wwPDB EM Validation Summary Report

Feb 14, 2023 – 02:18 PM JST

PDB ID	:	7VZG
EMDB ID	:	EMD-32228
Title	:	Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the larger form)
Authors	:	Huang, G.Q.; Dong, S.S.; Qin, X.C.; Sui, S.F.
Deposited on	:	2021-11-16
Resolution	:	2.61 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

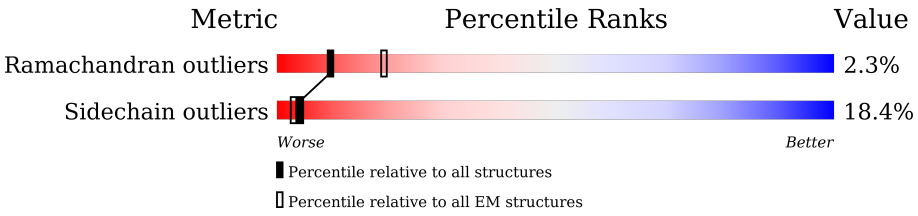
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.61 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	858	63% 31% 5%
1	a	858	67% 26% 7%
2	C	204	49% 36% 9% 5%
3	E	35	66% 29% 6%
3	e	35	71% 26%
4	F	35	43% 57%
4	f	35	71% 23% 6%
5	G	38	74% 16% 11%
5	g	38	74% 24%

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Mol	Chain	Length	Quality of chain
6	H	19	11% 100%
6	h	19	5% 100%
7	c	145	54% 32% 12%
8	B	76	14% 67% 29%
9	D	70	50% 83% 14%

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	CLA	A	910	X	-	-	-
12	CLA	A	911	X	-	-	-
13	LYC	c	201	-	X	-	-
15	85I	A	916	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 22458 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PscA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	854	Total	C	N	O	S	0	0
			6960	4602	1155	1170	33		
1	a	858	Total	C	N	O	S	0	0
			6984	4616	1160	1175	33		

- Molecule 2 is a protein called Cytochrome c, mono-and diheme variants.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	193	Total	C	N	O	S	0	0
			1474	900	277	288	9		

- Molecule 3 is a protein called PscE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	35	Total	C	N	O	S	0	0
			258	174	40	42	2		
3	e	35	Total	C	N	O	S	0	0
			258	174	40	42	2		

- Molecule 4 is a protein called PscF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	35	Total	C	N	O	S	0	0
			273	185	43	43	2		
4	f	35	Total	C	N	O	S	0	0
			273	185	43	43	2		

- Molecule 5 is a protein called PscG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

- Molecule 6 is a protein called undefined polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	19	Total	C	N	O	0	0
			95	57	19	19		
6	h	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 7 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	145	Total	C	N	O	S	0	0
			1096	679	200	210	7		

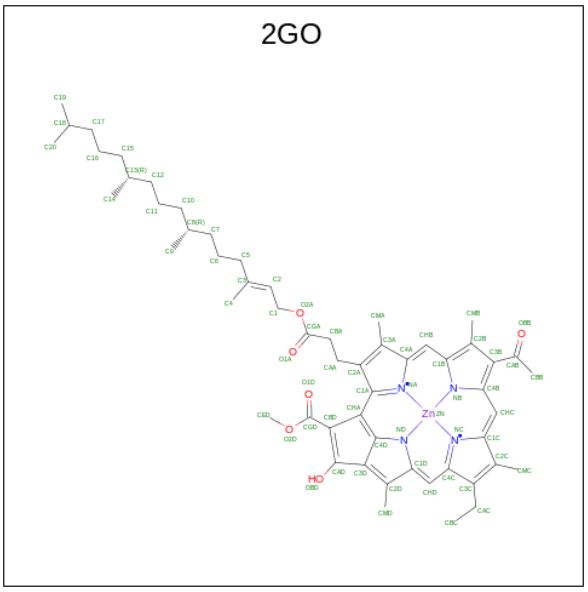
- Molecule 8 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	76	Total	C	N	O	S	0	0
			568	356	90	114	8		

- Molecule 9 is a protein called PscD'.

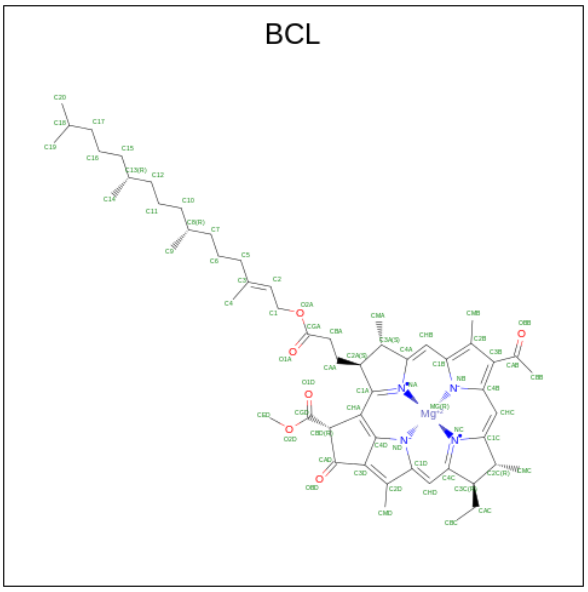
Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	60	Total	C	N	O	S	0	0
			520	330	92	96	2		

- Molecule 10 is [methyl 9-acetyl-14-ethyl-20-hydroxy-4,8,13,18-tetramethyl-3-{3-oxo-3-[(3 ,7,11,15-tetramethylhexadec-2-en-1-yl)oxy]propyl}-3,4,20,21-tetradehydrophorbine-21-ca rboxylatato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26]zinc (three-letter code: 2GO) (formula: $C_{55}H_{70}N_4O_6Zn$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	Zn	0
			66	55	4	6	1	
10	a	1	Total	C	N	O	Zn	0
			66	55	4	6	1	

- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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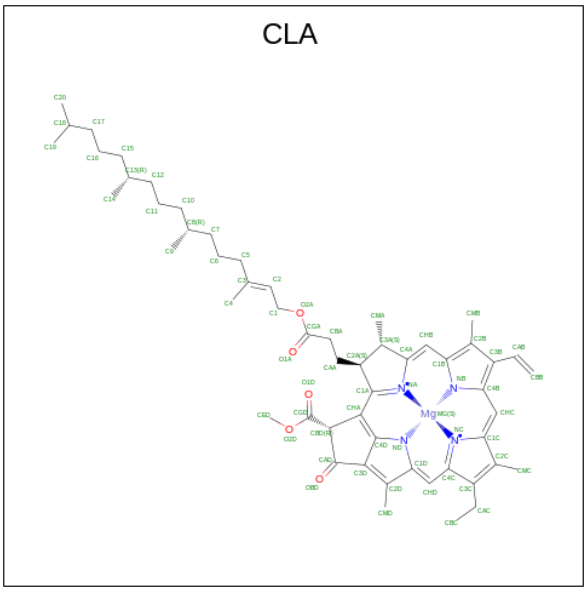
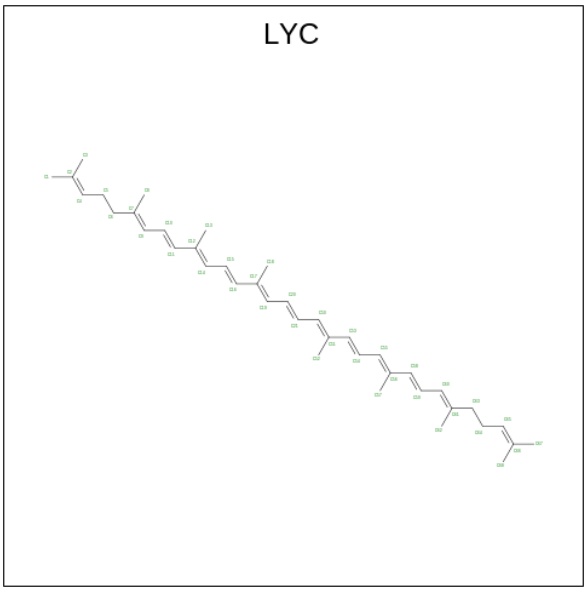
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	a	1	Total 51	C 41	Mg 1	N 4	O 5	0

- Molecule 13 is LYCOPENE (three-letter code: LYC) (formula: $C_{40}H_{56}$).

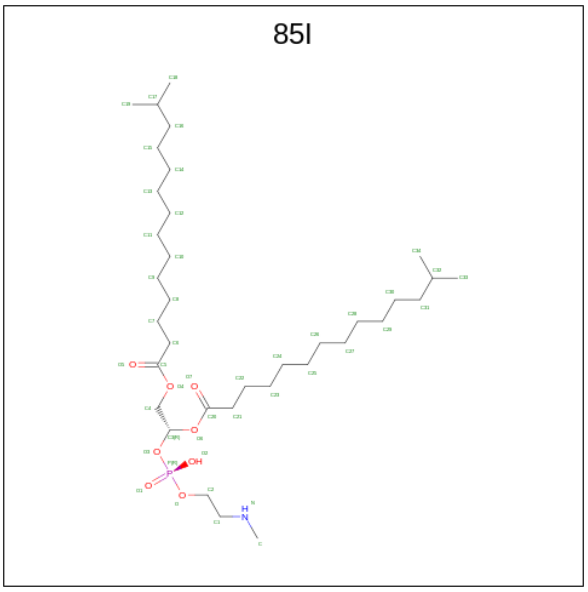


Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 40 40	0
13	c	1	Total C 40 40	0

- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total Ca 1 1	0
14	a	1	Total Ca 1 1	0

- Molecule 15 is [(2 {R})-2-[2-(methylamino)ethoxy-oxidanyl-phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (three-letter code: 85I) (formula: $C_{35}H_{70}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	a	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 16 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	A	13	Total	C	0
			240	240	
16	C	1	Total	C	0
			18	18	
16	E	2	Total	C	0
			26	26	
16	a	13	Total	C	0
			243	243	
16	c	1	Total	C	0
			8	8	

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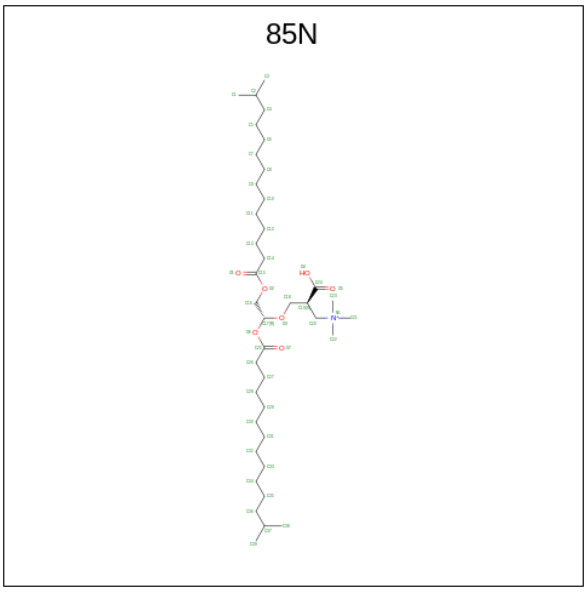
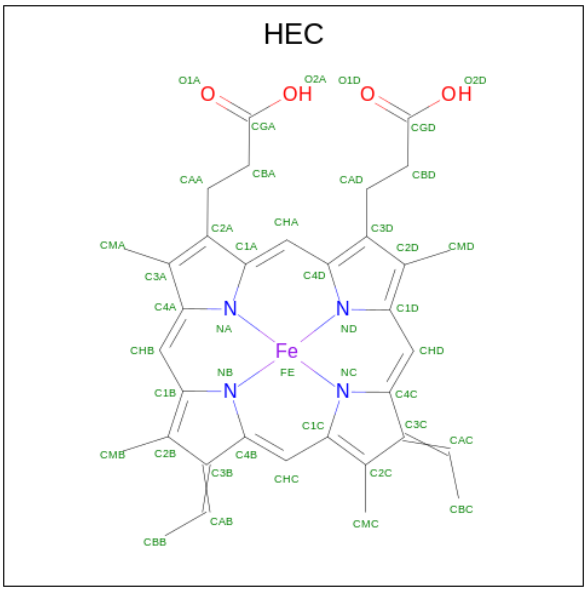
Mol	Chain	Residues	Atoms	AltConf
16	e	2	Total C 26 26	0

- Molecule 17 is [(2 {S})-2-[[(1 {R})-1,2-bis(13-methyltetradecanoyloxy)ethoxy]methyl]-3-oxidanyl-3-oxidanylidene-propyl]-trimethyl-azanium (three-letter code: 85N) (formula: $C_{39}H_{76}NO_7$) (labeled as "Ligand of Interest" by depositor).



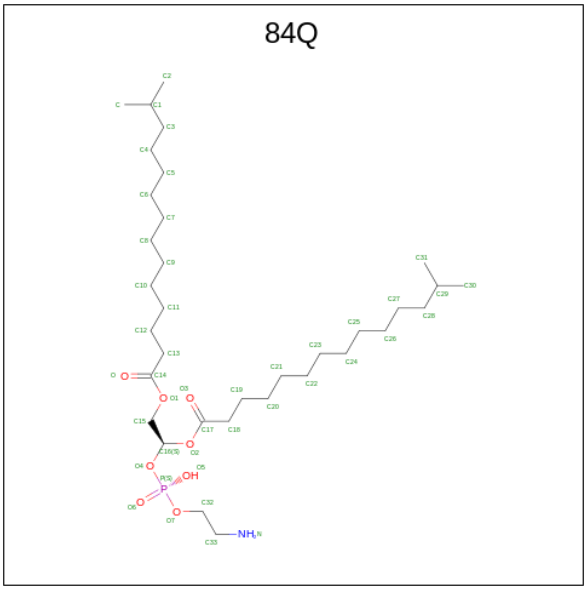
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C N O 47 39 1 7	0
17	G	1	Total C N O 38 30 1 7	0
17	a	1	Total C N O 47 39 1 7	0
17	g	1	Total C N O 38 30 1 7	0

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is [(2S)-2-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (three-letter code: 84Q) (formula: $C_{34}H_{68}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	E	1	Total	C	N	O	P	0
			44	34	1	8	1	

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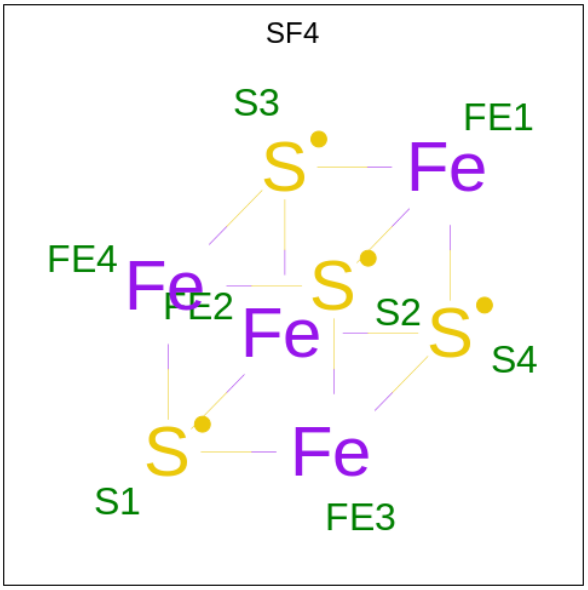
Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 20 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
20	a	1	Total	Fe	S	0
			8	4	4	
20	B	1	Total	Fe	S	0
			8	4	4	
20	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 21 is water.

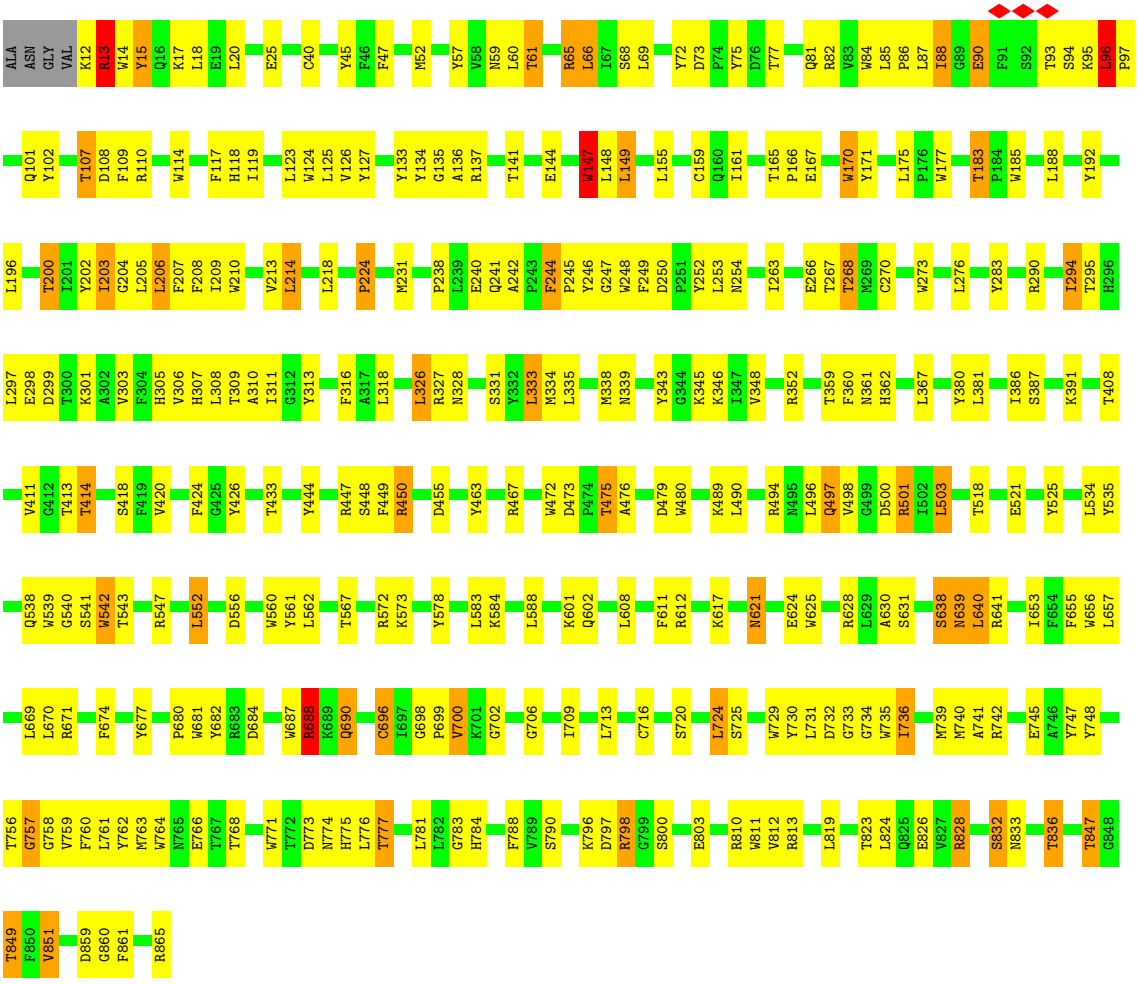
Mol	Chain	Residues	Atoms		AltConf
21	A	3	Total	O	0
			3	3	
21	a	3	Total	O	0
			3	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

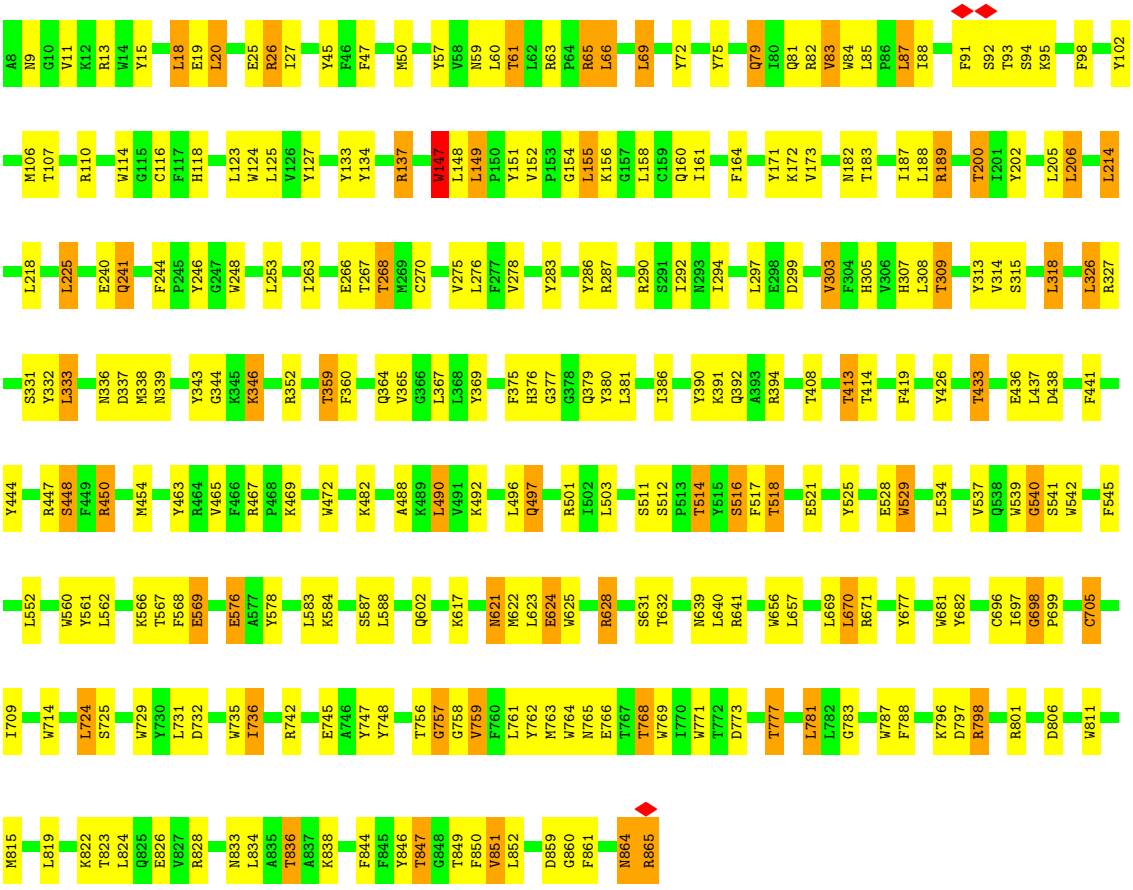
- Molecule 1: PscA

Chain A:



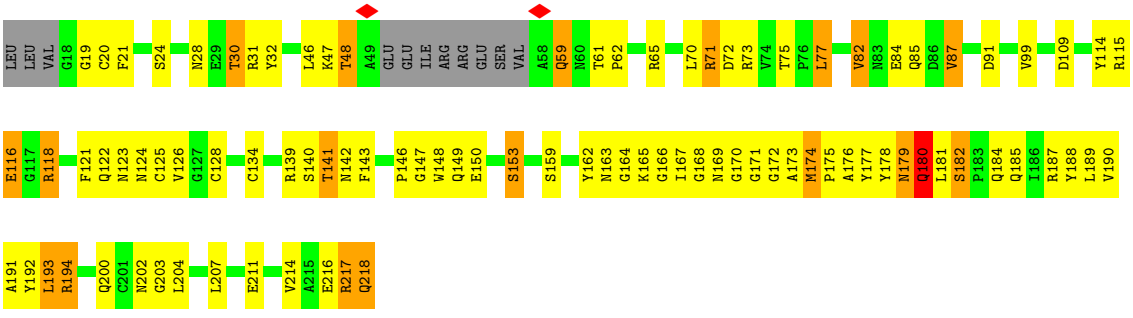
- Molecule 1: PscA

Chain a:



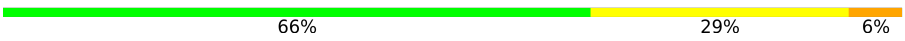
• Molecule 2: Cytochrome c, mono-and diheme variants

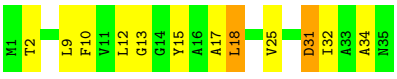
Chain C:



• Molecule 3: PscE

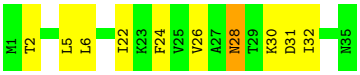
Chain E:





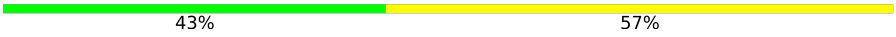
• Molecule 3: PscE

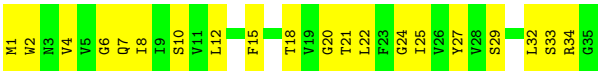
Chain e:



• Molecule 4: PscF

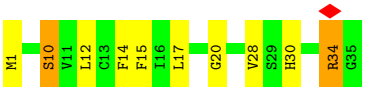
Chain F:





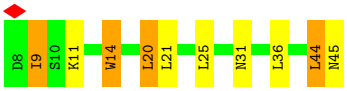
• Molecule 4: PscF

Chain f:



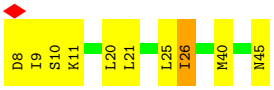
• Molecule 5: PscG

Chain G:



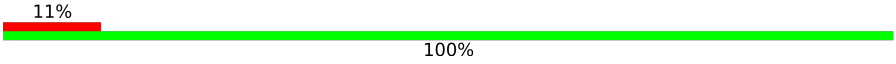
• Molecule 5: PscG

Chain g:



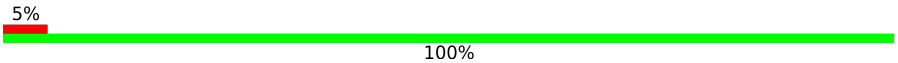
• Molecule 6: undefined polypeptide

Chain H:



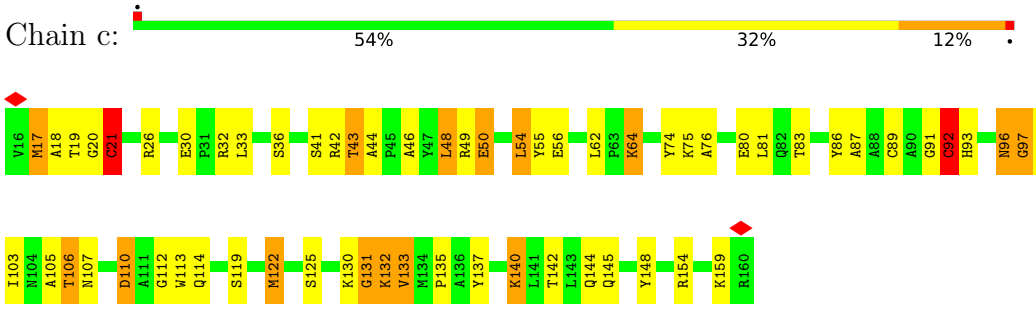
• Molecule 6: undefined polypeptide

Chain h:



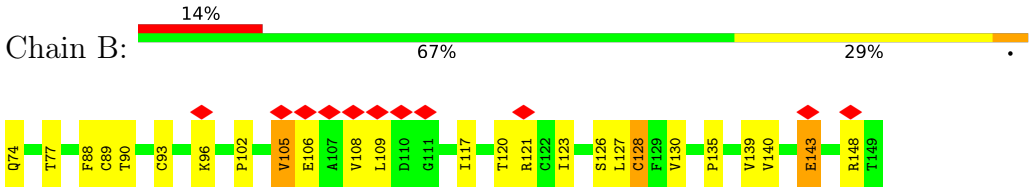
• Molecule 7: Cytochrome c domain-containing protein

Chain c:



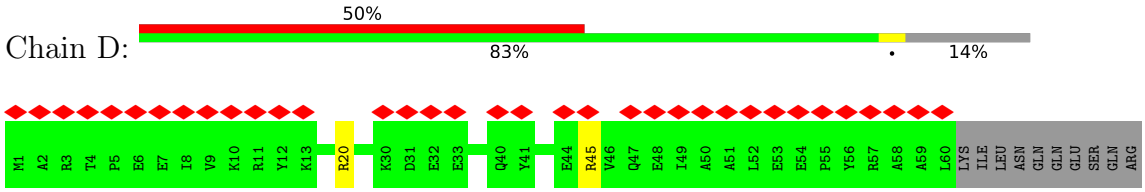
• Molecule 8: Photosystem P840 reaction center iron-sulfur protein

Chain B:



• Molecule 9: PscD'

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.381	Depositor
Minimum map value	-1.010	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	238.15, 238.15, 238.15	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, BCL, CLA, 84Q, CA, LYC, 85I, HEC, 85N, 2GO, SF4

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	1.97	235/7209 (3.3%)	1.33	86/9827 (0.9%)
1	a	1.85	195/7233 (2.7%)	1.28	90/9860 (0.9%)
2	C	2.35	99/1503 (6.6%)	1.67	34/2037 (1.7%)
3	E	2.16	9/262 (3.4%)	1.43	4/356 (1.1%)
3	e	1.50	2/262 (0.8%)	1.14	1/356 (0.3%)
4	F	2.28	15/279 (5.4%)	1.21	0/379
4	f	1.98	6/279 (2.2%)	1.28	1/379 (0.3%)
5	G	1.49	4/311 (1.3%)	1.60	6/421 (1.4%)
5	g	1.25	0/311	1.16	2/421 (0.5%)
7	c	2.54	75/1115 (6.7%)	1.79	36/1506 (2.4%)
8	B	0.79	0/578	1.11	3/789 (0.4%)
9	D	0.68	0/531	0.92	1/714 (0.1%)
All	All	1.93	640/19873 (3.2%)	1.35	264/27045 (1.0%)

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	1
1	a	0	4
2	C	0	2
7	c	0	1
All	All	0	8

The worst 5 of 640 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	539	TRP	C-O	-15.05	0.94	1.23
7	c	55	TYR	CD1-CE1	-13.98	1.18	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	55	TYR	CD2-CE2	-13.29	1.19	1.39
1	A	309	THR	CB-CG2	-13.11	1.09	1.52
1	A	758	GLY	C-O	-12.39	1.03	1.23

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	A	96	LEU	C-N-CD	-14.30	89.14	120.60
1	A	501	ARG	NE-CZ-NH2	12.92	126.76	120.30
7	c	26	ARG	NE-CZ-NH1	12.53	126.57	120.30
1	a	18	LEU	CA-CB-CG	12.52	144.09	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	639	ASN	Mainchain
2	C	141	THR	Mainchain
2	C	179	ASN	Mainchain
1	a	92	SER	Peptide
1	a	93	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	852/858 (99%)	792 (93%)	42 (5%)	18 (2%)	7 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	a	856/858 (100%)	798 (93%)	46 (5%)	12 (1%)	11 21
2	C	189/204 (93%)	174 (92%)	9 (5%)	6 (3%)	4 5
3	E	33/35 (94%)	31 (94%)	2 (6%)	0	100 100
3	e	33/35 (94%)	32 (97%)	0	1 (3%)	4 6
4	F	33/35 (94%)	31 (94%)	2 (6%)	0	100 100
4	f	33/35 (94%)	30 (91%)	2 (6%)	1 (3%)	4 6
5	G	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5 7
5	g	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
7	c	143/145 (99%)	127 (89%)	8 (6%)	8 (6%)	2 1
8	B	74/76 (97%)	43 (58%)	24 (32%)	7 (10%)	0 0
9	D	58/70 (83%)	58 (100%)	0	0	100 100
All	All	2376/2427 (98%)	2180 (92%)	142 (6%)	54 (2%)	9 10

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	97	PRO
1	A	147	TRP
1	A	170	TRP
1	A	346	LYS

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 PDB entries followed by that with respect to all EM entries.

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	718/720 (100%)	589 (82%)	129 (18%)	1 2
1	a	720/720 (100%)	585 (81%)	135 (19%)	1 2
2	C	155/166 (93%)	127 (82%)	28 (18%)	1 2
3	E	25/25 (100%)	23 (92%)	2 (8%)	12 23
3	e	25/25 (100%)	18 (72%)	7 (28%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	31/31 (100%)	25 (81%)	6 (19%)	1 2
4	f	31/31 (100%)	26 (84%)	5 (16%)	2 3
5	G	31/31 (100%)	25 (81%)	6 (19%)	1 2
5	g	31/31 (100%)	22 (71%)	9 (29%)	0 0
7	c	112/112 (100%)	91 (81%)	21 (19%)	1 2
8	B	65/65 (100%)	47 (72%)	18 (28%)	0 1
9	D	52/62 (84%)	51 (98%)	1 (2%)	57 78
All	All	1996/2019 (99%)	1629 (82%)	367 (18%)	4 2

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	303	VAL
1	a	736	ILE
1	a	386	ILE
1	a	552	LEU
1	a	836	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
7	c	96	ASN
7	c	109	GLN
1	A	825	GLN
1	A	808	GLN
7	c	144	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 81 ligands modelled in this entry, 2 are monoatomic and 32 are unknown - leaving 47 for Mogul analysis.

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	$\#\|Z\| > 2$
11	BCL	A	904	-	38,54,74	2.32	16 (42%)	45,91,115	2.92	22 (48%)
11	BCL	a	907	-	58,74,74	1.94	18 (31%)	69,115,115	3.75	24 (34%)
12	CLA	a	912	21	65,73,73	2.79	17 (26%)	76,113,113	3.23	38 (50%)
12	CLA	a	913	-	65,73,73	2.62	20 (30%)	76,113,113	4.02	34 (44%)
12	CLA	a	914	-	46,54,73	2.87	19 (41%)	53,90,113	3.60	27 (50%)
15	85I	a	920	-	43,44,44	2.22	2 (4%)	47,51,51	2.04	3 (6%)
12	CLA	A	933	-	51,59,73	2.87	18 (35%)	59,96,113	3.90	32 (54%)
11	BCL	A	902	-	58,74,74	2.34	18 (31%)	69,115,115	3.27	29 (42%)
10	2GO	a	903	1	65,74,74	3.45	20 (30%)	76,115,115	3.41	28 (36%)
11	BCL	A	908	-	58,74,74	2.32	23 (39%)	69,115,115	2.64	24 (34%)
18	HEC	C	301	2	32,50,50	2.95	17 (53%)	24,82,82	3.49	12 (50%)
17	85N	g	101	-	36,37,46	0.79	1 (2%)	40,45,55	0.58	0
18	HEC	c	202	7	32,50,50	2.84	14 (43%)	24,82,82	3.87	11 (45%)
11	BCL	A	907	-	53,69,74	3.09	23 (43%)	63,109,115	4.62	34 (53%)
11	BCL	a	904	-	58,74,74	2.22	15 (25%)	69,115,115	3.26	21 (30%)
12	CLA	A	910	-	65,73,73	2.10	21 (32%)	76,113,113	3.13	31 (40%)
13	LYC	c	201	-	39,39,39	1.65	9 (23%)	44,46,46	5.76	28 (63%)
15	85I	A	916	-	43,44,44	2.15	3 (6%)	47,51,51	2.32	7 (14%)
11	BCL	a	909	-	58,74,74	2.21	18 (31%)	69,115,115	3.75	21 (30%)
17	85N	a	902	-	45,46,46	0.59	0	50,55,55	0.43	0
19	84Q	a	921	-	42,43,43	1.35	2 (4%)	47,50,50	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	A	912	-	46,54,73	2.76	15 (32%)	53,90,113	4.13	29 (54%)
20	SF4	a	917	1	0,12,12	-	-	-		
15	85I	a	919	-	43,44,44	1.41	2 (4%)	47,51,51	1.66	3 (6%)
15	85I	A	917	-	43,44,44	1.57	2 (4%)	47,51,51	2.42	3 (6%)
11	BCL	A	909	-	58,74,74	2.96	22 (37%)	69,115,115	4.47	34 (49%)
11	BCL	A	906	1	44,60,74	2.27	9 (20%)	52,98,115	4.24	19 (36%)
12	CLA	A	911	-	65,73,73	2.71	22 (33%)	76,113,113	3.34	28 (36%)
11	BCL	a	905	-	58,74,74	2.38	14 (24%)	69,115,115	3.54	27 (39%)
15	85I	a	918	-	43,44,44	1.05	2 (4%)	47,51,51	1.69	4 (8%)
20	SF4	B	201	-	0,12,12	-	-	-		
10	2GO	A	901	1	65,74,74	3.57	18 (27%)	76,115,115	3.49	29 (38%)
11	BCL	a	906	-	38,54,74	2.51	15 (39%)	45,91,115	2.77	21 (46%)
11	BCL	a	911	-	58,74,74	2.51	16 (27%)	69,115,115	3.04	30 (43%)
19	84Q	E	101	-	42,43,43	2.09	10 (23%)	47,50,50	1.90	8 (17%)
11	BCL	a	910	-	58,74,74	3.13	15 (25%)	69,115,115	4.29	33 (47%)
15	85I	A	915	-	43,44,44	2.29	10 (23%)	47,51,51	2.44	7 (14%)
17	85N	A	932	-	45,46,46	1.04	1 (2%)	50,55,55	1.82	4 (8%)
13	LYC	A	913	-	39,39,39	2.05	11 (28%)	44,46,46	2.49	18 (40%)
12	CLA	a	915	-	51,59,73	2.93	17 (33%)	59,96,113	3.55	34 (57%)
17	85N	G	101	-	36,37,46	0.72	0	40,45,55	0.77	2 (5%)
11	BCL	a	908	1	58,74,74	2.44	20 (34%)	69,115,115	4.45	30 (43%)
11	BCL	A	905	-	58,74,74	2.40	17 (29%)	69,115,115	3.43	26 (37%)
12	CLA	a	901	21	65,73,73	2.66	21 (32%)	76,113,113	3.57	32 (42%)
11	BCL	A	903	-	58,74,74	2.60	18 (31%)	69,115,115	3.70	25 (36%)
20	SF4	B	202	8	0,12,12	-	-	-		
12	CLA	A	931	-	65,73,73	3.13	25 (38%)	76,113,113	4.31	38 (50%)

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
11	BCL	A	904	-	-	6/13/113/137	-
11	BCL	a	907	-	-	12/37/137/137	-
12	CLA	a	912	21	-	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	913	-	-	11/37/115/115	-
12	CLA	a	914	-	-	4/15/93/115	-
15	85I	a	920	-	-	29/47/48/48	-
12	CLA	A	933	-	-	4/21/99/115	-
11	BCL	A	902	-	-	16/37/137/137	-
10	2GO	a	903	1	-	9/37/97/97	-
11	BCL	A	908	-	-	14/37/137/137	-
18	HEC	C	301	2	-	3/10/54/54	-
17	85N	g	101	-	-	19/42/42/51	-
18	HEC	c	202	7	-	3/10/54/54	-
11	BCL	A	907	-	-	16/31/131/137	-
12	CLA	A	910	-	1/1/15/20	13/37/115/115	-
11	BCL	a	904	-	-	12/37/137/137	-
13	LYC	c	201	-	-	16/43/43/43	-
15	85I	A	916	-	1/1/6/7	29/47/48/48	-
11	BCL	a	909	-	-	13/37/137/137	-
17	85N	a	902	-	-	24/51/51/51	-
19	84Q	a	921	-	-	32/46/47/47	-
12	CLA	A	912	-	-	2/15/93/115	-
20	SF4	a	917	1	-	-	0/6/5/5
15	85I	a	919	-	-	36/47/48/48	-
15	85I	A	917	-	-	29/47/48/48	-
12	CLA	A	911	-	1/1/15/20	11/37/115/115	-
11	BCL	A	906	1	-	6/21/121/137	-
11	BCL	A	909	-	-	12/37/137/137	-
11	BCL	a	905	-	-	17/37/137/137	-
15	85I	a	918	-	-	21/47/48/48	-
20	SF4	B	201	-	-	-	0/6/5/5
10	2GO	A	901	1	-	4/37/97/97	-
11	BCL	a	906	-	-	6/13/113/137	-
11	BCL	a	911	-	-	5/37/137/137	-
19	84Q	E	101	-	-	27/46/47/47	-
11	BCL	a	910	-	-	11/37/137/137	-
15	85I	A	915	-	-	19/47/48/48	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	85N	A	932	-	-	18/51/51/51	-
13	LYC	A	913	-	-	1/43/43/43	-
12	CLA	a	915	-	-	7/21/99/115	-
17	85N	G	101	-	-	18/42/42/51	-
11	BCL	a	908	1	-	20/37/137/137	-
11	BCL	A	905	-	-	16/37/137/137	-
12	CLA	a	901	21	-	24/37/115/115	-
11	BCL	A	903	-	-	21/37/137/137	-
20	SF4	B	202	8	-	-	0/6/5/5
12	CLA	A	931	-	-	18/37/115/115	-

The worst 5 of 596 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	910	BCL	C4B-NB	-15.65	1.21	1.35
10	A	901	2GO	C4D-ND	-14.73	1.18	1.37
10	A	901	2GO	C2A-C3A	14.60	1.67	1.36
15	a	920	85I	O6-C3	-14.03	1.20	1.44
10	a	903	2GO	C3C-C2C	11.92	1.62	1.36

The worst 5 of 912 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	909	BCL	O2D-CGD-CBD	20.86	148.34	111.27
11	a	908	BCL	C4A-NA-C1A	18.75	115.13	106.71
11	A	906	BCL	O2D-CGD-CBD	18.23	143.66	111.27
12	A	931	CLA	O2D-CGD-CBD	18.08	143.39	111.27
11	a	907	BCL	C4A-NA-C1A	16.51	114.13	106.71

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	910	CLA	C8
12	A	911	CLA	C8
15	A	916	85I	C3

5 of 646 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	a	903	2GO	C1A-C2A-CAA-CBA

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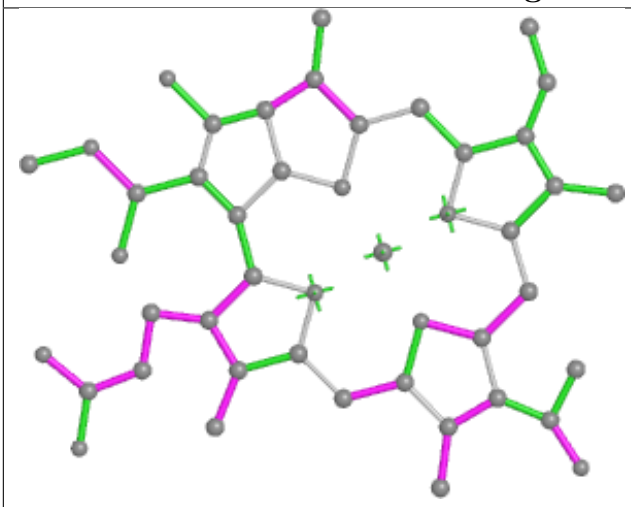
Mol	Chain	Res	Type	Atoms
11	A	902	BCL	C3A-C2A-CAA-CBA
11	A	902	BCL	C11-C12-C13-C14
11	A	903	BCL	C1A-C2A-CAA-CBA
11	A	903	BCL	C2-C3-C5-C6

There are no ring outliers.

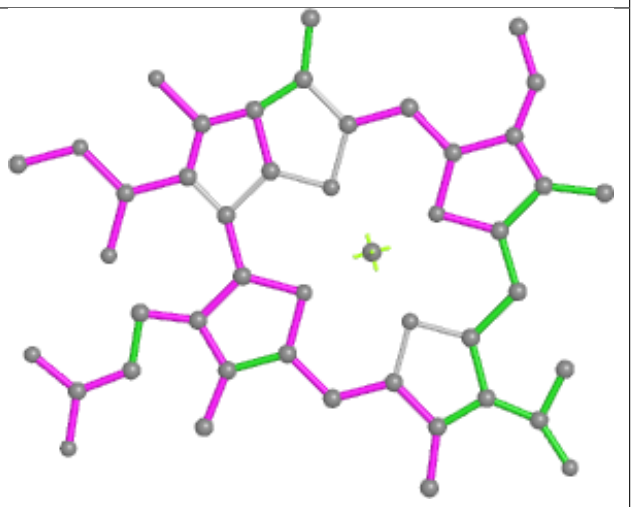
No monomer is involved in short contacts.

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.

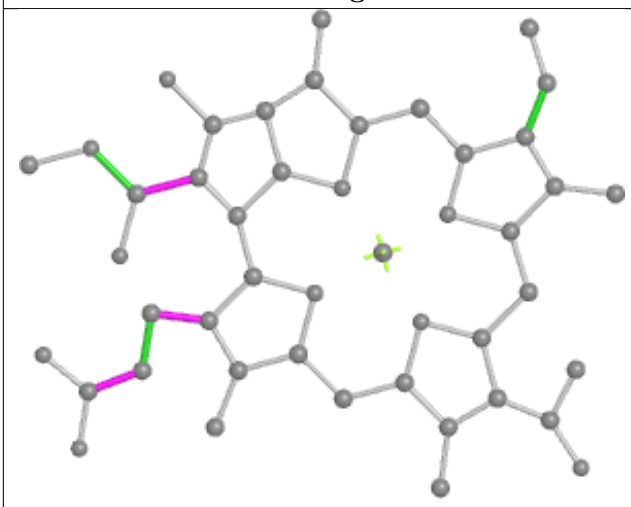
Ligand BCL A 904



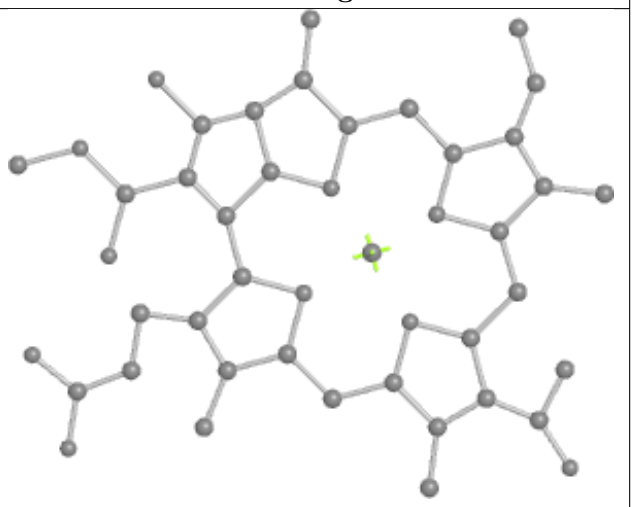
Bond lengths



Bond angles

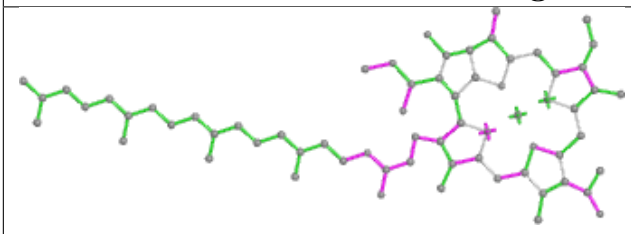


Torsions

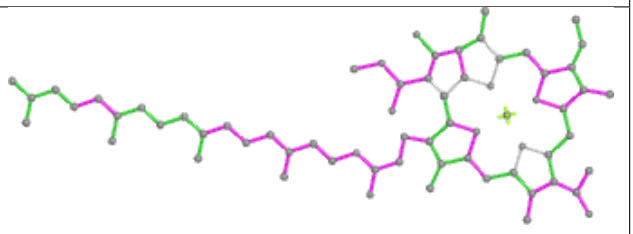


Rings

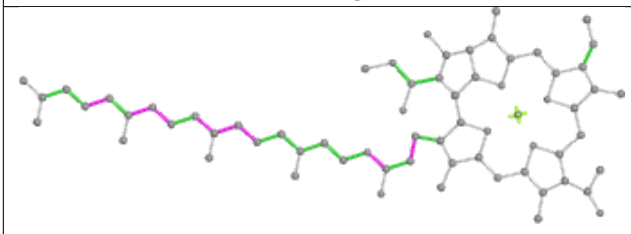
Ligand BCL a 907



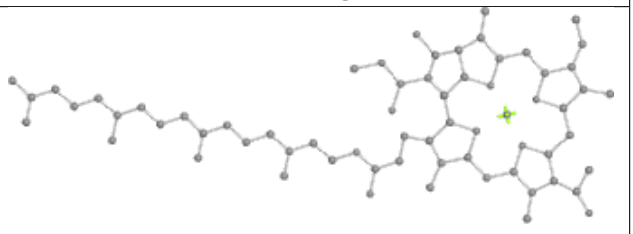
Bond lengths



Bond angles

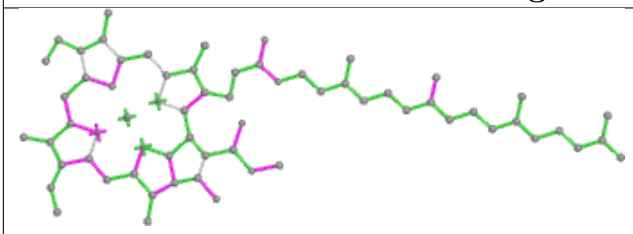


Torsions

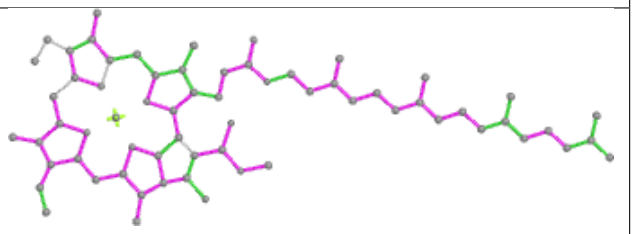


Rings

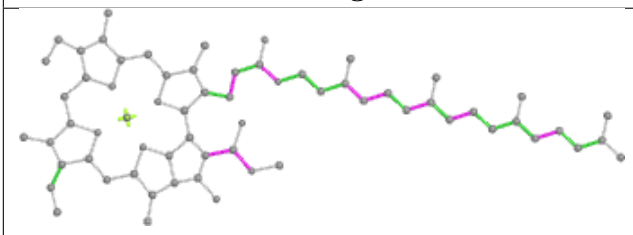
Ligand CLA a 912



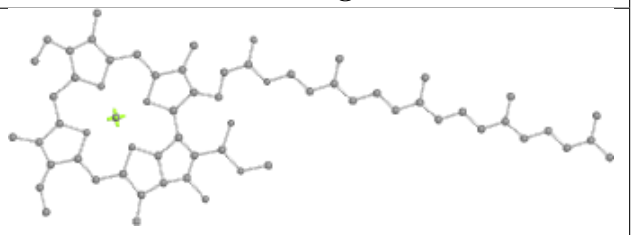
Bond lengths



Bond angles

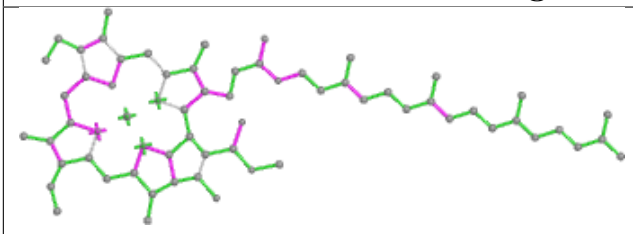


Torsions



Rings

Ligand CLA a 913



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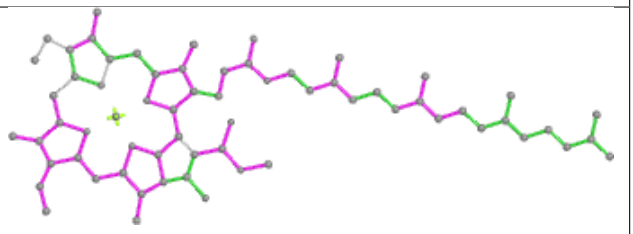
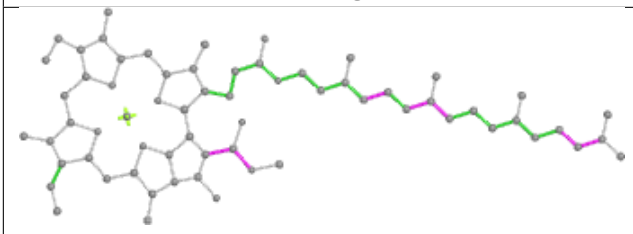
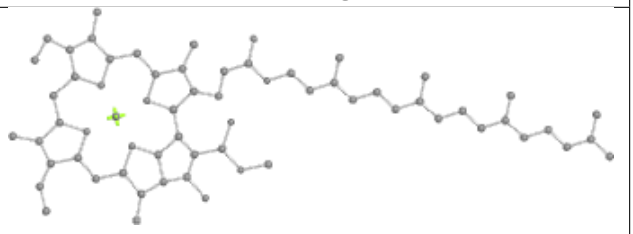


Bond angles

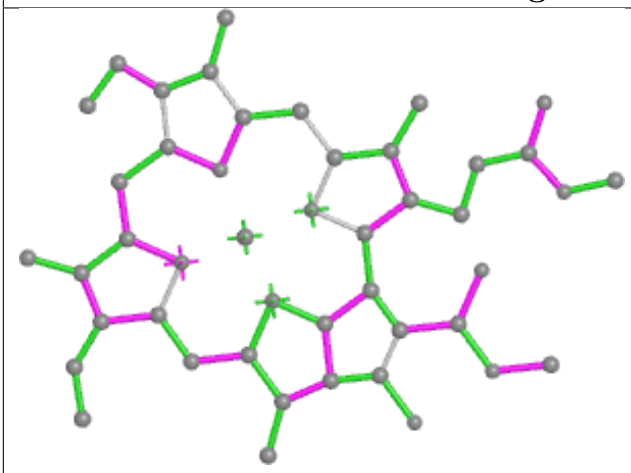


Torsions



Rings

Ligand CLA a 914



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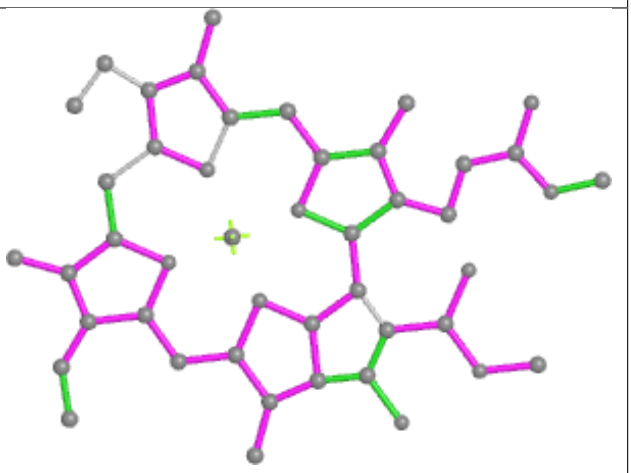
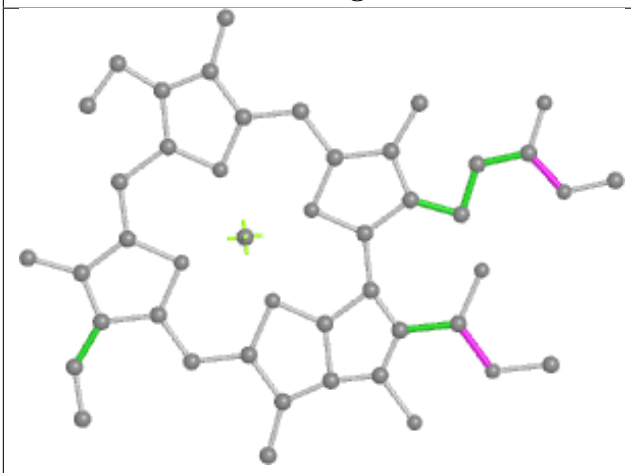
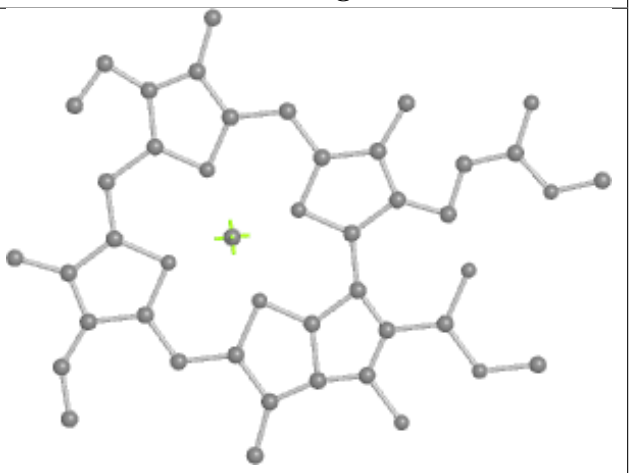


Bond angles

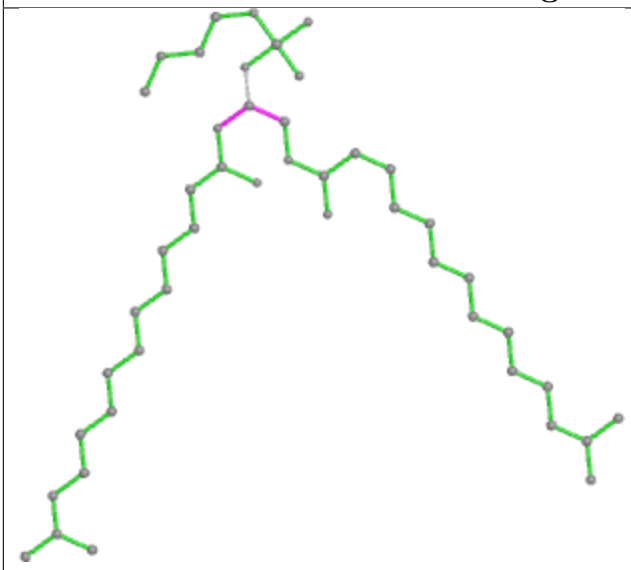


Torsions

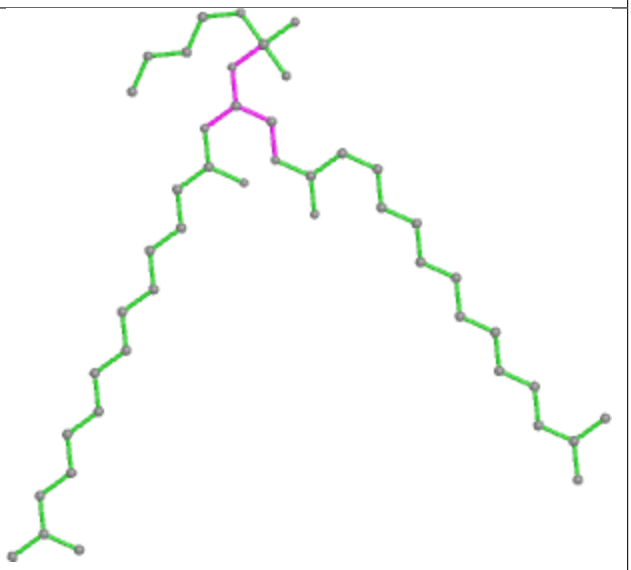


Rings

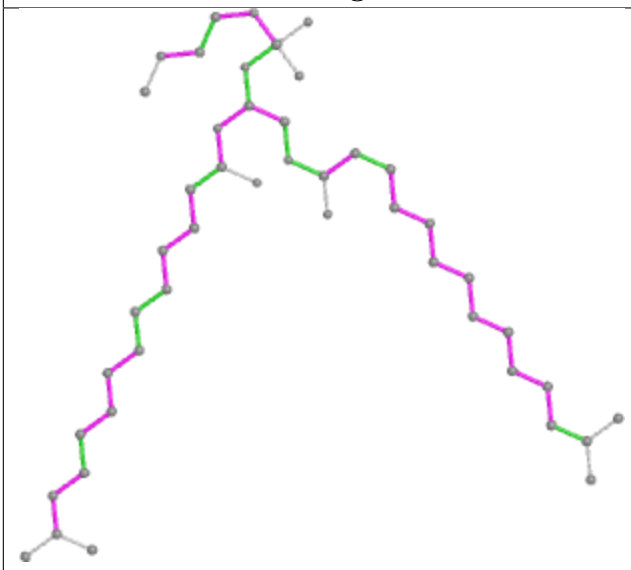
Ligand 85I a 920



Bond lengths



Bond angles



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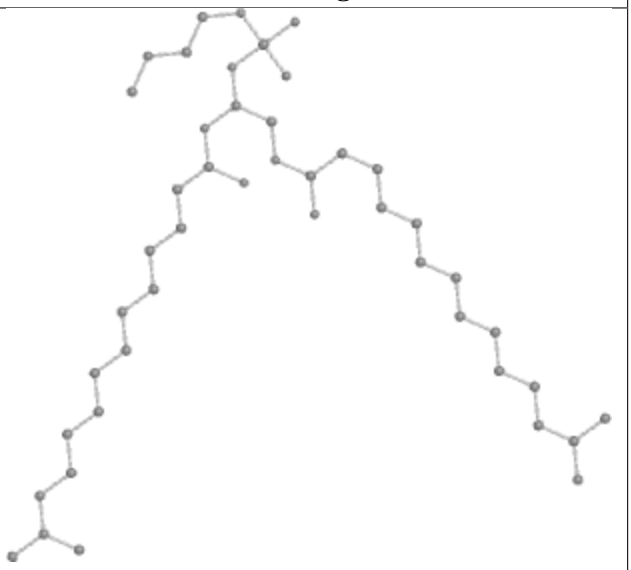
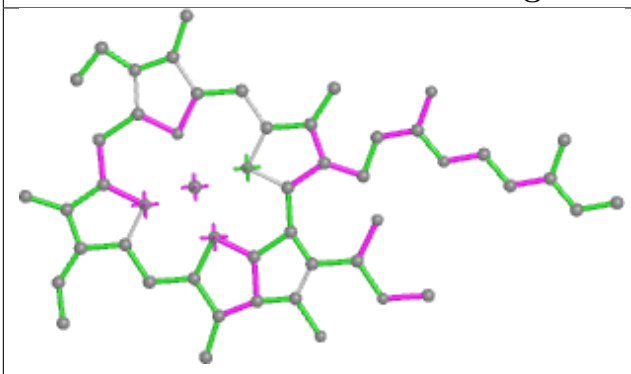


Rings

Ligand CLA A 933



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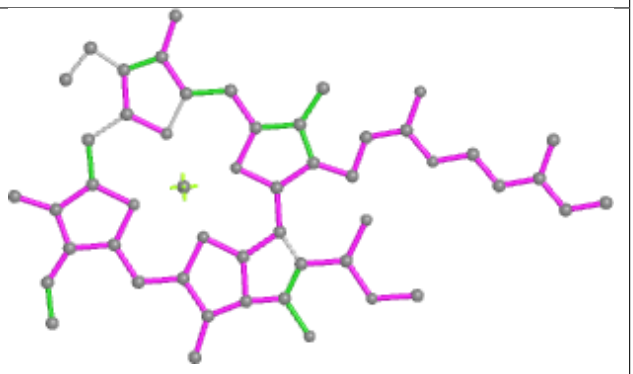
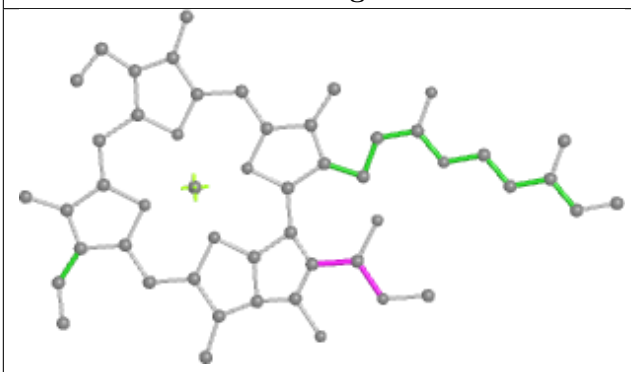
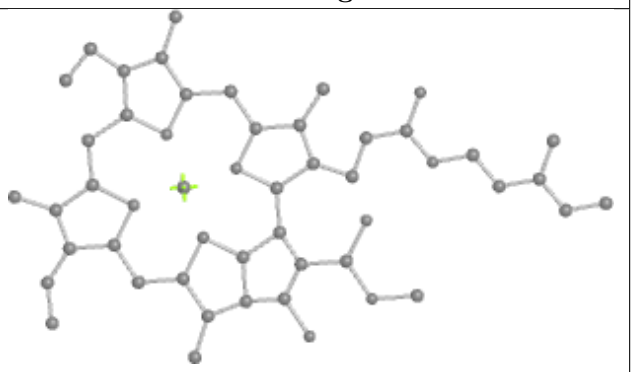


Bond angles

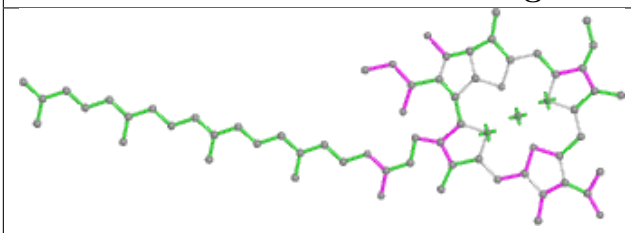


Torsions

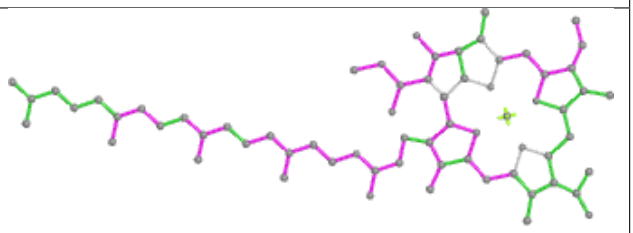


Rings

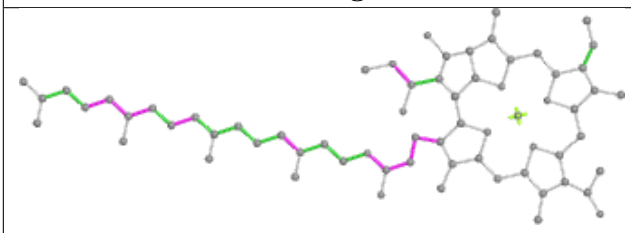
Ligand BCL A 902



Bond lengths



Bond angles



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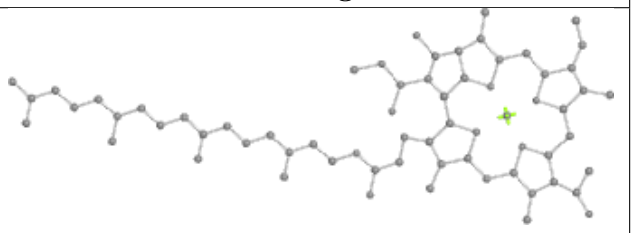
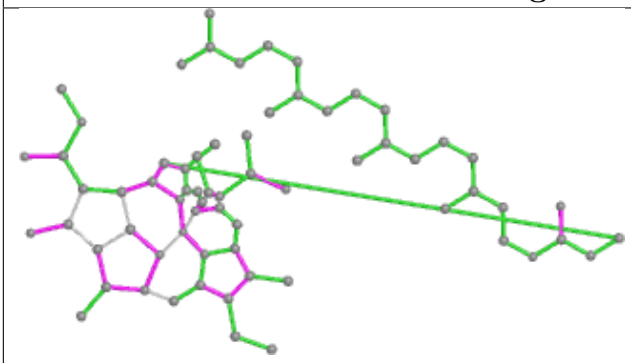


Rings

Ligand 2GO a 903



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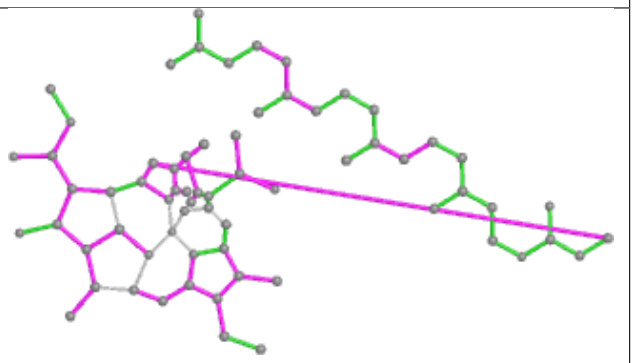
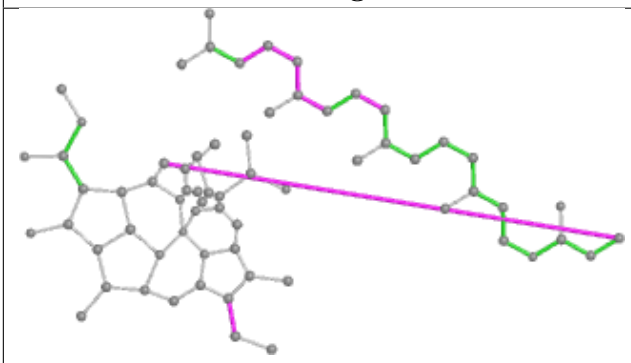
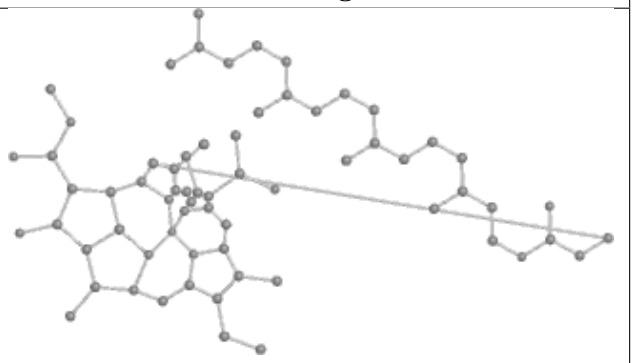


Bond angles

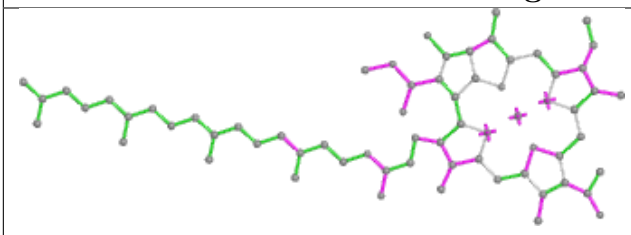


Torsions

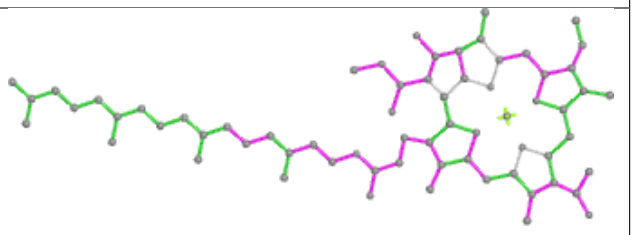


Rings

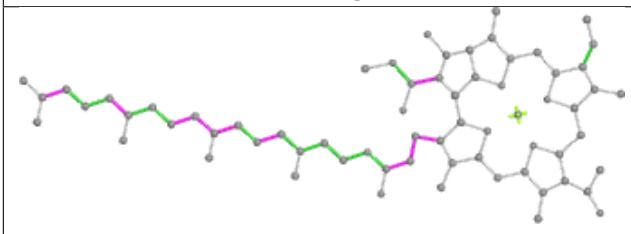
Ligand BCL A 908



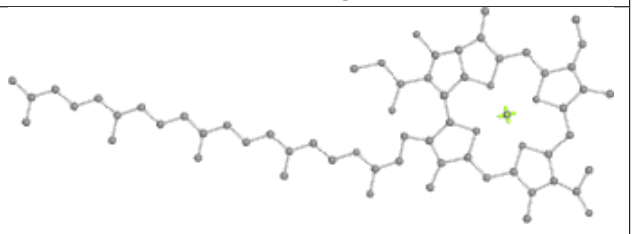
Bond lengths



Bond angles

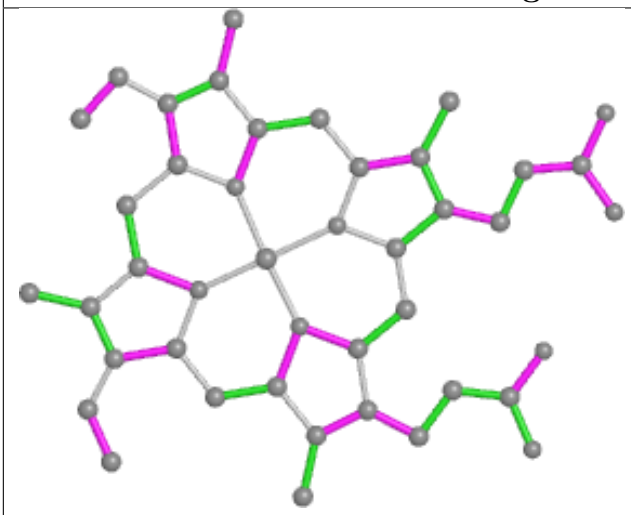


Torsions

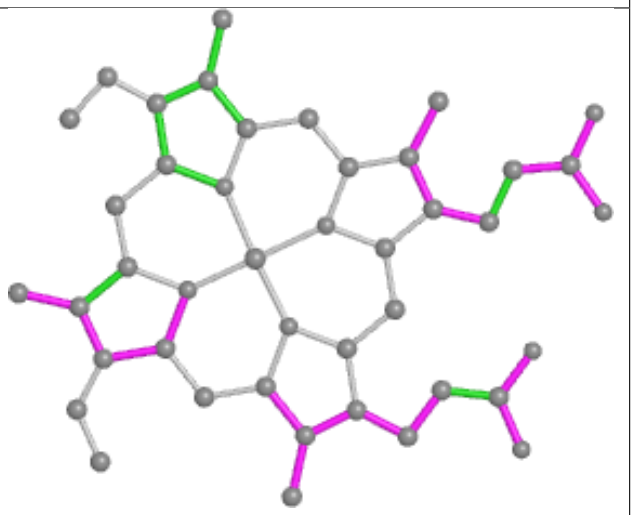


Rings

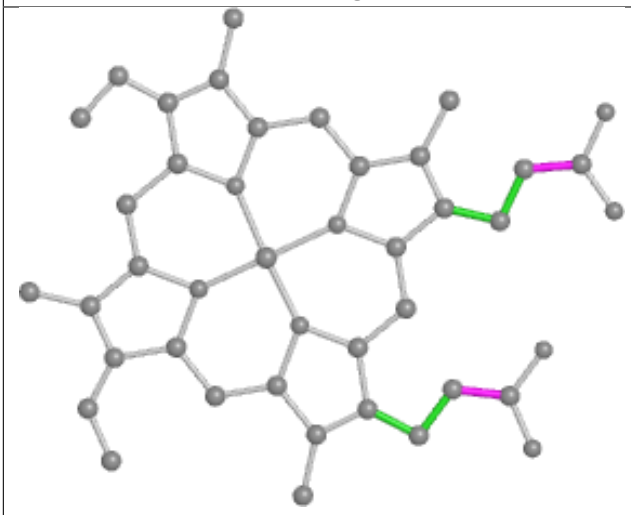
Ligand HEC C 301



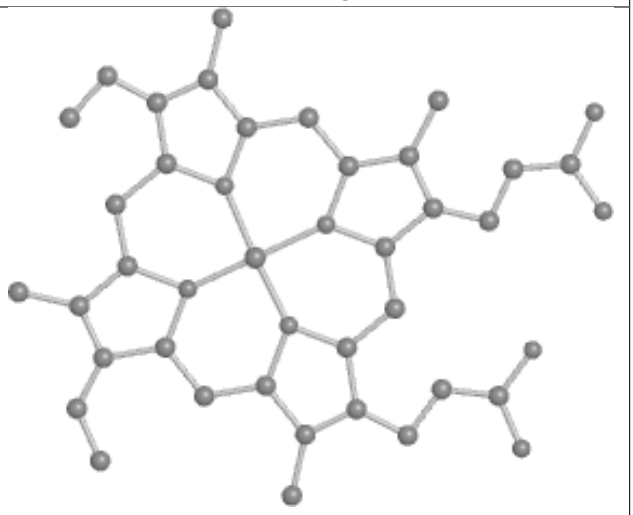
Bond lengths



Bond angles

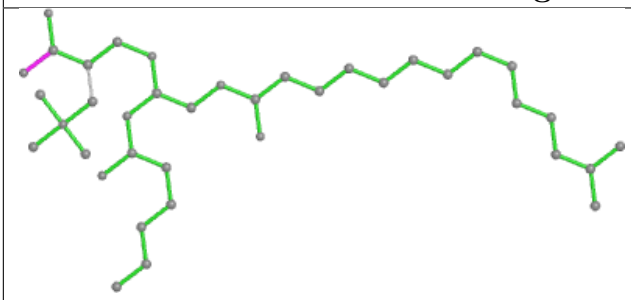


Torsions

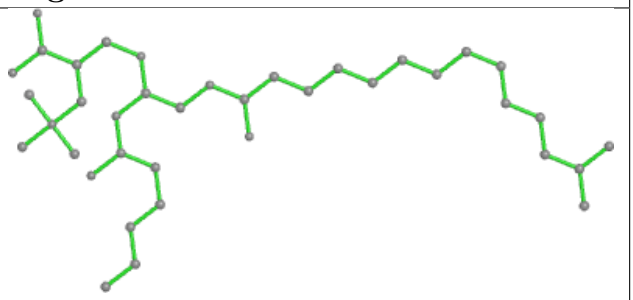


Rings

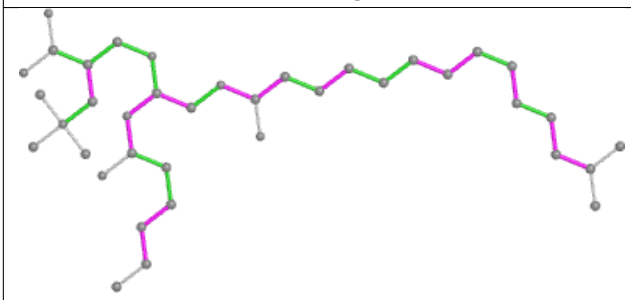
Ligand 85N g 101



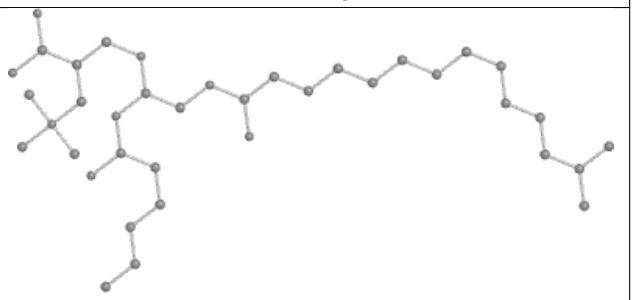
Bond lengths



Bond angles

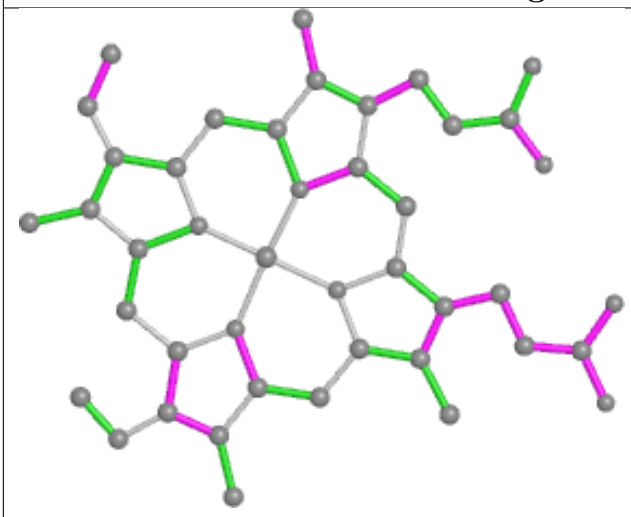


Torsions

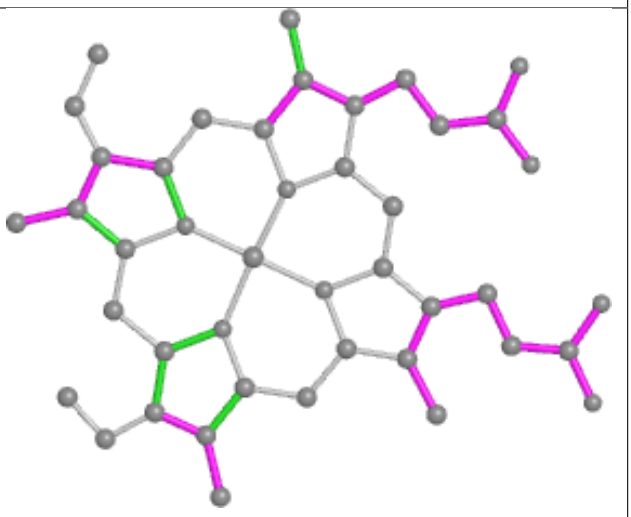


Rings

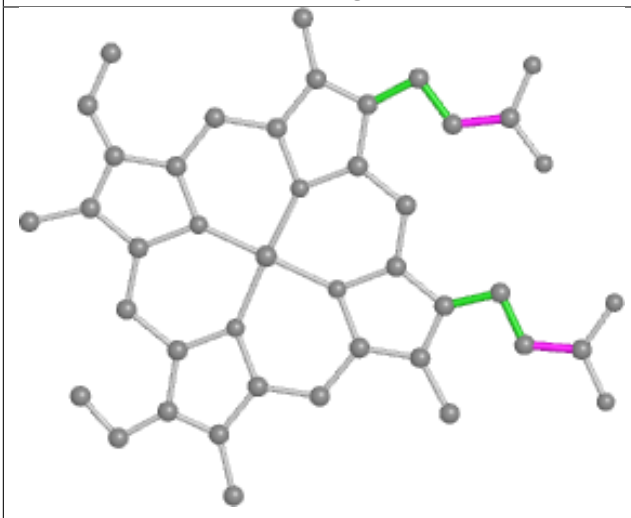
Ligand HEC c 202



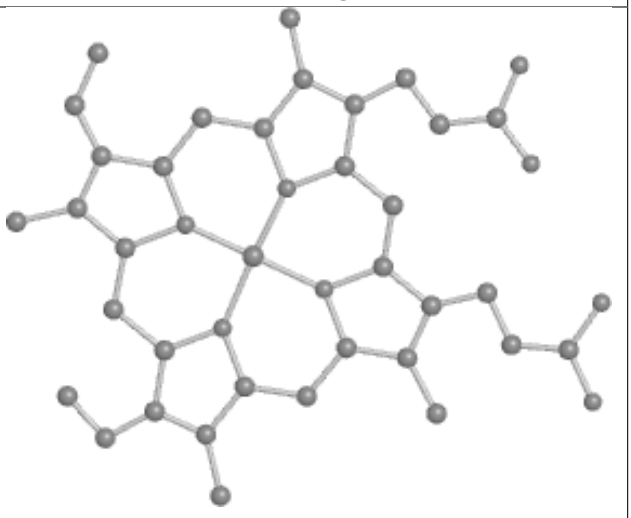
Bond lengths



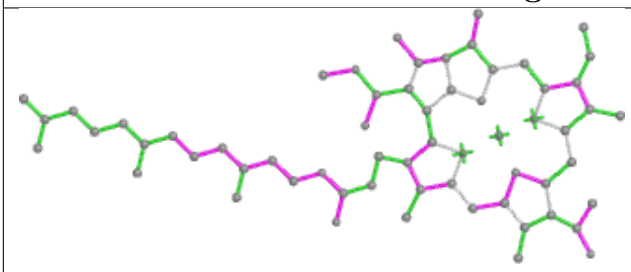
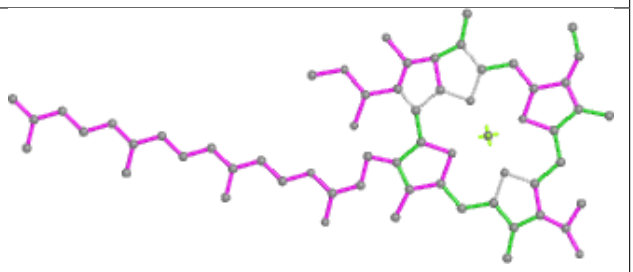
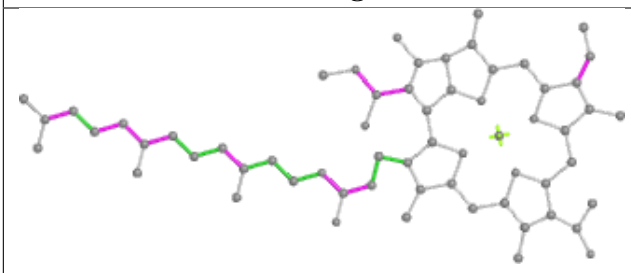
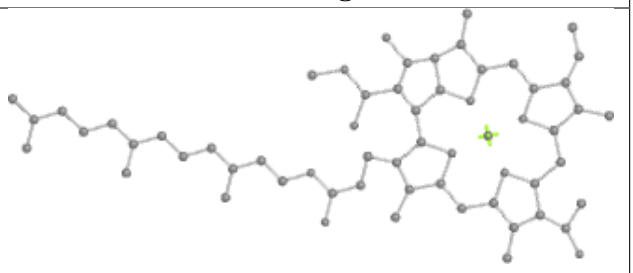
Bond angles

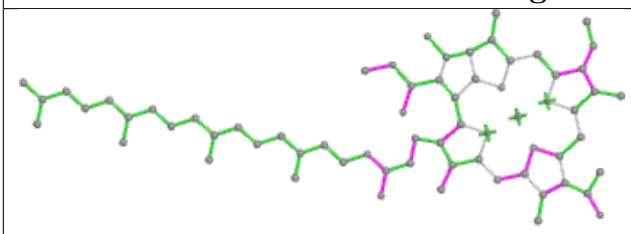
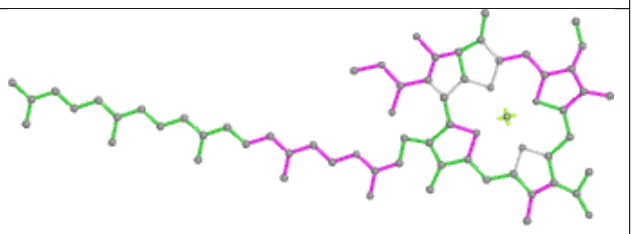
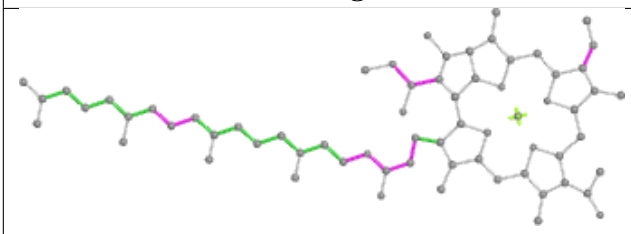
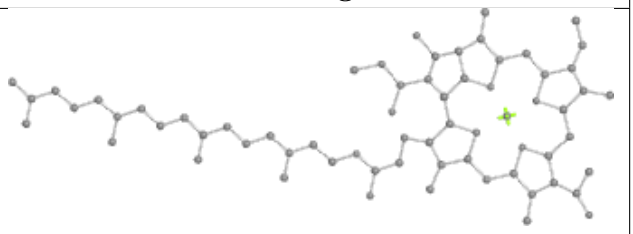


Torsions

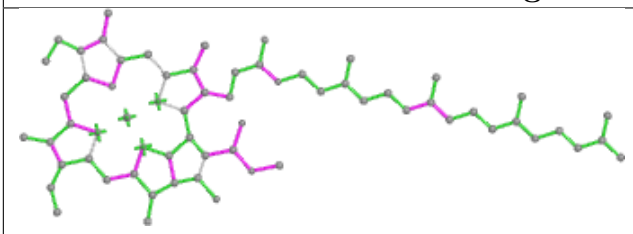


Rings

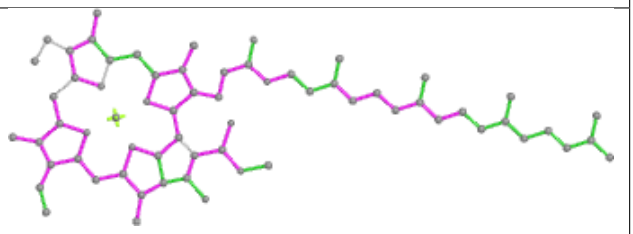
Ligand BCL A 907	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL a 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

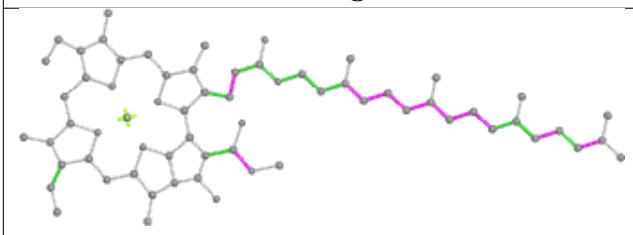
Ligand CLA A 910



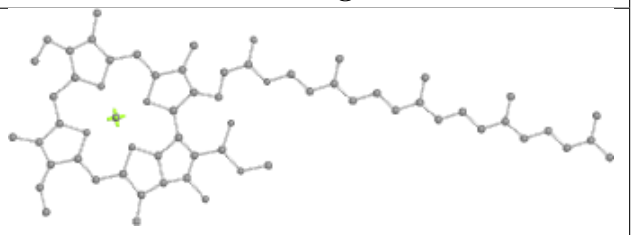
Bond lengths



Bond angles

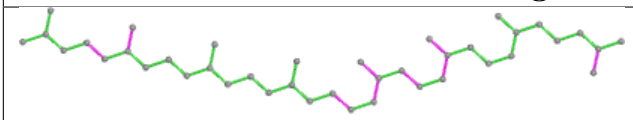


Torsions

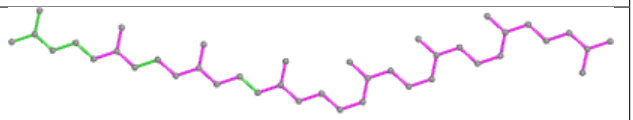


Rings

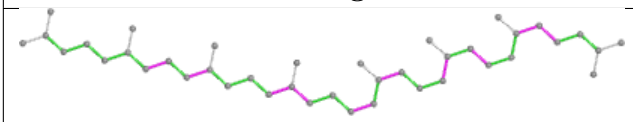
Ligand LYC c 201



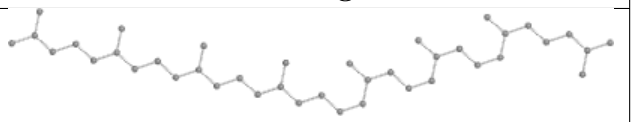
Bond lengths



Bond angles

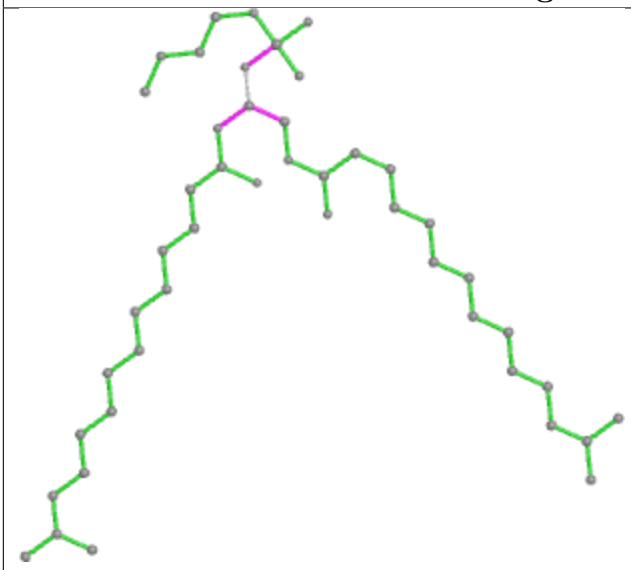


Torsions

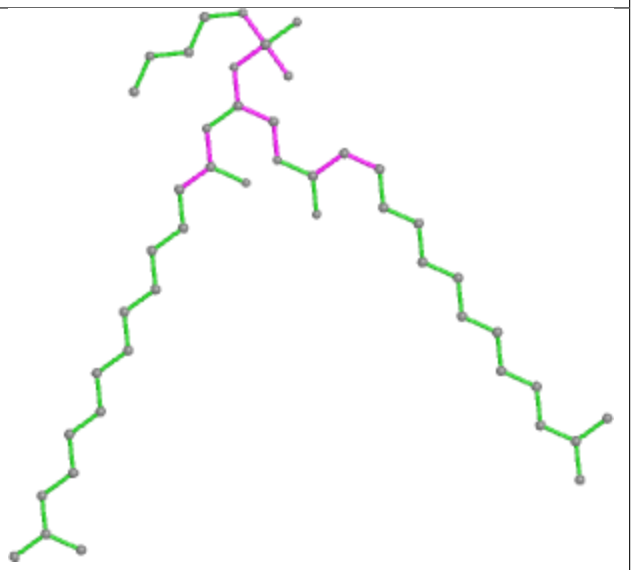


Rings

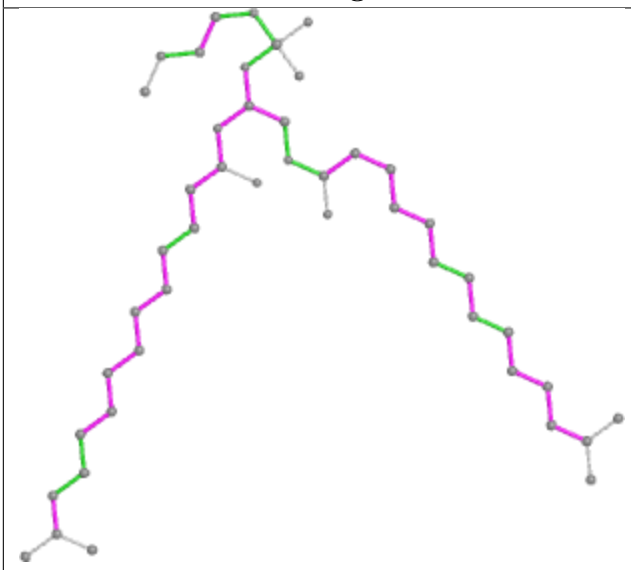
Ligand 85I A 916



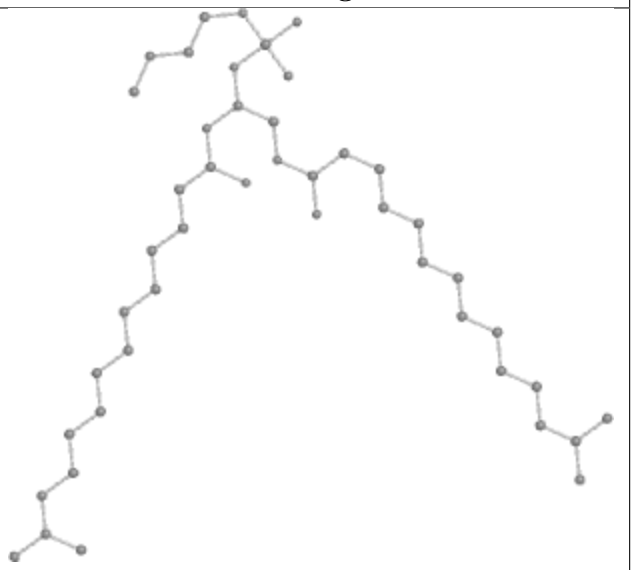
Bond lengths



Bond angles

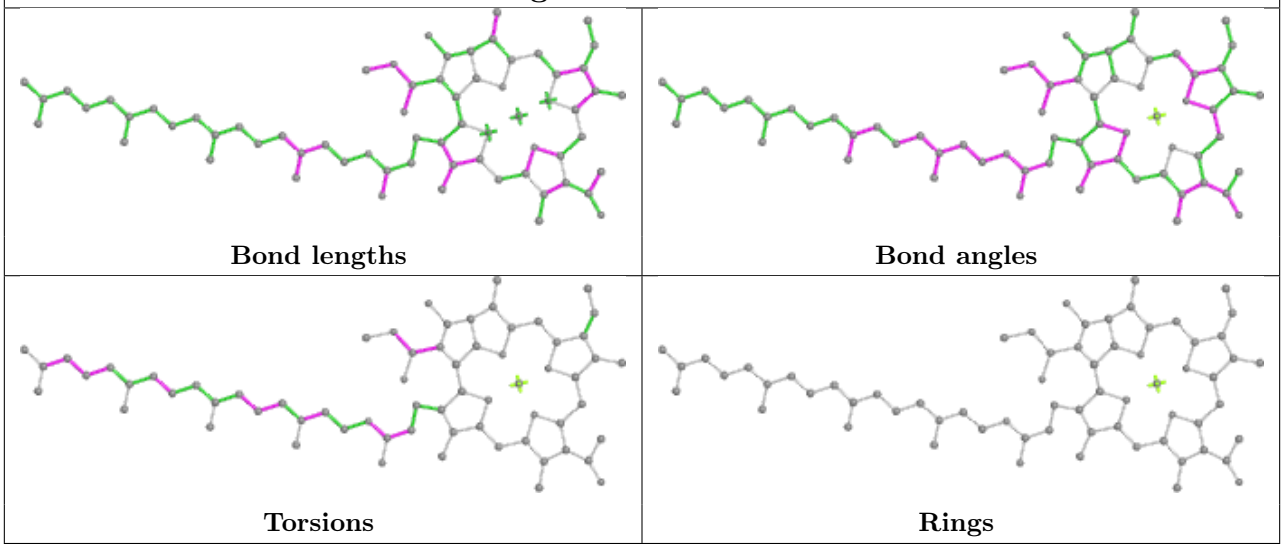


Torsions

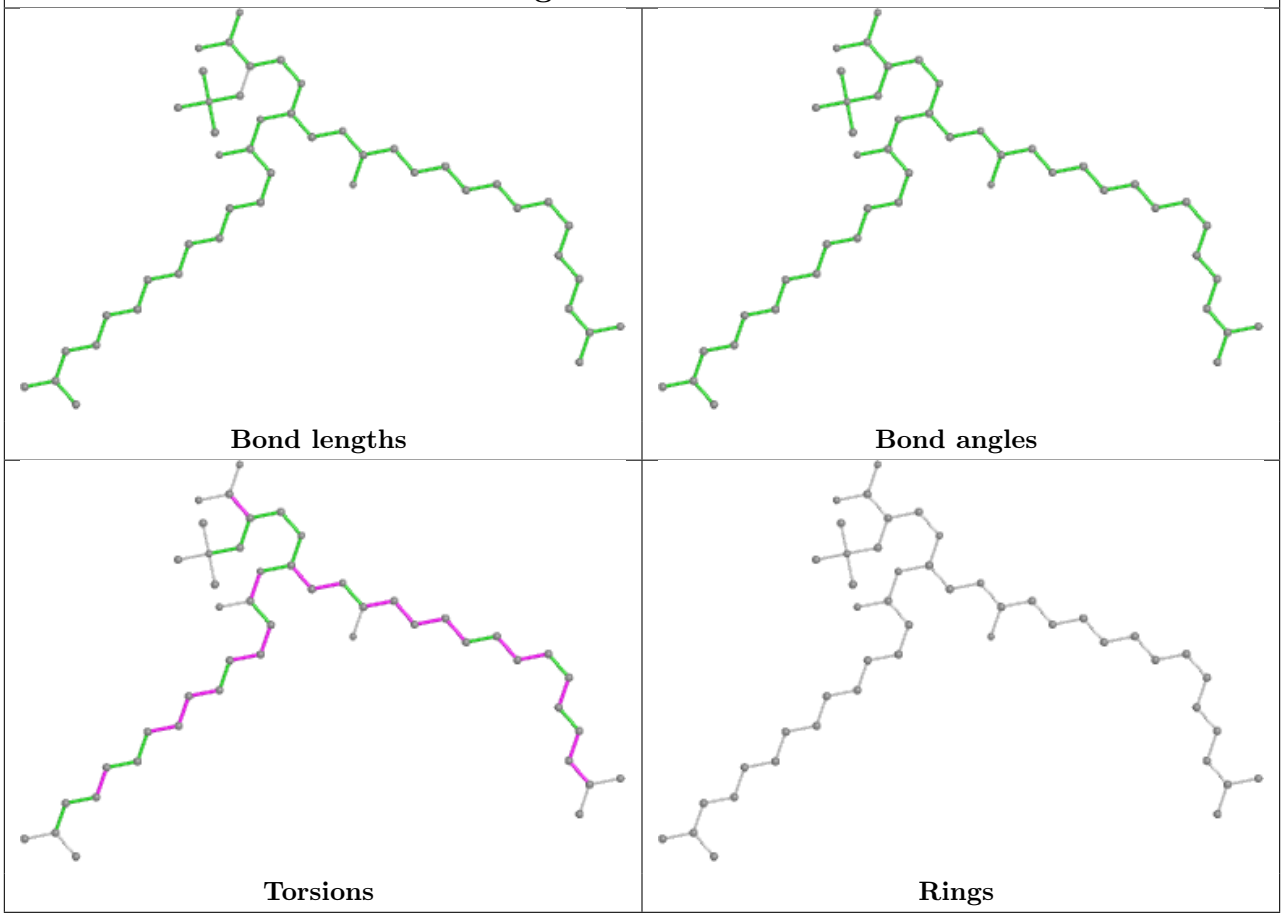


Rings

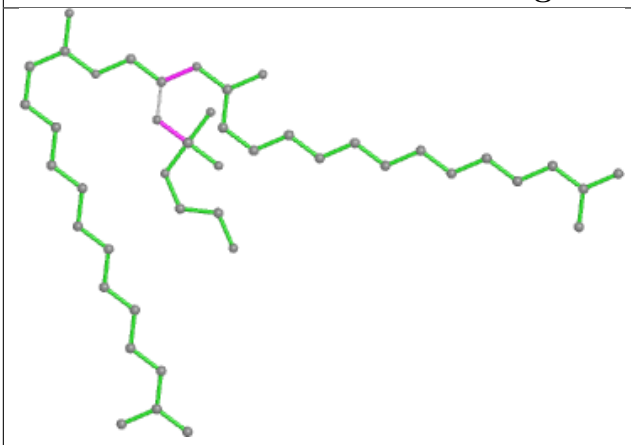
Ligand BCL a 909



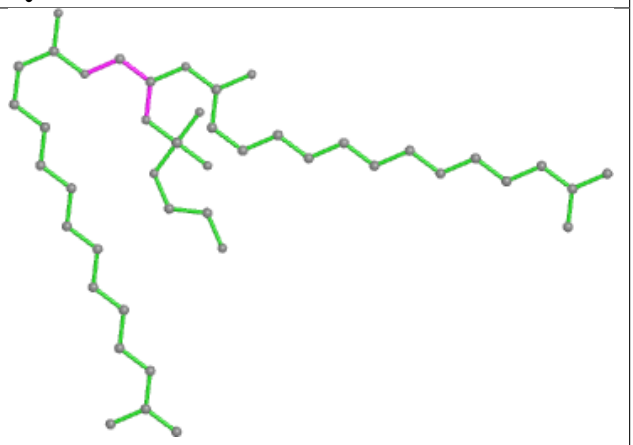
Ligand 85N a 902



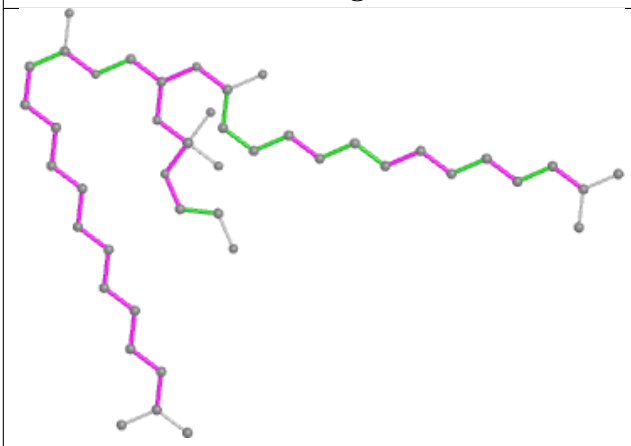
Ligand 84Q a 921



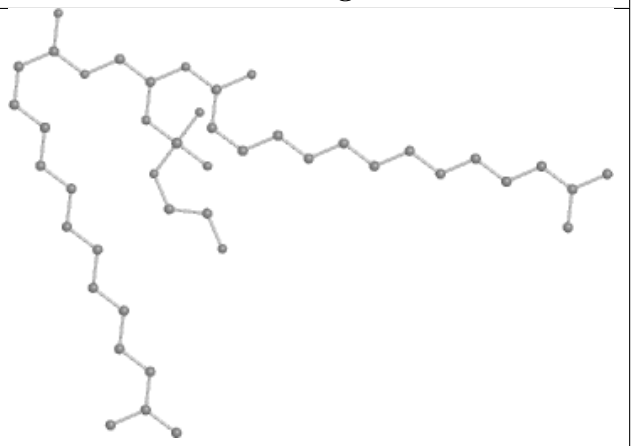
Bond lengths



Bond angles

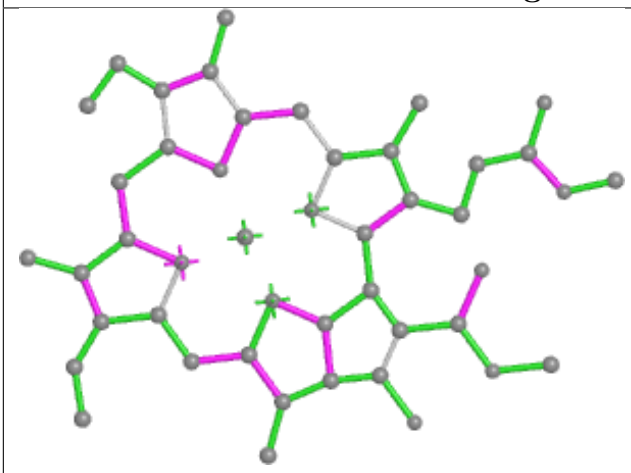


Torsions

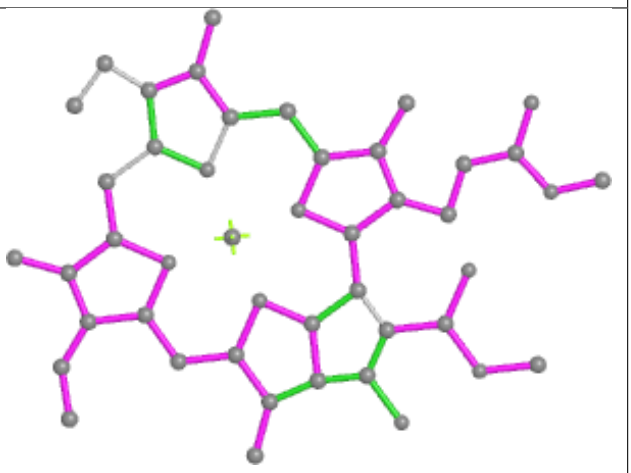


Rings

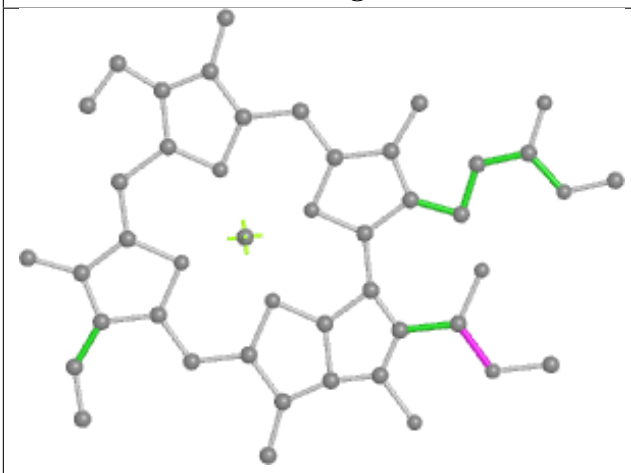
Ligand CLA A 912



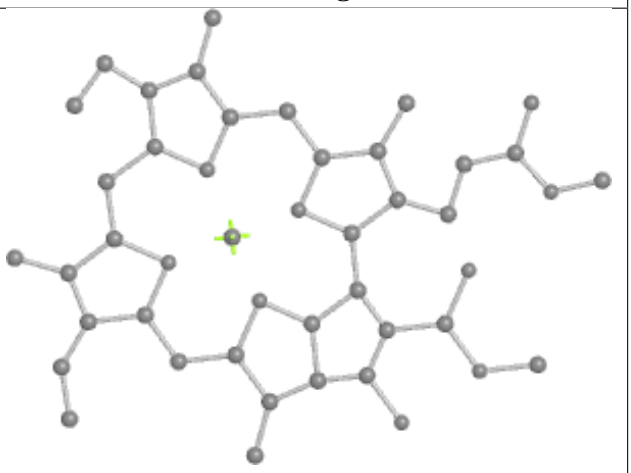
Bond lengths



Bond angles

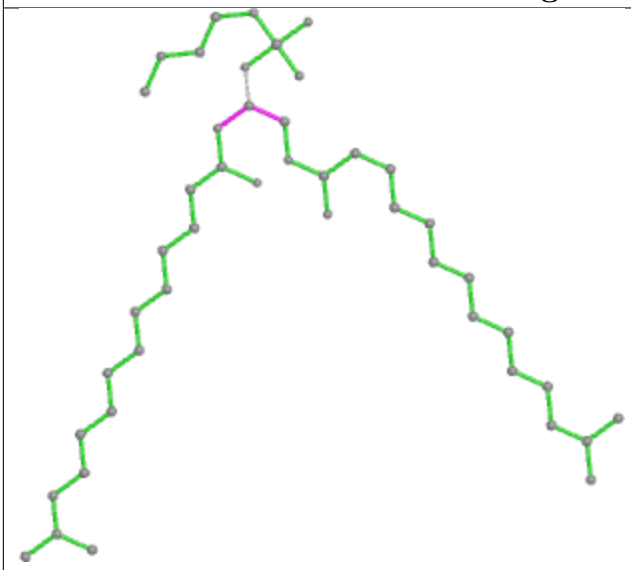


Torsions

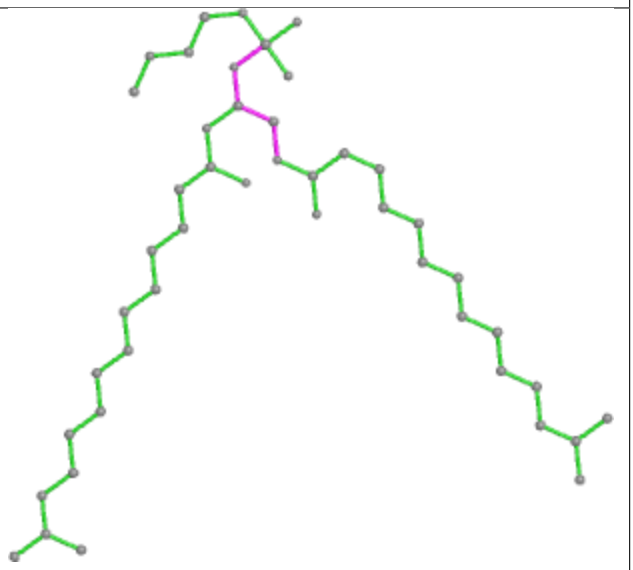


Rings

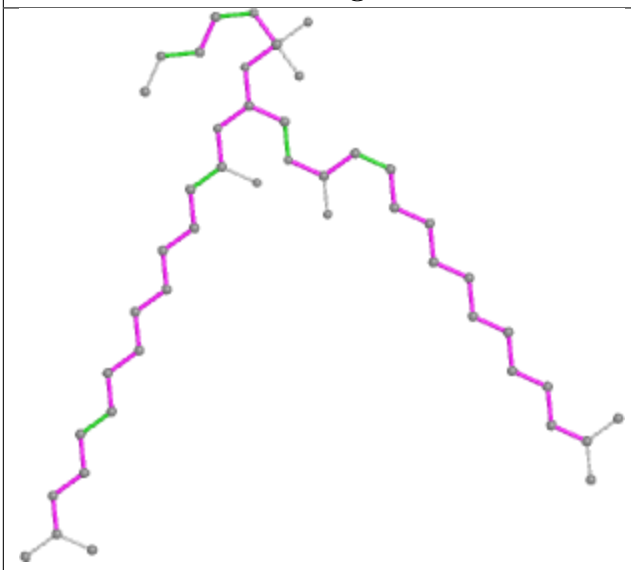
Ligand 85I a 919



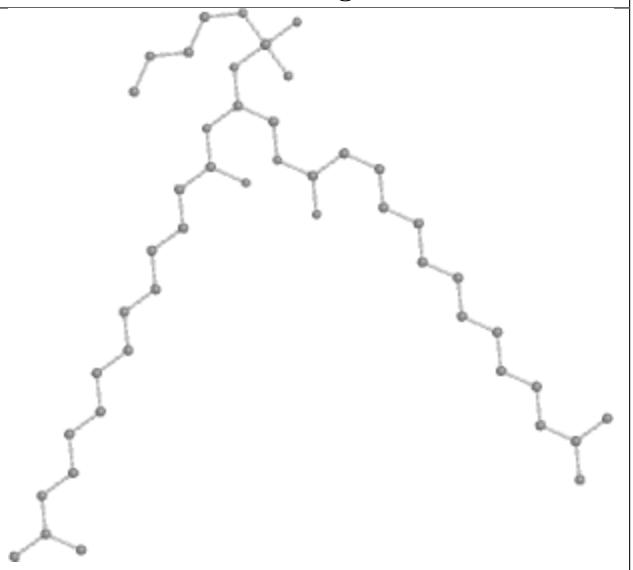
Bond lengths



Bond angles

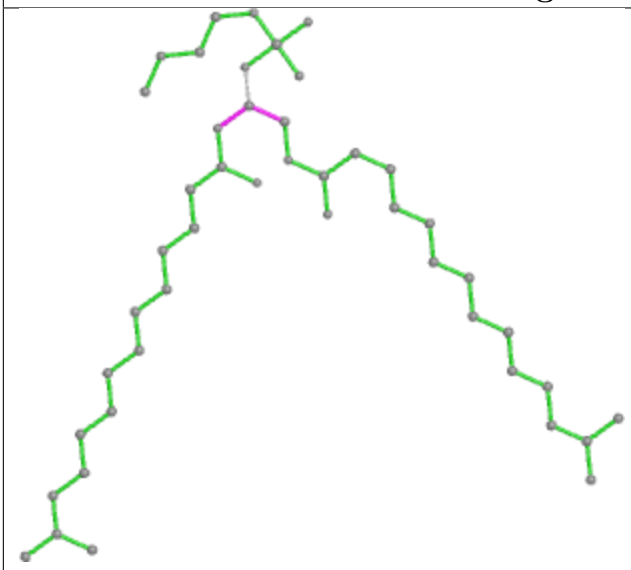


Torsions



Rings

Ligand 85I A 917



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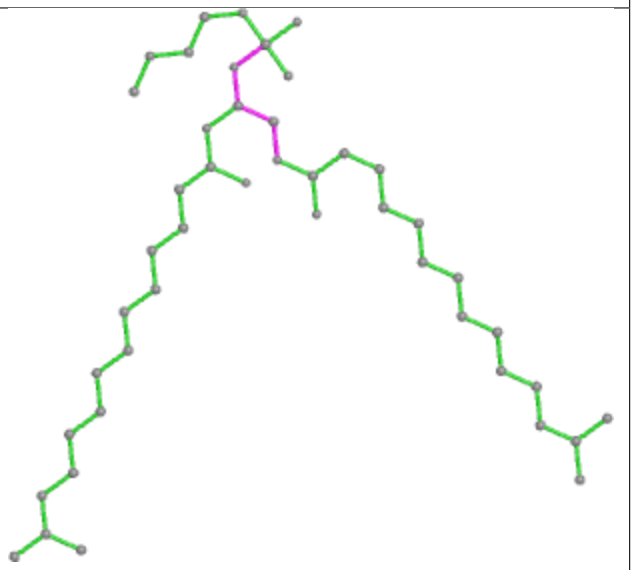
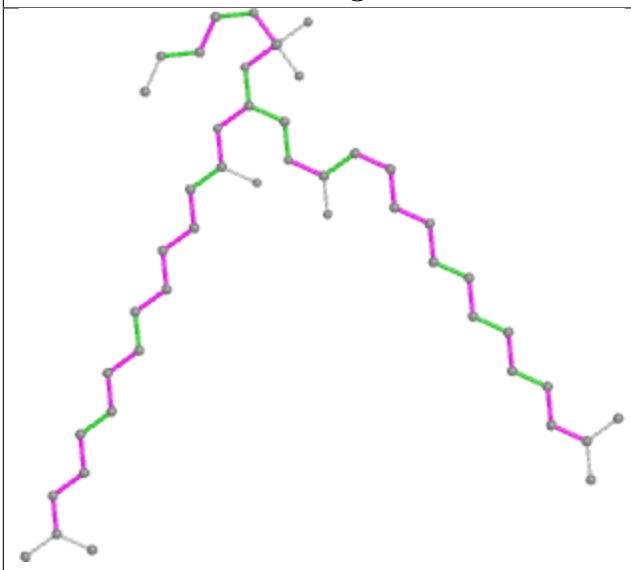
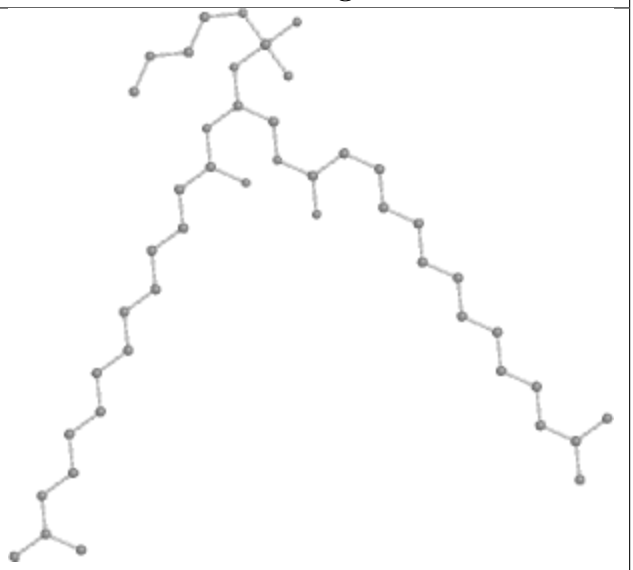


Bond angles

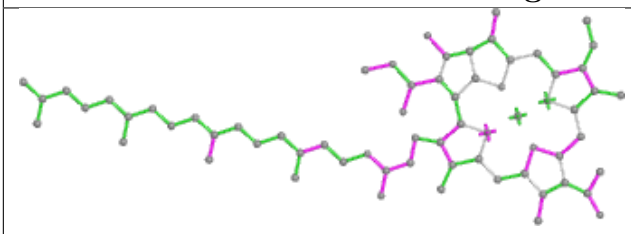


Torsions

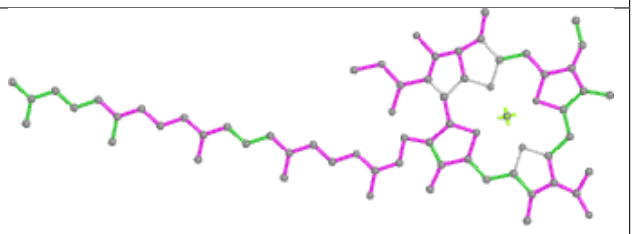


Rings

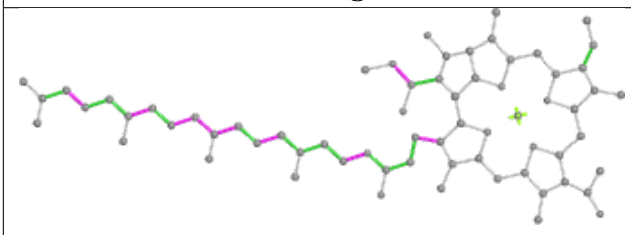
Ligand BCL A 909



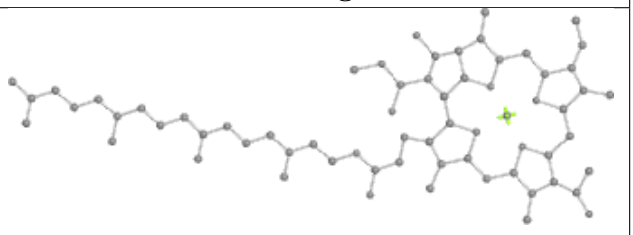
Bond lengths



Bond angles

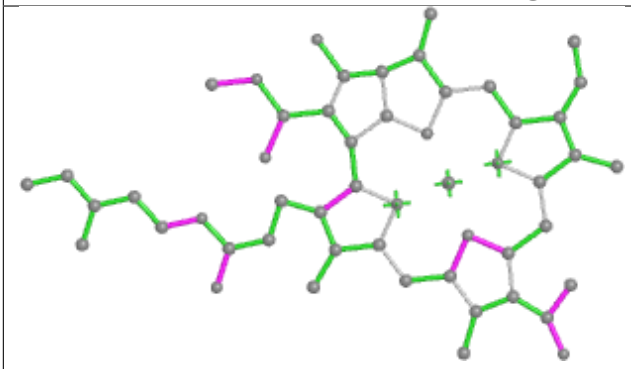


Torsions

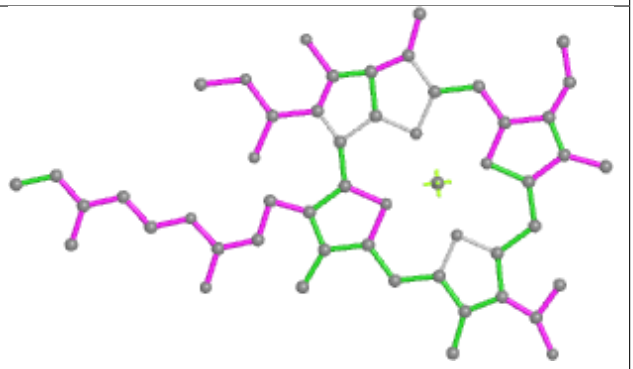


Rings

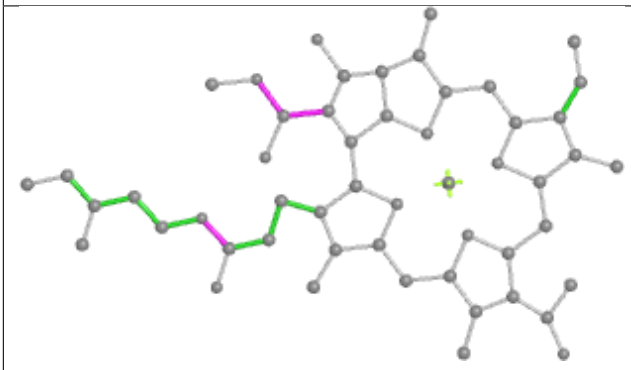
Ligand BCL A 906



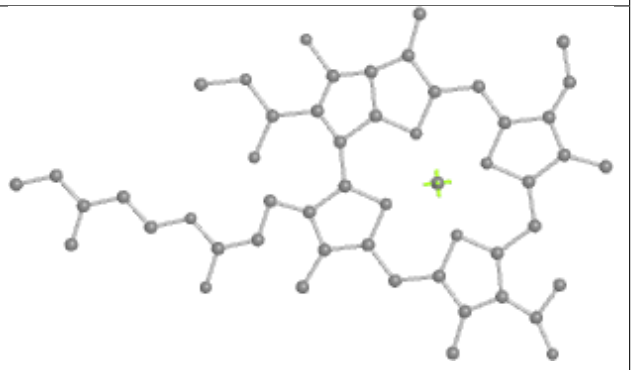
Bond lengths



Bond angles

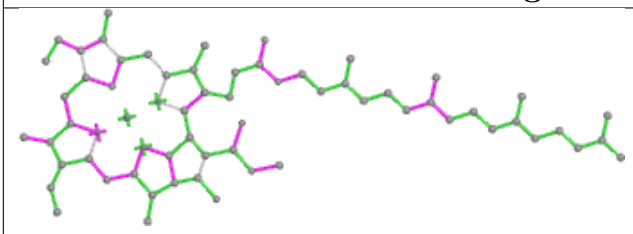


Torsions

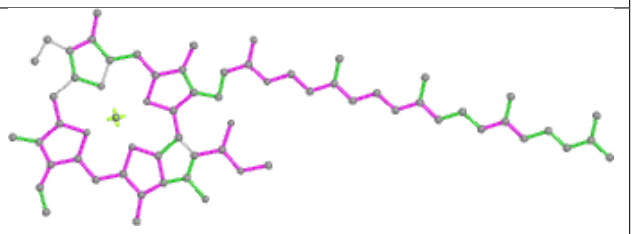


Rings

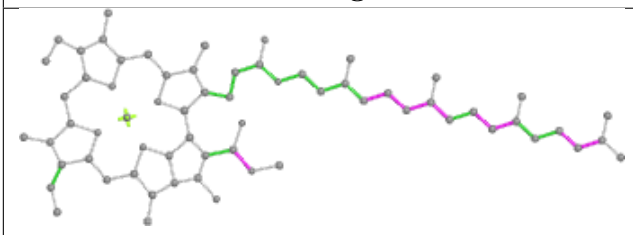
Ligand CLA A 911



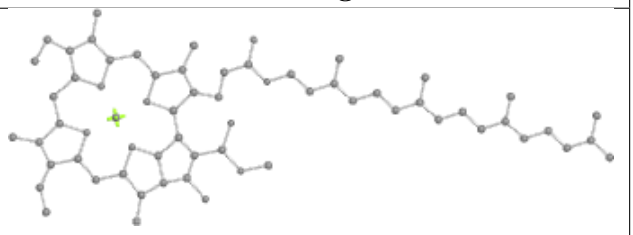
Bond lengths



Bond angles

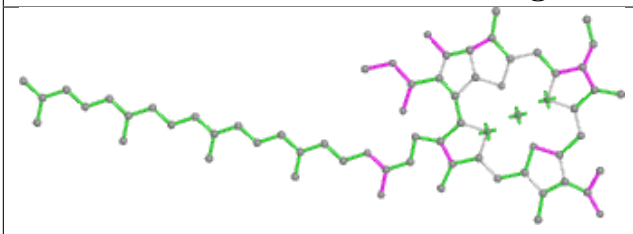


Torsions

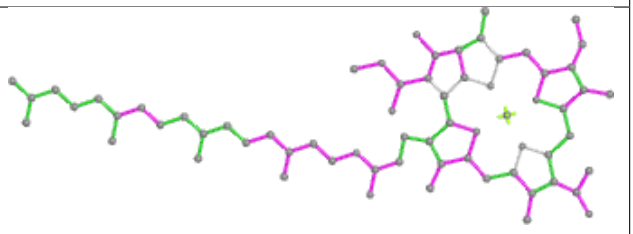


Rings

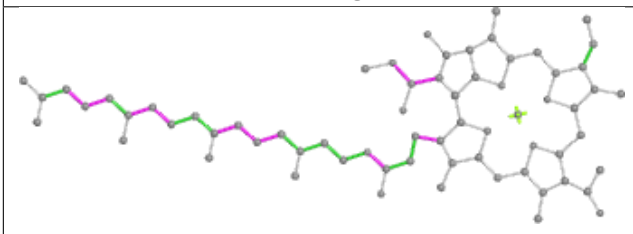
Ligand BCL a 905



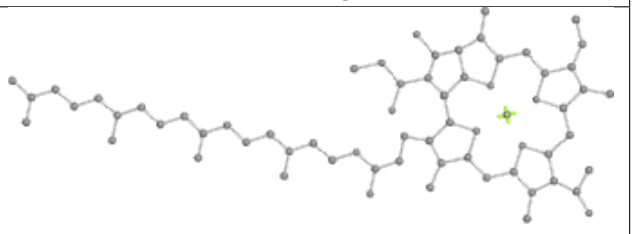
Bond lengths



Bond angles

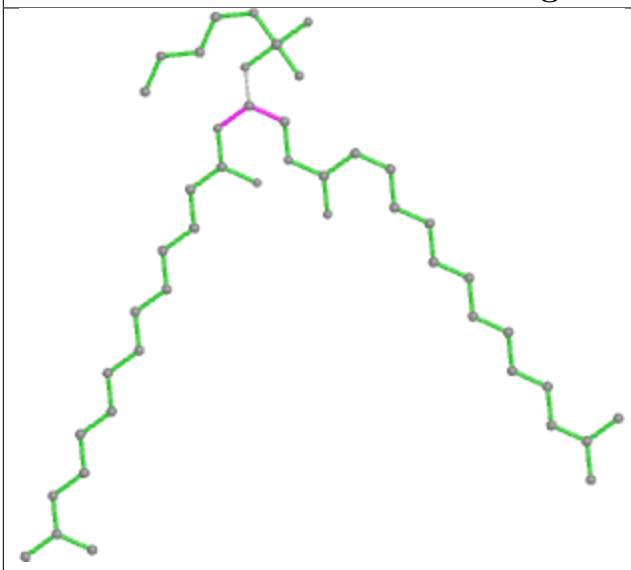


Torsions



Rings

Ligand 85I a 918



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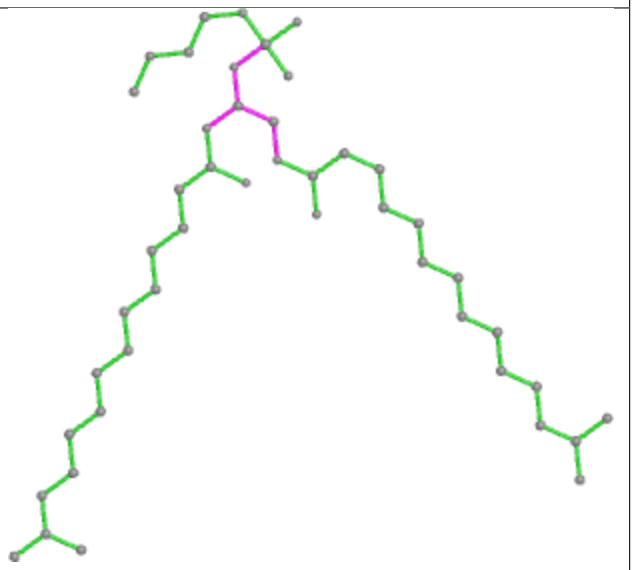
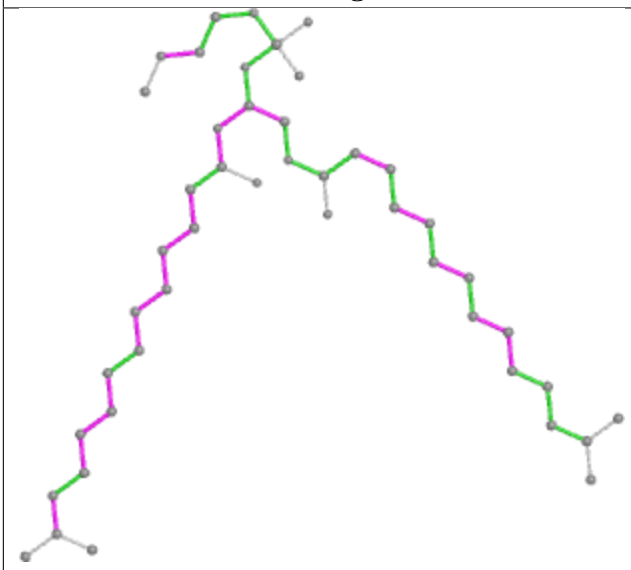


Bond angles



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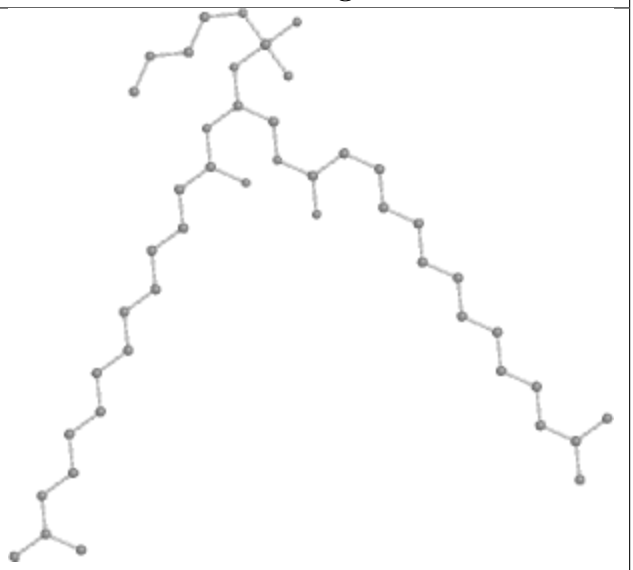
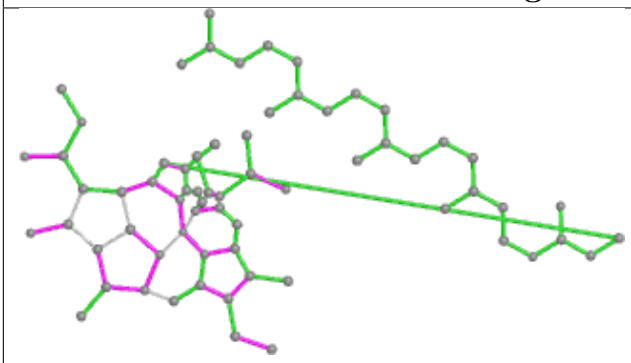
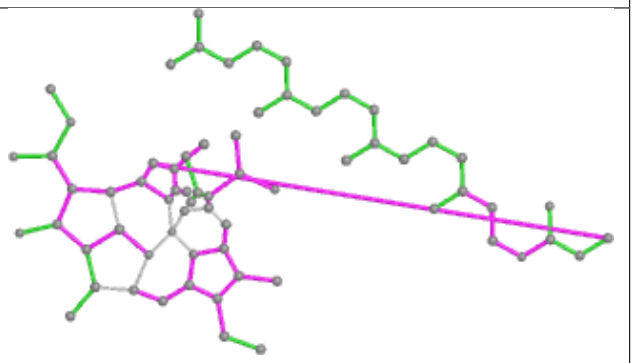


Rings

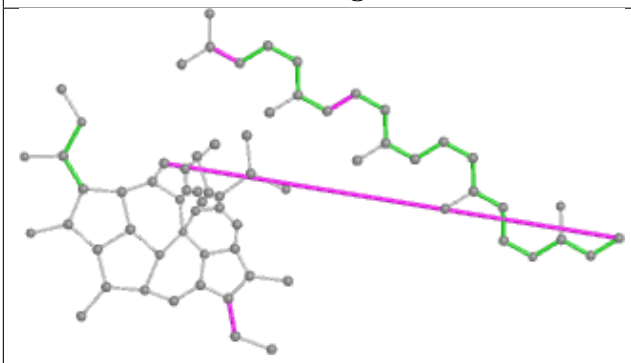
Ligand 2GO A 901



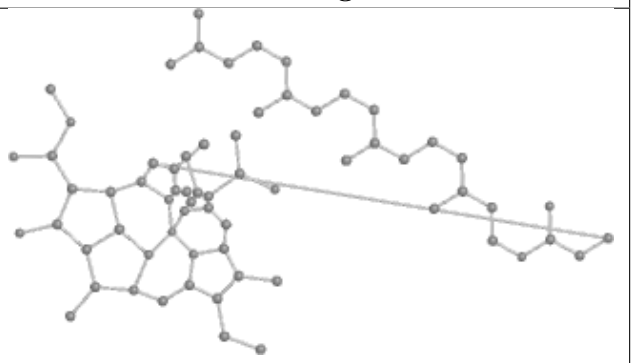
Bond lengths



Bond angles

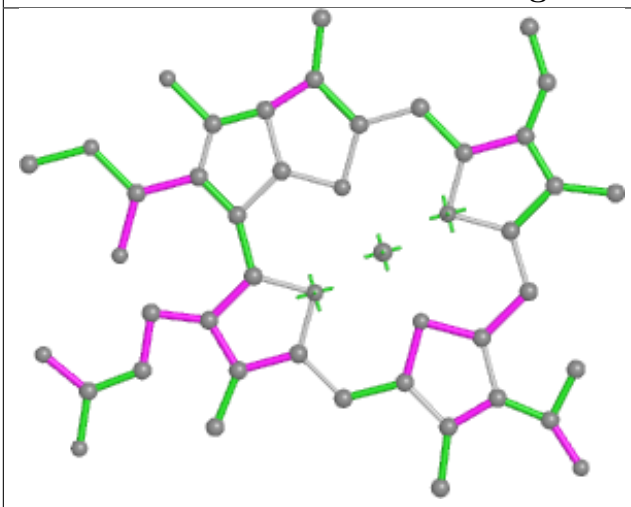


Torsions

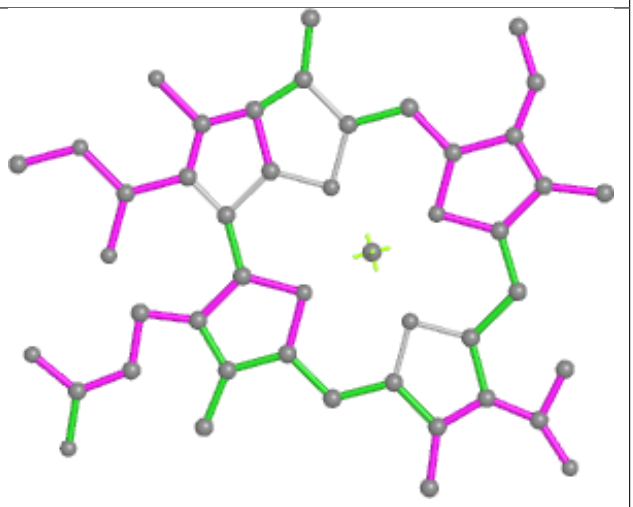


Rings

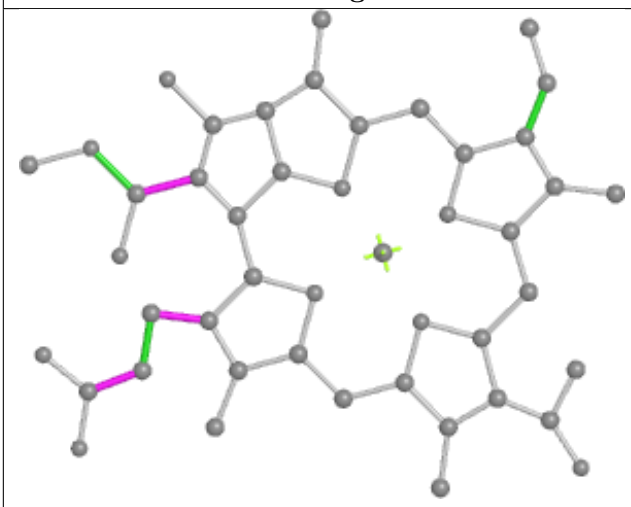
Ligand BCL a 906



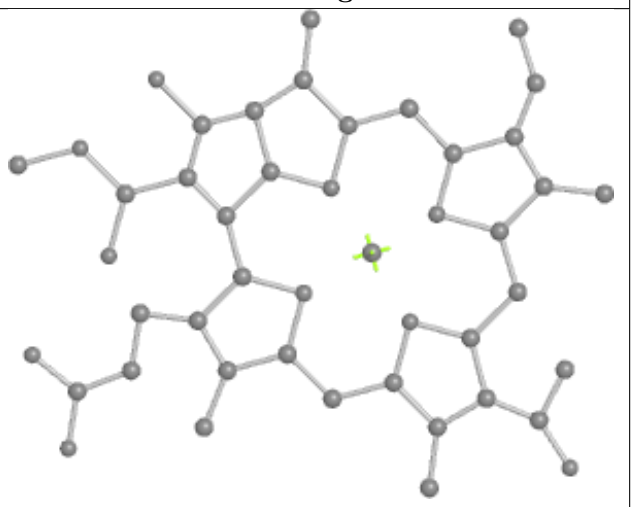
Bond lengths



Bond angles

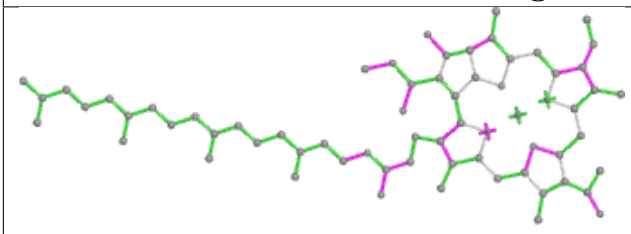


Torsions

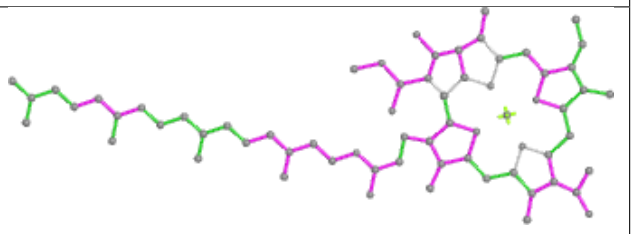


Rings

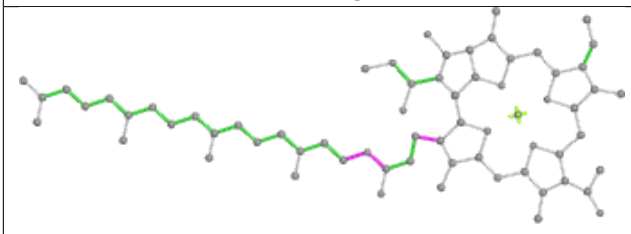
Ligand BCL a 911



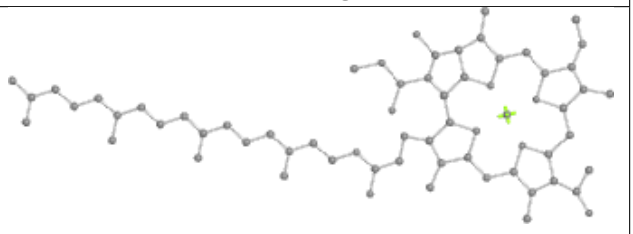
Bond lengths



Bond angles

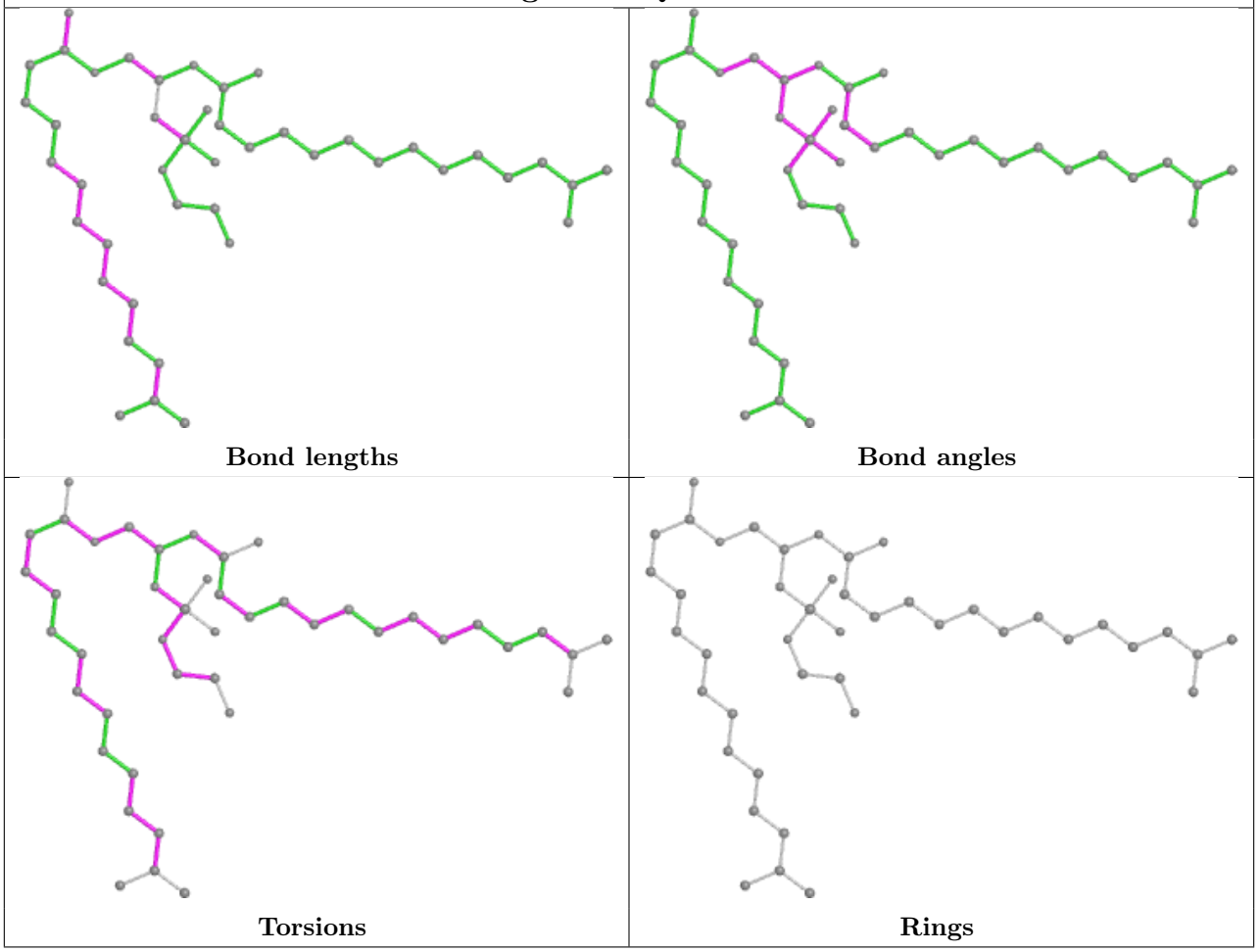


Torsions

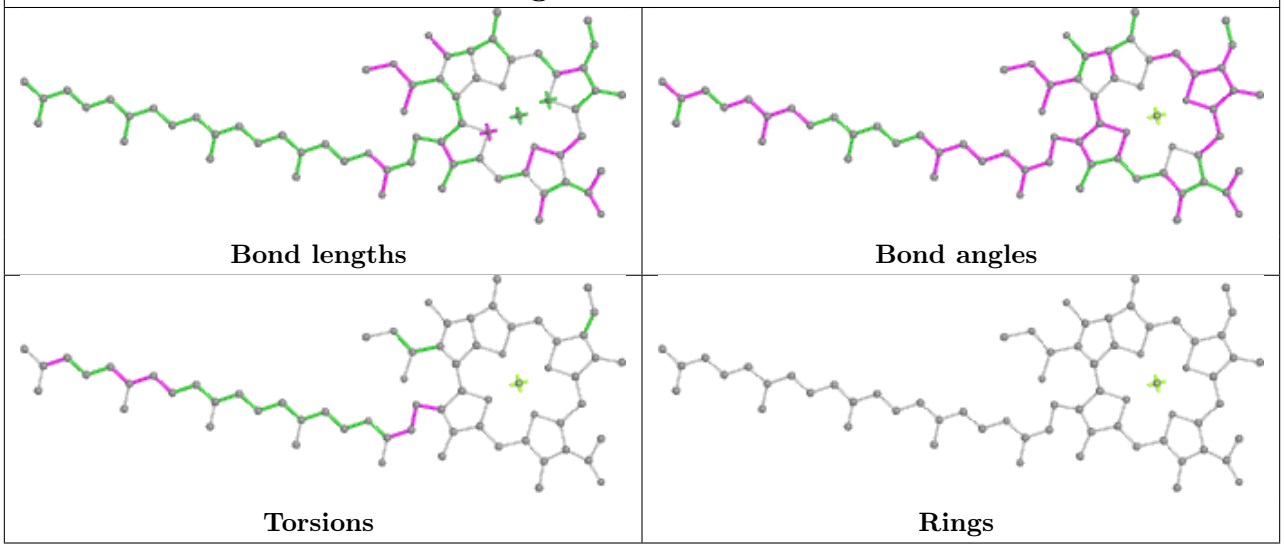


Rings

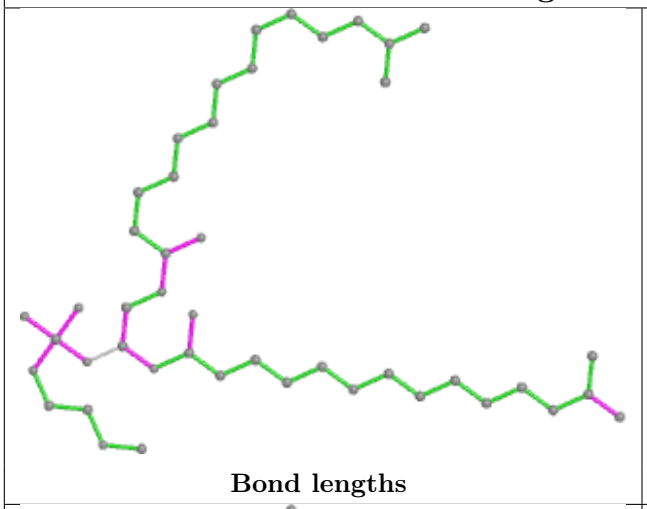
Ligand 84Q E 101



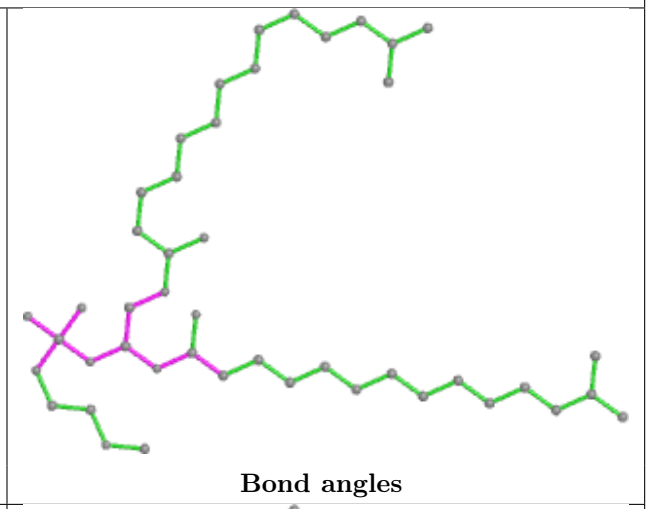
Ligand BCL a 910



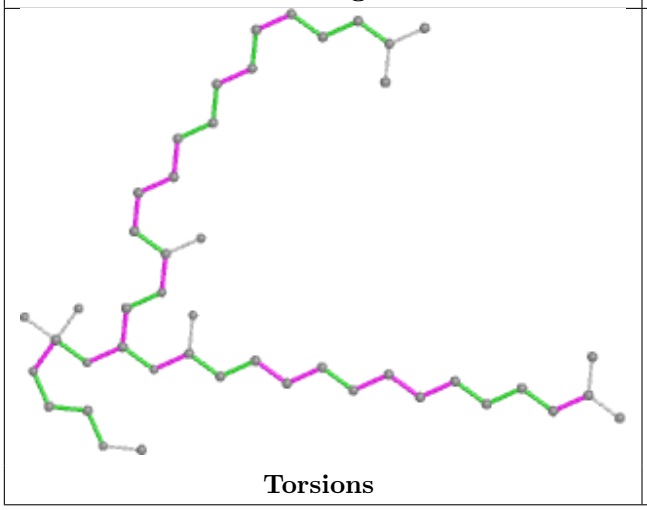
Ligand 85I A 915



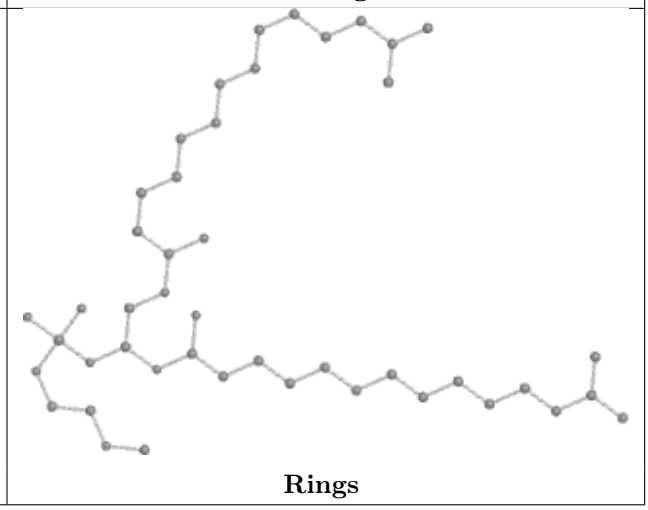
Bond lengths



Bond angles

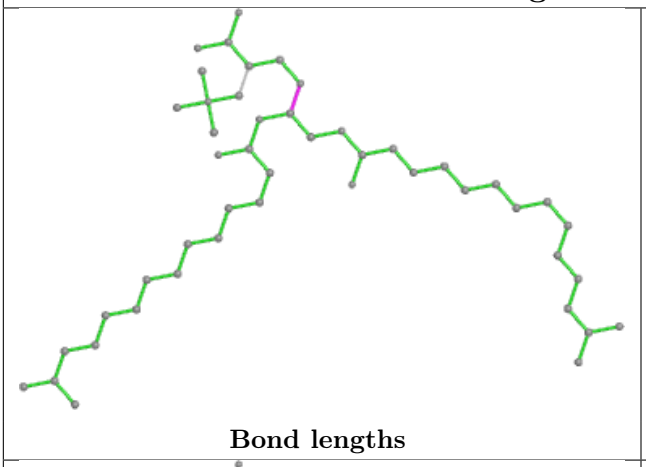


Torsions

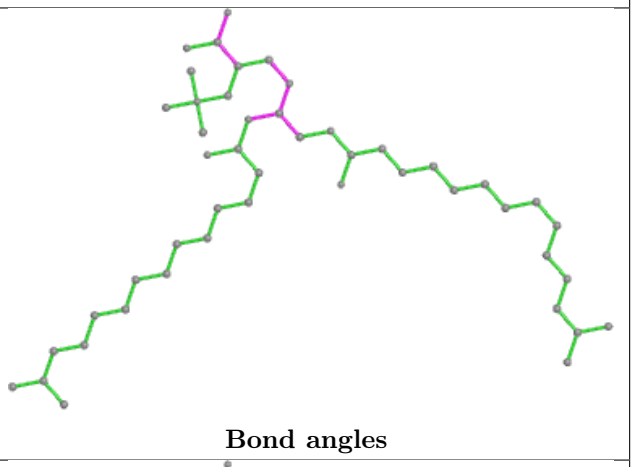


Rings

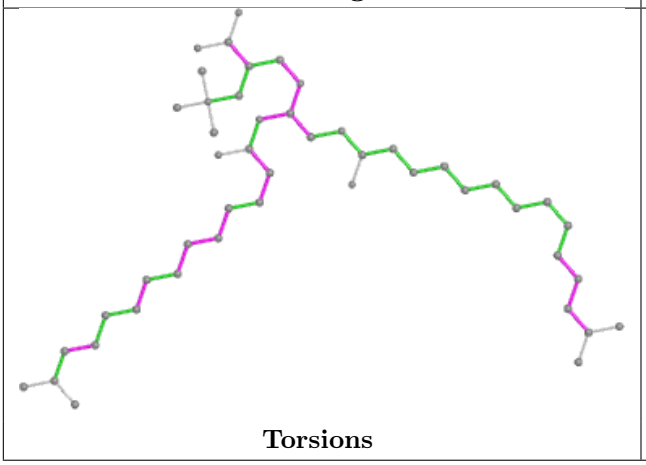
Ligand 85N A 932



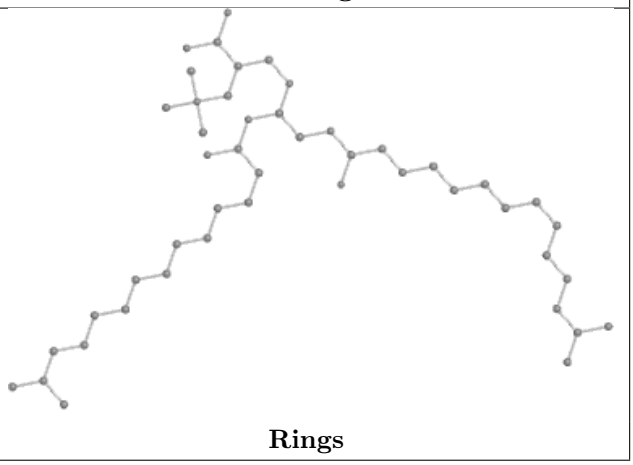
Bond lengths



Bond angles

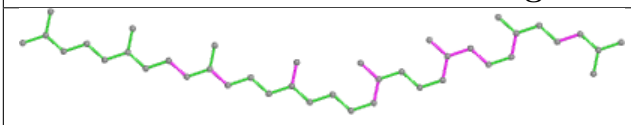


Torsions

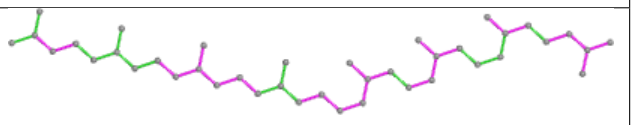


Rings

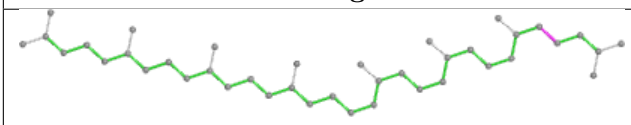
Ligand LYC A 913



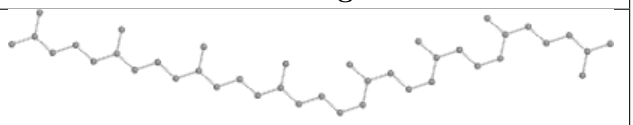
Bond lengths



Bond angles

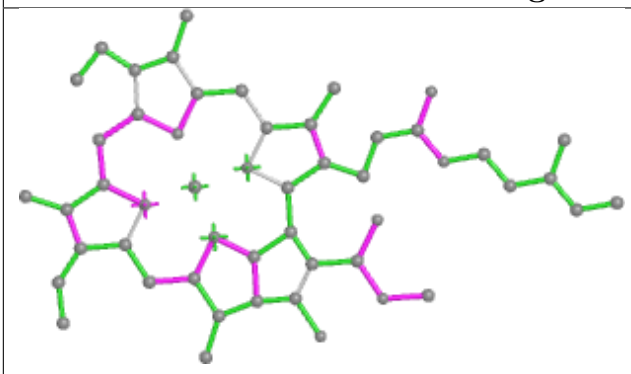


Torsions

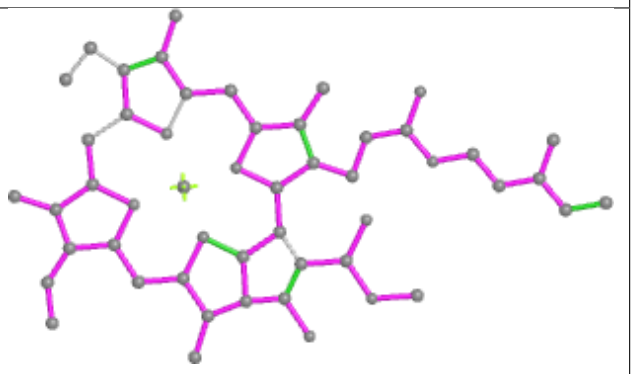


Rings

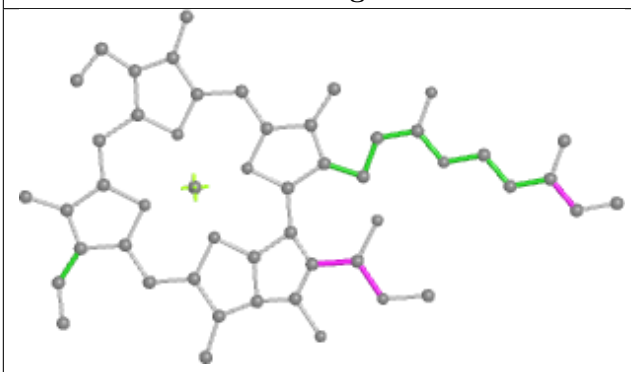
Ligand CLA a 915



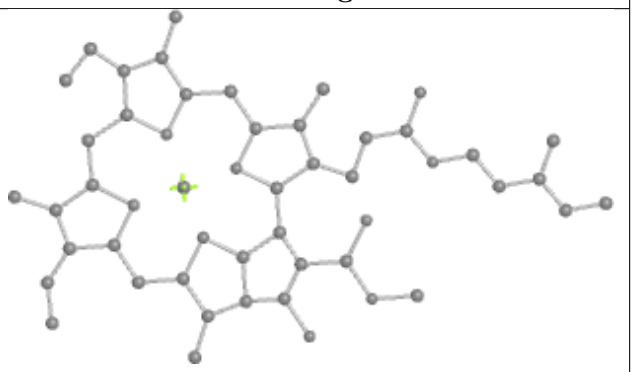
Bond lengths



Bond angles

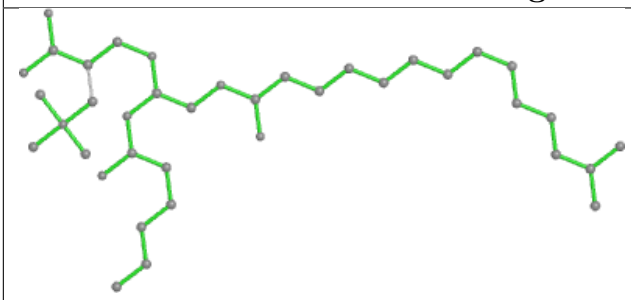


Torsions

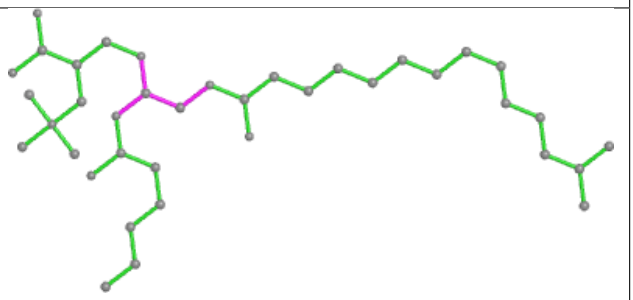


Rings

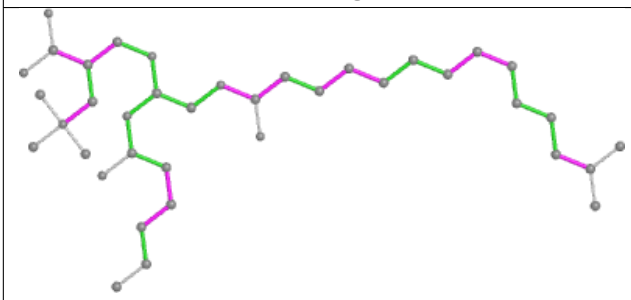
Ligand 85N G 101



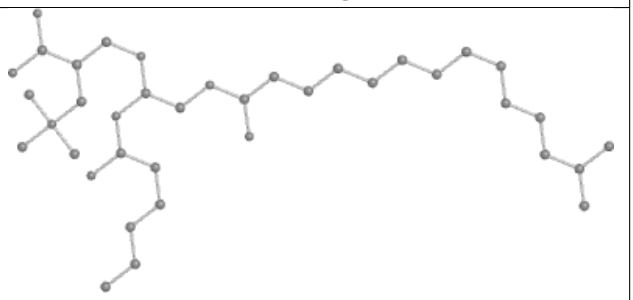
Bond lengths



Bond angles

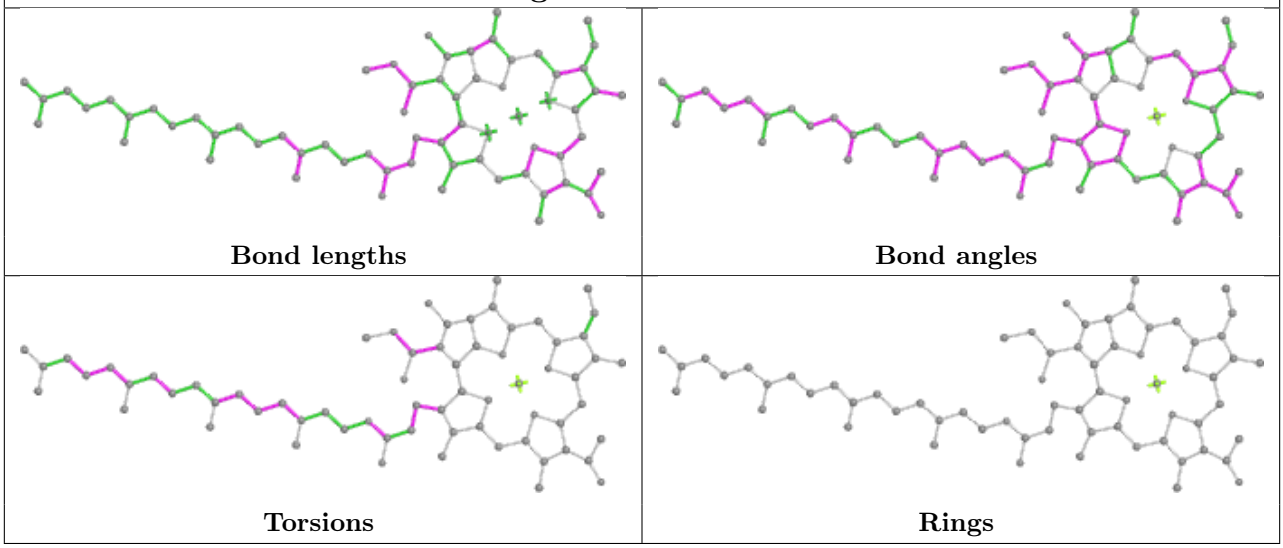


Torsions

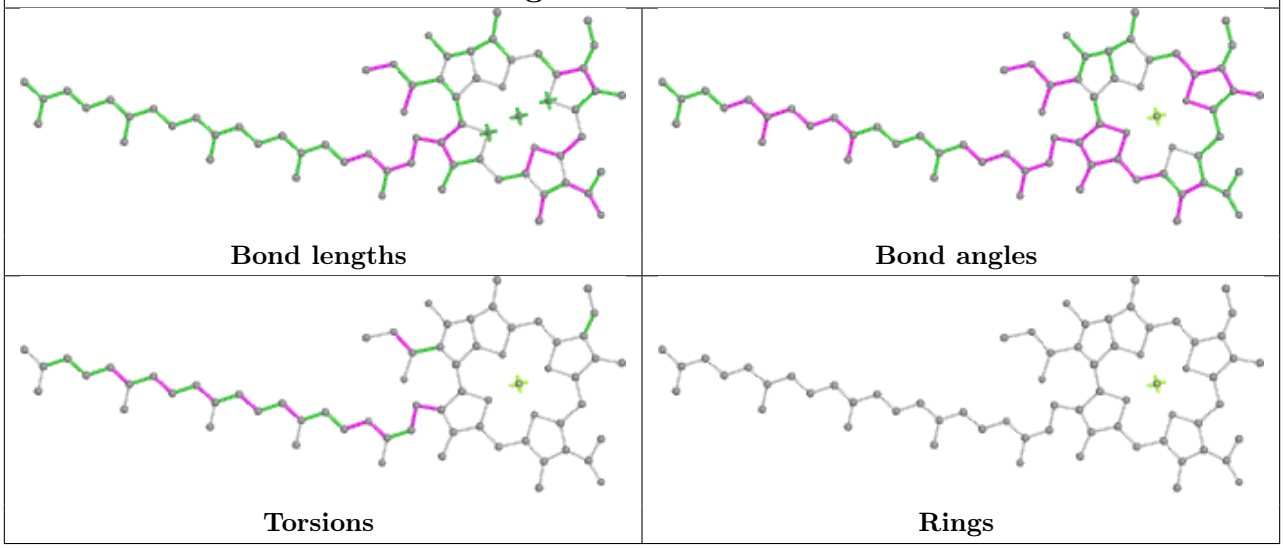


Rings

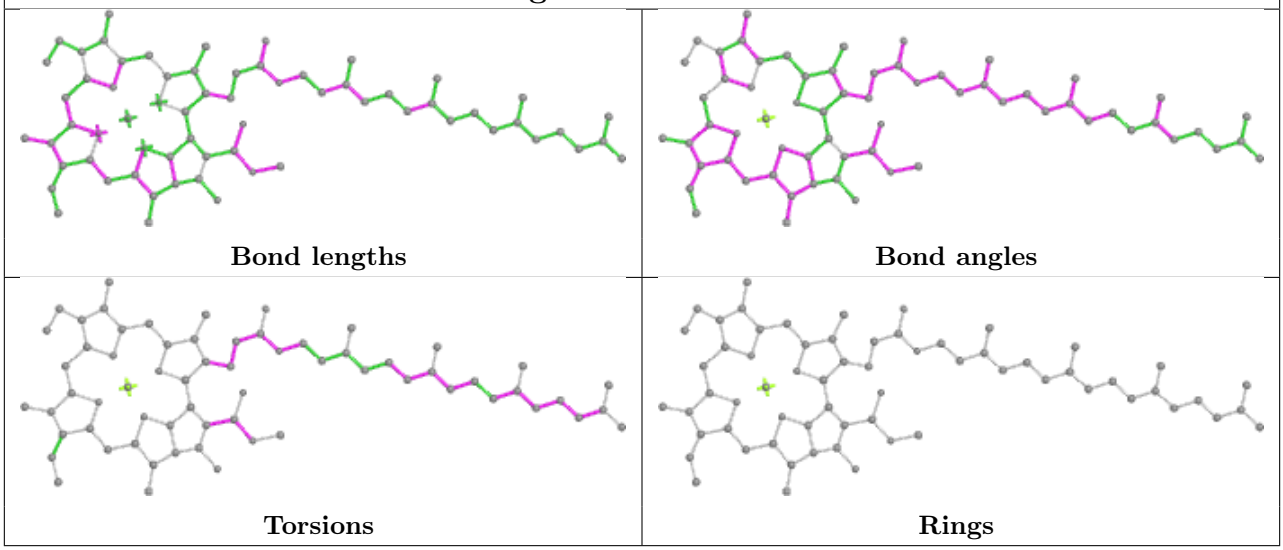
Ligand BCL a 908



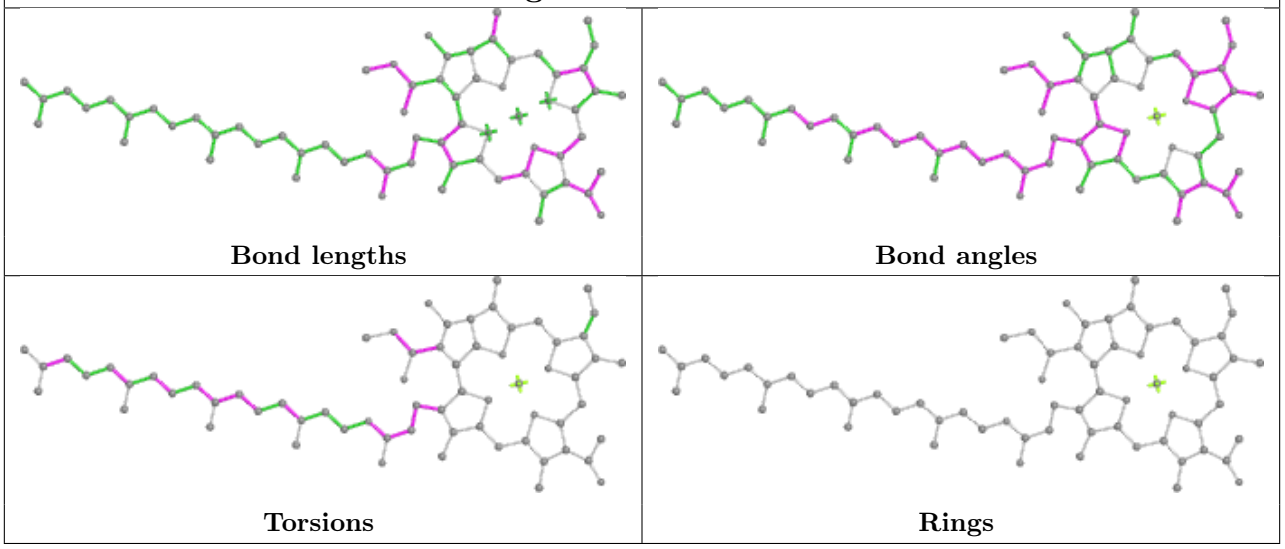
Ligand BCL A 905



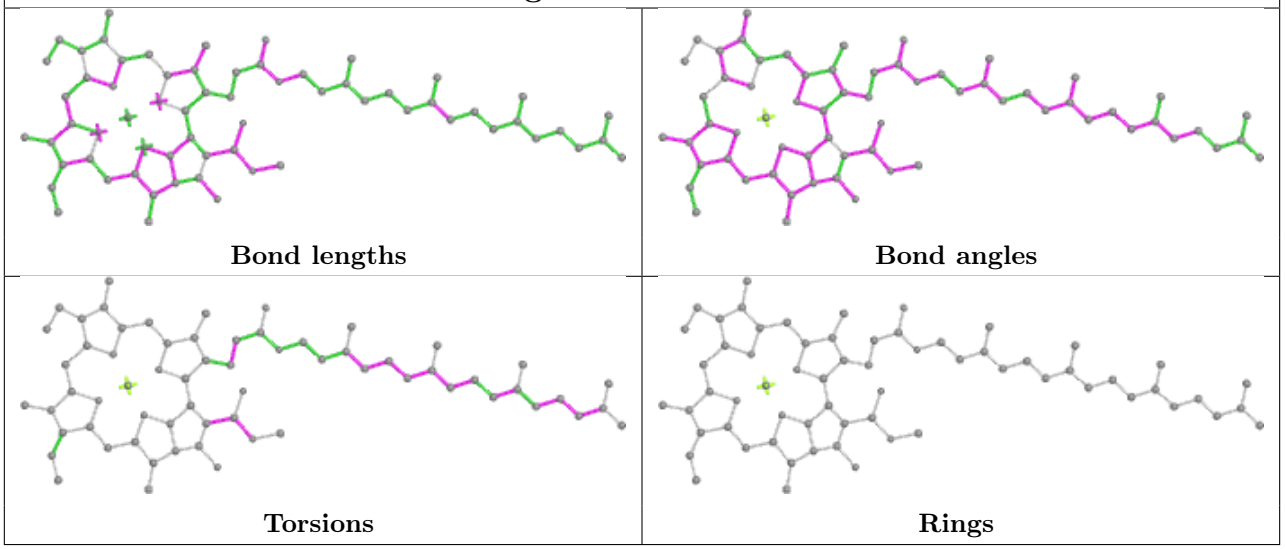
Ligand CLA a 901



Ligand BCL A 903



Ligand CLA A 931



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.

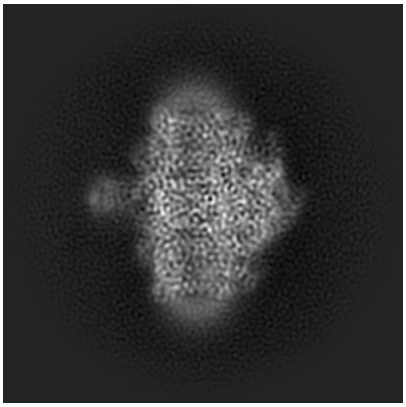
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32228. These allow visual inspection of the internal detail of the map and identification of artifacts.

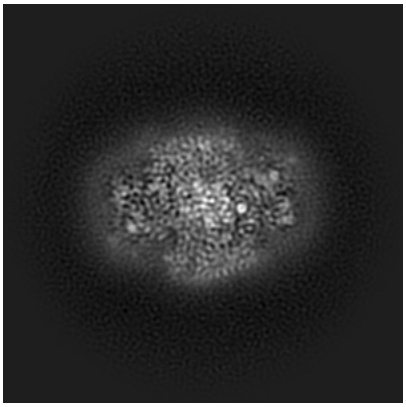
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

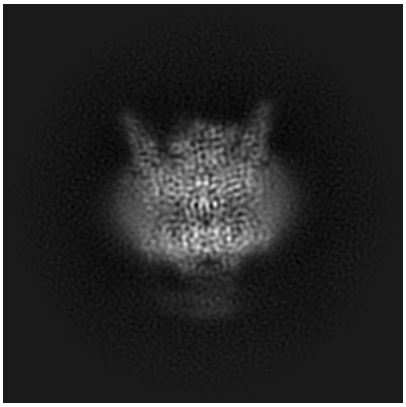
6.1.1 Primary map



X



Y

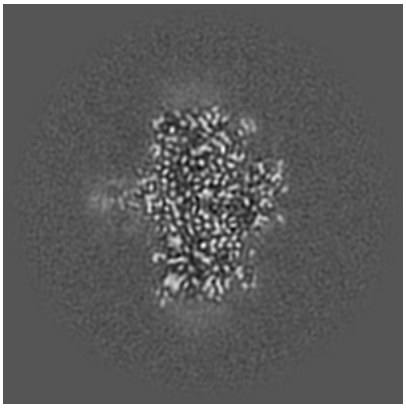


Z

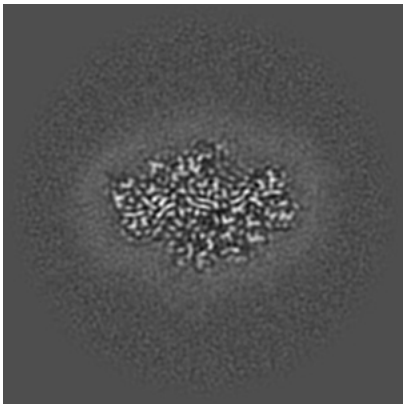
The images above show the map projected in three orthogonal directions.

6.2 Central slices

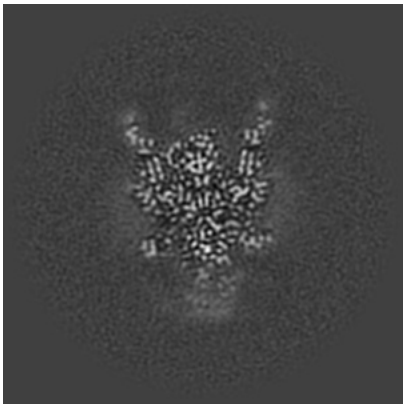
6.2.1 Primary map



X Index: 110



Y Index: 110

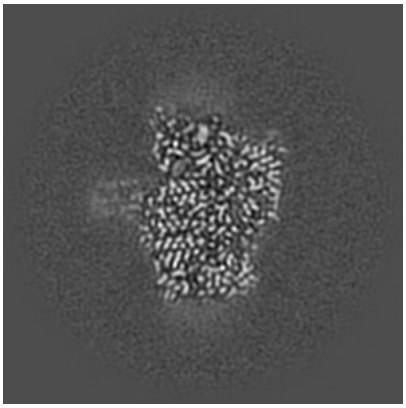


Z Index: 110

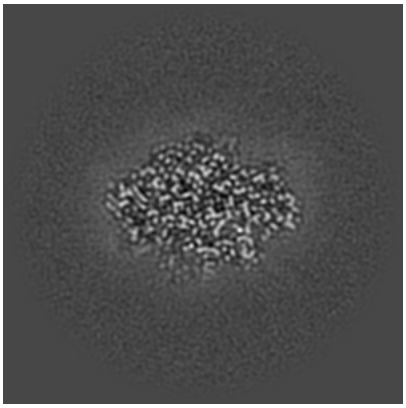
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

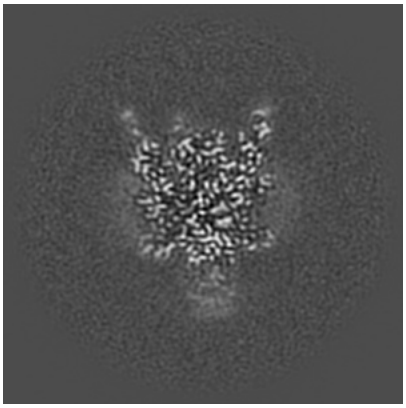
6.3.1 Primary map



X Index: 116



Y Index: 118

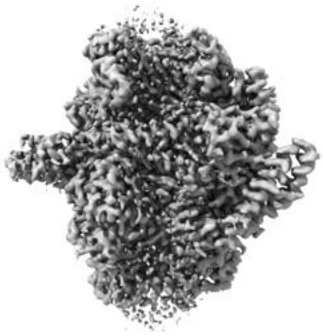


Z Index: 107

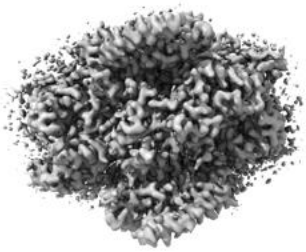
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

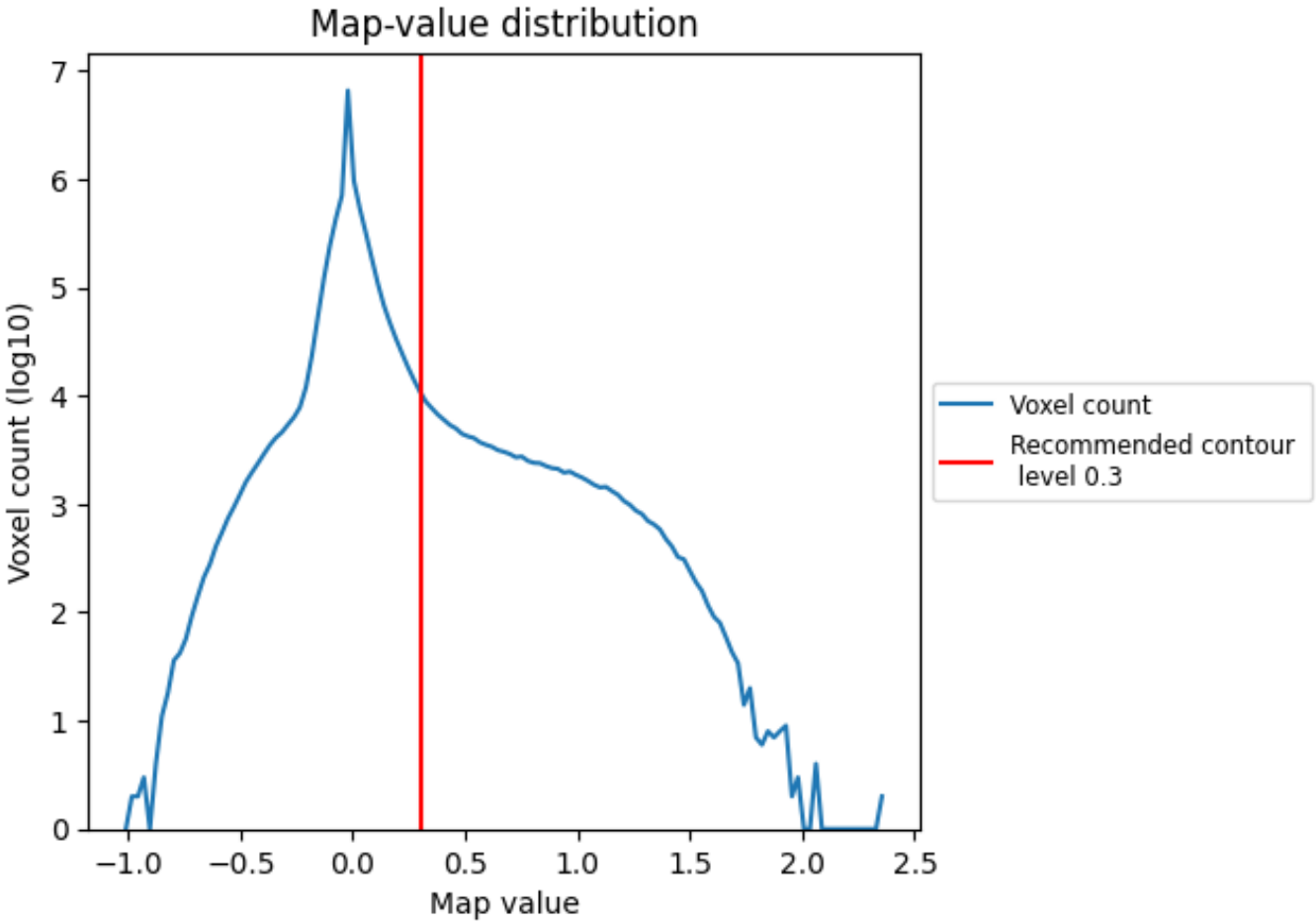
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

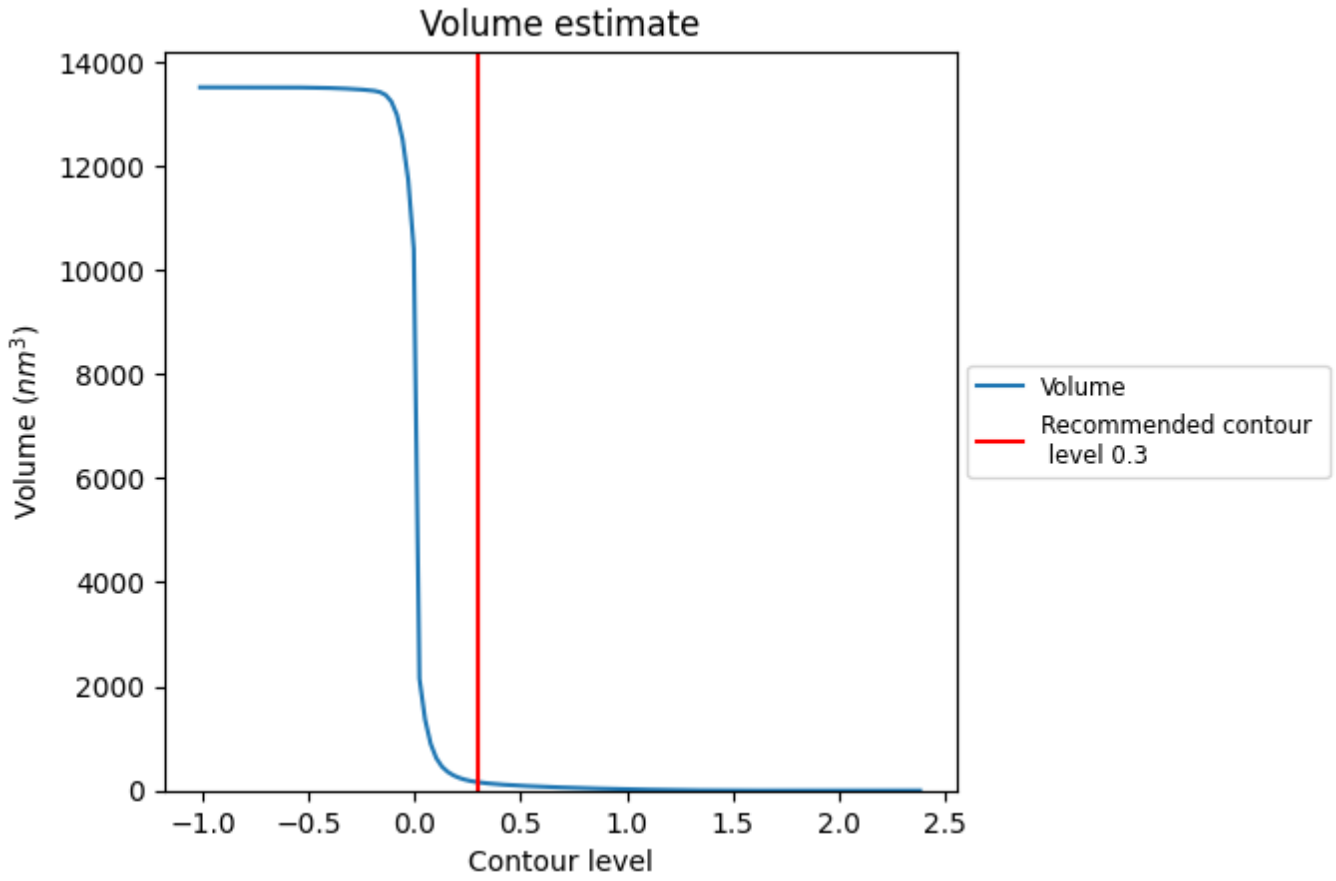
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

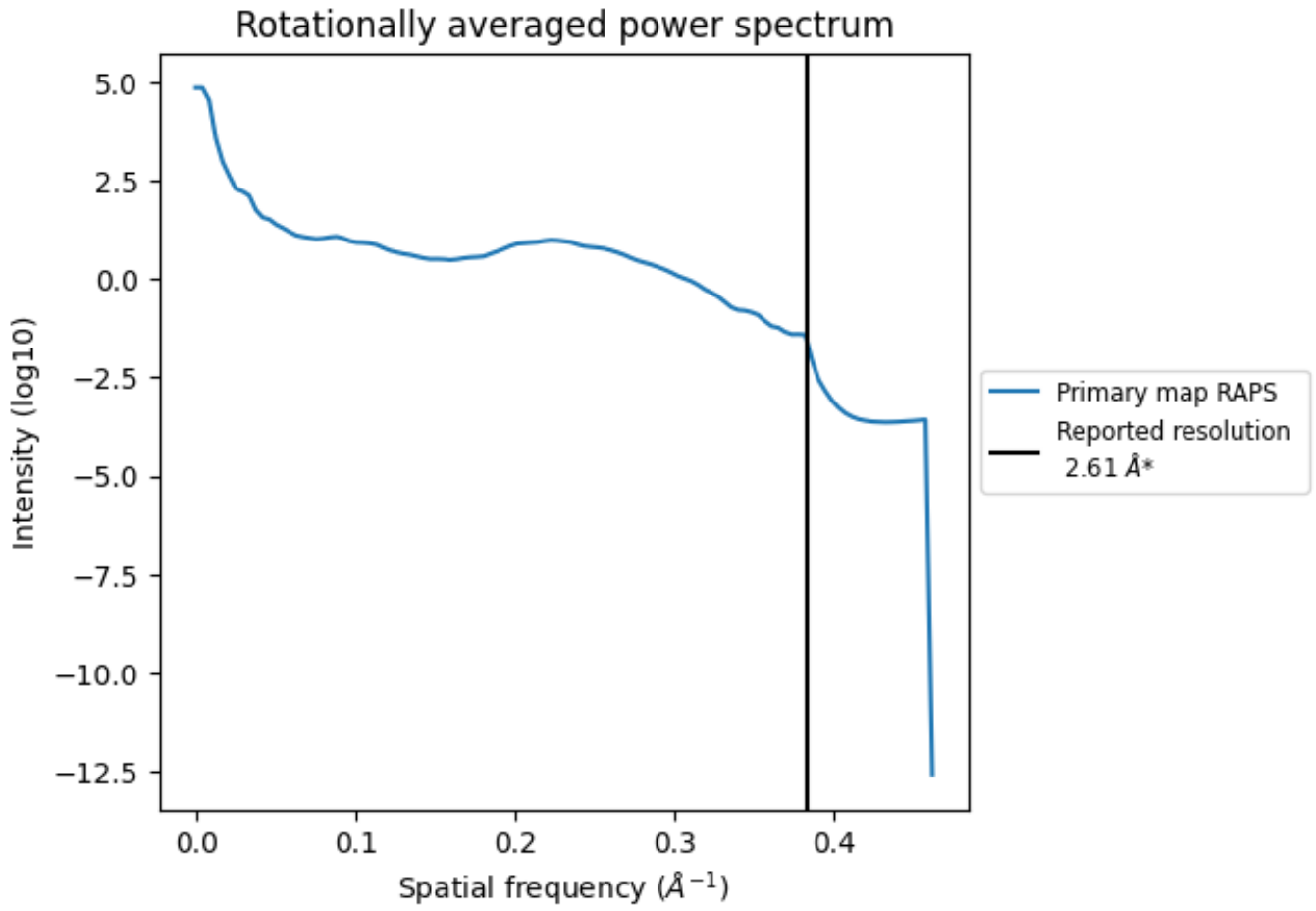
7.2 Volume estimate (i)



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 144 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.383 Å^{-1}

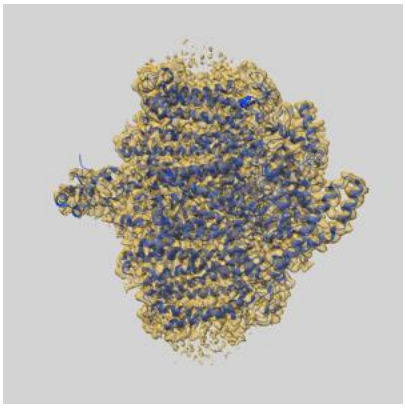
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

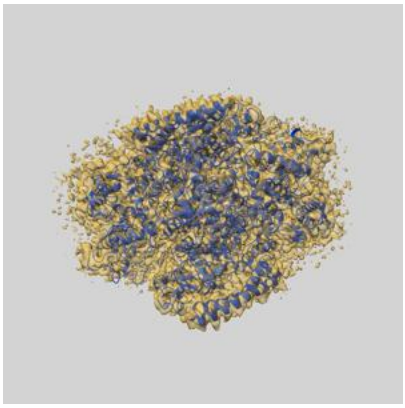
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32228 and PDB model 7VZG. Per-residue inclusion information can be found in section 3 on page 14.

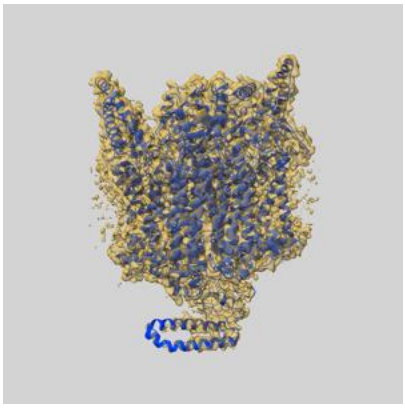
9.1 Map-model overlay



X



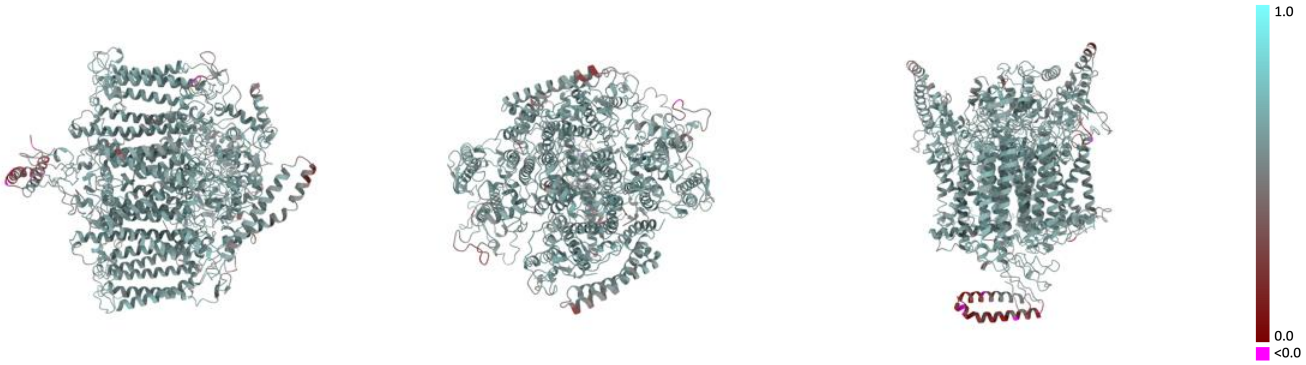
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

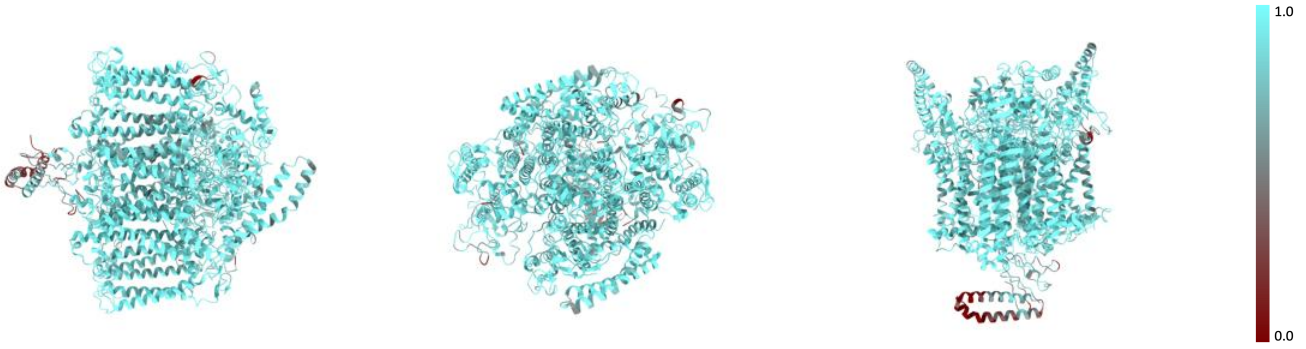
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

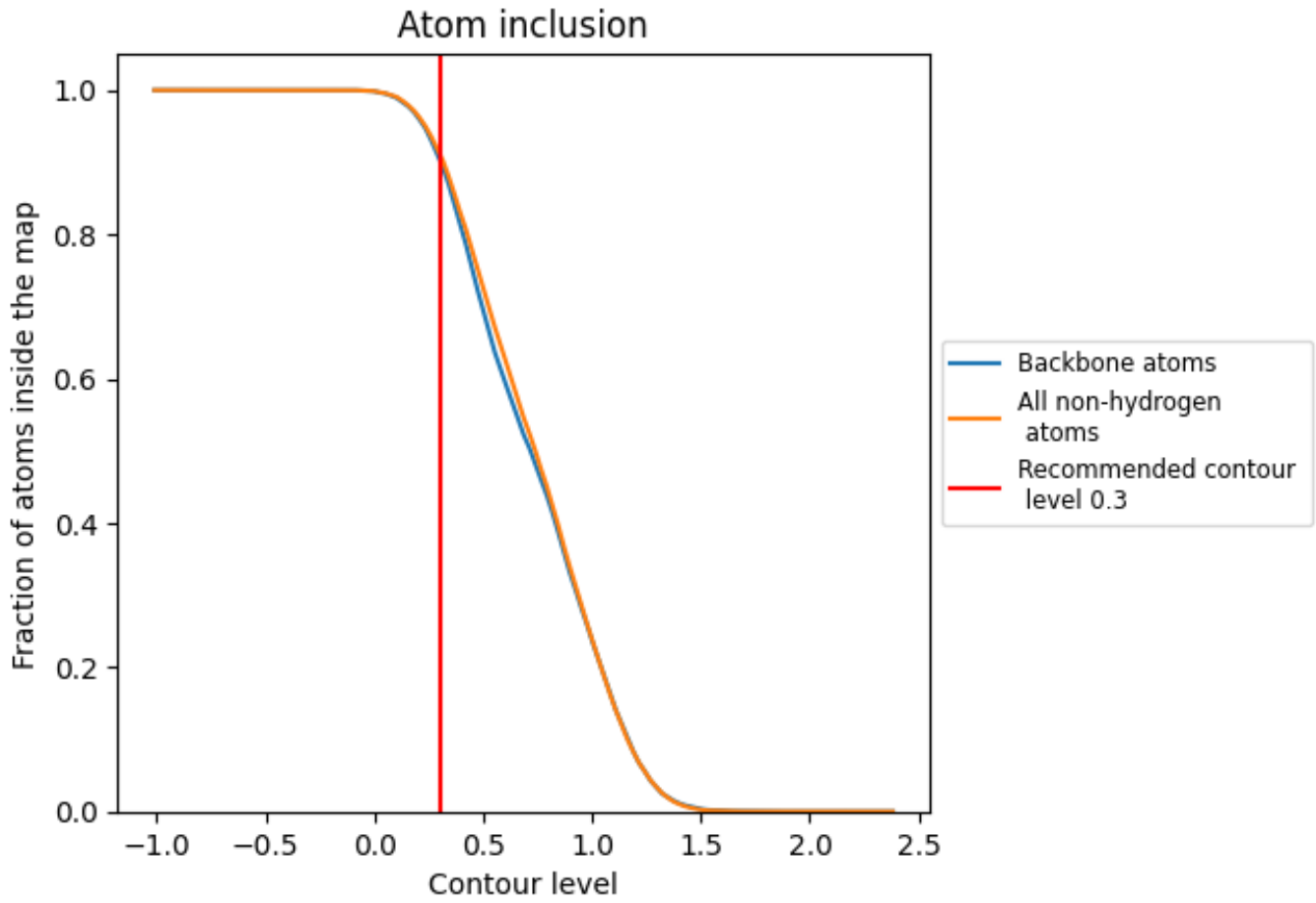
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9117	0.5780
A	0.9439	0.5910
B	0.6696	0.5210
C	0.9323	0.5780
D	0.3566	0.2470
E	0.9080	0.5740
F	0.9331	0.5960
G	0.7092	0.5340
H	0.8421	0.5600
a	0.9437	0.5910
c	0.9258	0.5760
e	0.8901	0.5780
f	0.9442	0.5880
g	0.8309	0.5940
h	0.8526	0.5770