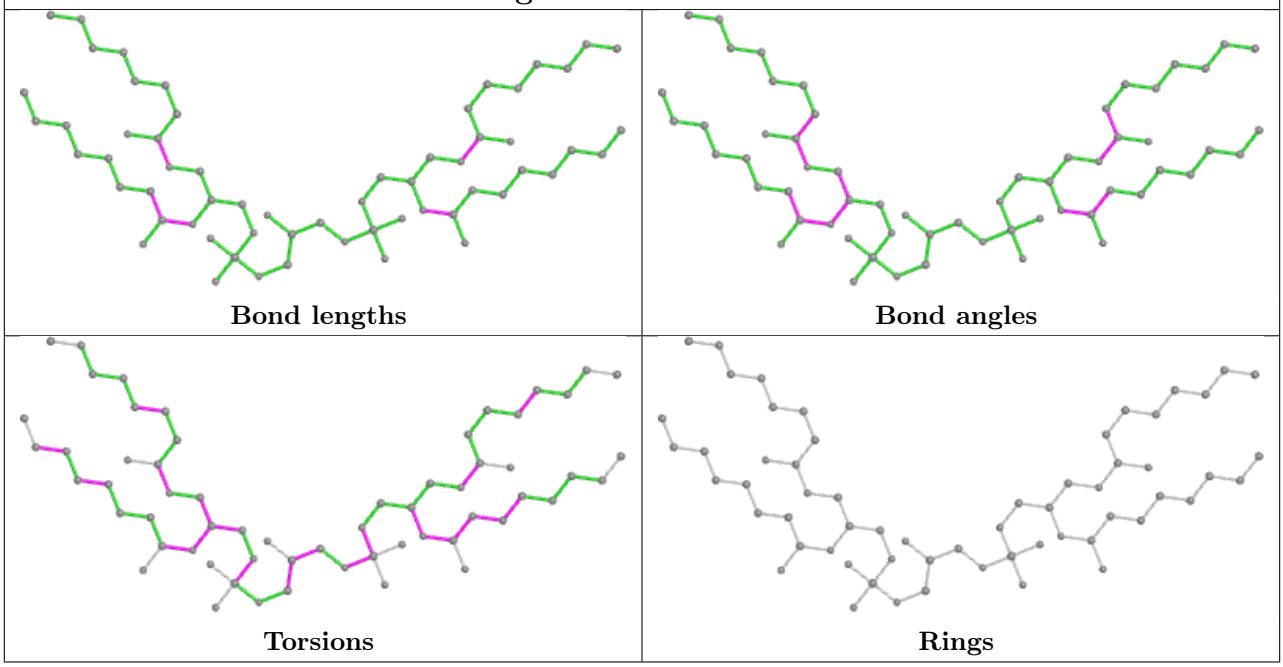
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	J	101	MC3	1	0
14	C	1002	HEM	1	0
17	D	1001	HEC	3	0
12	A	501	6PE	1	0

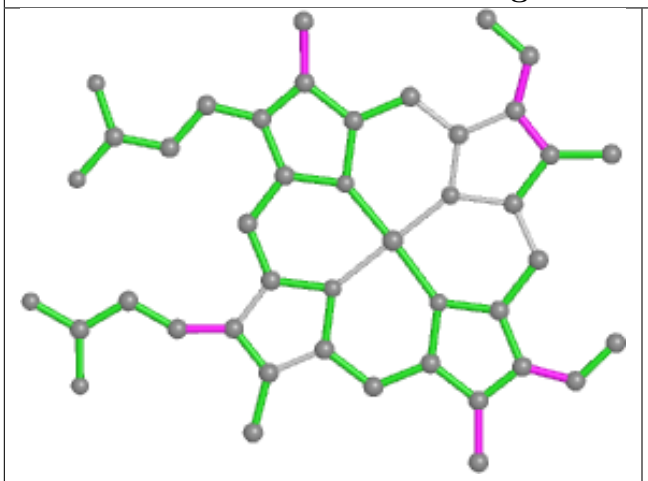
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

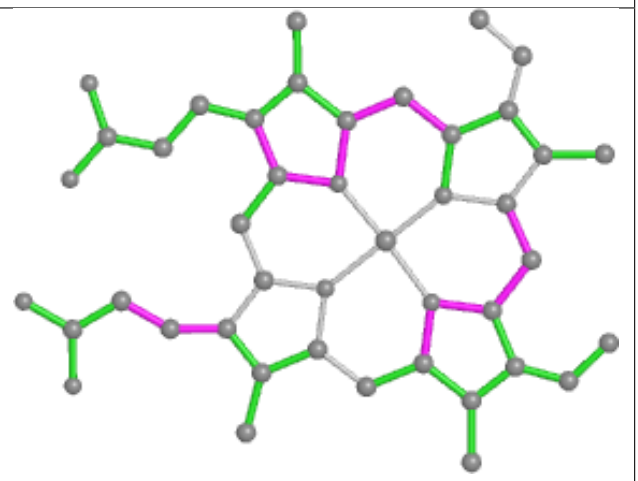
Ligand CDL D 1002



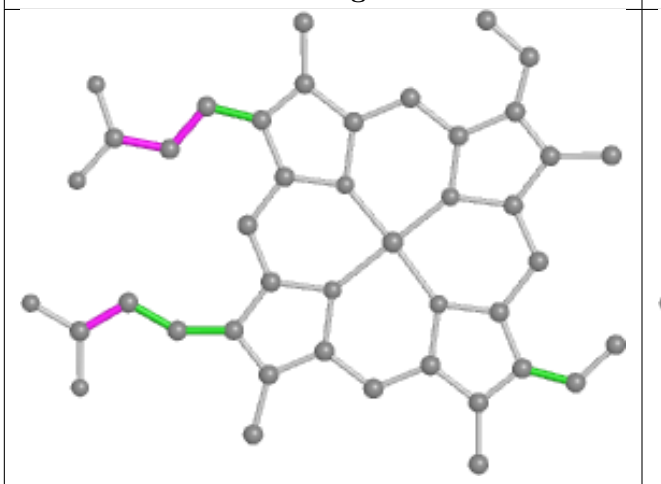
Ligand HEM C 1001



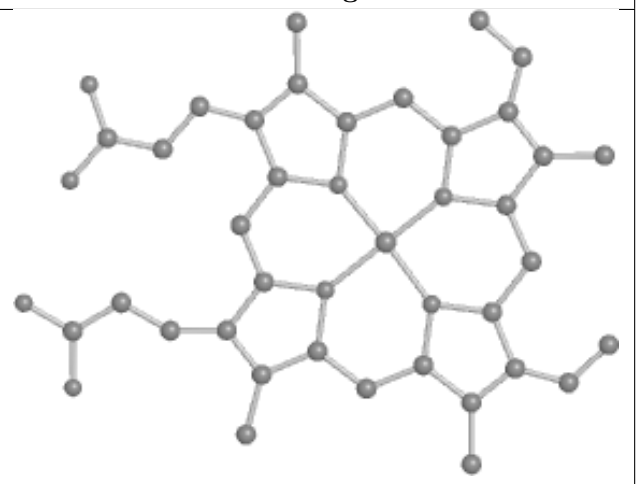
Bond lengths



Bond angles

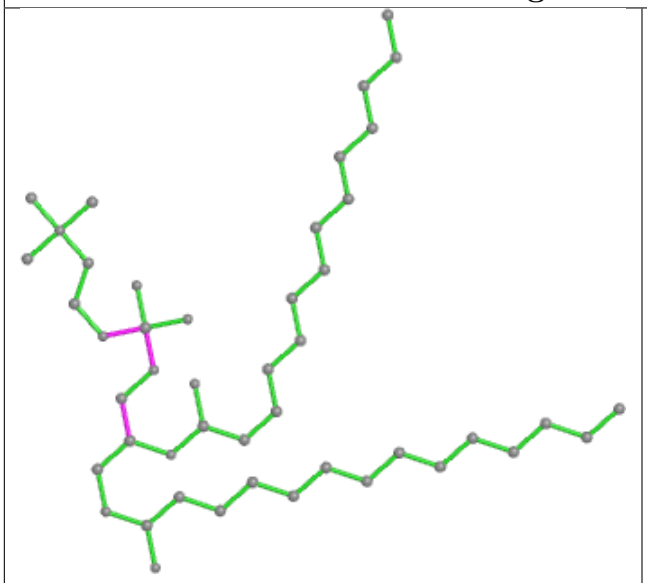


Torsions

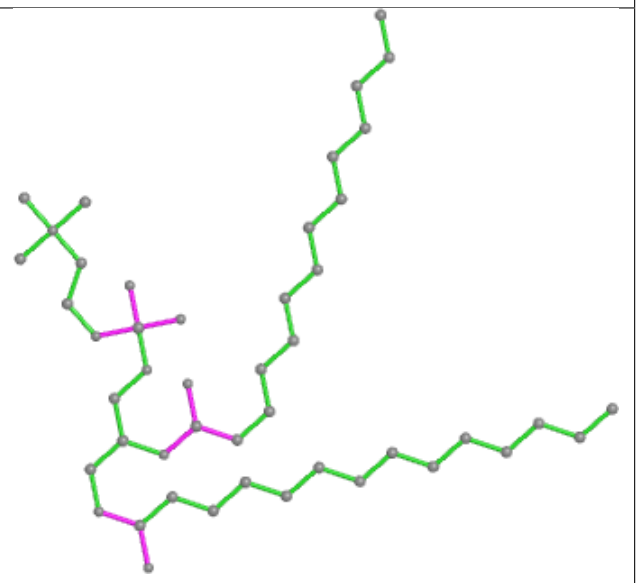


Rings

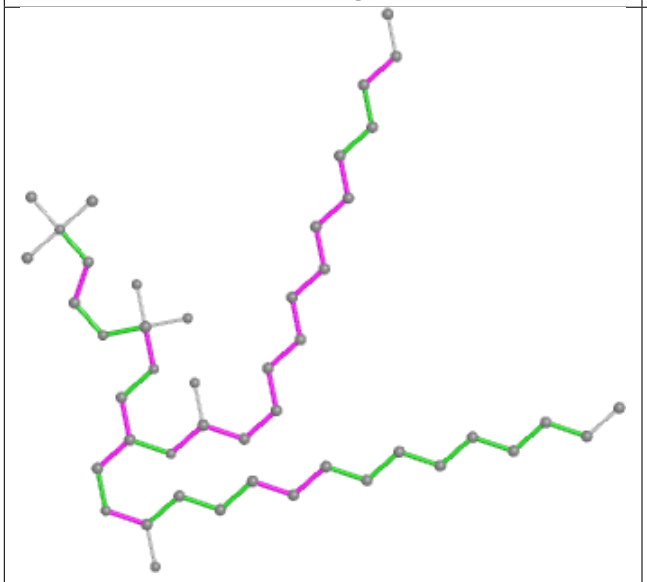
Ligand MC3 J 101



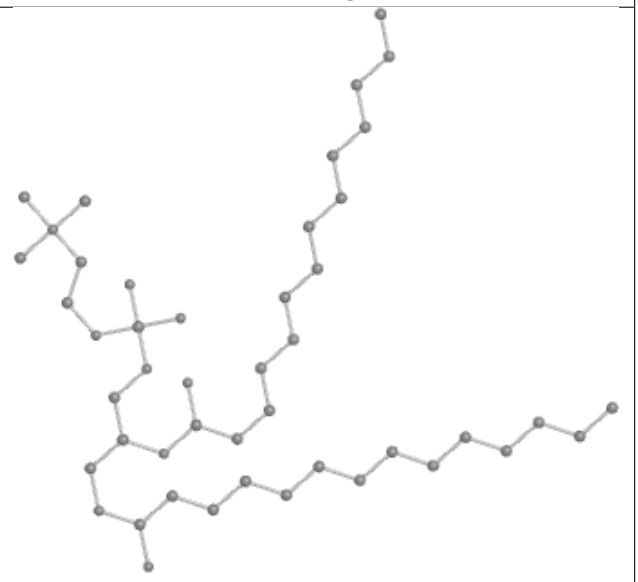
Bond lengths



Bond angles

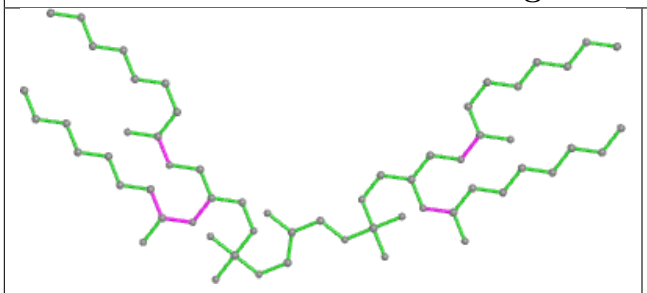


Torsions

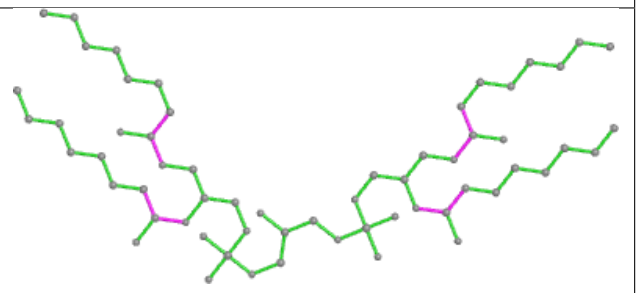


Rings

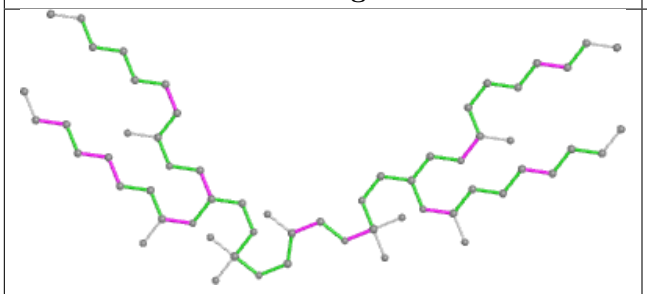
Ligand CDL G 101



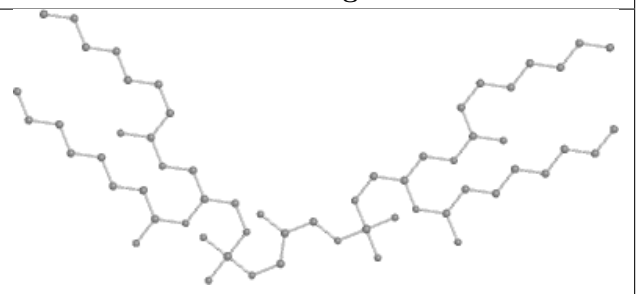
Bond lengths



Bond angles

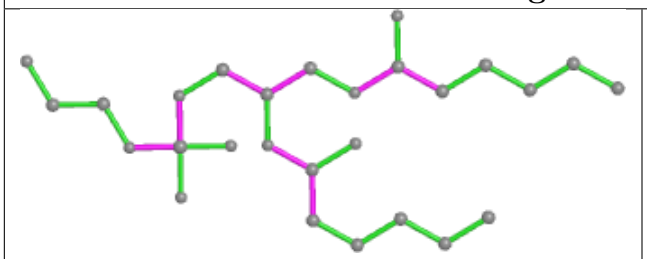


Torsions

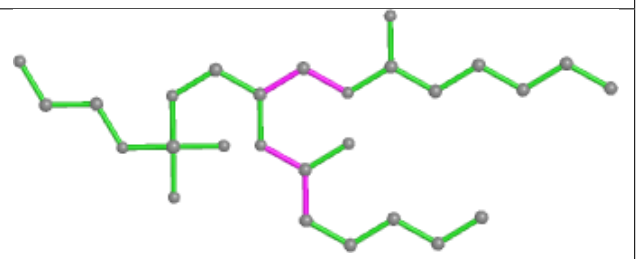


Rings

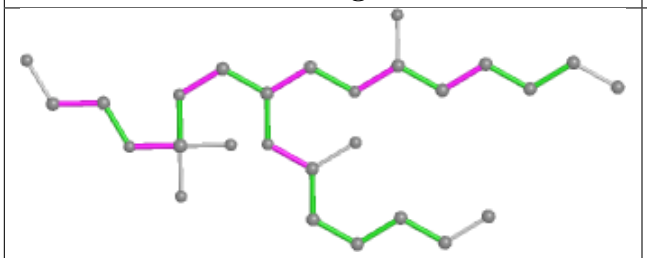
Ligand 6PE K 101



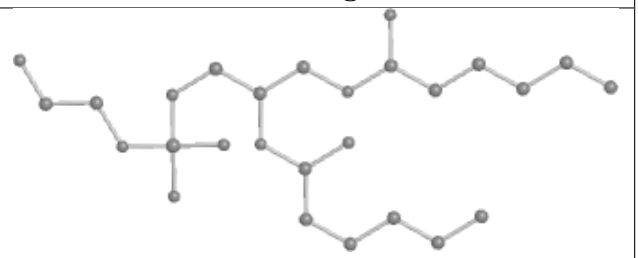
Bond lengths



Bond angles

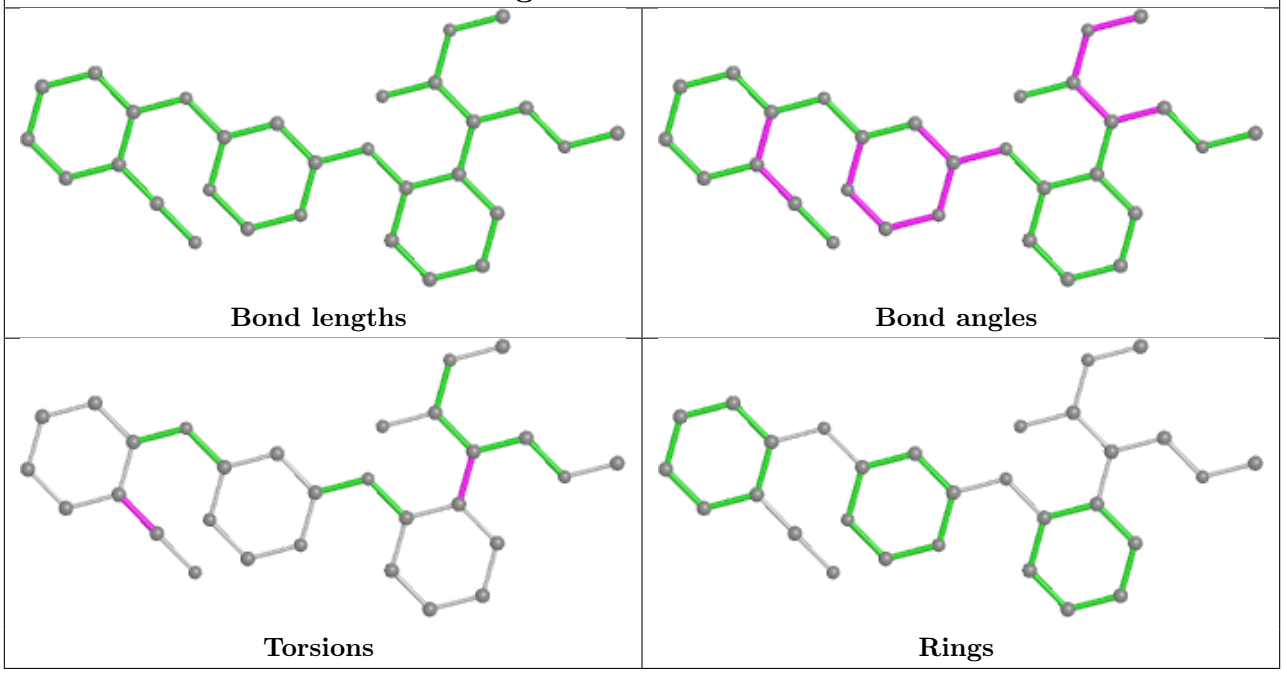


Torsions

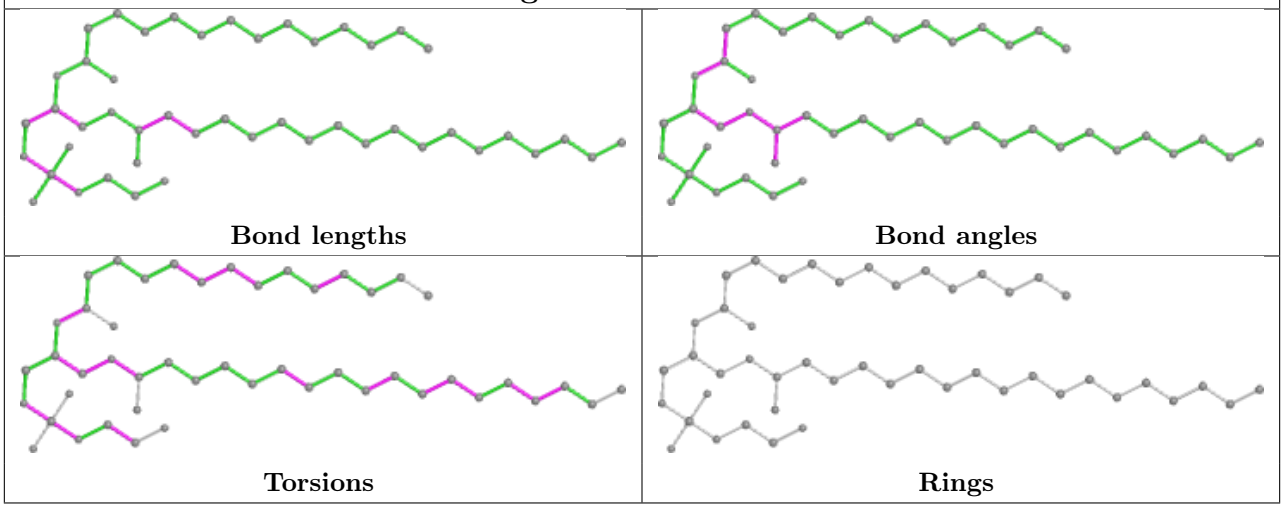


Rings

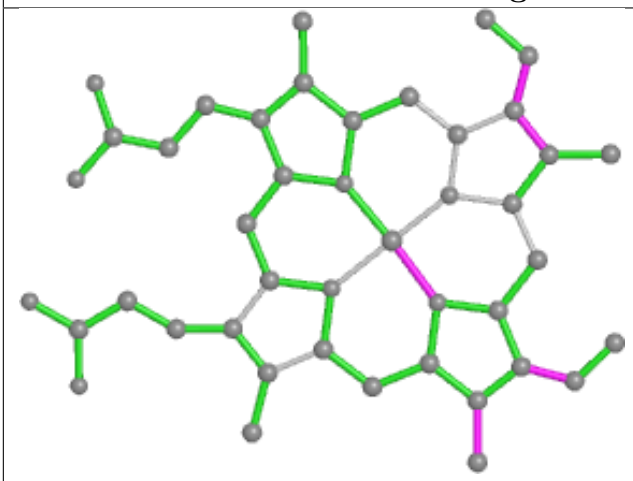
Ligand AZO C 1003



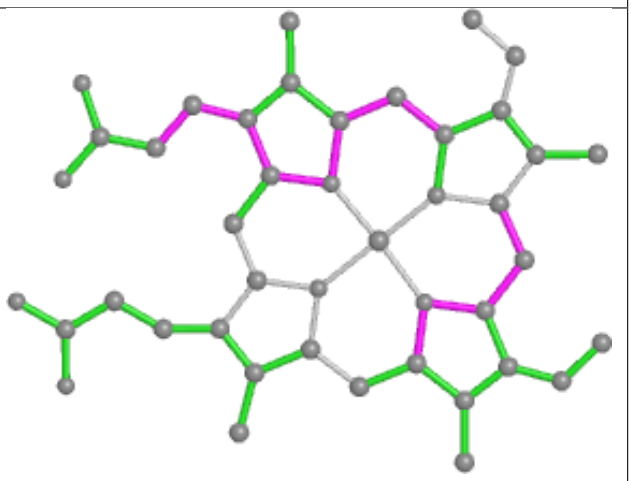
Ligand 8PE C 1004



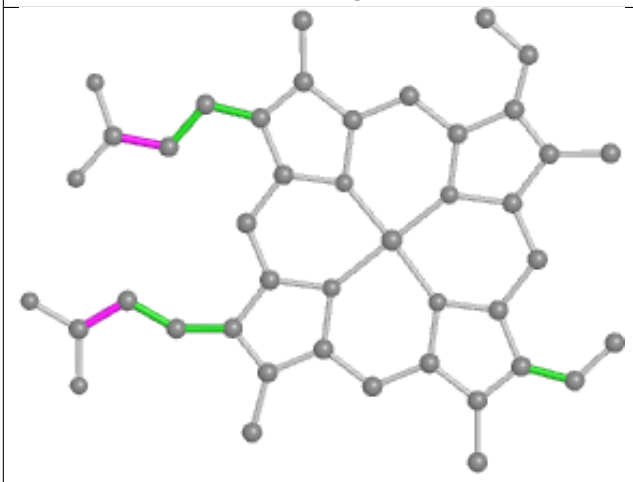
Ligand HEM C 1002



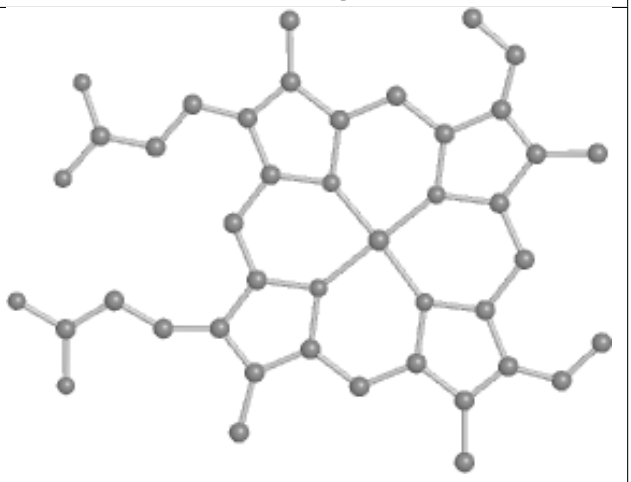
Bond lengths



Bond angles

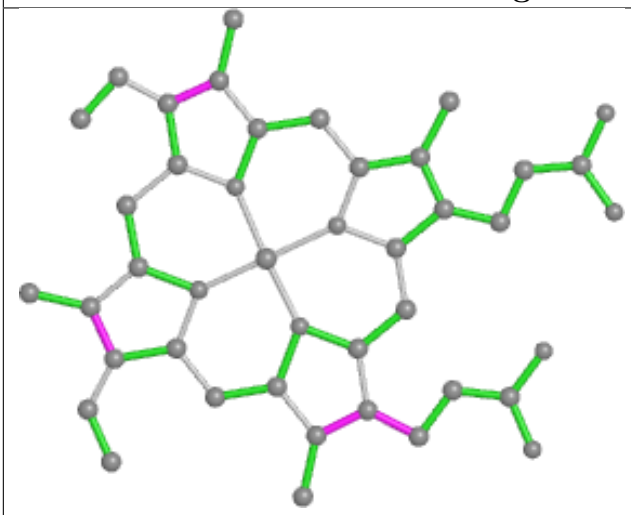


Torsions

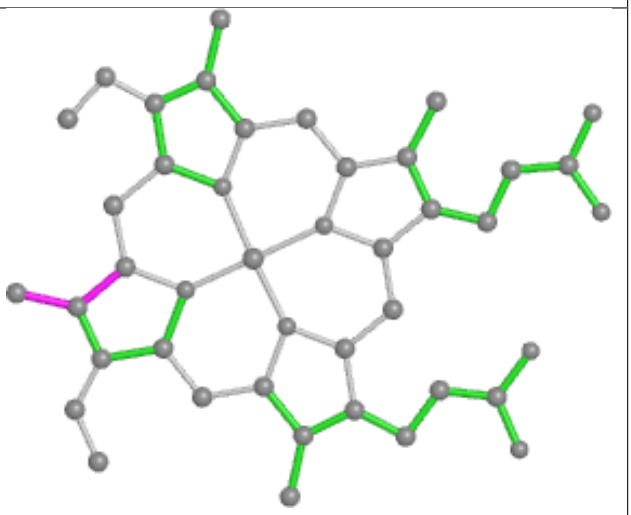


Rings

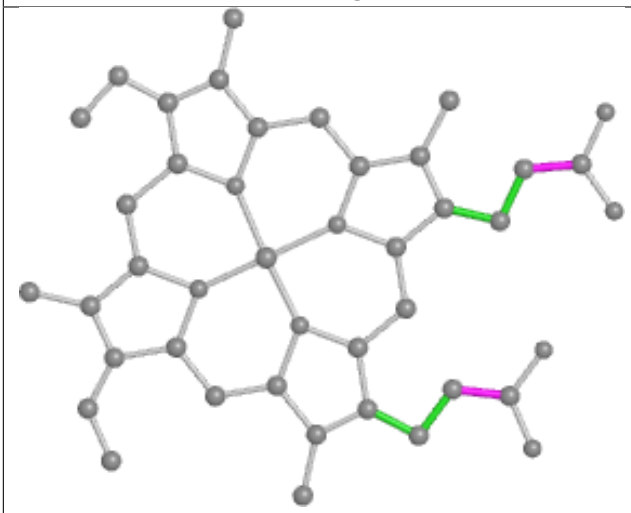
Ligand HEC D 1001



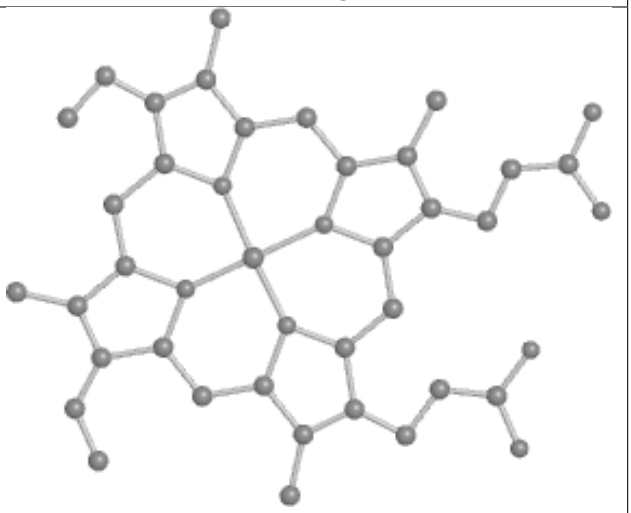
Bond lengths



Bond angles

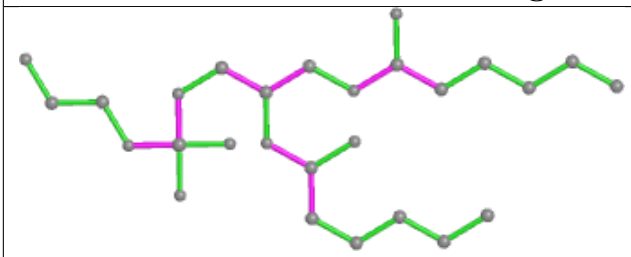


Torsions

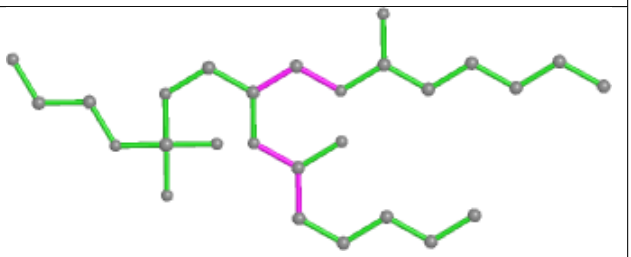


Rings

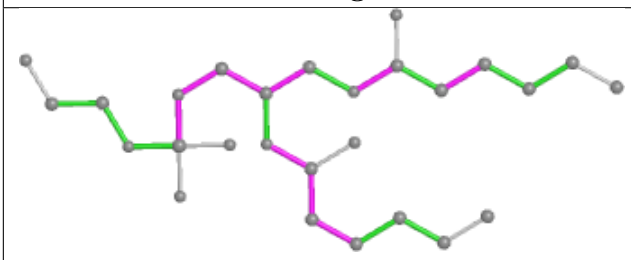
Ligand 6PE A 501



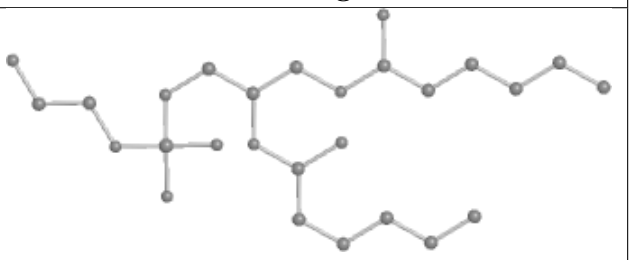
Bond lengths



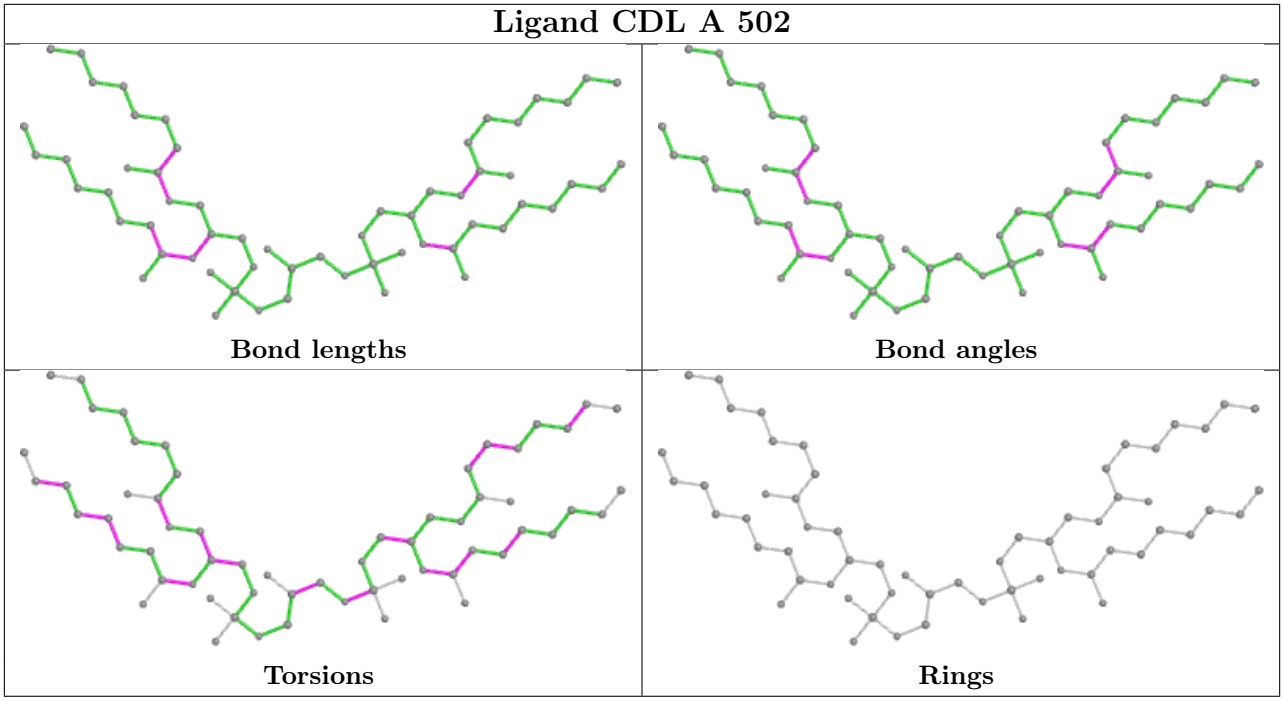
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	446/446 (100%)	0.31	24 (5%)	25	17	58, 83, 109, 183	0
2	B	425/439 (96%)	0.20	18 (4%)	36	26	51, 66, 93, 163	0
3	C	378/379 (99%)	0.33	13 (3%)	45	35	68, 99, 132, 151	0
4	D	241/241 (100%)	1.02	51 (21%)	0	0	72, 147, 168, 182	0
5	E	196/196 (100%)	3.07	113 (57%)	0	0	63, 71, 128, 158	124 (63%)
6	F	105/110 (95%)	0.35	8 (7%)	13	7	65, 85, 126, 141	0
7	G	75/80 (93%)	0.64	8 (10%)	6	3	67, 102, 138, 166	0
8	H	67/78 (85%)	1.82	25 (37%)	0	0	145, 159, 177, 181	0
9	I	34/78 (43%)	1.72	13 (38%)	0	0	75, 120, 148, 170	0
10	J	61/63 (96%)	1.25	15 (24%)	0	0	97, 128, 153, 172	0
11	K	52/55 (94%)	1.27	17 (32%)	0	0	95, 121, 153, 162	0
All	All	2080/2165 (96%)	0.77	305 (14%)	2	1	51, 89, 158, 183	124 (5%)

The worst 5 of 305 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	102	THR	14.5
5	E	114	VAL	12.9
10	J	1	VAL	11.3
5	E	144	CYS	10.2
5	E	154	GLY	9.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

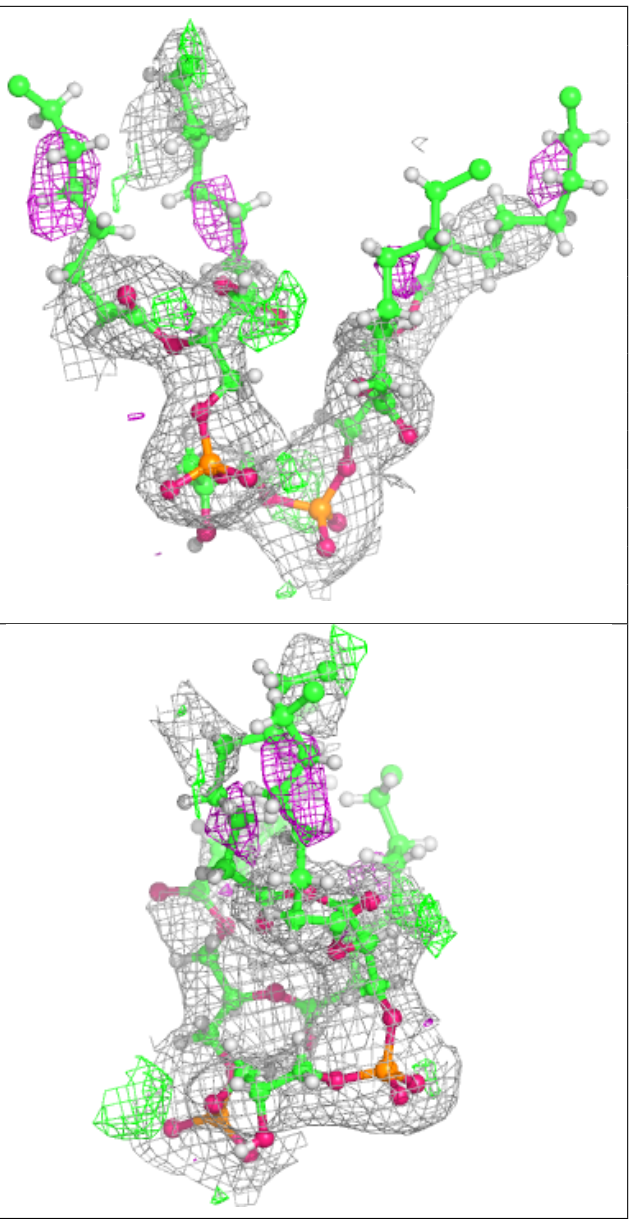
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G	101	60/100	0.71	0.38	94,115,138,139	0
12	6PE	K	101	27/27	0.73	0.42	132,162,168,168	0
19	MC3	J	101	46/46	0.75	0.40	96,119,143,144	0
13	CDL	D	1002	60/100	0.76	0.37	96,117,139,142	0
18	FES	E	1001	4/4	0.77	0.24	75,76,76,76	4
12	6PE	A	501	27/27	0.79	0.30	91,114,138,138	0
13	CDL	A	502	60/100	0.83	0.41	96,117,140,143	0
16	8PE	C	1004	47/47	0.85	0.38	74,98,129,132	0
17	HEC	D	1001	43/43	0.91	0.24	135,156,179,191	0
15	AZO	C	1003	30/30	0.92	0.31	99,113,137,157	0
14	HEM	C	1001	43/43	0.95	0.27	105,115,130,147	0
14	HEM	C	1002	43/43	0.96	0.20	70,86,111,117	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.

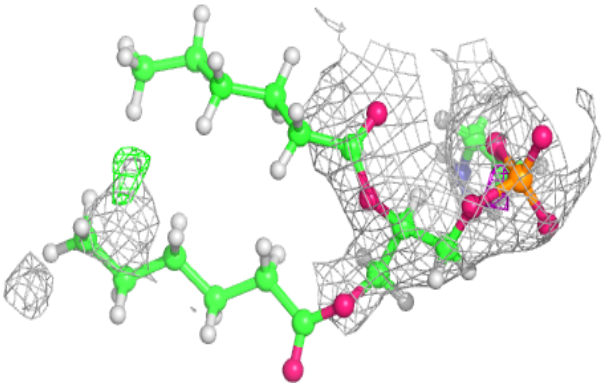
Electron density around CDL G 101:

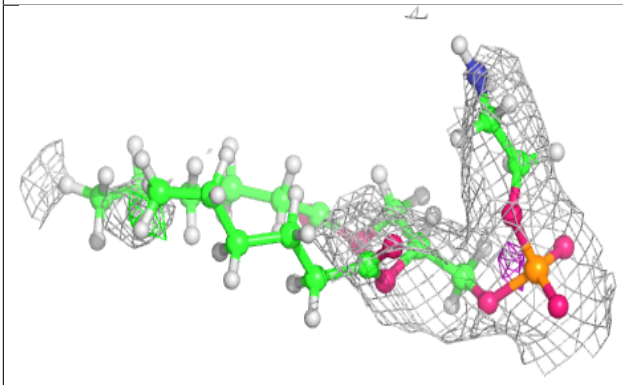
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

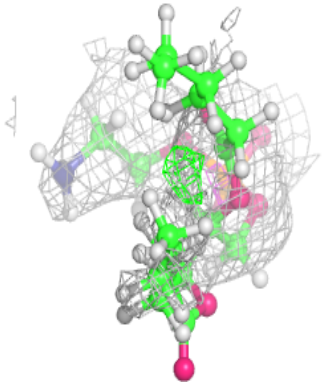


Electron density around 6PE K 101:

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

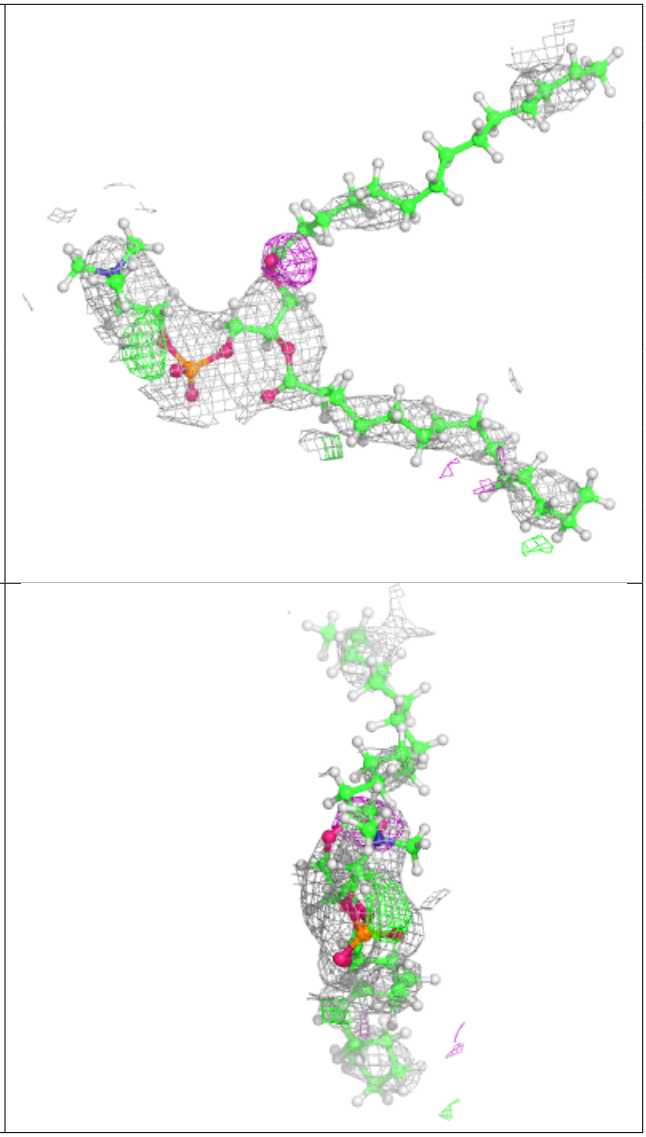






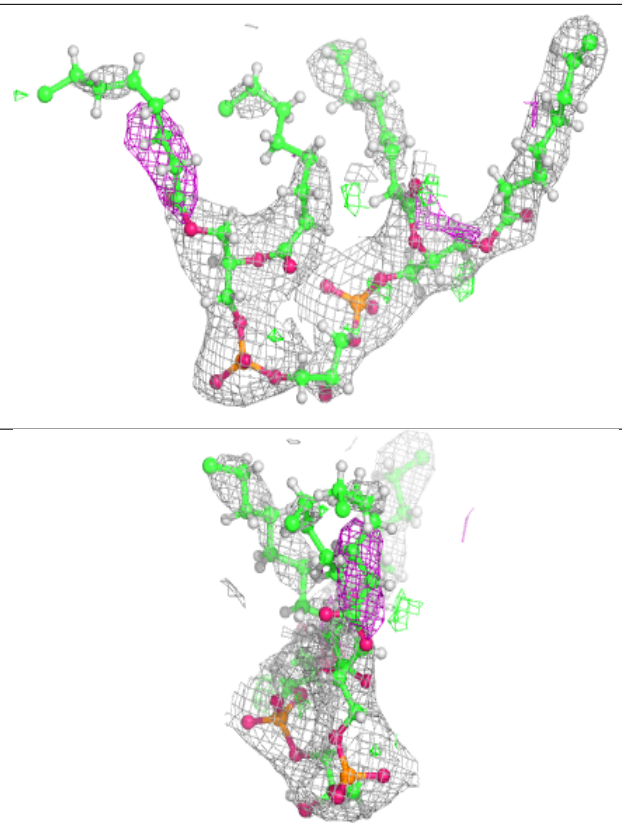
Electron density around MC3 J 101:

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



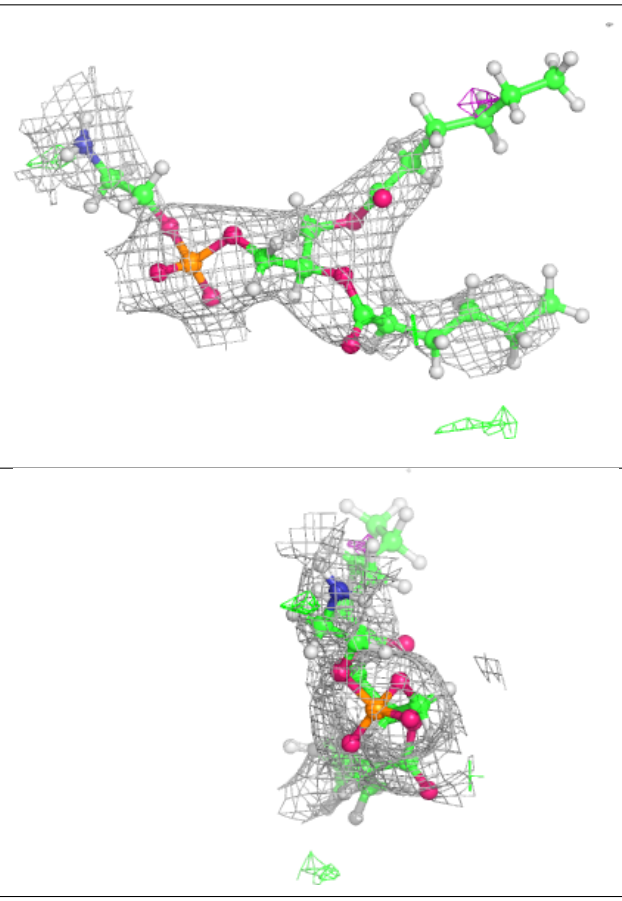
Electron density around CDL D 1002:

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



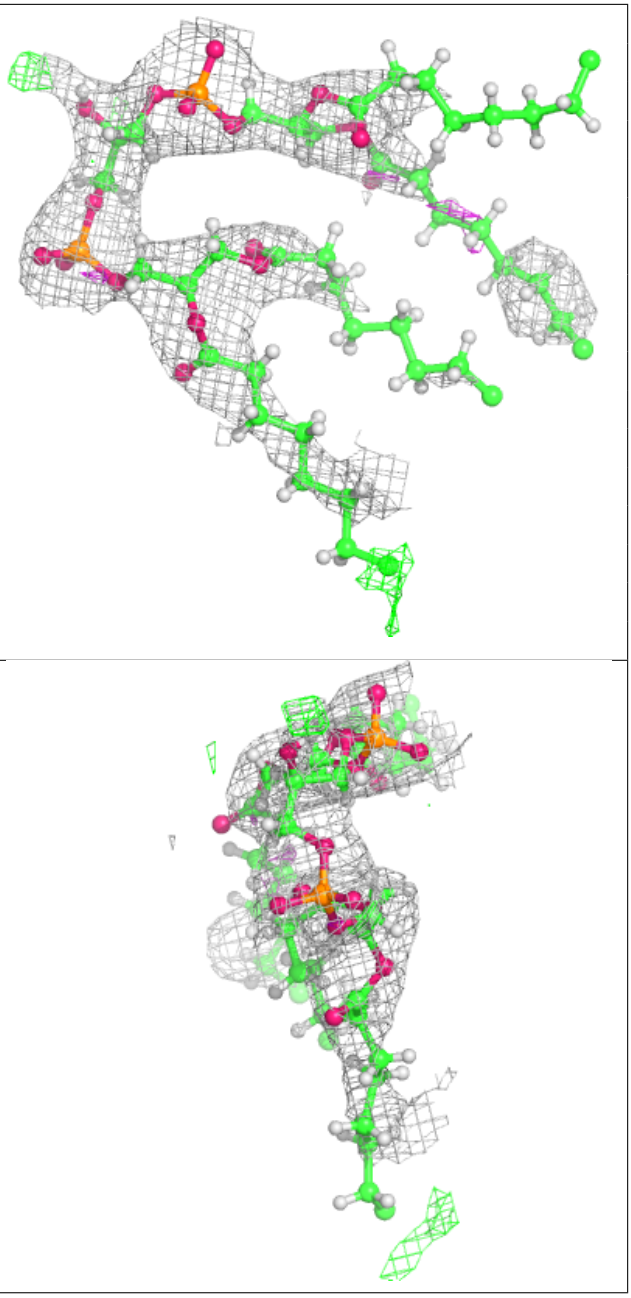
Electron density around 6PE A 501:

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



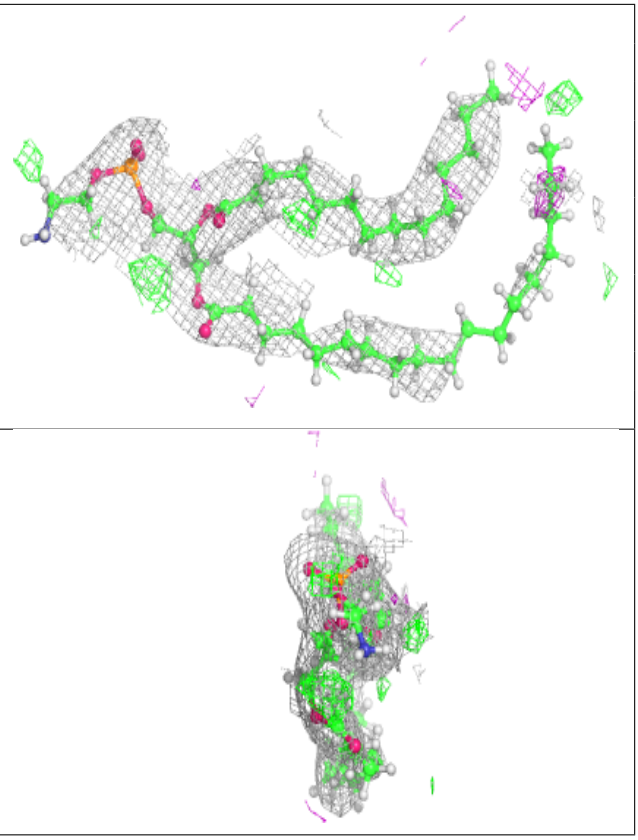
Electron density around CDL A 502:

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



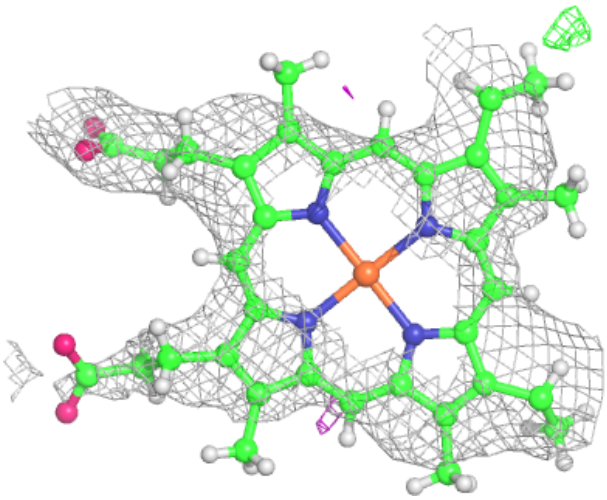
Electron density around 8PE C 1004:

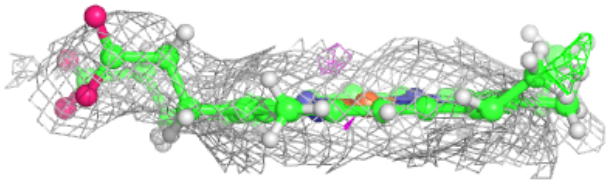
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

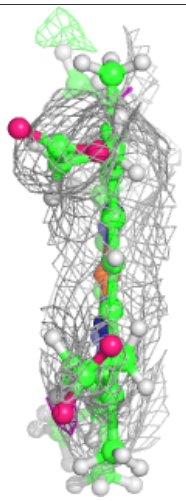


Electron density around HEC D 1001:

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

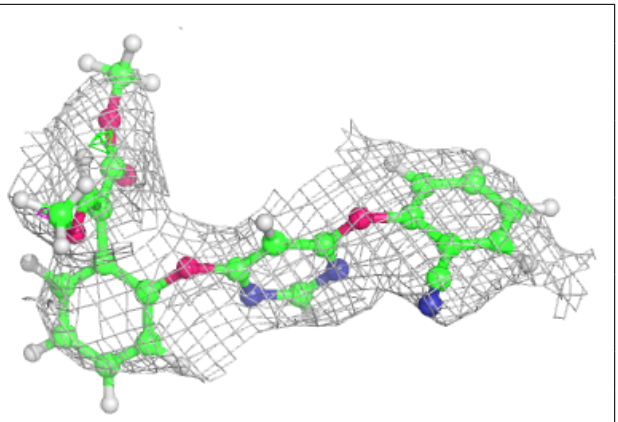


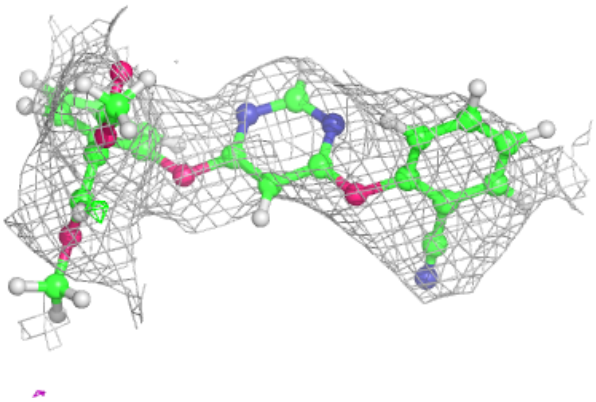


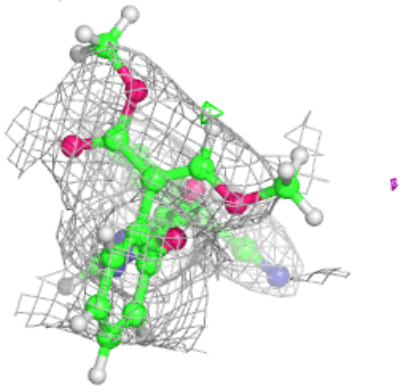


Electron density around AZO C 1003:

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

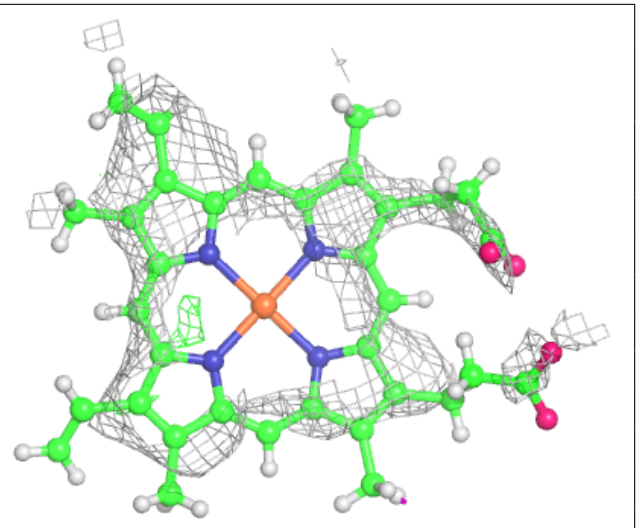


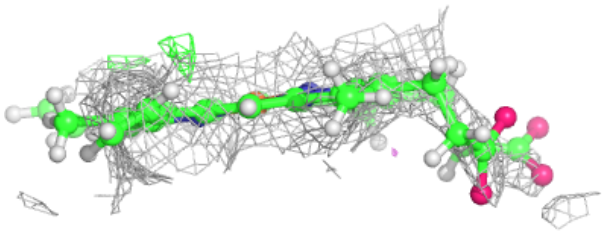


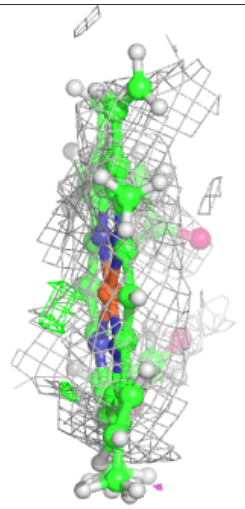


Electron density around HEM C 1001:

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

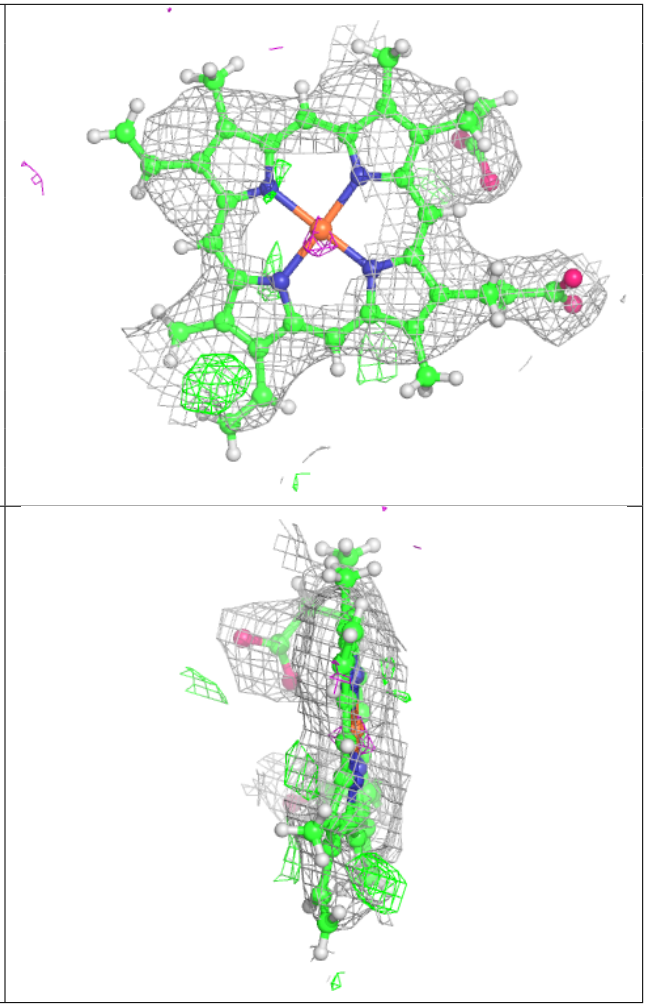






Electron density around HEM C 1002:

$2mF_o$-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.