wwPDB EM Validation Summary Report

Aug 27, 2026 – 07:59 pm BST

PDB ID	:	6T15 / pdb_00006t15
EMDB ID	:	EMD-10318
Title	:	The III2-IV(5B)1 respiratory supercomplex from S. cerevisiae
Authors	:	Marechal, A.; Pinotsis, N.; Hartley, A.
Deposited on	:	2019-10-03
Resolution	:	3.29 Å(reported)
Based on initial model	:	6HU9

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:

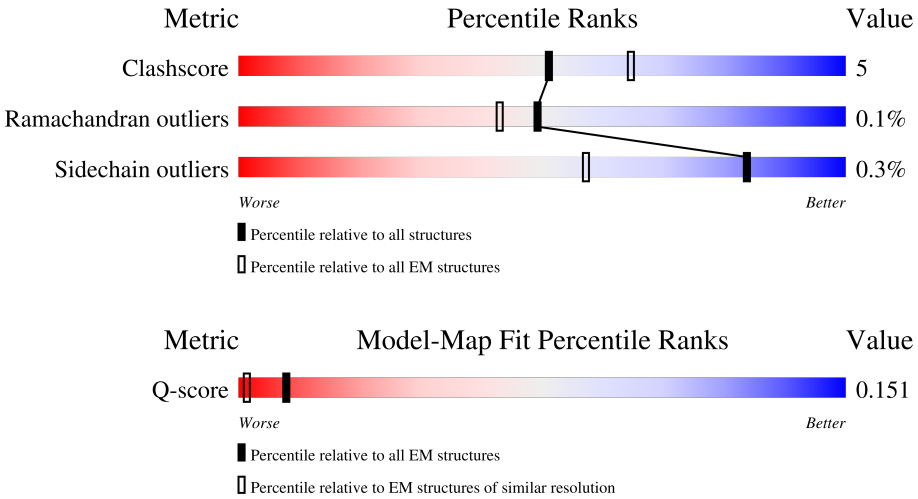
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13997 (2.91 - 3.91)

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	431	100% 89% 11%
1	L	431	100% 87% 13%
2	B	352	100% 87% 13%
2	M	352	100% 84% 16%

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Mol	Chain	Length	Quality of chain
3	C	385	100% 85% 15%
3	N	385	100% 85% 15%
4	D	248	100% 88% 12%
4	O	248	100% 84% 15%
5	E	185	100% 70% 29%
5	P	185	100% 77% 23%
6	F	147	51% 46% 5% 49%
6	Q	147	51% 47% 49%
7	G	127	99% 90% 9%
7	R	127	99% 88% 11%
8	H	94	99% 80% 19%
8	S	94	99% 88% 11%
9	I	66	86% 76% 11% 14%
9	T	66	86% 74% 12% 14%
10	J	77	99% 86% 13%
10	U	77	99% 83% 16%
11	a	534	81% 19%
12	b	236	85% 15%
13	c	269	80% 20%
14	d	130	75% 18% 7%
15	e	134	13% 91% 9%
16	f	108	86% 10%
17	g	59	93% 7%
18	h	51	90% 8%
19	i	55	91% 9%

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Mol	Chain	Length	Quality of chain
20	j	82	
21	k	131	
22	l	66	
23	m	224	

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
28	HEC	D	401	X	-	-	-
28	HEC	O	401	X	-	-	-

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 48966 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 CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	L	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6,COMPLEX III SUBUNIT VI,CYTOCHROME C1 NON-HEME 17 KDA PROTEIN,MITOCHONDRIAL HINGE PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total	C	N	O	0	0
			465	310	77	78		
9	T	57	Total	C	N	O	0	0
			465	310	77	78		

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10,COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	76	Total	C	N	O	S	0	0
			599	391	98	108	2		
10	U	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

- Molecule 11 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

- Molecule 12 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

- Molecule 13 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

- Molecule 14 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

- Molecule 15 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	134	Total	C	N	O	S	0	0
			1083	694	188	199	2		

- Molecule 16 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	104	Total	C	N	O	S	0	0
			866	554	141	170	1		

- Molecule 17 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	59	Total	C	N	O	0	0
			484	328	83	73		

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	51	Total	C	N	O	S	0	0
			409	278	66	64	1		

- Molecule 19 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	77	Total	C	N	O	S	0	0
			642	410	109	118	5		

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	118	Total	C	N	O	S	0	0
			967	626	167	171	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799

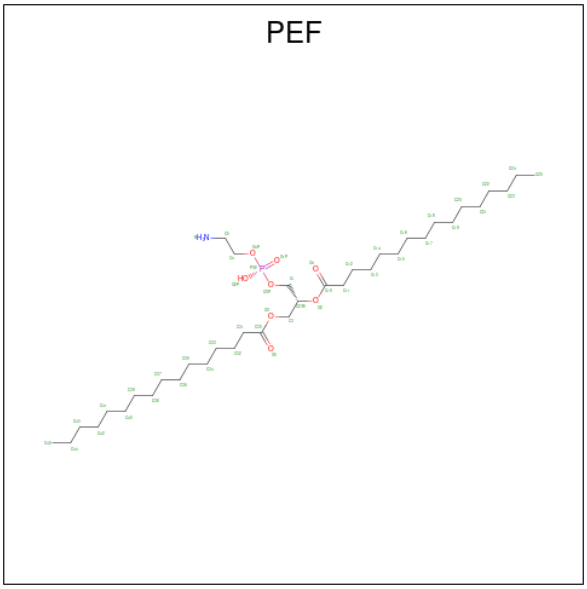
- Molecule 22 is a protein called COX26; SYNONYM: Uncharacterized protein YDR119W-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 23 is a protein called RCF2; SYNONYM: Respiratory supercomplex factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	99	Total	C	N	O	S	0	0
			799	511	140	144	4		

- Molecule 24 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



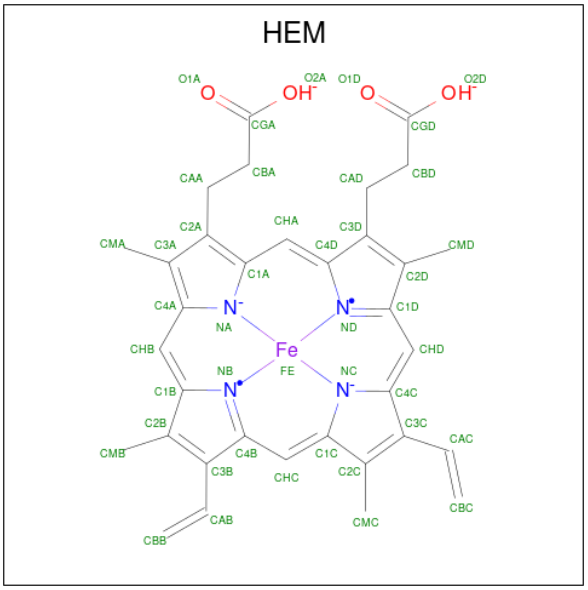
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
24	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
24	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
24	E	1	Total	C	N	O	P	0
			43	33	1	8	1	
24	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
24	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
24	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
24	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
24	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
24	P	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	S	1	Total	C	N	O	P	0
			36	26	1	8	1	
24	U	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
24	a	1	Total	C	N	O	P	0
			33	23	1	8	1	
24	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
24	b	1	Total	C	N	O	P	0
			33	23	1	8	1	
24	c	1	Total	C	N	O	P	0
			36	26	1	8	1	
24	c	1	Total	C	N	O	P	0
			41	31	1	8	1	
24	e	1	Total	C	N	O	P	0
			42	32	1	8	1	

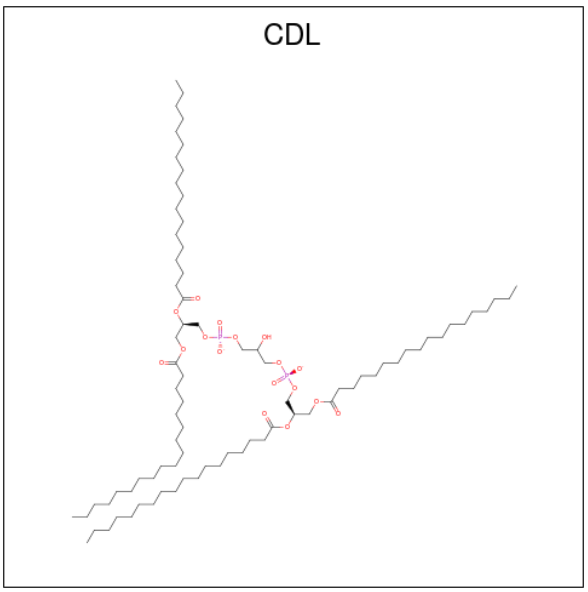
- Molecule 25 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

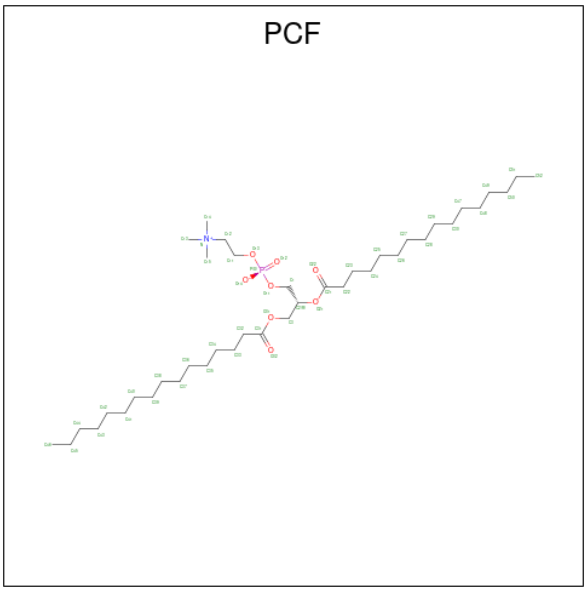
- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand

of Interest" by depositor).



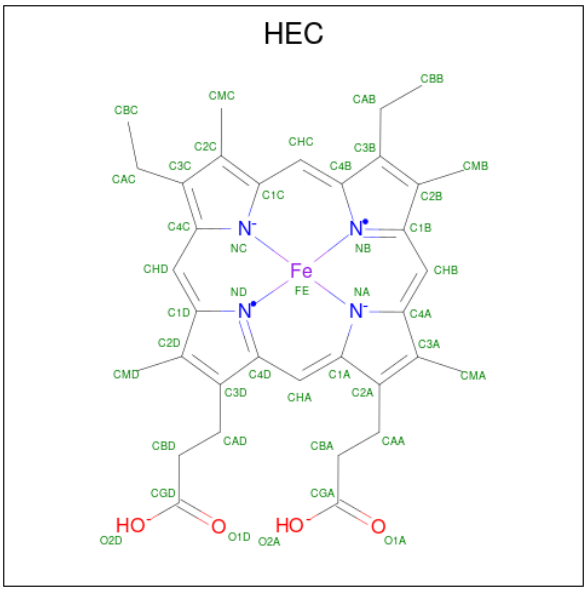
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			55	36	17	2	
26	D	1	Total	C	O	P	0
			67	48	17	2	
26	H	1	Total	C	O	P	0
			53	34	17	2	
26	L	1	Total	C	O	P	0
			58	39	17	2	
26	N	1	Total	C	O	P	0
			66	47	17	2	
26	O	1	Total	C	O	P	0
			71	52	17	2	
26	S	1	Total	C	O	P	0
			53	34	17	2	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$).



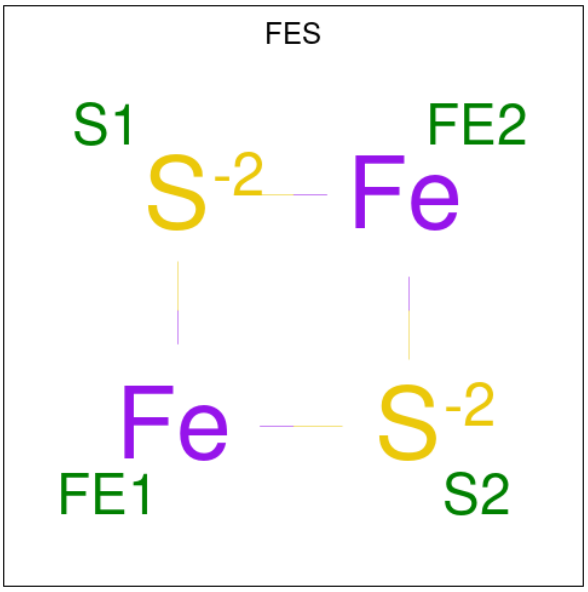
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	I	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	T	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 28 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

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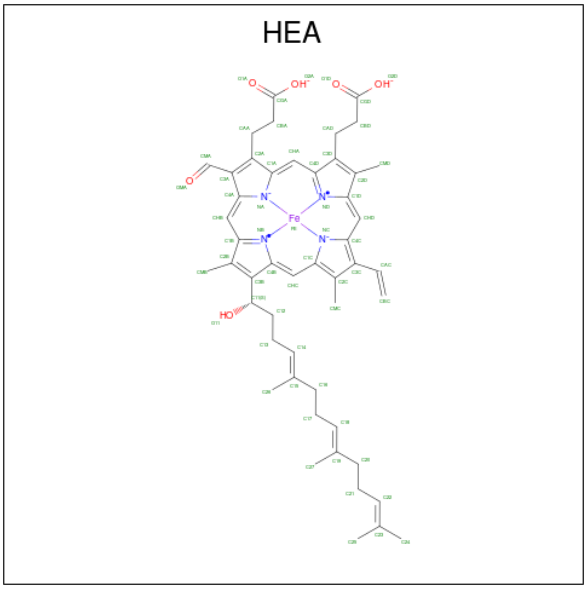
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Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Cu	0
			1	1	

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

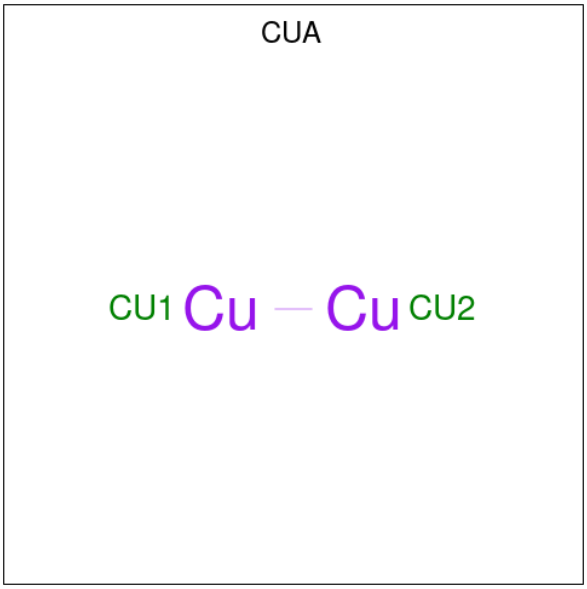


Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Mg	0
			1	1	

- Molecule 33 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
33	b	1	Total Cu 2 2	0

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
34	d	1	Total Zn 1 1	0

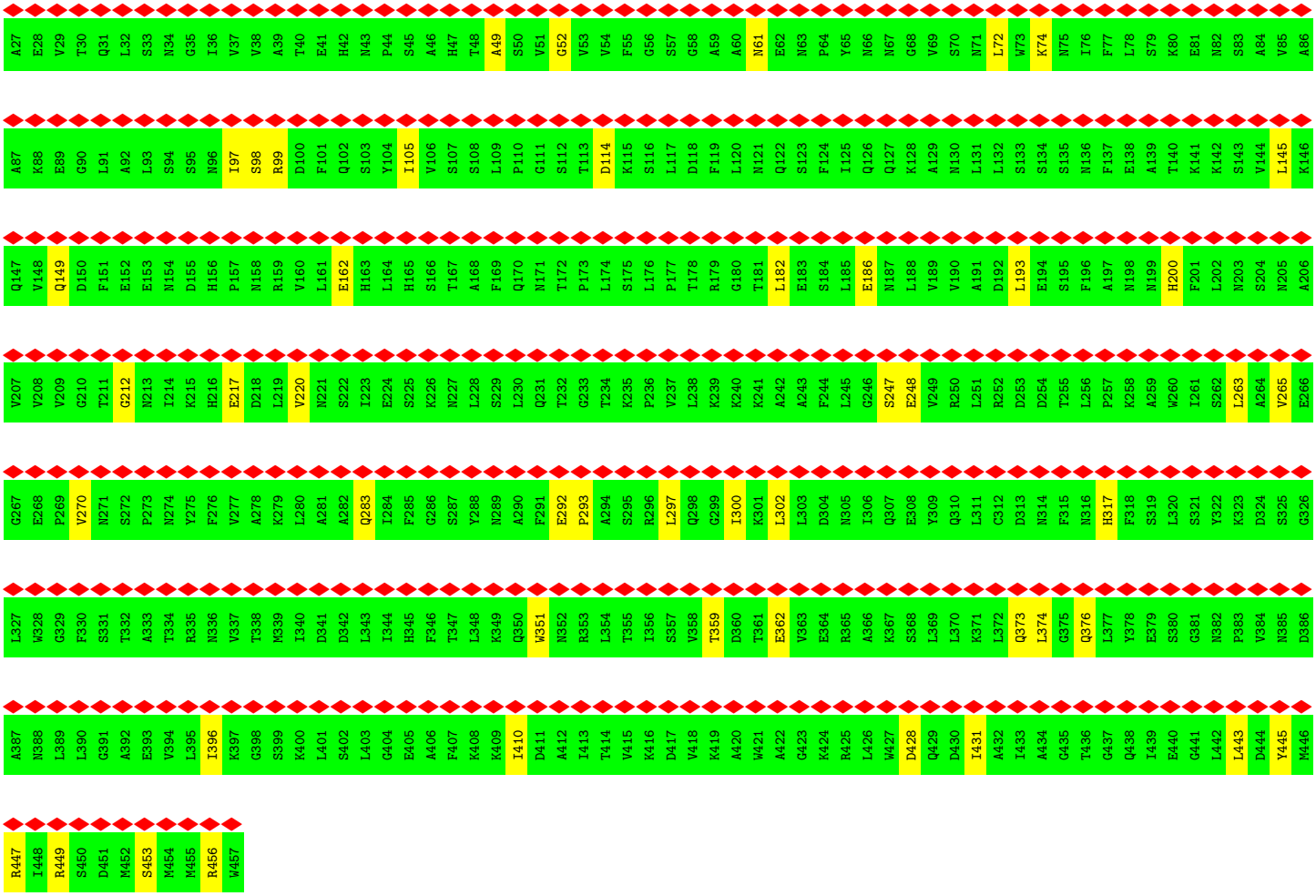
3 Residue-property plots (i)

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 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: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

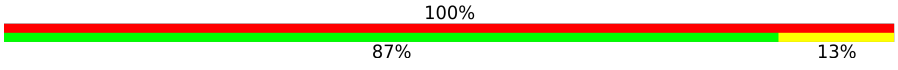
Chain A:





• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

Chain L:



A27 E28 V29 T30 Q31 L32 S33 N34 G35 I36 V37 V38 A39 T40 E41 H42 N43 P44 S45 A46 H47 T48 A49 S50 V51 G52 V53 V54 F55 G56 S57 G58 A59 A60 N61 E62 N63 P64 Y65 N66 N67 G68 V69 S70 N71 L72 W73 K74 N75 I76 F77 L78 S79 K80 E81 N82 S83 A84 V85 A86

A87 K88 E89 G90 L91 A92 L93 S94 S96 N96 I97 S98 R99 D100 F101 Q102 S103 Y104 I105 V106 S107 S108 L109 P110 G111 S112 T113 D114 K115 S116 L117 D118 F119 L120 N121 Q122 S123 F124 I125 Q126 Q127 K128 A129 N130 L131 L132 S133 S134 S135 N136 F137 E138 A139 T140 K141 K142 S143 V144 L145 K146

Q147 V148 Q149 D150 F151 E152 E153 N154 D155 H156 P157 N158 R159 V160 L161 E162 H163 L164 H165 S166 T167 A168 F169 Q170 N171 T172 P173 L174 S175 L176 P177 T178 R179 G180 T181 L182 E183 S184 L185 E186 N187 L188 V189 V190 A191 D192 L193 E194 S195 F196 A197 N198 N199 H200 F201 L202 N203 S204 N205 A206

V207 V208 V209 G210 T211 G212 N213 I214 K215 H216 E217 D218 L219 V220 N221 S222 I223 E224 S225 K226 N227 L228 S229 L230 Q231 T232 G233 T234 K235 P236 V237 L238 K239 K240 K241 A242 A243 F244 L245 G246 S247 E248 V249 R250 L251 R252 D253 D254 T255 L256 P257 K258 A259 W260 I261 S262 L263 A264 V265 E266

G267 E268 P269 V270 N271 S272 P273 N274 Y275 F276 V277 A278 K279 L280 A281 A282 Q283 I284 F285 G286 S287 Y288 N289 A290 F291 E292 P293 A294 S295 R296 L297 Q298 G299 I300 K301 L302 L303 D304 N305 I306 Q307 E308 Y309 Q310 L311 C312 D313 N314 F315 N316 H317 F318 S319 L320 S321 Y322 K323 D324 S325 G326

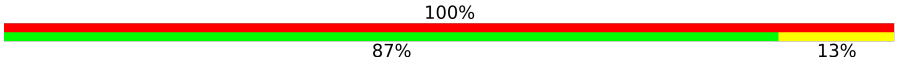
L327 W328 G329 F330 S331 T332 A333 T334 R335 N336 V337 T338 M339 I340 D341 D342 L343 I344 H345 F346 T347 L348 K349 Q350 W351 N352 R353 L354 T355 I356 S357 V358 T359 D360 T361 E362 V363 E364 R365 A366 K367 S368 L369 L370 K371 L372 Q373 L374 G375 Q376 L377 Y378 E379 S380 G381 N382 P383 V384 N385 D386

A387 N388 L389 L390 G391 A392 E393 V394 L395 I396 K397 G398 S399 K400 L401 S402 L403 G404 E405 A406 F407 K408 K409 I410 D411 A412 I413 T414 V415 K416 D417 V418 K419 A420 W421 A422 G423 K424 R425 L426 W427 D428 Q429 D430 I431 A432 I433 A434 G435 T436 G437 Q438 I439 E440 G441 L442 L443 D444 Y445 M446

R447 I448 R449 S450 D451 M452 S453 M454 M455 R456 W457

• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:

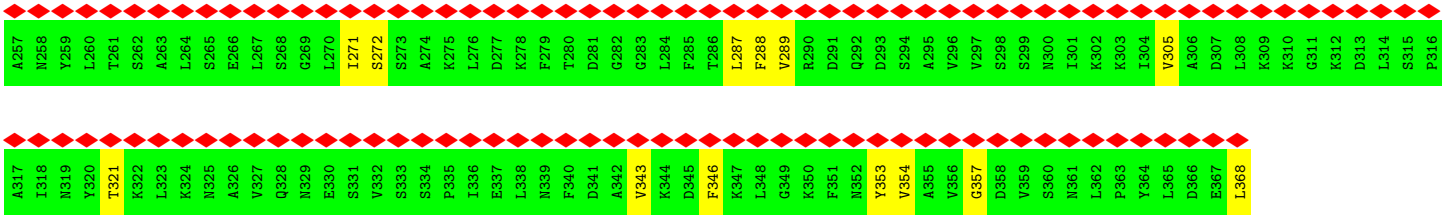


L17 T18 V19 S20 A21 R22 D23 A24 P25 T26 K27 I28 S29 T30 L31 A32 V33 K34 V35 H36 G37 G38 S39 R40 Y41 A42 T43 K44 D45 G46 V47 A48 H49 L50 L51 N52 R53 F54 N55 F56 Q57 N58 T59 N60 T61 R62 S63 A64 L65 K66 L67 V68 R69 E70 S71 E72 L73 L74 G75 G76

T77 F78 K79 S80 T81 L82 D83 R84 E85 Y86 I87 T88 L89 K90 A91 T92 F93 L94 K95 D96 D97 L98 P99 Y100 Y101 V102 N103 A104 L105 A106 D107 V108 L109 Y110 K111 T112 A113 F114 K115 P116 H117 E118 L119 T120 E121 S122 V123 L124 P125 A126 A127 R128 Y129 D130 Y131 A132 V133 A134 E135 Q136

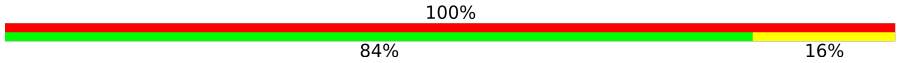
C137 P138 V139 K140 S141 A142 E143 D144 Q145 L146 Y147 A148 I149 T150 F151 R152 K153 G154 L155 G156 N157 P158 L159 L160 Y161 D162 G163 V164 E165 R166 V167 S168 L169 Q170 D171 I172 K173 D174 F175 A176 D177 K178 V179 Y180 T181 K182 E183 N184 L185 E186 V187 S188 G189 E190 N191 V192 V193 E194 A195 D196

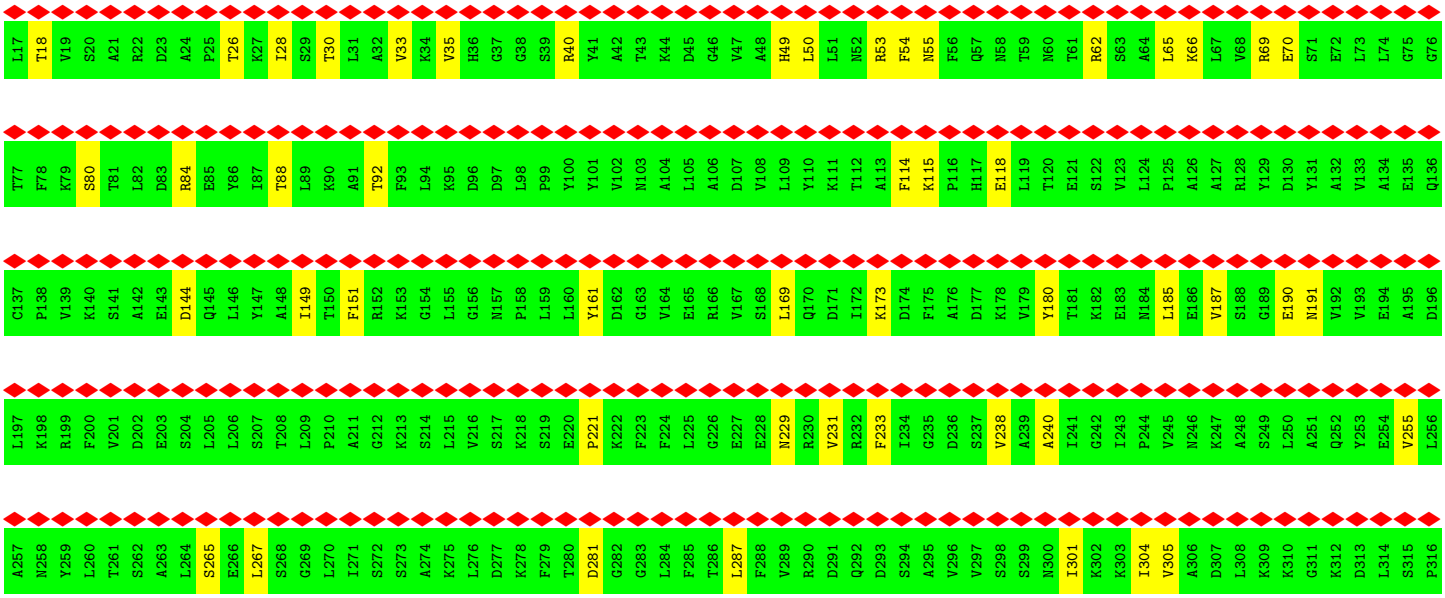
L197 K198 R199 F200 V201 D202 E203 S204 L205 L206 S207 T208 L209 P210 A211 G212 K213 S214 L215 V216 S217 K218 S219 E220 P221 K222 F223 F224 L225 G226 E227 E228 N229 R230 V231 R232 F233 I234 G235 D236 S237 V238 A239 A240 I241 G242 I243 P244 V245 N246 K247 A248 S249 L250 A251 Q252 Y253 E254 V255 L256



• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain M:

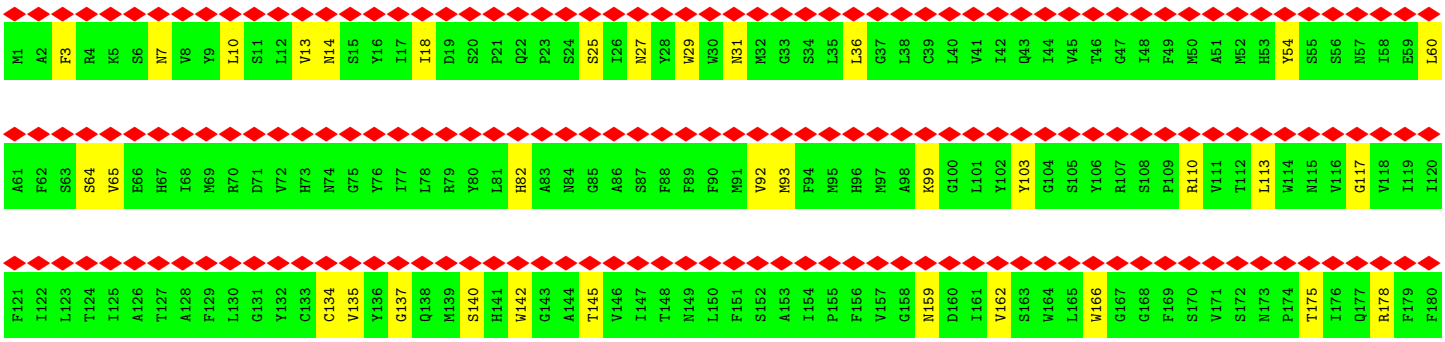


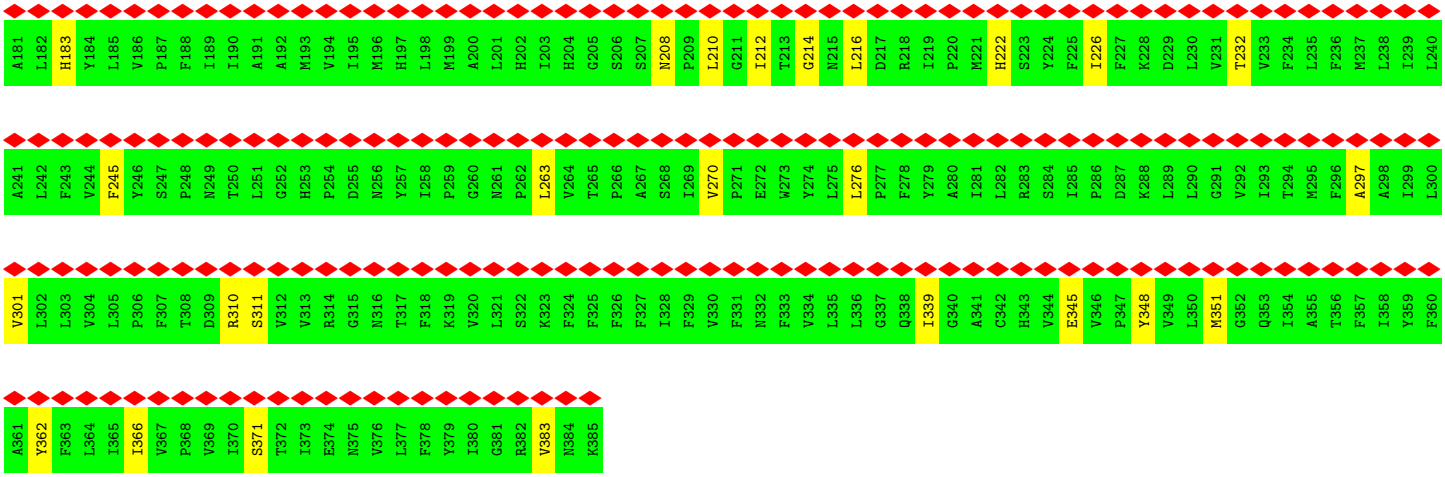


• Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2

Chain C:



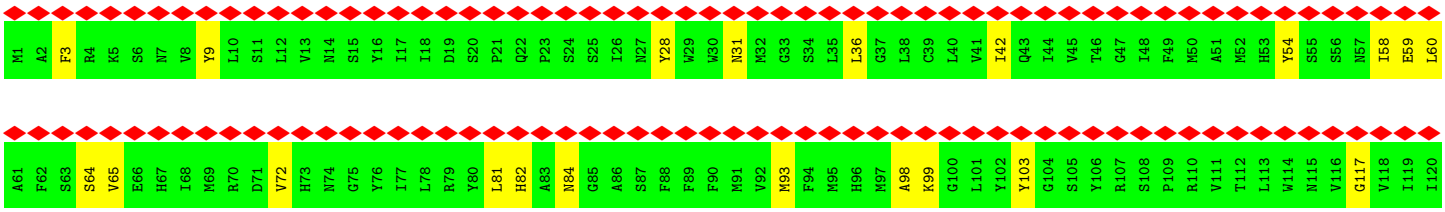




• Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2

Chain N:





• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1

Chain D:



M62 T63 A64 A65 E66 H67 G68 L69 H70 A71 P72 A73 Y74 A75 W76 S77 H78 M79 G80 P81 F82 E83 T84 F85 D86 H87 A88 S89 I90 R91 R92 G93 Y94 Q95 V96 Y97 R98 E99 V100 C101 A102 A103 C104 H105 S106 L107 D108 R109 V110 A111 W112 R113 T114 L115 V116 G117 V118 S119 H120 T121

N122 E123 E124 V125 R126 N127 M128 A129 E130 E131 F132 E133 Y134 D135 D136 E137 P138 D139 E140 Q141 G142 N143 P144 K145 K146 R147 P148 G149 K150 L151 S152 D153 Y154 I155 P156 G157 P158 Y159 P160 N161 E162 Q163 A164 A165 R166 A167 A168 N169 Q170 G171 A172 L173 P174 P175 D176 L177 S178 L179 I180 V181

K182 A183 R184 H185 G186 G187 C188 D189 Y190 I191 F192 S193 L194 L195 T196 G197 Y198 P199 D200 E201 P202 P203 A204 G205 V206 A207 L208 P209 P210 G211 S212 N213 Y214 N215 P216 Y217 F218 P219 G220 G221 S222 I223 A224 M225 A226 R227 V228 L229 F230 D231 D232 M233 V234 E235 Y236 E237 D238 G239 T240 P241

A242 T243 T244 S245 Q246 M247 A248 K249 D250 V251 T252 T253 F254 L255 N256 W257 C258 A259 E260 P261 E262 H263 D264 E265 R266 K267 R268 L269 G270 L271 K272 T273 V274 I275 I276 L277 S278 S279 L280 Y281 L282 L283 S284 I285 W286 V287 K288 K289 F290 K291 W292 A293 G294 I295 K296 T297 R298 K299 F300 V301

F302 N303 P304 P305 K306 P307 R308 LYS

• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1

Chain O:



M62 T63 A64 A65 E66 H67 G68 L69 H70 A71 P72 A73 Y74 A75 W76 S77 H78 N79 G80 P81 F82 E83 T84 F85 D86 H87 A88 S89 I90 R91 R92 G93 Y94 Q95 V96 Y97 R98 E99 V100 C101 A102 A103 C104 H105 S106 L107 D108 R109 V110 A111 W112 R113 T114 L115 V116 G117 V118 S119 H120 T121

N122 E123 E124 V125 R126 N127 M128 A129 E130 E131 F132 E133 Y134 D135 D136 E137 P138 D139 E140 Q141 G142 N143 P144 K145 K146 R147 P148 G149 K150 L151 S152 D153 Y154 I155 P156 G157 P158 Y159 P160 N161 E162 Q163 A164 A165 R166 A167 A168 N169 Q170 G171 A172 L173 P174 P175 D176 L177 S178 L179 I180 V181

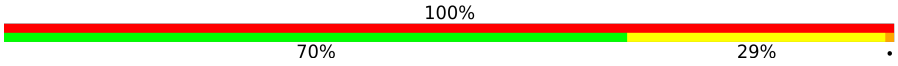
K182 A183 R184 H185 G186 G187 C188 D189 Y190 I191 F192 S193 L194 L195 T196 G197 Y198 P199 D200 E201 P202 P203 A204 G205 V206 A207 L208 P209 P210 G211 S212 N213 Y214 N215 P216 Y217 F218 P219 G220 G221 S222 I223 A224 M225 A226 R227 V228 L229 F230 D231 D232 M233 V234 E235 Y236 E237 D238 G239 T240 P241

A242 T243 T244 S245 Q246 M247 A248 K249 D250 V251 T252 T253 F254 L255 N256 W257 C258 A259 E260 P261 E262 H263 D264 E265 R266 K267 R268 L269 G270 L271 K272 T273 V274 I275 I276 L277 S278 S279 L280 Y281 L282 L283 S284 I285 W286 V287 K288 K289 F290 K291 W292 A293 G294 I295 K296 T297 R298 K299 F300 V301

F302 N303 P304 P305 K306 P307 R308 LYS

• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E:

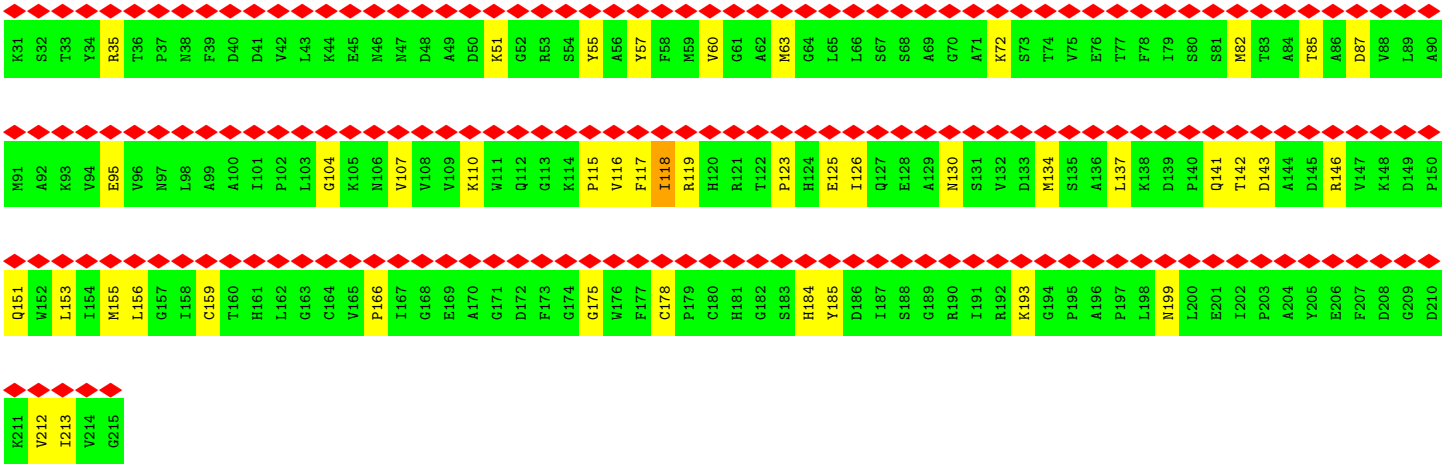




• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

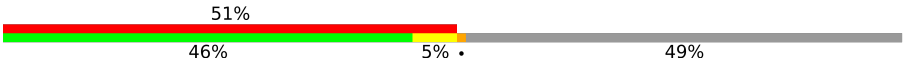
Chain P:

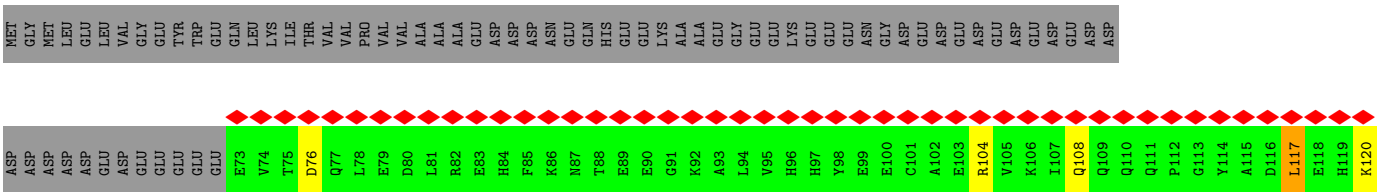


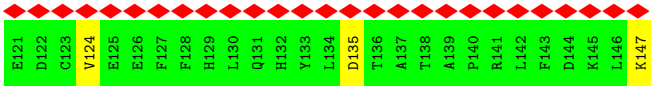


• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6,COMPLEX III SUBUNIT VI,CYTOCHROME C1 NON-HEME 17 KDA PROTEIN,MITOCHONDRIAL HINGE PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN

Chain F:



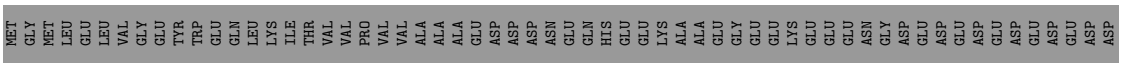


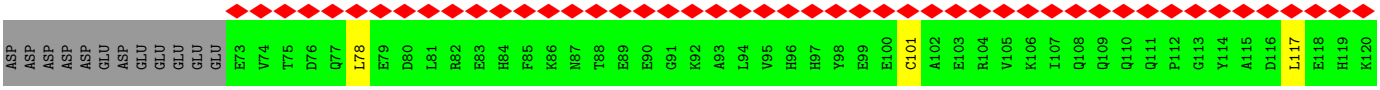


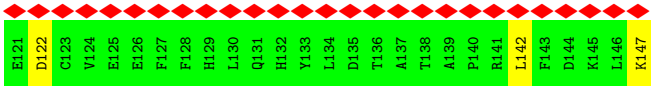
• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6,COMPLEX III SUBUNIT VI,CYTOCHROME C1 NON-HEME 17 KDA PROTE IN,MITOCHONDRIAL HINGE PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN

Chain Q:



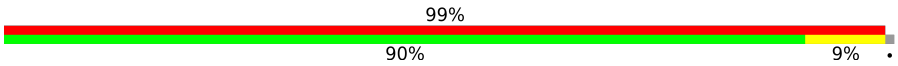


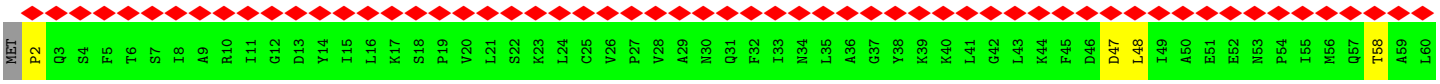


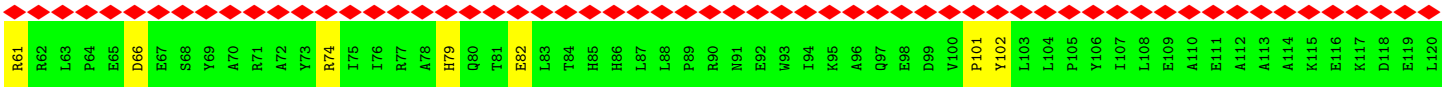


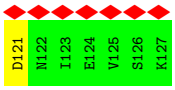
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN

Chain G:



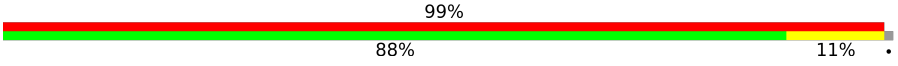


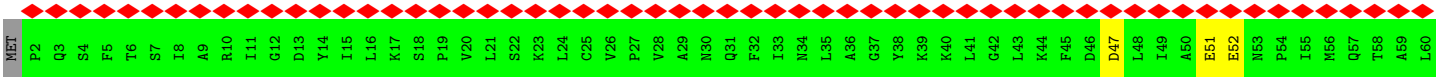


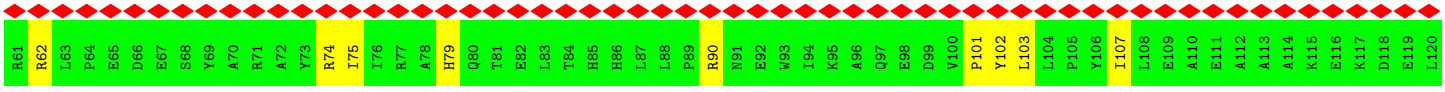


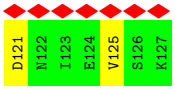
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN

Chain R:



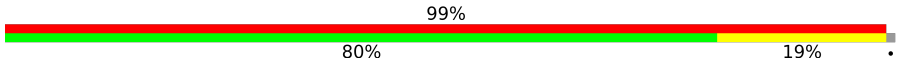


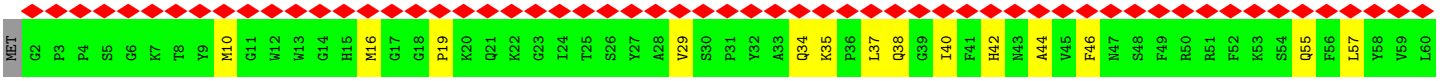


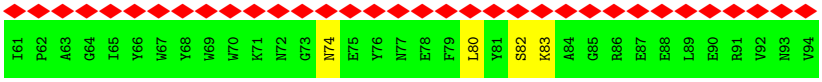


• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain H:

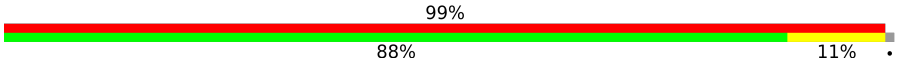


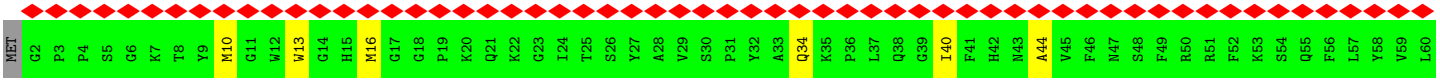


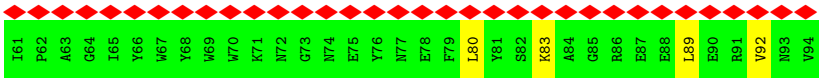


• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain S:



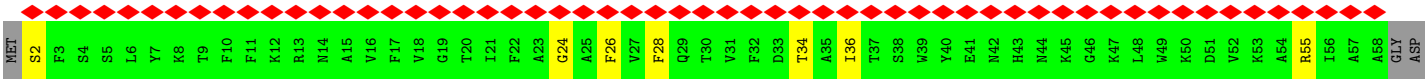




• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

Chain I:



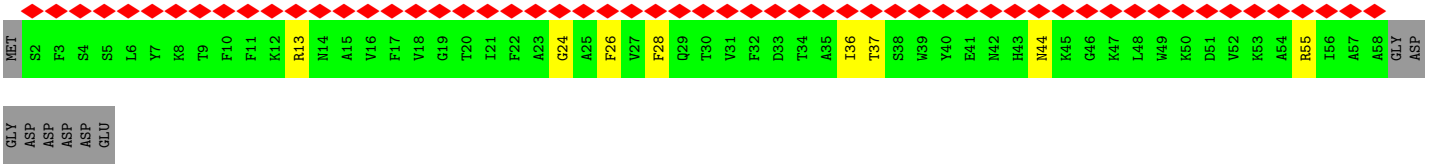




• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

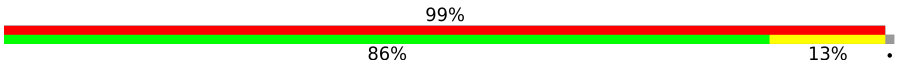
Chain T:

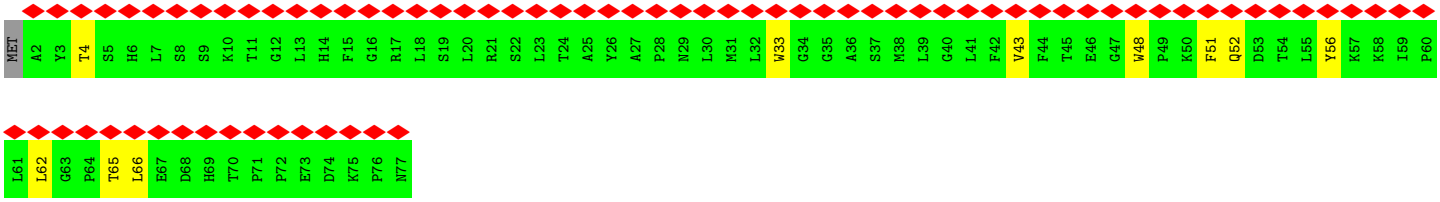




• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10,COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN

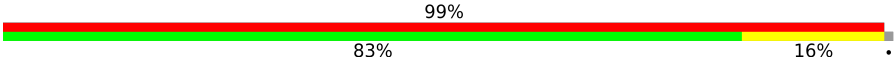
Chain J:

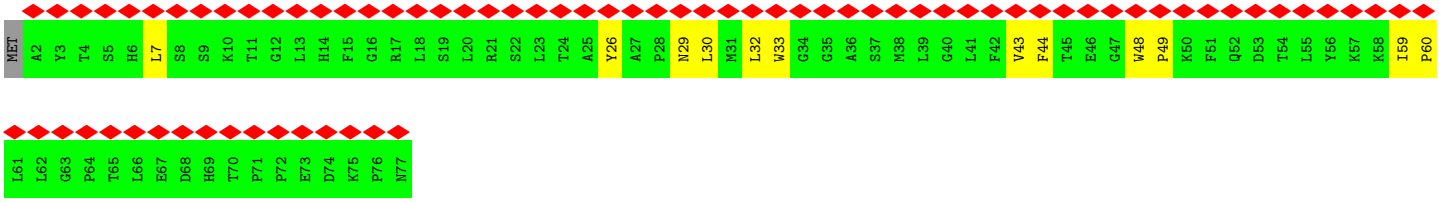




• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10,COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN

Chain U:

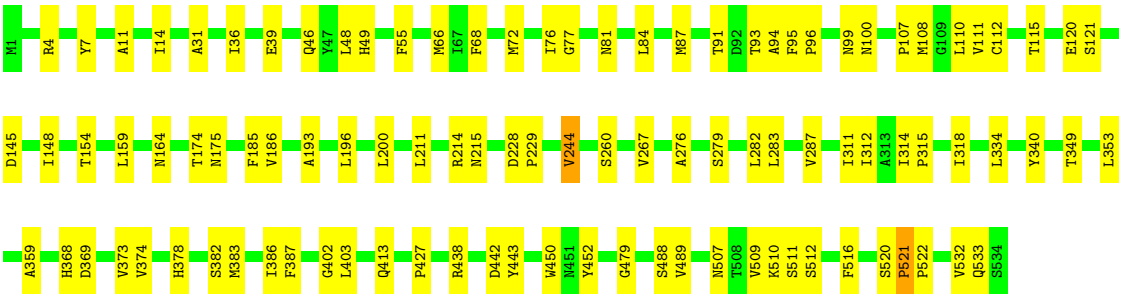




• Molecule 11: CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1

Chain a:

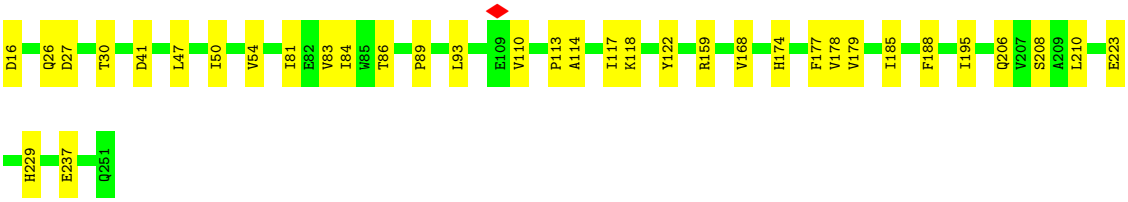




• Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2

Chain b:

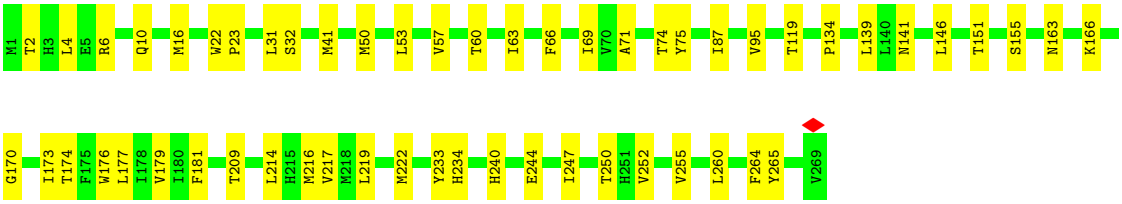




• Molecule 13: CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3

Chain c:





• Molecule 14: CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4

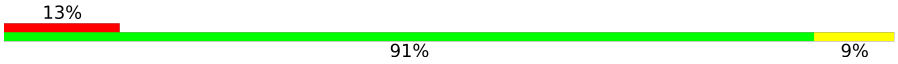
Chain d:

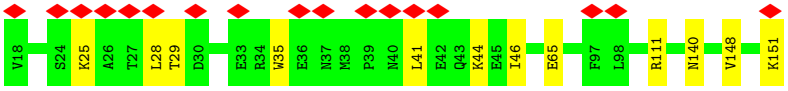




• Molecule 15: CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B

Chain e:

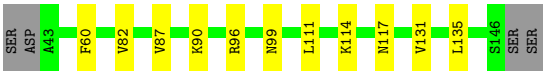




• Molecule 16: CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6

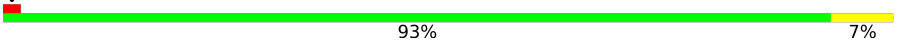
Chain f:

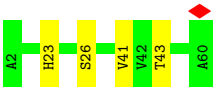




• Molecule 17: CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7

Chain g:





• Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h:

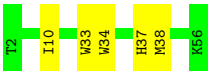




• Molecule 19: CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9

Chain i:

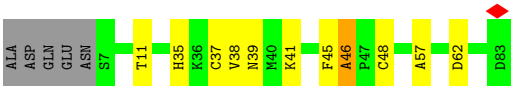




• Molecule 20: Cytochrome c oxidase subunit 6B

Chain j:

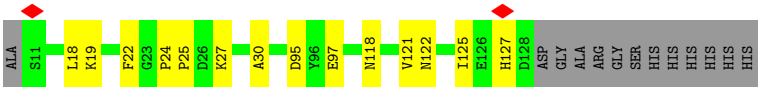




• Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13

Chain k:

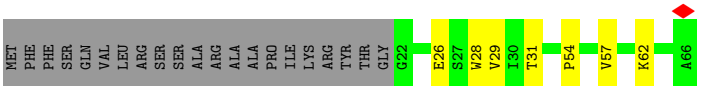




• Molecule 22: COX26; SYNONYM: Uncharacterized protein YDR119W-A

Chain l:



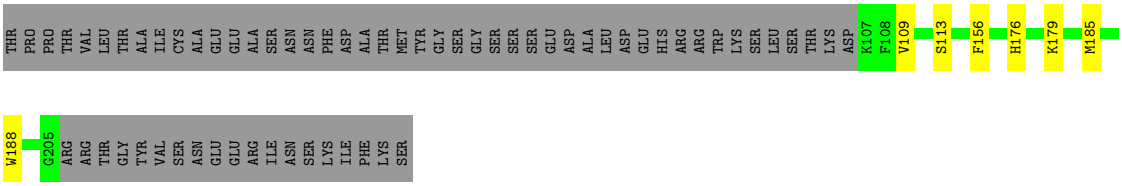


• Molecule 23: RCF2; SYNONYM: Respiratory supercomplex factor 2

Chain m:






THR PRO PRO THR VAL LEU THR ALA ILE CYS ALA GLU GLU ALA SER ASN ASN PHE ASP ALA THR MET TYR GLY SER GLY SER SER GLU ASP ALA LEU ASP GLU HIS ARG ARG TRP LYS SER LEU SER THR LYS ASP
K107 F108 V109 S113 F156 H176 K179 M185
W188 G205 ARG ARG THR GLY TYR VAL SER ASN GLU GLU ARG ILE ASN SER LYS ILE PHE LYS SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73042	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 ($e^-/Å^2$)	56.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.004	Depositor
Minimum map value	-1.391	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.424	Depositor
Map size (Å)	402.432, 402.432, 402.432	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PEF, MG, HEC, ZN, PCF, CU, CUA, HEA, CDL, FES

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	0.21	0/3406	0.49	0/4615
1	L	0.22	0/3406	0.53	0/4615
2	B	0.22	0/2781	0.50	0/3764
2	M	0.22	0/2781	0.51	0/3764
3	C	0.26	0/3192	0.59	1/4354 (0.0%)
3	N	0.26	0/3192	0.57	0/4354
4	D	0.20	0/2012	0.44	0/2740
4	O	0.21	0/2012	0.44	0/2740
5	E	0.28	0/1444	0.65	2/1957 (0.1%)
5	P	0.30	0/1444	0.67	0/1957
6	F	0.31	0/647	0.71	2/870 (0.2%)
6	Q	0.28	0/647	0.67	2/870 (0.2%)
7	G	0.24	0/1040	0.54	0/1408
7	R	0.22	0/1040	0.47	0/1408
8	H	0.19	0/804	0.44	0/1088
8	S	0.22	0/804	0.48	0/1088
9	I	0.22	0/479	0.48	0/646
9	T	0.20	0/479	0.47	0/646
10	J	0.21	0/619	0.52	0/841
10	U	0.26	0/619	0.58	0/841
11	a	0.29	0/4290	0.66	1/5857 (0.0%)
12	b	0.26	0/1941	0.66	0/2653
13	c	0.27	0/2218	0.62	0/3036
14	d	0.26	0/932	0.61	0/1269
15	e	0.24	0/1111	0.59	0/1503
16	f	0.28	0/884	0.56	0/1196
17	g	0.30	0/500	0.70	1/681 (0.1%)
18	h	0.25	0/424	0.68	2/569 (0.4%)
19	i	0.25	0/468	0.56	0/626
20	j	0.31	0/664	0.75	1/899 (0.1%)
21	k	0.24	0/1002	0.55	0/1364
22	l	0.25	0/372	0.64	0/502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
23	m	0.29	0/813	0.64	0/1093
All	All	0.25	0/48467	0.57	12/65814 (0.0%)

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	L	0	1
2	B	0	1
3	N	0	1
5	E	0	1
5	P	0	1
11	a	0	4
13	c	0	1
14	d	0	1
21	k	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	j	46	ALA	N-CA-C	10.14	117.34	108.22
11	a	14	ILE	N-CA-C	-6.09	106.86	112.96
18	h	77	ALA	CA-C-N	5.71	131.98	121.70
18	h	77	ALA	C-N-CA	5.71	131.98	121.70
6	F	117	LEU	CA-C-N	5.64	132.30	121.54

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	220	GLU	Peptide
5	E	167	ILE	Peptide
1	L	444	ASP	Peptide
3	N	345	GLU	Peptide
5	P	125	GLU	Peptide

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	3345	0	3323	29	0
1	L	3345	0	3323	37	0
2	B	2735	0	2774	30	0
2	M	2735	0	2774	35	0
3	C	3090	0	3127	42	0
3	N	3090	0	3129	45	0
4	D	1951	0	1874	22	0
4	O	1951	0	1874	28	0
5	E	1411	0	1386	30	0
5	P	1411	0	1386	29	0
6	F	633	0	587	7	0
6	Q	633	0	587	4	0
7	G	1019	0	1034	11	0
7	R	1019	0	1034	11	0
8	H	773	0	736	14	0
8	S	773	0	735	8	0
9	I	465	0	459	6	0
9	T	465	0	459	7	0
10	J	599	0	594	8	0
10	U	599	0	594	9	0
11	a	4162	0	4189	66	0
12	b	1889	0	1866	26	0
13	c	2146	0	2137	38	0
14	d	913	0	910	20	0
15	e	1083	0	1081	9	0
16	f	866	0	834	6	0
17	g	484	0	517	2	0
18	h	409	0	408	5	0
19	i	456	0	469	4	0
20	j	642	0	586	7	0
21	k	967	0	933	11	0
22	l	361	0	363	4	0
23	m	799	0	819	4	0
24	A	31	0	35	2	0
24	C	83	0	113	3	0
24	E	43	0	62	2	0
24	H	32	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	29	0	31	0	0
24	L	36	0	43	1	0
24	N	83	0	118	3	0
24	P	42	0	60	1	0
24	S	36	0	48	1	0
24	U	47	0	73	0	0
24	a	33	0	39	1	0
24	b	73	0	95	1	0
24	c	77	0	100	2	0
24	e	42	0	60	1	0
25	C	86	0	60	3	0
25	N	86	0	60	5	0
26	C	55	0	52	0	0
26	D	67	0	78	1	0
26	H	53	0	50	3	0
26	L	58	0	60	2	0
26	N	66	0	75	4	0
26	O	71	0	89	2	0
26	S	53	0	50	2	0
27	C	50	0	80	0	0
27	I	39	0	52	0	0
27	N	39	0	55	3	0
27	S	32	0	38	0	0
27	T	50	0	80	1	0
27	e	36	0	44	3	0
28	D	43	0	31	1	0
28	O	43	0	31	3	0
29	E	4	0	0	0	0
29	P	4	0	0	1	0
30	a	1	0	0	0	0
31	a	120	0	105	9	0
32	a	1	0	0	0	0
33	b	2	0	0	0	0
34	d	1	0	0	0	0
All	All	48966	0	48905	533	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 5.

The worst 5 of 533 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)
19:i:34:TRP:O	19:i:38:MET:HB2	1.84	0.78
11:a:66:MET:HG2	31:a:602:HEA:HBC1	1.65	0.76
2:M:50:LEU:O	2:M:54:PHE:HB2	1.84	0.75
5:E:118:ILE:HA	5:E:153:LEU:O	1.87	0.72
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.74	0.69

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 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	429/431 (100%)	397 (92%)	32 (8%)	0	100	100
1	L	429/431 (100%)	394 (92%)	35 (8%)	0	100	100
2	B	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
2	M	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
3	C	383/385 (100%)	363 (95%)	20 (5%)	0	100	100
3	N	383/385 (100%)	357 (93%)	26 (7%)	0	100	100
4	D	245/248 (99%)	239 (98%)	6 (2%)	0	100	100
4	O	245/248 (99%)	241 (98%)	4 (2%)	0	100	100
5	E	183/185 (99%)	163 (89%)	20 (11%)	0	100	100
5	P	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
6	F	73/147 (50%)	68 (93%)	5 (7%)	0	100	100
6	Q	73/147 (50%)	70 (96%)	3 (4%)	0	100	100
7	G	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
7	R	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
8	H	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
8	S	91/94 (97%)	85 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
9	T	55/66 (83%)	55 (100%)	0	0	100	100
10	J	74/77 (96%)	70 (95%)	4 (5%)	0	100	100
10	U	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
11	a	532/534 (100%)	490 (92%)	40 (8%)	2 (0%)	30	60
12	b	234/236 (99%)	214 (92%)	20 (8%)	0	100	100
13	c	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	30	60
14	d	119/130 (92%)	101 (85%)	18 (15%)	0	100	100
15	e	132/134 (98%)	123 (93%)	9 (7%)	0	100	100
16	f	102/108 (94%)	96 (94%)	6 (6%)	0	100	100
17	g	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
18	h	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
20	j	75/82 (92%)	67 (89%)	8 (11%)	0	100	100
21	k	116/131 (88%)	103 (89%)	13 (11%)	0	100	100
22	l	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
23	m	97/224 (43%)	91 (94%)	6 (6%)	0	100	100
All	All	5890/6303 (93%)	5521 (94%)	366 (6%)	3 (0%)	49	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	a	121	SER
11	a	521	PRO
13	c	23	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	370/370 (100%)	370 (100%)	0	100	100
1	L	370/370 (100%)	370 (100%)	0	100	100
2	B	301/301 (100%)	300 (100%)	1 (0%)	86	86
2	M	301/301 (100%)	300 (100%)	1 (0%)	86	86
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	337 (100%)	1 (0%)	86	86
4	D	205/206 (100%)	205 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	150 (99%)	1 (1%)	76	80
5	P	151/151 (100%)	149 (99%)	2 (1%)	61	74
6	F	68/131 (52%)	68 (100%)	0	100	100
6	Q	68/131 (52%)	67 (98%)	1 (2%)	57	72
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	109 (99%)	1 (1%)	70	78
8	H	77/78 (99%)	77 (100%)	0	100	100
8	S	77/78 (99%)	77 (100%)	0	100	100
9	I	47/54 (87%)	47 (100%)	0	100	100
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	65 (100%)	0	100	100
10	U	65/66 (98%)	65 (100%)	0	100	100
11	a	447/447 (100%)	446 (100%)	1 (0%)	87	88
12	b	209/209 (100%)	209 (100%)	0	100	100
13	c	228/228 (100%)	228 (100%)	0	100	100
14	d	102/111 (92%)	101 (99%)	1 (1%)	68	76
15	e	115/115 (100%)	114 (99%)	1 (1%)	70	78
16	f	92/96 (96%)	91 (99%)	1 (1%)	65	76
17	g	50/50 (100%)	50 (100%)	0	100	100
18	h	41/41 (100%)	41 (100%)	0	100	100
19	i	46/46 (100%)	46 (100%)	0	100	100
20	j	69/73 (94%)	69 (100%)	0	100	100
21	k	104/113 (92%)	104 (100%)	0	100	100
22	l	36/53 (68%)	35 (97%)	1 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	m	84/191 (44%)	84 (100%)	0	100 100
All	All	5087/5385 (94%)	5074 (100%)	13 (0%)	84 86

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	R	125	VAL
11	a	244	VAL
22	l	29	VAL
15	e	148	VAL
16	f	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
15	e	115	ASN
16	f	44	HIS
1	L	121	ASN
1	L	102	GLN
17	g	13	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 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	$\#\|Z\| > 2$
29	FES	P	301	5	0,4,4	-	-	-		
33	CUA	b	301	12	0,1,1	-	-	-		
24	PEF	c	302	-	40,40,46	1.02	2 (5%)	43,45,51	1.04	1 (2%)
24	PEF	c	301	-	35,35,46	1.08	2 (5%)	38,40,51	1.14	3 (7%)
26	CDL	N	603	26	65,65,99	1.12	4 (6%)	71,77,111	1.16	6 (8%)
27	PCF	e	202	15	35,35,49	1.13	2 (5%)	41,43,57	1.06	3 (7%)
24	PEF	N	605	-	38,38,46	1.08	2 (5%)	41,43,51	0.99	2 (4%)
26	CDL	D	402	-	66,66,99	1.12	4 (6%)	72,78,111	1.19	6 (8%)
29	FES	E	301	5	0,4,4	-	-	-		
25	HEM	C	601	3	50,50,50	1.60	10 (20%)	66,82,82	1.74	14 (21%)
24	PEF	J	101	-	28,28,46	1.22	2 (7%)	31,33,51	1.18	2 (6%)
24	PEF	C	605	-	42,42,46	1.01	2 (4%)	45,47,51	1.15	3 (6%)
24	PEF	E	302	-	42,42,46	1.01	2 (4%)	45,47,51	1.10	3 (6%)
27	PCF	S	103	8	31,31,49	1.19	2 (6%)	37,39,57	1.09	4 (10%)
28	HEC	O	401	4	50,50,50	2.90	27 (54%)	68,82,82	2.69	29 (42%)
24	PEF	P	302	-	41,41,46	1.00	2 (4%)	44,46,51	1.04	3 (6%)
26	CDL	O	402	26	70,70,99	1.09	4 (5%)	76,82,111	1.22	6 (7%)
26	CDL	H	601	-	52,52,99	1.26	4 (7%)	58,64,111	1.26	5 (8%)
24	PEF	A	501	1	30,30,46	1.17	2 (6%)	33,35,51	1.12	3 (9%)
24	PEF	S	102	-	35,35,46	1.08	2 (5%)	38,40,51	1.11	3 (7%)
24	PEF	a	605	11	32,32,46	1.16	2 (6%)	35,37,51	1.19	3 (8%)
27	PCF	T	101	-	49,49,49	0.97	2 (4%)	55,57,57	1.02	3 (5%)
25	HEM	N	601	3	50,50,50	1.60	9 (18%)	66,82,82	1.72	13 (19%)
25	HEM	N	602	3	50,50,50	1.60	8 (16%)	66,82,82	1.70	16 (24%)
26	CDL	L	501	-	57,57,99	1.21	4 (7%)	63,69,111	1.20	4 (6%)
27	PCF	I	101	24	38,38,49	1.07	2 (5%)	44,46,57	1.08	4 (9%)
24	PEF	C	604	27	39,39,46	1.04	2 (5%)	42,44,51	1.10	3 (7%)
24	PEF	b	302	-	39,39,46	1.04	2 (5%)	42,44,51	1.05	2 (4%)
28	HEC	D	401	4	50,50,50	2.89	28 (56%)	68,82,82	2.65	28 (41%)
31	HEA	a	603	11	66,67,67	2.42	25 (37%)	78,103,103	2.73	34 (43%)
26	CDL	S	101	-	52,52,99	1.26	4 (7%)	58,64,111	1.25	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PEF	H	602	-	31,31,46	1.16	2 (6%)	34,36,51	1.24	4 (11%)
31	HEA	a	602	11	66,67,67	2.39	24 (36%)	78,103,103	2.63	34 (43%)
25	HEM	C	602	3	50,50,50	1.62	8 (16%)	66,82,82	1.71	16 (24%)
27	PCF	N	606	-	38,38,49	1.10	2 (5%)	44,46,57	1.05	3 (6%)
24	PEF	b	303	-	32,32,46	1.12	2 (6%)	35,37,51	1.23	4 (11%)
24	PEF	U	101	-	46,46,46	0.96	2 (4%)	49,51,51	1.03	2 (4%)
26	CDL	C	603	1,3	54,54,99	1.16	4 (7%)	60,66,111	1.24	5 (8%)
24	PEF	N	604	-	43,43,46	0.97	2 (4%)	46,48,51	1.05	3 (6%)
27	PCF	C	606	-	49,49,49	0.96	2 (4%)	55,57,57	1.00	4 (7%)
24	PEF	e	201	-	41,41,46	1.03	2 (4%)	44,46,51	0.97	2 (4%)
24	PEF	L	502	1	35,35,46	1.08	2 (5%)	38,40,51	1.14	4 (10%)

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
29	FES	P	301	5	-	-	0/1/1/1
24	PEF	c	302	-	-	11/44/44/50	-
24	PEF	c	301	-	-	10/39/39/50	-
26	CDL	N	603	26	-	11/76/76/110	-
27	PCF	e	202	15	-	7/39/39/53	-
24	PEF	N	605	-	-	10/42/42/50	-
26	CDL	D	402	-	-	29/77/77/110	-
29	FES	E	301	5	-	-	0/1/1/1
25	HEM	C	601	3	-	10/14/54/54	-
24	PEF	J	101	-	-	15/32/32/50	-
24	PEF	C	605	-	-	13/46/46/50	-
27	PCF	S	103	8	-	8/35/35/53	-
28	HEC	O	401	4	1/1/3/7	7/14/54/54	-
24	PEF	P	302	-	-	13/45/45/50	-
26	CDL	O	402	26	-	19/81/81/110	-
26	CDL	H	601	-	-	19/63/63/110	-
24	PEF	A	501	1	-	7/34/34/50	-
24	PEF	S	102	-	-	10/39/39/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEF	a	605	11	-	6/36/36/50	-
27	PCF	T	101	-	-	9/53/53/53	-
25	HEM	N	601	3	-	10/14/54/54	-
25	HEM	N	602	3	-	6/14/54/54	-
26	CDL	L	501	-	-	19/68/68/110	-
27	PCF	I	101	24	-	6/42/42/53	-
24	PEF	C	604	27	-	9/43/43/50	-
28	HEC	D	401	4	1/1/3/7	4/14/54/54	-
24	PEF	b	302	-	-	19/43/43/50	-
31	HEA	a	603	11	-	6/36/76/76	-
24	PEF	e	201	-	-	13/45/45/50	-
26	CDL	S	101	-	-	23/63/63/110	-
24	PEF	H	602	-	-	6/35/35/50	-
31	HEA	a	602	11	-	14/36/76/76	-
25	HEM	C	602	3	-	6/14/54/54	-
27	PCF	N	606	-	-	11/42/42/53	-
24	PEF	b	303	-	-	14/36/36/50	-
24	PEF	U	101	-	-	14/50/50/50	-
26	CDL	C	603	1,3	-	21/64/64/110	-
24	PEF	N	604	-	-	9/47/47/50	-
27	PCF	C	606	-	-	15/53/53/53	-
24	PEF	E	302	-	-	14/46/46/50	-
24	PEF	L	502	1	-	15/39/39/50	-

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	401	HEC	C3B-C2B	5.64	1.48	1.36
28	D	401	HEC	C3B-C2B	5.63	1.48	1.36
31	a	602	HEA	FE-NB	5.51	2.11	1.94
31	a	603	HEA	FE-NB	5.46	2.11	1.94
31	a	602	HEA	C3B-C2B	5.41	1.46	1.34

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	603	HEA	C3D-C4D-ND	6.65	116.80	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	603	HEA	C2D-C1D-ND	6.36	117.38	109.84
31	a	602	HEA	C3C-C4C-NC	6.29	114.12	110.25
31	a	603	HEA	C3C-C4C-NC	6.12	114.01	110.25
31	a	602	HEA	C3D-C4D-ND	6.08	116.24	110.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	D	401	HEC	NA
28	O	401	HEC	NA

5 of 468 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	501	PEF	C1-O3P-P-O1P
24	A	501	PEF	C1-O3P-P-O2P
24	A	501	PEF	C1-O3P-P-O4P
24	C	605	PEF	C11-C10-O2-C2
24	C	605	PEF	O4-C10-O2-C2

There are no ring outliers.

32 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	P	301	FES	1	0
24	c	302	PEF	1	0
24	c	301	PEF	1	0
26	N	603	CDL	4	0
27	e	202	PCF	3	0
24	N	605	PEF	1	0
26	D	402	CDL	1	0
25	C	601	HEM	2	0
24	C	605	PEF	1	0
24	E	302	PEF	2	0
28	O	401	HEC	3	0
24	P	302	PEF	1	0
26	O	402	CDL	2	0
26	H	601	CDL	3	0
24	A	501	PEF	2	0
24	S	102	PEF	1	0
24	a	605	PEF	1	0
27	T	101	PCF	1	0

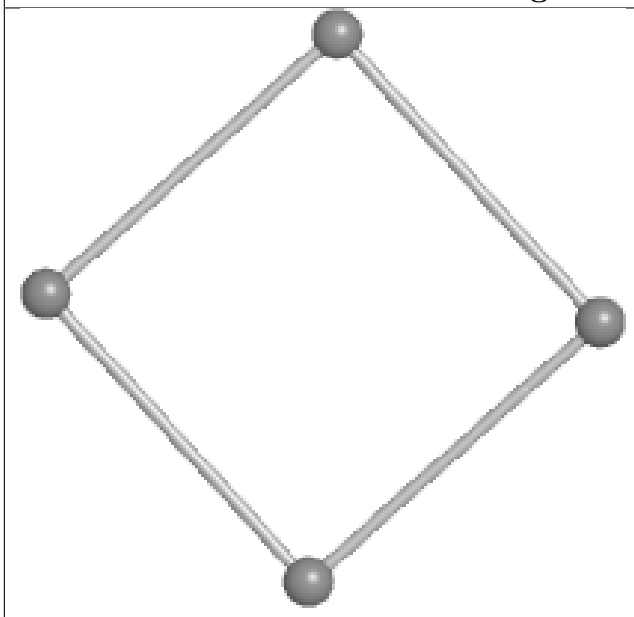
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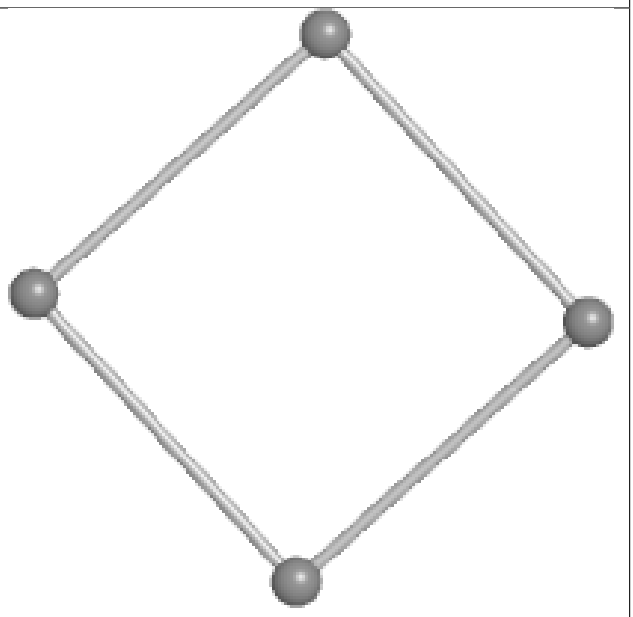
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	601	HEM	3	0
25	N	602	HEM	2	0
26	L	501	CDL	2	0
24	C	604	PEF	2	0
24	b	302	PEF	1	0
28	D	401	HEC	1	0
31	a	603	HEA	8	0
26	S	101	CDL	2	0
31	a	602	HEA	1	0
25	C	602	HEM	1	0
27	N	606	PCF	3	0
24	N	604	PEF	2	0
24	e	201	PEF	1	0
24	L	502	PEF	1	0

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.

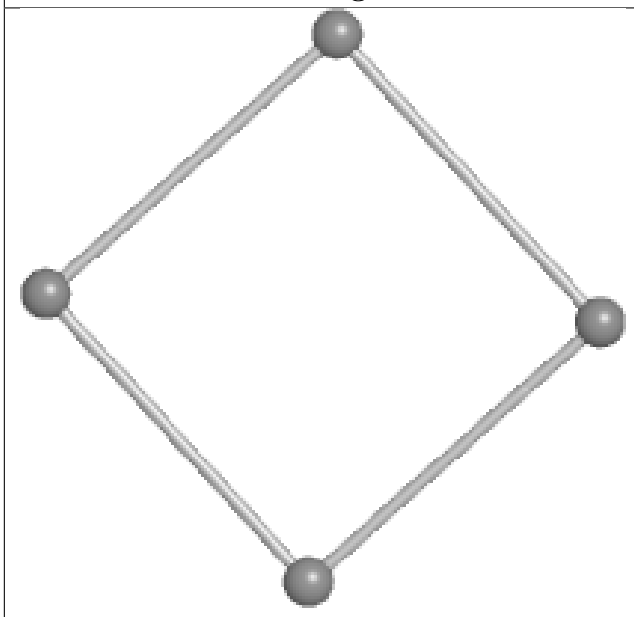
Ligand FES P 301



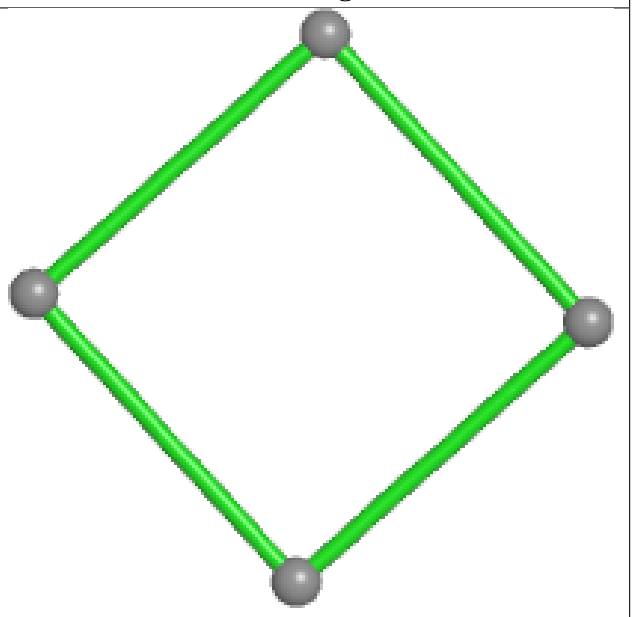
Bond lengths



Bond angles



Torsions



Rings

Ligand CUA b 301



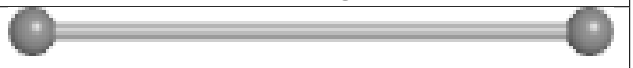
Bond lengths



Bond angles

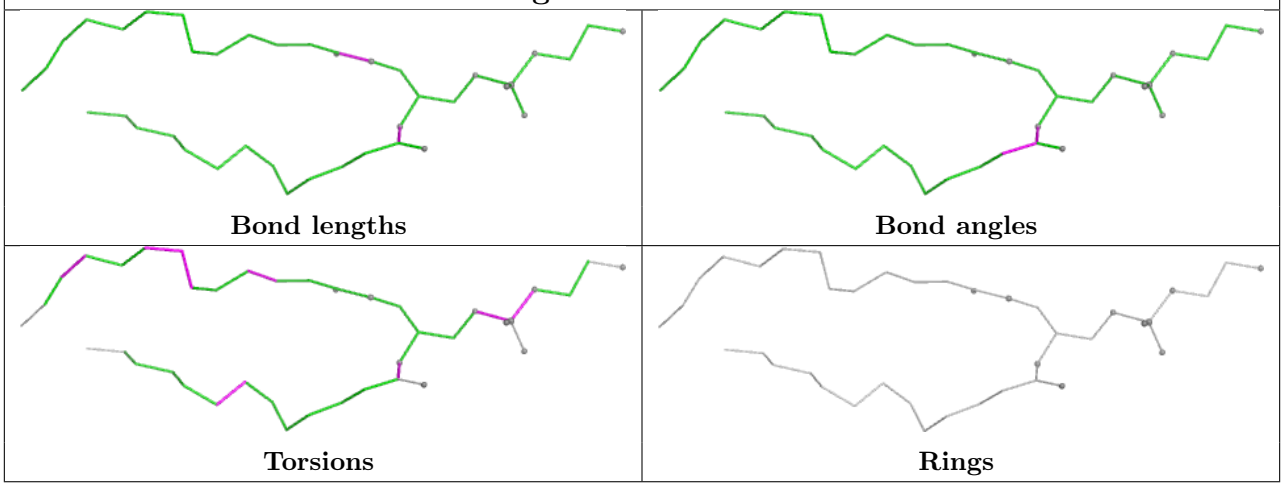


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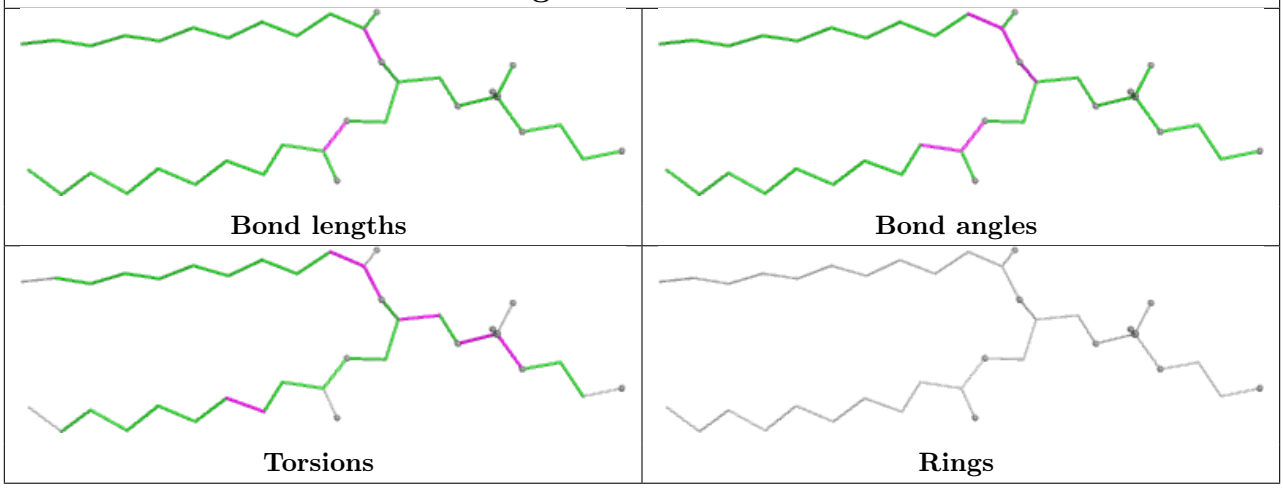


Rings

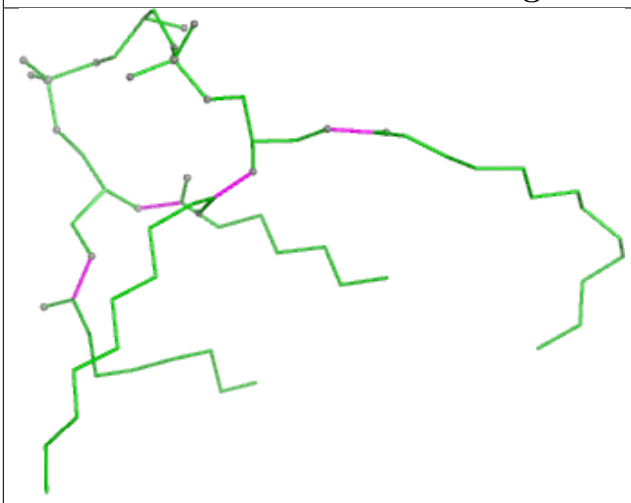
Ligand PEF c 302



Ligand PEF c 301



Ligand CDL N 603



Bond lengths



Bond angles

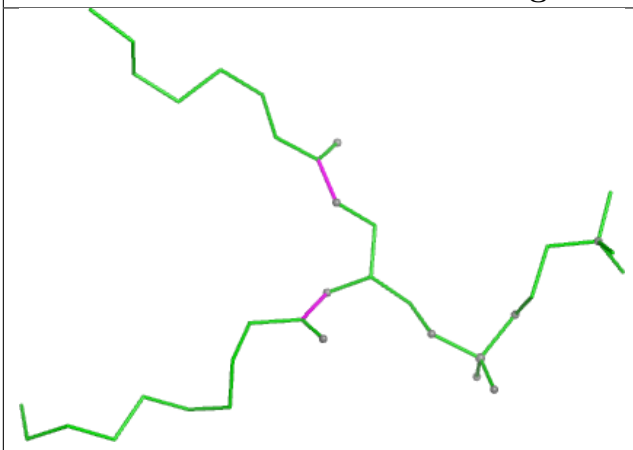


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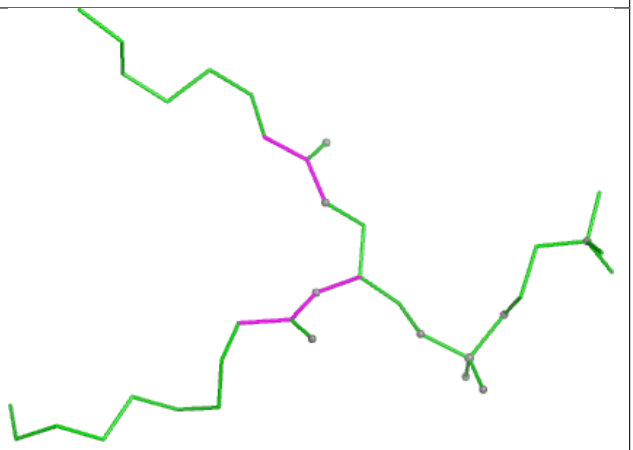


Rings

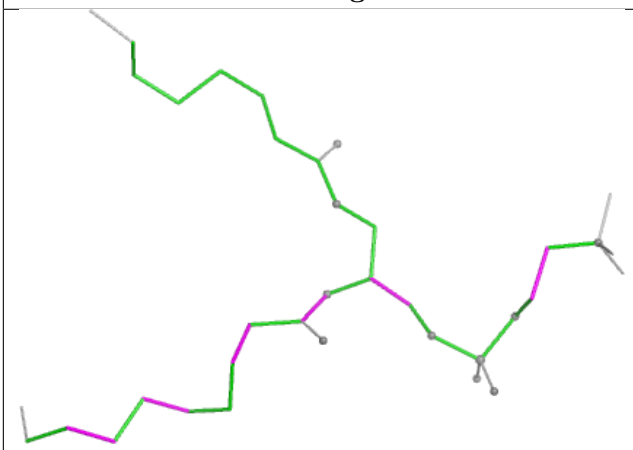
Ligand PCF e 202



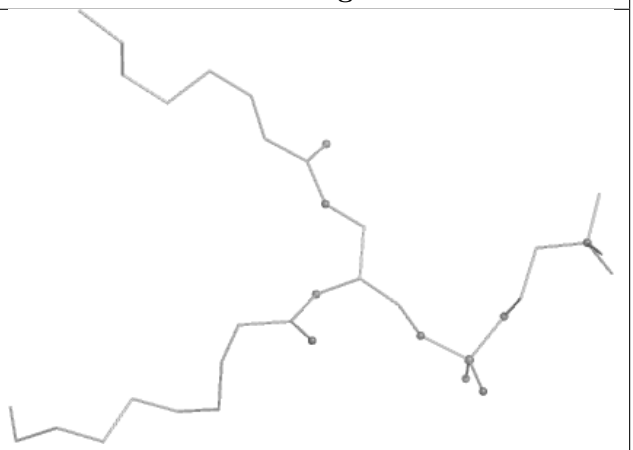
Bond lengths



Bond angles

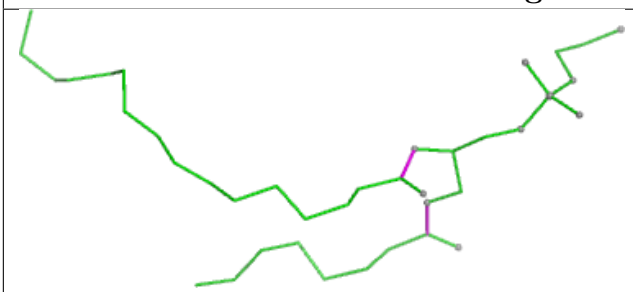


Torsions

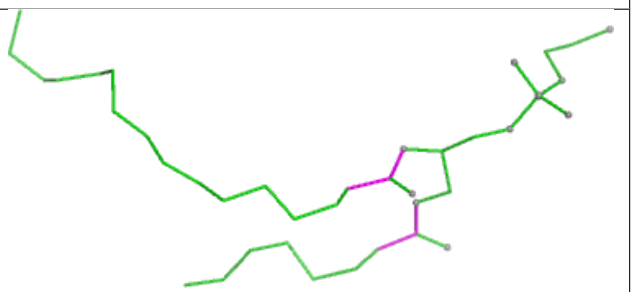


Rings

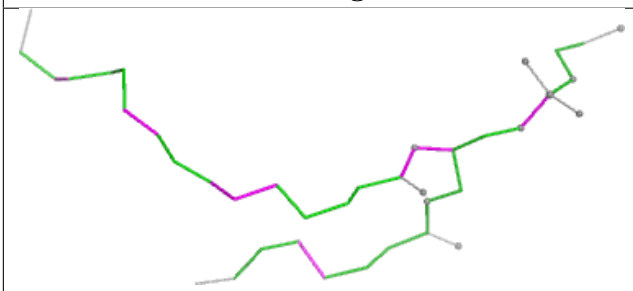
Ligand PEF N 605



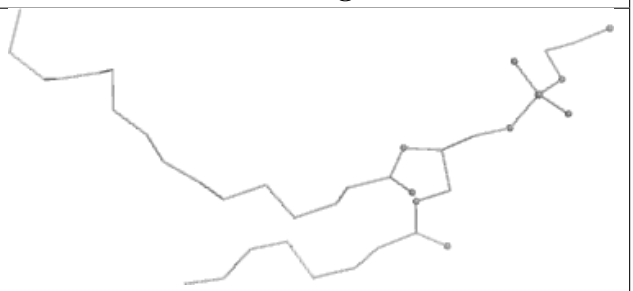
Bond lengths



Bond angles

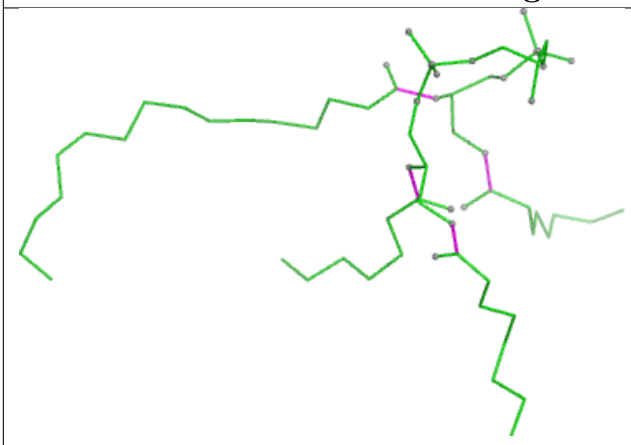


Torsions

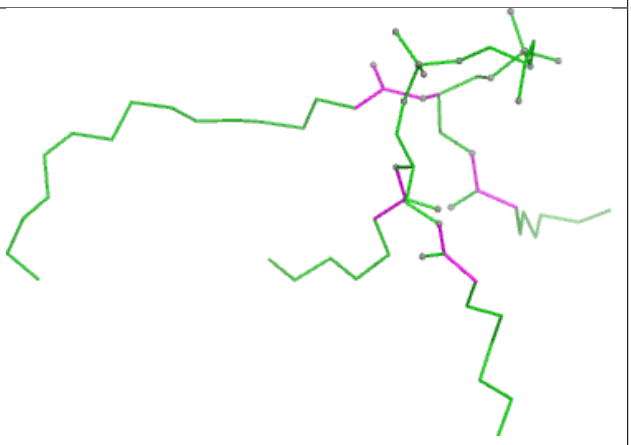


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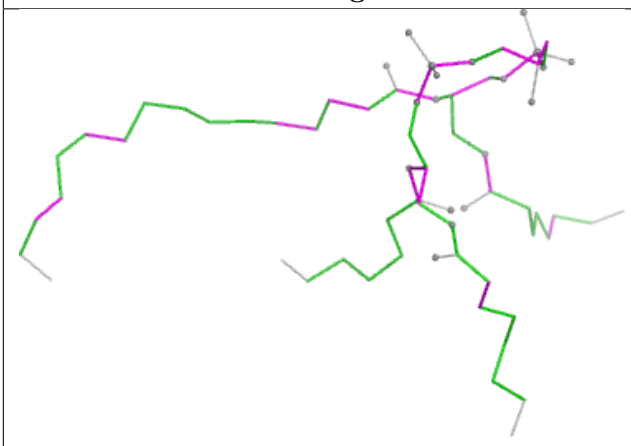
Ligand CDL D 402



Bond lengths



Bond angles

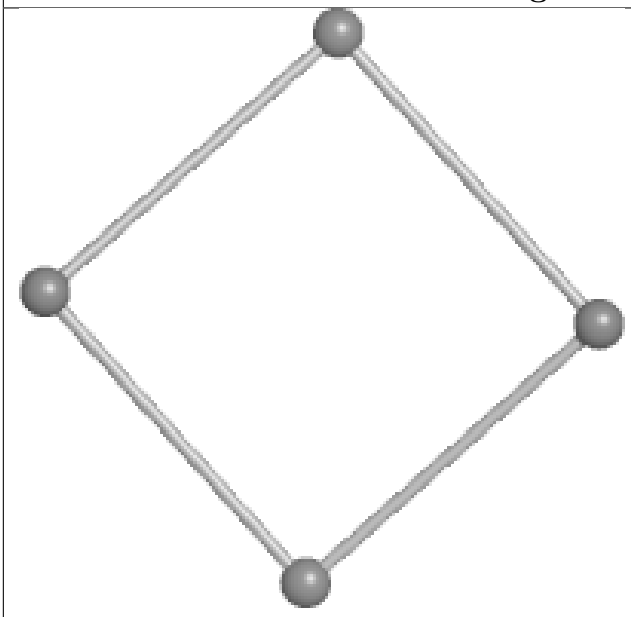


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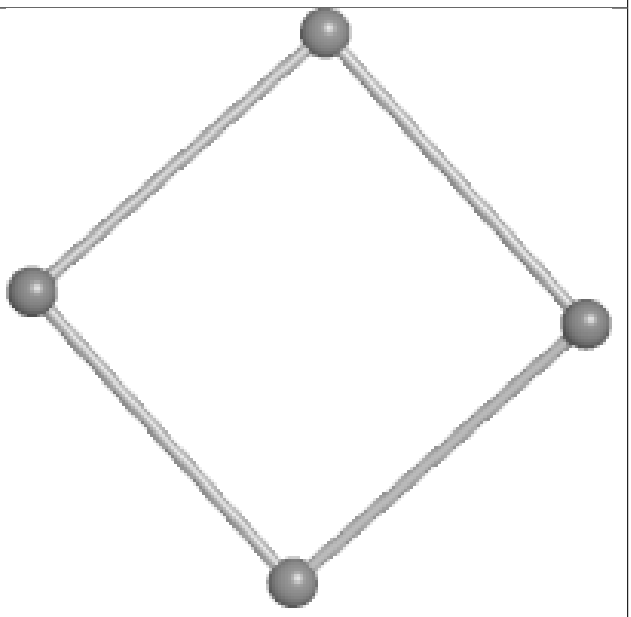


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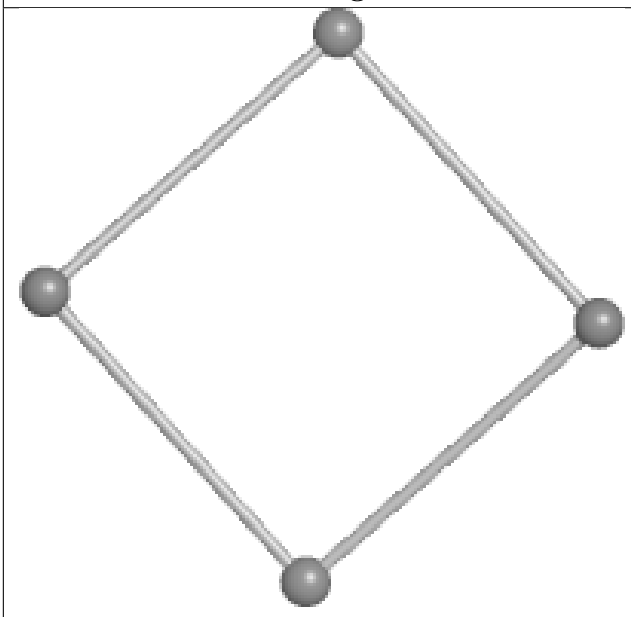
Ligand FES E 301



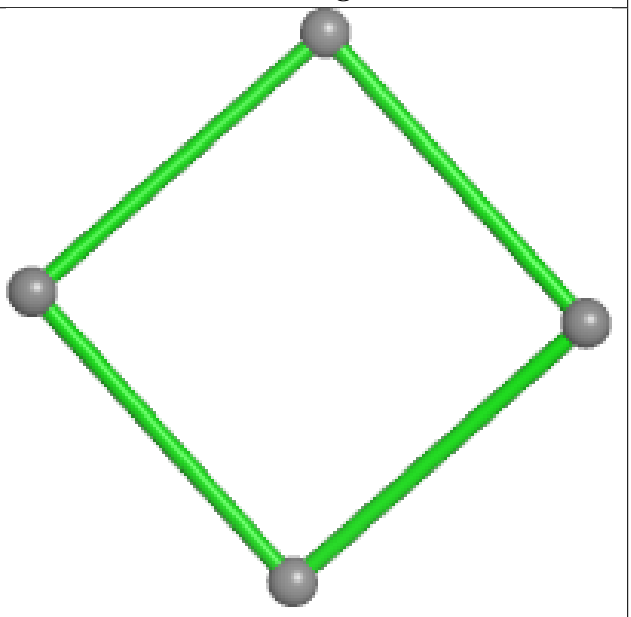
Bond lengths



Bond angles

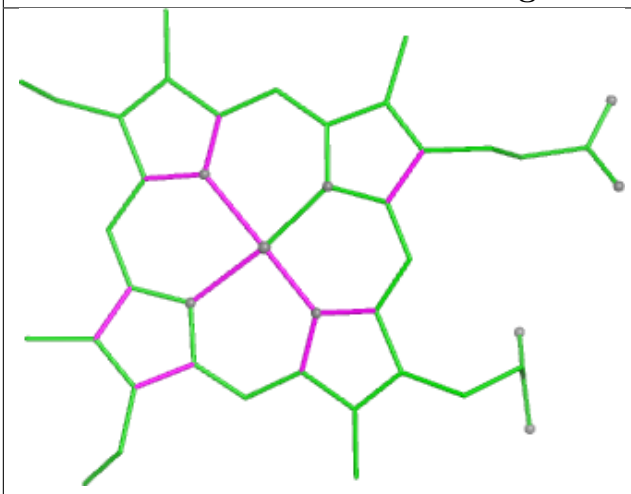


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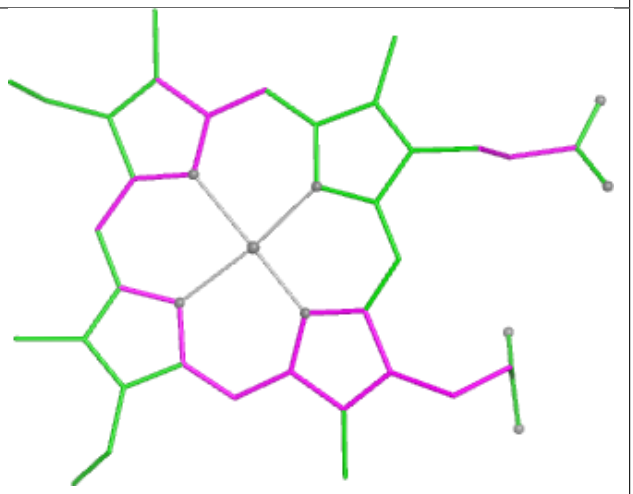


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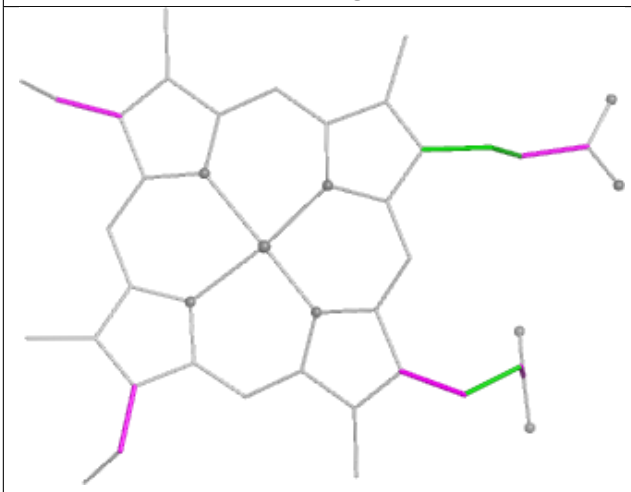
Ligand HEM C 601



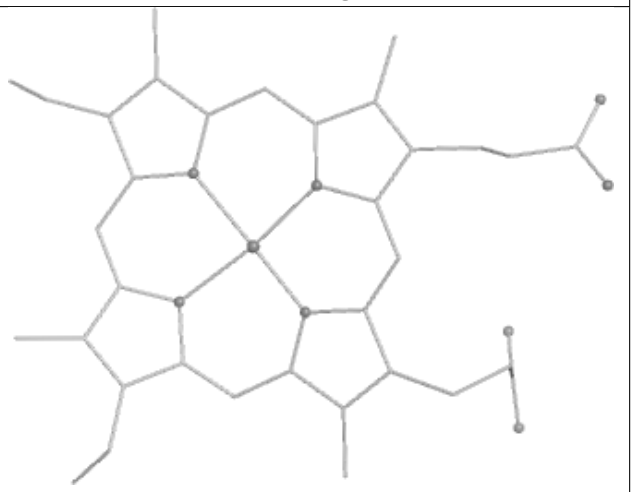
Bond lengths



Bond angles

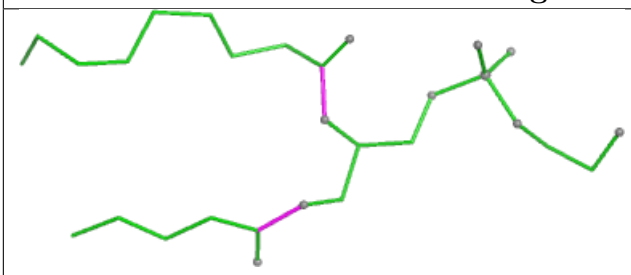


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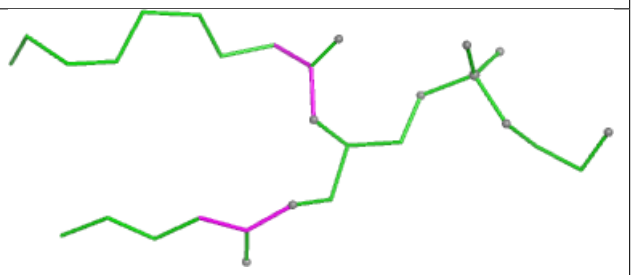


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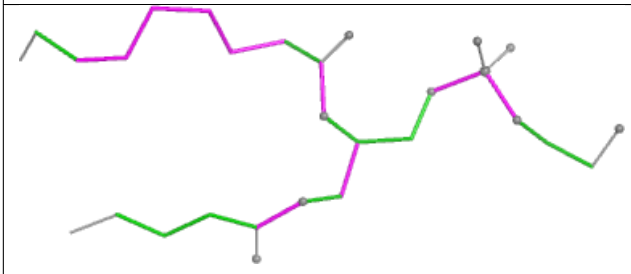
Ligand PEF J 101



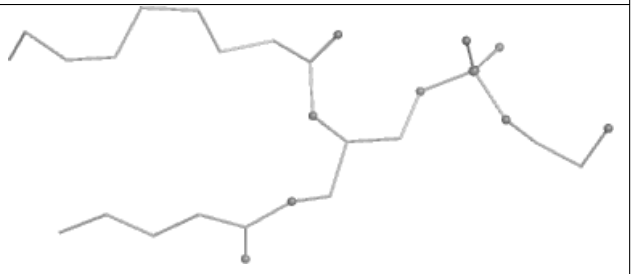
Bond lengths



Bond angles

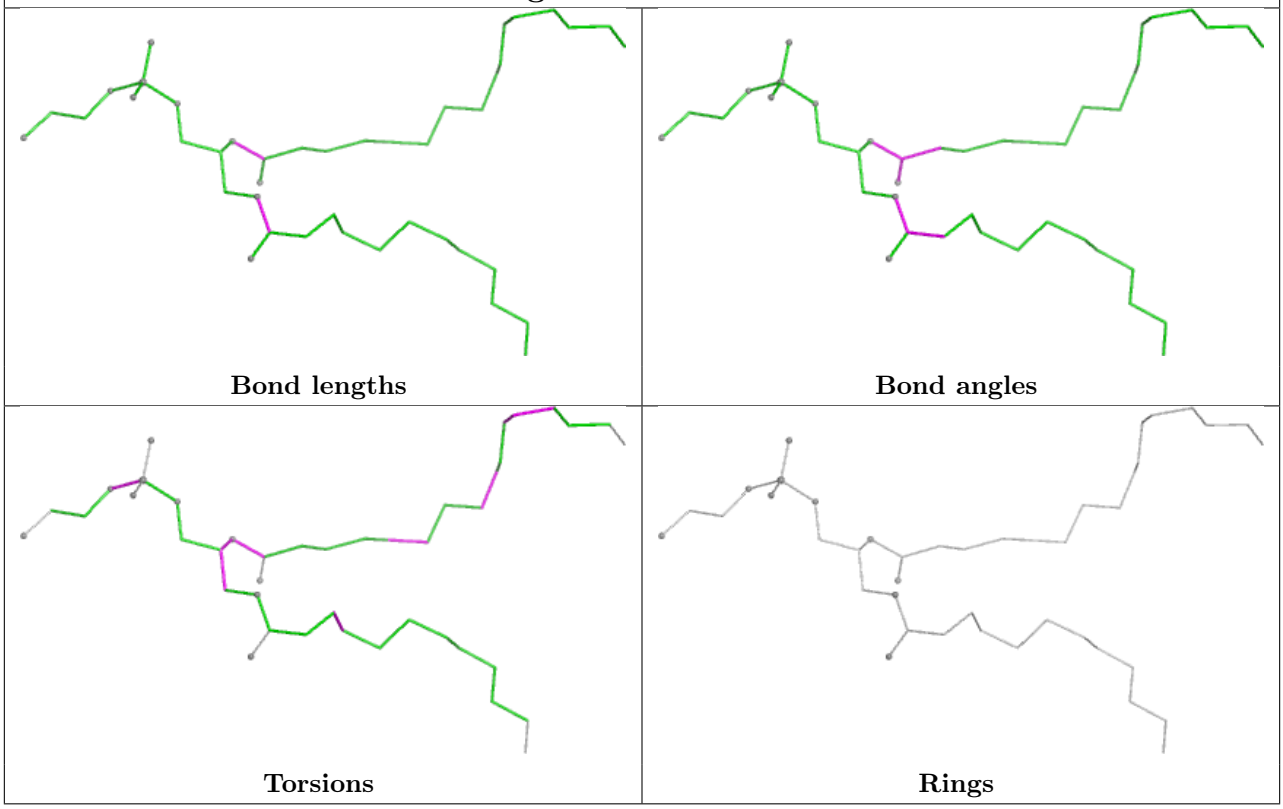


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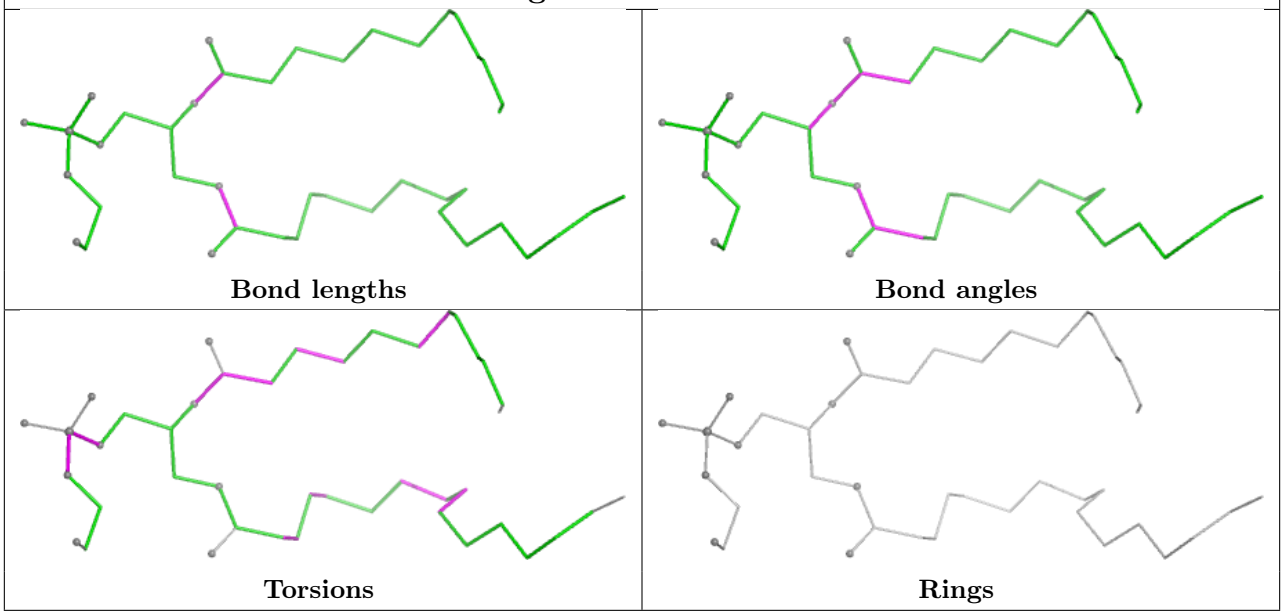


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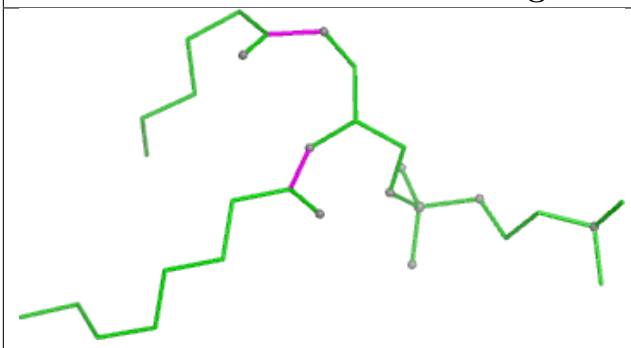
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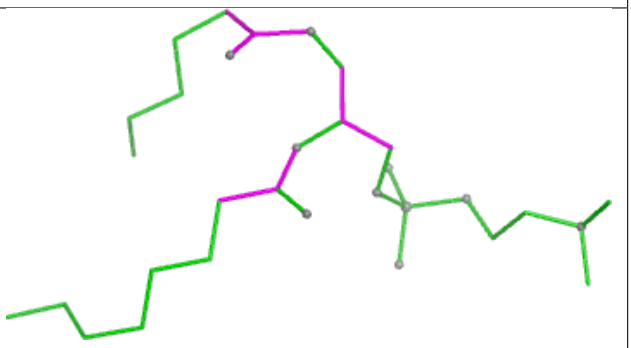
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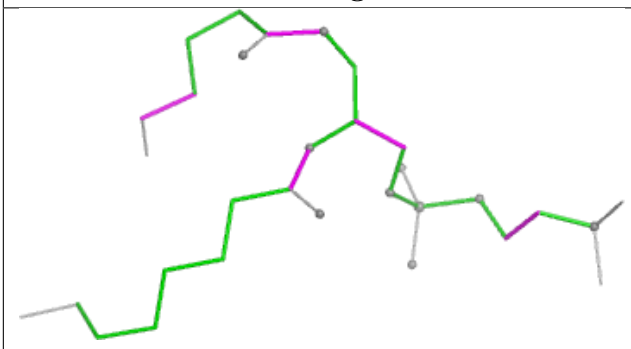
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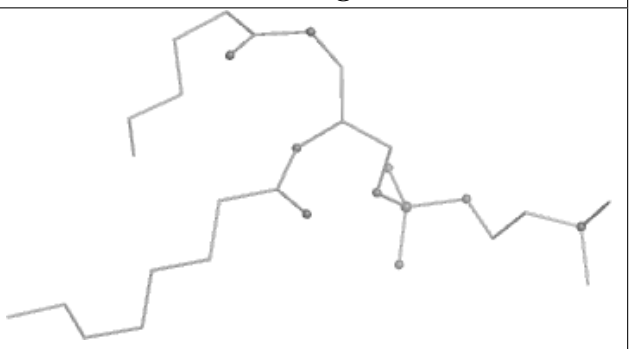
Bond lengths



Bond angles

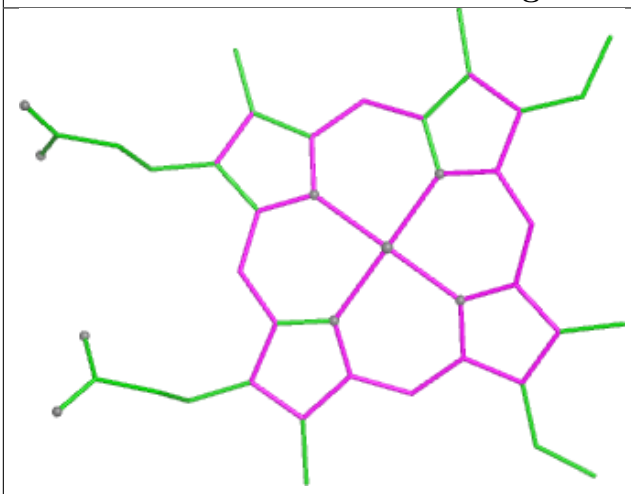


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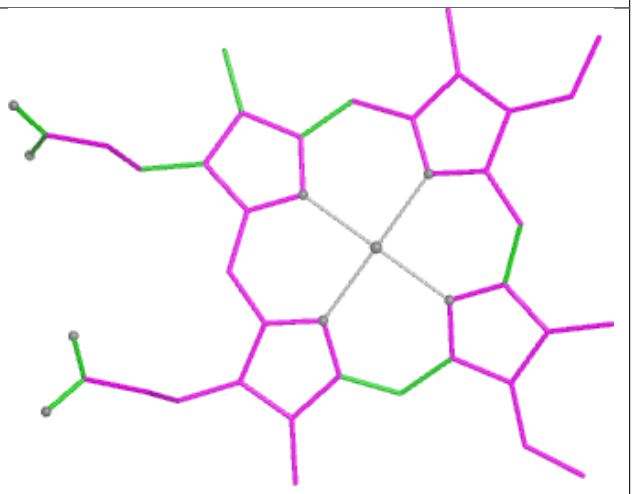


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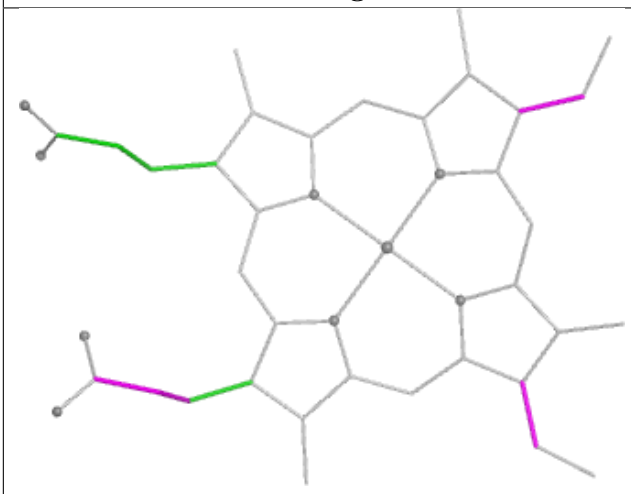
Ligand HEC O 401



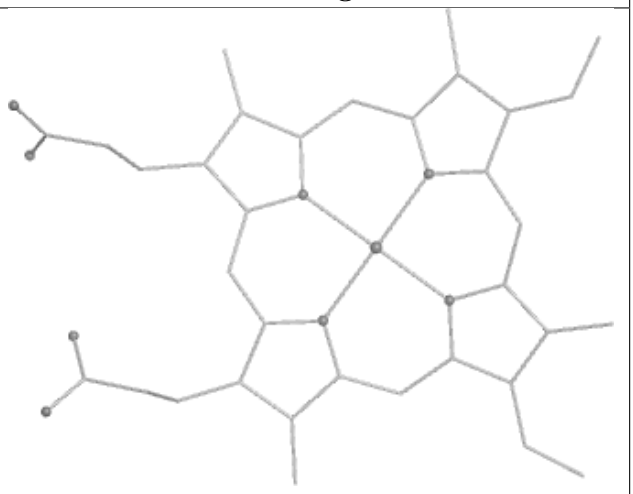
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Bond angles

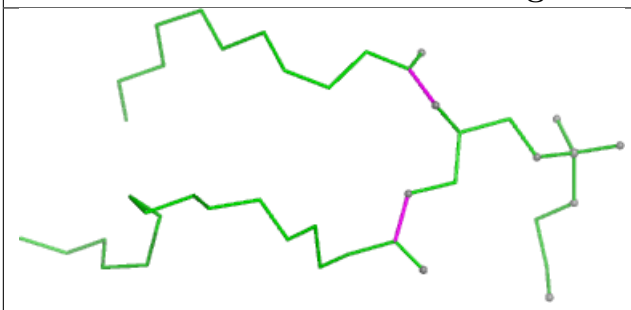


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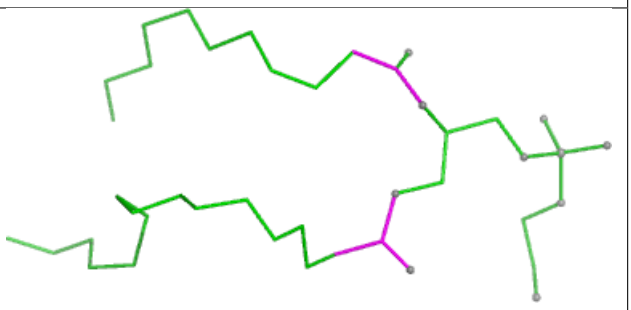


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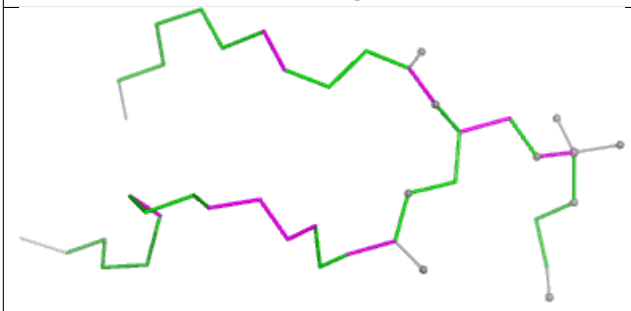
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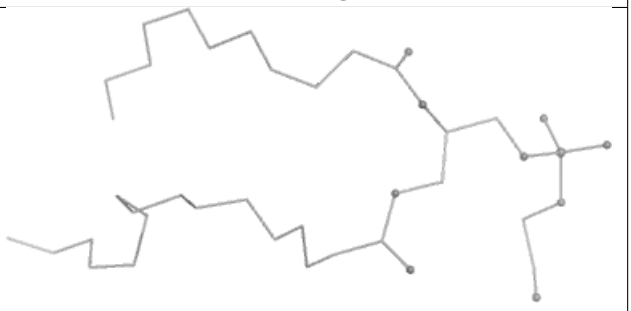
Bond lengths



Bond angles

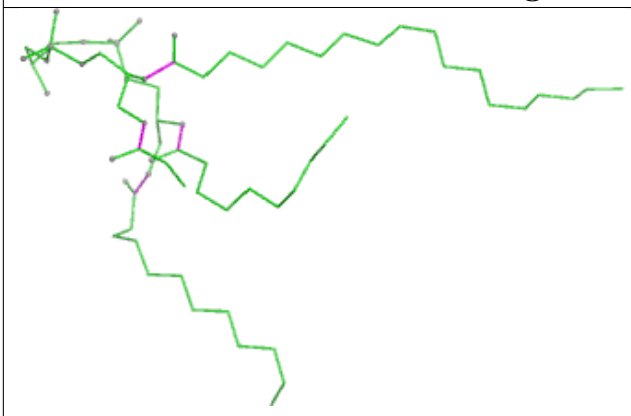


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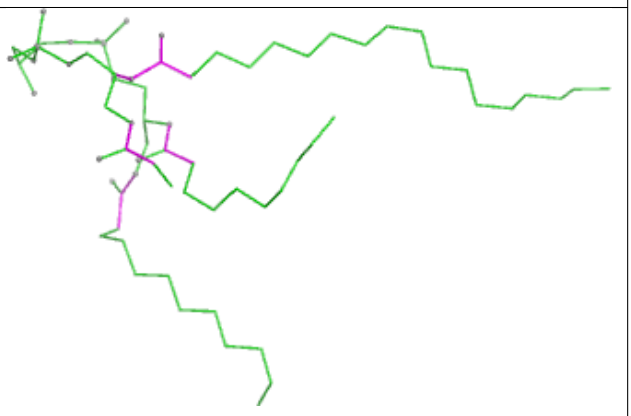


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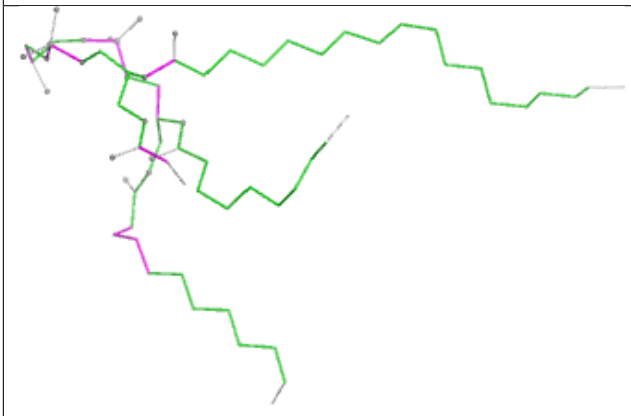
Ligand CDL O 402



Bond lengths



Bond angles

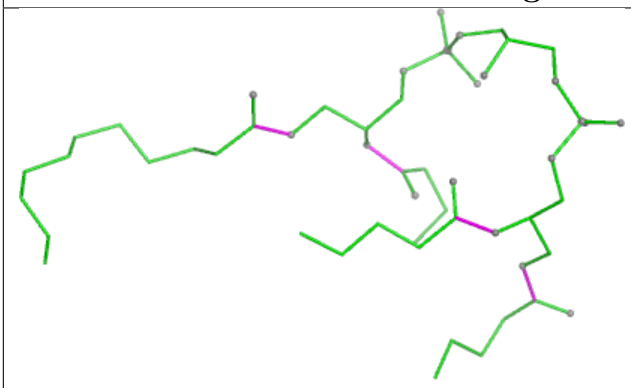


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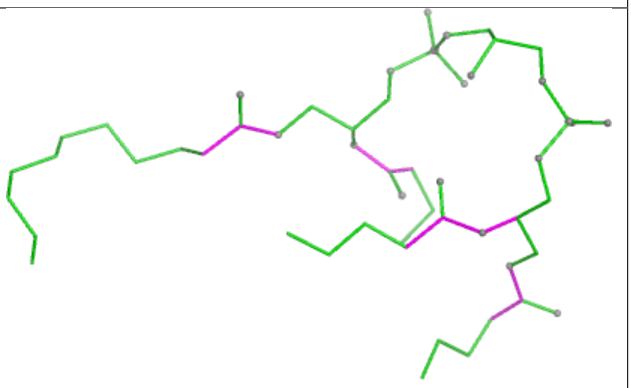


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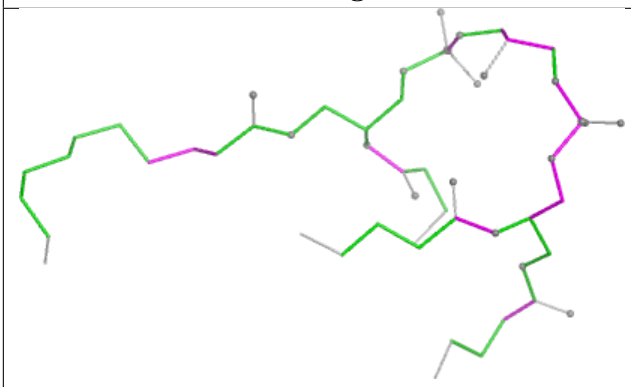
Ligand CDL H 601



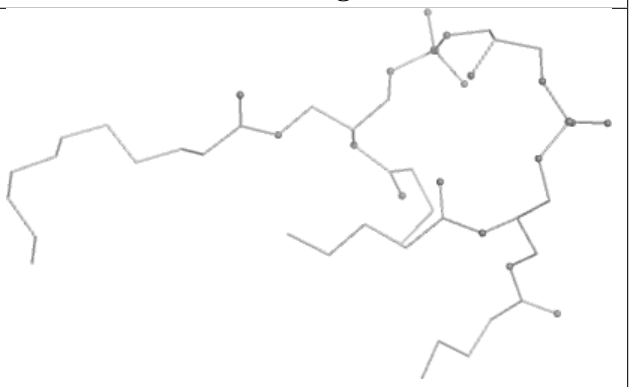
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Bond angles

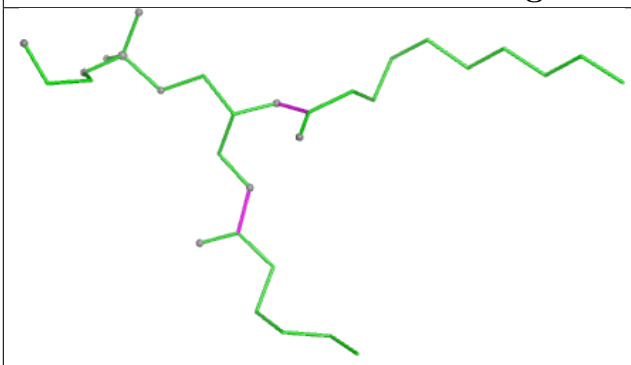


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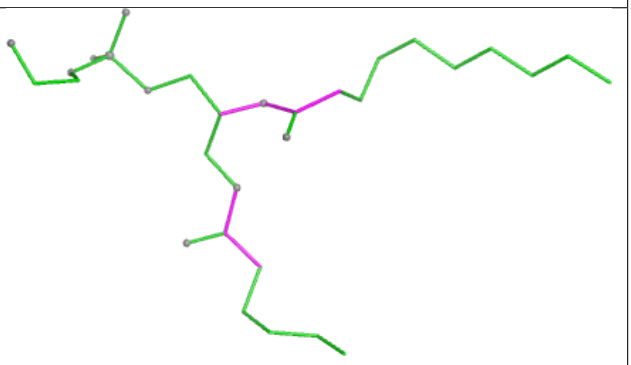


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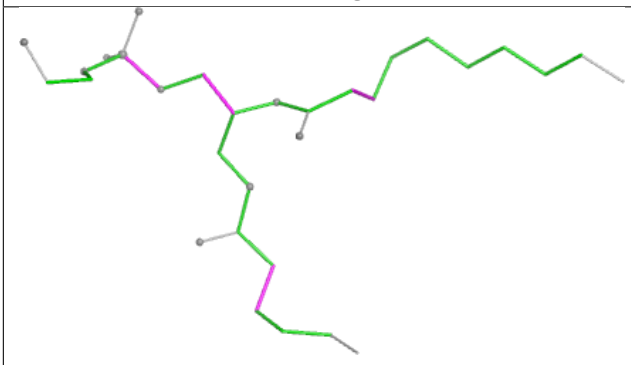
Ligand PEF A 501



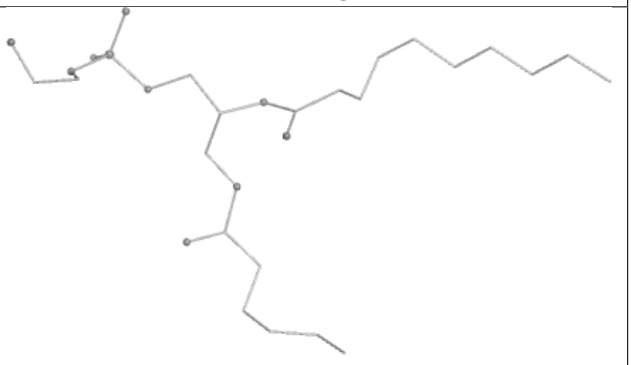
Bond lengths



Bond angles

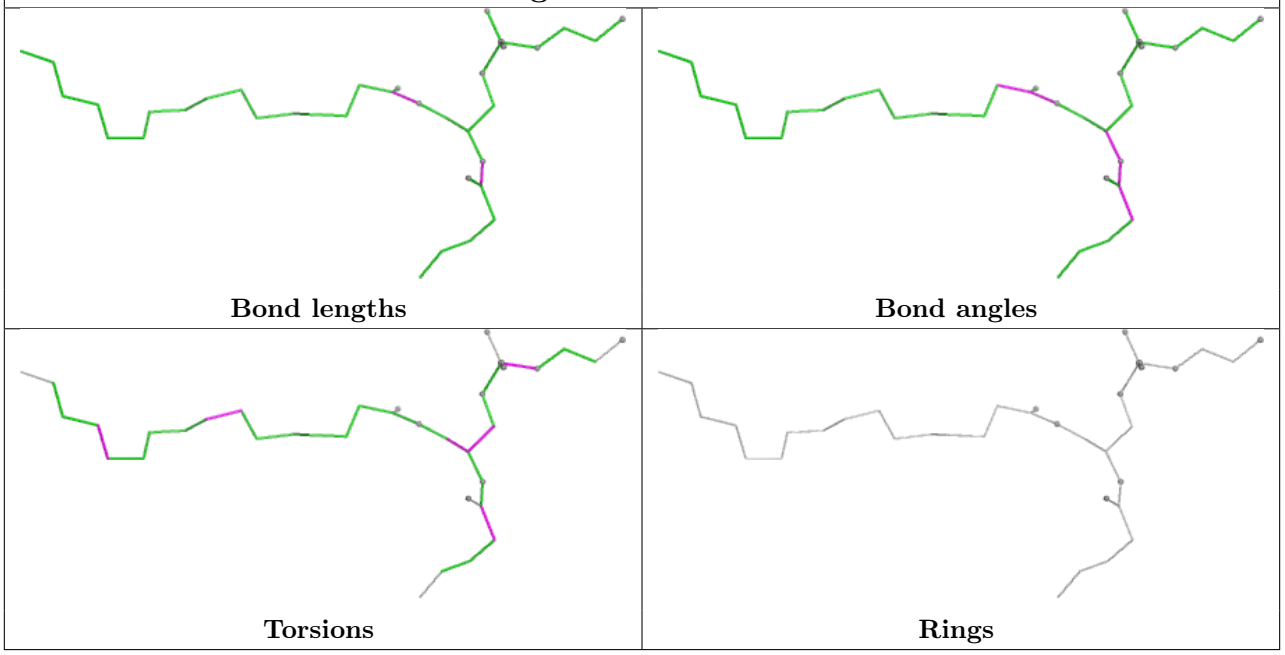


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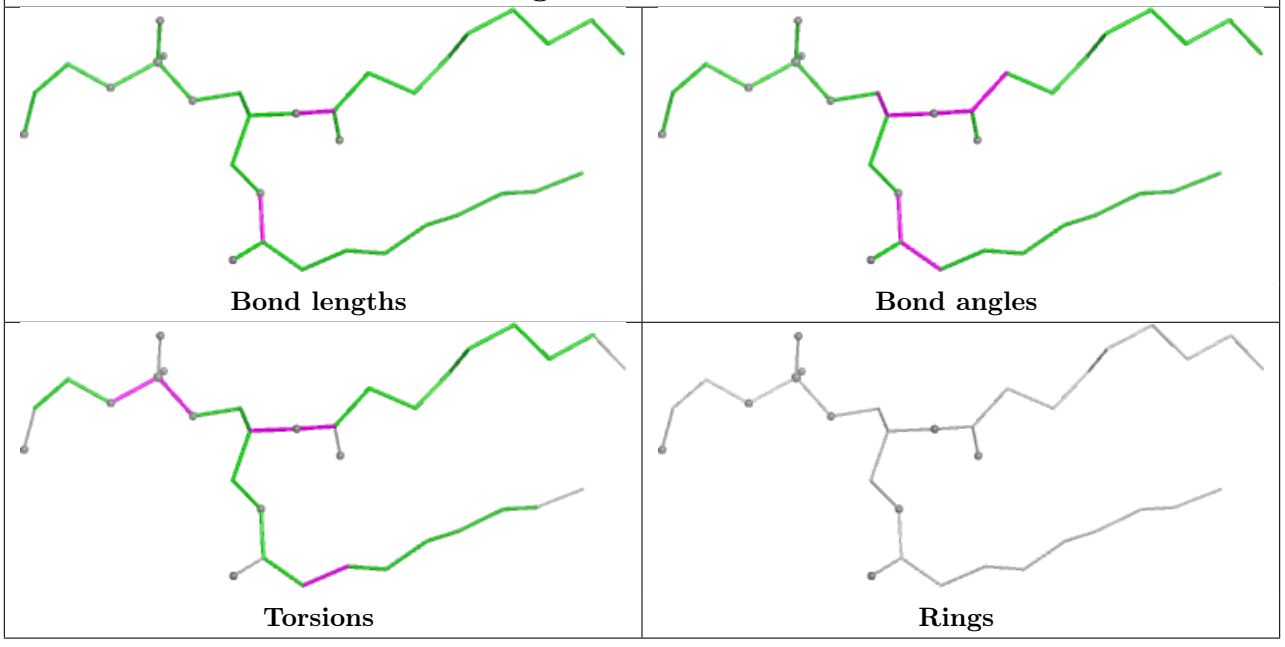


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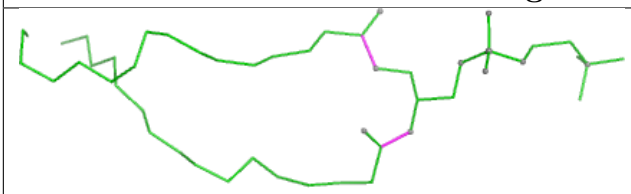
Ligand PEF S 102



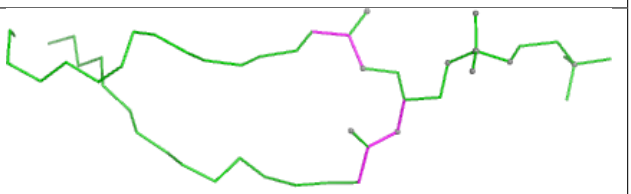
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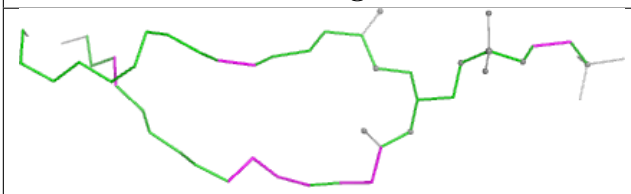
Ligand PCF T 101



Bond lengths



Bond angles

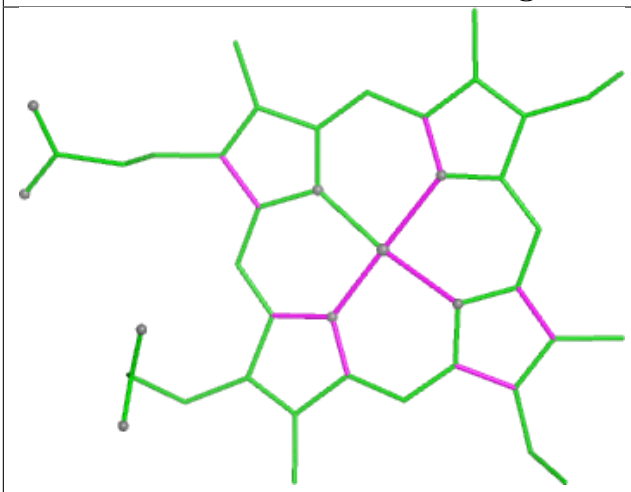


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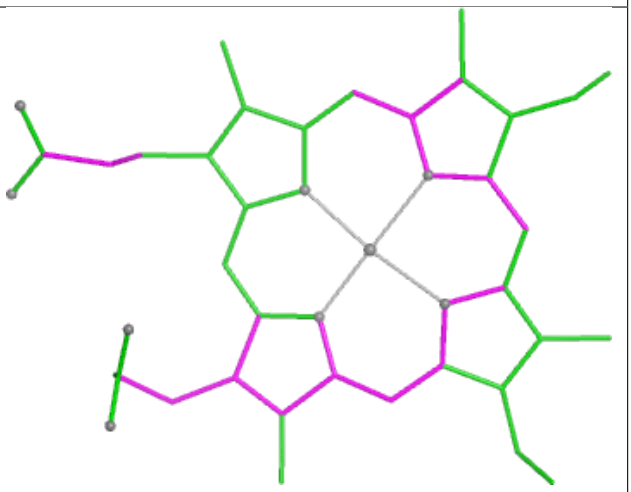


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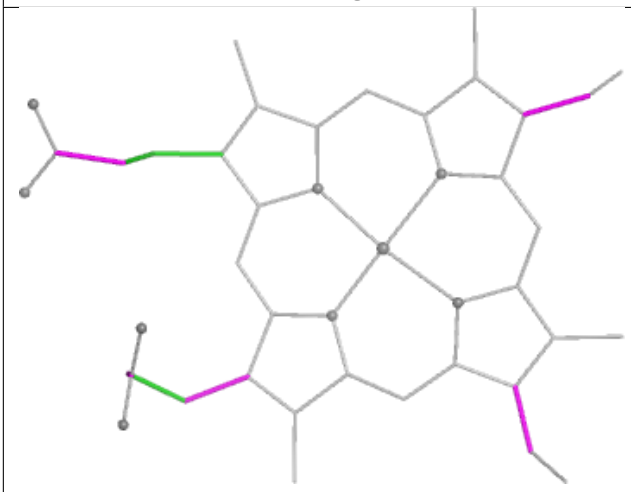
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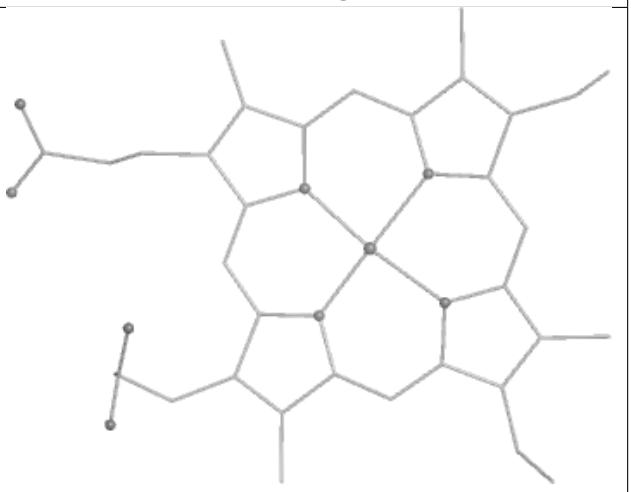
Bond lengths



Bond angles

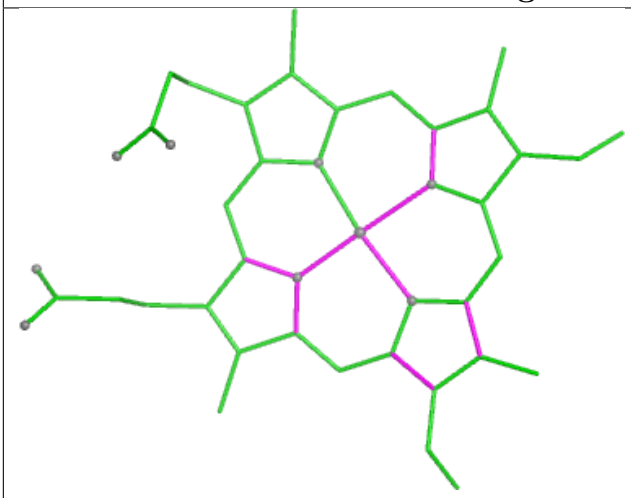


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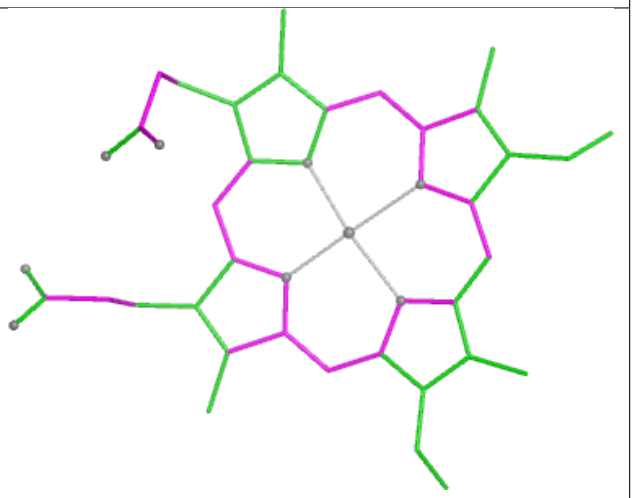


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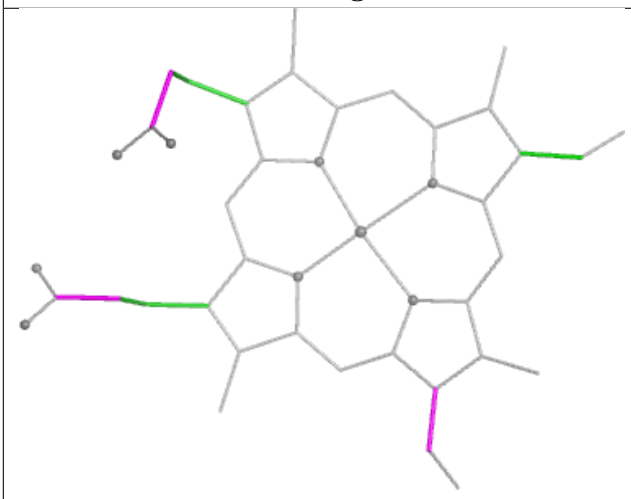
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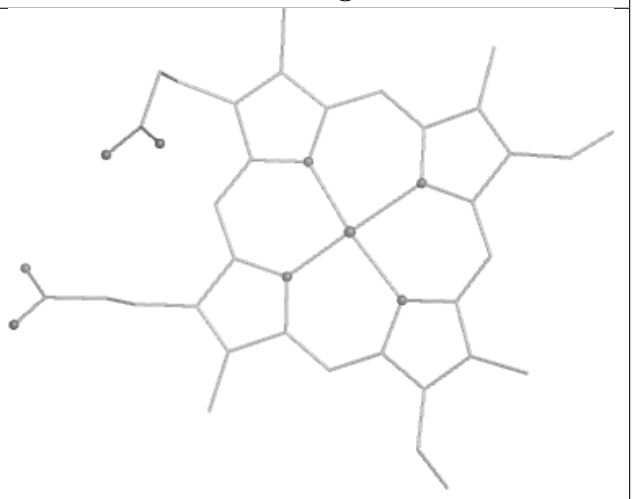
Bond lengths



Bond angles

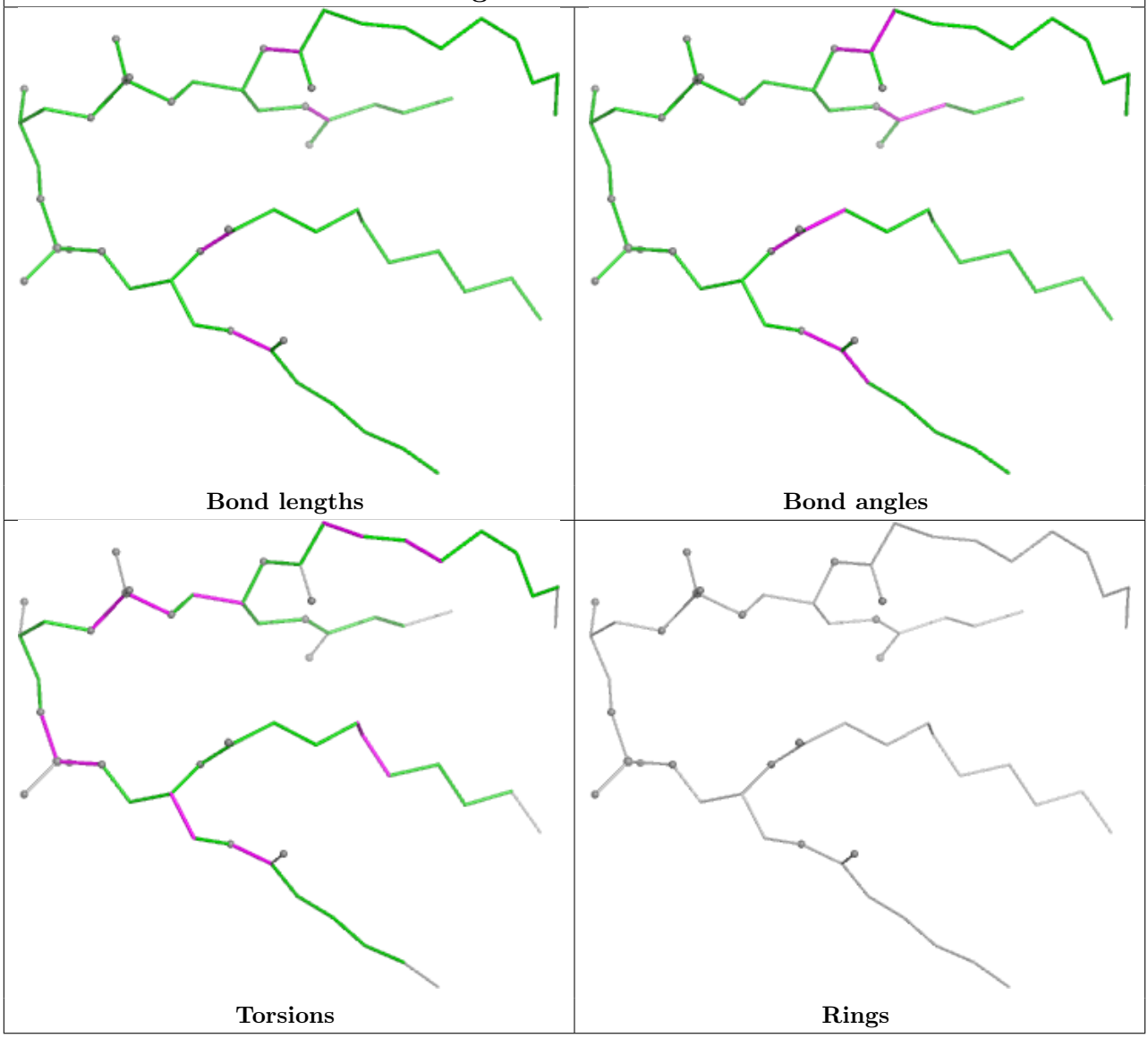


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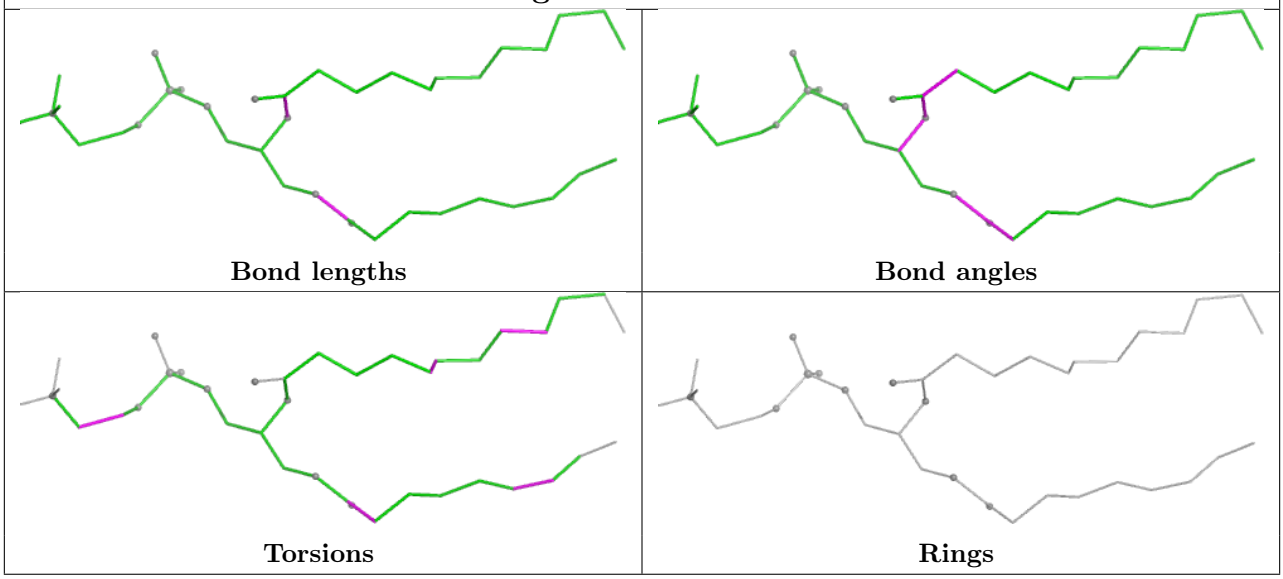


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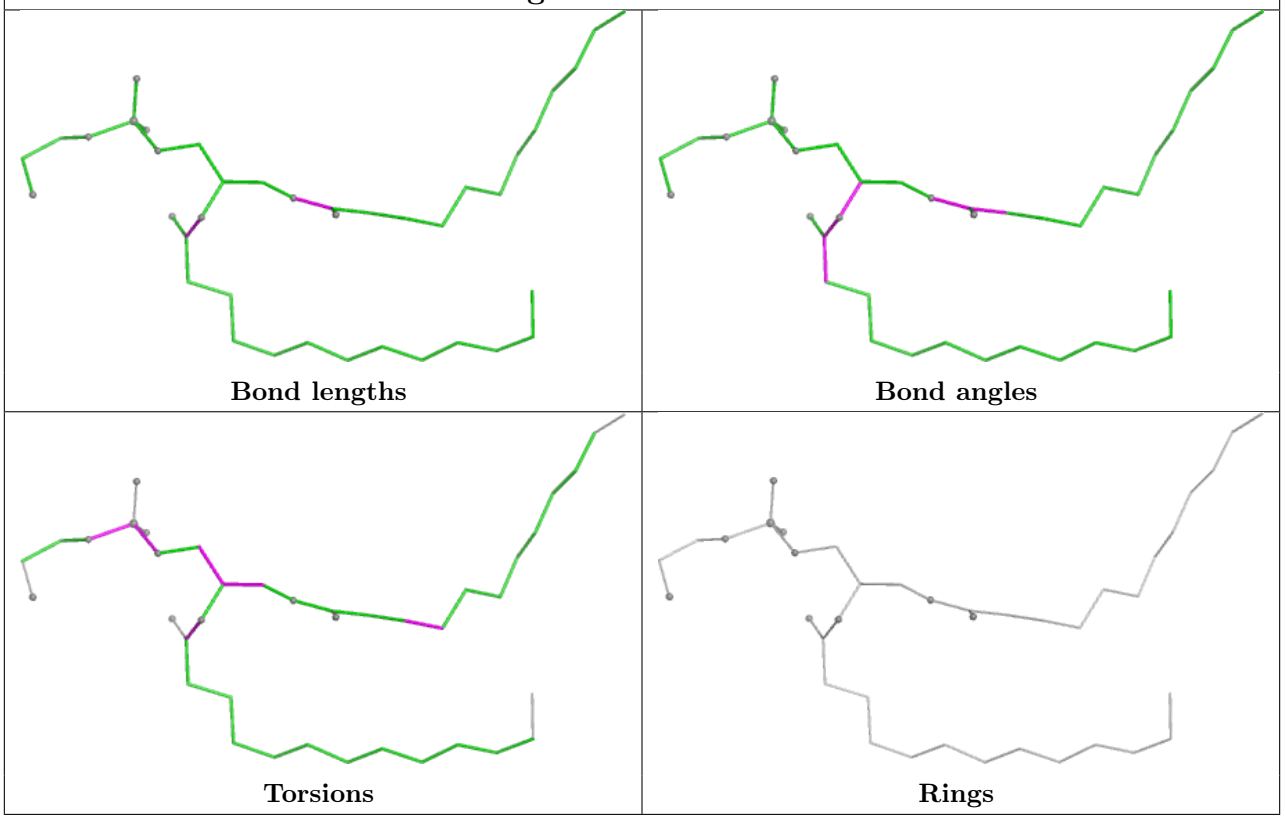
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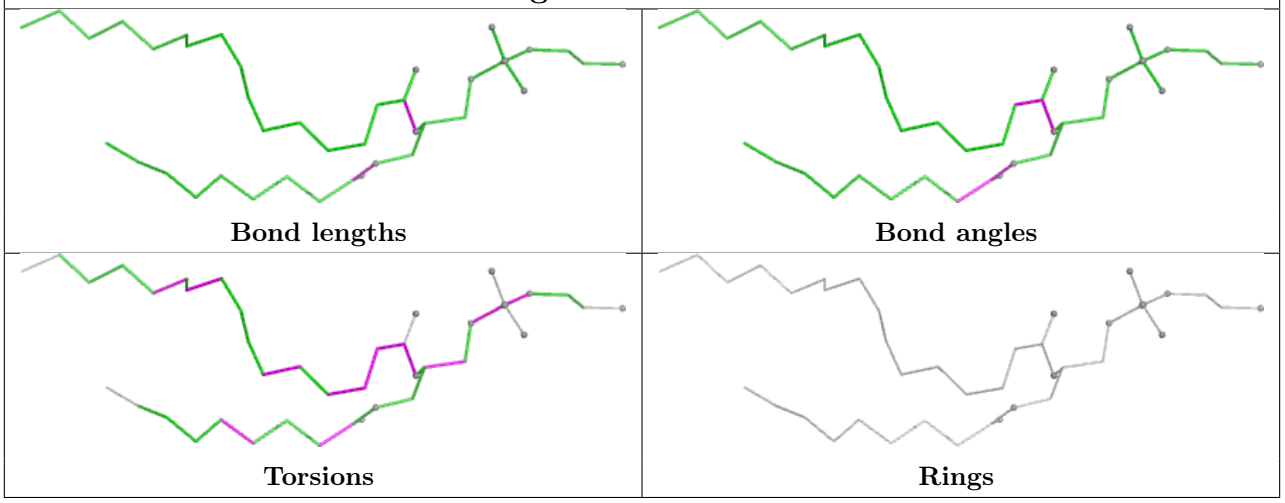
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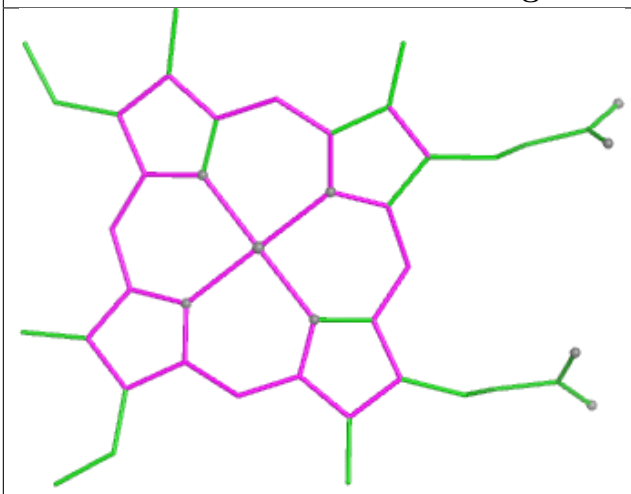
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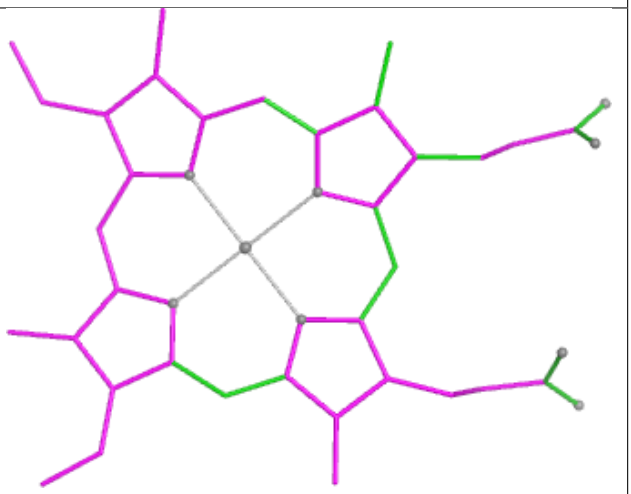
Ligand PEF b 302



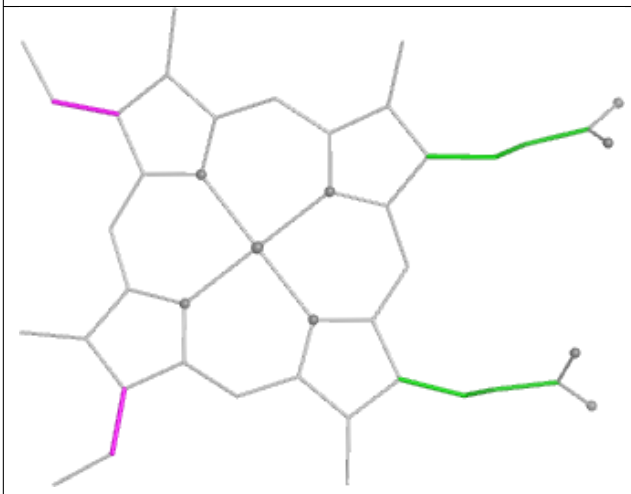
Ligand HEC D 401



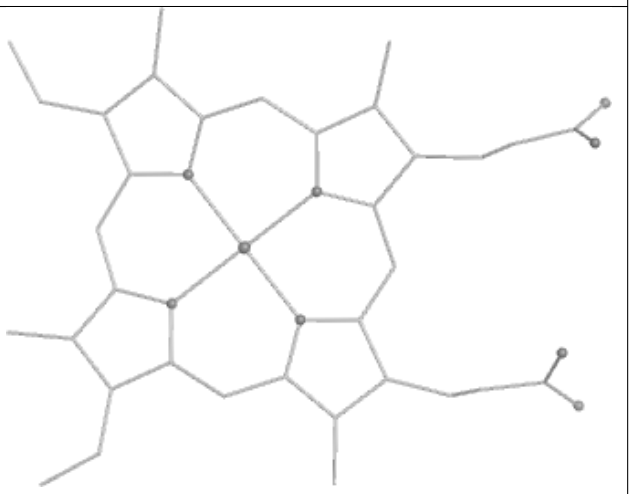
Bond lengths



Bond angles

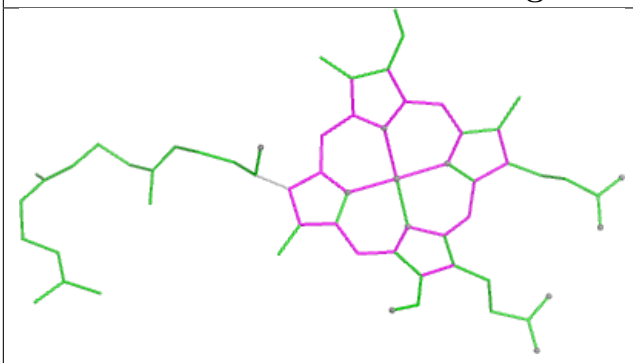


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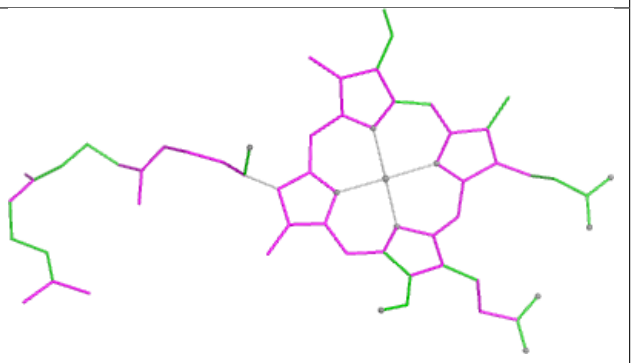


Rings

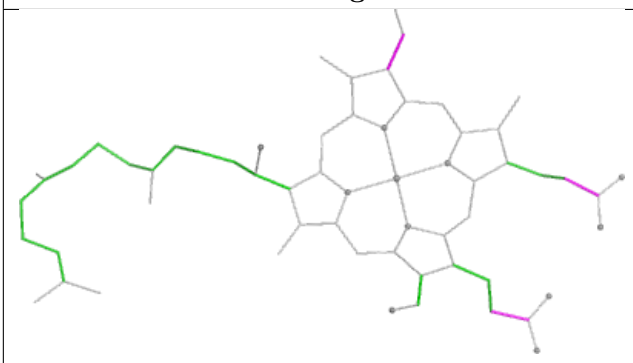
Ligand HEA a 603



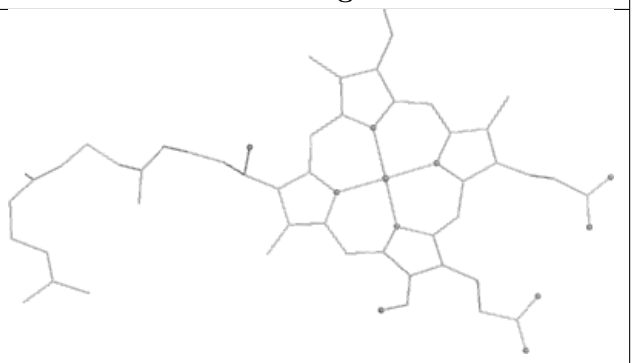
Bond lengths



Bond angles

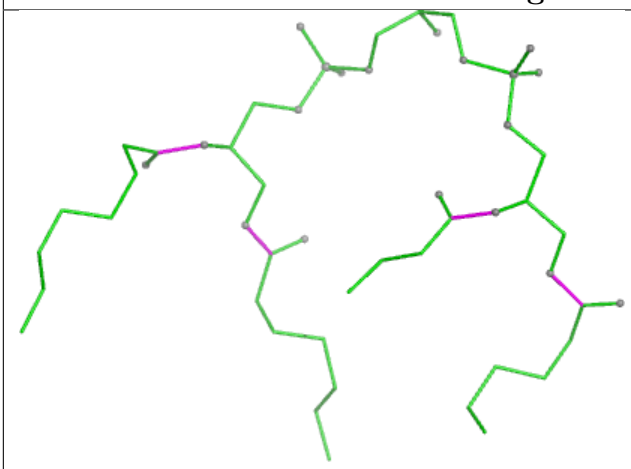


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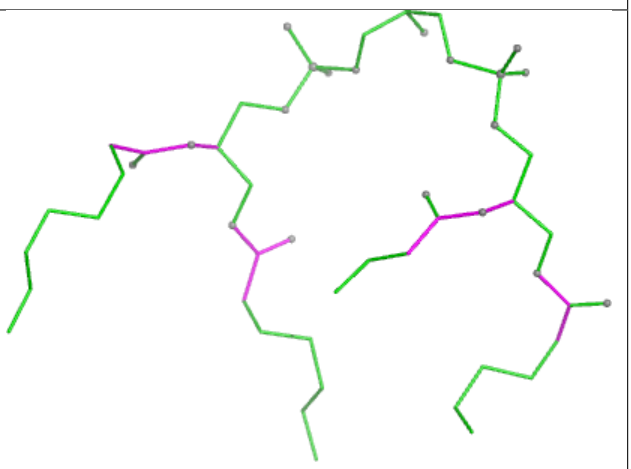


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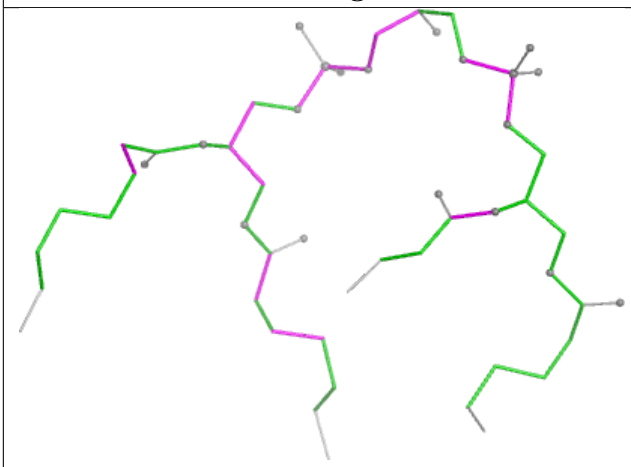
Ligand CDL S 101



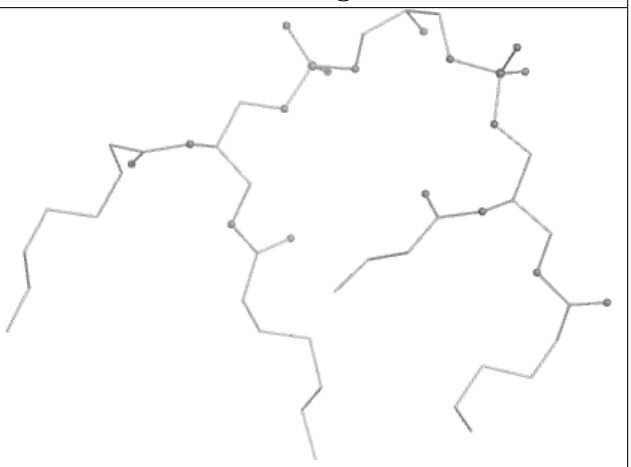
Bond lengths



Bond angles

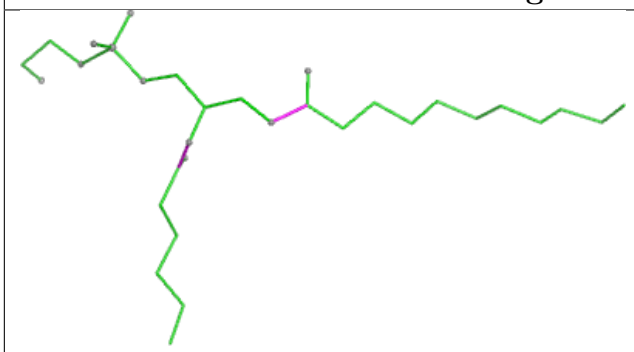


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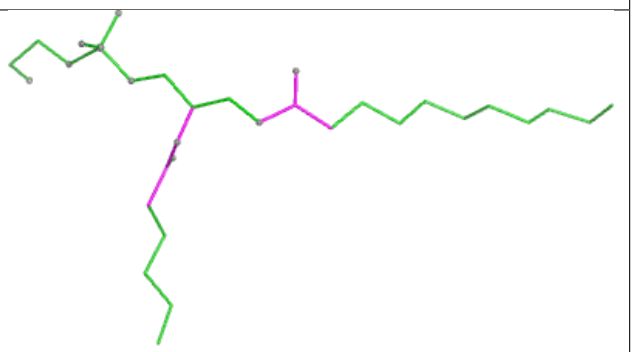


Rings

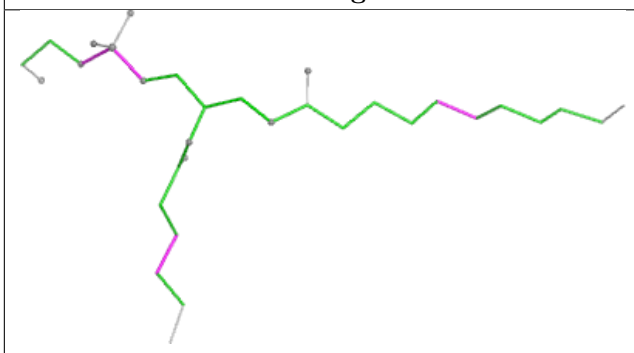
Ligand PEF H 602



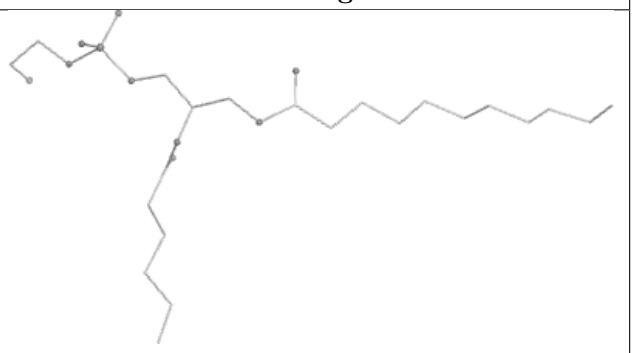
Bond lengths



Bond angles

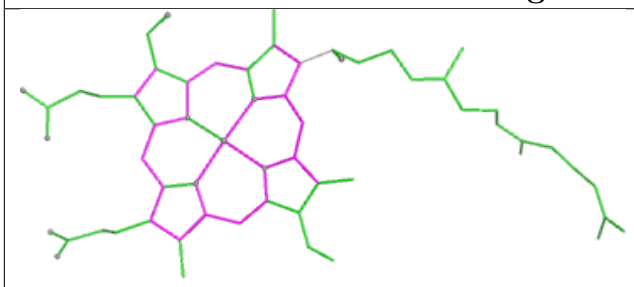


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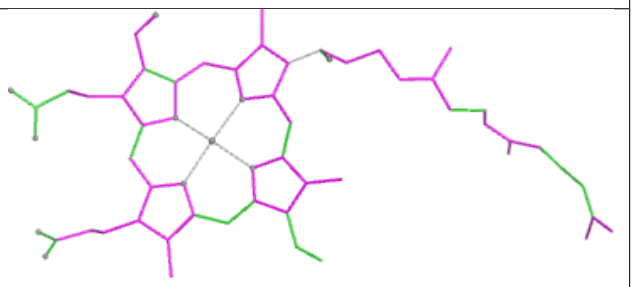


Rings

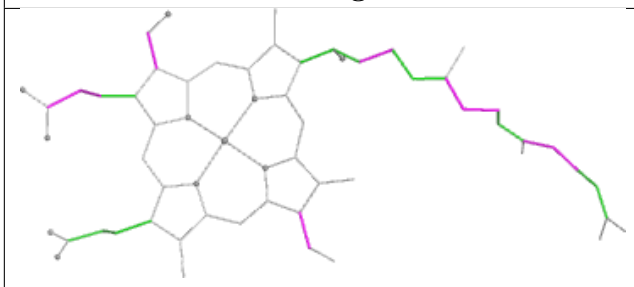
Ligand HEA a 602



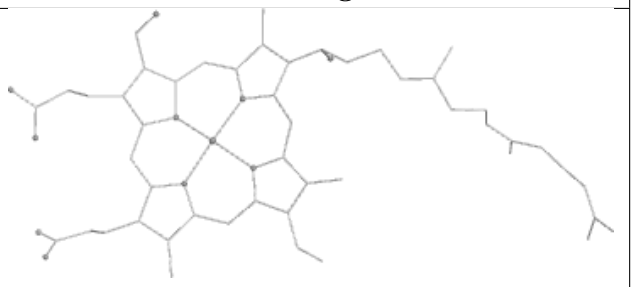
Bond lengths



Bond angles

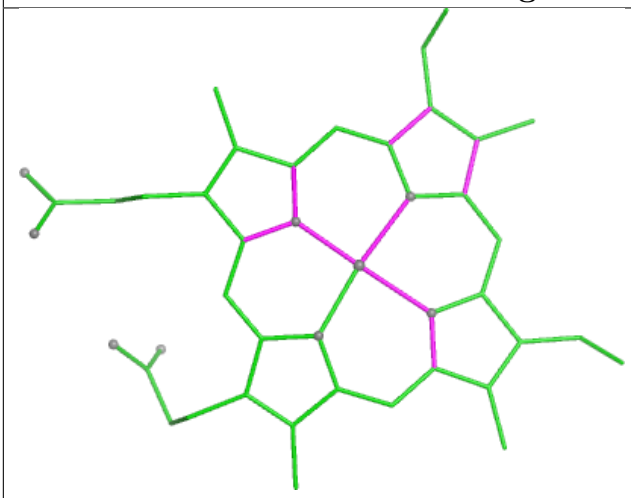


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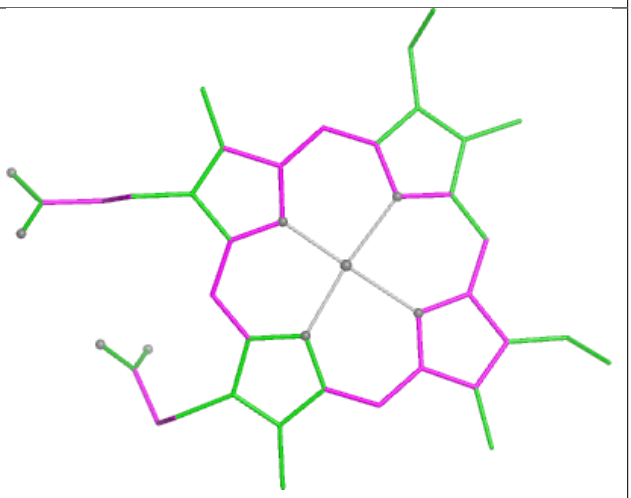


Rings

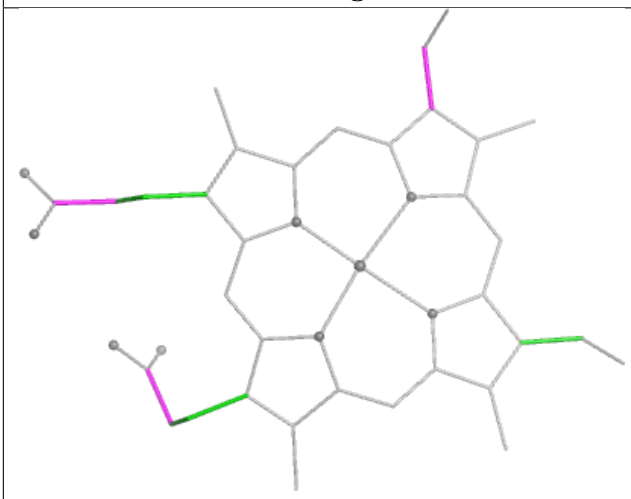
Ligand HEM C 602



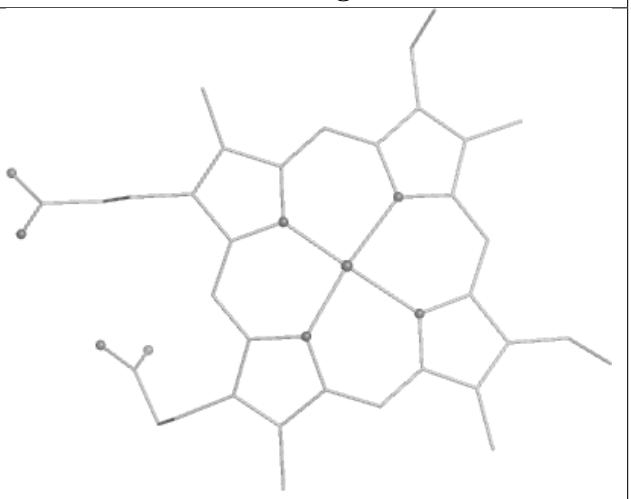
Bond lengths



Bond angles

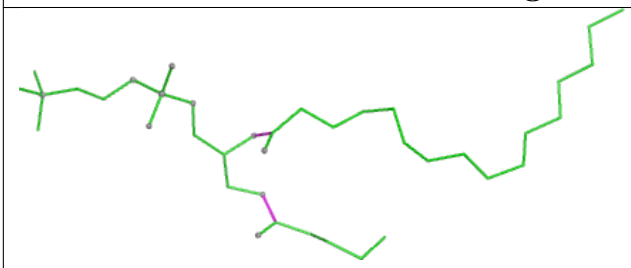


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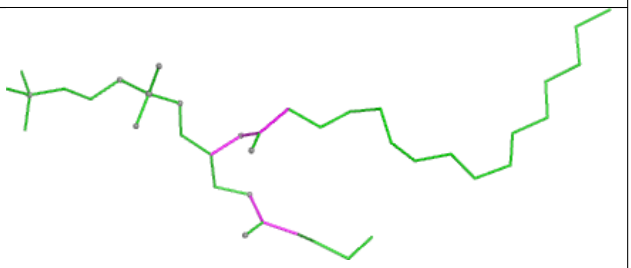


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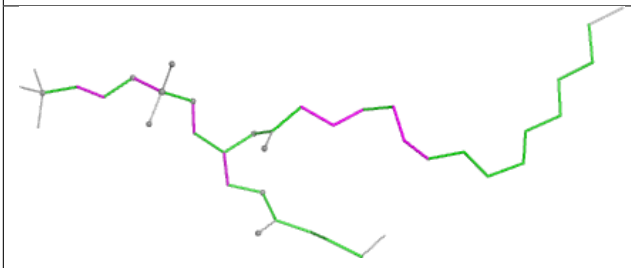
Ligand PCF N 606



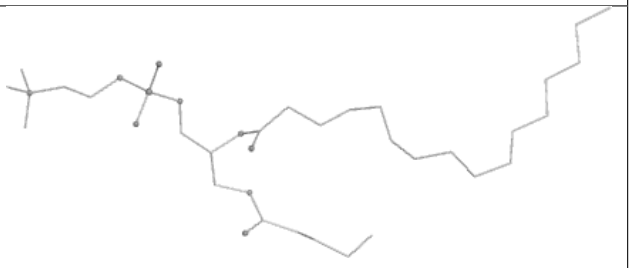
Bond lengths



Bond angles

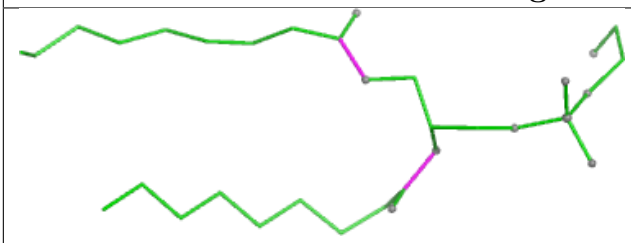


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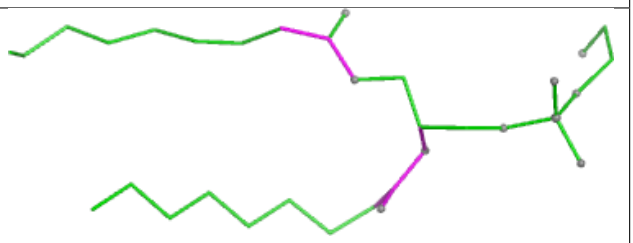


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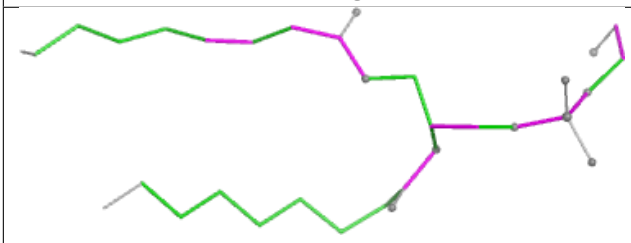
Ligand PEF b 303



Bond lengths



Bond angles

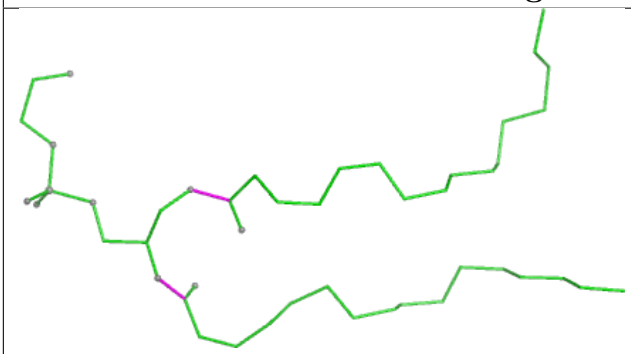


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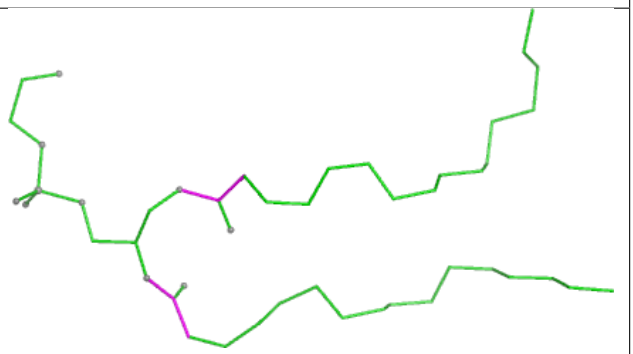


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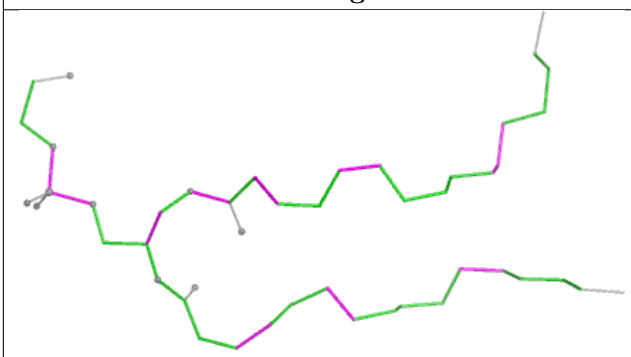
Ligand PEF U 101



Bond lengths



Bond angles

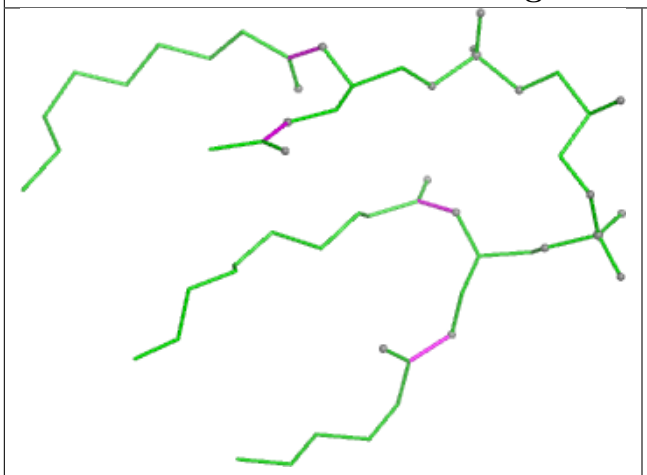


Torsions



Rings

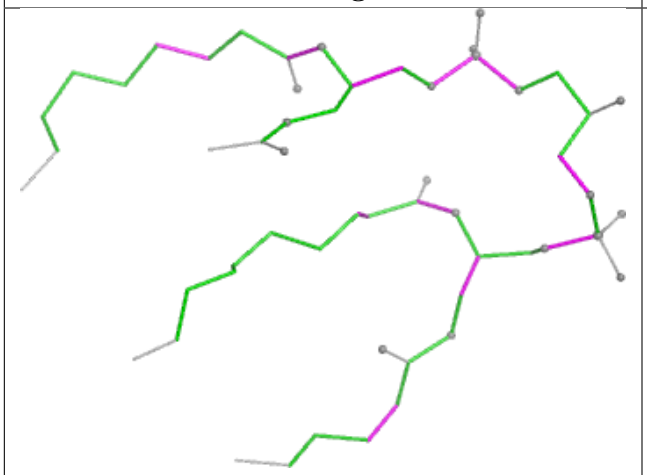
Ligand CDL C 603



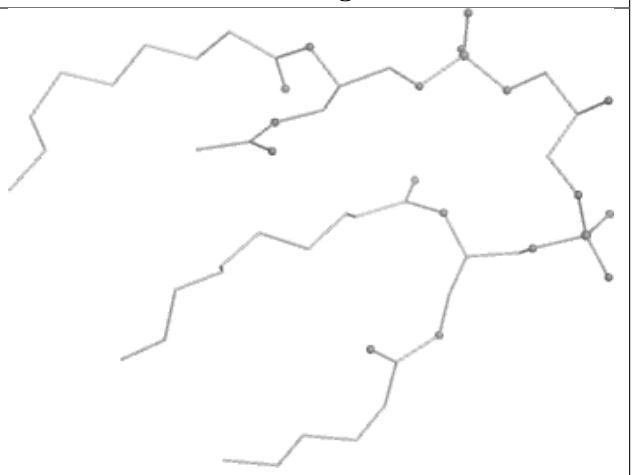
Bond lengths



Bond angles

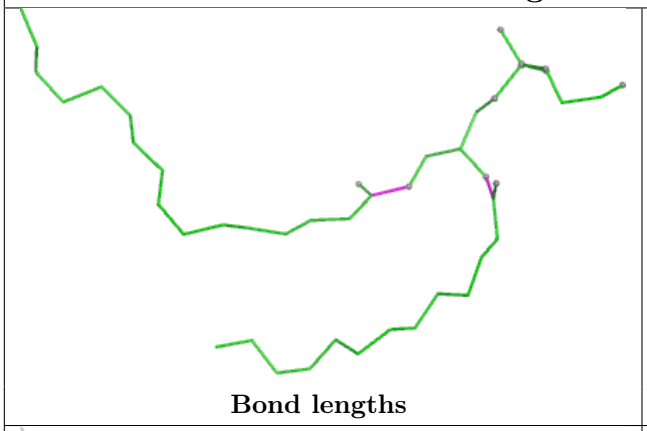


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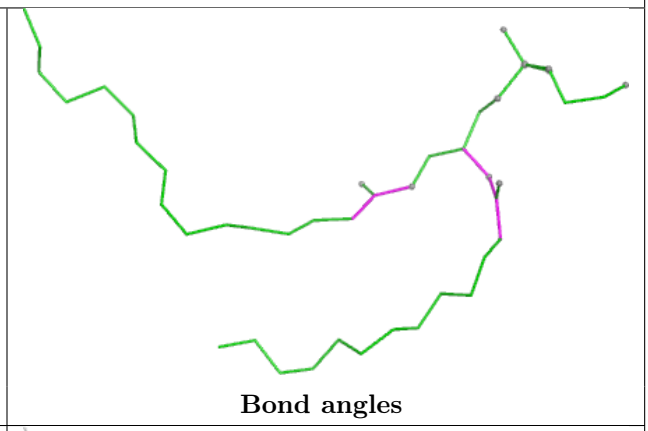


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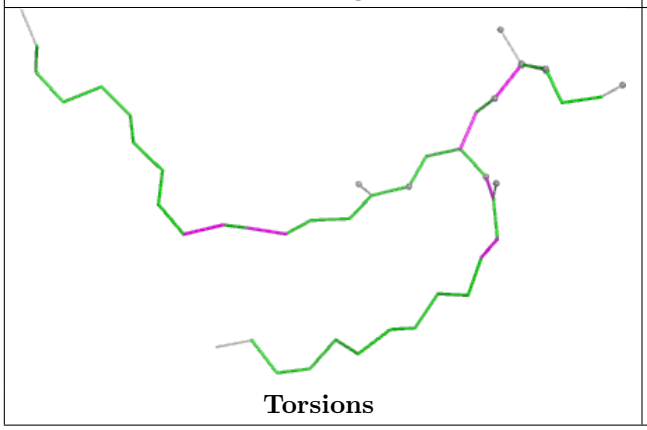
Ligand PEF N 604



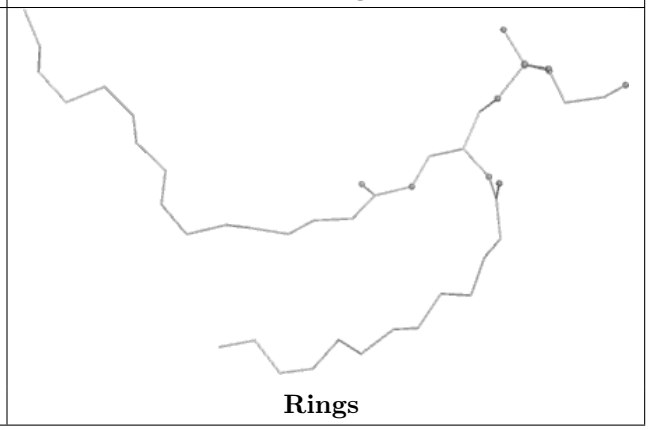
Bond lengths



Bond angles

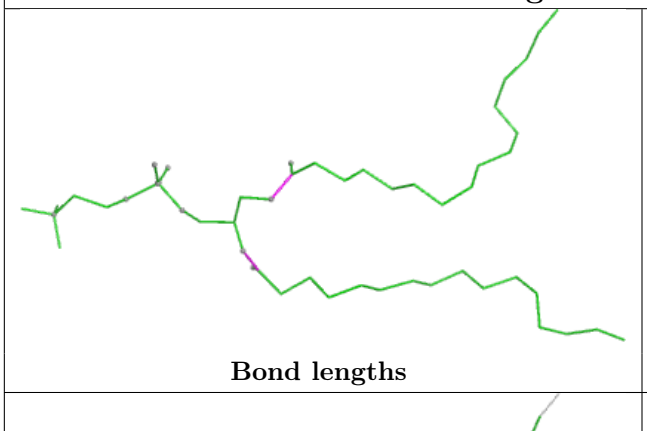


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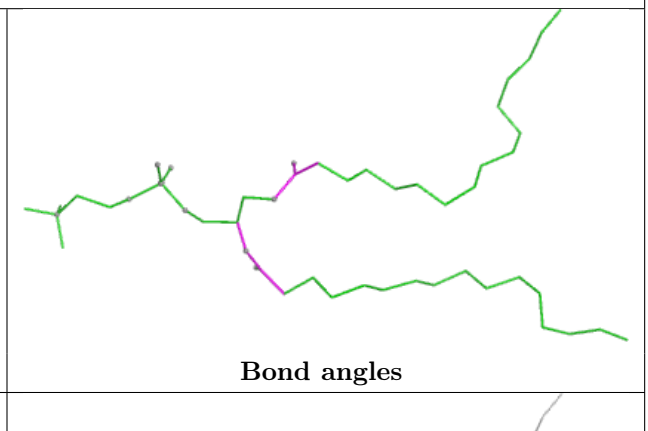


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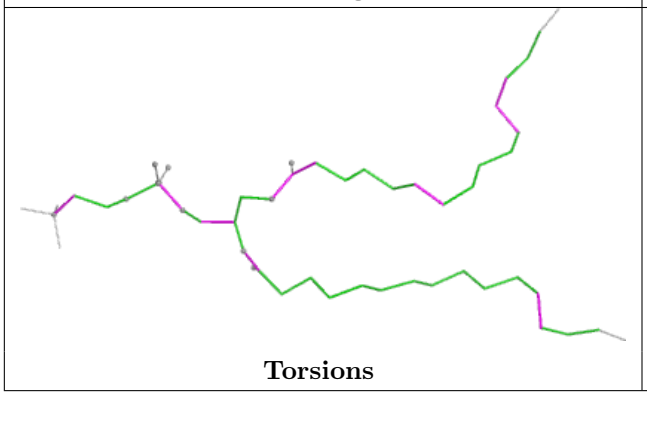
Ligand PCF C 606



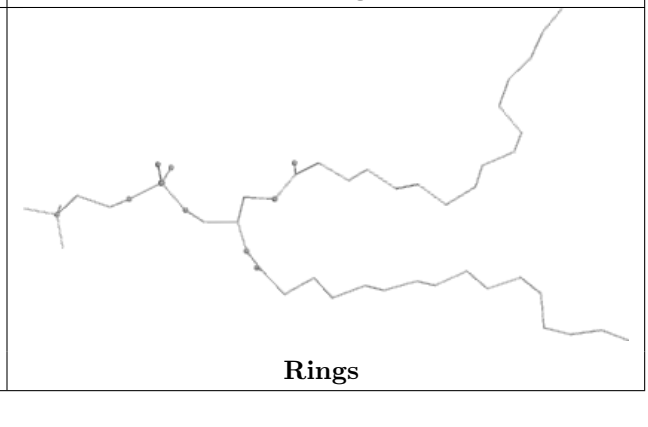
Bond lengths



Bond angles

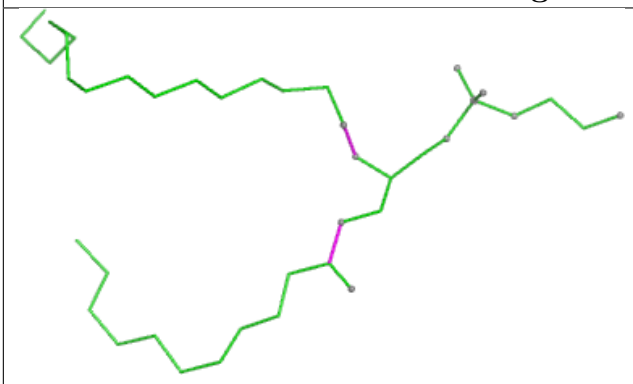


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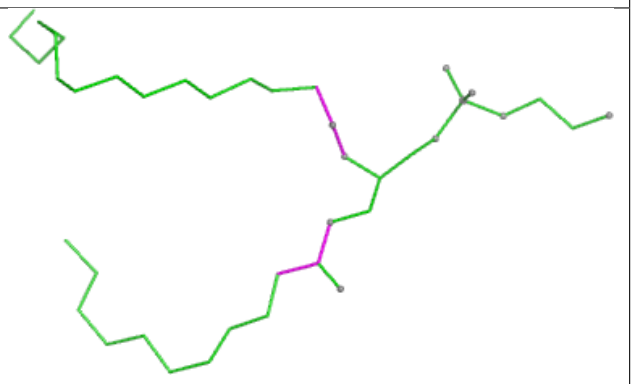


Rings

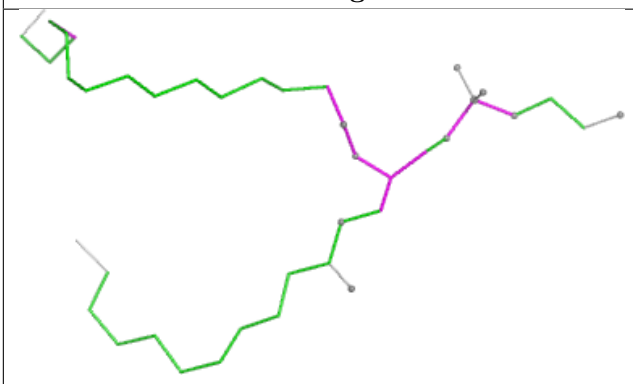
Ligand PEF e 201



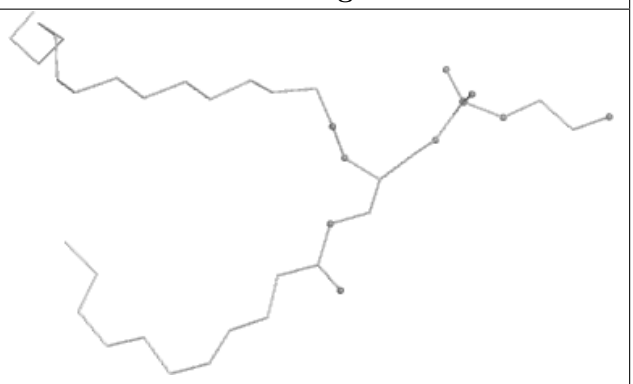
Bond lengths



Bond angles

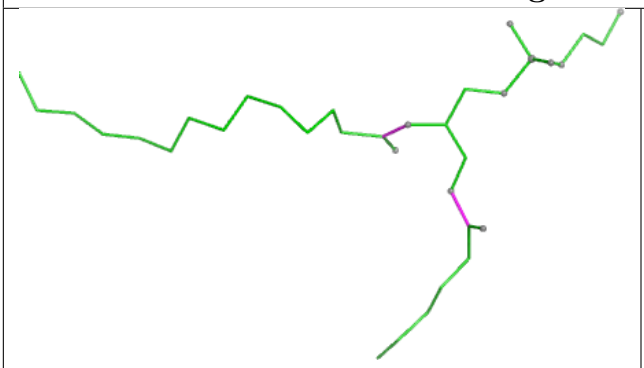


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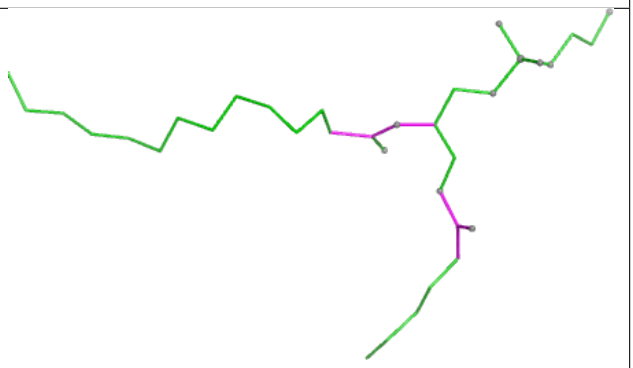


Rings

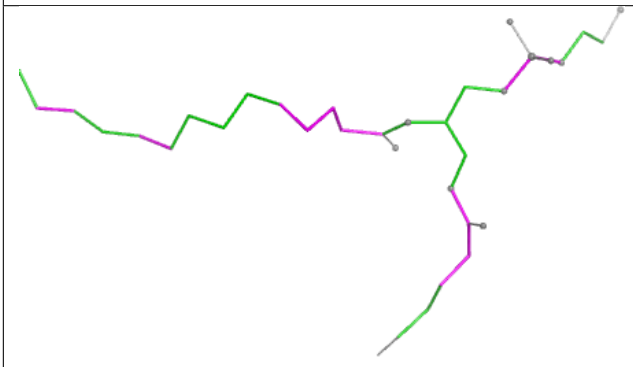
Ligand PEF L 502



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.

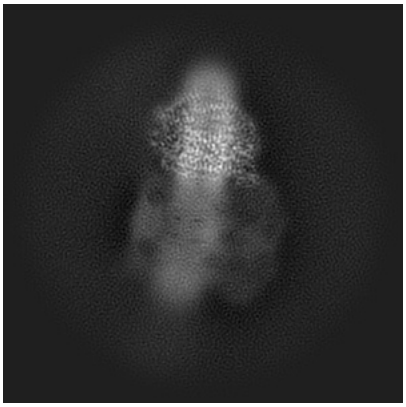
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10318. These allow visual inspection of the internal detail of the map and identification of artifacts.

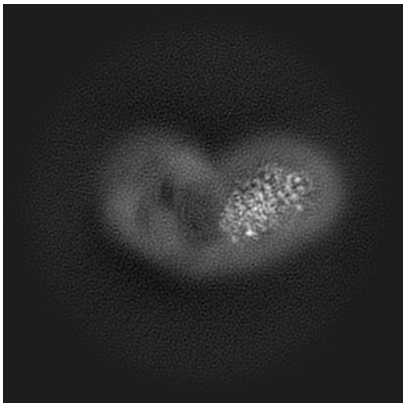
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

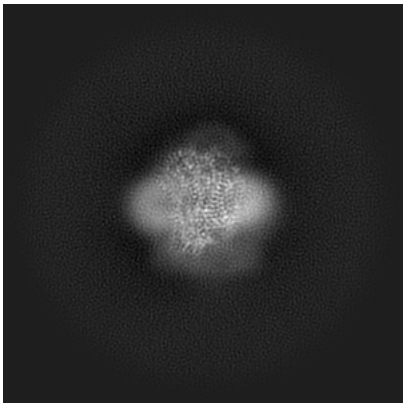
6.1.1 Primary map



X



Y

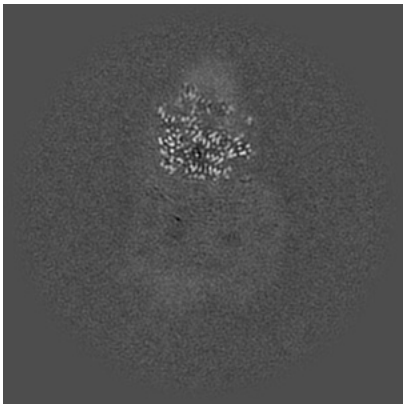


Z

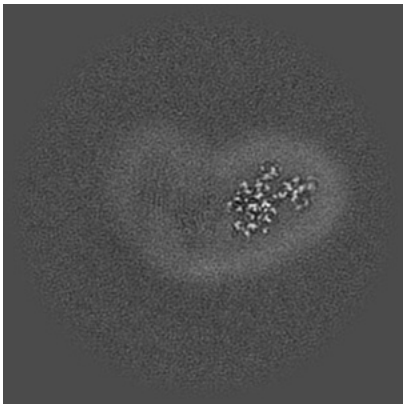
The images above show the map projected in three orthogonal directions.

6.2 Central slices

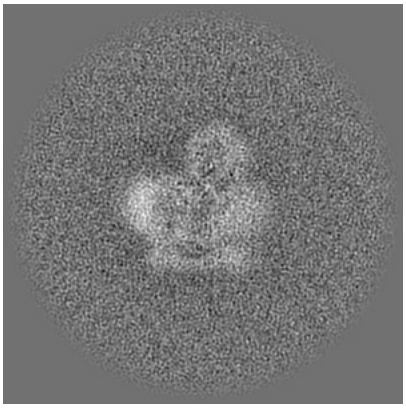
6.2.1 Primary map



X Index: 192



Y Index: 192

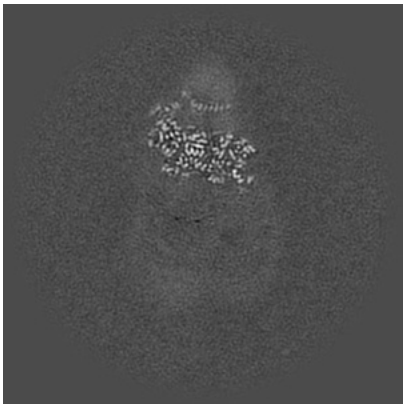


Z Index: 192

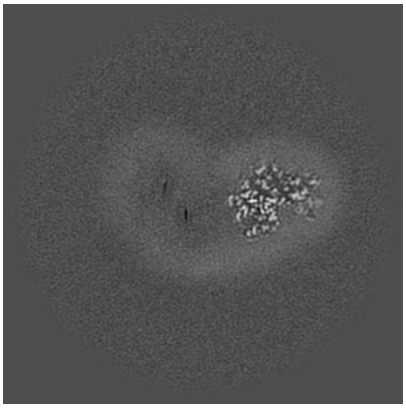
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

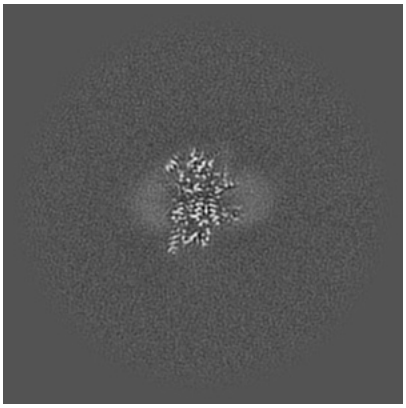
6.3.1 Primary map



X Index: 186



Y Index: 184

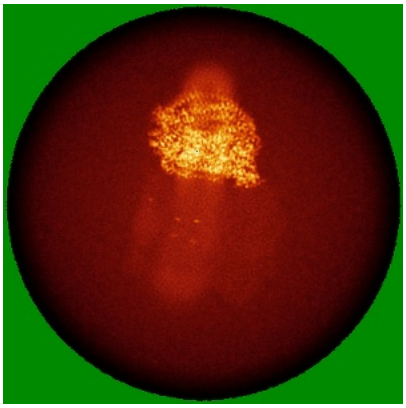


Z Index: 241

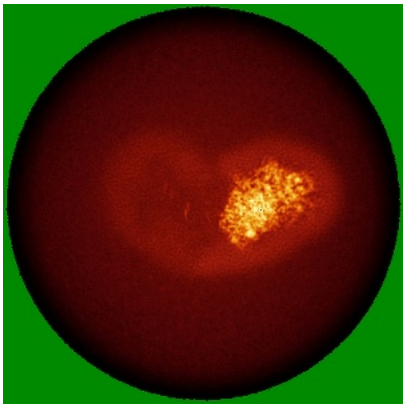
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

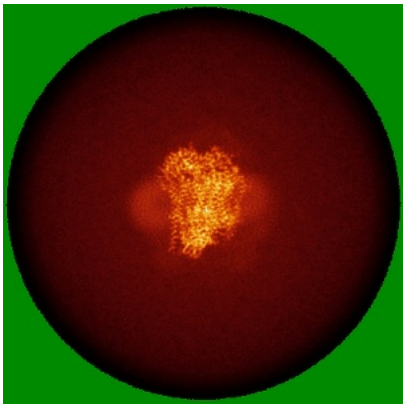
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.424. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

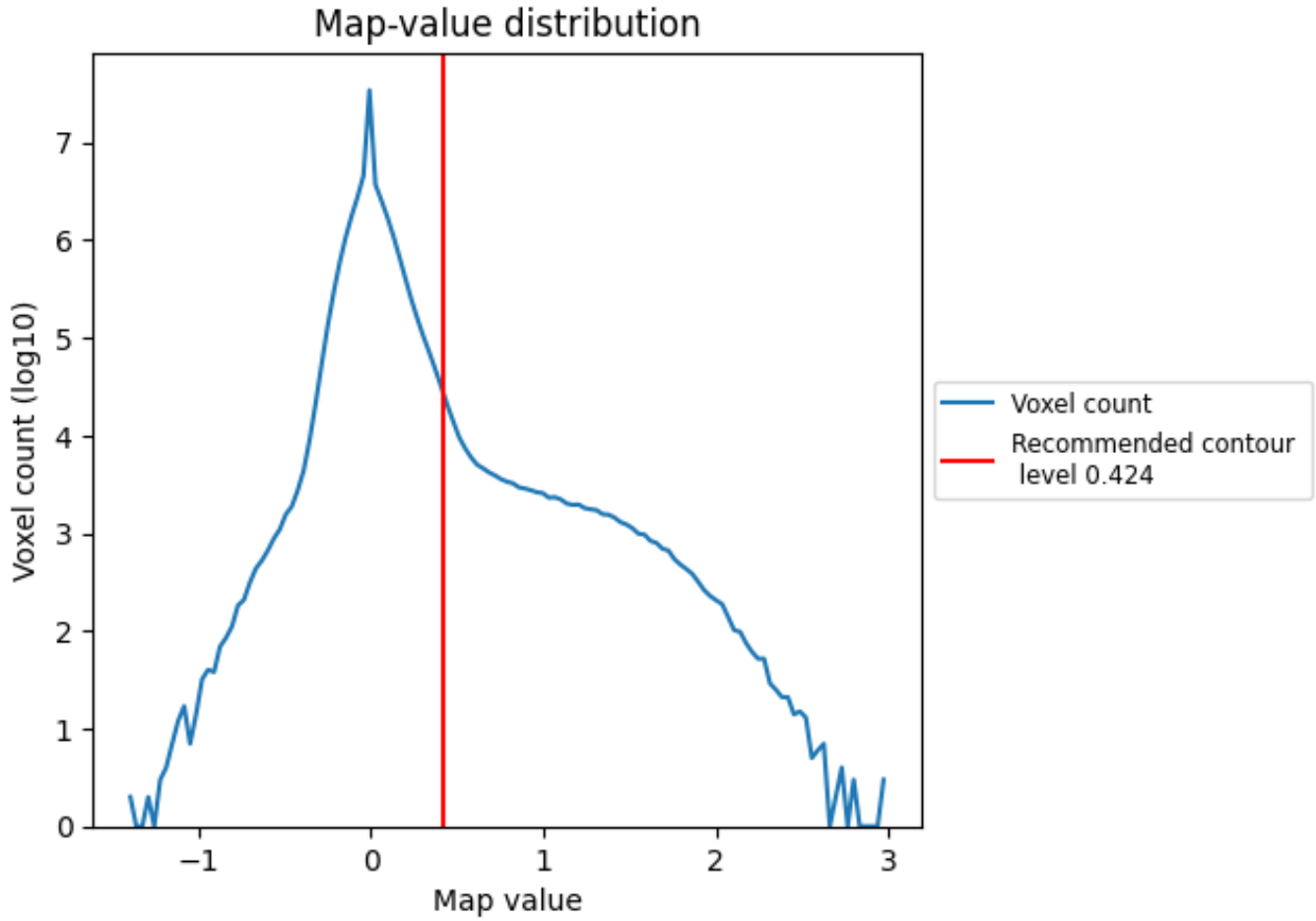
6.6 Mask visualisation (i)

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

7 Map analysis

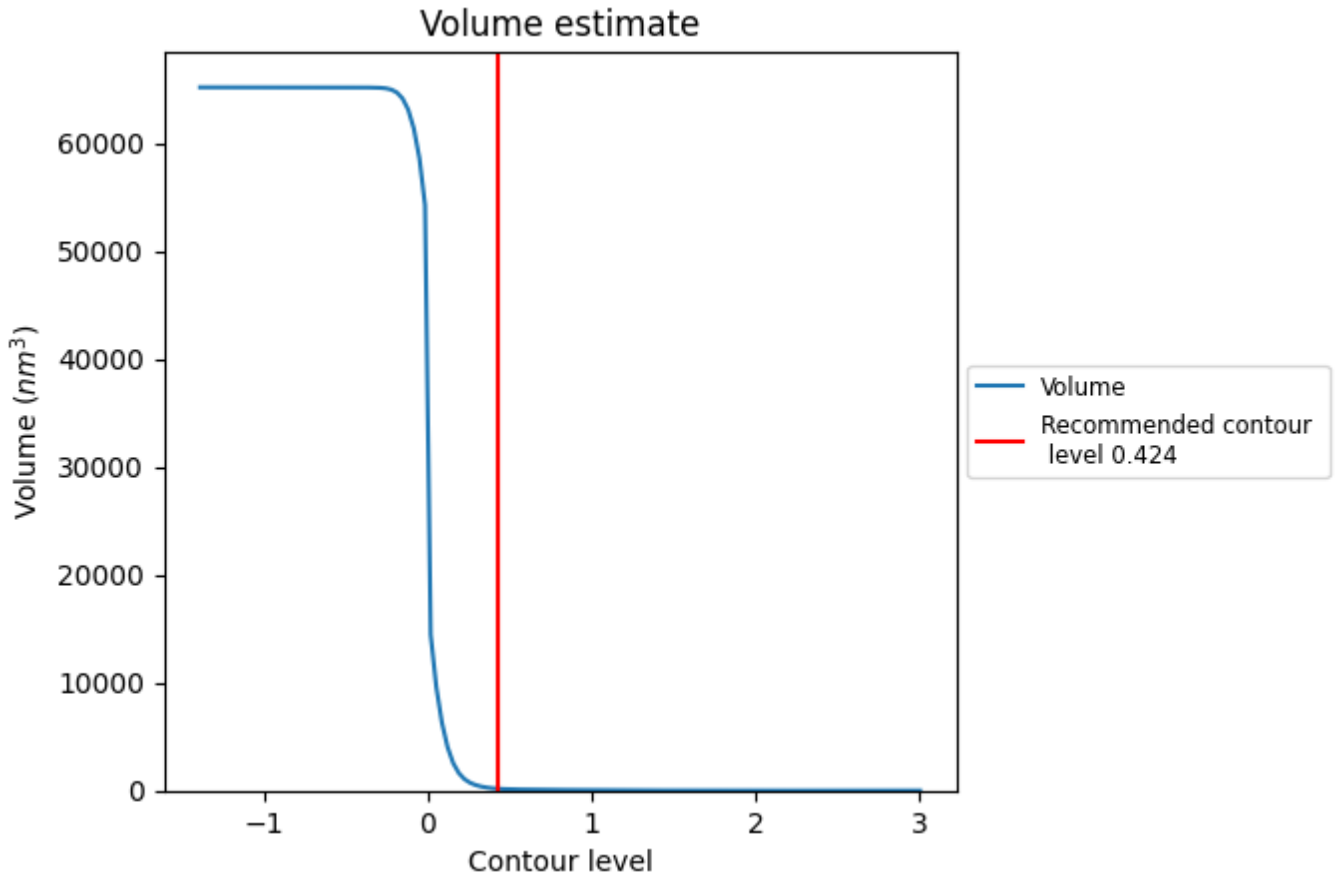
This section contains the results of statistical analysis of the map.

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.

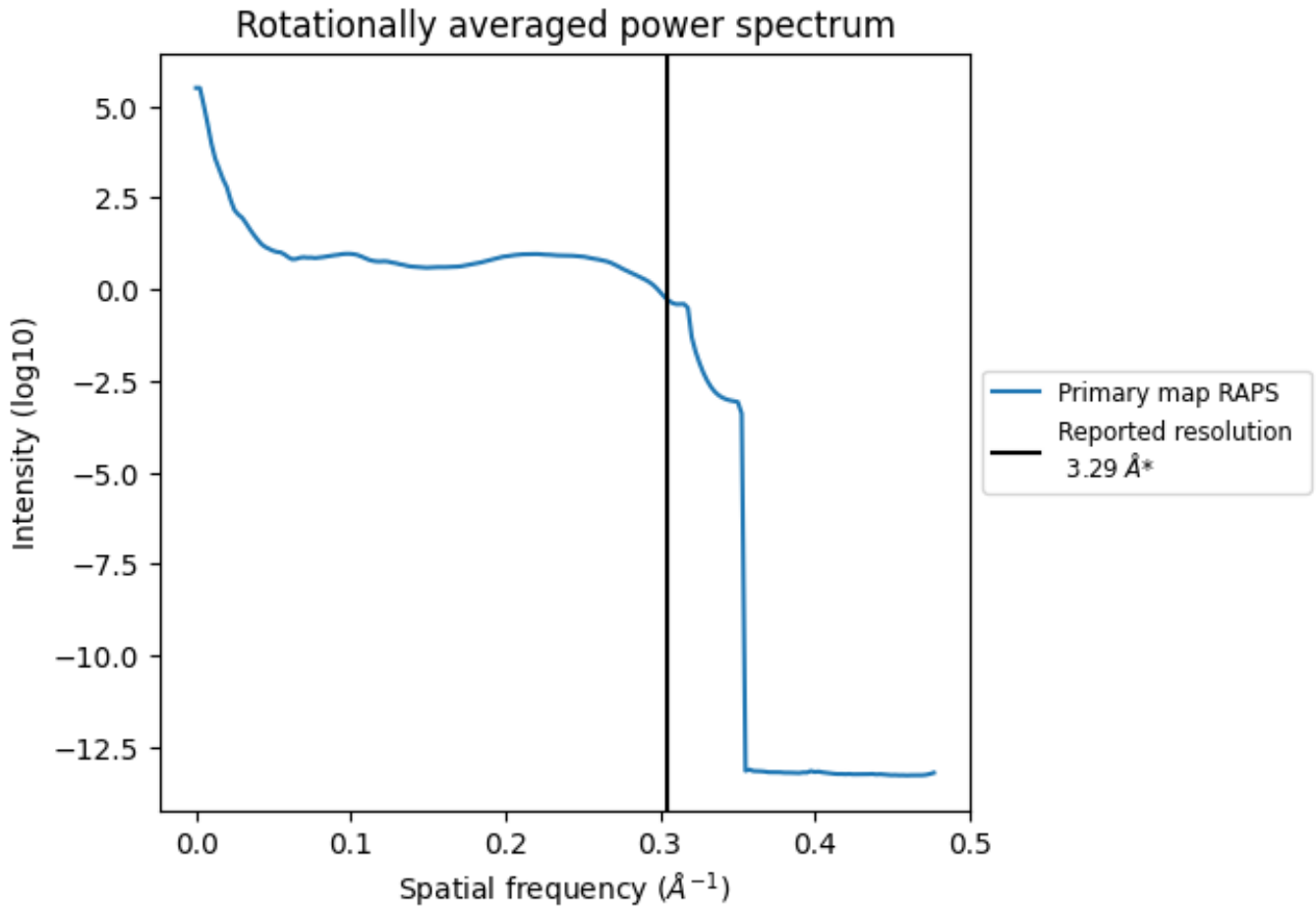
7.2 Volume estimate (i)



The volume at the recommended contour level is 174 nm^3; this corresponds to an approximate mass of 158 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)

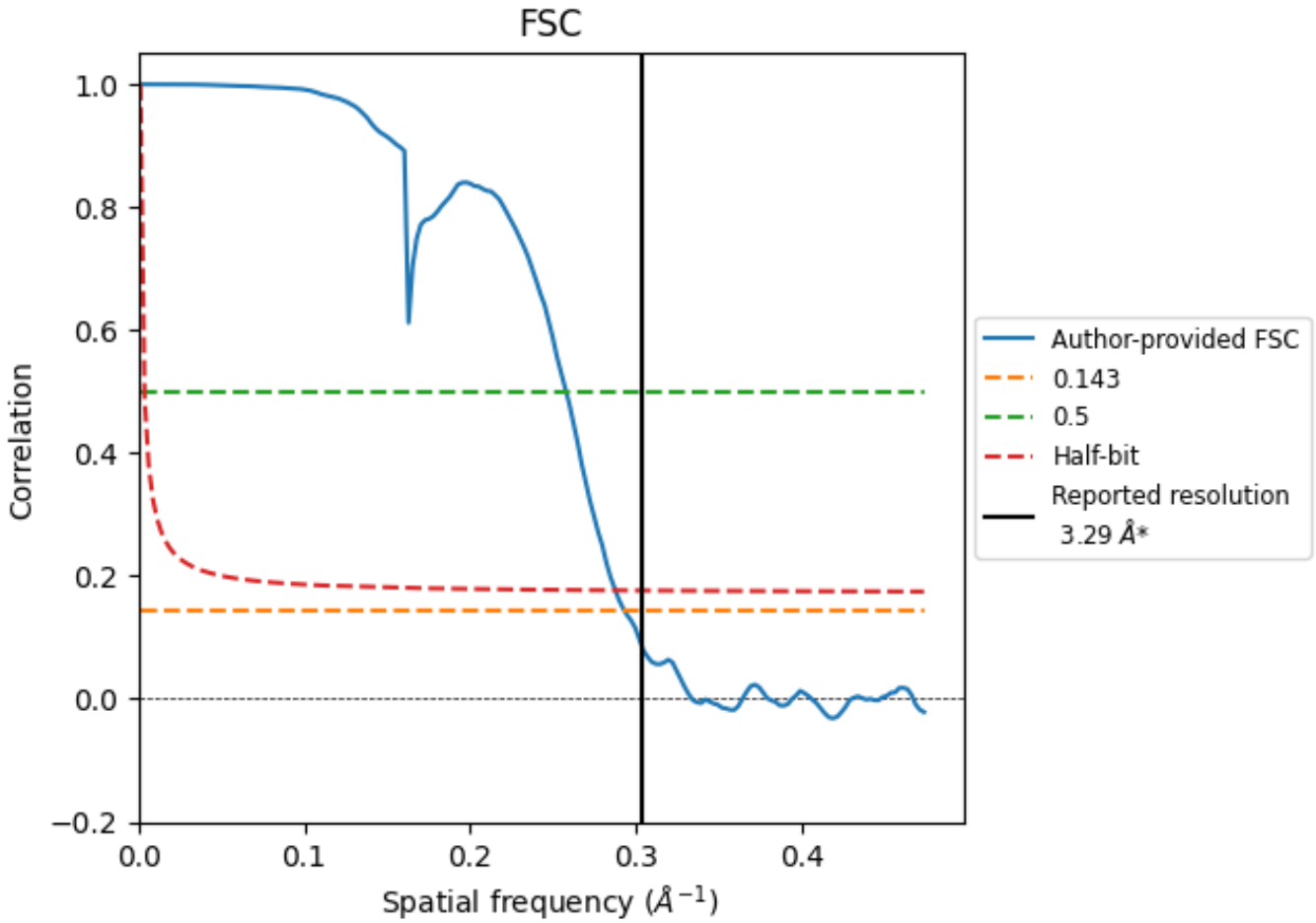


*Reported resolution corresponds to spatial frequency of 0.304 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.304 Å^{-1}

8.2 Resolution estimates (i)

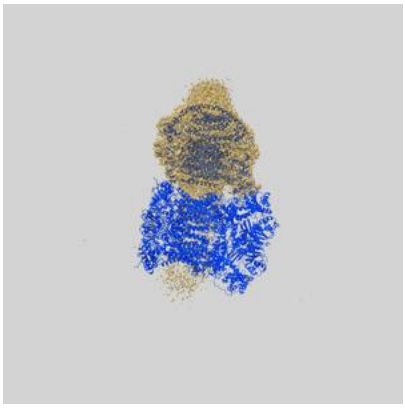
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.41	3.88	3.48
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

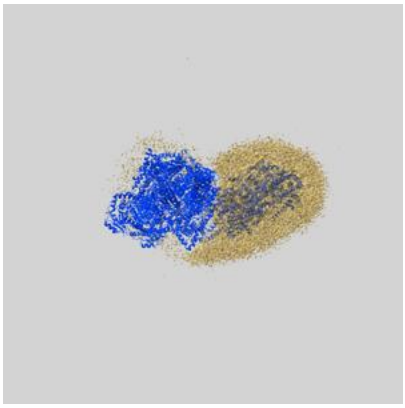
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10318 and PDB model 6T15. Per-residue inclusion information can be found in section 3 on page 17.

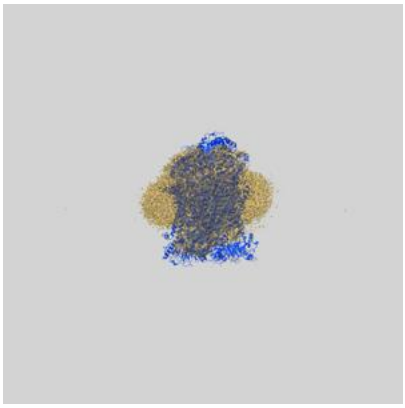
9.1 Map-model overlay



X



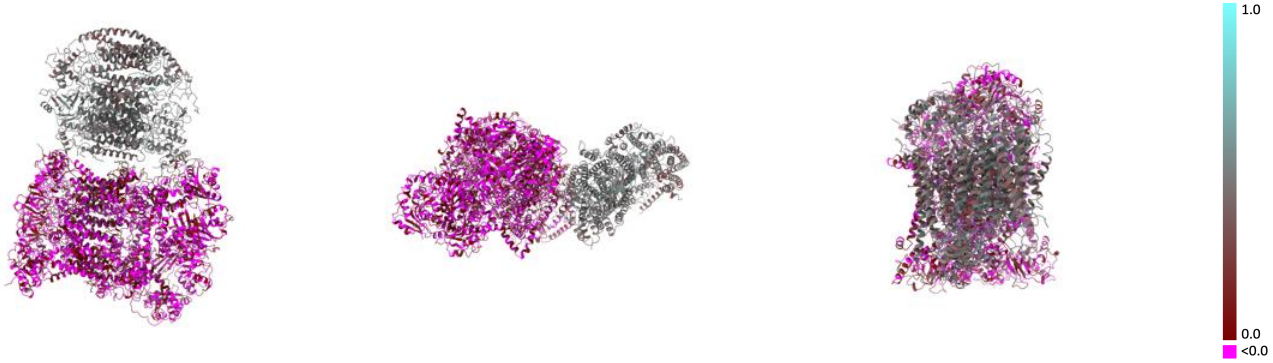
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.424 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.

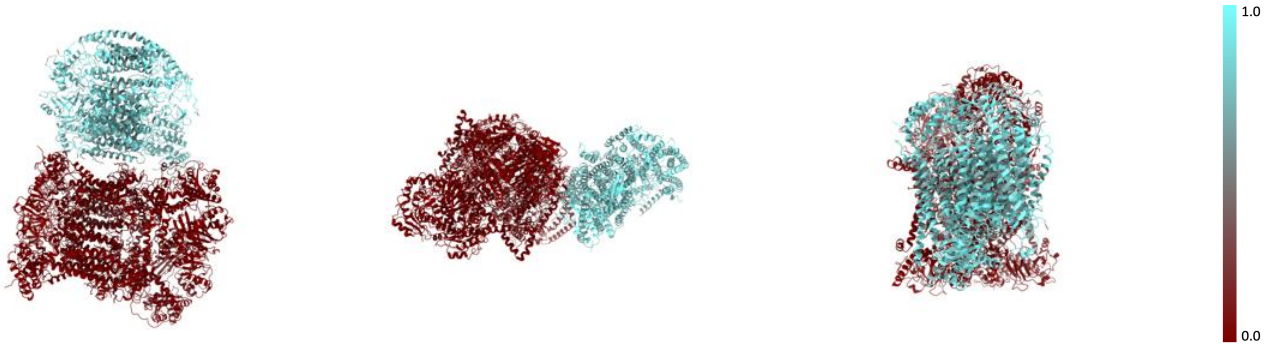
9.2 Q-score mapped to coordinate model



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.

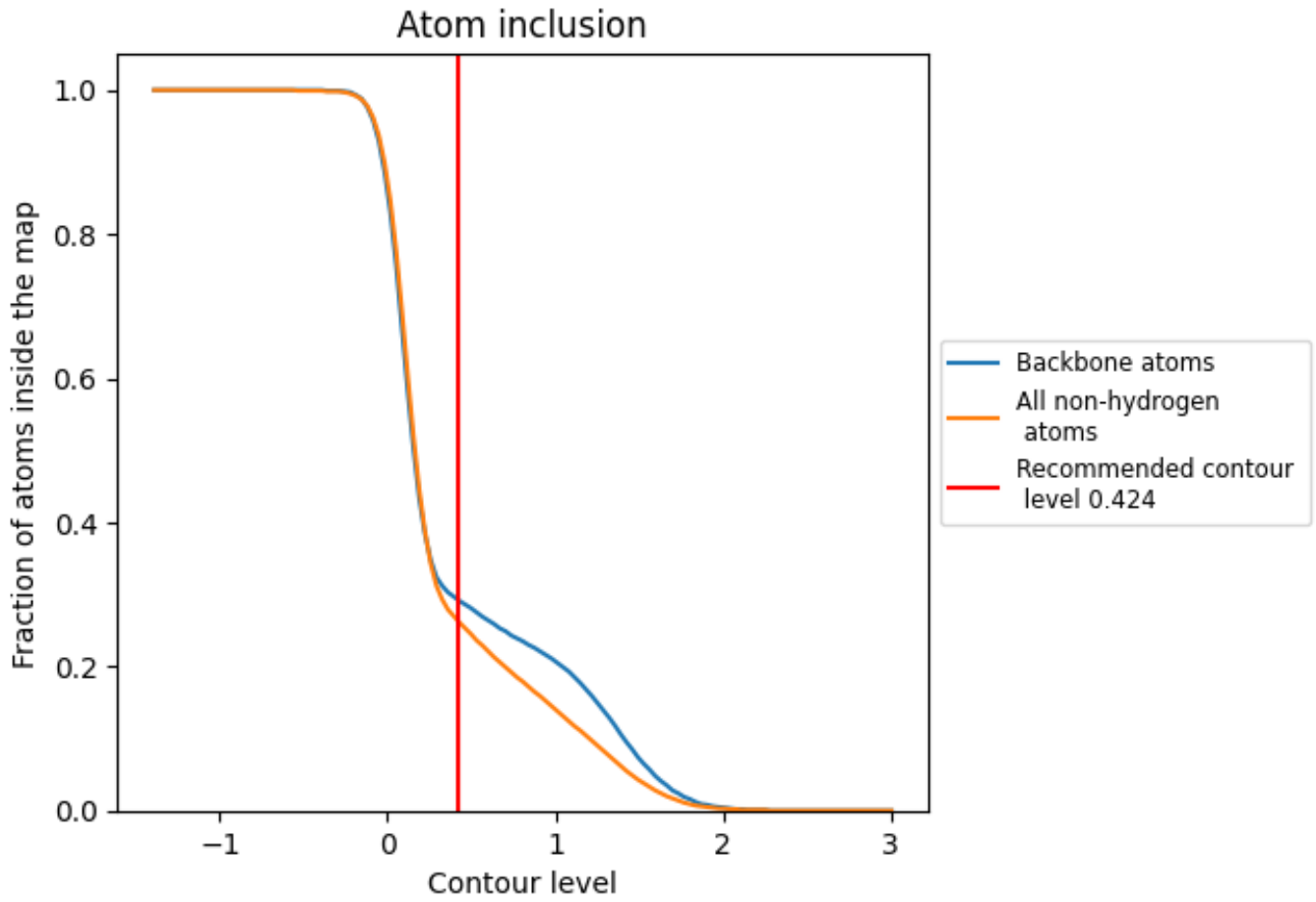
9.3 Atom inclusion mapped to coordinate model



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 (0.424).

9.4 Atom inclusion (i)



At the recommended contour level, 29% of all backbone atoms, 26% 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 (0.424) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2620	0.1510
A	0.0000	-0.0120
B	0.0000	-0.0220
C	0.0010	-0.0200
D	0.0000	-0.0080
E	0.0030	0.0720
F	0.0000	0.0100
G	0.0000	-0.0100
H	0.0000	0.0110
I	0.0000	0.0150
J	0.0030	0.0320
L	0.0020	0.0170
M	0.0000	-0.0140
N	0.0010	0.0040
O	0.0010	0.0200
P	0.0040	0.0560
Q	0.0000	0.0360
R	0.0000	-0.0030
S	0.0050	0.0550
T	0.0020	0.0320
U	0.0080	0.0530
a	0.8290	0.4840
b	0.8270	0.4750
c	0.8200	0.4630
d	0.8740	0.4750
e	0.7480	0.4390
f	0.8390	0.4470
g	0.8520	0.4730
h	0.8440	0.4610
i	0.8260	0.4400
j	0.8400	0.4460
k	0.8330	0.4310
l	0.8220	0.4540
m	0.7720	0.3910

