Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 03:21 am BST

PDB ID	:	7QHO
EMDB ID	:	EMD-13977
Title	:	Cytochrome bcc-aa3 supercomplex (respiratory supercomplex III2/IV2) from Corynebacterium glutamicum (as isolated)
Authors	:	Kao, W.-C.; Hunte, C.
Deposited on	:	2021-12-13
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation 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:

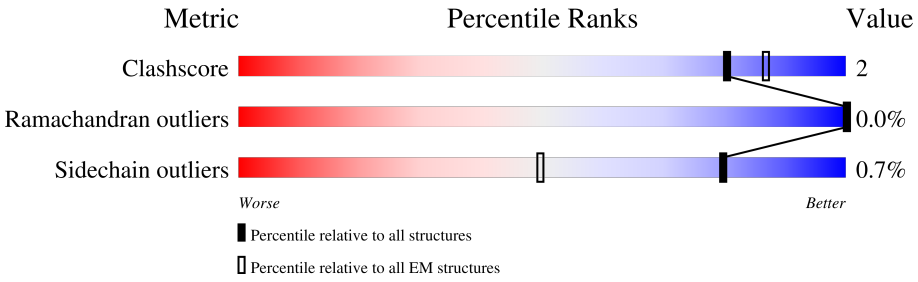
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	408	92% 7% •
1	N	408	91% 7% •
2	B	539	92% 7% •
2	O	539	91% 8% •
3	C	283	78% • • 18%
3	P	283	78% • • 18%
4	D	594	91% 6% •
4	Q	594	90% 6% •

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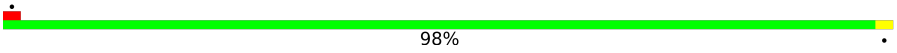
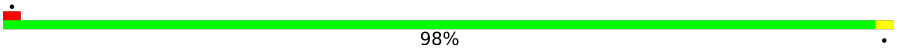
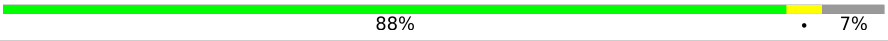
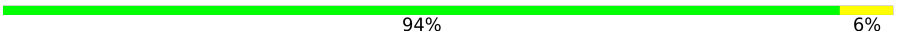
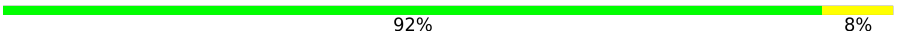
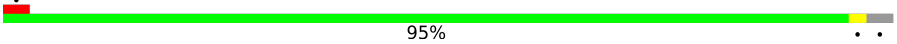
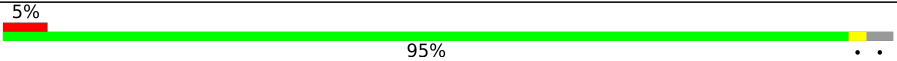
Mol	Chain	Length	Quality of chain
5	E	331	
5	R	331	
6	F	205	
6	S	205	
7	G	143	
7	T	143	
8	H	163	
8	U	163	
9	I	147	
9	V	147	
10	J	112	
10	W	112	
11	K	73	
11	X	73	
12	L	65	
12	Y	65	
13	M	168	
13	Z	168	

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
25	HAS	D	601	X	-	-	-
25	HAS	D	602	X	-	-	-
25	HAS	Q	601	X	-	-	-
25	HAS	Q	602	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 95954 atoms, of which 47460 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 bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	402	Total	C	H	N	O	S	0	0
			6206	1998	3070	536	586	16		
1	N	402	Total	C	H	N	O	S	0	0
			6206	1998	3070	536	586	16		

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	534	Total	C	H	N	O	S	5	0
			8491	2775	4268	707	719	22		
2	O	534	Total	C	H	N	O	S	5	0
			8491	2775	4268	707	719	22		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	233	Total	C	H	N	O	S	0	0
			3418	1083	1680	302	343	10		
3	P	233	Total	C	H	N	O	S	0	0
			3418	1083	1680	302	343	10		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	574	Total	C	H	N	O	S	0	0
			8994	3023	4458	733	748	32		
4	Q	574	Total	C	H	N	O	S	0	0
			8994	3023	4458	733	748	32		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	586	ALA	-	expression tag	UNP Q79VD7
D	587	TRP	-	expression tag	UNP Q79VD7
D	588	SER	-	expression tag	UNP Q79VD7
D	589	HIS	-	expression tag	UNP Q79VD7
D	590	PRO	-	expression tag	UNP Q79VD7
D	591	GLN	-	expression tag	UNP Q79VD7
D	592	PHE	-	expression tag	UNP Q79VD7
D	593	GLU	-	expression tag	UNP Q79VD7
D	594	LYS	-	expression tag	UNP Q79VD7
Q	585	ALA	-	expression tag	UNP Q79VD7
Q	586	ALA	-	expression tag	UNP Q79VD7
Q	587	TRP	-	expression tag	UNP Q79VD7
Q	588	SER	-	expression tag	UNP Q79VD7
Q	589	HIS	-	expression tag	UNP Q79VD7
Q	590	PRO	-	expression tag	UNP Q79VD7
Q	591	GLN	-	expression tag	UNP Q79VD7
Q	592	PHE	-	expression tag	UNP Q79VD7
Q	593	GLU	-	expression tag	UNP Q79VD7
Q	594	LYS	-	expression tag	UNP Q79VD7

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	331	Total	C	H	N	O	S	0	0
			5066	1660	2468	429	498	11		
5	R	331	Total	C	H	N	O	S	0	0
			5066	1660	2468	429	498	11		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	190	Total	C	H	N	O	S	0	0
			2981	992	1495	236	251	7		
6	S	190	Total	C	H	N	O	S	0	0
			2981	992	1495	236	251	7		

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	143	Total	C	H	N	O	S	0	0
			2201	728	1106	167	191	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	143	Total	C	H	N	O	S	0	0
			2201	728	1106	167	191	9		

- Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	154	Total	C	H	N	O	S	0	0
			2182	686	1058	185	250	3		
8	U	154	Total	C	H	N	O	S	0	0
			2182	686	1058	185	250	3		

- Molecule 9 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	129	Total	C	H	N	O	S	0	0
			2059	664	1031	182	181	1		
9	V	129	Total	C	H	N	O	S	0	0
			2059	664	1031	182	181	1		

- Molecule 10 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	100	Total	C	H	N	O	S	0	0
			1547	498	780	132	134	3		
10	W	100	Total	C	H	N	O	S	0	0
			1547	498	780	132	134	3		

- Molecule 11 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total	C	H	N	O	0	0
			864	286	413	78	87		
11	X	57	Total	C	H	N	O	0	0
			864	286	413	78	87		

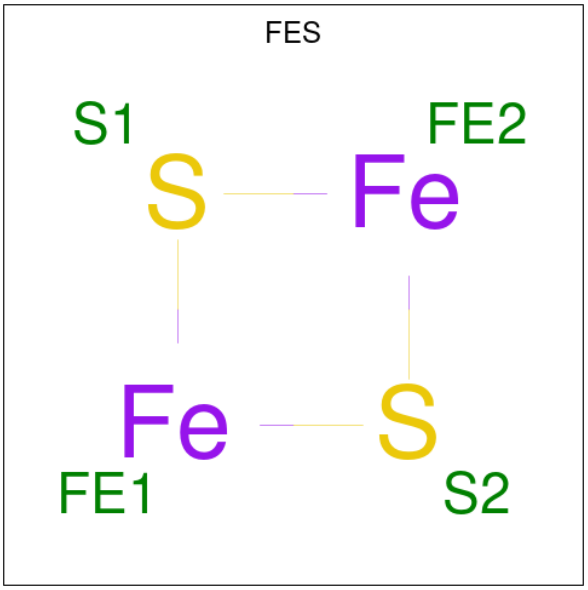
- Molecule 12 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		
12	Y	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		

- Molecule 13 is a protein called Thiamine biosynthesis protein X.

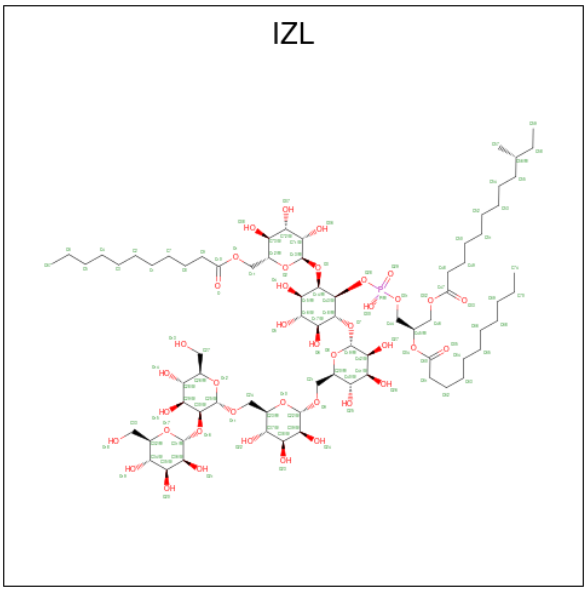
Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	25	Total	C	H	N	O	S	0	0
			372	114	179	36	42	1		
13	Z	25	Total	C	H	N	O	S	0	0
			372	114	179	36	42	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



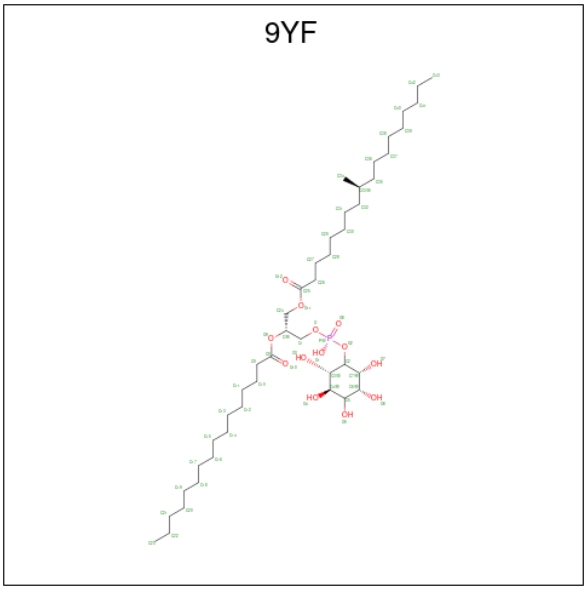
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	Fe	S		0
			4	2	2		
14	N	1	Total	Fe	S		0
			4	2	2		

- Molecule 15 is [(2 {R})-3-[[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (three-letter code: IZL) (formula: $C_{74}H_{133}O_{39}P$) (labeled as "Ligand of Interest" by depositor).



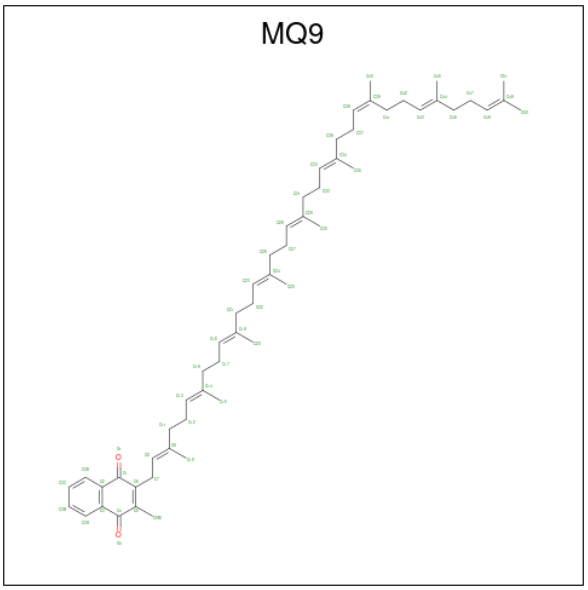
Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	H	O	P	0
			212	63	109	39	1	
15	N	1	Total	C	H	O	P	0
			212	63	109	39	1	

- Molecule 16 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula: $C_{44}H_{85}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



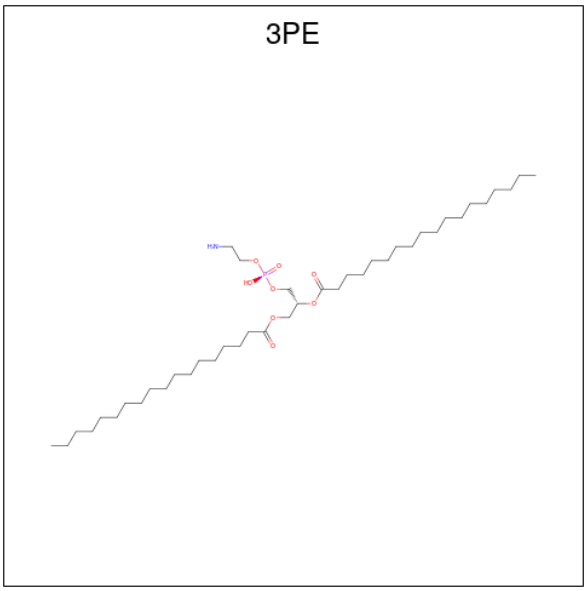
Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	H	O	P	0
			66	22	30	13	1	
16	B	1	Total	C	H	O	P	0
			60	20	26	13	1	
16	N	1	Total	C	H	O	P	0
			66	22	30	13	1	
16	U	1	Total	C	H	O	P	0
			60	20	26	13	1	

- Molecule 17 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



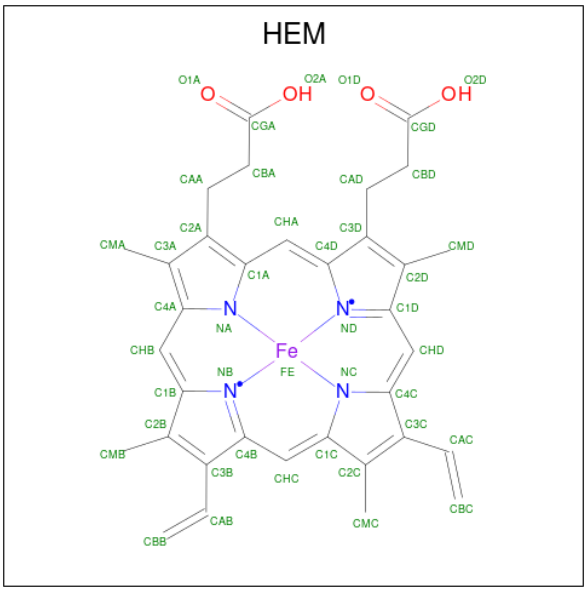
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	H	O	0
			52	24	26	2	
17	B	1	Total	C	H	O	0
			46	21	23	2	
17	B	1	Total	C	H	O	0
			46	21	23	2	
17	N	1	Total	C	H	O	0
			52	24	26	2	
17	O	1	Total	C	H	O	0
			46	21	23	2	
17	O	1	Total	C	H	O	0
			46	21	23	2	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



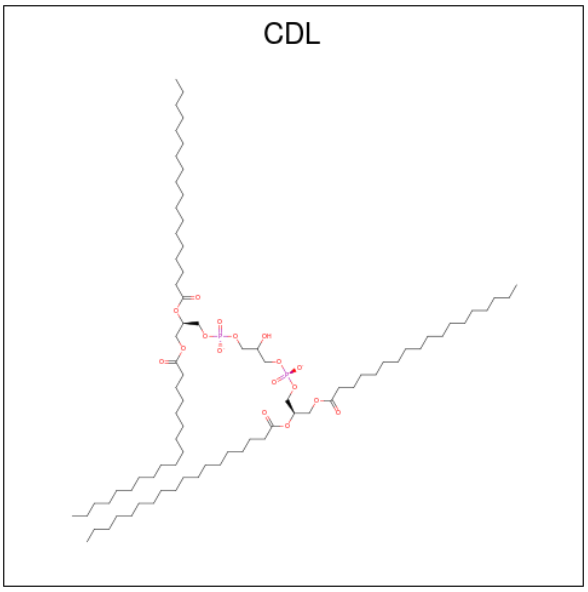
Mol	Chain	Residues	Atoms						AltConf
18	A	1	Total	C	H	N	O	P	0
			66	28	28	1	8	1	
18	D	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	E	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	F	1	Total	C	H	N	O	P	0
			54	22	22	1	8	1	
18	J	1	Total	C	H	N	O	P	0
			111	37	64	1	8	1	
18	N	1	Total	C	H	N	O	P	0
			66	28	28	1	8	1	
18	Q	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	R	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	S	1	Total	C	H	N	O	P	0
			54	22	22	1	8	1	
18	W	1	Total	C	H	N	O	P	0
			111	37	64	1	8	1	

- Molecule 19 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



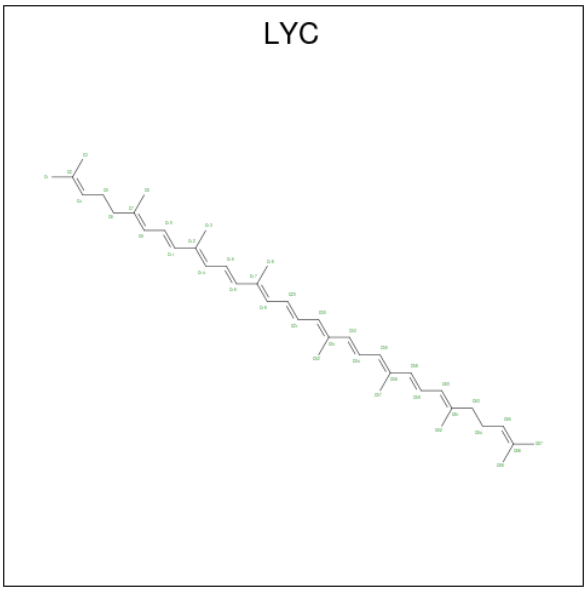
Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



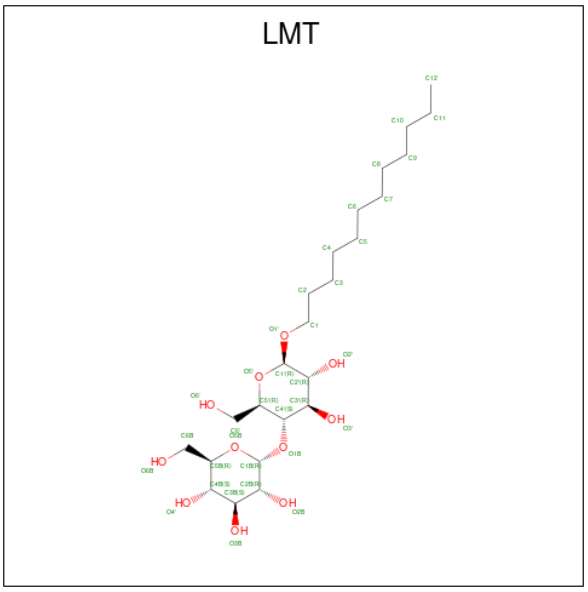
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	H	O	P	0
			72	26	27	17	2	
20	C	1	Total	C	H	O	P	0
			113	46	48	17	2	
20	D	1	Total	C	H	O	P	0
			161	58	84	17	2	
20	D	1	Total	C	H	O	P	0
			128	44	65	17	2	
20	F	1	Total	C	H	O	P	0
			94	38	37	17	2	
20	G	1	Total	C	H	O	P	0
			104	43	42	17	2	
20	I	1	Total	C	H	O	P	0
			107	38	50	17	2	
20	O	1	Total	C	H	O	P	0
			72	26	27	17	2	
20	P	1	Total	C	H	O	P	0
			113	46	48	17	2	
20	Q	1	Total	C	H	O	P	0
			161	58	84	17	2	
20	Q	1	Total	C	H	O	P	0
			128	44	65	17	2	
20	S	1	Total	C	H	O	P	0
			94	38	37	17	2	
20	S	1	Total	C	H	O	P	0
			104	43	42	17	2	
20	V	1	Total	C	H	O	P	0
			107	38	50	17	2	

- Molecule 21 is LYCOPENE (three-letter code: LYC) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	H	0
			96	40	56	
21	O	1	Total	C	H	0
			96	40	56	

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	H	O	0
			71	21	39	11	

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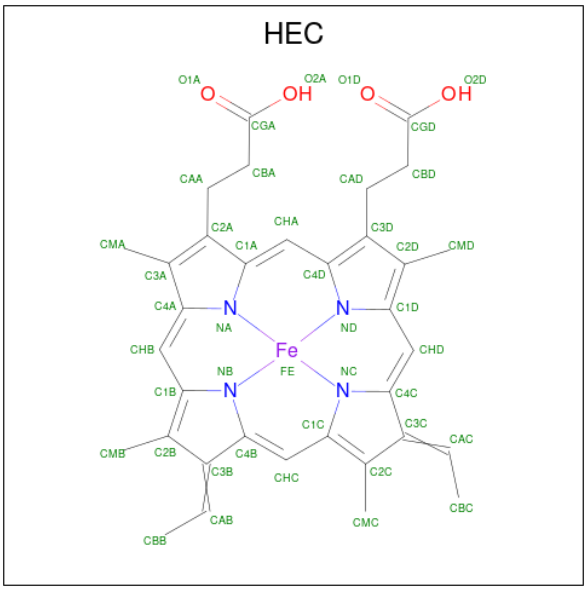
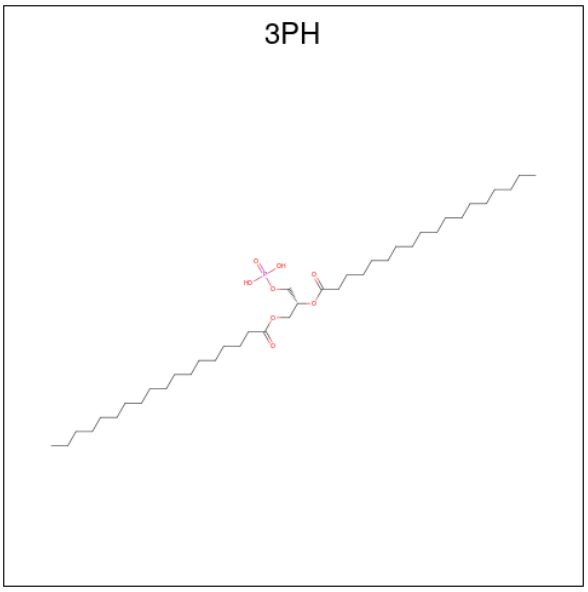
Mol	Chain	Residues	Atoms				AltConf
22	O	1	Total	C	H	O	0
			71	21	39	11	

- Molecule 23 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



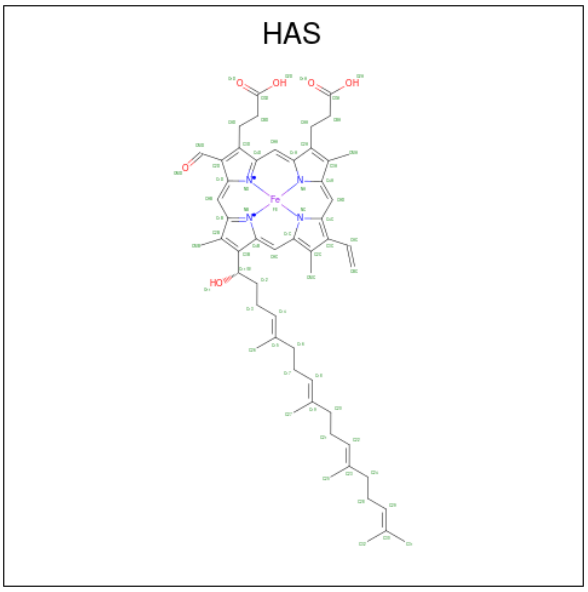
Mol	Chain	Residues	Atoms						AltConf
23	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
23	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
23	P	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
23	P	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 24 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	H	O	P	0
			90	29	52	8	1	
24	T	1	Total	C	H	O	P	0
			90	29	52	8	1	

- Molecule 25 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	

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Mol	Chain	Residues	Atoms						AltConf
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	

- Molecule 26 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Cu	0
			1	1	
26	Q	1	Total	Cu	0
			1	1	

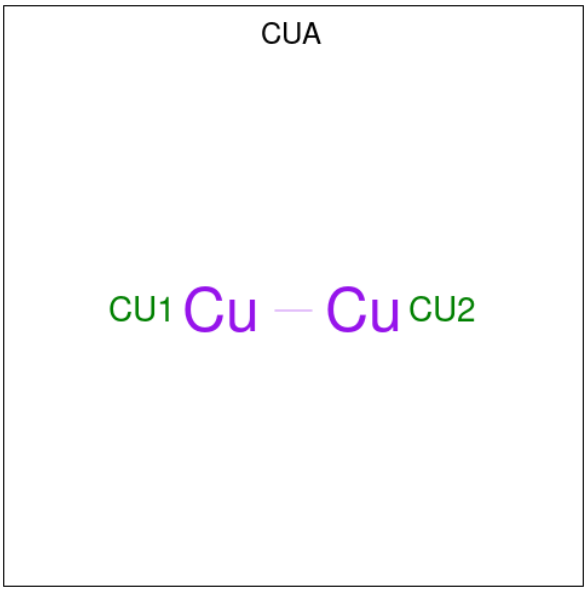
- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total	Ca	0
			1	1	
27	Q	1	Total	Ca	0
			1	1	

- Molecule 28 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

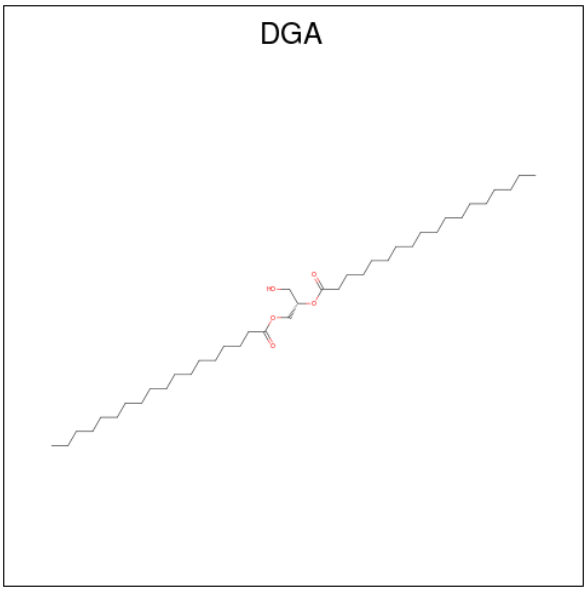
Mol	Chain	Residues	Atoms		AltConf
28	E	1	Total	Mn	0
			1	1	
28	R	1	Total	Mn	0
			1	1	

- Molecule 29 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



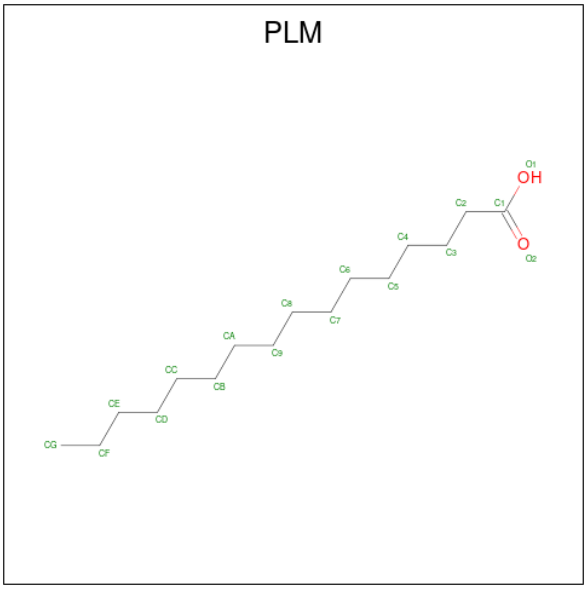
Mol	Chain	Residues	Atoms	AltConf
29	E	1	Total Cu 1 1	0
29	E	1	Total Cu 1 1	0
29	R	1	Total Cu 1 1	0
29	R	1	Total Cu 1 1	0

- Molecule 30 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
30	E	1	Total C O 20 16 4	0
30	H	1	Total C O 17 13 4	0
30	M	1	Total C O 22 18 4	0
30	R	1	Total C O 20 16 4	0
30	U	1	Total C O 17 13 4	0
30	Z	1	Total C O 22 18 4	0

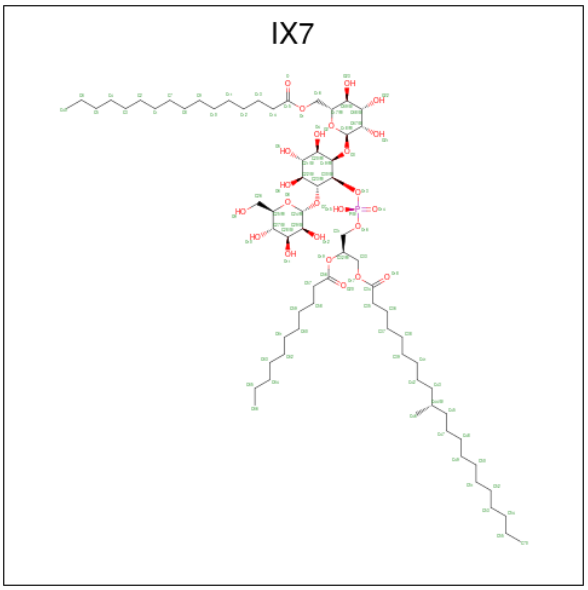
- Molecule 31 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
31	H	1	Total C H O 35 14 20 1	0
31	M	1	Total C H O 9 4 4 1	0
31	U	1	Total C H O 35 14 20 1	0
31	Z	1	Total C H O 9 4 4 1	0

- Molecule 32 is [(2 {R})-3-[[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {

S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {S})-10-methylhenicosanoate (three-letter code: IX7) (formula: $C_{70}H_{131}O_{24}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	I	1	Total	C	H	O	P	0
			155	47	83	24	1	
32	R	1	Total	C	H	O	P	0
			155	47	83	24	1	

- Molecule 33 is water.

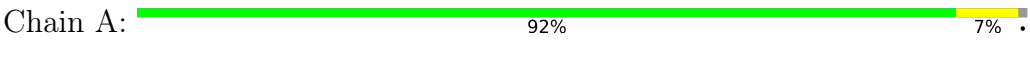
Mol	Chain	Residues	Atoms		AltConf
33	B	2	Total	O	0
			2	2	
33	D	2	Total	O	0
			2	2	
33	E	1	Total	O	0
			1	1	
33	O	2	Total	O	0
			2	2	
33	Q	2	Total	O	0
			2	2	
33	R	1	Total	O	0
			1	1	

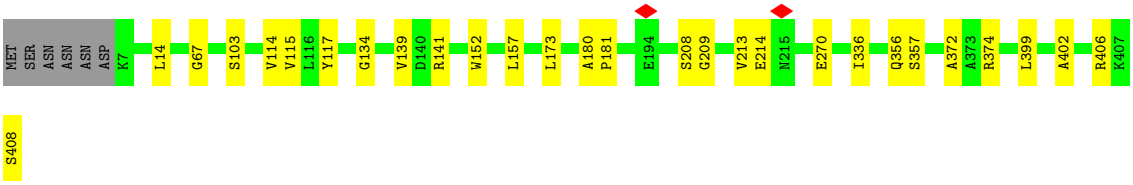
3 Residue-property plots (i)

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 bc1 complex Rieske iron-sulfur subunit

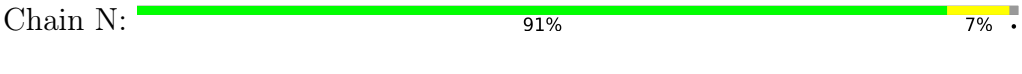
Chain A:

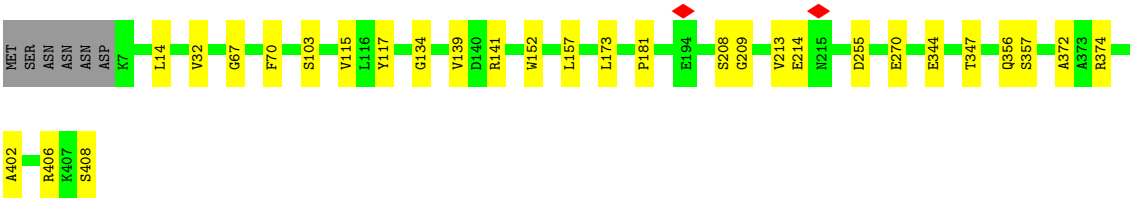




• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

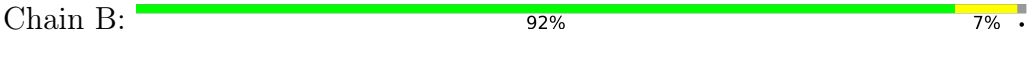
Chain N:

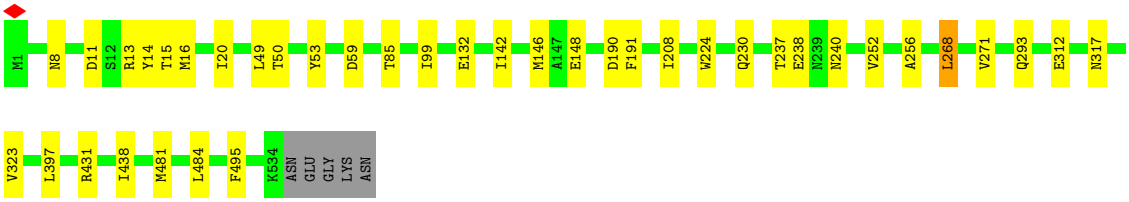




• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

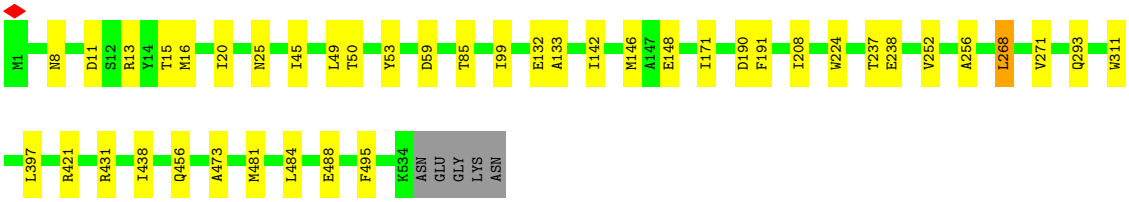
Chain B:



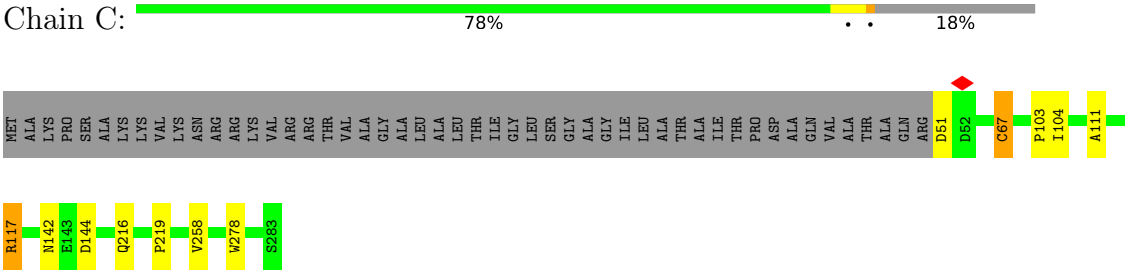


• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

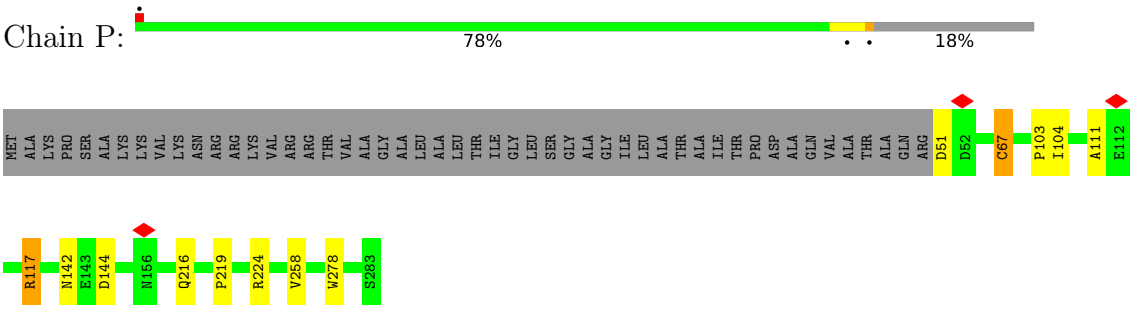
Chain O:



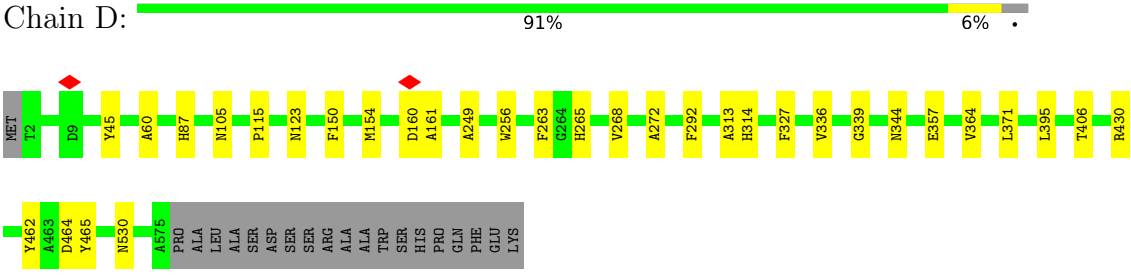
• Molecule 3: Cytochrome bc1 complex cytochrome c subunit



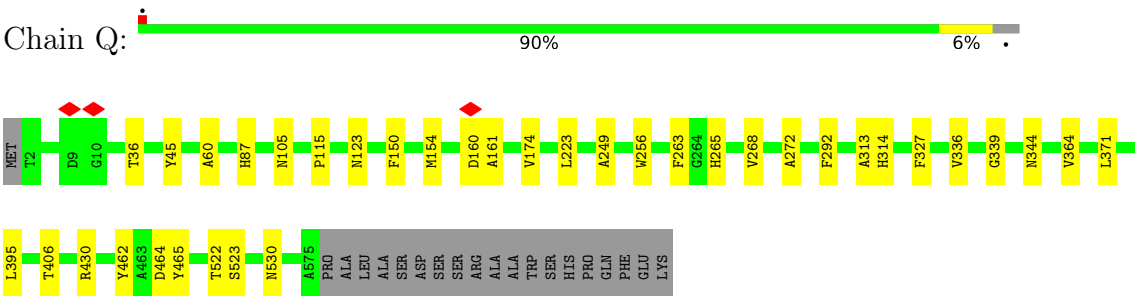
• Molecule 3: Cytochrome bc1 complex cytochrome c subunit



• Molecule 4: Cytochrome c oxidase subunit 1

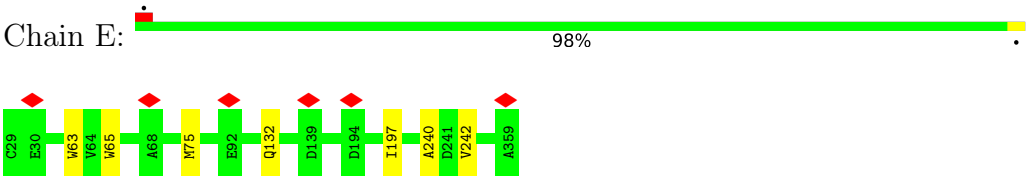


• Molecule 4: Cytochrome c oxidase subunit 1



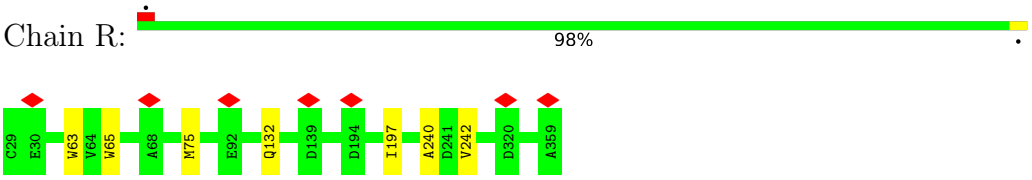
• Molecule 5: Cytochrome c oxidase subunit 2

Chain E:



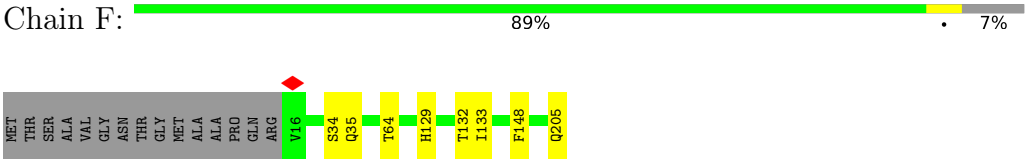
• Molecule 5: Cytochrome c oxidase subunit 2

Chain R:



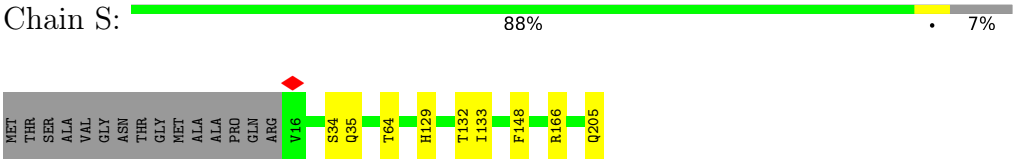
• Molecule 6: Cytochrome c oxidase subunit 3

Chain F:



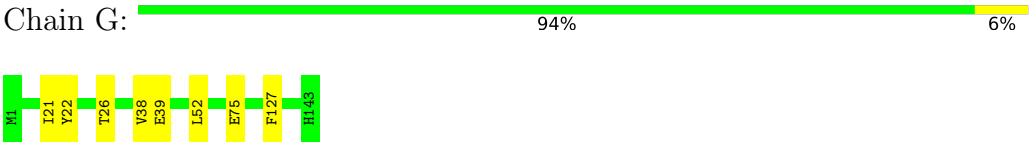
• Molecule 6: Cytochrome c oxidase subunit 3

Chain S:



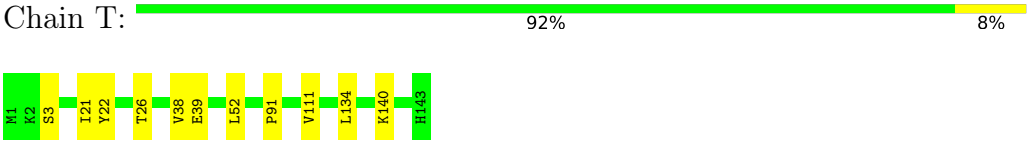
• Molecule 7: Cytochrome c oxidase polypeptide 4

Chain G:



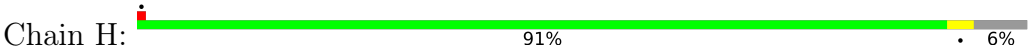
• Molecule 7: Cytochrome c oxidase polypeptide 4

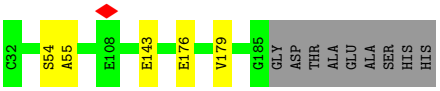
Chain T:



• Molecule 8: Uncharacterized protein Cgl2664/cg2949

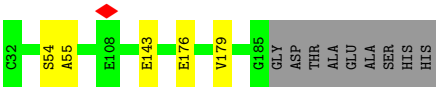
Chain H:





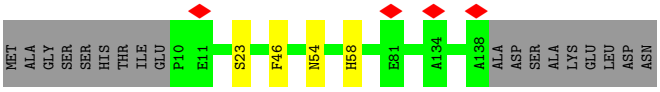
• Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain U:



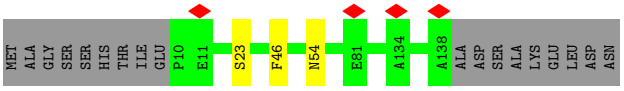
• Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211

Chain I:



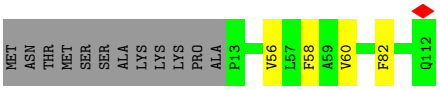
• Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211

Chain V:



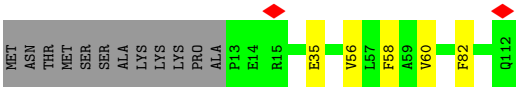
• Molecule 10: Hypothetical membrane protein

Chain J:



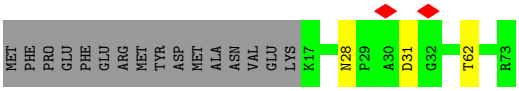
• Molecule 10: Hypothetical membrane protein

Chain W:



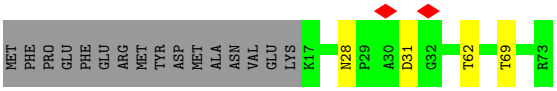
• Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

Chain K:



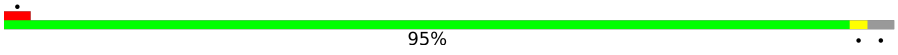
• Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

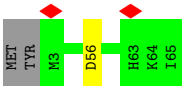
Chain X:



• Molecule 12: Hypothetical membrane protein

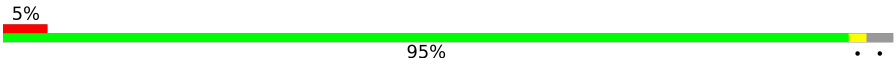
Chain L:

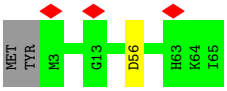




• Molecule 12: Hypothetical membrane protein

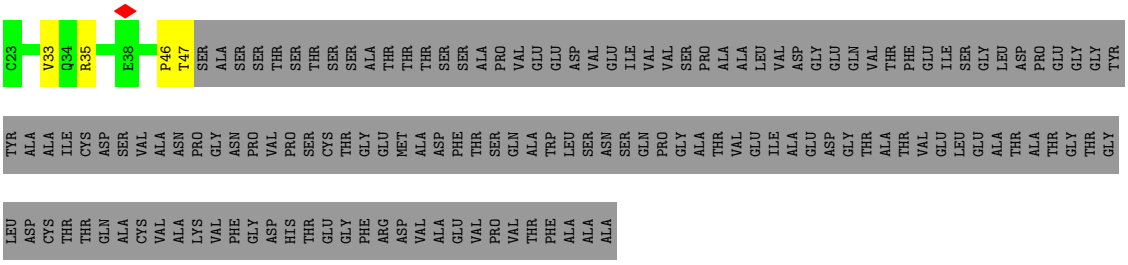
Chain Y:





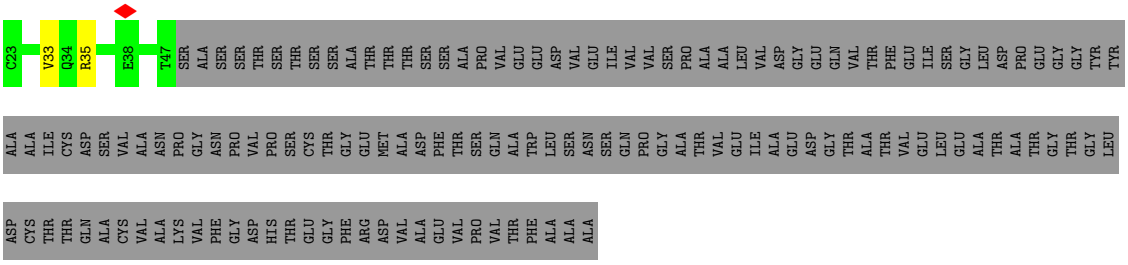
• Molecule 13: Thiamine biosynthesis protein X

Chain M:



• Molecule 13: Thiamine biosynthesis protein X

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	51060	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 ($e^-/Å^2$)	49.95	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.056	Depositor
Minimum map value	-0.798	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	232.20001, 249.48001, 162.0	wwPDB
Map dimensions	150, 231, 215	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LYC, CU, IZL, HEC, CA, DGA, MQ9, 3PH, 3PE, 9YF, CUA, PLM, LMT, HEM, IX7, HAS, FES, MN, CDL

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	0.37	0/3216	0.63	0/4375
1	N	0.37	0/3216	0.63	0/4375
2	B	0.40	0/4361	0.61	0/5944
2	O	0.40	0/4361	0.61	0/5944
3	C	0.29	0/1770	0.58	0/2394
3	P	0.29	0/1770	0.58	0/2394
4	D	0.31	0/4705	0.55	0/6419
4	Q	0.31	0/4705	0.55	0/6419
5	E	0.30	0/2671	0.55	0/3642
5	R	0.30	0/2671	0.55	0/3642
6	F	0.30	0/1528	0.51	0/2081
6	S	0.30	0/1528	0.51	0/2081
7	G	0.31	0/1126	0.50	0/1529
7	T	0.31	0/1126	0.50	0/1529
8	H	0.29	0/1138	0.57	0/1558
8	U	0.29	0/1138	0.57	0/1558
9	I	0.27	0/1057	0.57	0/1444
9	V	0.27	0/1057	0.57	0/1444
10	J	0.27	0/786	0.56	0/1068
10	W	0.27	0/786	0.56	0/1068
11	K	0.32	0/468	0.54	0/640
11	X	0.32	0/468	0.54	0/640
12	L	0.26	0/453	0.49	0/616
12	Y	0.26	0/453	0.49	0/616
13	M	0.27	0/197	0.57	0/271
13	Z	0.28	0/197	0.57	0/271
All	All	0.33	0/46952	0.57	0/63962

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3136	3070	3070	35	0
1	N	3136	3070	3070	30	0
2	B	4223	4268	4252	35	0
2	O	4223	4268	4252	38	0
3	C	1738	1680	1680	11	0
3	P	1738	1680	1680	12	0
4	D	4536	4458	4459	19	0
4	Q	4536	4458	4459	22	0
5	E	2598	2468	2468	5	0
5	R	2598	2468	2468	5	0
6	F	1486	1495	1494	5	0
6	S	1486	1495	1494	6	0
7	G	1095	1106	1106	6	0
7	T	1095	1106	1106	11	0
8	H	1124	1058	1057	3	0
8	U	1124	1058	1057	3	0
9	I	1028	1031	1031	3	0
9	V	1028	1031	1031	2	0
10	J	767	780	780	2	0
10	W	767	780	780	4	0
11	K	451	413	413	3	0
11	X	451	413	413	5	0
12	L	445	470	469	1	0
12	Y	445	470	469	1	0
13	M	193	179	179	2	0
13	Z	193	179	179	1	0
14	A	4	0	0	1	0
14	N	4	0	0	1	0
15	A	103	109	0	4	0
15	N	103	109	0	3	0
16	A	36	30	0	0	0
16	B	34	26	0	0	0
16	N	36	30	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	34	26	0	0	0
17	A	26	26	26	8	0
17	B	46	46	42	0	0
17	N	26	26	26	6	0
17	O	46	46	42	2	0
18	A	38	28	53	8	0
18	D	31	26	36	1	0
18	E	31	26	36	0	0
18	F	32	22	38	1	0
18	J	47	64	71	1	0
18	N	38	28	53	9	0
18	Q	31	26	36	1	0
18	R	31	26	36	0	0
18	S	32	22	38	1	0
18	W	47	64	71	1	0
19	B	86	60	60	1	0
19	O	86	60	60	1	0
20	B	45	27	34	1	0
20	C	65	48	74	2	0
20	D	140	149	171	0	0
20	F	57	37	58	0	0
20	G	62	42	68	3	0
20	I	57	50	61	0	0
20	O	45	27	34	1	0
20	P	65	48	74	2	0
20	Q	140	149	171	1	0
20	S	119	79	126	2	0
20	V	57	50	61	0	0
21	B	40	56	56	2	0
21	O	40	56	56	2	0
22	B	32	39	37	3	0
22	O	32	39	37	3	0
23	C	86	60	60	7	0
23	P	86	60	60	7	0
24	C	38	52	48	0	0
24	T	38	52	48	0	0
25	D	130	124	124	5	0
25	Q	130	124	124	4	0
26	D	1	0	0	0	0
26	Q	1	0	0	0	0
27	D	1	0	0	0	0
27	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	E	1	0	0	0	0
28	R	1	0	0	0	0
29	E	2	0	0	0	0
29	R	2	0	0	0	0
30	E	20	0	21	1	0
30	H	17	0	15	0	0
30	M	22	0	25	0	0
30	R	20	0	21	1	0
30	U	17	0	15	0	0
30	Z	22	0	25	1	0
31	H	15	20	20	0	0
31	M	5	4	4	0	0
31	U	15	20	20	0	0
31	Z	5	4	4	0	0
32	I	72	83	0	2	0
32	R	72	83	0	1	0
33	B	2	0	0	0	0
33	D	2	0	0	0	0
33	E	1	0	0	0	0
33	O	2	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
All	All	48494	47460	47392	239	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 2.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:504:MQ9:H5M1	2:O:50:THR:HG23	1.65	0.79
15:N:504:IZL:O30	15:N:504:IZL:O33	2.07	0.72
25:Q:601:HAS:HMC1	25:Q:601:HAS:HBC1	1.72	0.72
15:A:502:IZL:O30	15:A:502:IZL:O33	2.07	0.71
25:D:601:HAS:HMC1	25:D:601:HAS:HBC1	1.72	0.71
1:A:134:GLY:O	2:O:15:THR:HG22	1.91	0.71
2:B:13:ARG:NH1	2:O:132:GLU:OE1	2.25	0.69
2:B:15:THR:HG22	1:N:134:GLY:O	1.93	0.69
25:Q:602:HAS:HBC1	25:Q:602:HAS:HMC1	1.75	0.68
25:D:602:HAS:HMC1	25:D:602:HAS:HBC1	1.75	0.68
32:I:202:IX7:O2	32:I:202:IX7:O4	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:CYS:HA	23:P:302:HEC:HMC3	1.76	0.66
3:C:67:CYS:HA	23:C:302:HEC:HMC3	1.76	0.66
32:R:406:IX7:O2	32:R:406:IX7:O4	2.13	0.66
18:A:505:3PE:H2F2	1:N:117:TYR:CD2	2.30	0.65
2:B:50:THR:HG23	17:N:501:MQ9:H5M1	1.76	0.65
18:A:505:3PE:H2C2	2:O:252:VAL:HG21	1.78	0.65
23:C:302:HEC:HBC3	23:C:302:HEC:HMC1	1.79	0.65
2:B:252:VAL:HG21	18:N:502:3PE:H2C2	1.78	0.65
23:P:302:HEC:HMC1	23:P:302:HEC:HBC3	1.79	0.65
17:A:504:MQ9:H5M1	2:O:50:THR:CG2	2.28	0.63
4:D:339:GLY:HA2	25:D:602:HAS:H273	1.79	0.63
4:Q:430:ARG:NH1	12:Y:56:ASP:OD2	2.32	0.63
4:Q:339:GLY:HA2	25:Q:602:HAS:H273	1.80	0.63
4:D:115:PRO:O	4:D:530:ASN:ND2	2.33	0.62
1:A:157:LEU:HD11	18:A:505:3PE:H2G1	1.81	0.62
4:D:430:ARG:NH1	12:L:56:ASP:OD2	2.32	0.62
4:Q:115:PRO:O	4:Q:530:ASN:ND2	2.33	0.61
1:N:157:LEU:HD11	18:N:502:3PE:H2G1	1.83	0.60
2:O:484:LEU:HD13	11:X:62:THR:CG2	2.32	0.60
2:B:484:LEU:HD13	11:K:62:THR:CG2	2.32	0.60
4:D:160:ASP:OD1	4:D:161:ALA:N	2.36	0.58
4:Q:160:ASP:OD1	4:Q:161:ALA:N	2.36	0.58
18:A:505:3PE:H2I3	1:N:117:TYR:CG	2.39	0.58
6:S:148:PHE:CE1	18:S:301:3PE:H2A2	2.39	0.58
1:A:181:PRO:HD2	17:A:504:MQ9:H3D	1.84	0.58
3:P:142:ASN:ND2	3:P:144:ASP:OD2	2.37	0.58
7:T:21:ILE:HD11	10:W:82:PHE:CE2	2.39	0.58
3:C:142:ASN:ND2	3:C:144:ASP:OD2	2.37	0.57
6:F:148:PHE:CE1	18:F:301:3PE:H2A2	2.39	0.57
1:A:117:TYR:CD2	18:N:502:3PE:H2F2	2.40	0.57
1:A:157:LEU:HD22	1:N:117:TYR:OH	2.04	0.57
1:A:357:SER:OG	14:A:501:FES:S1	2.58	0.57
2:O:268:LEU:HA	2:O:271:VAL:HG12	1.85	0.57
4:D:249:ALA:HB3	5:E:197:ILE:HG21	1.85	0.57
2:B:268:LEU:HA	2:B:271:VAL:HG12	1.85	0.57
1:A:141:ARG:NH1	2:O:11:ASP:OD2	2.38	0.56
7:T:21:ILE:HD11	10:W:82:PHE:CZ	2.39	0.56
4:Q:249:ALA:HB3	5:R:197:ILE:HG21	1.86	0.56
11:X:28:ASN:ND2	11:X:31:ASP:OD2	2.39	0.56
11:K:28:ASN:ND2	11:K:31:ASP:OD2	2.39	0.56
1:A:14:LEU:HD11	1:N:139:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG22	1:N:14:LEU:HD11	1.87	0.55
1:A:117:TYR:OH	1:N:157:LEU:HD22	2.07	0.55
2:B:11:ASP:OD2	1:N:141:ARG:NH1	2.39	0.55
1:N:374:ARG:NH2	1:N:402:ALA:HB2	2.22	0.55
18:A:505:3PE:H2I3	1:N:117:TYR:CB	2.37	0.54
1:A:181:PRO:HG2	17:A:504:MQ9:H3D	1.88	0.54
1:A:374:ARG:NH2	1:A:402:ALA:HB2	2.22	0.54
23:P:302:HEC:HMB1	23:P:302:HEC:HBB3	1.90	0.54
1:N:356:GLN:HG3	2:O:397:LEU:HD21	1.90	0.54
23:C:302:HEC:HMB1	23:C:302:HEC:HBB3	1.90	0.53
2:O:142:ILE:HG23	21:O:607:LYC:H672	1.91	0.53
2:B:142:ILE:HG23	21:B:606:LYC:H672	1.91	0.53
2:O:20:ILE:HD11	22:O:601:LMT:H62	1.91	0.52
1:A:67:GLY:HA3	1:N:173:LEU:HD12	1.92	0.52
3:C:104:ILE:HD11	3:C:111:ALA:HB2	1.91	0.52
4:Q:364:VAL:CG1	18:Q:607:3PE:H241	2.39	0.52
2:B:20:ILE:HD11	22:B:608:LMT:H62	1.91	0.52
4:D:364:VAL:CG1	18:D:607:3PE:H241	2.39	0.52
1:N:181:PRO:HD2	17:N:501:MQ9:H3D	1.93	0.51
3:P:104:ILE:HD11	3:P:111:ALA:HB2	1.91	0.51
3:C:51:ASP:OD1	3:C:51:ASP:N	2.44	0.51
2:O:473:ALA:HB1	11:X:69:THR:HG22	1.92	0.51
4:D:154:MET:O	4:D:256:TRP:NE1	2.44	0.51
4:D:292:PHE:O	4:D:344:ASN:ND2	2.44	0.51
1:A:181:PRO:CD	17:A:504:MQ9:H3D	2.41	0.51
1:A:374:ARG:NH1	2:B:312:GLU:OE2	2.42	0.51
4:Q:292:PHE:O	4:Q:344:ASN:ND2	2.44	0.51
4:D:272:ALA:HA	4:D:406:THR:HG21	1.93	0.50
4:Q:154:MET:O	4:Q:256:TRP:NE1	2.44	0.50
1:N:255:ASP:HA	3:P:224:ARG:HD3	1.94	0.50
4:Q:272:ALA:HA	4:Q:406:THR:HG21	1.93	0.50
1:A:173:LEU:HD12	1:N:67:GLY:HA3	1.93	0.50
4:D:265:HIS:O	4:D:268:VAL:HG22	2.11	0.50
3:P:51:ASP:OD1	3:P:51:ASP:N	2.44	0.50
2:O:59:ASP:HB3	2:O:85:THR:HG21	1.94	0.50
2:B:132:GLU:OE1	2:O:13:ARG:NH1	2.45	0.49
2:O:311:TRP:CE3	30:Z:201:DGA:HA32	2.48	0.49
4:Q:265:HIS:O	4:Q:268:VAL:HG22	2.11	0.49
6:S:64:THR:OG1	6:S:205:GLN:OE1	2.30	0.49
1:A:356:GLN:HG3	2:B:397:LEU:HD21	1.93	0.49
2:B:49:LEU:HB3	17:N:501:MQ9:H5M3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD21	18:A:505:3PE:H2D1	1.95	0.49
6:F:64:THR:OG1	6:F:205:GLN:OE1	2.30	0.49
23:C:302:HEC:HMC1	23:C:302:HEC:CBC	2.43	0.48
20:S:303:CDL:OA7	20:S:303:CDL:H512	2.13	0.48
2:B:59:ASP:HB3	2:B:85:THR:HG21	1.94	0.48
20:G:201:CDL:OA7	20:G:201:CDL:H512	2.13	0.48
1:A:336:ILE:HD11	2:B:323:VAL:HG21	1.95	0.48
2:O:484:LEU:HD13	11:X:62:THR:HG22	1.96	0.48
23:P:302:HEC:HMC1	23:P:302:HEC:CBC	2.43	0.48
4:Q:174:VAL:HG11	7:T:111:VAL:HG23	1.94	0.48
1:A:181:PRO:HG2	17:A:504:MQ9:C3D	2.43	0.48
1:N:208:SER:OG	1:N:209:GLY:N	2.47	0.48
1:A:208:SER:OG	1:A:209:GLY:N	2.47	0.48
1:A:214:GLU:OE2	15:A:502:IZL:O20	2.32	0.48
4:Q:371:LEU:HD13	5:R:75:MET:HE2	1.95	0.48
5:R:63:TRP:CE3	30:R:404:DGA:HB52	2.49	0.48
8:U:54:SER:OG	8:U:55:ALA:N	2.47	0.48
5:E:63:TRP:CE3	30:E:404:DGA:HB52	2.49	0.48
1:N:214:GLU:OE2	15:N:504:IZL:O20	2.32	0.48
4:Q:371:LEU:HD13	5:R:75:MET:CE	2.44	0.48
4:D:371:LEU:HD13	5:E:75:MET:HE2	1.95	0.47
8:H:54:SER:OG	8:H:55:ALA:N	2.47	0.47
3:P:103:PRO:HB3	23:P:302:HEC:HMC2	1.96	0.47
4:D:371:LEU:HD13	5:E:75:MET:CE	2.44	0.47
1:A:270:GLU:OE1	1:A:270:GLU:N	2.48	0.47
3:C:103:PRO:HB3	23:C:302:HEC:HMC2	1.96	0.47
2:B:148:GLU:HB2	2:B:208:ILE:HG21	1.97	0.47
1:N:157:LEU:HD21	18:N:502:3PE:H2D1	1.96	0.47
2:B:190:ASP:OD1	2:B:191:PHE:N	2.47	0.47
3:C:219:PRO:HD3	23:C:303:HEC:HBC2	1.97	0.46
20:O:606:CDL:H512	20:P:301:CDL:HA61	1.96	0.46
1:A:181:PRO:CG	17:A:504:MQ9:H3D	2.45	0.46
4:Q:60:ALA:HB2	4:Q:87:HIS:CE1	2.50	0.46
4:D:60:ALA:HB2	4:D:87:HIS:CE1	2.50	0.46
2:B:49:LEU:CB	17:N:501:MQ9:H5M3	2.45	0.46
2:O:190:ASP:OD1	2:O:191:PHE:N	2.47	0.46
20:B:605:CDL:H512	20:C:301:CDL:HA61	1.96	0.46
4:D:395:LEU:HD11	25:D:602:HAS:HHA	1.98	0.46
2:O:148:GLU:HB2	2:O:208:ILE:HG21	1.97	0.46
1:N:270:GLU:N	1:N:270:GLU:OE1	2.48	0.46
3:P:117:ARG:NH2	5:R:240:ALA:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:438:ILE:HG21	2:O:481:MET:HE3	1.98	0.46
3:P:219:PRO:HD3	23:P:303:HEC:HBC2	1.97	0.45
1:A:115:VAL:HG23	2:B:256:ALA:HB1	1.98	0.45
1:N:357:SER:OG	14:N:503:FES:S1	2.58	0.45
2:O:456:GLN:NE2	11:X:62:THR:OG1	2.50	0.45
2:B:293:GLN:OE1	3:C:258:VAL:HG23	2.17	0.45
1:N:406:ARG:NH1	1:N:408:SER:OXT	2.48	0.45
1:A:117:TYR:CB	18:N:502:3PE:H2I3	2.45	0.45
1:A:406:ARG:NH1	1:A:408:SER:OXT	2.48	0.45
1:N:115:VAL:HG23	2:O:256:ALA:HB1	1.98	0.45
1:A:372:ALA:O	9:I:54:ASN:ND2	2.49	0.45
4:Q:36:THR:OG1	7:T:91:PRO:O	2.35	0.45
1:A:114:VAL:HA	18:N:502:3PE:H2I2	1.99	0.45
3:C:117:ARG:NH2	5:E:240:ALA:O	2.49	0.45
7:G:26:THR:HG23	7:G:38:VAL:HA	1.99	0.45
3:C:216:GLN:NE2	23:C:303:HEC:O2D	2.47	0.44
13:M:33:VAL:HG12	13:M:35:ARG:H	1.82	0.44
4:Q:395:LEU:HD11	25:Q:602:HAS:HHA	1.98	0.44
7:T:26:THR:HG23	7:T:38:VAL:HA	1.99	0.44
1:A:152:TRP:HA	18:A:505:3PE:H292	1.97	0.44
4:Q:313:ALA:HB3	4:Q:327:PHE:CE1	2.52	0.44
4:Q:336:VAL:HB	18:W:201:3PE:H2I3	2.00	0.44
4:D:336:VAL:HB	18:J:201:3PE:H2I3	2.00	0.44
4:D:313:ALA:HB3	4:D:327:PHE:CE1	2.52	0.44
7:G:22:TYR:OH	7:G:39:GLU:OE2	2.28	0.44
13:Z:33:VAL:HG12	13:Z:35:ARG:H	1.82	0.44
2:O:293:GLN:OE1	3:P:258:VAL:HG23	2.17	0.44
2:B:49:LEU:HD23	17:N:501:MQ9:H101	1.98	0.43
7:G:127:PHE:CE1	20:G:201:CDL:H531	2.53	0.43
13:M:46:PRO:O	13:M:47:THR:OG1	2.30	0.43
2:B:20:ILE:CD1	22:B:608:LMT:H62	2.49	0.43
2:B:50:THR:CG2	17:N:501:MQ9:H5M1	2.44	0.43
1:N:152:TRP:HA	18:N:502:3PE:H292	1.99	0.43
2:B:438:ILE:HG21	2:B:481:MET:HE3	2.01	0.43
2:B:484:LEU:HD13	11:K:62:THR:HG22	2.00	0.43
2:O:8:ASN:HB2	22:O:601:LMT:O2'	2.19	0.43
9:I:58:HIS:ND1	32:I:202:IX7:O15	2.52	0.43
20:P:301:CDL:H121	20:P:301:CDL:H732	2.00	0.43
2:B:431:ARG:NH2	9:I:23:SER:OG	2.46	0.43
10:W:56:VAL:O	10:W:60:VAL:HG22	2.18	0.43
8:U:176:GLU:O	8:U:179:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:502:IZL:O8	15:A:502:IZL:O6	2.37	0.42
8:H:176:GLU:O	8:H:179:VAL:HG22	2.19	0.42
1:A:180:ALA:HB3	1:N:70:PHE:HE2	1.83	0.42
6:F:34:SER:O	7:G:52:LEU:HD12	2.18	0.42
2:O:20:ILE:CD1	22:O:601:LMT:H62	2.48	0.42
7:G:75:GLU:OE1	7:G:75:GLU:N	2.50	0.42
1:N:372:ALA:O	9:V:54:ASN:ND2	2.53	0.42
20:C:301:CDL:H121	20:C:301:CDL:H732	2.01	0.42
15:A:502:IZL:O24	2:B:317:ASN:OD1	2.37	0.42
2:B:8:ASN:HB2	22:B:608:LMT:O2'	2.20	0.42
2:O:431:ARG:NH2	9:V:23:SER:OG	2.46	0.42
3:C:278:TRP:HB2	20:G:201:CDL:HB61	2.02	0.42
10:J:56:VAL:O	10:J:60:VAL:HG22	2.18	0.42
15:N:504:IZL:O6	15:N:504:IZL:O8	2.37	0.42
1:A:117:TYR:CG	18:N:502:3PE:H2I3	2.55	0.42
6:S:129:HIS:O	6:S:129:HIS:ND1	2.52	0.42
1:A:213:VAL:HG12	1:A:213:VAL:O	2.20	0.42
3:C:111:ALA:HB3	3:C:216:GLN:NE2	2.35	0.42
6:F:129:HIS:O	6:F:129:HIS:ND1	2.52	0.42
6:S:132:THR:OG1	6:S:133:ILE:N	2.53	0.42
8:H:143:GLU:N	8:H:143:GLU:OE1	2.53	0.41
3:P:216:GLN:NE2	23:P:303:HEC:O2D	2.47	0.41
1:N:344:GLU:OE1	1:N:347:THR:OG1	2.30	0.41
2:O:53:TYR:CD1	2:O:99:ILE:HG21	2.55	0.41
3:P:111:ALA:HB3	3:P:216:GLN:NE2	2.35	0.41
6:F:132:THR:OG1	6:F:133:ILE:N	2.53	0.41
6:S:166:ARG:HG2	7:T:134:LEU:HD23	2.03	0.41
1:N:32:VAL:HG11	2:O:25:ASN:HB3	2.02	0.41
1:N:213:VAL:O	1:N:213:VAL:HG12	2.20	0.41
2:O:237:THR:OG1	2:O:238:GLU:N	2.53	0.41
2:B:146:MET:SD	21:B:606:LYC:H683	2.61	0.41
2:O:59:ASP:CB	2:O:85:THR:HG21	2.51	0.41
19:B:603:HEM:HMC2	19:B:603:HEM:HBC2	2.02	0.41
2:B:14:TYR:OH	2:O:133:ALA:CB	2.69	0.41
2:B:53:TYR:CD1	2:B:99:ILE:HG21	2.55	0.41
2:B:230:GLN:NE2	2:B:240:ASN:O	2.54	0.41
2:O:488:GLU:OE2	7:T:140:LYS:N	2.50	0.41
4:Q:105:ASN:OD1	4:Q:123:ASN:ND2	2.54	0.41
2:O:45:ILE:O	2:O:49:LEU:HD13	2.20	0.41
2:O:146:MET:SD	21:O:607:LYC:H683	2.61	0.41
4:Q:223:LEU:HD23	7:T:52:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:143:GLU:OE1	8:U:143:GLU:N	2.53	0.41
25:D:602:HAS:HHD	25:D:602:HAS:HMA1	1.93	0.41
3:P:278:TRP:HB2	20:S:303:CDL:HB61	2.02	0.41
4:Q:464:ASP:OD1	4:Q:465:TYR:N	2.54	0.41
6:S:34:SER:O	7:T:52:LEU:HD12	2.20	0.41
2:B:237:THR:OG1	2:B:238:GLU:N	2.53	0.40
1:N:152:TRP:CE3	18:N:502:3PE:H261	2.56	0.40
2:B:14:TYR:OH	2:O:133:ALA:HB2	2.21	0.40
4:D:357:GLU:OE1	4:D:357:GLU:N	2.48	0.40
2:O:171:ILE:HD13	17:O:602:MQ9:H72	2.03	0.40
1:A:152:TRP:CE3	18:A:505:3PE:H261	2.56	0.40
2:B:59:ASP:CB	2:B:85:THR:HG21	2.51	0.40
7:T:22:TYR:OH	7:T:39:GLU:OE2	2.28	0.40
2:O:171:ILE:HD13	17:O:602:MQ9:C7	2.52	0.40
2:O:421:ARG:NH1	20:Q:606:CDL:OB3	2.50	0.40
19:O:604:HEM:HMC2	19:O:604:HEM:HBC2	2.02	0.40
4:Q:522:THR:OG1	4:Q:523:SER:N	2.54	0.40
7:T:3:SER:OG	10:W:35:GLU:OE1	2.39	0.40
1:A:399:LEU:HD23	1:A:399:LEU:H	1.86	0.40
17:A:504:MQ9:H5M3	2:O:49:LEU:HB3	2.04	0.40
4:D:105:ASN:OD1	4:D:123:ASN:ND2	2.54	0.40
4:D:464:ASP:OD1	4:D:465:TYR:N	2.54	0.40
7:G:21:ILE:HD11	10:J:82:PHE:CE2	2.56	0.40

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	400/408 (98%)	376 (94%)	24 (6%)	0	100	100
1	N	400/408 (98%)	376 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	537/539 (100%)	525 (98%)	12 (2%)	0	100	100
2	O	537/539 (100%)	524 (98%)	13 (2%)	0	100	100
3	C	231/283 (82%)	219 (95%)	12 (5%)	0	100	100
3	P	231/283 (82%)	219 (95%)	12 (5%)	0	100	100
4	D	572/594 (96%)	556 (97%)	16 (3%)	0	100	100
4	Q	572/594 (96%)	556 (97%)	16 (3%)	0	100	100
5	E	329/331 (99%)	311 (94%)	17 (5%)	1 (0%)	37	68
5	R	329/331 (99%)	311 (94%)	17 (5%)	1 (0%)	37	68
6	F	188/205 (92%)	187 (100%)	1 (0%)	0	100	100
6	S	188/205 (92%)	187 (100%)	1 (0%)	0	100	100
7	G	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
7	T	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
8	H	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
8	U	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
9	I	127/147 (86%)	120 (94%)	7 (6%)	0	100	100
9	V	127/147 (86%)	120 (94%)	7 (6%)	0	100	100
10	J	98/112 (88%)	96 (98%)	2 (2%)	0	100	100
10	W	98/112 (88%)	96 (98%)	2 (2%)	0	100	100
11	K	55/73 (75%)	54 (98%)	1 (2%)	0	100	100
11	X	55/73 (75%)	54 (98%)	1 (2%)	0	100	100
12	L	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
12	Y	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
13	M	23/168 (14%)	23 (100%)	0	0	100	100
13	Z	23/168 (14%)	23 (100%)	0	0	100	100
All	All	5828/6462 (90%)	5623 (96%)	203 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	242	VAL
5	R	242	VAL

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	326/332 (98%)	325 (100%)	1 (0%)	91	95
1	N	326/332 (98%)	325 (100%)	1 (0%)	91	95
2	B	442/441 (100%)	437 (99%)	5 (1%)	70	84
2	O	442/441 (100%)	437 (99%)	5 (1%)	70	84
3	C	177/212 (84%)	175 (99%)	2 (1%)	70	84
3	P	177/212 (84%)	175 (99%)	2 (1%)	70	84
4	D	472/488 (97%)	467 (99%)	5 (1%)	70	84
4	Q	472/488 (97%)	467 (99%)	5 (1%)	70	84
5	E	274/274 (100%)	272 (99%)	2 (1%)	81	90
5	R	274/274 (100%)	272 (99%)	2 (1%)	81	90
6	F	156/166 (94%)	155 (99%)	1 (1%)	84	91
6	S	156/166 (94%)	155 (99%)	1 (1%)	84	91
7	G	114/114 (100%)	114 (100%)	0	100	100
7	T	114/114 (100%)	114 (100%)	0	100	100
8	H	127/133 (96%)	127 (100%)	0	100	100
8	U	127/133 (96%)	127 (100%)	0	100	100
9	I	111/125 (89%)	110 (99%)	1 (1%)	75	88
9	V	111/125 (89%)	110 (99%)	1 (1%)	75	88
10	J	80/90 (89%)	79 (99%)	1 (1%)	65	82
10	W	80/90 (89%)	79 (99%)	1 (1%)	65	82
11	K	48/63 (76%)	48 (100%)	0	100	100
11	X	48/63 (76%)	48 (100%)	0	100	100
12	L	43/45 (96%)	43 (100%)	0	100	100
12	Y	43/45 (96%)	43 (100%)	0	100	100
13	M	25/135 (18%)	25 (100%)	0	100	100
13	Z	25/135 (18%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4790/5236 (92%)	4754 (99%)	36 (1%)	80 89

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	SER
2	B	16	MET
2	B	224[A]	TRP
2	B	224[B]	TRP
2	B	268	LEU
2	B	495	PHE
3	C	67	CYS
3	C	117	ARG
4	D	45	TYR
4	D	150	PHE
4	D	263	PHE
4	D	314	HIS
4	D	462	TYR
5	E	65	TRP
5	E	132	GLN
6	F	35	GLN
9	I	46	PHE
10	J	58	PHE
1	N	103	SER
2	O	16	MET
2	O	224[A]	TRP
2	O	224[B]	TRP
2	O	268	LEU
2	O	495	PHE
3	P	67	CYS
3	P	117	ARG
4	Q	45	TYR
4	Q	150	PHE
4	Q	263	PHE
4	Q	314	HIS
4	Q	462	TYR
5	R	65	TRP
5	R	132	GLN
6	S	35	GLN
9	V	46	PHE
10	W	58	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	A	287	HIS
1	N	232	HIS
1	N	287	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 78 ligands modelled in this entry, 6 are monoatomic and 4 are modelled with single atom - leaving 68 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	$\#\|Z\| > 2$
17	MQ9	B	601	-	24,24,59	0.44	0	30,33,75	0.61	1 (3%)
17	MQ9	N	501	-	27,27,59	0.96	1 (3%)	33,36,75	1.72	2 (6%)
20	CDL	B	605	-	44,44,99	0.42	0	50,56,111	0.43	0
23	HEC	C	302	3	32,50,50	1.22	2 (6%)	24,82,82	1.82	6 (25%)
18	3PE	N	502	-	37,37,50	0.39	0	40,42,55	0.72	1 (2%)
16	9YF	N	505	-	36,36,58	0.35	0	46,48,71	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	HEC	C	303	3	32,50,50	1.40	2 (6%)	24,82,82	1.91	6 (25%)
30	DGA	E	404	-	19,19,43	0.27	0	21,21,45	0.26	0
16	9YF	A	503	-	36,36,58	0.35	0	46,48,71	0.51	0
19	HEM	B	602	2	41,50,50	1.10	2 (4%)	45,82,82	1.18	4 (8%)
17	MQ9	A	504	-	27,27,59	0.96	1 (3%)	33,36,75	1.72	2 (6%)
24	3PH	C	304	-	36,36,47	0.28	0	39,40,52	0.55	1 (2%)
22	LMT	B	608	-	33,33,36	0.40	0	44,44,47	0.74	1 (2%)
30	DGA	R	404	-	19,19,43	0.27	0	21,21,45	0.26	0
18	3PE	J	201	-	46,46,50	0.32	0	49,51,55	0.31	0
19	HEM	O	604	2	41,50,50	1.12	2 (4%)	45,82,82	1.15	2 (4%)
20	CDL	D	606	-	62,62,99	0.38	0	68,74,111	0.36	0
20	CDL	S	302	-	56,56,99	0.38	0	62,68,111	0.33	0
23	HEC	P	302	3	32,50,50	1.21	2 (6%)	24,82,82	1.83	6 (25%)
20	CDL	C	301	-	64,64,99	0.37	0	70,76,111	0.36	0
20	CDL	S	303	-	61,61,99	0.38	0	67,73,111	0.39	0
24	3PH	T	201	-	36,36,47	0.28	0	39,40,52	0.55	1 (2%)
18	3PE	F	301	-	31,31,50	0.40	0	34,36,55	0.68	1 (2%)
22	LMT	O	601	-	33,33,36	0.40	0	44,44,47	0.74	1 (2%)
31	PLM	U	202	8	13,13,17	0.25	0	11,11,17	0.18	0
15	IZL	N	504	-	108,108,119	0.40	0	150,152,163	1.04	11 (7%)
30	DGA	U	201	-	16,16,43	0.29	0	18,18,45	0.20	0
20	CDL	V	201	-	56,56,99	0.38	0	62,68,111	0.34	0
16	9YF	U	203	-	34,34,58	0.38	0	44,46,71	0.37	0
20	CDL	O	606	-	44,44,99	0.42	0	50,56,111	0.43	0
30	DGA	M	201	-	21,21,43	0.27	0	23,23,45	0.23	0
32	IX7	I	202	-	74,74,97	0.30	0	97,99,123	0.83	6 (6%)
20	CDL	F	302	-	56,56,99	0.38	0	62,68,111	0.33	0
25	HAS	D	602	4	69,72,72	1.18	6 (8%)	73,109,109	1.62	14 (19%)
31	PLM	M	202	13	4,4,17	0.33	0	3,3,17	0.46	0
18	3PE	S	301	-	31,31,50	0.40	0	34,36,55	0.68	1 (2%)
14	FES	N	503	1	0,4,4	-	-	-		
20	CDL	Q	605	-	76,76,99	0.35	0	82,88,111	0.50	1 (1%)
18	3PE	D	607	-	30,30,50	0.38	0	33,35,55	0.33	0
18	3PE	A	505	-	37,37,50	0.39	0	40,42,55	0.72	1 (2%)
19	HEM	B	603	2	41,50,50	1.12	2 (4%)	45,82,82	1.15	2 (4%)
15	IZL	A	502	-	108,108,119	0.40	0	150,152,163	1.04	11 (7%)
16	9YF	B	607	-	34,34,58	0.38	0	44,46,71	0.36	0
18	3PE	E	405	-	30,30,50	0.38	0	33,35,55	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	HEM	O	603	2	41,50,50	1.10	2 (4%)	45,82,82	1.18	4 (8%)
20	CDL	D	605	-	76,76,99	0.35	0	82,88,111	0.50	1 (1%)
20	CDL	P	301	-	64,64,99	0.37	0	70,76,111	0.36	0
31	PLM	Z	202	13	4,4,17	0.33	0	3,3,17	0.46	0
20	CDL	G	201	-	61,61,99	0.38	0	67,73,111	0.39	0
25	HAS	D	601	4	69,72,72	1.18	5 (7%)	73,109,109	1.45	12 (16%)
17	MQ9	O	605	-	24,24,59	0.40	0	30,33,75	0.66	1 (3%)
18	3PE	R	405	-	30,30,50	0.38	0	33,35,55	0.35	0
23	HEC	P	303	3	32,50,50	1.40	2 (6%)	24,82,82	1.92	6 (25%)
25	HAS	Q	602	4	69,72,72	1.18	5 (7%)	73,109,109	1.62	14 (19%)
20	CDL	Q	606	-	62,62,99	0.38	0	68,74,111	0.36	0
32	IX7	R	406	-	74,74,97	0.30	0	97,99,123	0.83	6 (6%)
30	DGA	Z	201	-	21,21,43	0.27	0	23,23,45	0.23	0
21	LYC	O	607	-	39,39,39	0.20	0	44,46,46	0.39	0
14	FES	A	501	1	0,4,4	-	-	-		
31	PLM	H	202	8	13,13,17	0.25	0	11,11,17	0.18	0
17	MQ9	B	604	-	24,24,59	0.40	0	30,33,75	0.67	1 (3%)
21	LYC	B	606	-	39,39,39	0.19	0	44,46,46	0.39	0
30	DGA	H	201	-	16,16,43	0.29	0	18,18,45	0.20	0
20	CDL	I	201	-	56,56,99	0.38	0	62,68,111	0.34	0
25	HAS	Q	601	4	69,72,72	1.18	5 (7%)	73,109,109	1.45	12 (16%)
18	3PE	W	201	-	46,46,50	0.32	0	49,51,55	0.31	0
18	3PE	Q	607	-	30,30,50	0.38	0	33,35,55	0.33	0
17	MQ9	O	602	-	24,24,59	0.44	0	30,33,75	0.61	1 (3%)

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
17	MQ9	B	601	-	-	3/11/31/73	0/2/2/2
17	MQ9	N	501	-	-	6/15/35/73	0/2/2/2
20	CDL	B	605	-	-	7/54/54/110	-
23	HEC	C	302	3	-	3/10/54/54	-
18	3PE	N	502	-	-	25/41/41/54	-
16	9YF	N	505	-	-	6/31/55/78	0/1/1/1
23	HEC	C	303	3	-	0/10/54/54	-
30	DGA	E	404	-	-	0/20/20/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	9YF	A	503	-	-	6/31/55/78	0/1/1/1
19	HEM	B	602	2	-	3/12/54/54	-
17	MQ9	A	504	-	-	6/15/35/73	0/2/2/2
24	3PH	C	304	-	-	8/37/37/49	-
22	LMT	B	608	-	-	3/18/58/61	0/2/2/2
30	DGA	R	404	-	-	0/20/20/45	-
18	3PE	J	201	-	-	7/50/50/54	-
19	HEM	O	604	2	-	2/12/54/54	-
20	CDL	D	606	-	-	21/73/73/110	-
20	CDL	S	302	-	-	19/67/67/110	-
23	HEC	P	302	3	-	3/10/54/54	-
20	CDL	C	301	-	-	16/75/75/110	-
20	CDL	S	303	-	-	19/72/72/110	-
24	3PH	T	201	-	-	8/37/37/49	-
18	3PE	F	301	-	-	16/35/35/54	-
22	LMT	O	601	-	-	3/18/58/61	0/2/2/2
31	PLM	U	202	8	-	0/8/9/15	-
15	IZL	N	504	-	-	34/73/197/208	0/6/6/6
30	DGA	U	201	-	-	1/17/17/45	-
20	CDL	V	201	-	-	19/67/67/110	-
16	9YF	U	203	-	-	5/29/53/78	0/1/1/1
20	CDL	O	606	-	-	7/54/54/110	-
30	DGA	M	201	-	-	3/22/22/45	-
32	IX7	I	202	-	-	29/58/122/146	0/3/3/3
20	CDL	F	302	-	-	19/67/67/110	-
25	HAS	D	602	4	1/1/18/18	12/40/82/82	-
31	PLM	M	202	13	-	0/1/2/15	-
18	3PE	S	301	-	-	16/35/35/54	-
14	FES	N	503	1	-	-	0/1/1/1
20	CDL	Q	605	-	-	27/87/87/110	-
18	3PE	D	607	-	-	5/34/34/54	-
18	3PE	A	505	-	-	25/41/41/54	-
19	HEM	B	603	2	-	2/12/54/54	-
15	IZL	A	502	-	-	34/73/197/208	0/6/6/6
16	9YF	B	607	-	-	5/29/53/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	E	405	-	-	1/34/34/54	-
19	HEM	O	603	2	-	3/12/54/54	-
20	CDL	D	605	-	-	27/87/87/110	-
20	CDL	P	301	-	-	16/75/75/110	-
31	PLM	Z	202	13	-	0/1/2/15	-
25	HAS	D	601	4	1/1/18/18	9/40/82/82	-
20	CDL	G	201	-	-	19/72/72/110	-
17	MQ9	O	605	-	-	0/11/31/73	0/2/2/2
25	HAS	Q	602	4	1/1/18/18	12/40/82/82	-
18	3PE	R	405	-	-	1/34/34/54	-
23	HEC	P	303	3	-	0/10/54/54	-
20	CDL	Q	606	-	-	21/73/73/110	-
32	IX7	R	406	-	-	29/58/122/146	0/3/3/3
30	DGA	Z	201	-	-	3/22/22/45	-
21	LYC	O	607	-	-	3/43/43/43	-
14	FES	A	501	1	-	-	0/1/1/1
31	PLM	H	202	8	-	0/8/9/15	-
17	MQ9	B	604	-	-	0/11/31/73	0/2/2/2
21	LYC	B	606	-	-	3/43/43/43	-
30	DGA	H	201	-	-	1/17/17/45	-
20	CDL	I	201	-	-	19/67/67/110	-
25	HAS	Q	601	4	1/1/18/18	9/40/82/82	-
18	3PE	W	201	-	-	8/50/50/54	-
18	3PE	Q	607	-	-	5/34/34/54	-
17	MQ9	O	602	-	-	3/11/31/73	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	602	HAS	OMD-CMD	4.95	1.33	1.22
25	Q	602	HAS	OMD-CMD	4.93	1.33	1.22
25	D	601	HAS	OMD-CMD	4.91	1.33	1.22
25	Q	601	HAS	OMD-CMD	4.89	1.33	1.22
23	P	303	HEC	C3C-C2C	-4.80	1.35	1.40
23	C	303	HEC	C3C-C2C	-4.78	1.35	1.40
23	C	303	HEC	C2B-C3B	-4.61	1.35	1.40
23	P	303	HEC	C2B-C3B	-4.61	1.35	1.40
23	C	302	HEC	C3C-C2C	-4.06	1.36	1.40
23	P	302	HEC	C3C-C2C	-4.06	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	504	MQ9	C6-C5	3.91	1.42	1.35
17	N	501	MQ9	C6-C5	3.88	1.42	1.35
23	C	302	HEC	C2B-C3B	-3.79	1.36	1.40
23	P	302	HEC	C2B-C3B	-3.68	1.36	1.40
25	Q	601	HAS	CMD-C2D	3.27	1.52	1.45
25	D	601	HAS	CMD-C2D	3.24	1.52	1.45
19	B	602	HEM	C3C-C2C	-3.02	1.36	1.40
19	O	604	HEM	C3C-C2C	-3.00	1.36	1.40
25	D	602	HAS	CMD-C2D	2.99	1.51	1.45
19	O	603	HEM	C3C-C2C	-2.99	1.36	1.40
25	Q	602	HAS	CMD-C2D	2.98	1.51	1.45
19	B	603	HEM	C3C-C2C	-2.97	1.36	1.40
25	D	601	HAS	C3C-C2C	-2.91	1.36	1.40
25	Q	601	HAS	C3C-C2C	-2.91	1.36	1.40
25	Q	602	HAS	C3C-C2C	-2.72	1.36	1.40
25	D	602	HAS	C3C-C2C	-2.70	1.36	1.40
25	Q	601	HAS	C3C-CAC	2.68	1.53	1.47
25	D	601	HAS	C3C-CAC	2.65	1.53	1.47
25	Q	602	HAS	C3C-CAC	2.60	1.53	1.47
25	D	602	HAS	C3C-CAC	2.59	1.53	1.47
19	B	603	HEM	C3C-CAC	2.39	1.52	1.47
19	O	604	HEM	C3C-CAC	2.39	1.52	1.47
19	B	602	HEM	C3C-CAC	2.36	1.52	1.47
25	D	601	HAS	CHD-C4A	2.35	1.38	1.35
19	O	603	HEM	C3C-CAC	2.34	1.52	1.47
25	Q	601	HAS	CHD-C4A	2.28	1.38	1.35
25	Q	602	HAS	CHD-C4A	2.23	1.38	1.35
25	D	602	HAS	CHD-C4A	2.22	1.38	1.35
25	D	602	HAS	FE-NA	2.00	2.03	1.95

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	504	MQ9	C8-C7-C6	8.57	135.14	112.05
17	N	501	MQ9	C8-C7-C6	8.56	135.12	112.05
25	Q	602	HAS	C26-C15-C16	4.49	122.83	115.27
25	D	602	HAS	C26-C15-C16	4.46	122.78	115.27
23	C	302	HEC	CMB-C2B-C1B	-4.29	121.88	128.46
23	P	302	HEC	CMB-C2B-C1B	-4.28	121.89	128.46
25	Q	602	HAS	CMC-C2C-C1C	-4.23	121.96	128.46
25	D	602	HAS	CMC-C2C-C1C	-4.23	121.96	128.46
23	P	302	HEC	CMB-C2B-C3B	3.94	130.45	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	303	HEC	CMB-C2B-C1B	-3.92	122.43	128.46
23	C	302	HEC	CMB-C2B-C3B	3.92	130.43	125.82
23	C	303	HEC	CMB-C2B-C1B	-3.91	122.46	128.46
25	Q	601	HAS	C25-C23-C24	3.83	121.71	115.27
25	D	602	HAS	CAA-C2A-C3A	3.81	134.98	127.88
25	D	601	HAS	C25-C23-C24	3.81	121.68	115.27
25	Q	602	HAS	CAA-C2A-C3A	3.80	134.96	127.88
23	C	303	HEC	CMB-C2B-C3B	3.64	130.10	125.82
23	P	303	HEC	CMB-C2B-C3B	3.64	130.09	125.82
23	C	303	HEC	CBA-CAA-C2A	-3.59	106.55	112.60
23	P	303	HEC	CBA-CAA-C2A	-3.59	106.55	112.60
15	A	502	IZL	O16-C30-C25	-3.54	99.75	108.61
25	Q	602	HAS	OMD-CMD-C2D	-3.54	117.68	125.69
15	N	504	IZL	O16-C30-C25	-3.54	99.77	108.61
25	D	602	HAS	OMD-CMD-C2D	-3.53	117.71	125.69
23	P	303	HEC	CBD-CAD-C3D	-3.46	106.71	112.62
23	C	303	HEC	CBD-CAD-C3D	-3.46	106.72	112.62
25	Q	602	HAS	C26-C15-C14	-3.44	114.86	123.68
25	D	602	HAS	C26-C15-C14	-3.42	114.91	123.68
25	D	602	HAS	CAA-C2A-C1A	-3.27	118.72	124.89
25	Q	602	HAS	CAA-C2A-C1A	-3.27	118.73	124.89
19	B	603	HEM	CMC-C2C-C3C	3.26	130.78	124.68
19	O	604	HEM	CMC-C2C-C3C	3.25	130.76	124.68
25	Q	601	HAS	OMD-CMD-C2D	-3.21	118.44	125.69
25	D	601	HAS	OMD-CMD-C2D	-3.19	118.47	125.69
25	Q	602	HAS	CMC-C2C-C3C	3.19	130.64	124.68
25	D	602	HAS	CMC-C2C-C3C	3.19	130.64	124.68
25	D	601	HAS	C16-C15-C14	3.17	127.53	121.12
25	Q	601	HAS	C16-C15-C14	3.17	127.52	121.12
15	N	504	IZL	O11-C24-C23	-3.16	103.20	109.05
15	A	502	IZL	O11-C24-C23	-3.15	103.22	109.05
25	D	601	HAS	CMC-C2C-C1C	-3.12	123.67	128.46
25	Q	601	HAS	CMC-C2C-C1C	-3.08	123.72	128.46
15	A	502	IZL	O34-C45-C46	3.05	119.43	108.40
15	N	504	IZL	O34-C45-C46	3.03	119.38	108.40
25	D	601	HAS	C25-C23-C22	-3.01	115.96	123.68
25	Q	601	HAS	C25-C23-C22	-3.00	115.98	123.68
15	N	504	IZL	O2-C13-C71	2.99	116.67	110.35
15	A	502	IZL	O2-C13-C71	2.98	116.67	110.35
15	A	502	IZL	C13-C71-C72	2.98	116.21	110.00
15	N	504	IZL	C13-C71-C72	2.97	116.19	110.00
17	B	604	MQ9	C7-C6-C1	-2.95	115.34	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O	605	MQ9	C7-C6-C1	-2.93	115.37	118.50
25	Q	601	HAS	C17-C18-C19	-2.91	120.65	127.66
23	P	302	HEC	CMC-C2C-C1C	-2.90	124.00	128.46
23	C	302	HEC	CMC-C2C-C1C	-2.90	124.00	128.46
25	D	601	HAS	C17-C18-C19	-2.90	120.69	127.66
25	Q	601	HAS	C26-C15-C14	-2.89	116.26	123.68
25	D	601	HAS	C26-C15-C14	-2.88	116.28	123.68
22	O	601	LMT	O2'-C2'-C3'	-2.86	103.74	110.35
22	B	608	LMT	O2'-C2'-C3'	-2.85	103.77	110.35
25	D	601	HAS	C32-C30-C31	2.74	120.66	114.60
25	Q	601	HAS	C32-C30-C31	2.73	120.64	114.60
23	P	302	HEC	CMC-C2C-C3C	2.72	129.02	125.82
23	P	303	HEC	CMD-C2D-C1D	-2.68	124.34	128.46
23	C	302	HEC	CMC-C2C-C3C	2.68	128.97	125.82
23	C	303	HEC	CMD-C2D-C1D	-2.65	124.39	128.46
15	A	502	IZL	C72-C73-C12	-2.65	105.51	110.24
18	F	301	3PE	O21-C2-C3	2.65	117.99	108.40
15	N	504	IZL	C72-C73-C12	-2.65	105.52	110.24
18	S	301	3PE	O21-C2-C3	2.65	117.99	108.40
25	Q	602	HAS	C25-C23-C24	2.63	119.70	115.27
25	D	602	HAS	C25-C23-C24	2.62	119.67	115.27
15	A	502	IZL	C25-C30-C29	2.61	114.88	110.38
19	O	603	HEM	CMC-C2C-C3C	2.61	129.56	124.68
19	B	602	HEM	CMC-C2C-C3C	2.61	129.56	124.68
15	N	504	IZL	C25-C30-C29	2.59	114.84	110.38
15	A	502	IZL	O32-C46-C45	2.59	115.97	108.43
15	N	504	IZL	O32-C46-C45	2.59	115.96	108.43
15	N	504	IZL	C38-C37-C23	-2.53	105.72	110.24
15	A	502	IZL	C38-C37-C23	-2.52	105.75	110.24
32	I	202	IX7	P-O13-C30	2.51	128.55	119.41
32	R	406	IX7	P-O13-C30	2.51	128.54	119.41
23	P	303	HEC	CMC-C2C-C1C	-2.50	124.62	128.46
23	C	303	HEC	CMC-C2C-C1C	-2.50	124.62	128.46
25	D	602	HAS	CMA-C3A-C4A	-2.49	120.32	124.71
23	C	302	HEC	CBD-CAD-C3D	-2.49	108.37	112.62
25	Q	602	HAS	CMA-C3A-C4A	-2.49	120.33	124.71
23	P	302	HEC	CMD-C2D-C1D	-2.49	124.64	128.46
25	Q	602	HAS	CMA-C3A-C2A	2.48	132.85	126.12
19	O	603	HEM	C4B-CHC-C1C	2.48	125.83	122.56
23	C	302	HEC	CMD-C2D-C1D	-2.47	124.66	128.46
20	Q	605	CDL	OB6-CB4-CB3	2.47	117.36	108.40
25	D	602	HAS	CMA-C3A-C2A	2.47	132.83	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	605	CDL	OB6-CB4-CB3	2.47	117.34	108.40
23	P	302	HEC	CBD-CAD-C3D	-2.47	108.41	112.62
19	B	602	HEM	C4B-CHC-C1C	2.45	125.80	122.56
32	R	406	IX7	O6-C22-C21	-2.43	104.72	110.35
25	D	601	HAS	C20-C19-C18	2.42	126.02	121.12
32	I	202	IX7	O6-C22-C21	-2.42	104.76	110.35
19	B	602	HEM	C1B-NB-C4B	2.42	107.57	105.07
25	Q	601	HAS	C20-C19-C18	2.41	125.99	121.12
17	N	501	MQ9	C5M-C5-C4	-2.37	112.35	116.27
17	A	504	MQ9	C5M-C5-C4	-2.35	112.37	116.27
19	O	603	HEM	C1B-NB-C4B	2.35	107.50	105.07
32	I	202	IX7	O2-C17-C16	2.31	111.33	106.67
32	R	406	IX7	O2-C17-C16	2.30	111.31	106.67
17	O	602	MQ9	C7-C6-C1	-2.28	116.06	118.50
17	B	601	MQ9	C7-C6-C1	-2.28	116.06	118.50
18	N	502	3PE	O21-C2-C3	-2.25	100.27	108.40
18	A	505	3PE	O21-C2-C3	-2.23	100.33	108.40
15	A	502	IZL	C24-C23-C37	2.20	116.68	112.09
15	N	504	IZL	C24-C23-C37	2.19	116.66	112.09
25	D	602	HAS	C21-C22-C23	-2.19	122.40	127.66
25	Q	602	HAS	C21-C22-C23	-2.18	122.40	127.66
19	O	604	HEM	C4D-ND-C1D	2.18	107.32	105.07
19	B	603	HEM	C4D-ND-C1D	2.16	107.31	105.07
15	N	504	IZL	C31-O17-C32	2.12	117.86	113.69
32	I	202	IX7	C24-O7-C23	2.11	123.19	117.96
15	A	502	IZL	C31-O17-C32	2.11	117.83	113.69
25	D	601	HAS	C4B-NB-C1B	2.11	107.25	105.07
32	R	406	IX7	C24-O7-C23	2.10	123.16	117.96
19	B	602	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
25	D	602	HAS	C32-C30-C29	-2.09	116.61	122.65
24	C	304	3PH	P-O11-C1	2.08	124.03	118.30
25	D	601	HAS	CMC-C2C-C3C	2.08	128.57	124.68
19	O	603	HEM	CAD-CBD-CGD	-2.08	109.12	113.60
25	Q	602	HAS	C32-C30-C31	2.08	119.20	114.60
25	Q	601	HAS	C4B-NB-C1B	2.08	107.22	105.07
24	T	201	3PH	P-O11-C1	2.08	124.02	118.30
25	Q	602	HAS	C32-C30-C29	-2.08	116.65	122.65
25	D	601	HAS	CAA-CBA-CGA	-2.07	109.14	113.60
25	Q	601	HAS	CAA-CBA-CGA	-2.07	109.14	113.60
25	Q	601	HAS	CMC-C2C-C3C	2.07	128.55	124.68
25	D	602	HAS	C32-C30-C31	2.07	119.17	114.60
25	Q	602	HAS	C4B-NB-C1B	2.07	107.21	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	R	406	IX7	C16-C17-C69	2.06	116.40	112.09
32	I	202	IX7	C16-C17-C69	2.05	116.37	112.09
25	D	602	HAS	C4B-NB-C1B	2.02	107.16	105.07
32	R	406	IX7	O15-P-O14	2.01	122.16	112.24
32	I	202	IX7	O15-P-O14	2.00	122.15	112.24

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	D	601	HAS	NA
25	D	602	HAS	NA
25	Q	601	HAS	NA
25	Q	602	HAS	NA

All (625) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	502	IZL	O34-C45-C46-O32
15	A	502	IZL	C61-C60-O34-C45
15	A	502	IZL	O35-C60-O34-C45
15	A	502	IZL	C44-O31-P-O28
15	N	504	IZL	O34-C45-C46-O32
15	N	504	IZL	C61-C60-O34-C45
15	N	504	IZL	O35-C60-O34-C45
15	N	504	IZL	C44-O31-P-O28
16	A	503	9YF	C2-O2-P-O1
16	B	607	9YF	C1-O-P-O2
16	B	607	9YF	C1-O-P-O8
16	N	505	9YF	C2-O2-P-O1
16	U	203	9YF	C1-O-P-O2
16	U	203	9YF	C1-O-P-O8
18	A	505	3PE	C1-O11-P-O12
18	A	505	3PE	C1-O11-P-O14
18	A	505	3PE	O13-C11-C12-N
18	F	301	3PE	C11-O13-P-O12
18	F	301	3PE	C11-O13-P-O14
18	J	201	3PE	C11-O13-P-O12
18	N	502	3PE	C1-O11-P-O12
18	N	502	3PE	C1-O11-P-O14
18	N	502	3PE	O13-C11-C12-N
18	S	301	3PE	C11-O13-P-O12
18	S	301	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
18	W	201	3PE	C11-O13-P-O12
20	C	301	CDL	CB2-OB2-PB2-OB3
20	C	301	CDL	CB3-OB5-PB2-OB2
20	C	301	CDL	CB3-OB5-PB2-OB3
20	C	301	CDL	CB3-OB5-PB2-OB4
20	D	605	CDL	CA2-C1-CB2-OB2
20	D	605	CDL	CA3-OA5-PA1-OA3
20	D	605	CDL	CA3-OA5-PA1-OA4
20	D	606	CDL	CA2-OA2-PA1-OA3
20	D	606	CDL	CA3-OA5-PA1-OA3
20	D	606	CDL	CB2-OB2-PB2-OB3
20	F	302	CDL	C1-CA2-OA2-PA1
20	F	302	CDL	CA2-OA2-PA1-OA4
20	F	302	CDL	CB3-OB5-PB2-OB2
20	F	302	CDL	CB3-OB5-PB2-OB3
20	F	302	CDL	CB3-OB5-PB2-OB4
20	G	201	CDL	CA2-OA2-PA1-OA3
20	G	201	CDL	CB2-OB2-PB2-OB4
20	I	201	CDL	CA2-OA2-PA1-OA4
20	I	201	CDL	CB3-OB5-PB2-OB3
20	I	201	CDL	CB4-CB3-OB5-PB2
20	P	301	CDL	CB2-OB2-PB2-OB3
20	P	301	CDL	CB3-OB5-PB2-OB2
20	P	301	CDL	CB3-OB5-PB2-OB3
20	P	301	CDL	CB3-OB5-PB2-OB4
20	Q	605	CDL	CA2-C1-CB2-OB2
20	Q	605	CDL	CA3-OA5-PA1-OA3
20	Q	605	CDL	CA3-OA5-PA1-OA4
20	Q	606	CDL	CA2-OA2-PA1-OA3
20	Q	606	CDL	CA3-OA5-PA1-OA3
20	Q	606	CDL	CB2-OB2-PB2-OB3
20	S	302	CDL	C1-CA2-OA2-PA1
20	S	302	CDL	CA2-OA2-PA1-OA4
20	S	302	CDL	CB3-OB5-PB2-OB2
20	S	302	CDL	CB3-OB5-PB2-OB3
20	S	302	CDL	CB3-OB5-PB2-OB4
20	S	303	CDL	CA2-OA2-PA1-OA3
20	S	303	CDL	CB2-OB2-PB2-OB4
20	V	201	CDL	CA2-OA2-PA1-OA4
20	V	201	CDL	CB3-OB5-PB2-OB3
20	V	201	CDL	CB4-CB3-OB5-PB2
24	C	304	3PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
24	C	304	3PH	C1-O11-P-O14
24	T	201	3PH	C1-O11-P-O13
24	T	201	3PH	C1-O11-P-O14
25	D	601	HAS	C22-C23-C24-C28
25	D	601	HAS	C25-C23-C24-C28
25	D	602	HAS	C1A-C2A-CAA-CBA
25	D	602	HAS	C11-C12-C13-C14
25	D	602	HAS	C14-C15-C16-C17
25	D	602	HAS	C26-C15-C16-C17
25	Q	601	HAS	C22-C23-C24-C28
25	Q	601	HAS	C25-C23-C24-C28
25	Q	602	HAS	C1A-C2A-CAA-CBA
25	Q	602	HAS	C11-C12-C13-C14
25	Q	602	HAS	C14-C15-C16-C17
25	Q	602	HAS	C26-C15-C16-C17
30	H	201	DGA	OG1-CG1-CG2-OG2
30	M	201	DGA	OG1-CG1-CG2-OG2
30	U	201	DGA	OG1-CG1-CG2-OG2
30	Z	201	DGA	OG1-CG1-CG2-OG2
32	I	202	IX7	O1-C16-C17-C69
32	I	202	IX7	C57-C56-O19-C32
32	I	202	IX7	C31-O16-P-O14
32	R	406	IX7	O1-C16-C17-C69
32	R	406	IX7	C57-C56-O19-C32
32	R	406	IX7	C31-O16-P-O14
32	I	202	IX7	O8-C24-O7-C23
32	R	406	IX7	O8-C24-O7-C23
15	A	502	IZL	O-C10-O1-C11
15	N	504	IZL	O-C10-O1-C11
32	I	202	IX7	O20-C56-O19-C32
32	R	406	IX7	O20-C56-O19-C32
15	A	502	IZL	C48-C47-O32-C46
15	N	504	IZL	C48-C47-O32-C46
25	D	602	HAS	C3A-C2A-CAA-CBA
25	Q	602	HAS	C3A-C2A-CAA-CBA
15	A	502	IZL	C9-C10-O1-C11
15	N	504	IZL	C9-C10-O1-C11
18	A	505	3PE	C32-C31-O31-C3
18	N	502	3PE	C32-C31-O31-C3
15	A	502	IZL	O12-C26-C27-O13
15	N	504	IZL	O12-C26-C27-O13
32	I	202	IX7	O1-C16-C17-O2

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Mol	Chain	Res	Type	Atoms
32	R	406	IX7	O1-C16-C17-O2
18	A	505	3PE	O32-C31-O31-C3
18	N	502	3PE	O32-C31-O31-C3
20	D	605	CDL	O1-C1-CB2-OB2
20	Q	605	CDL	O1-C1-CB2-OB2
20	D	605	CDL	C1-CB2-OB2-PB2
20	I	201	CDL	C1-CA2-OA2-PA1
20	Q	605	CDL	C1-CB2-OB2-PB2
20	V	201	CDL	C1-CA2-OA2-PA1
15	A	502	IZL	C28-C26-C27-O13
15	N	504	IZL	C28-C26-C27-O13
15	A	502	IZL	O33-C47-O32-C46
15	N	504	IZL	O33-C47-O32-C46
17	A	504	MQ9	C9-C11-C12-C13
17	A	504	MQ9	C14-C16-C17-C18
17	B	601	MQ9	C9-C11-C12-C13
17	N	501	MQ9	C9-C11-C12-C13
17	N	501	MQ9	C14-C16-C17-C18
17	O	602	MQ9	C9-C11-C12-C13
25	D	602	HAS	C19-C20-C21-C22
25	Q	602	HAS	C19-C20-C21-C22
15	A	502	IZL	C53-C54-C55-C56
15	N	504	IZL	C53-C54-C55-C56
18	A	505	3PE	C31-C32-C33-C34
18	N	502	3PE	C31-C32-C33-C34
20	F	302	CDL	OA6-CA4-CA6-OA8
20	S	302	CDL	OA6-CA4-CA6-OA8
21	B	606	LYC	C57-C56-C58-C59
21	O	607	LYC	C57-C56-C58-C59
32	I	202	IX7	C12-C13-C14-C15
32	R	406	IX7	C12-C13-C14-C15
20	C	301	CDL	CA7-C31-C32-C33
20	P	301	CDL	CA7-C31-C32-C33
25	D	601	HAS	C15-C16-C17-C18
25	D	601	HAS	C23-C24-C28-C29
25	D	602	HAS	C23-C24-C28-C29
25	Q	601	HAS	C15-C16-C17-C18
25	Q	602	HAS	C23-C24-C28-C29
18	A	505	3PE	C1-O11-P-O13
18	F	301	3PE	C1-O11-P-O13
18	F	301	3PE	C11-O13-P-O11
18	N	502	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
18	S	301	3PE	C1-O11-P-O13
18	S	301	3PE	C11-O13-P-O11
20	D	605	CDL	CA3-OA5-PA1-OA2
20	D	606	CDL	CA2-OA2-PA1-OA5
20	D	606	CDL	CA3-OA5-PA1-OA2
20	F	302	CDL	CA2-OA2-PA1-OA5
20	G	201	CDL	CB3-OB5-PB2-OB2
20	I	201	CDL	CA3-OA5-PA1-OA2
20	Q	605	CDL	CA3-OA5-PA1-OA2
20	Q	606	CDL	CA2-OA2-PA1-OA5
20	Q	606	CDL	CA3-OA5-PA1-OA2
20	S	302	CDL	CA2-OA2-PA1-OA5
20	S	303	CDL	CB3-OB5-PB2-OB2
20	V	201	CDL	CA3-OA5-PA1-OA2
32	I	202	IX7	C31-O16-P-O13
32	R	406	IX7	C31-O16-P-O13
32	I	202	IX7	C29-C24-O7-C23
32	R	406	IX7	C29-C24-O7-C23
20	G	201	CDL	CB5-C51-C52-C53
20	S	303	CDL	CB5-C51-C52-C53
16	A	503	9YF	C2-O2-P-O
16	N	505	9YF	C2-O2-P-O
18	A	505	3PE	C22-C21-O21-C2
18	N	502	3PE	C22-C21-O21-C2
20	D	605	CDL	C51-CB5-OB6-CB4
20	Q	605	CDL	C51-CB5-OB6-CB4
32	I	202	IX7	C61-C62-C63-C64
32	R	406	IX7	C61-C62-C63-C64
18	A	505	3PE	C2B-C2C-C2D-C2E
18	N	502	3PE	C2B-C2C-C2D-C2E
20	F	302	CDL	CB7-C71-C72-C73
20	S	302	CDL	CB7-C71-C72-C73
18	A	505	3PE	C2F-C2G-C2H-C2I
18	N	502	3PE	C2F-C2G-C2H-C2I
20	D	606	CDL	C12-C13-C14-C15
20	Q	605	CDL	C52-C53-C54-C55
20	Q	606	CDL	C12-C13-C14-C15
20	D	605	CDL	C52-C53-C54-C55
15	A	502	IZL	C48-C49-C50-C51
15	N	504	IZL	C48-C49-C50-C51
32	I	202	IX7	C10-C11-C12-C13
32	R	406	IX7	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	Q	601	HAS	C23-C24-C28-C29
20	D	606	CDL	C13-C14-C15-C16
20	Q	606	CDL	C13-C14-C15-C16
32	I	202	IX7	C57-C58-C59-C60
32	R	406	IX7	C57-C58-C59-C60
19	B	602	HEM	C2A-CAA-CBA-CGA
19	O	603	HEM	C2A-CAA-CBA-CGA
15	A	502	IZL	O17-C32-C33-O18
15	N	504	IZL	O17-C32-C33-O18
15	A	502	IZL	C34-C32-C33-O18
15	N	504	IZL	C34-C32-C33-O18
20	D	605	CDL	OB7-CB5-OB6-CB4
20	Q	605	CDL	OB7-CB5-OB6-CB4
20	D	605	CDL	C51-C52-C53-C54
20	Q	605	CDL	C51-C52-C53-C54
18	F	301	3PE	O22-C21-O21-C2
18	S	301	3PE	O22-C21-O21-C2
32	I	202	IX7	C35-C36-C37-C38
32	R	406	IX7	C35-C36-C37-C38
18	F	301	3PE	C22-C21-O21-C2
18	S	301	3PE	C22-C21-O21-C2
18	A	505	3PE	O22-C21-O21-C2
18	N	502	3PE	O22-C21-O21-C2
18	A	505	3PE	C29-C2A-C2B-C2C
18	N	502	3PE	C29-C2A-C2B-C2C
20	B	605	CDL	OB6-CB4-CB6-OB8
20	O	606	CDL	OB6-CB4-CB6-OB8
20	D	606	CDL	C18-C19-C20-C21
20	Q	606	CDL	C18-C19-C20-C21
22	B	608	LMT	O5'-C5'-C6'-O6'
22	O	601	LMT	O5'-C5'-C6'-O6'
15	A	502	IZL	C50-C51-C52-C53
15	N	504	IZL	C50-C51-C52-C53
20	D	606	CDL	C33-C34-C35-C36
20	Q	606	CDL	C33-C34-C35-C36
17	A	504	MQ9	C6-C7-C8-C9
17	N	501	MQ9	C6-C7-C8-C9
18	A	505	3PE	C25-C26-C27-C28
18	N	502	3PE	C25-C26-C27-C28
18	W	201	3PE	C24-C25-C26-C27
22	B	608	LMT	C3-C4-C5-C6
22	O	601	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	J	201	3PE	C24-C25-C26-C27
32	I	202	IX7	C59-C60-C61-C62
32	R	406	IX7	C59-C60-C61-C62
15	A	502	IZL	C44-C45-C46-O32
15	N	504	IZL	C44-C45-C46-O32
20	C	301	CDL	CB5-C51-C52-C53
20	P	301	CDL	CB5-C51-C52-C53
18	E	405	3PE	C21-C22-C23-C24
18	R	405	3PE	C21-C22-C23-C24
32	I	202	IX7	C63-C64-C65-C66
32	R	406	IX7	C63-C64-C65-C66
18	F	301	3PE	C3-C2-O21-C21
18	S	301	3PE	C3-C2-O21-C21
25	D	601	HAS	C11-C12-C13-C14
25	Q	601	HAS	C11-C12-C13-C14
18	A	505	3PE	C26-C27-C28-C29
18	N	502	3PE	C26-C27-C28-C29
20	D	605	CDL	C55-C56-C57-C58
20	Q	605	CDL	C55-C56-C57-C58
32	I	202	IX7	O2-C18-O3-C19
32	R	406	IX7	O2-C18-O3-C19
15	A	502	IZL	O2-C13-O3-C14
15	N	504	IZL	O2-C13-O3-C14
18	S	301	3PE	C24-C25-C26-C27
20	I	201	CDL	C24-C25-C26-C27
20	V	201	CDL	C24-C25-C26-C27
18	F	301	3PE	C24-C25-C26-C27
15	N	504	IZL	C17-C18-O7-C19
15	A	502	IZL	C17-C18-O7-C19
21	B	606	LYC	C55-C56-C58-C59
21	O	607	LYC	C55-C56-C58-C59
20	D	605	CDL	OA5-CA3-CA4-CA6
20	Q	605	CDL	OA5-CA3-CA4-CA6
15	A	502	IZL	C47-C48-C49-C50
15	N	504	IZL	C47-C48-C49-C50
15	N	504	IZL	C43-C18-O7-C19
20	C	301	CDL	C1-CA2-OA2-PA1
20	D	606	CDL	C1-CA2-OA2-PA1
20	G	201	CDL	C1-CA2-OA2-PA1
20	G	201	CDL	C1-CB2-OB2-PB2
20	P	301	CDL	C1-CA2-OA2-PA1
20	Q	606	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
20	S	303	CDL	C1-CA2-OA2-PA1
20	S	303	CDL	C1-CB2-OB2-PB2
24	C	304	3PH	C2-C1-O11-P
24	T	201	3PH	C2-C1-O11-P
15	A	502	IZL	C43-C18-O7-C19
20	B	605	CDL	CB3-CB4-CB6-OB8
20	F	302	CDL	CA3-CA4-CA6-OA8
20	O	606	CDL	CB3-CB4-CB6-OB8
20	S	302	CDL	CA3-CA4-CA6-OA8
16	A	503	9YF	C2-O2-P-O8
16	N	505	9YF	C2-O2-P-O8
20	F	302	CDL	CB2-OB2-PB2-OB5
20	S	302	CDL	CB2-OB2-PB2-OB5
18	D	607	3PE	O11-C1-C2-O21
18	Q	607	3PE	O11-C1-C2-O21
20	D	605	CDL	OB5-CB3-CB4-OB6
20	Q	605	CDL	OB5-CB3-CB4-OB6
24	C	304	3PH	O11-C1-C2-O21
24	T	201	3PH	O11-C1-C2-O21
15	A	502	IZL	C49-C50-C51-C52
15	N	504	IZL	C49-C50-C51-C52
20	B	605	CDL	CB4-CB3-OB5-PB2
20	C	301	CDL	CB4-CB3-OB5-PB2
20	O	606	CDL	CB4-CB3-OB5-PB2
20	P	301	CDL	CB4-CB3-OB5-PB2
24	C	304	3PH	C22-C21-O21-C2
24	T	201	3PH	C22-C21-O21-C2
18	D	607	3PE	O11-C1-C2-C3
18	Q	607	3PE	O11-C1-C2-C3
24	C	304	3PH	O11-C1-C2-C3
24	T	201	3PH	O11-C1-C2-C3
32	I	202	IX7	O16-C31-C32-C33
32	R	406	IX7	O16-C31-C32-C33
15	A	502	IZL	C46-C45-O34-C60
15	N	504	IZL	C46-C45-O34-C60
32	I	202	IX7	C34-C35-C36-C37
16	B	607	9YF	C-C1-O-P
16	U	203	9YF	C-C1-O-P
20	F	302	CDL	CB4-CB3-OB5-PB2
20	S	302	CDL	CB4-CB3-OB5-PB2
20	D	605	CDL	OA5-CA3-CA4-OA6
20	Q	605	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
32	I	202	IX7	O16-C31-C32-O19
32	R	406	IX7	O16-C31-C32-O19
32	R	406	IX7	C34-C35-C36-C37
20	D	606	CDL	OB6-CB4-CB6-OB8
20	Q	606	CDL	OB6-CB4-CB6-OB8
18	A	505	3PE	C2A-C2B-C2C-C2D
18	N	502	3PE	C2A-C2B-C2C-C2D
17	B	601	MQ9	C12-C11-C9-C10
17	O	602	MQ9	C12-C11-C9-C10
18	A	505	3PE	C28-C29-C2A-C2B
18	N	502	3PE	C28-C29-C2A-C2B
32	I	202	IX7	O8-C25-C26-O9
32	R	406	IX7	O8-C25-C26-O9
20	C	301	CDL	CA5-C11-C12-C13
20	P	301	CDL	CA5-C11-C12-C13
20	G	201	CDL	CA2-OA2-PA1-OA5
20	G	201	CDL	CB2-OB2-PB2-OB5
20	I	201	CDL	CA2-OA2-PA1-OA5
20	S	303	CDL	CA2-OA2-PA1-OA5
20	S	303	CDL	CB2-OB2-PB2-OB5
20	V	201	CDL	CA2-OA2-PA1-OA5
20	Q	606	CDL	C19-C20-C21-C22
15	A	502	IZL	C45-C44-O31-P
15	N	504	IZL	C45-C44-O31-P
18	D	607	3PE	C2-C1-O11-P
18	Q	607	3PE	C2-C1-O11-P
20	B	605	CDL	CA4-CA3-OA5-PA1
20	D	605	CDL	C1-CA2-OA2-PA1
20	D	606	CDL	CA4-CA3-OA5-PA1
20	G	201	CDL	CA4-CA3-OA5-PA1
20	O	606	CDL	CA4-CA3-OA5-PA1
20	Q	605	CDL	C1-CA2-OA2-PA1
20	Q	606	CDL	CA4-CA3-OA5-PA1
20	S	303	CDL	CA4-CA3-OA5-PA1
18	N	502	3PE	C23-C24-C25-C26
20	D	606	CDL	C19-C20-C21-C22
15	A	502	IZL	C44-O31-P-O30
15	N	504	IZL	C44-O31-P-O30
18	F	301	3PE	C1-O11-P-O12
18	F	301	3PE	C1-O11-P-O14
18	S	301	3PE	C1-O11-P-O12
18	S	301	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
20	D	606	CDL	CA2-OA2-PA1-OA4
20	D	606	CDL	CA3-OA5-PA1-OA4
20	F	302	CDL	CA2-OA2-PA1-OA3
20	G	201	CDL	CB3-OB5-PB2-OB3
20	I	201	CDL	CA2-OA2-PA1-OA3
20	I	201	CDL	CA3-OA5-PA1-OA3
20	I	201	CDL	CB3-OB5-PB2-OB4
20	Q	606	CDL	CA2-OA2-PA1-OA4
20	Q	606	CDL	CA3-OA5-PA1-OA4
20	S	302	CDL	CA2-OA2-PA1-OA3
20	S	303	CDL	CB3-OB5-PB2-OB3
20	V	201	CDL	CA2-OA2-PA1-OA3
20	V	201	CDL	CA3-OA5-PA1-OA3
20	V	201	CDL	CB3-OB5-PB2-OB4
32	I	202	IX7	C31-O16-P-O15
32	R	406	IX7	C31-O16-P-O15
20	G	201	CDL	OA5-CA3-CA4-CA6
20	S	303	CDL	OA5-CA3-CA4-CA6
18	A	505	3PE	C23-C24-C25-C26
18	A	505	3PE	C12-C11-O13-P
18	F	301	3PE	C12-C11-O13-P
18	J	201	3PE	C12-C11-O13-P
18	N	502	3PE	C12-C11-O13-P
18	S	301	3PE	C12-C11-O13-P
18	W	201	3PE	C12-C11-O13-P
20	D	605	CDL	C57-C58-C59-C60
32	I	202	IX7	C11-C10-C9-C8
20	Q	605	CDL	C57-C58-C59-C60
25	D	601	HAS	O11-C11-C3B-C4B
25	Q	601	HAS	O11-C11-C3B-C4B
32	R	406	IX7	C11-C10-C9-C8
20	D	605	CDL	C31-C32-C33-C34
20	Q	605	CDL	C31-C32-C33-C34
15	A	502	IZL	C63-C64-C65-C66
15	N	504	IZL	C63-C64-C65-C66
18	F	301	3PE	C25-C26-C27-C28
15	A	502	IZL	C54-C55-C56-C57
15	N	504	IZL	C54-C55-C56-C57
18	S	301	3PE	C25-C26-C27-C28
32	I	202	IX7	C67-C18-O3-C19
32	R	406	IX7	C67-C18-O3-C19
18	N	502	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	A	505	3PE	C22-C23-C24-C25
20	D	606	CDL	OB5-CB3-CB4-CB6
20	Q	606	CDL	OB5-CB3-CB4-CB6
20	I	201	CDL	CB2-C1-CA2-OA2
20	V	201	CDL	CB2-C1-CA2-OA2
32	I	202	IX7	C30-C19-O3-C18
32	R	406	IX7	C30-C19-O3-C18
15	A	502	IZL	C62-C63-C64-C65
20	D	606	CDL	OB5-CB3-CB4-OB6
20	Q	606	CDL	OB5-CB3-CB4-OB6
15	N	504	IZL	C62-C63-C64-C65
17	B	601	MQ9	C12-C11-C9-C8
17	O	602	MQ9	C12-C11-C9-C8
15	A	502	IZL	C61-C62-C63-C64
20	F	302	CDL	CB4-CB6-OB8-CB7
20	S	302	CDL	CB4-CB6-OB8-CB7
18	A	505	3PE	C11-O13-P-O11
18	N	502	3PE	C11-O13-P-O11
20	B	605	CDL	CA2-OA2-PA1-OA5
20	B	605	CDL	CA3-OA5-PA1-OA2
20	C	301	CDL	CB2-OB2-PB2-OB5
20	D	605	CDL	CB2-OB2-PB2-OB5
20	D	606	CDL	CB2-OB2-PB2-OB5
20	O	606	CDL	CA2-OA2-PA1-OA5
20	O	606	CDL	CA3-OA5-PA1-OA2
20	P	301	CDL	CB2-OB2-PB2-OB5
20	Q	605	CDL	CB2-OB2-PB2-OB5
20	Q	606	CDL	CB2-OB2-PB2-OB5
15	N	504	IZL	C61-C62-C63-C64
20	I	201	CDL	C32-C31-CA7-OA8
20	V	201	CDL	C32-C31-CA7-OA8
20	D	605	CDL	C54-C55-C56-C57
20	Q	605	CDL	C54-C55-C56-C57
15	A	502	IZL	C71-C13-O3-C14
20	D	605	CDL	C58-C59-C60-C61
20	Q	605	CDL	C58-C59-C60-C61
16	A	503	9YF	C-C1-O-P
16	N	505	9YF	C-C1-O-P
18	F	301	3PE	C2-C1-O11-P
18	S	301	3PE	C2-C1-O11-P
20	Q	606	CDL	C1-CB2-OB2-PB2
15	N	504	IZL	C71-C13-O3-C14

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Mol	Chain	Res	Type	Atoms
21	B	606	LYC	C63-C64-C65-C66
21	O	607	LYC	C63-C64-C65-C66
32	R	406	IX7	C20-C19-O3-C18
32	I	202	IX7	C20-C19-O3-C18
18	A	505	3PE	C2D-C2E-C2F-C2G
18	N	502	3PE	C2D-C2E-C2F-C2G
20	D	605	CDL	C74-C75-C76-C77
20	Q	605	CDL	C74-C75-C76-C77
20	C	301	CDL	C33-C34-C35-C36
20	P	301	CDL	C33-C34-C35-C36
20	I	201	CDL	C32-C31-CA7-OA9
20	V	201	CDL	C32-C31-CA7-OA9
20	G	201	CDL	C51-C52-C53-C54
20	D	606	CDL	C1-CB2-OB2-PB2
20	S	303	CDL	C51-C52-C53-C54
17	A	504	MQ9	C16-C17-C18-C19
17	N	501	MQ9	C16-C17-C18-C19
16	B	607	9YF	C2-O2-P-O1
16	B	607	9YF	C2-O2-P-O8
16	U	203	9YF	C2-O2-P-O1
16	U	203	9YF	C2-O2-P-O8
20	D	605	CDL	CB3-CB4-OB6-CB5
20	D	606	CDL	CB6-CB4-OB6-CB5
20	I	201	CDL	CB6-CB4-OB6-CB5
20	Q	605	CDL	CB3-CB4-OB6-CB5
20	Q	606	CDL	CB6-CB4-OB6-CB5
20	V	201	CDL	CB6-CB4-OB6-CB5
20	I	201	CDL	CB3-OB5-PB2-OB2
20	V	201	CDL	CB3-OB5-PB2-OB2
20	F	302	CDL	C1-CB2-OB2-PB2
20	S	302	CDL	C1-CB2-OB2-PB2
15	A	502	IZL	C7-C8-C9-C10
15	N	504	IZL	C7-C8-C9-C10
20	D	606	CDL	CA5-C11-C12-C13
20	Q	606	CDL	CA5-C11-C12-C13
24	C	304	3PH	O22-C21-O21-C2
24	T	201	3PH	O22-C21-O21-C2
15	N	504	IZL	C52-C53-C54-C55
15	A	502	IZL	C52-C53-C54-C55
18	A	505	3PE	C32-C33-C34-C35
18	N	502	3PE	C32-C33-C34-C35
25	D	602	HAS	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	Q	601	HAS	CAD-CBD-CGD-O1D
25	Q	602	HAS	CAA-CBA-CGA-O2A
20	B	605	CDL	C52-C51-CB5-OB6
20	O	606	CDL	C52-C51-CB5-OB6
20	F	302	CDL	O1-C1-CA2-OA2
20	S	302	CDL	O1-C1-CA2-OA2
25	D	601	HAS	CAD-CBD-CGD-O1D
18	D	607	3PE	C21-C22-C23-C24
18	Q	607	3PE	C21-C22-C23-C24
20	D	605	CDL	OB5-CB3-CB4-CB6
20	Q	605	CDL	OB5-CB3-CB4-CB6
15	A	502	IZL	C54-C55-C56-C58
15	N	504	IZL	C54-C55-C56-C58
17	A	504	MQ9	C12-C11-C9-C8
17	N	501	MQ9	C12-C11-C9-C8
20	Q	605	CDL	C38-C39-C40-C41
20	D	605	CDL	C38-C39-C40-C41
20	I	201	CDL	C12-C11-CA5-OA6
20	V	201	CDL	C12-C11-CA5-OA6
16	A	503	9YF	O11-C25-C26-C27
16	N	505	9YF	O11-C25-C26-C27
20	D	605	CDL	C72-C71-CB7-OB8
20	Q	605	CDL	C72-C71-CB7-OB8
25	D	602	HAS	C27-C19-C20-C21
25	Q	602	HAS	C27-C19-C20-C21
20	G	201	CDL	C32-C31-CA7-OA8
20	S	303	CDL	C32-C31-CA7-OA8
32	I	202	IX7	C11-C12-C13-C14
32	R	406	IX7	C11-C12-C13-C14
20	G	201	CDL	CA6-CA4-OA6-CA5
20	I	201	CDL	CB3-CB4-OB6-CB5
20	S	303	CDL	CA6-CA4-OA6-CA5
20	V	201	CDL	CB3-CB4-OB6-CB5
22	O	601	LMT	C5'-C4'-O1B-C1B
20	Q	605	CDL	C71-C72-C73-C74
22	B	608	LMT	C5'-C4'-O1B-C1B
20	D	605	CDL	C71-C72-C73-C74
18	J	201	3PE	C2-C1-O11-P
18	W	201	3PE	C2-C1-O11-P
24	C	304	3PH	C1-O11-P-O12
24	T	201	3PH	C1-O11-P-O12
25	D	602	HAS	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	Q	602	HAS	CAA-CBA-CGA-O1A
19	B	602	HEM	CAA-CBA-CGA-O2A
19	O	603	HEM	CAA-CBA-CGA-O2A
17	A	504	MQ9	C12-C11-C9-C10
17	N	501	MQ9	C12-C11-C9-C10
32	I	202	IX7	C13-C14-C15-O1
32	R	406	IX7	C13-C14-C15-O1
20	C	301	CDL	OA6-CA4-CA6-OA8
20	P	301	CDL	OA6-CA4-CA6-OA8
18	A	505	3PE	O21-C21-C22-C23
18	J	201	3PE	O21-C21-C22-C23
18	N	502	3PE	O21-C21-C22-C23
18	W	201	3PE	O21-C21-C22-C23
20	C	301	CDL	C72-C71-CB7-OB8
20	G	201	CDL	C12-C11-CA5-OA6
20	P	301	CDL	C72-C71-CB7-OB8
20	S	303	CDL	C12-C11-CA5-OA6
32	I	202	IX7	C19-C30-O13-P
32	R	406	IX7	C19-C30-O13-P
20	C	301	CDL	C74-C75-C76-C77
20	P	301	CDL	C74-C75-C76-C77
25	D	601	HAS	CAD-CBD-CGD-O2D
25	Q	601	HAS	CAD-CBD-CGD-O2D
15	A	502	IZL	O32-C47-C48-C49
25	D	601	HAS	C16-C17-C18-C19
25	Q	601	HAS	C16-C17-C18-C19
15	N	504	IZL	O32-C47-C48-C49
18	F	301	3PE	O31-C31-C32-C33
18	S	301	3PE	O31-C31-C32-C33
23	P	302	HEC	CAD-CBD-CGD-O2D
20	S	303	CDL	C32-C31-CA7-OA9
19	B	602	HEM	CAA-CBA-CGA-O1A
19	O	603	HEM	CAA-CBA-CGA-O1A
23	C	302	HEC	CAD-CBD-CGD-O2D
20	G	201	CDL	C32-C31-CA7-OA9
18	A	505	3PE	O22-C21-C22-C23
20	I	201	CDL	C12-C11-CA5-OA7
20	V	201	CDL	C12-C11-CA5-OA7
18	F	301	3PE	O32-C31-C32-C33
18	S	301	3PE	O32-C31-C32-C33
20	D	605	CDL	C72-C71-CB7-OB9
18	F	301	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
18	S	301	3PE	C1-C2-C3-O31
16	A	503	9YF	O12-C25-C26-C27
16	N	505	9YF	O12-C25-C26-C27
18	N	502	3PE	O22-C21-C22-C23
20	Q	605	CDL	C72-C71-CB7-OB9
20	F	302	CDL	C72-C71-CB7-OB8
20	S	302	CDL	C72-C71-CB7-OB8
18	A	505	3PE	C11-O13-P-O14
18	J	201	3PE	C11-O13-P-O14
18	N	502	3PE	C11-O13-P-O14
18	W	201	3PE	C11-O13-P-O14
20	F	302	CDL	CA3-OA5-PA1-OA3
20	F	302	CDL	CB2-OB2-PB2-OB3
20	G	201	CDL	CB2-OB2-PB2-OB3
20	I	201	CDL	CA3-OA5-PA1-OA4
20	S	302	CDL	CA3-OA5-PA1-OA3
20	S	302	CDL	CB2-OB2-PB2-OB3
20	S	303	CDL	CB2-OB2-PB2-OB3
20	V	201	CDL	CA3-OA5-PA1-OA4
32	I	202	IX7	C13-C14-C15-O
32	R	406	IX7	C13-C14-C15-O
20	G	201	CDL	C12-C11-CA5-OA7
20	S	303	CDL	C12-C11-CA5-OA7
23	C	302	HEC	CAD-CBD-CGD-O1D
23	P	302	HEC	CAD-CBD-CGD-O1D
25	D	602	HAS	CAD-CBD-CGD-O2D
25	Q	602	HAS	CAD-CBD-CGD-O2D
15	A	502	IZL	C44-C45-O34-C60
15	N	504	IZL	C44-C45-O34-C60
18	D	607	3PE	C12-C11-O13-P
18	Q	607	3PE	C12-C11-O13-P
20	G	201	CDL	CA3-CA4-OA6-CA5
20	S	303	CDL	CA3-CA4-OA6-CA5
19	B	603	HEM	CAD-CBD-CGD-O1D
19	O	604	HEM	CAD-CBD-CGD-O1D
20	F	302	CDL	C12-C11-CA5-OA6
20	S	302	CDL	C12-C11-CA5-OA6
19	B	603	HEM	CAD-CBD-CGD-O2D
19	O	604	HEM	CAD-CBD-CGD-O2D
23	C	302	HEC	CAA-CBA-CGA-O2A
23	P	302	HEC	CAA-CBA-CGA-O2A
20	C	301	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
20	P	301	CDL	C52-C51-CB5-OB6
30	M	201	DGA	OG2-CB1-CB2-CB3
30	Z	201	DGA	OG2-CB1-CB2-CB3
20	C	301	CDL	C72-C71-CB7-OB9
20	P	301	CDL	C72-C71-CB7-OB9
30	M	201	DGA	OG1-CA1-CA2-CA3
30	Z	201	DGA	OG1-CA1-CA2-CA3
18	W	201	3PE	C2F-C2G-C2H-C2I
18	J	201	3PE	O22-C21-C22-C23
18	W	201	3PE	O22-C21-C22-C23
25	D	602	HAS	CAD-CBD-CGD-O1D
25	Q	602	HAS	CAD-CBD-CGD-O1D

There are no ring outliers.

41 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	501	MQ9	6	0
20	B	605	CDL	1	0
23	C	302	HEC	5	0
18	N	502	3PE	9	0
23	C	303	HEC	2	0
30	E	404	DGA	1	0
17	A	504	MQ9	8	0
22	B	608	LMT	3	0
30	R	404	DGA	1	0
18	J	201	3PE	1	0
19	O	604	HEM	1	0
23	P	302	HEC	5	0
20	C	301	CDL	2	0
20	S	303	CDL	2	0
18	F	301	3PE	1	0
22	O	601	LMT	3	0
15	N	504	IZL	3	0
20	O	606	CDL	1	0
32	I	202	IX7	2	0
25	D	602	HAS	4	0
18	S	301	3PE	1	0
14	N	503	FES	1	0
18	D	607	3PE	1	0
18	A	505	3PE	8	0
19	B	603	HEM	1	0

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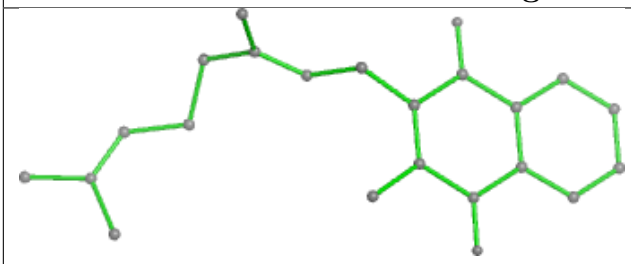
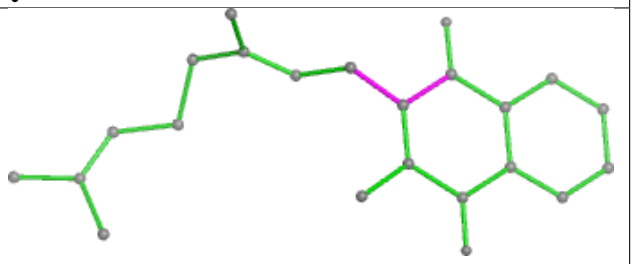
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	502	IZL	4	0
20	P	301	CDL	2	0
20	G	201	CDL	3	0
25	D	601	HAS	1	0
23	P	303	HEC	2	0
25	Q	602	HAS	3	0
20	Q	606	CDL	1	0
32	R	406	IX7	1	0
30	Z	201	DGA	1	0
21	O	607	LYC	2	0
14	A	501	FES	1	0
21	B	606	LYC	2	0
25	Q	601	HAS	1	0
18	W	201	3PE	1	0
18	Q	607	3PE	1	0
17	O	602	MQ9	2	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.

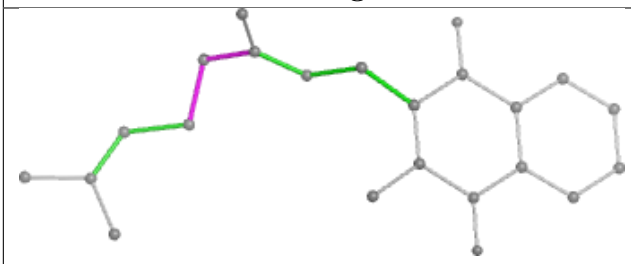
Ligand MQ9 B 601



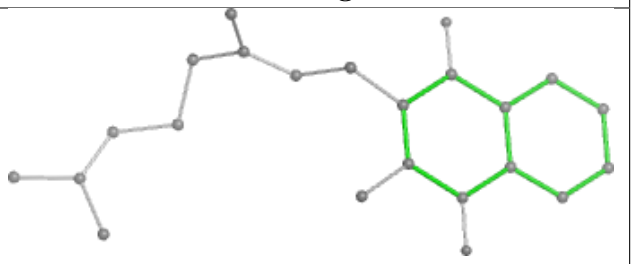
Bond lengths



Bond angles

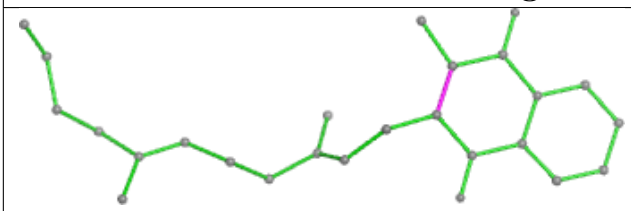


Torsions

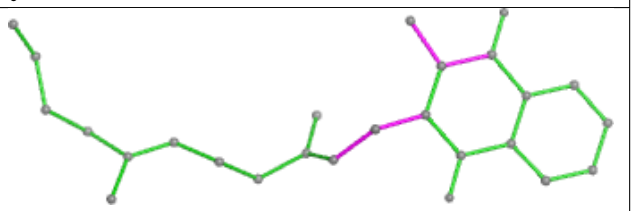


Rings

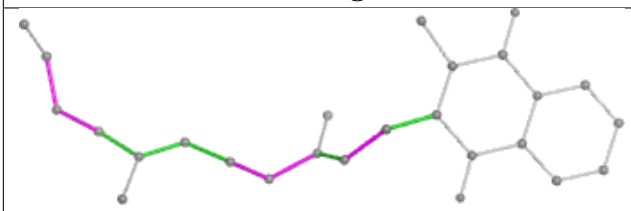
Ligand MQ9 N 501



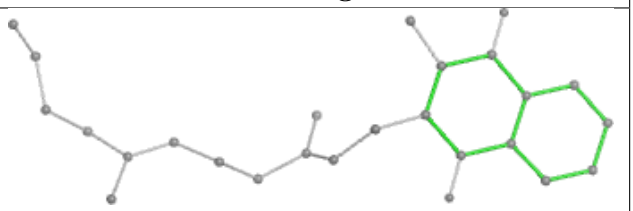
Bond lengths



Bond angles

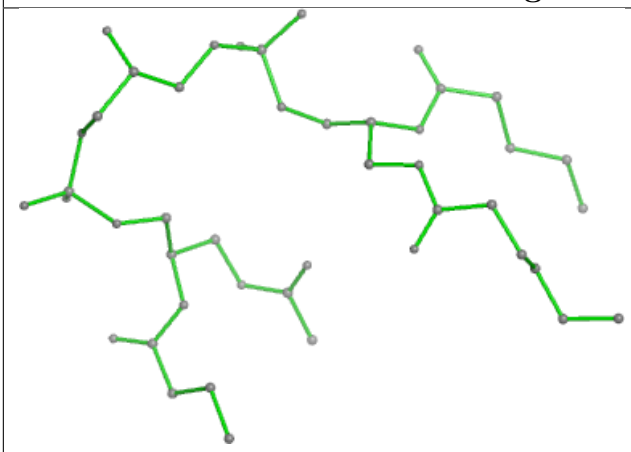


Torsions

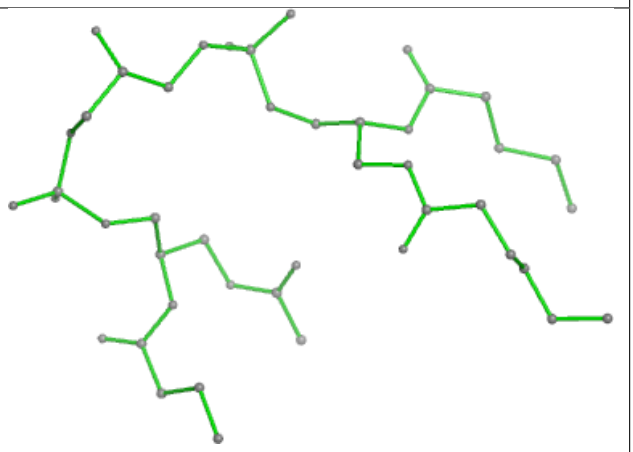


Rings

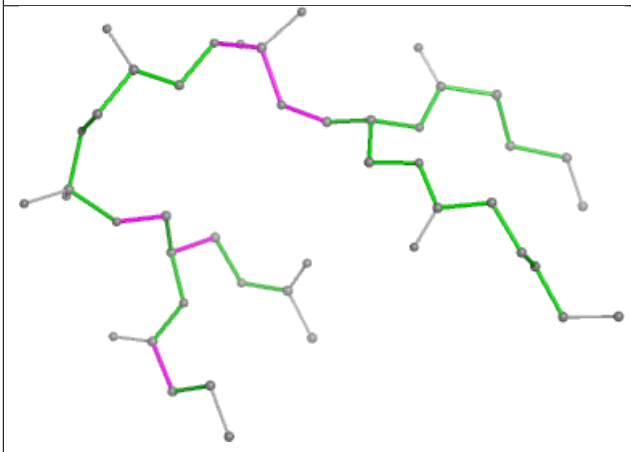
Ligand CDL B 605



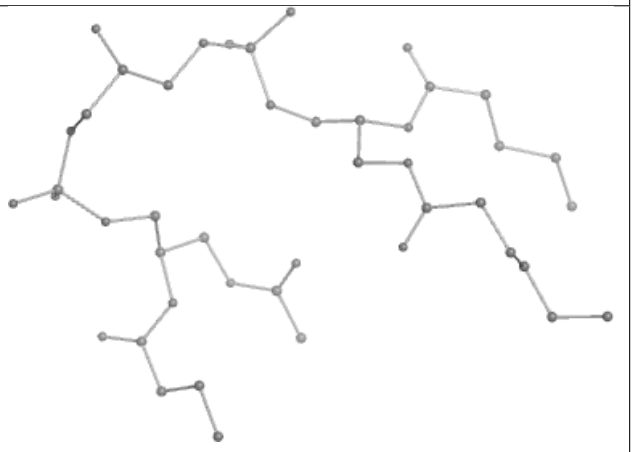
Bond lengths



Bond angles

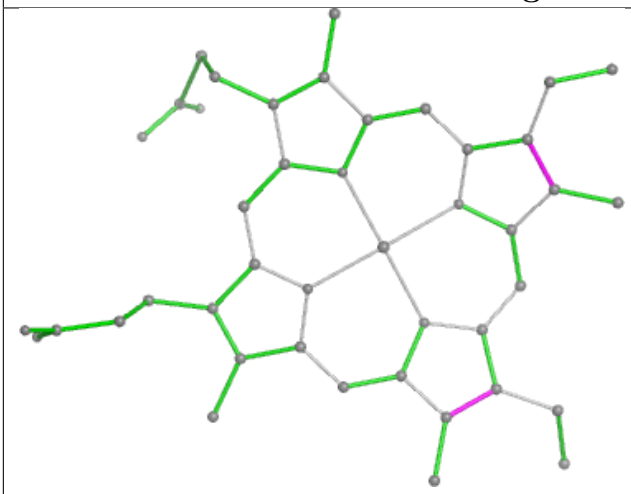


Torsions

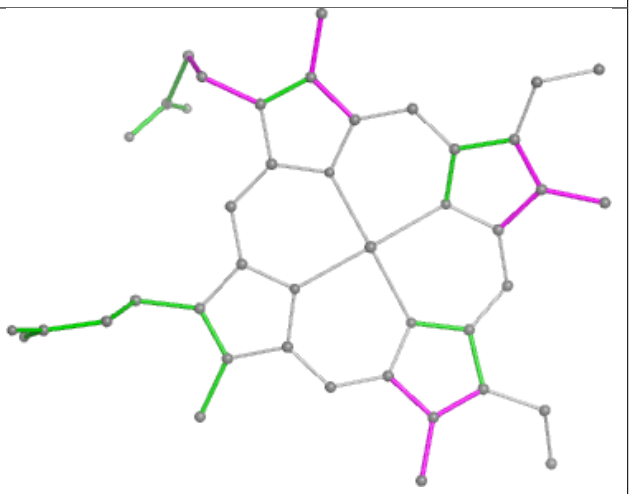


Rings

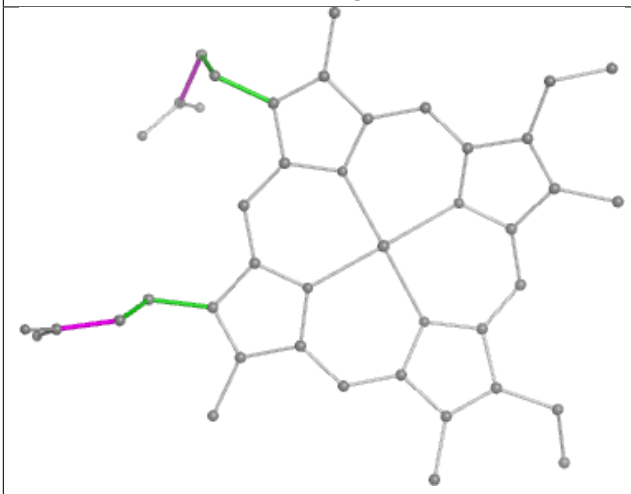
Ligand HEC C 302



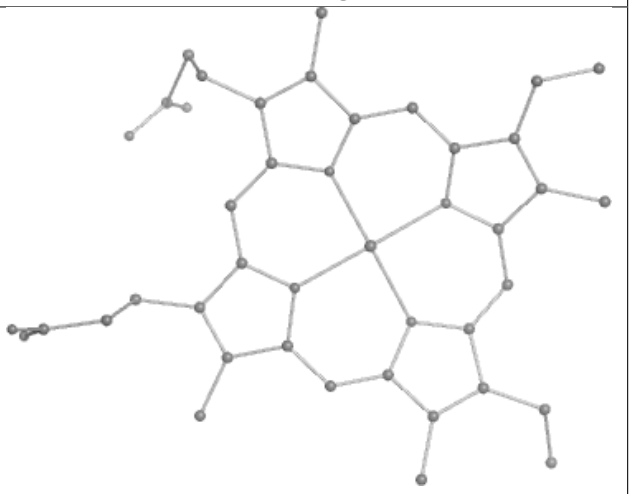
Bond lengths



Bond angles

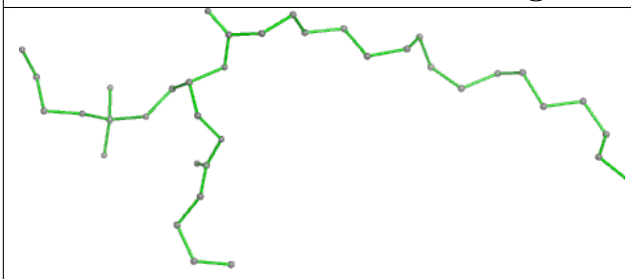


Torsions

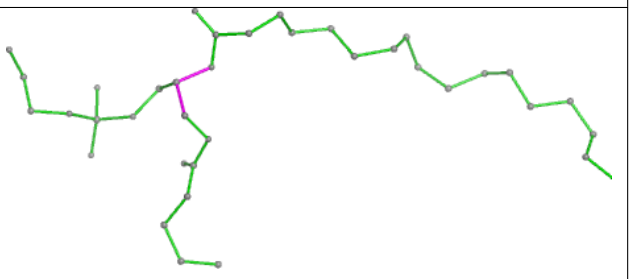


Rings

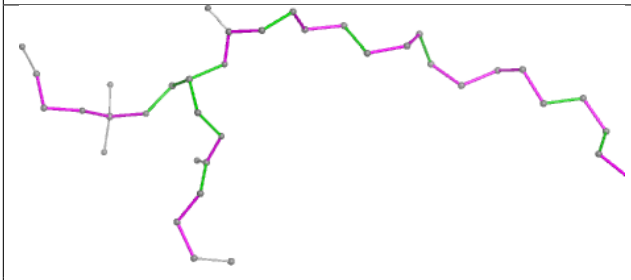
Ligand 3PE N 502



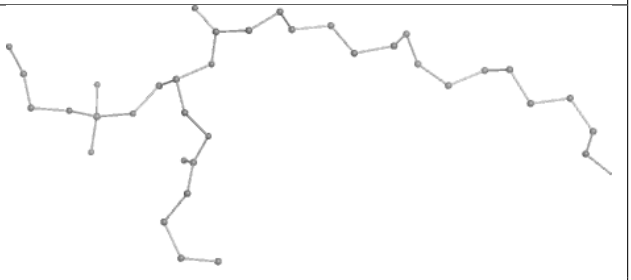
Bond lengths



Bond angles

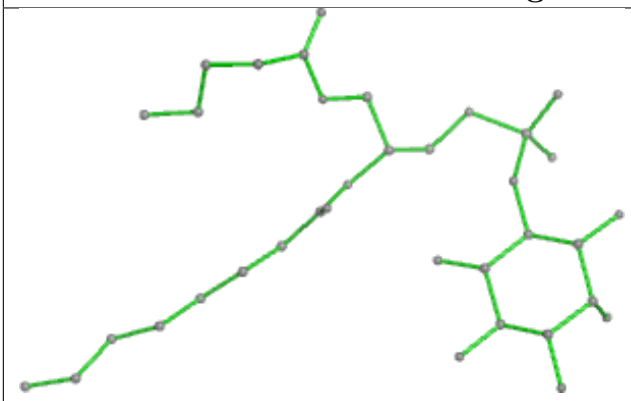


Torsions

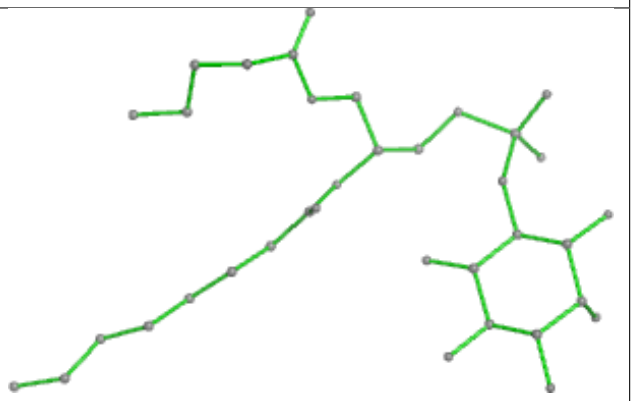


Rings

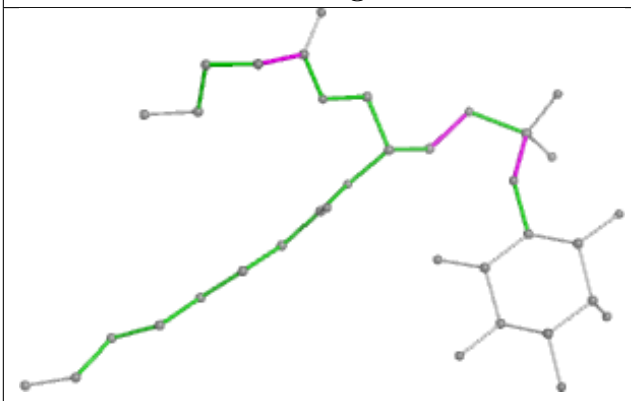
Ligand 9YF N 505



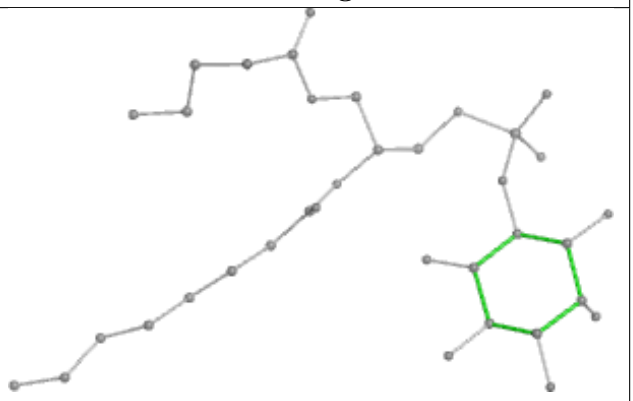
Bond lengths



Bond angles

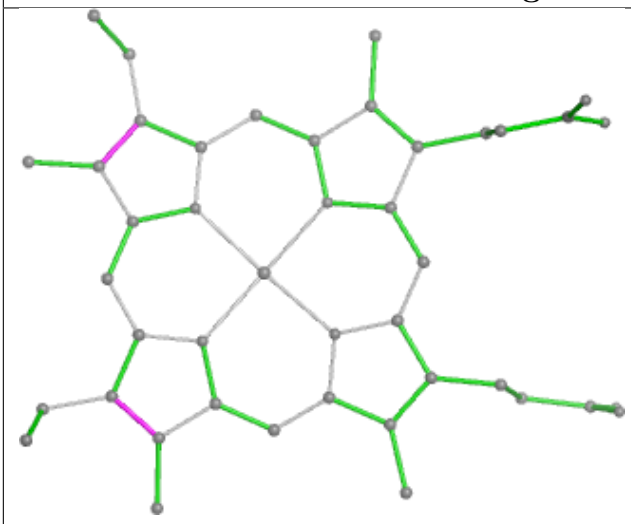


Torsions



Rings

Ligand HEC C 303



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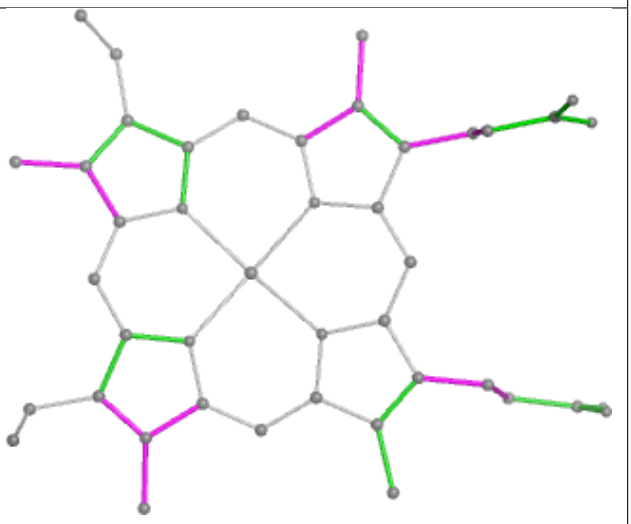
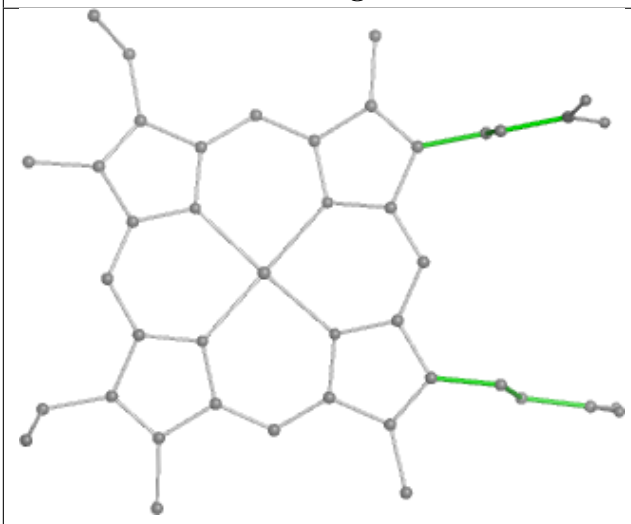
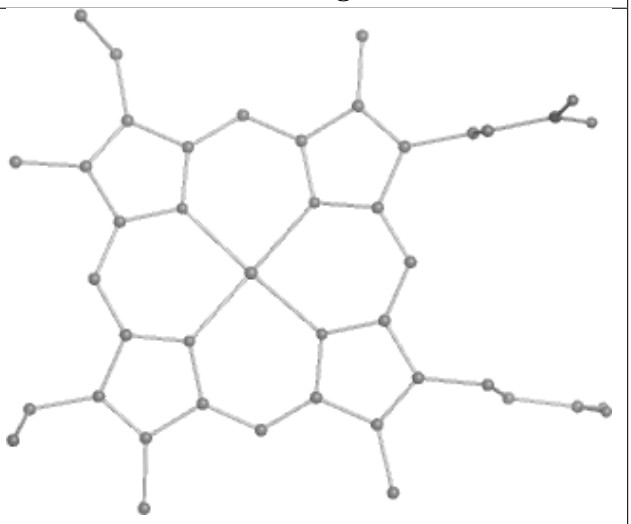


Bond angles

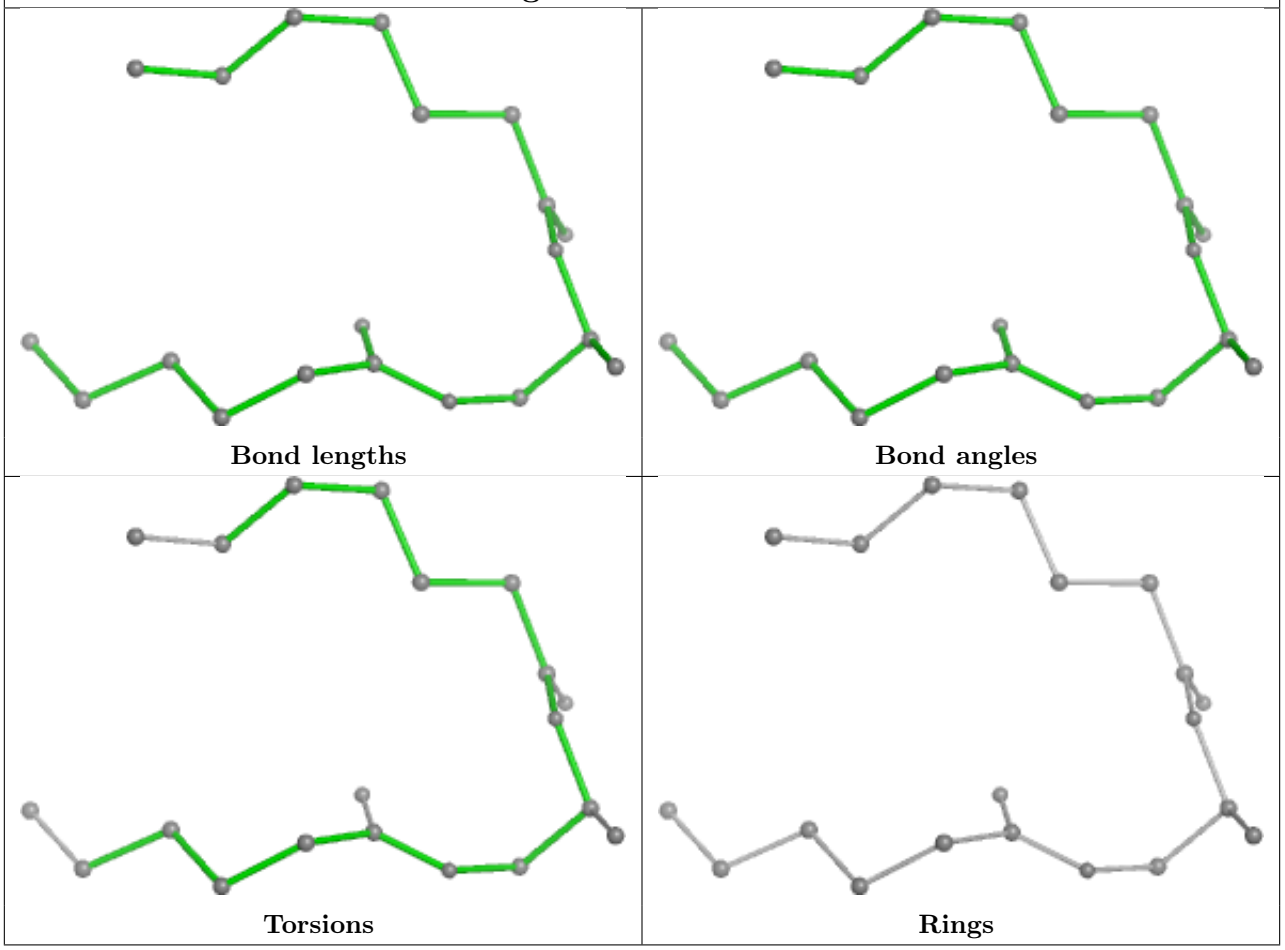


Torsions

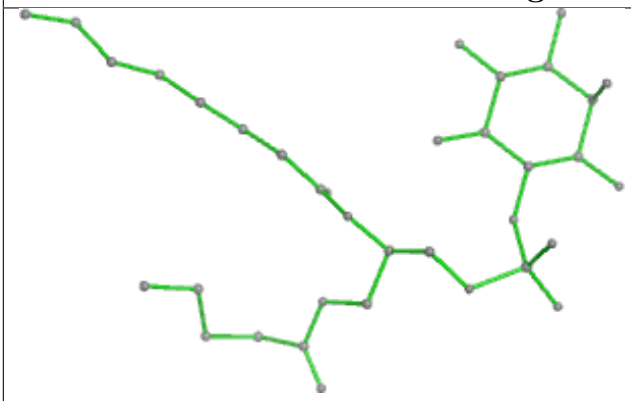


Rings

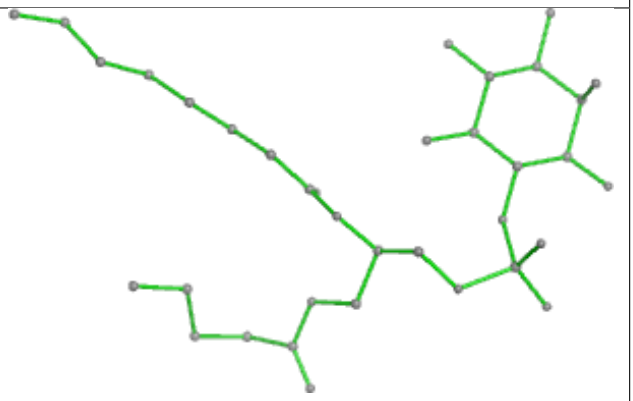
Ligand DGA E 404



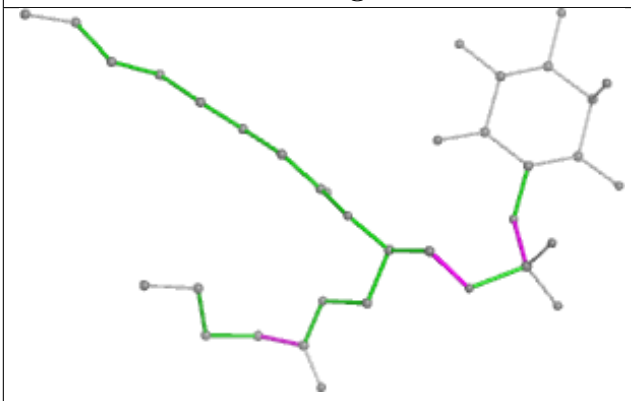
Ligand 9YF A 503



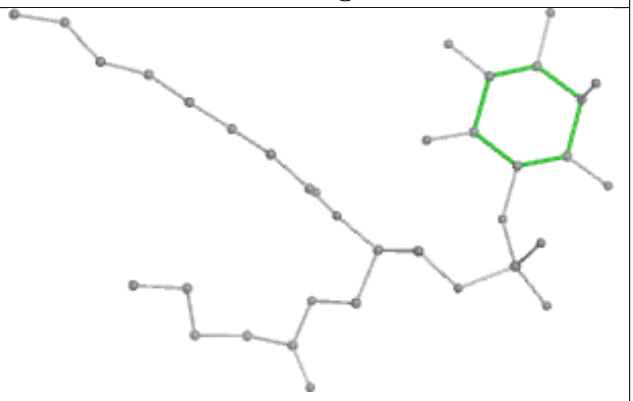
Bond lengths



Bond angles

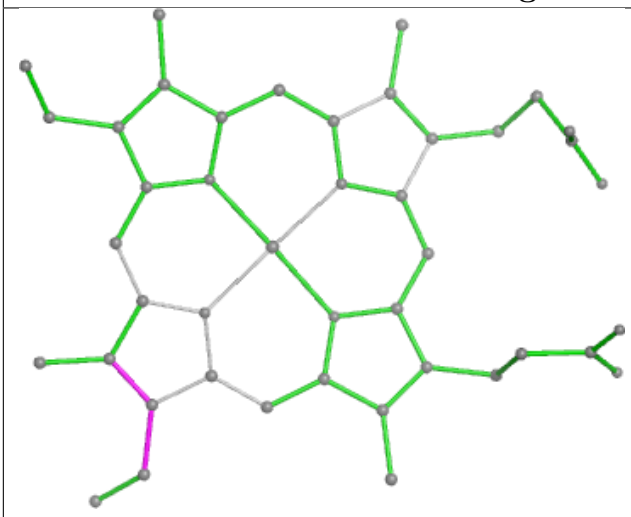


Torsions

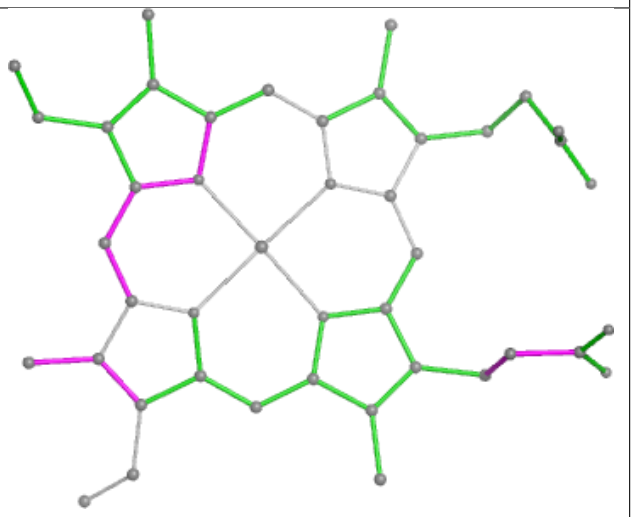


Rings

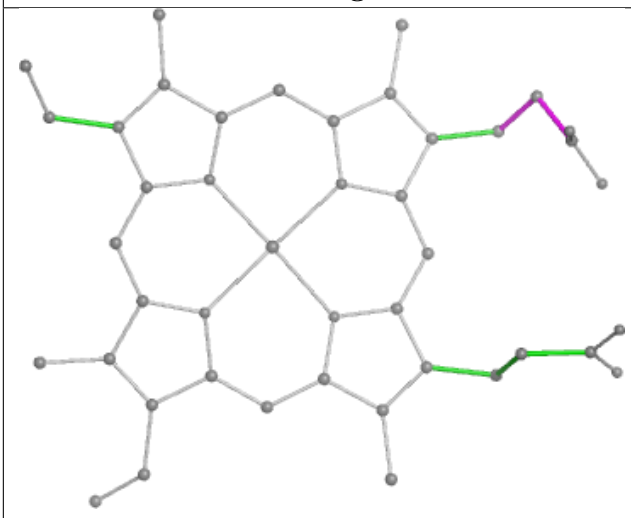
Ligand HEM B 602



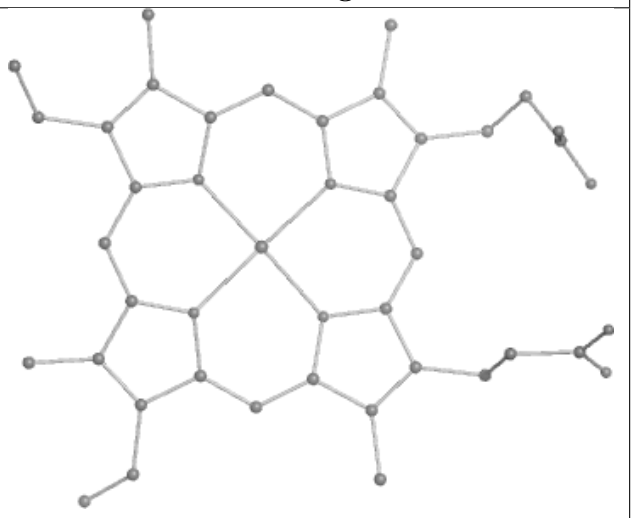
Bond lengths



Bond angles

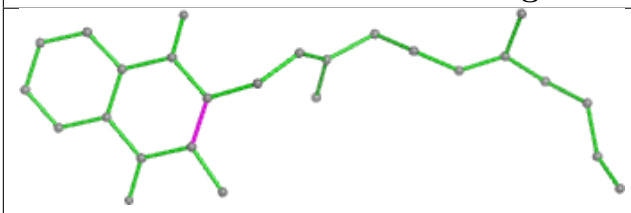


Torsions

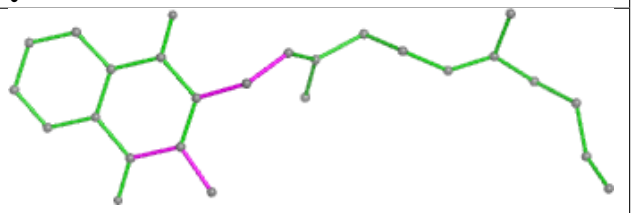


Rings

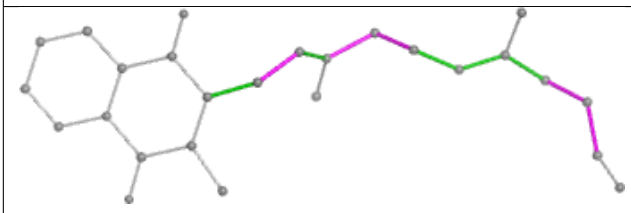
Ligand MQ9 A 504



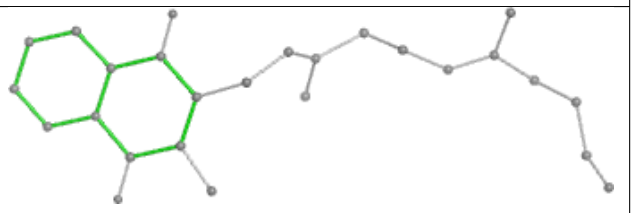
Bond lengths



Bond angles

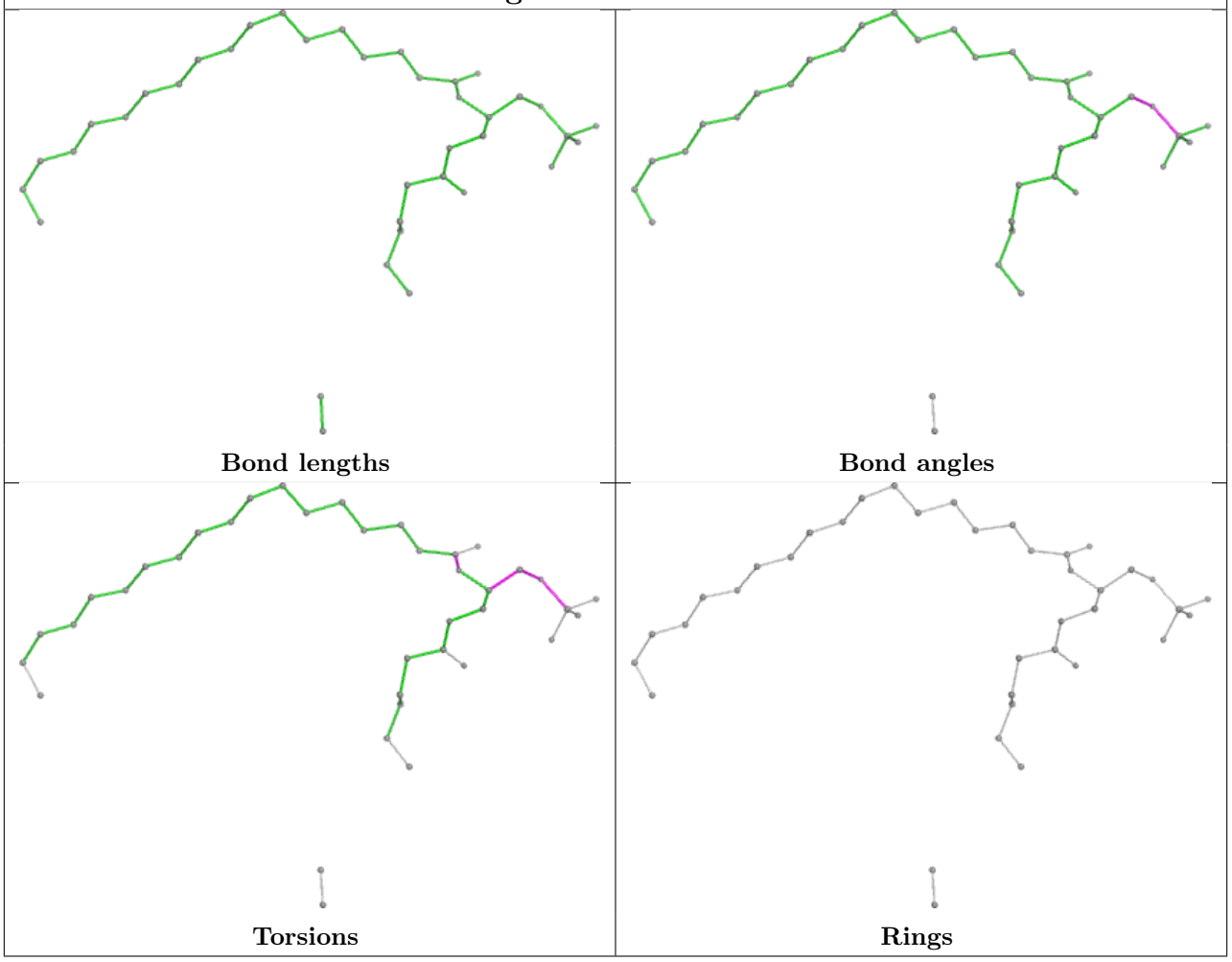


Torsions

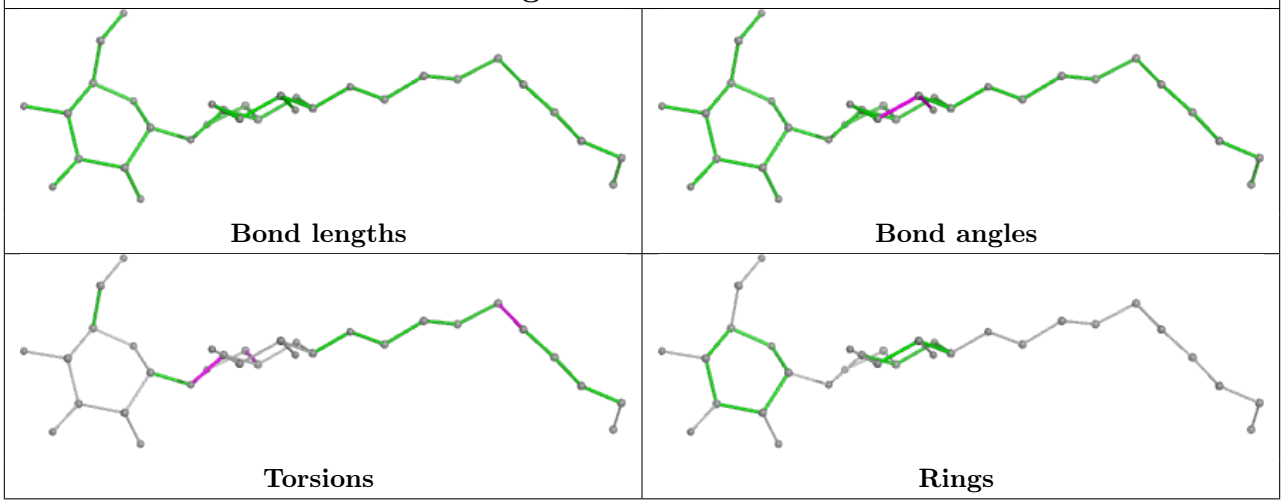


Rings

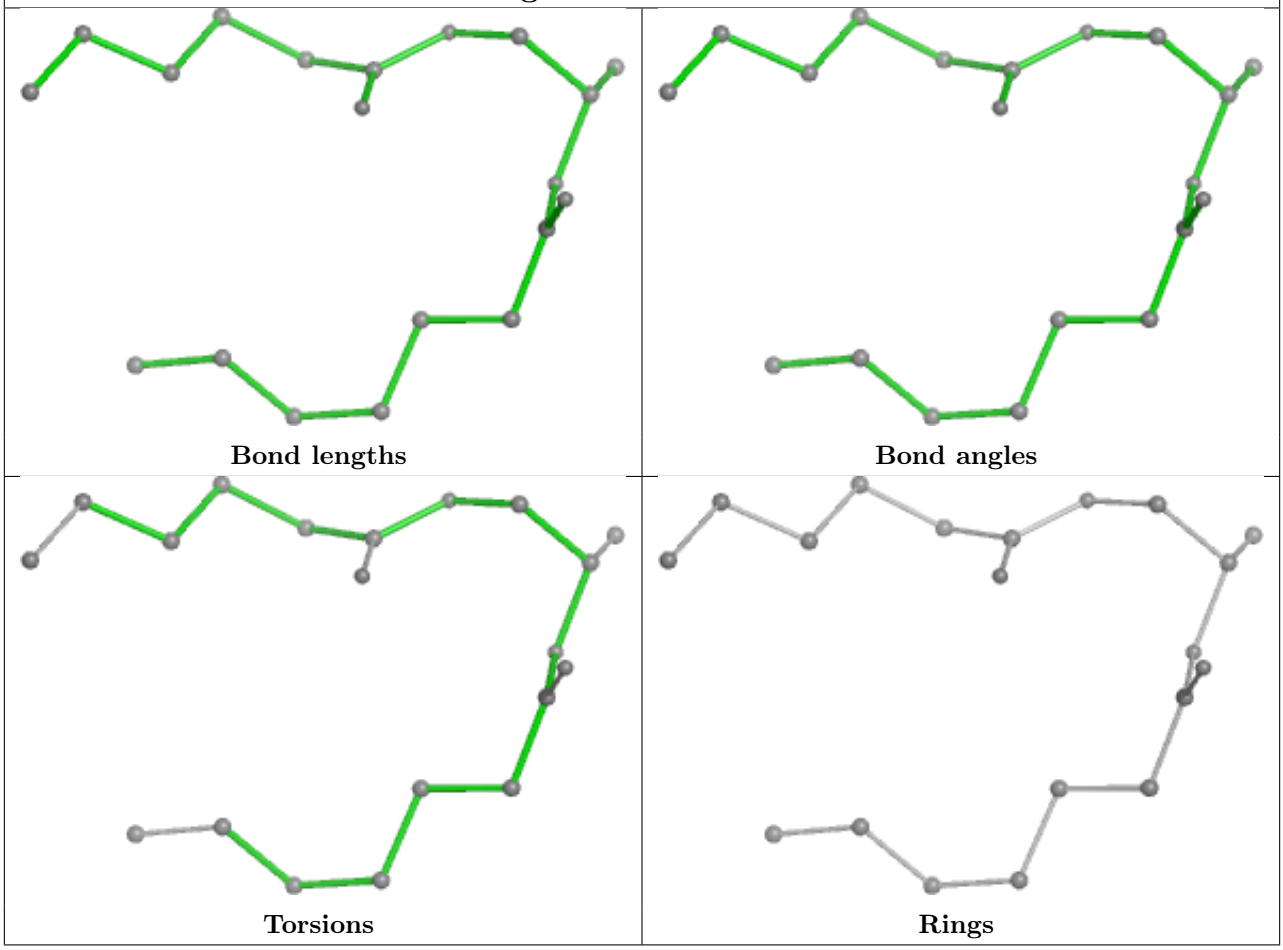
Ligand 3PH C 304



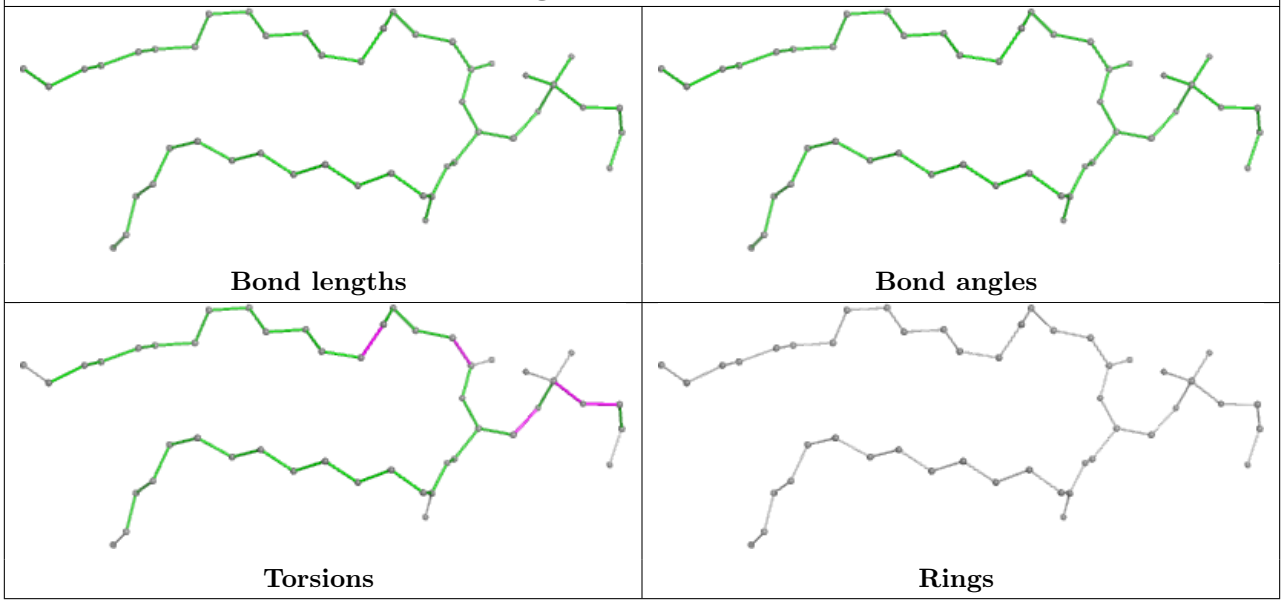
Ligand LMT B 608



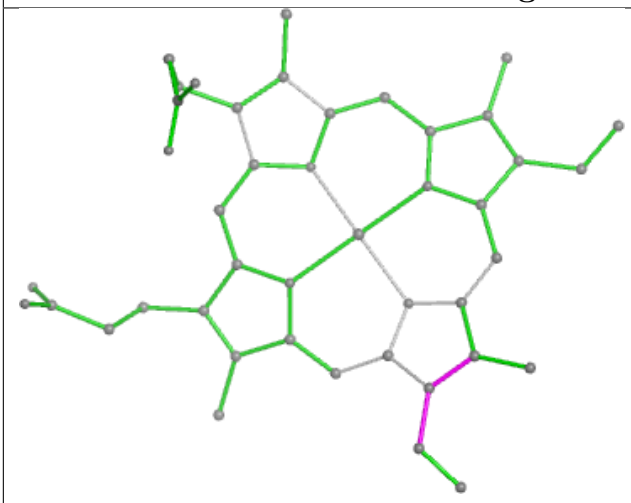
Ligand DGA R 404



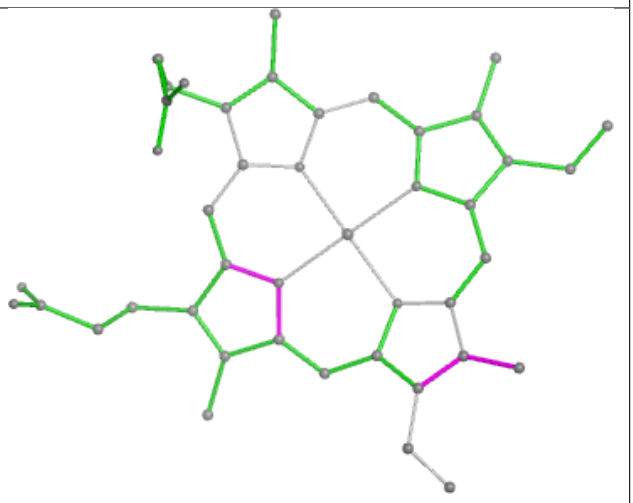
Ligand 3PE J 201



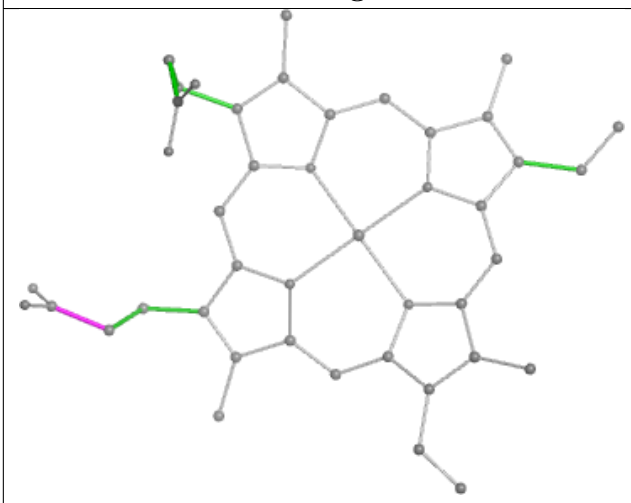
Ligand HEM O 604



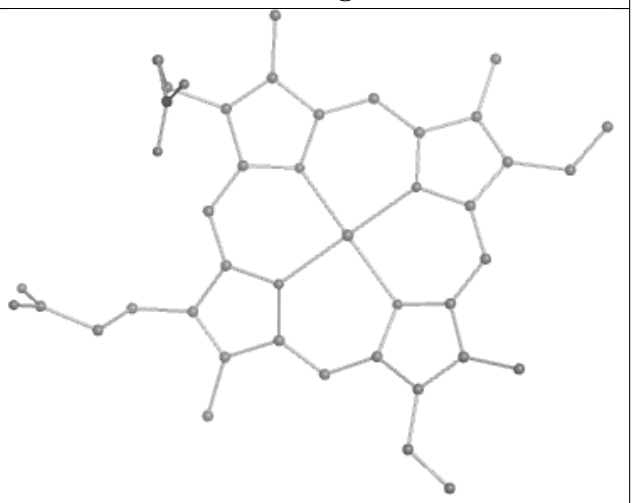
Bond lengths



Bond angles

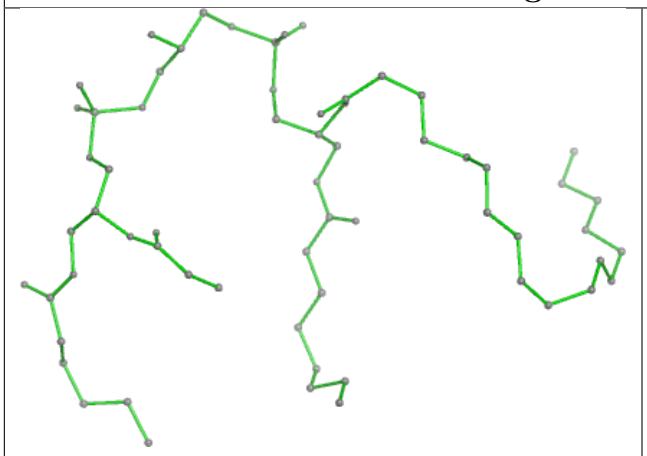


Torsions

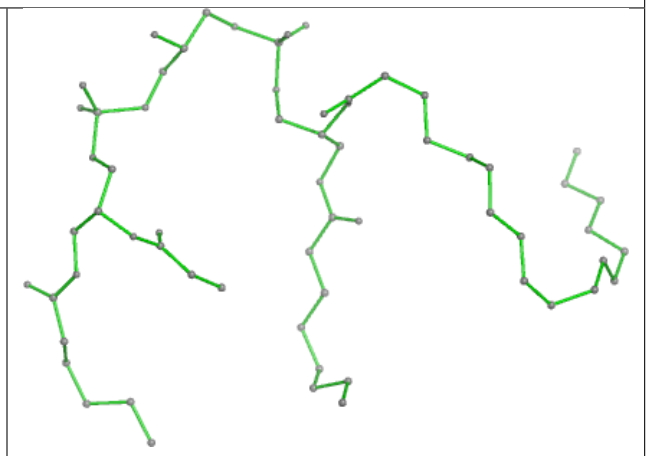


Rings

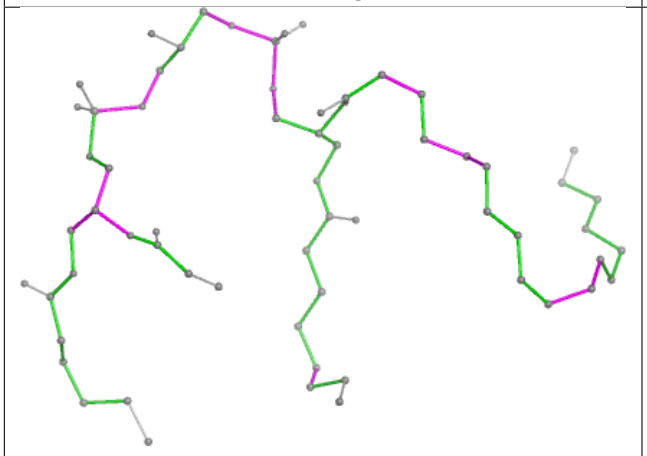
Ligand CDL D 606



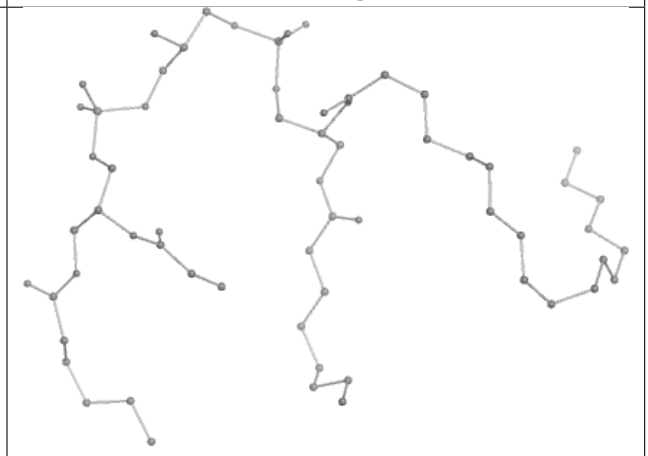
Bond lengths



Bond angles

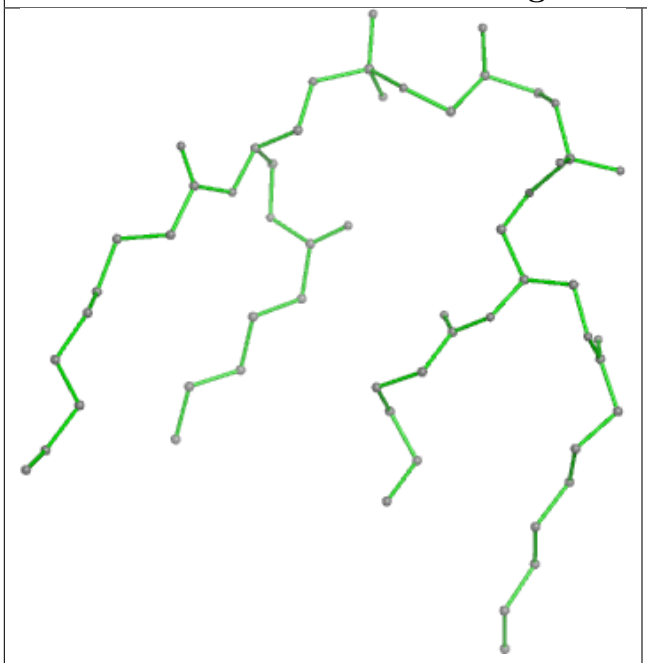


Torsions

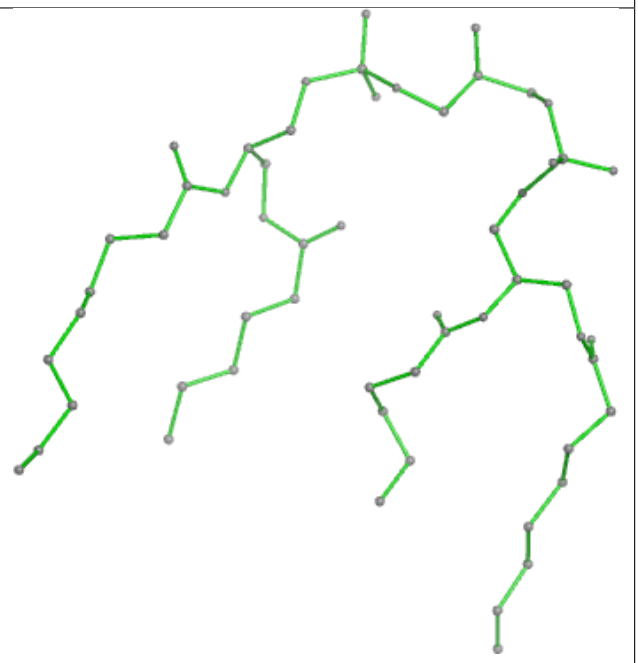


Rings

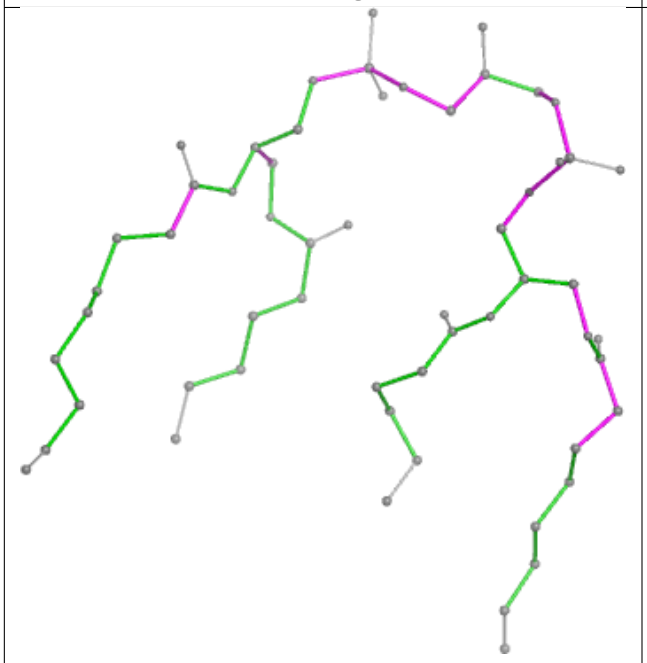
Ligand CDL S 302



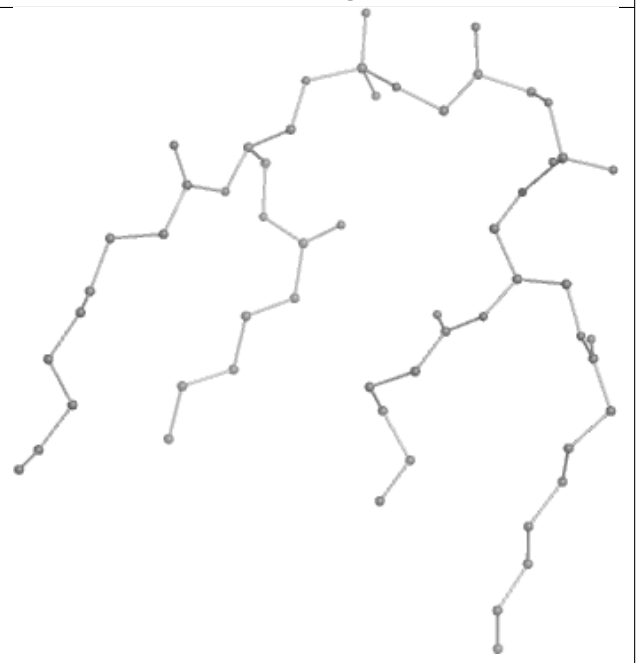
Bond lengths



Bond angles

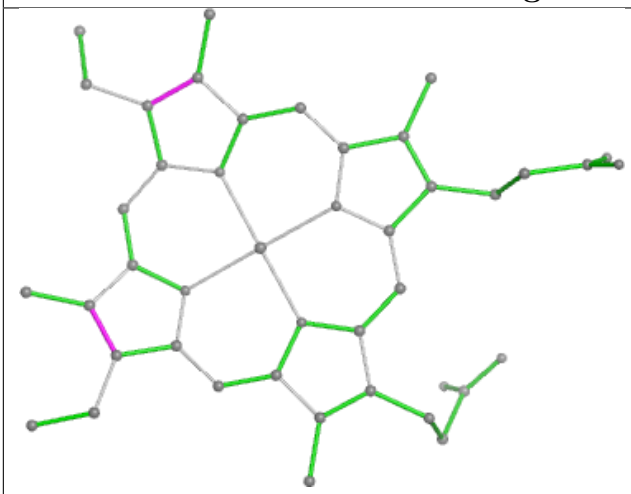


Torsions

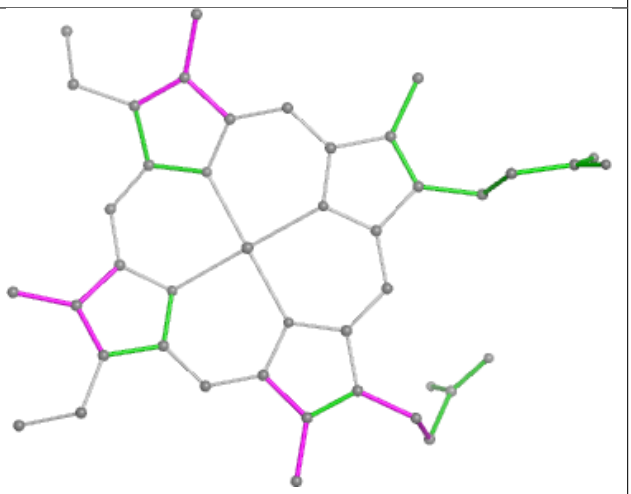


Rings

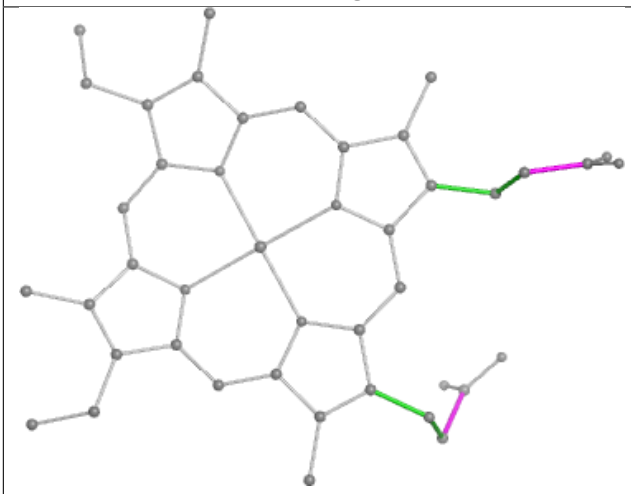
Ligand HEC P 302



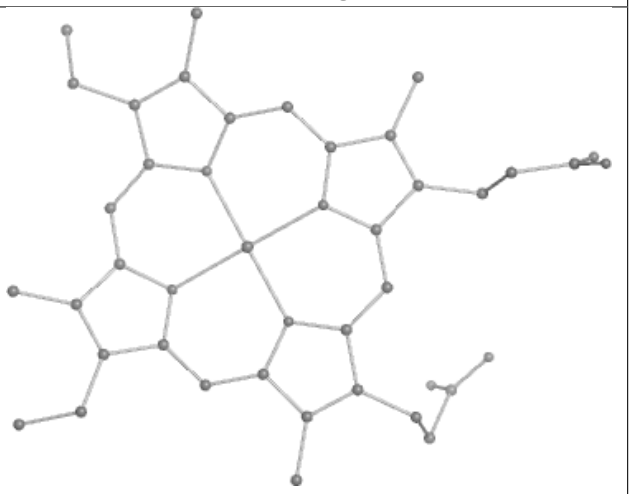
Bond lengths



Bond angles

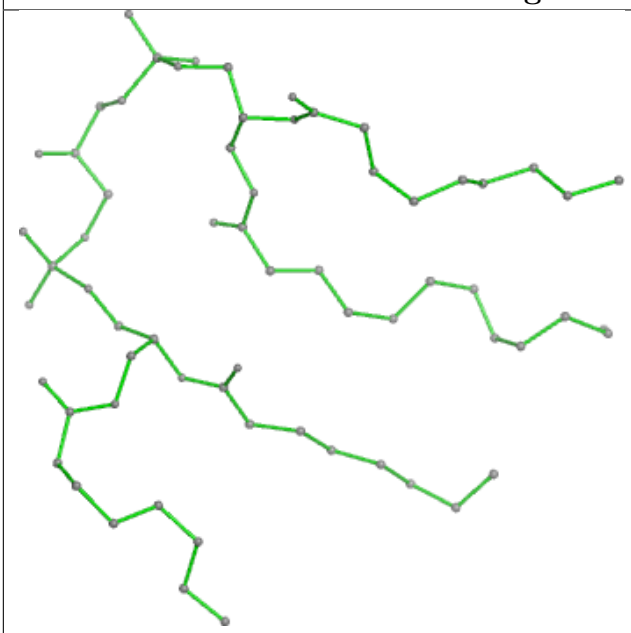


Torsions

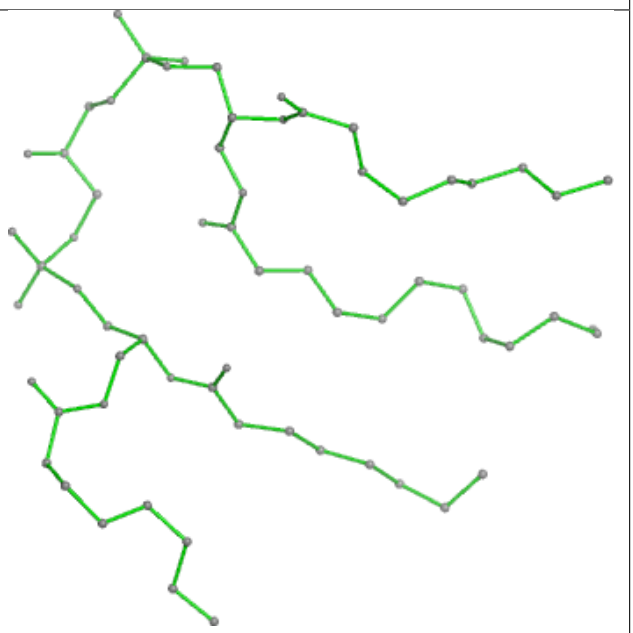


Rings

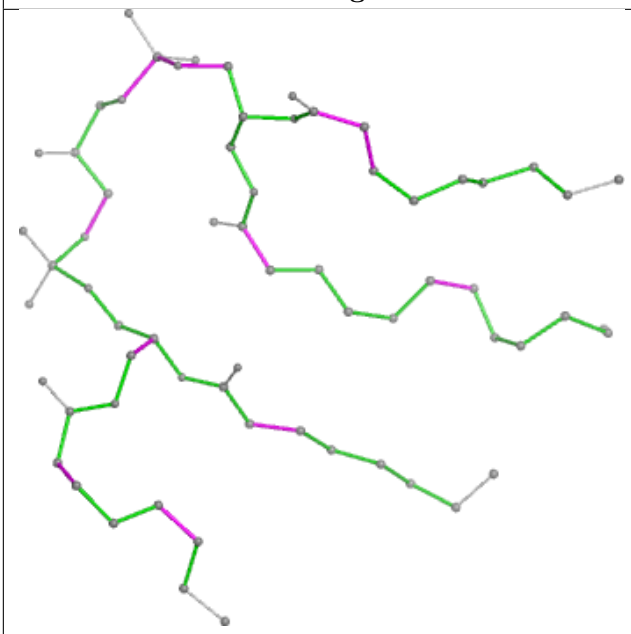
Ligand CDL C 301



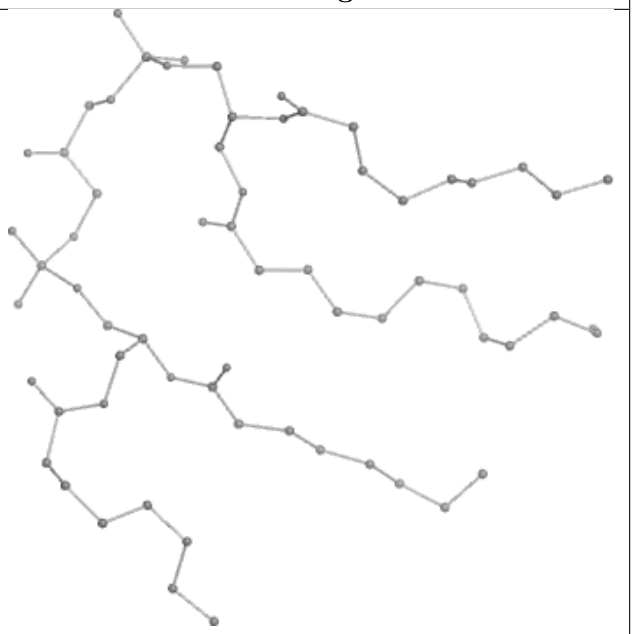
Bond lengths



Bond angles

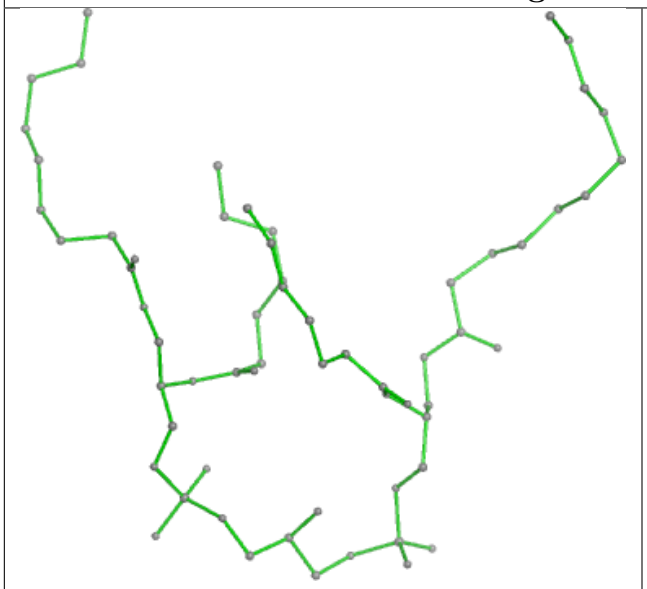


Torsions

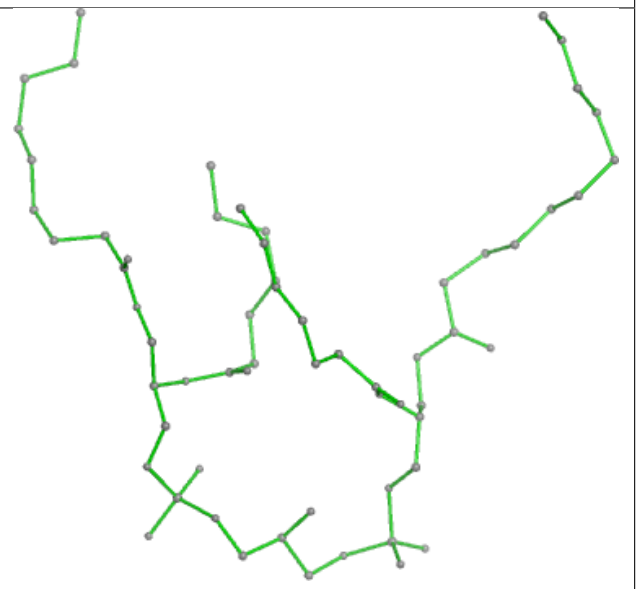


Rings

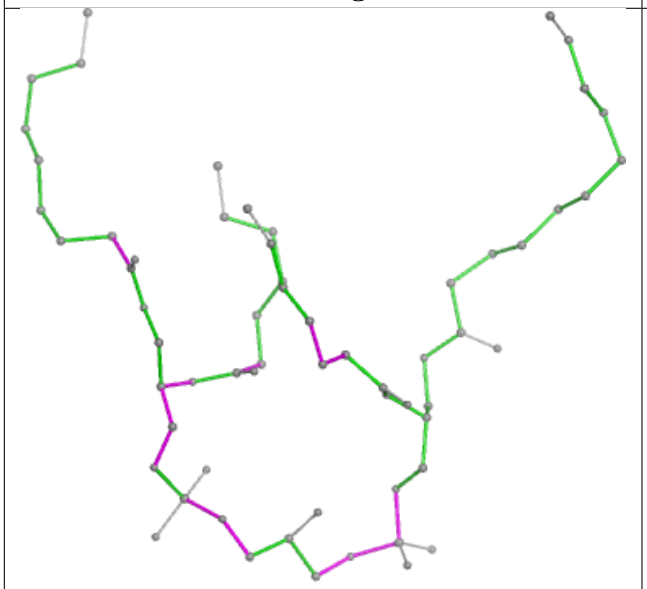
Ligand CDL S 303



Bond lengths



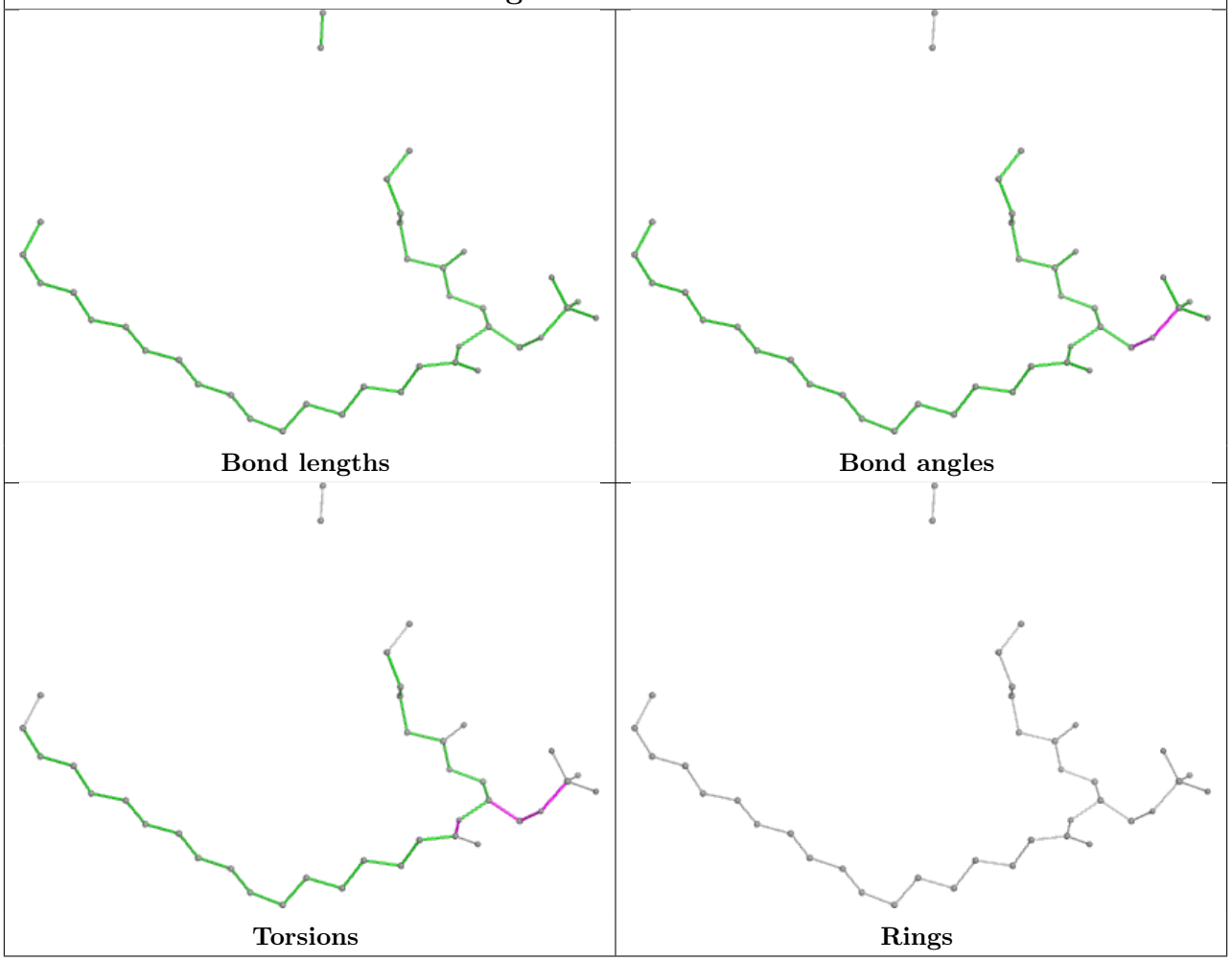
Bond angles



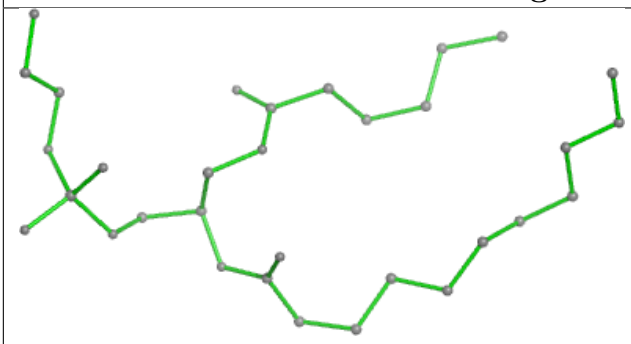
Torsions

Rings

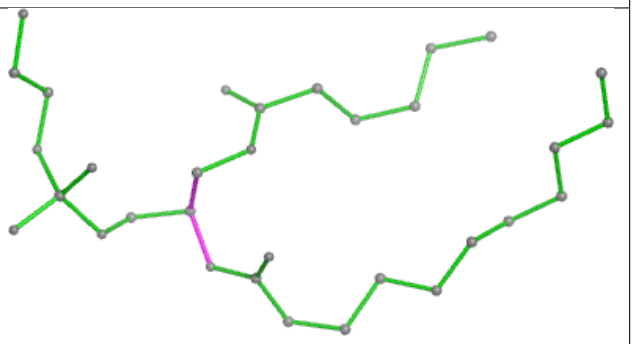
Ligand 3PH T 201



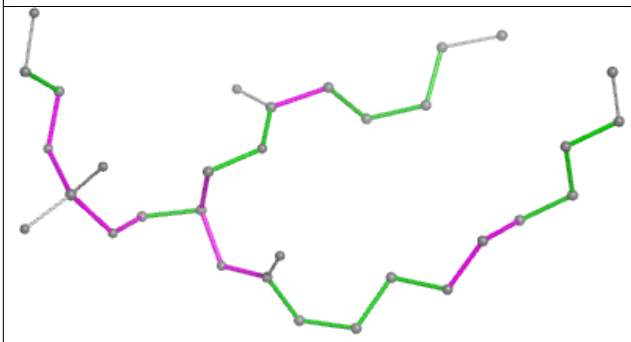
Ligand 3PE F 301



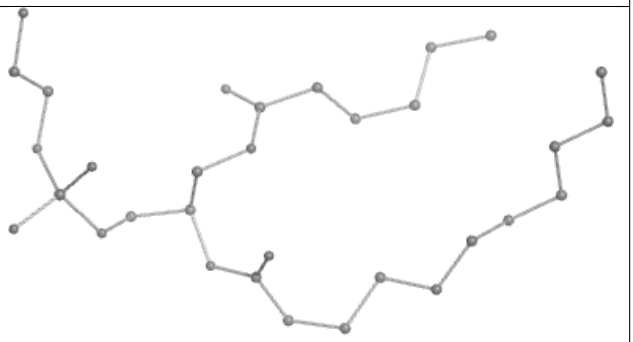
Bond lengths



Bond angles

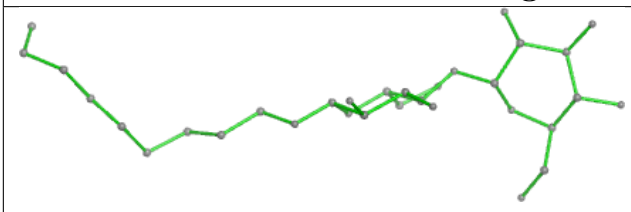


Torsions

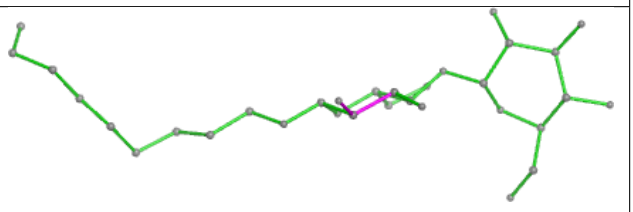


Rings

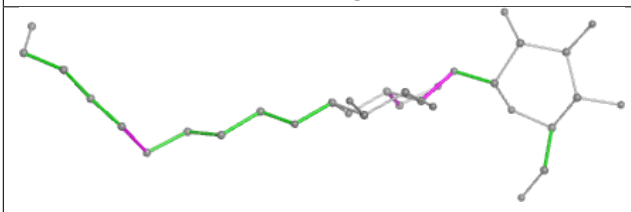
Ligand LMT O 601



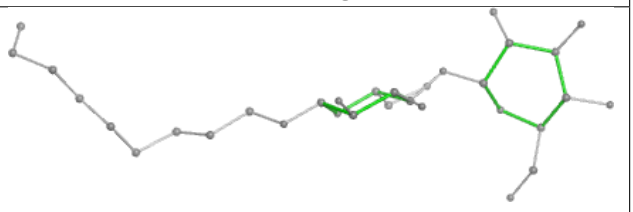
Bond lengths



Bond angles

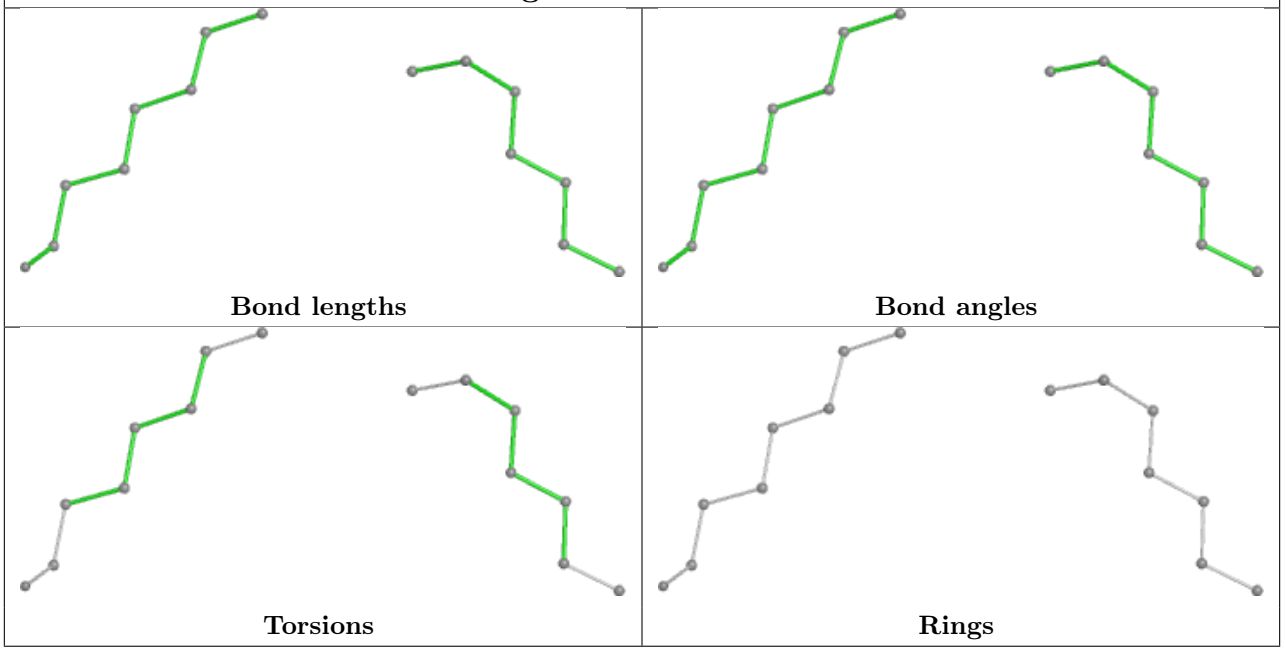


Torsions

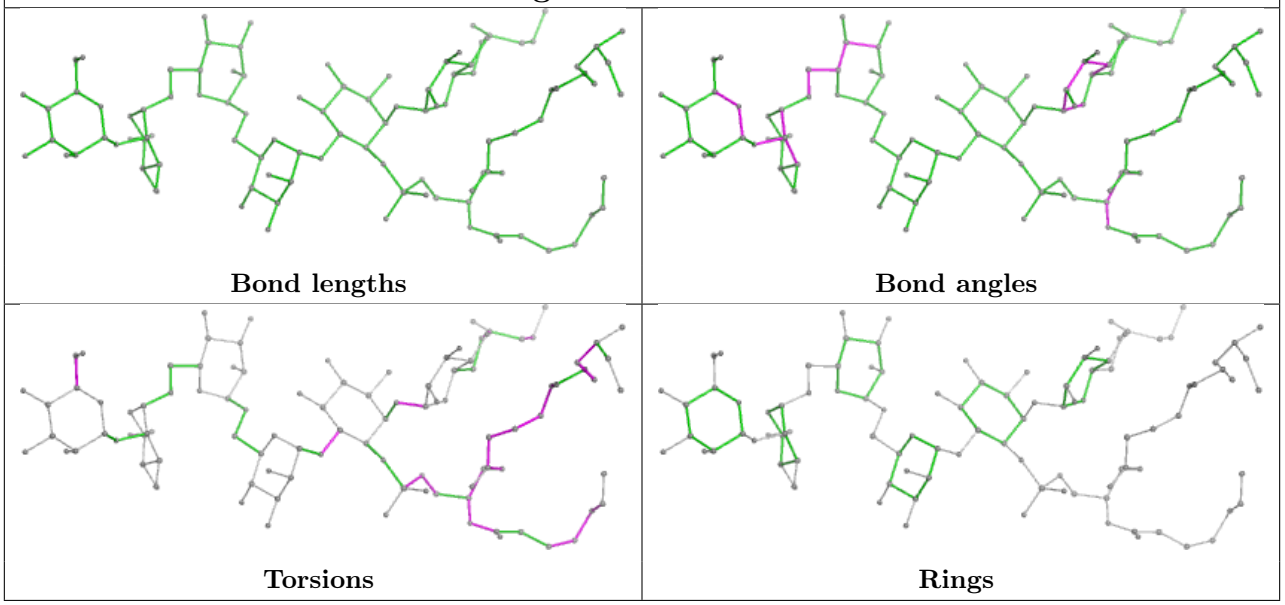


Rings

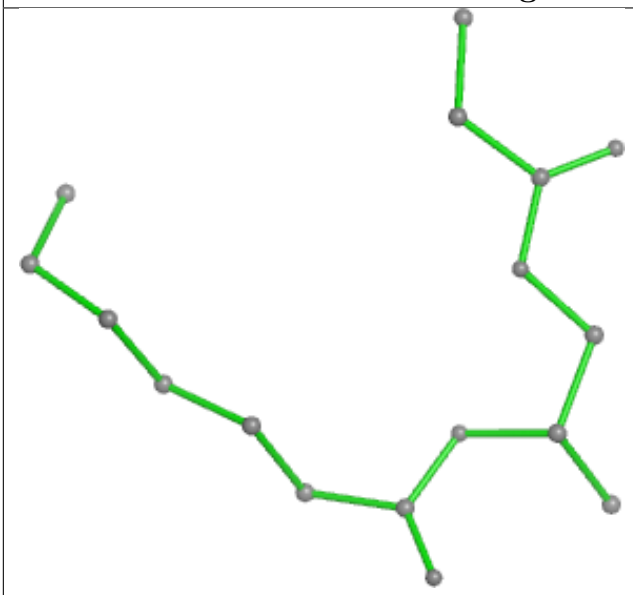
Ligand PLM U 202



Ligand IZL N 504



Ligand DGA U 201



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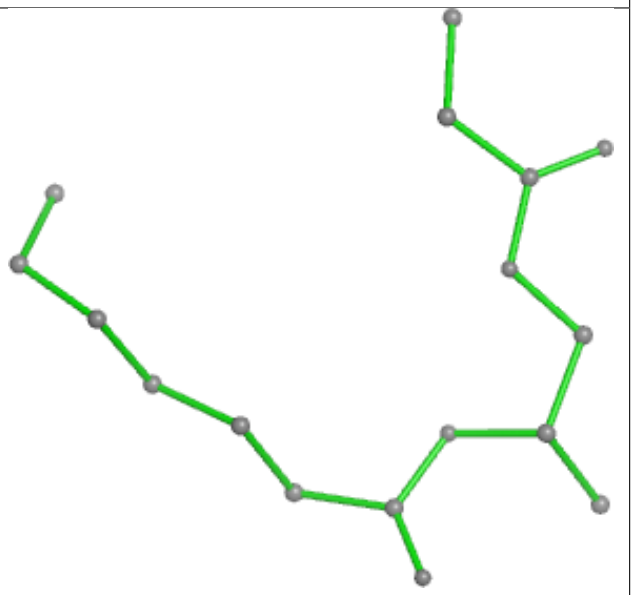
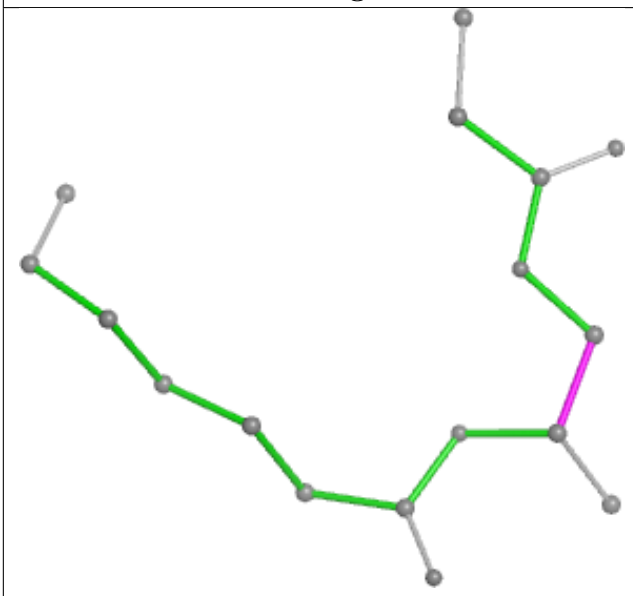
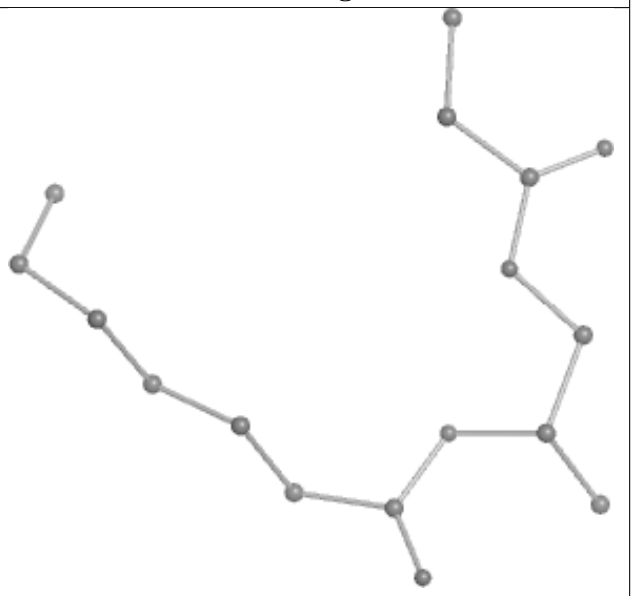


Bond angles

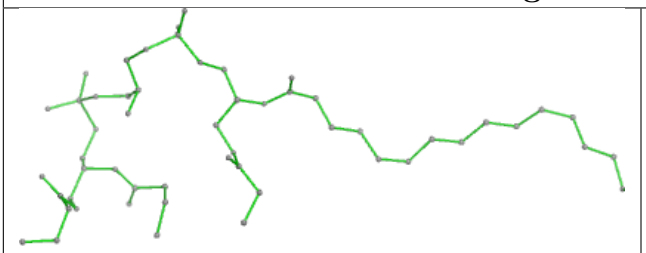


Torsions

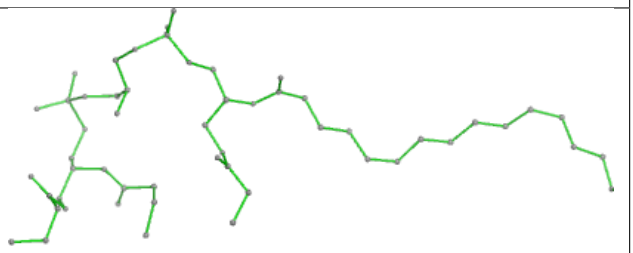


Rings

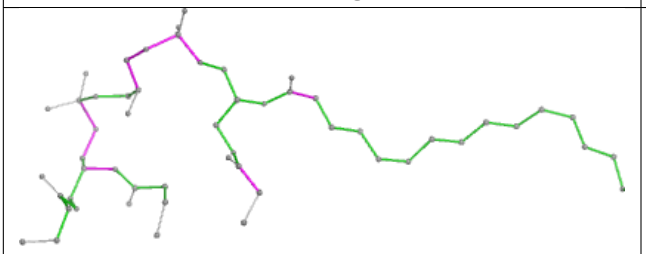
Ligand CDL V 201



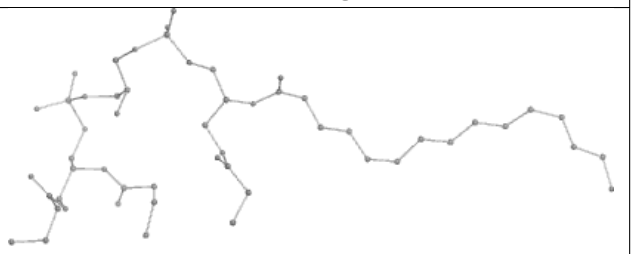
Bond lengths



Bond angles

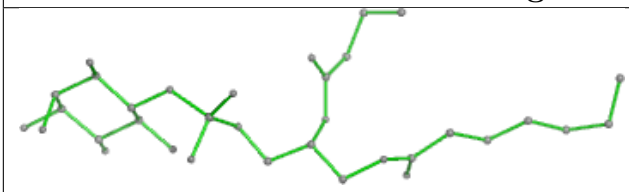


Torsions

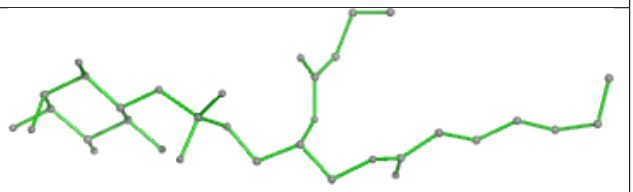


Rings

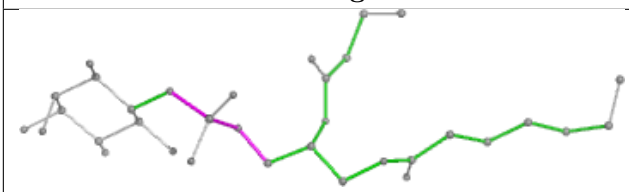
Ligand 9YF U 203



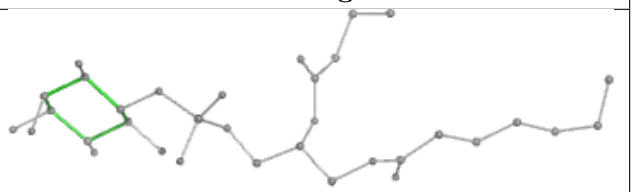
Bond lengths



Bond angles

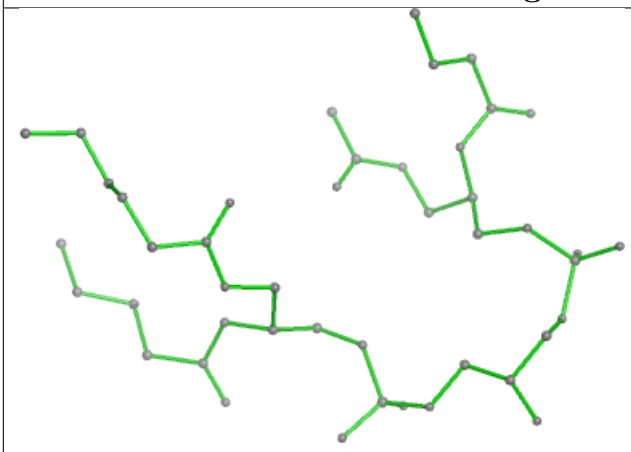


Torsions

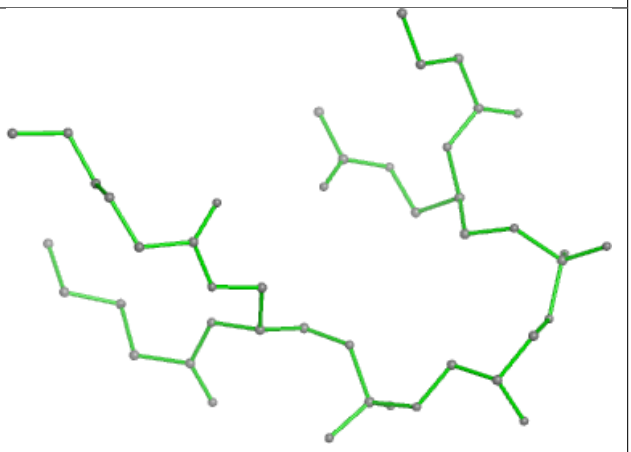


Rings

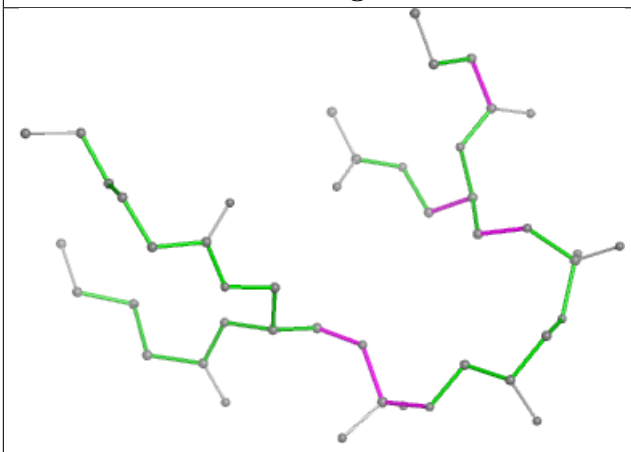
Ligand CDL O 606



Bond lengths



Bond angles



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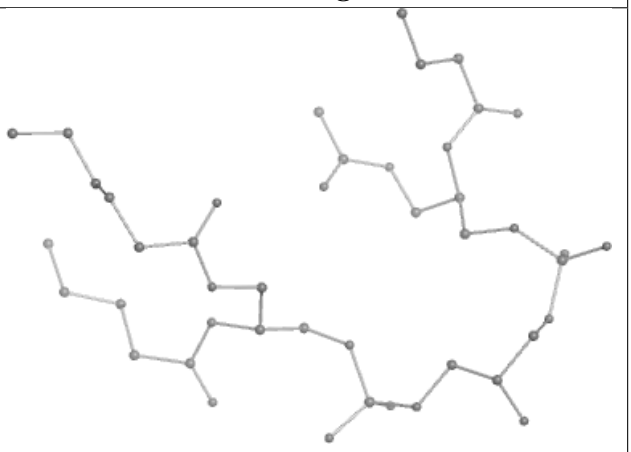
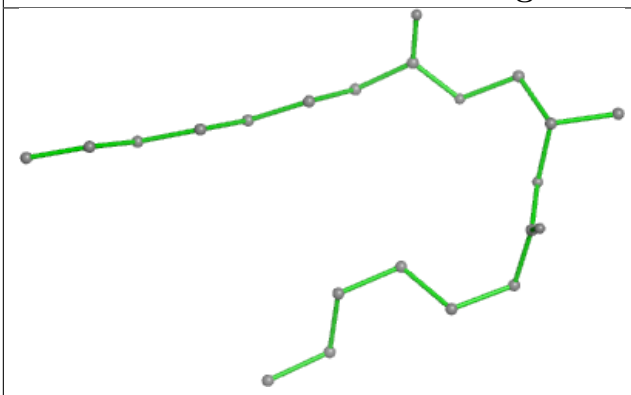


Rings

Ligand DGA M 201



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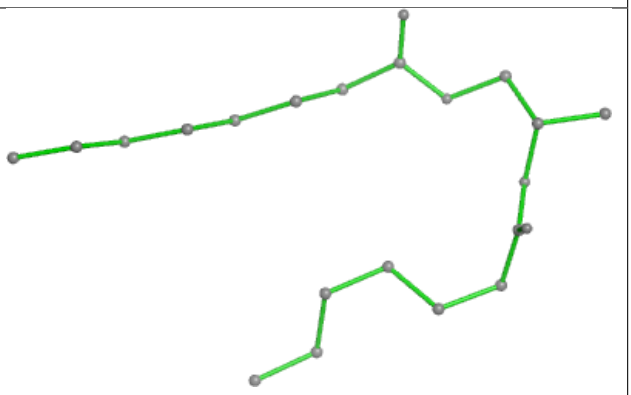
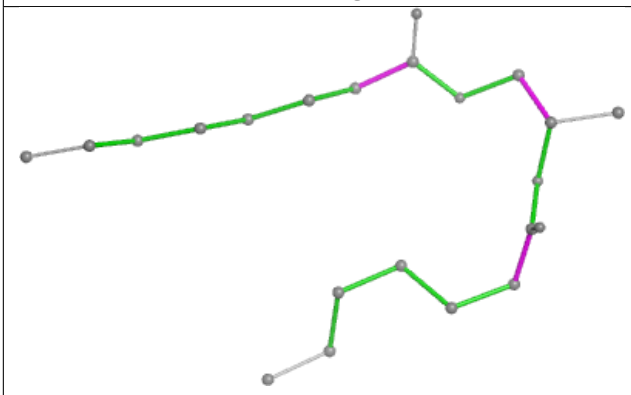


Bond angles



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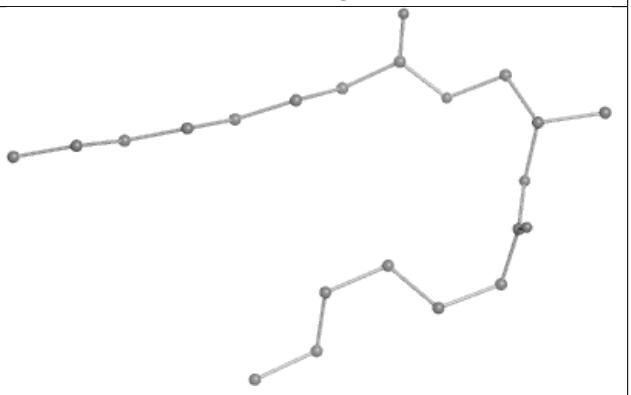
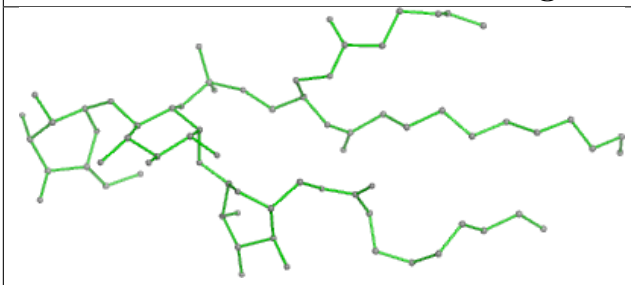


Rings

Ligand IX7 I 202



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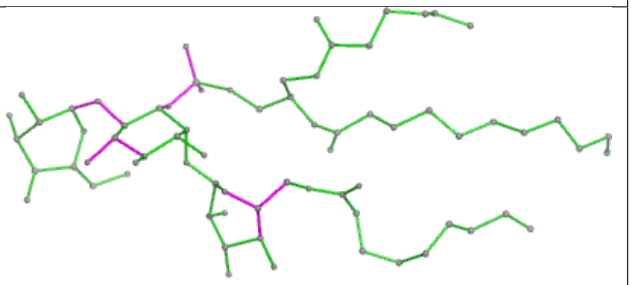
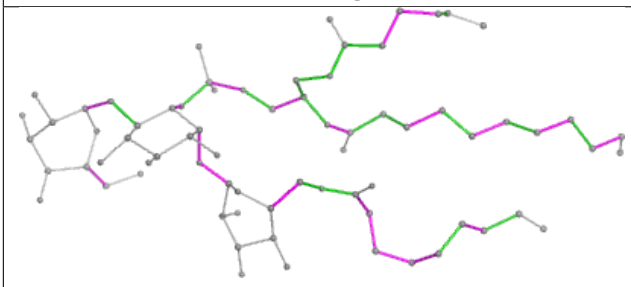
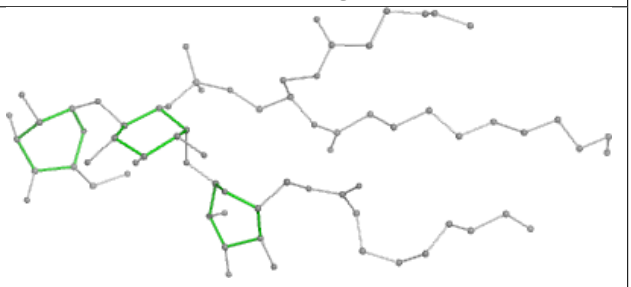


Bond angles

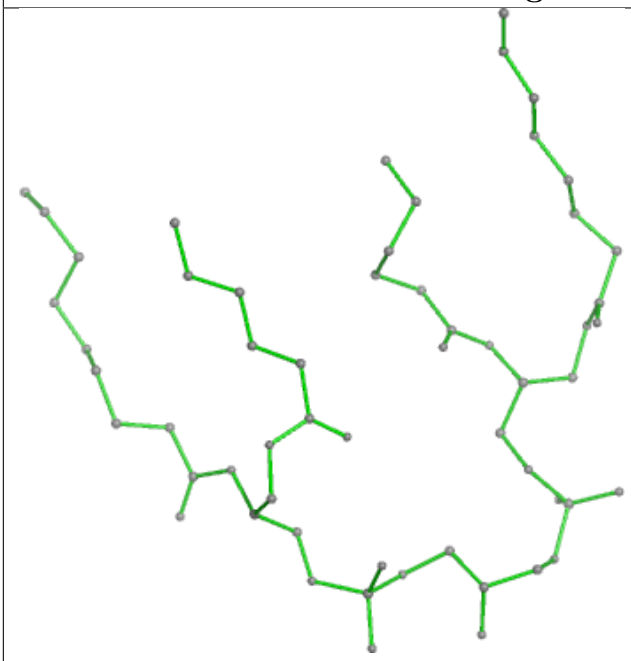


Torsions

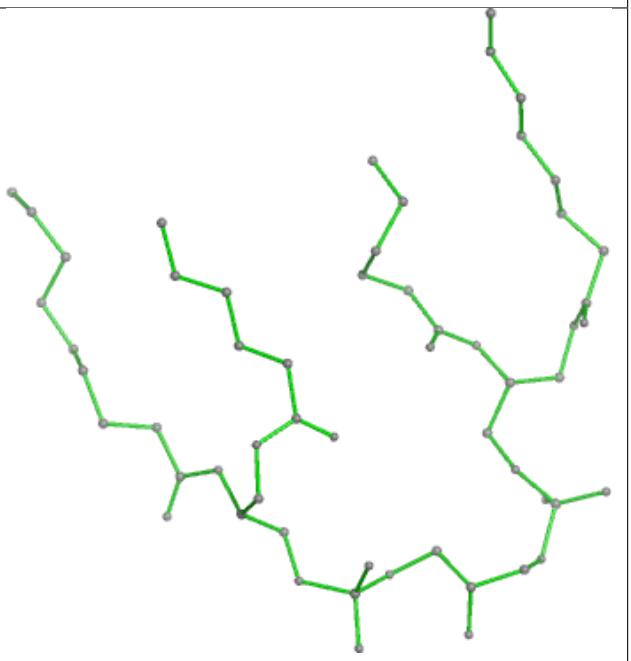


Rings

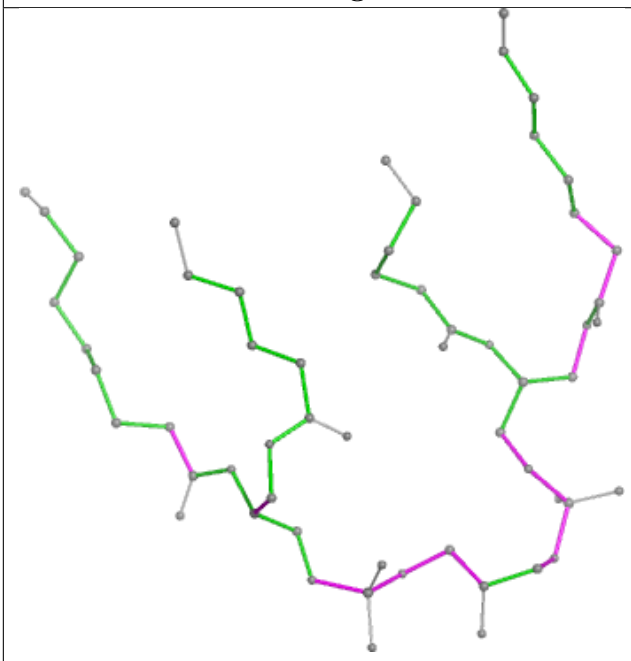
Ligand CDL F 302



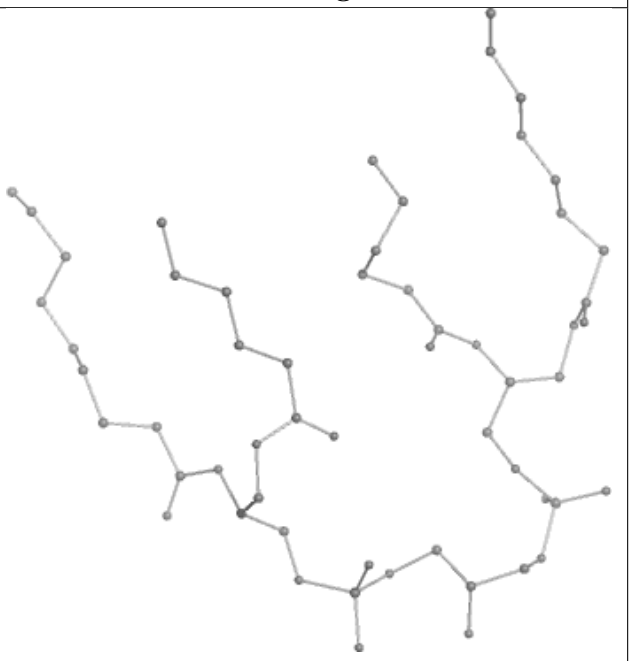
Bond lengths



Bond angles

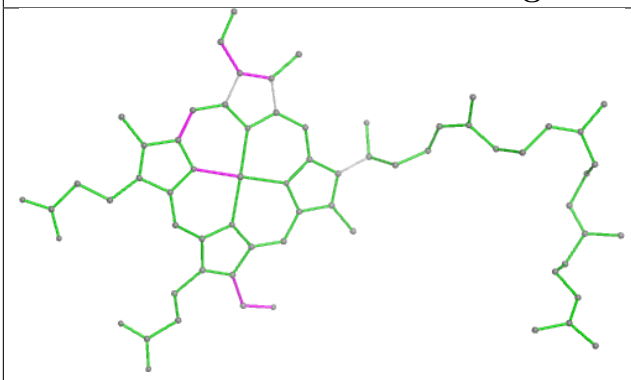


Torsions

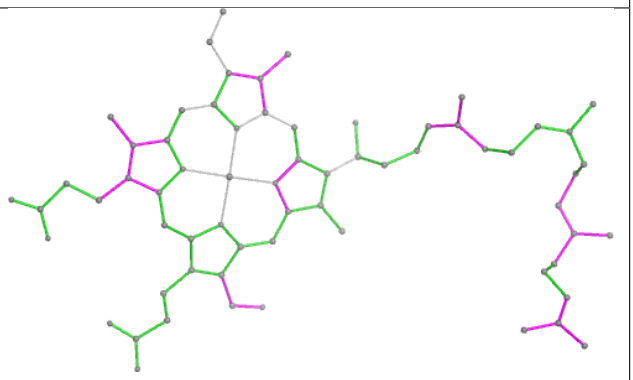


Rings

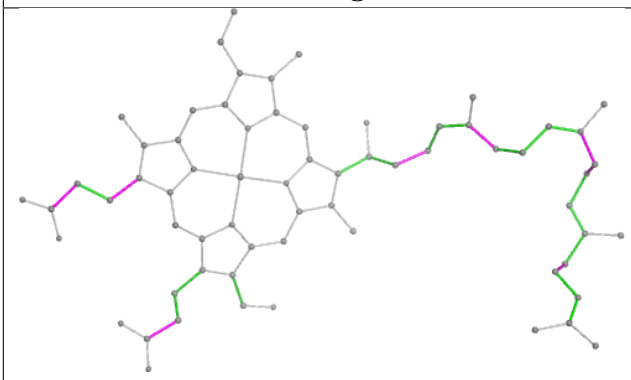
Ligand HAS D 602



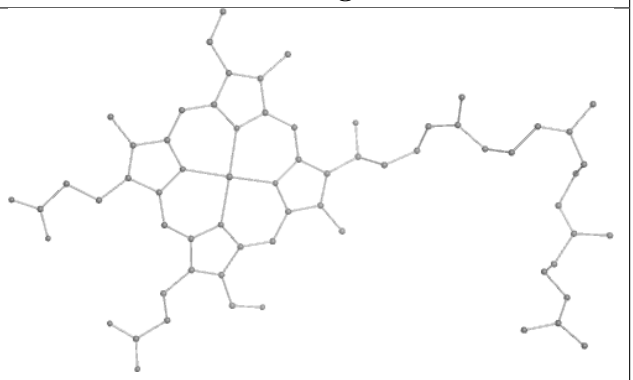
Bond lengths



Bond angles

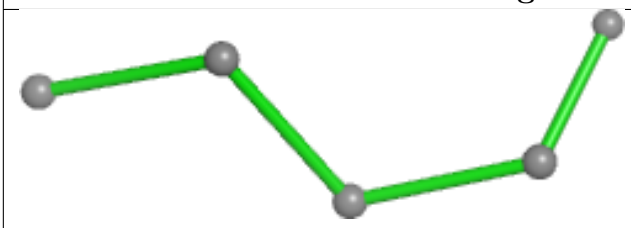


Torsions

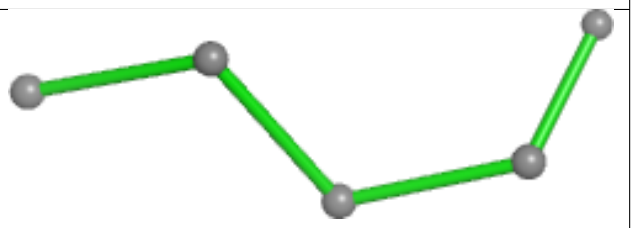


Rings

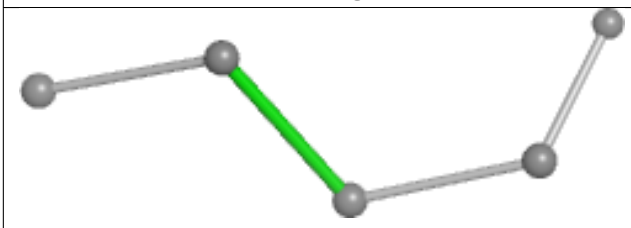
Ligand PLM M 202



Bond lengths



Bond angles



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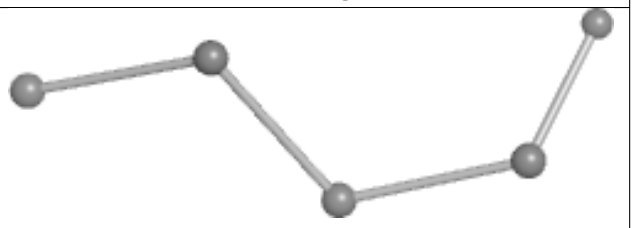
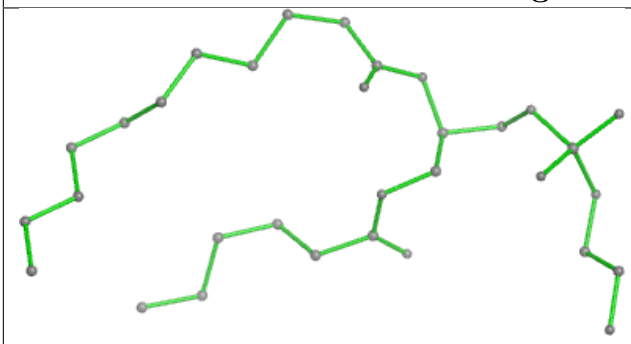


Rings

Ligand 3PE S 301



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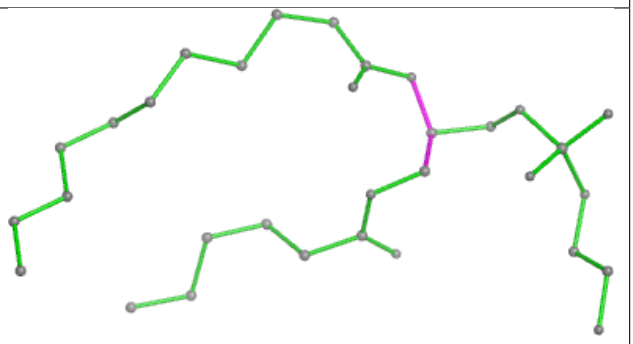
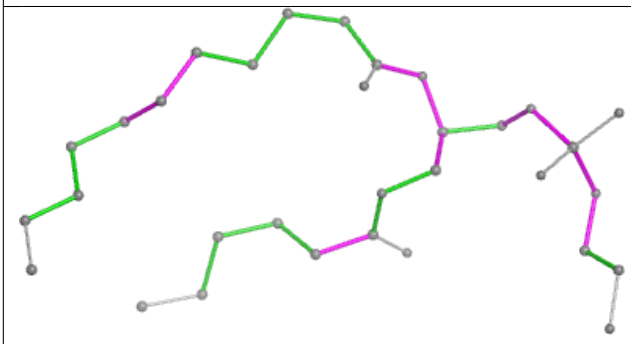
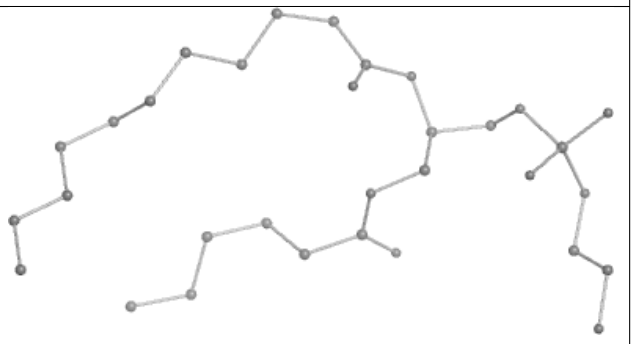


Bond angles

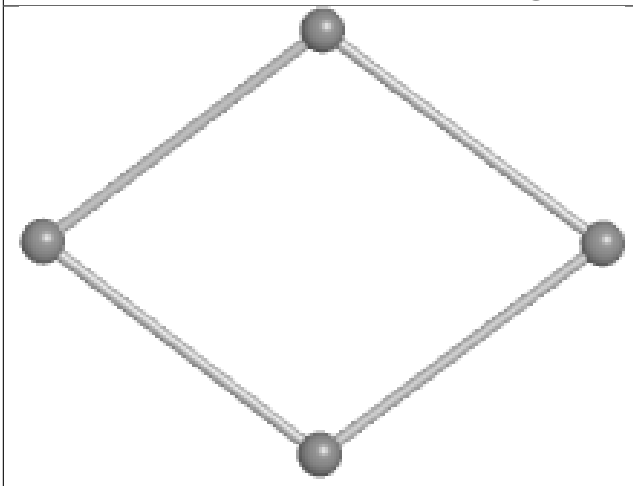


Torsions

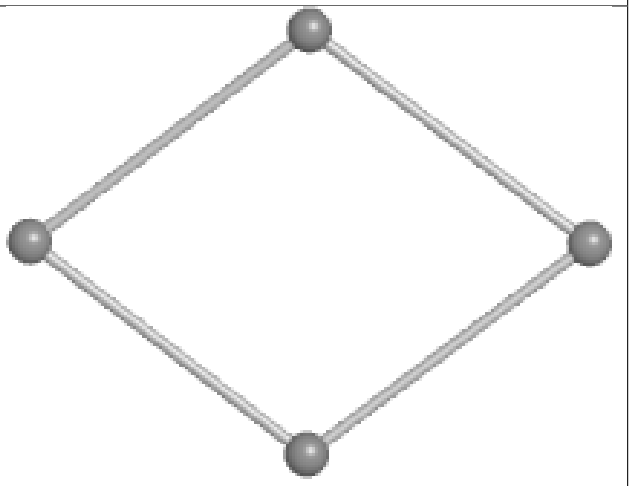


Rings

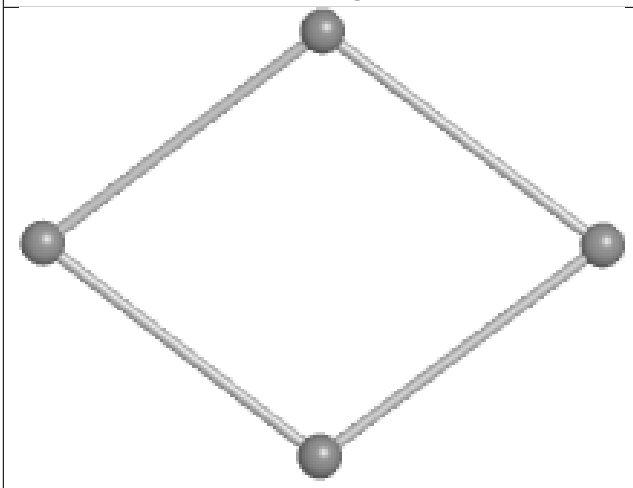
Ligand FES N 503



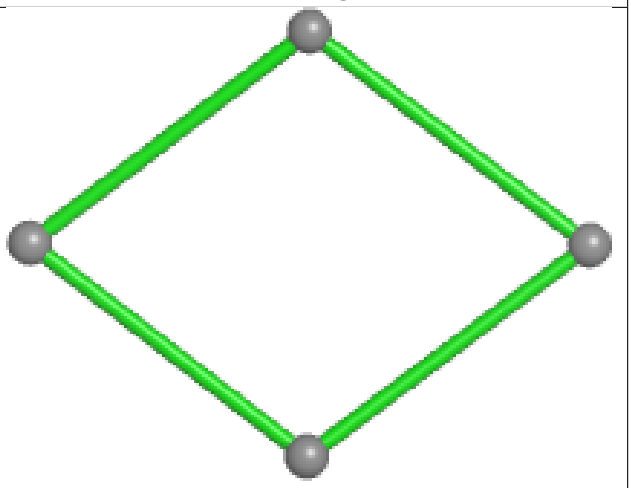
Bond lengths



Bond angles

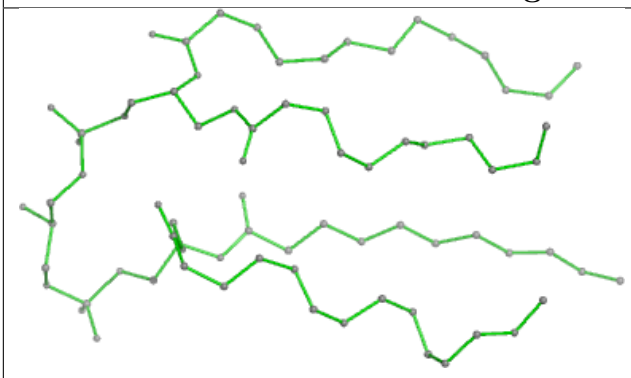


Torsions

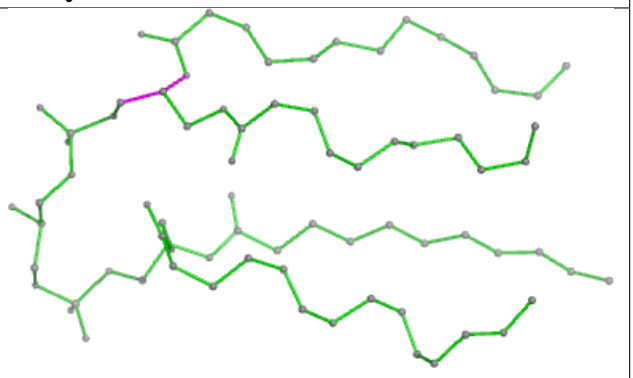


Rings

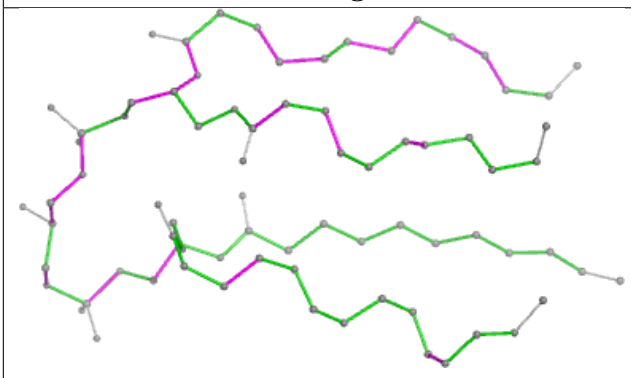
Ligand CDL Q 605



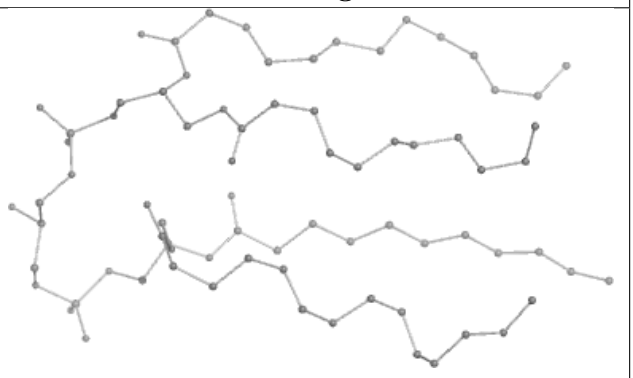
Bond lengths



Bond angles

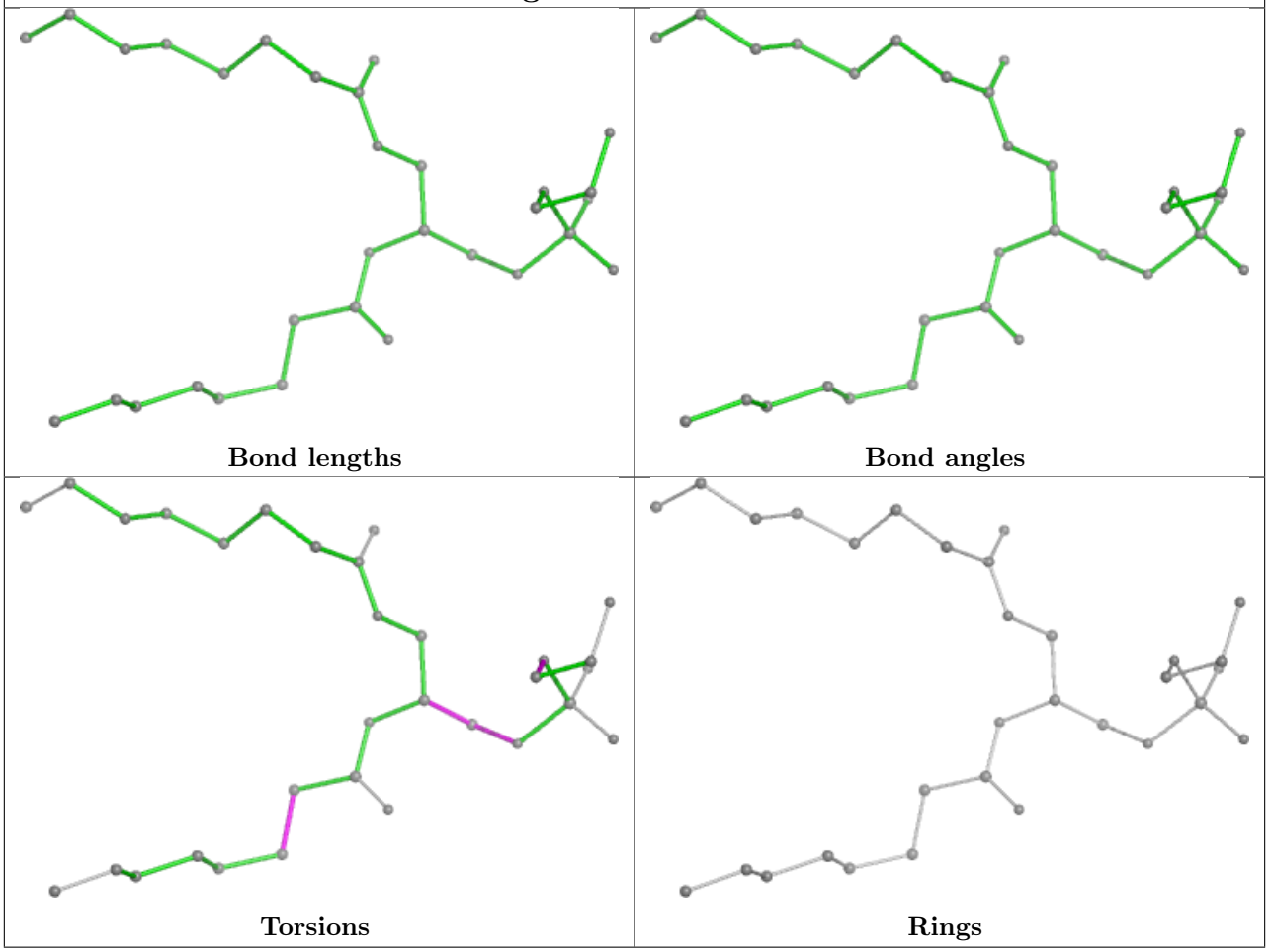


Torsions

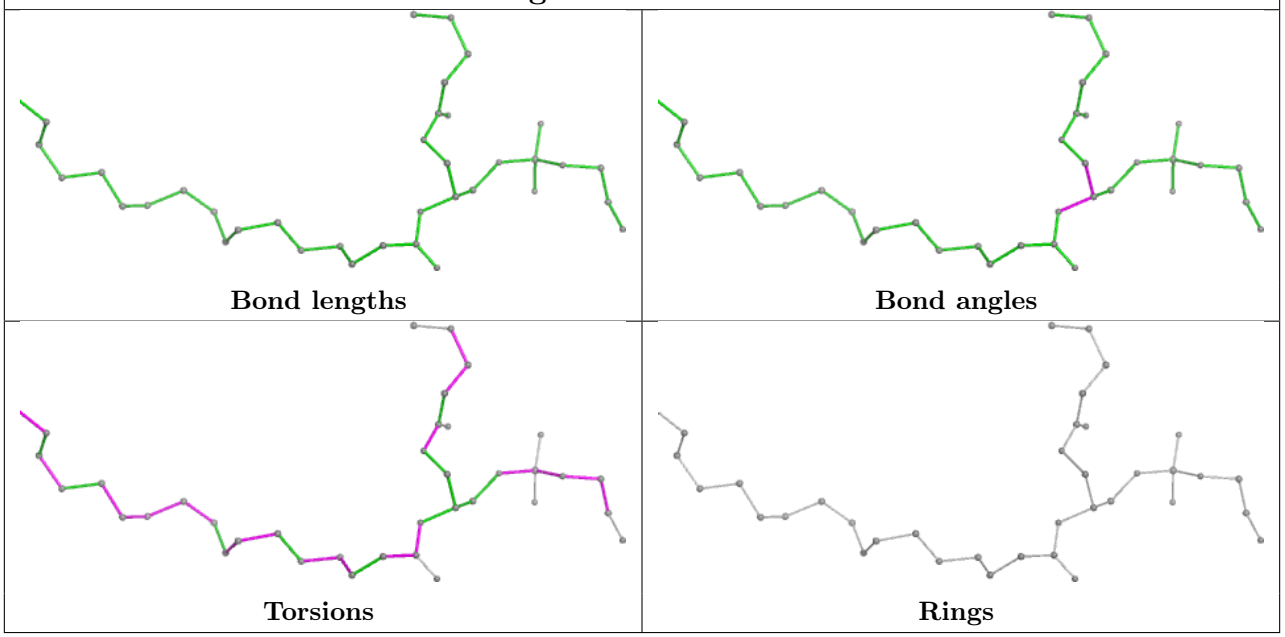


Rings

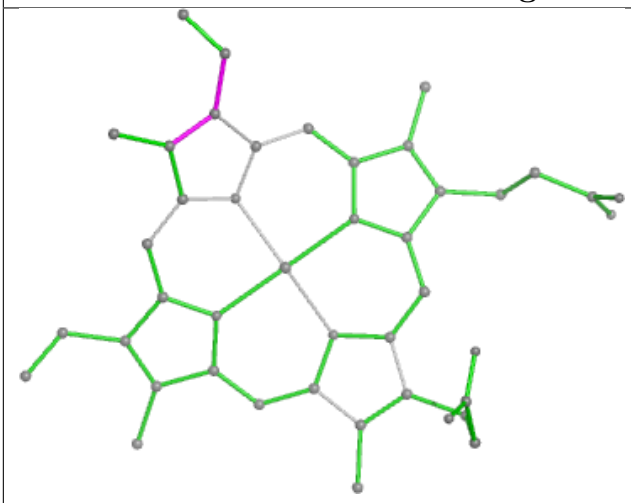
Ligand 3PE D 607



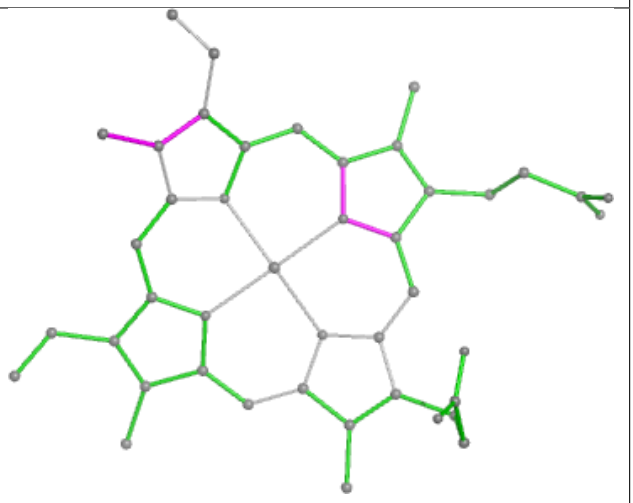
Ligand 3PE A 505



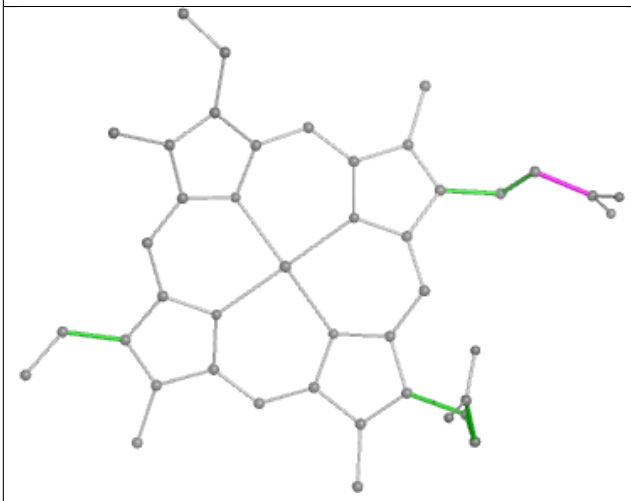
Ligand HEM B 603



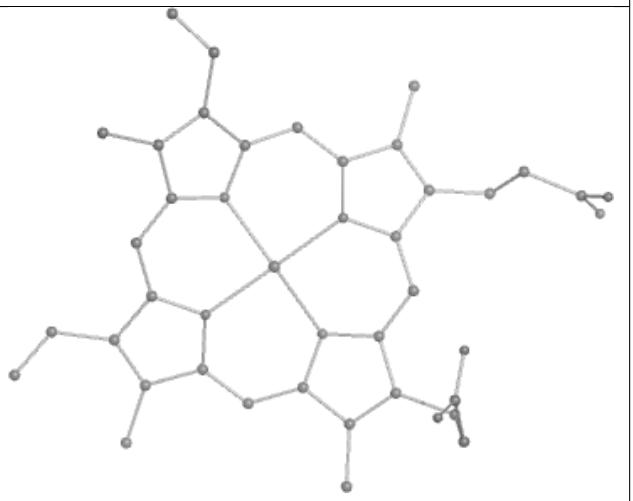
Bond lengths



Bond angles

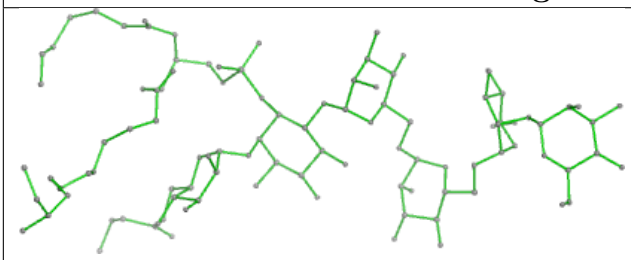


Torsions



Rings

Ligand IZL A 502



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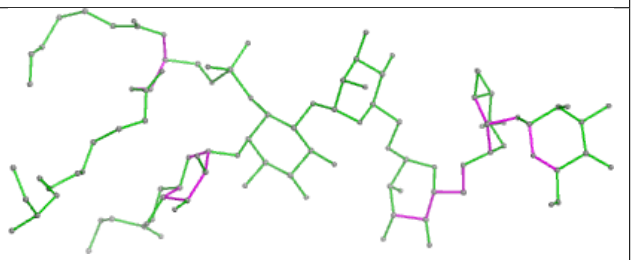
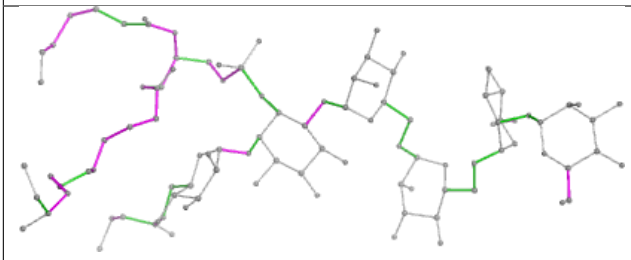
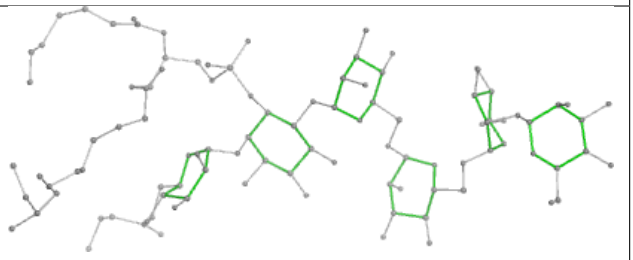


Bond angles

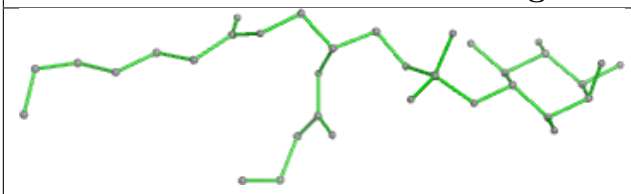


Torsions

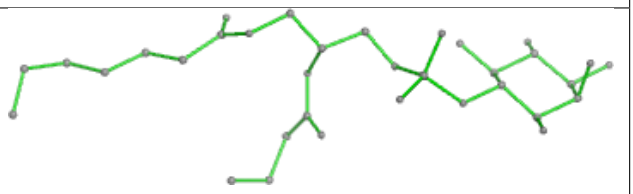


Rings

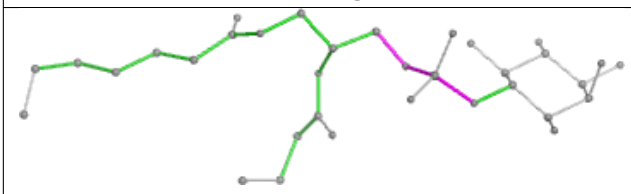
Ligand 9YF B 607



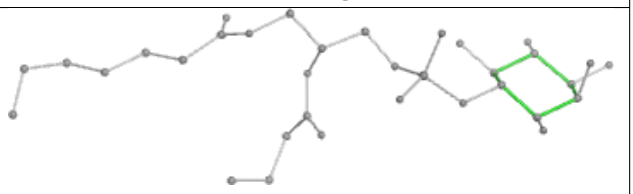
Bond lengths



Bond angles

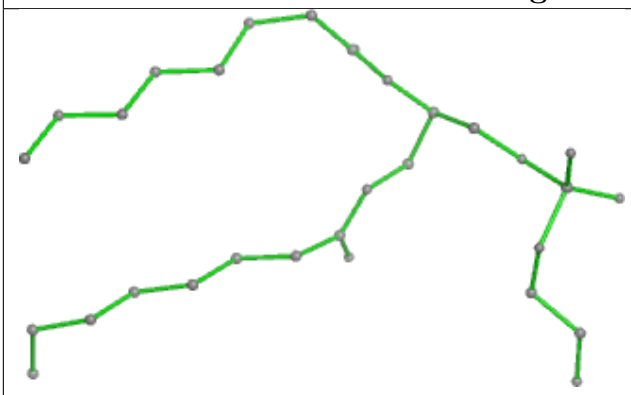


Torsions

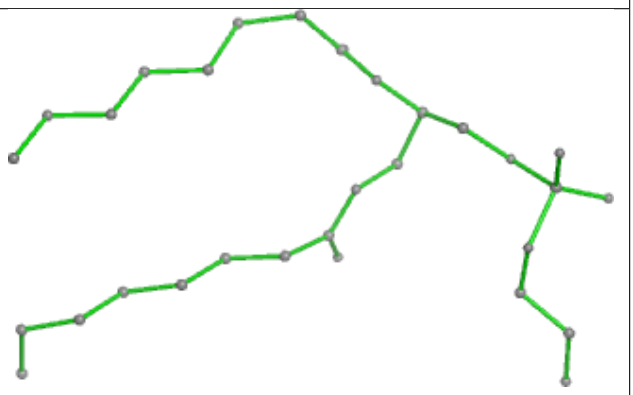


Rings

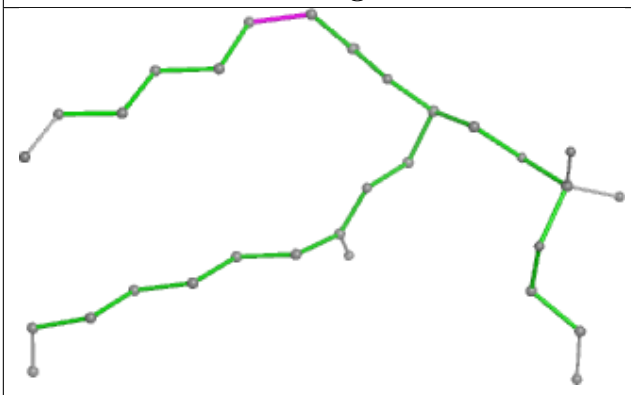
Ligand 3PE E 405



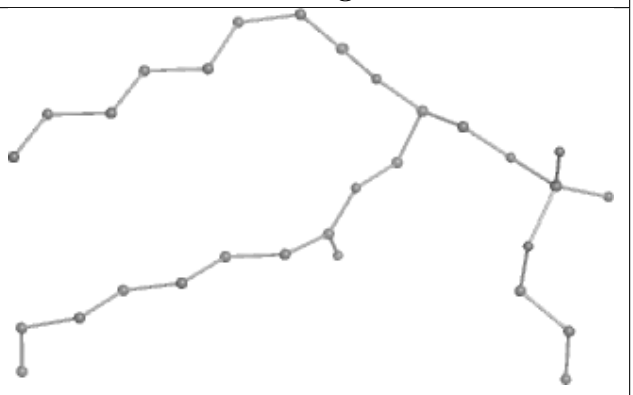
Bond lengths



Bond angles

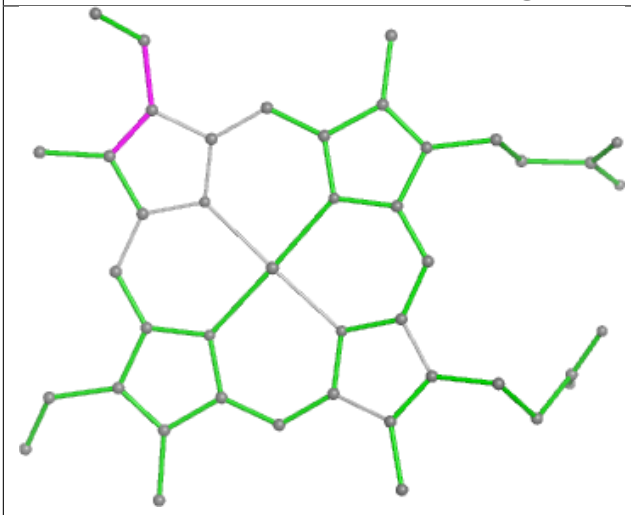


Torsions

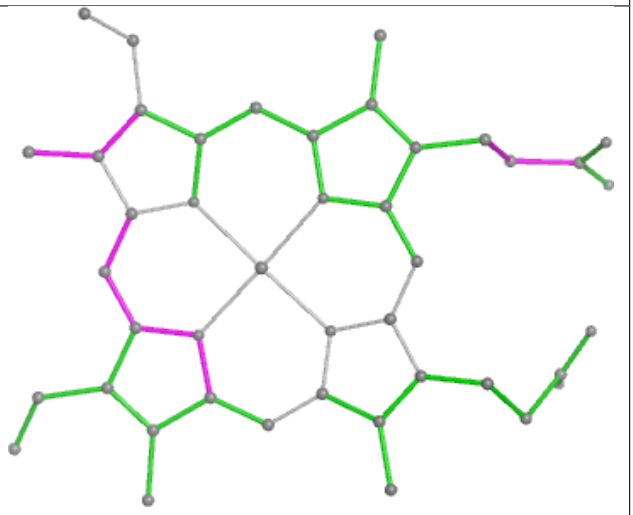


Rings

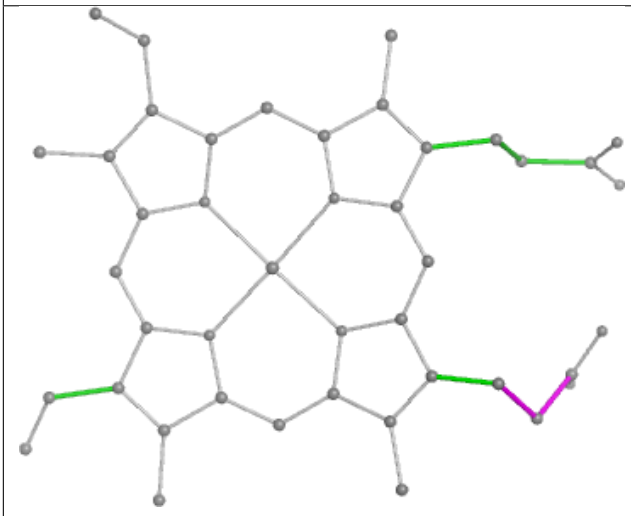
Ligand HEM O 603



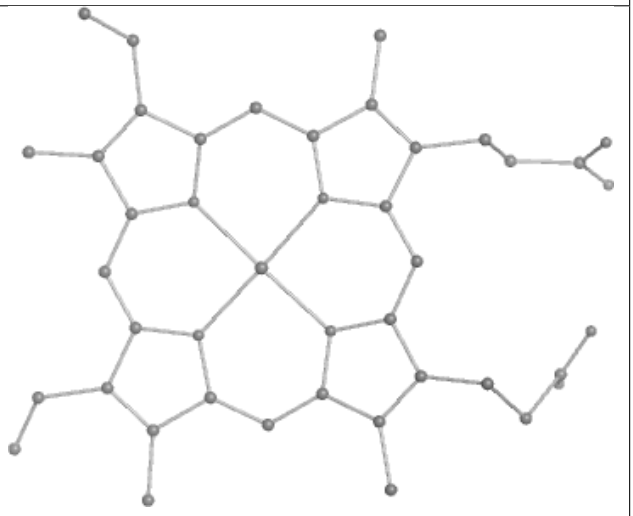
Bond lengths



Bond angles

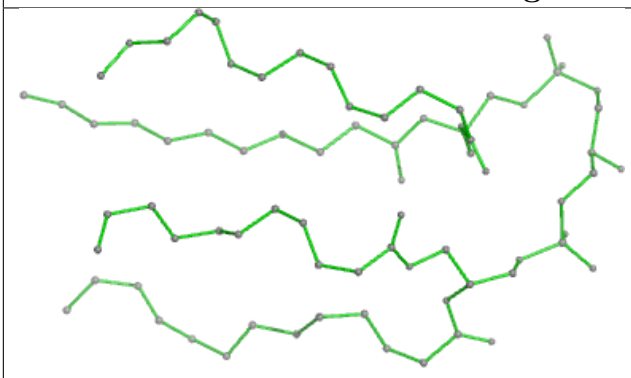


Torsions



Rings

Ligand CDL D 605



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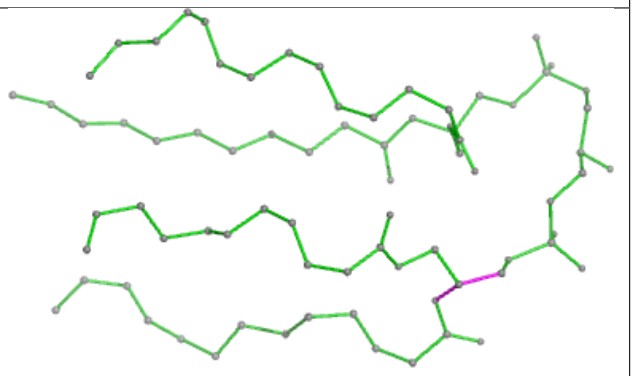
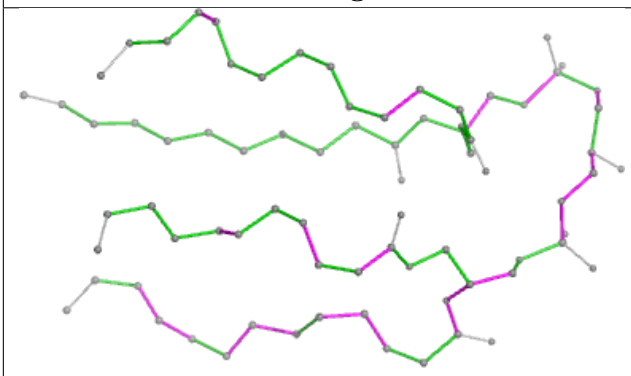


Bond angles



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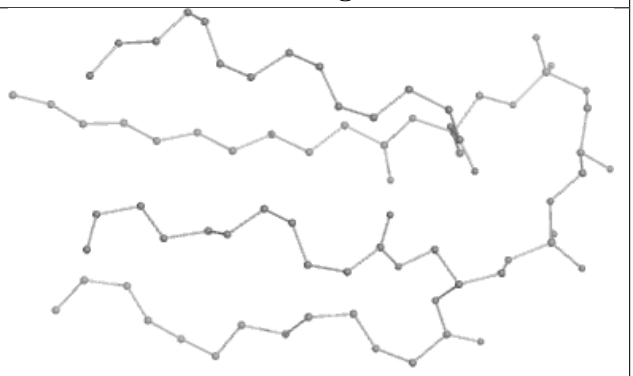
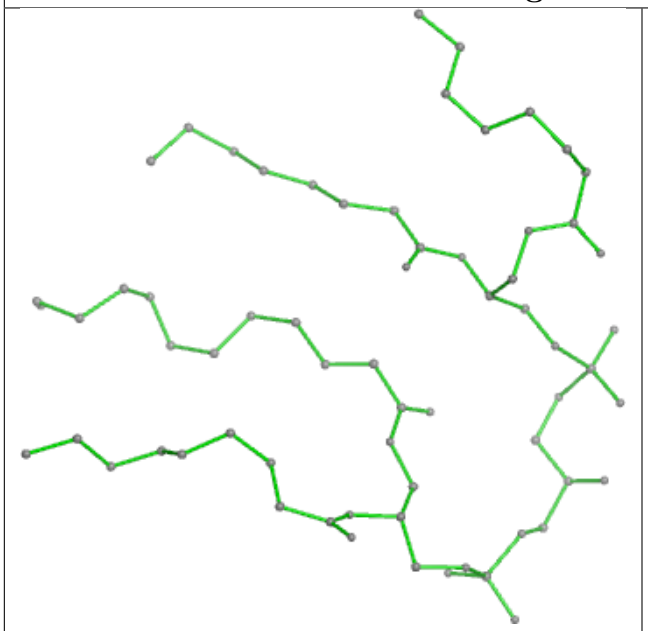
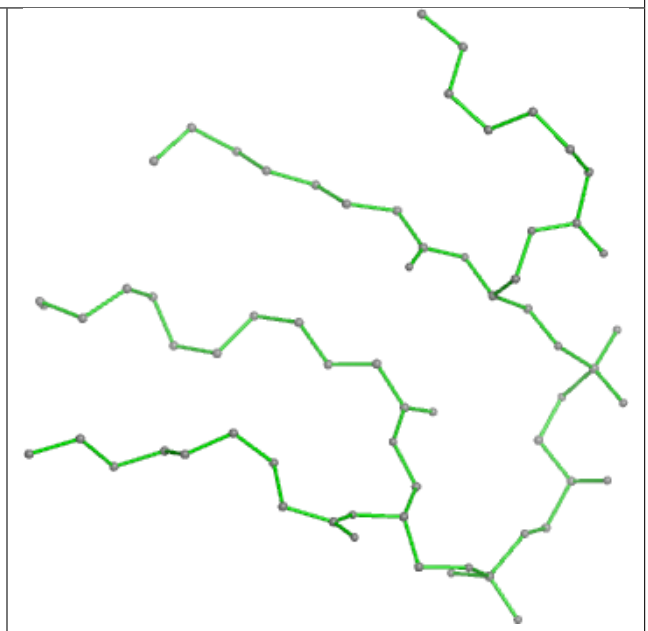


Rings

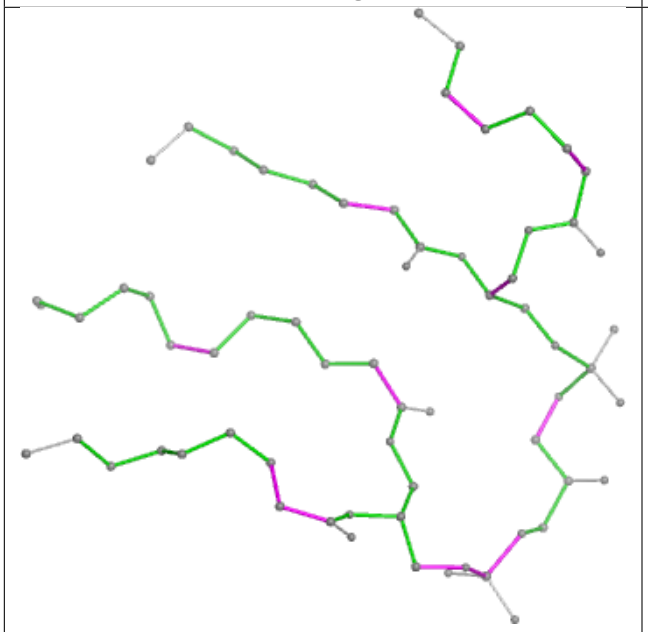
Ligand CDL P 301



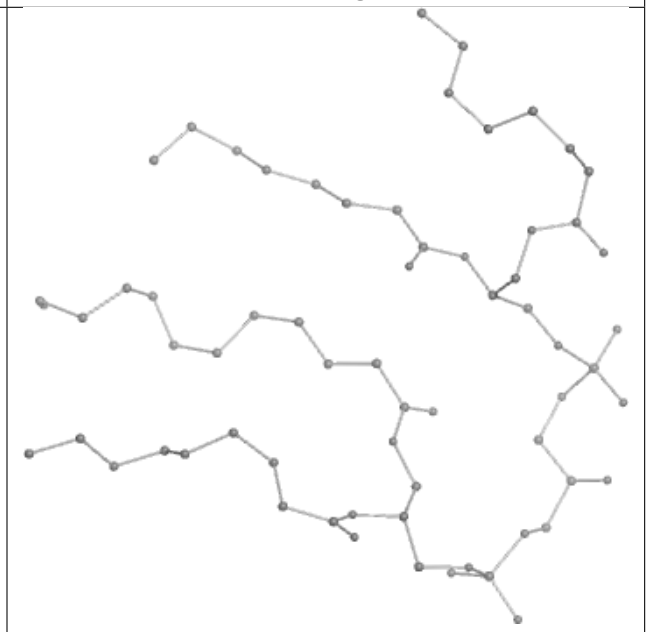
Bond lengths



Bond angles

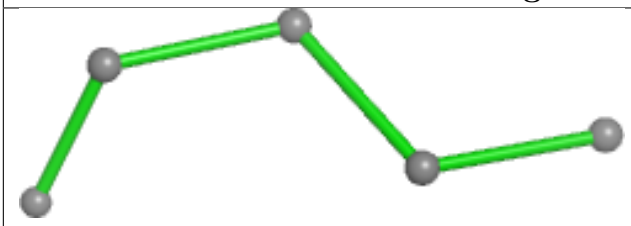


Torsions

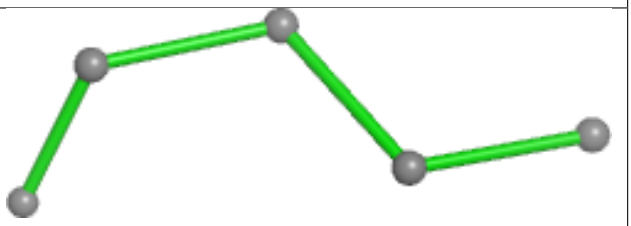


Rings

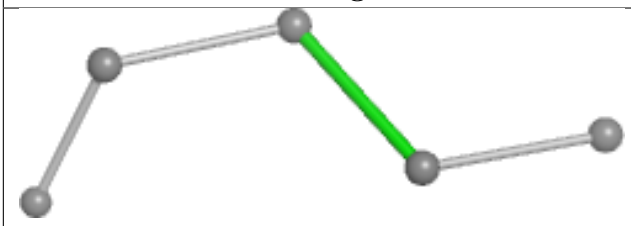
Ligand PLM Z 202



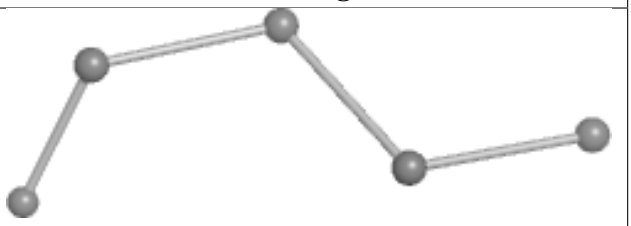
Bond lengths



Bond angles



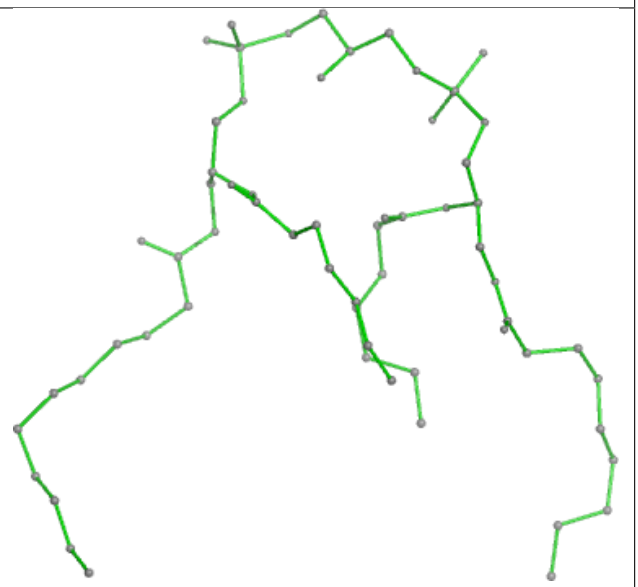
Torsions



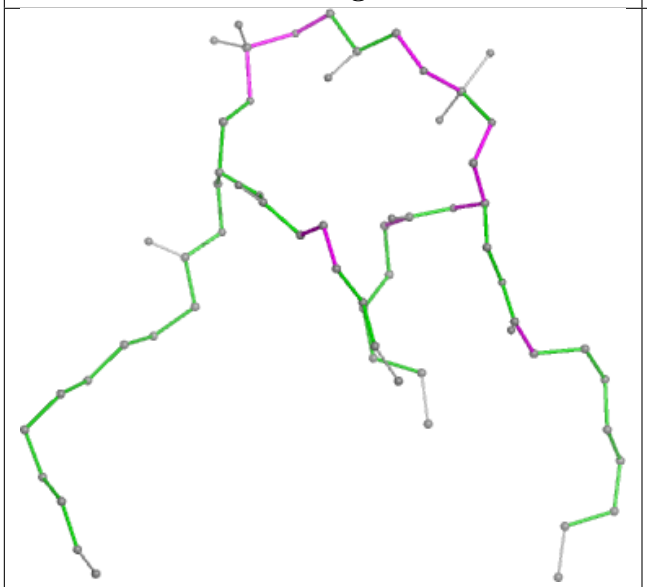
Rings

Ligand CDL G 201

Bond lengths



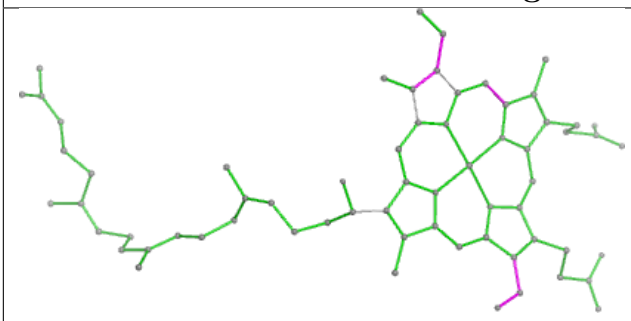
Bond angles



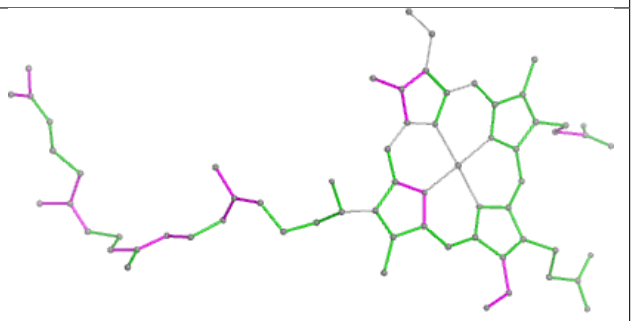
Torsions

Rings

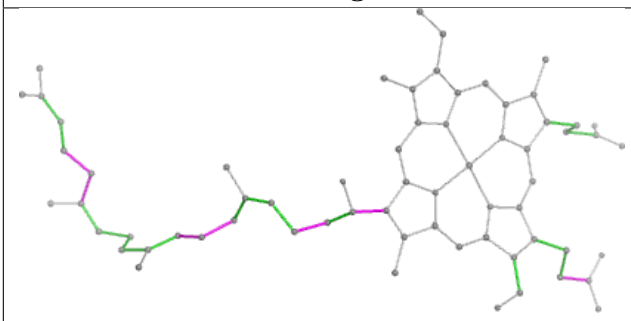
Ligand HAS D 601



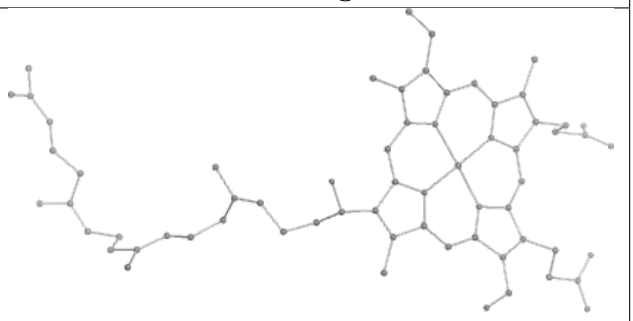
Bond lengths



Bond angles

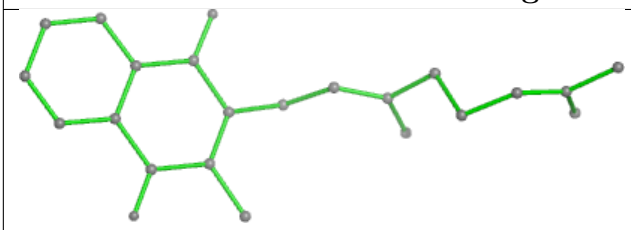


Torsions

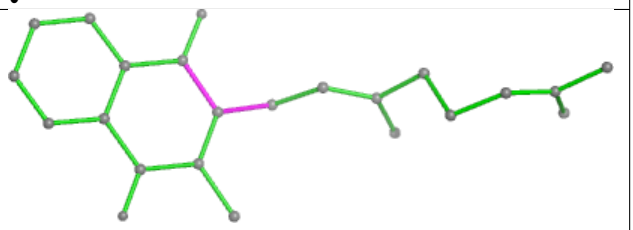


Rings

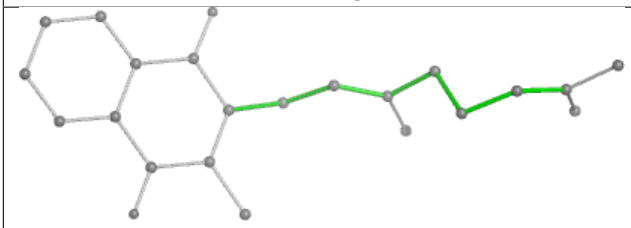
Ligand MQ9 O 605



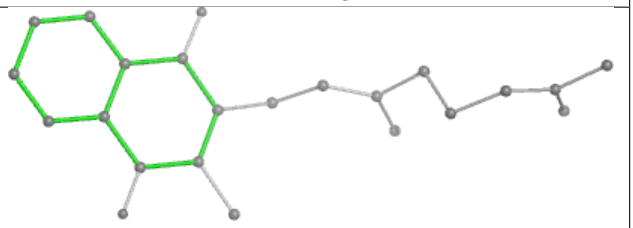
Bond lengths



Bond angles

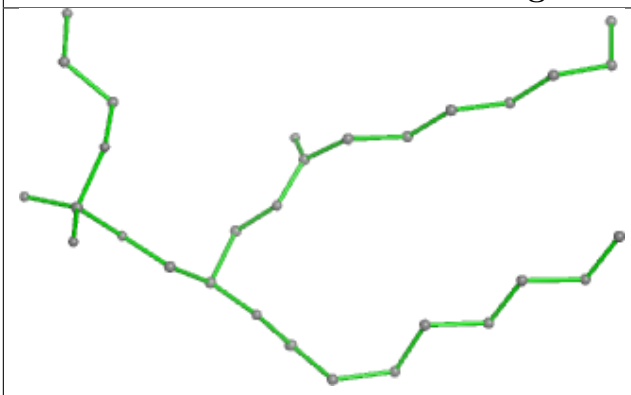


Torsions



Rings

Ligand 3PE R 405



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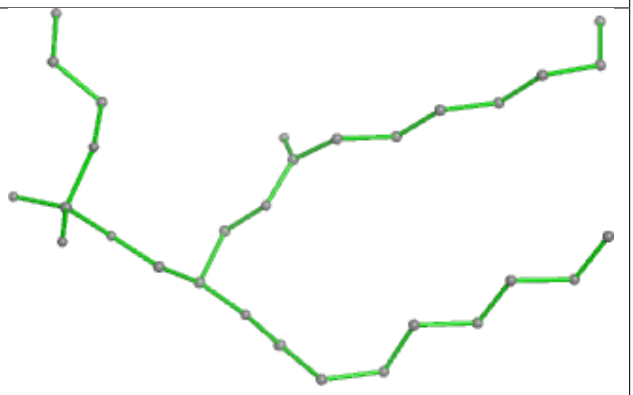
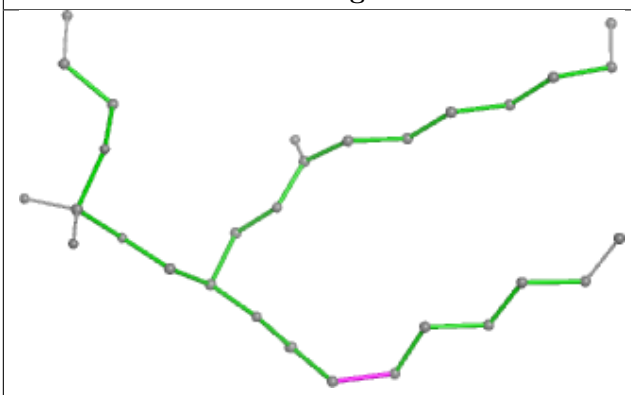
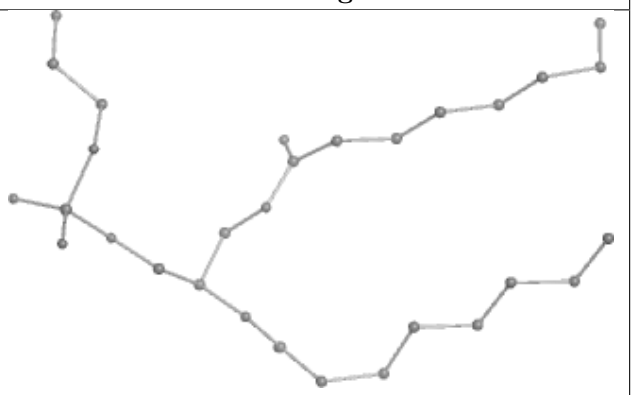


Bond angles

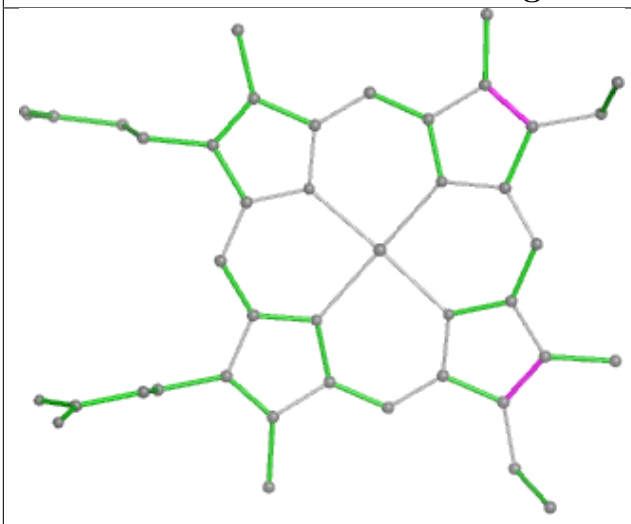


Torsions

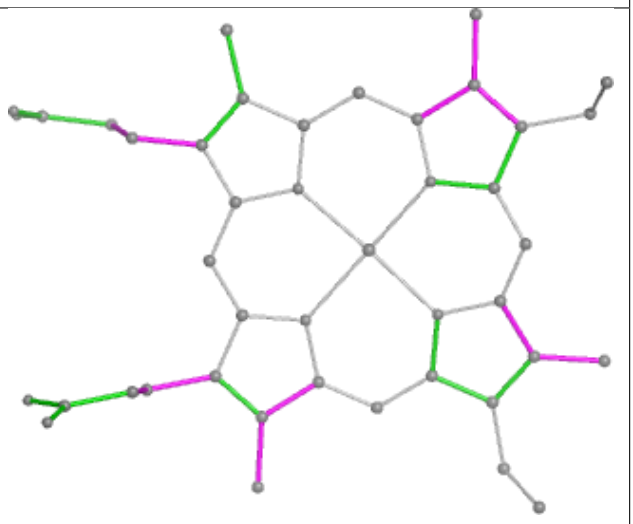


Rings

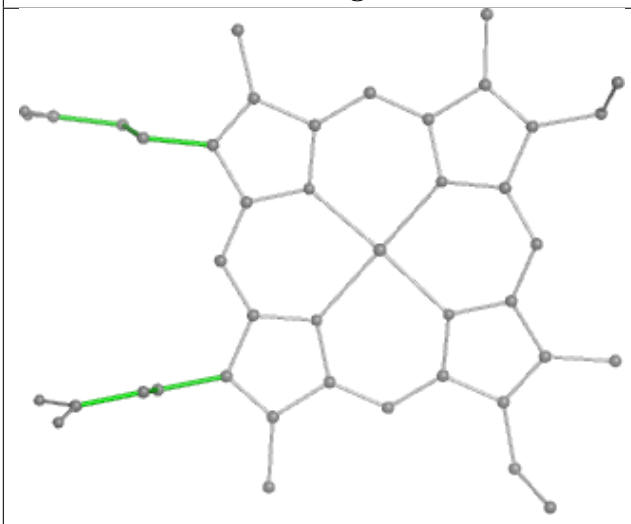
Ligand HEC P 303



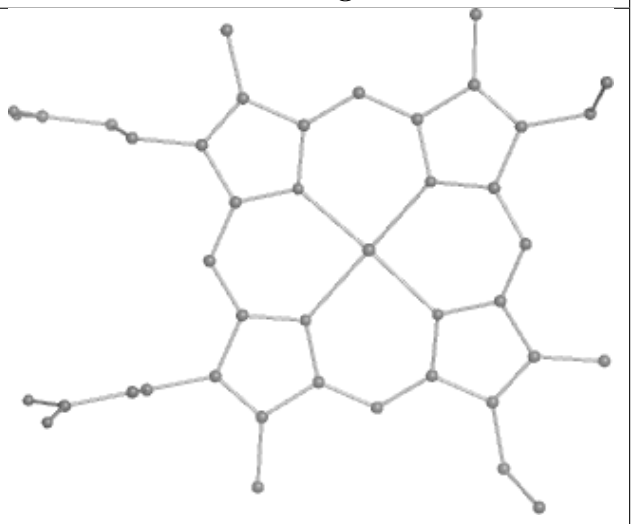
Bond lengths



Bond angles

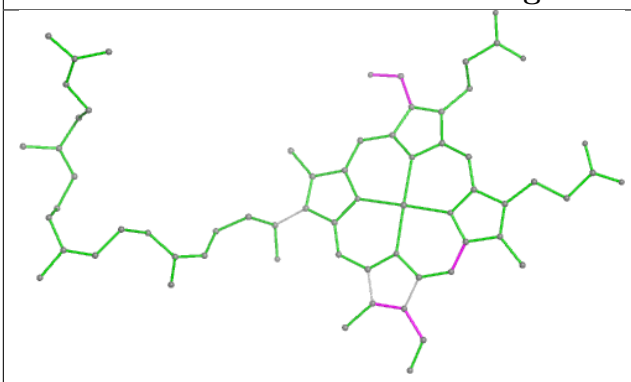


Torsions

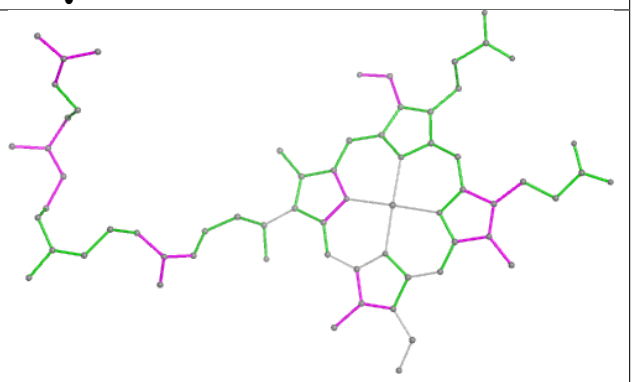


Rings

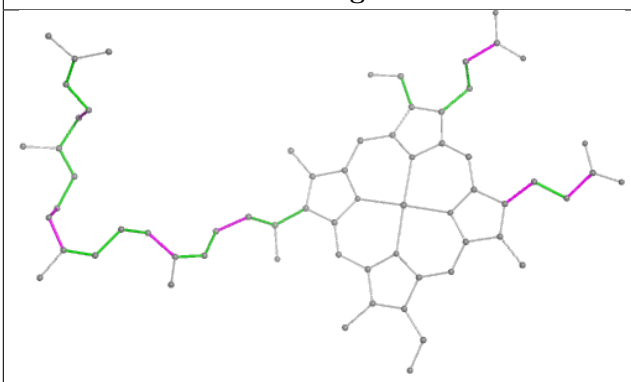
Ligand HAS Q 602



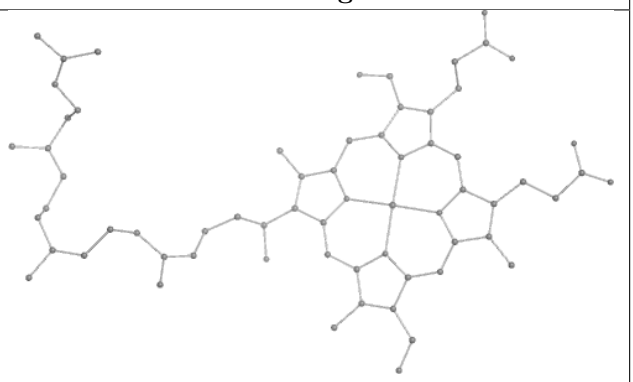
Bond lengths



Bond angles

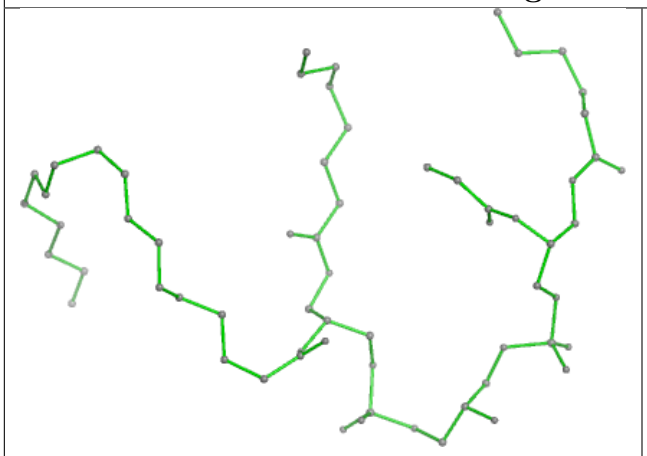


Torsions



Rings

Ligand CDL Q 606



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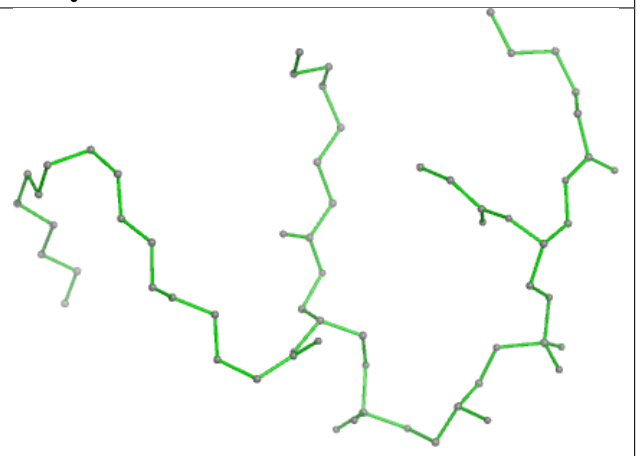
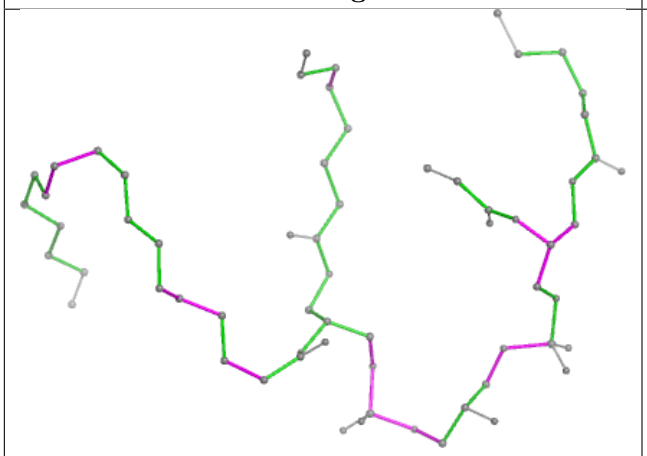
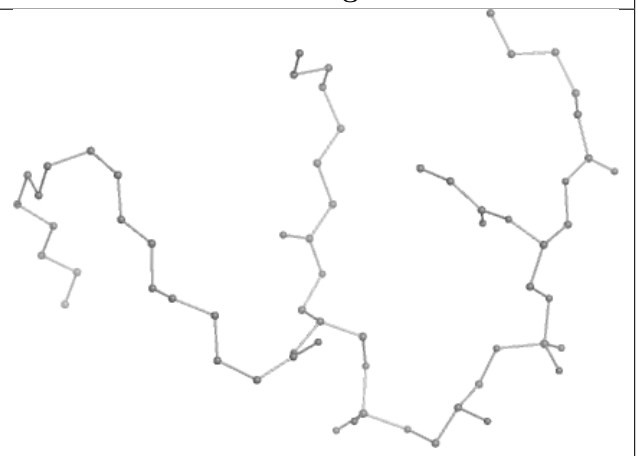


Bond angles

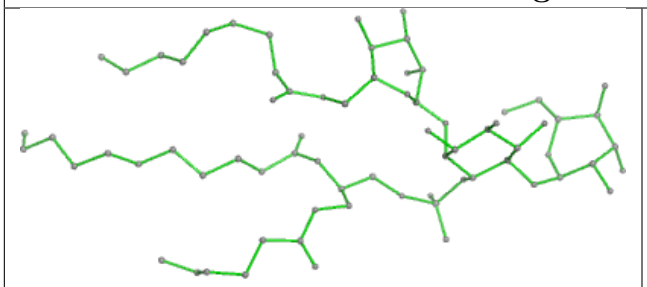


Torsions

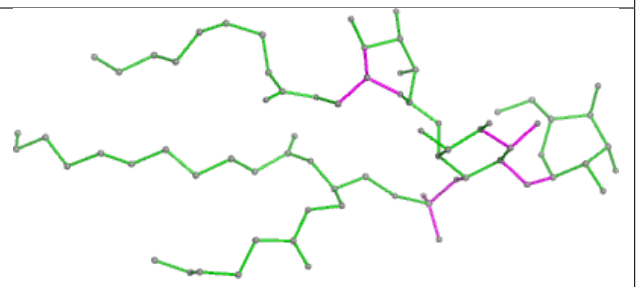


Rings

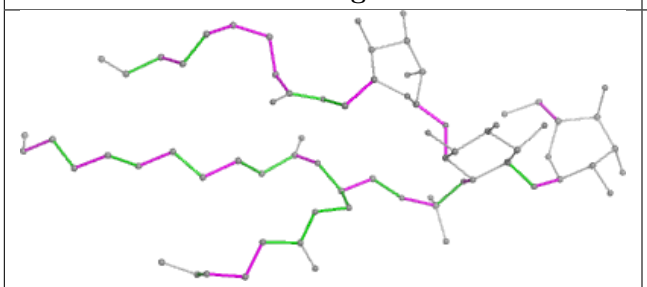
Ligand IX7 R 406



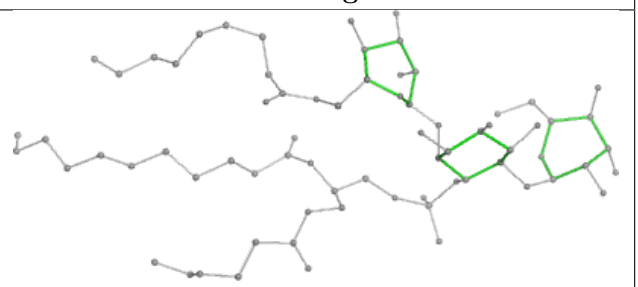
Bond lengths



Bond angles

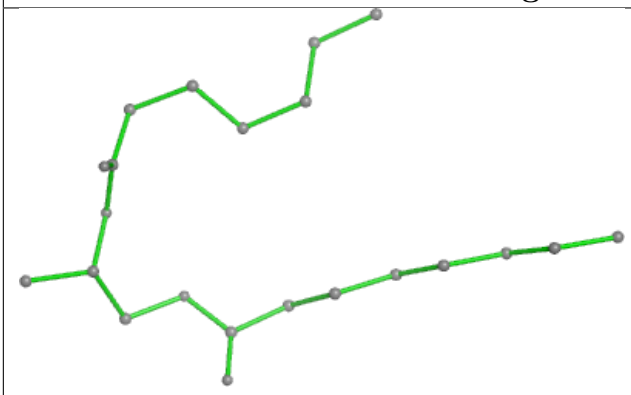


Torsions

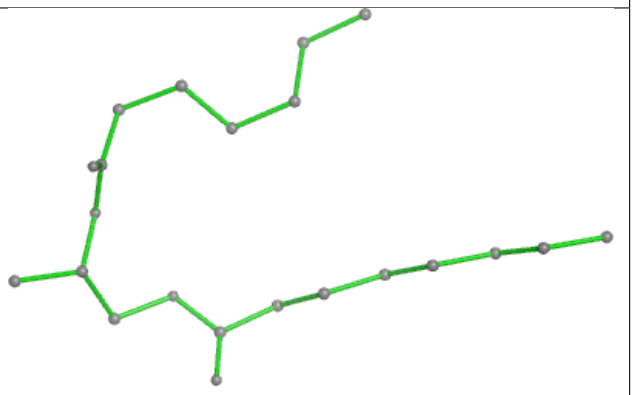


Rings

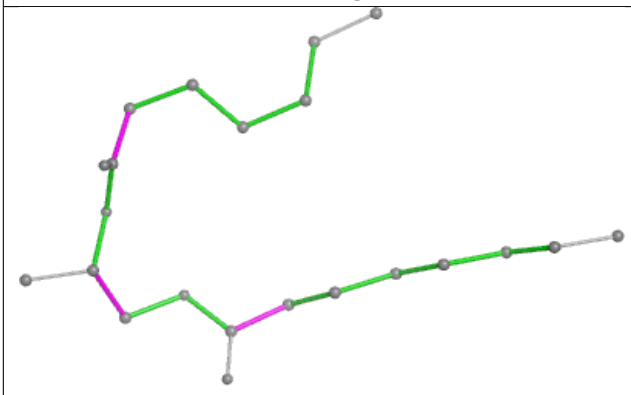
Ligand DGA Z 201



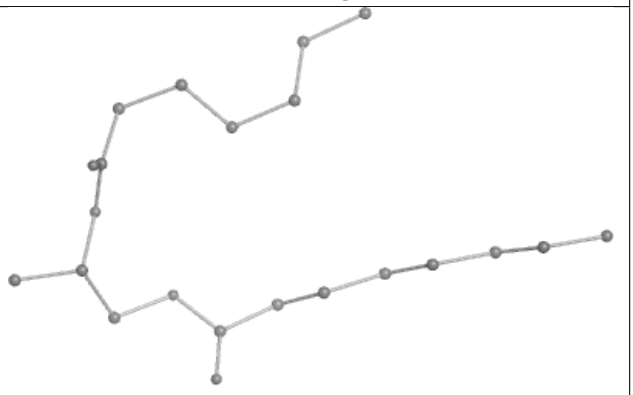
Bond lengths



Bond angles

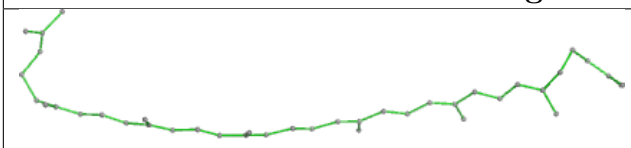


Torsions

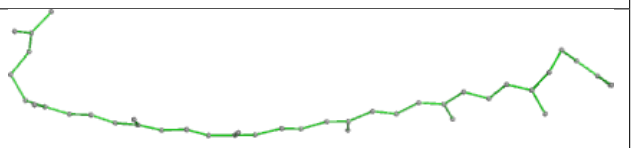


Rings

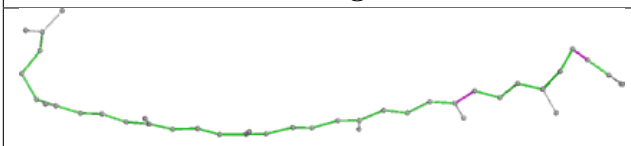
Ligand LYC O 607



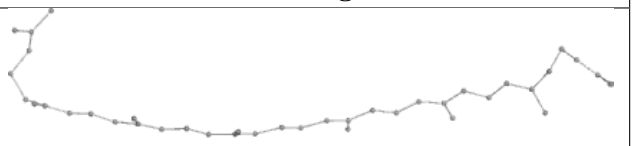
Bond lengths



Bond angles

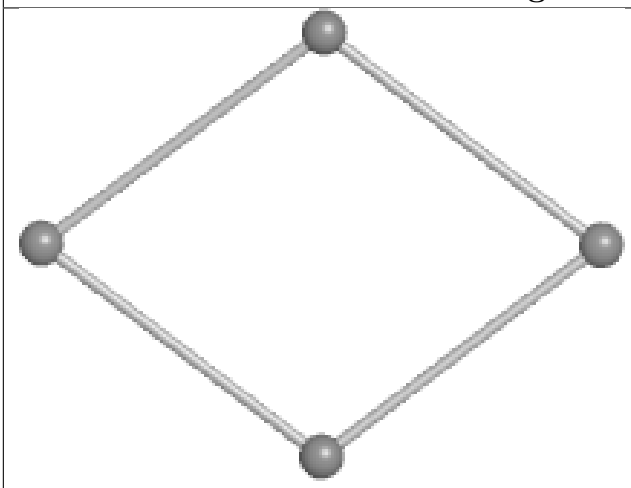


Torsions

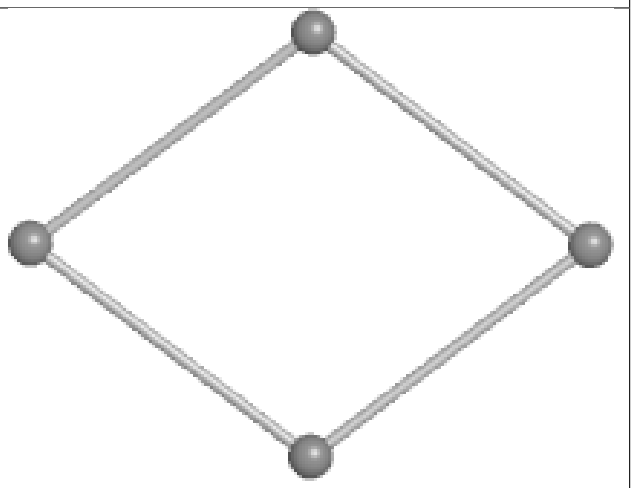


Rings

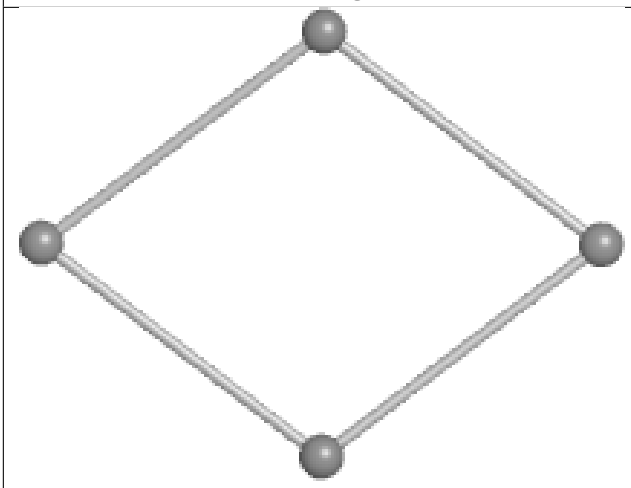
Ligand FES A 501



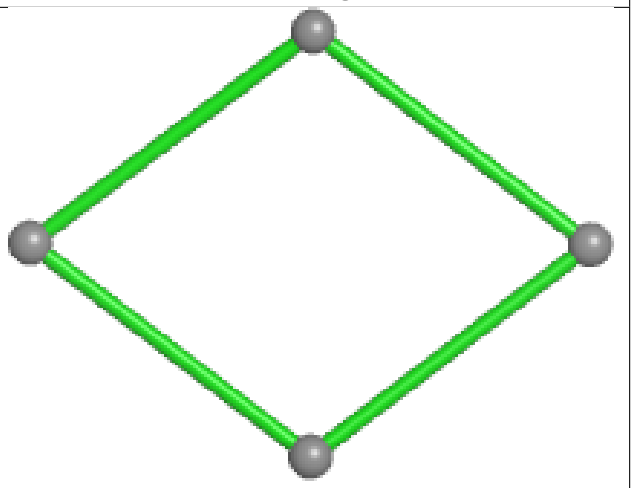
Bond lengths



Bond angles

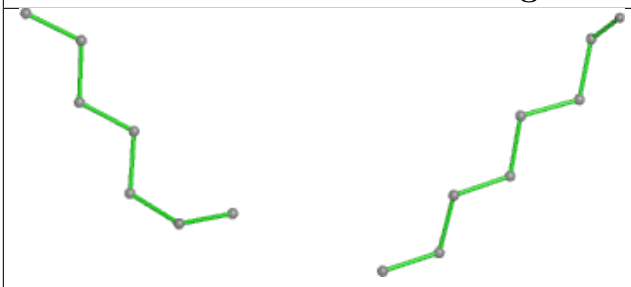


Torsions



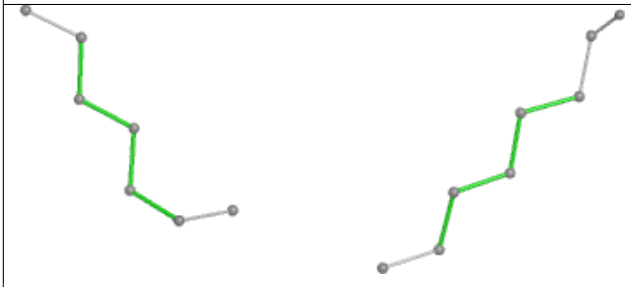
Rings

Ligand PLM H 202

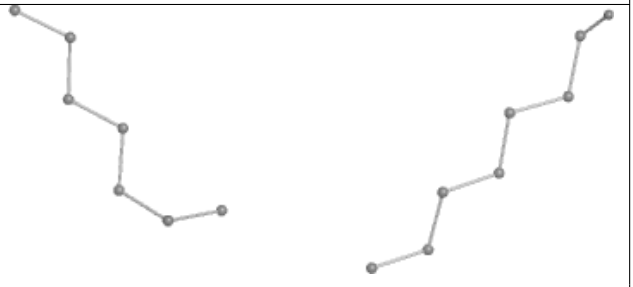


Bond lengths

Bond angles

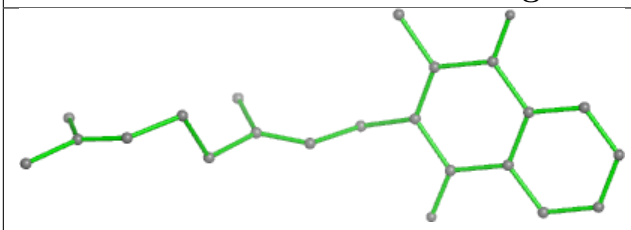


Torsions

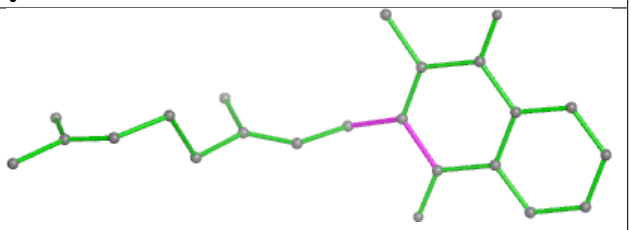


Rings

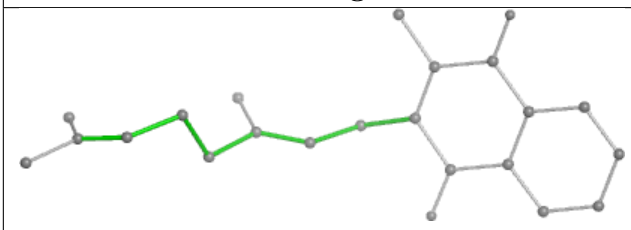
Ligand MQ9 B 604



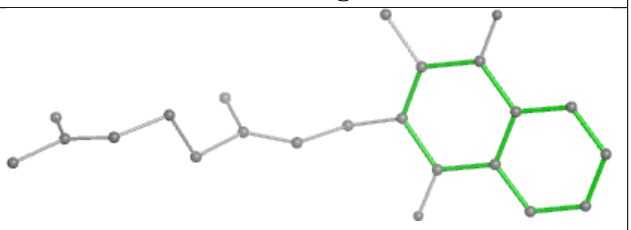
Bond lengths



Bond angles

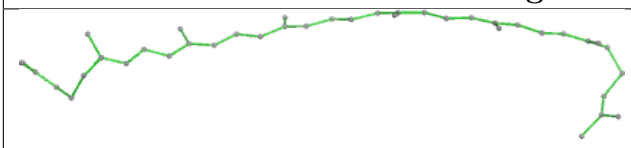


Torsions

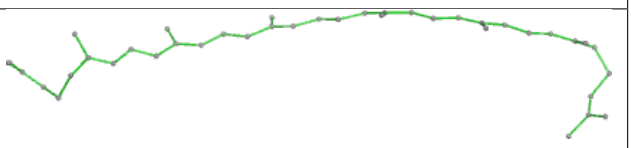


Rings

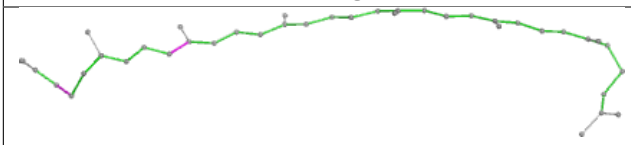
Ligand LYC B 606



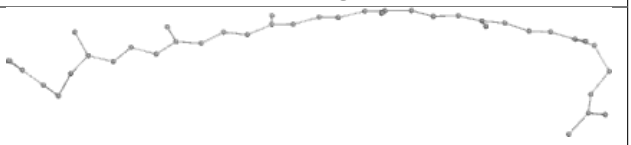
Bond lengths



Bond angles

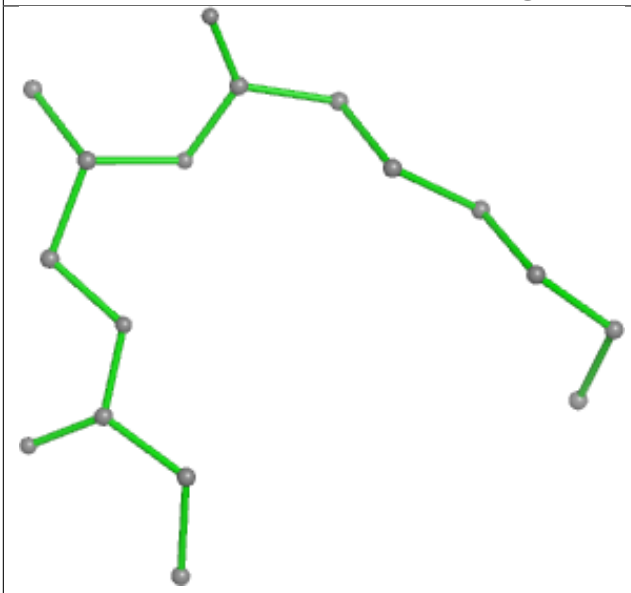


Torsions

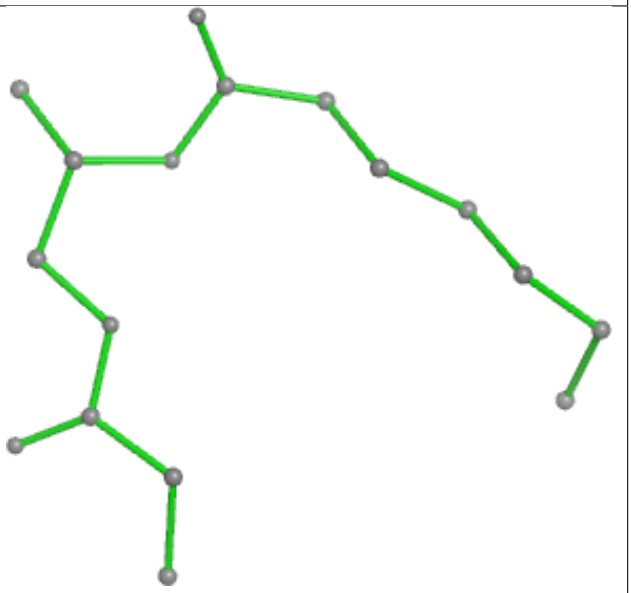


Rings

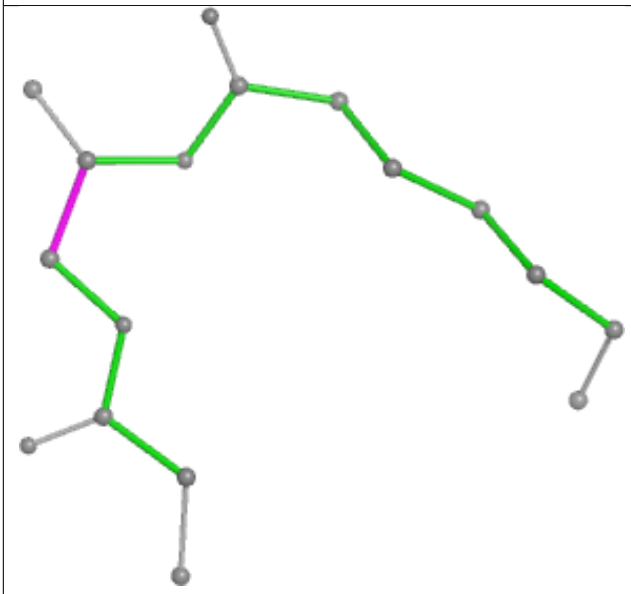
Ligand DGA H 201



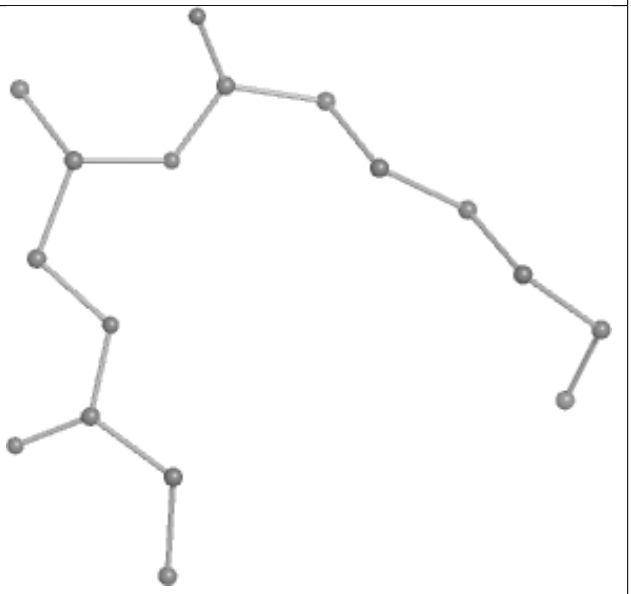
Bond lengths



Bond angles

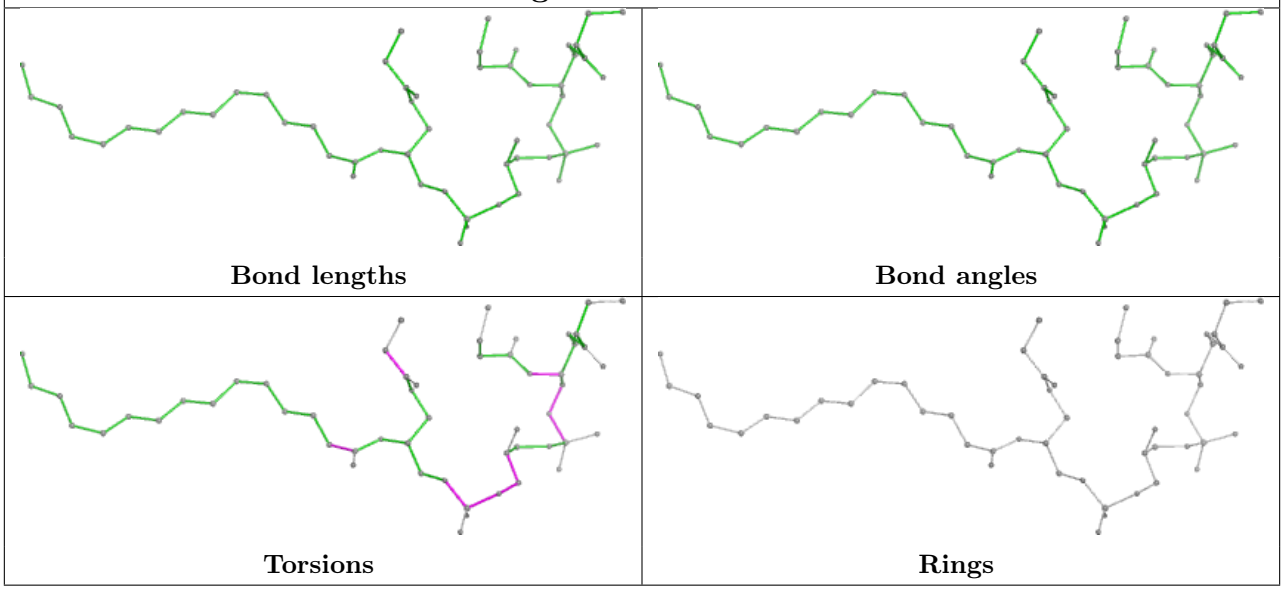


Torsions

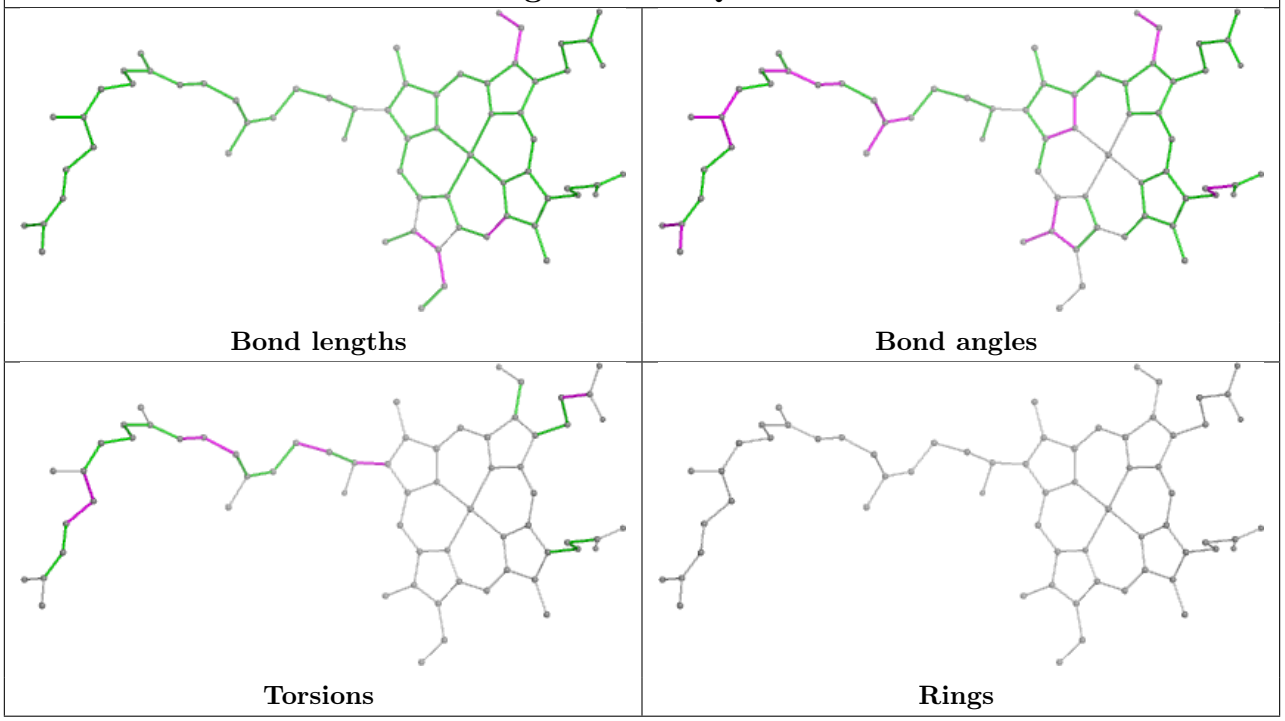


Rings

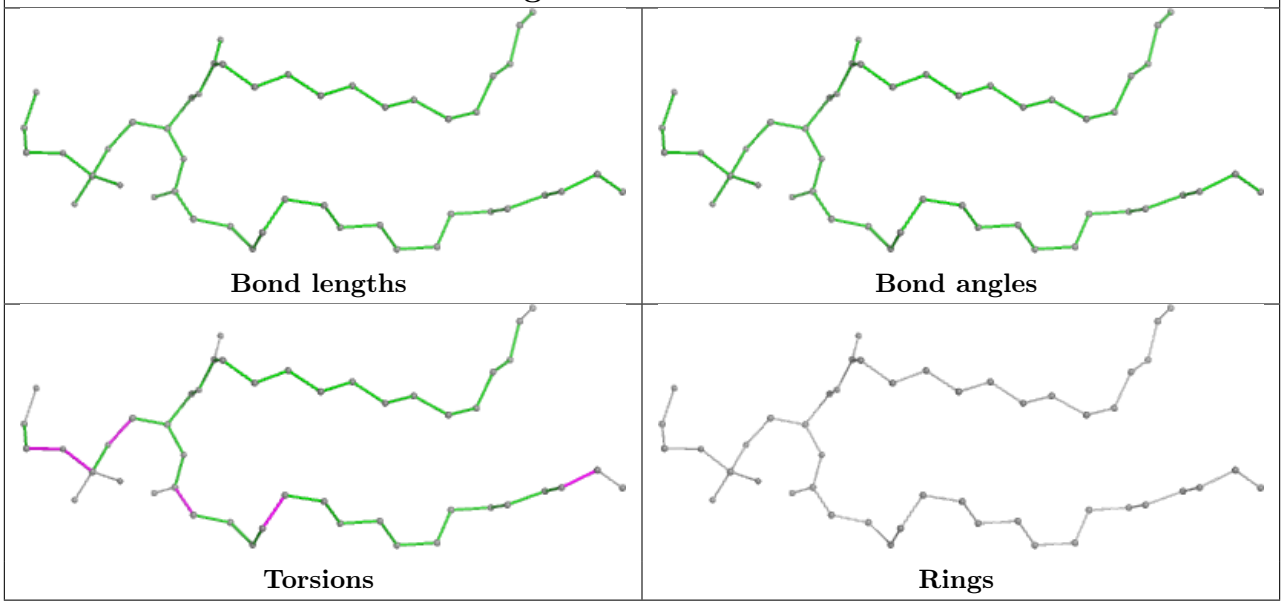
Ligand CDL I 201



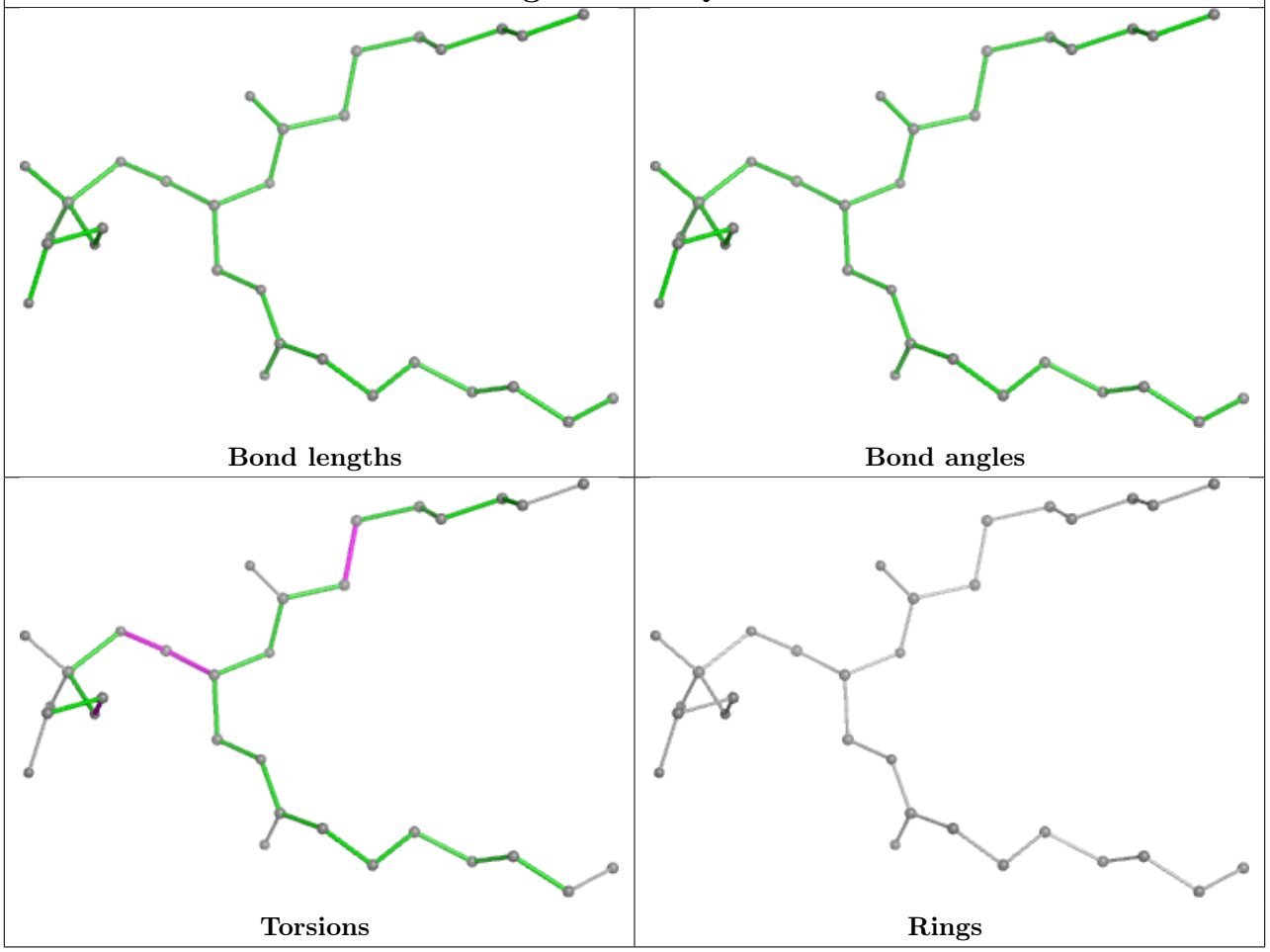
Ligand HAS Q 601



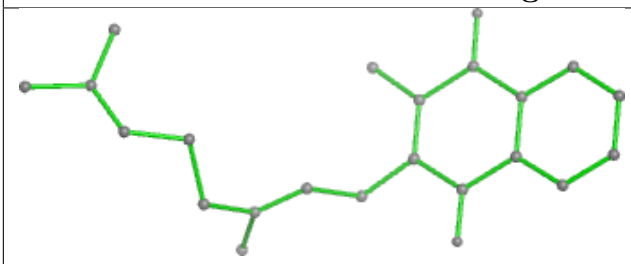
Ligand 3PE W 201



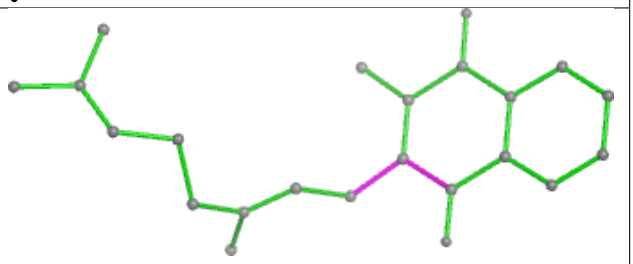
Ligand 3PE Q 607



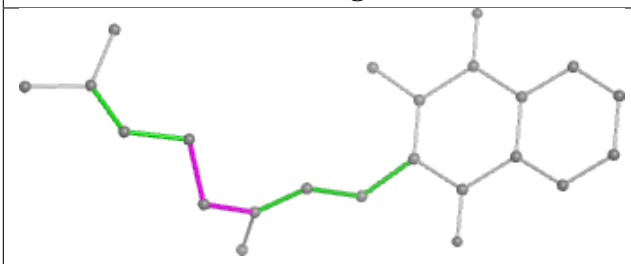
Ligand MQ9 O 602



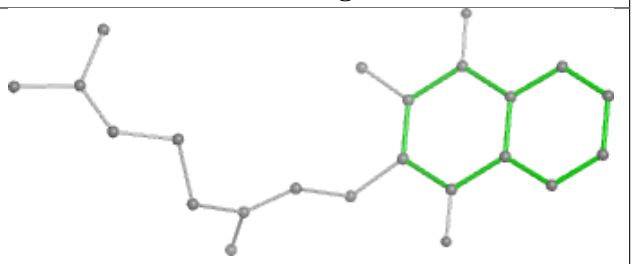
Bond lengths



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.

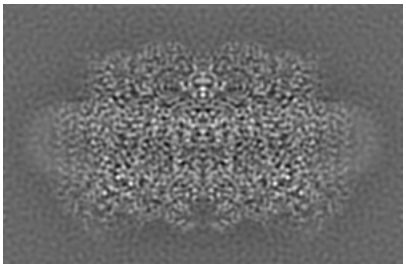
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13977. These allow visual inspection of the internal detail of the map and identification of artifacts.

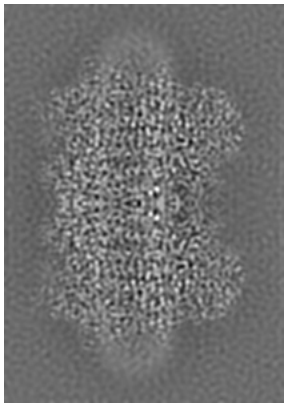
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

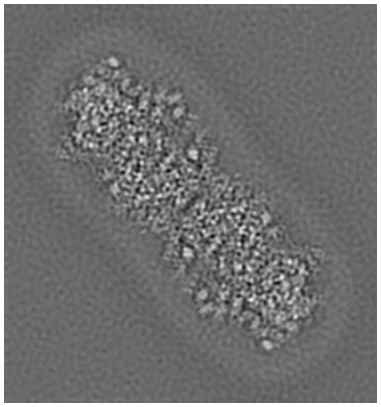
6.1.1 Primary map



X



Y

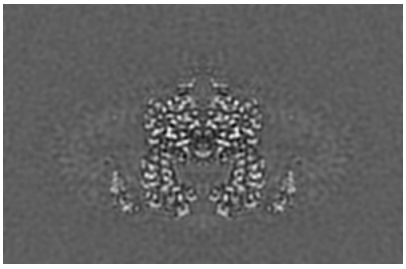


Z

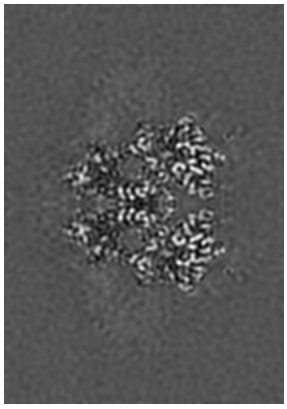
The images above show the map projected in three orthogonal directions.

6.2 Central slices

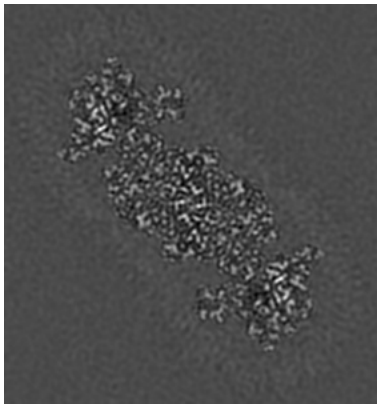
6.2.1 Primary map



X Index: 107



Y Index: 115

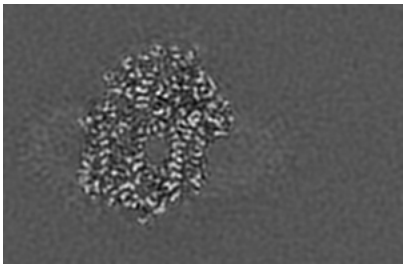


Z Index: 75

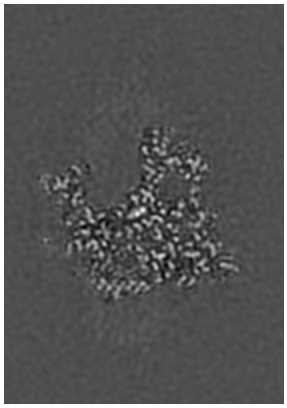
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

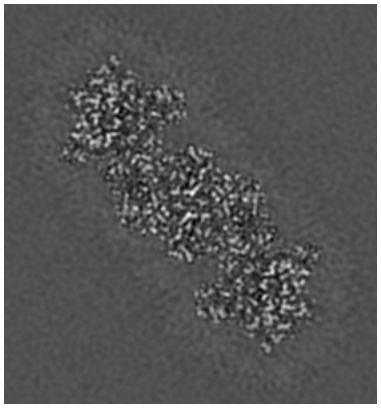
6.3.1 Primary map



X Index: 136



Y Index: 123

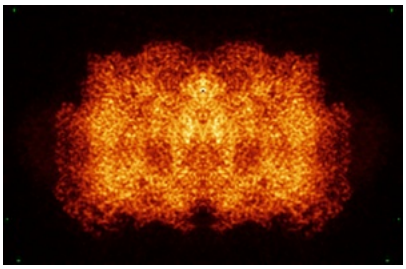


Z Index: 79

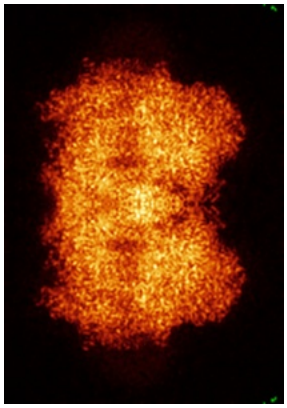
The images above show the largest variance slices of the map in three orthogonal directions.

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

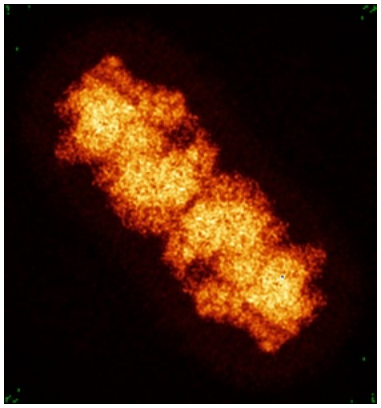
6.4.1 Primary map



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 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

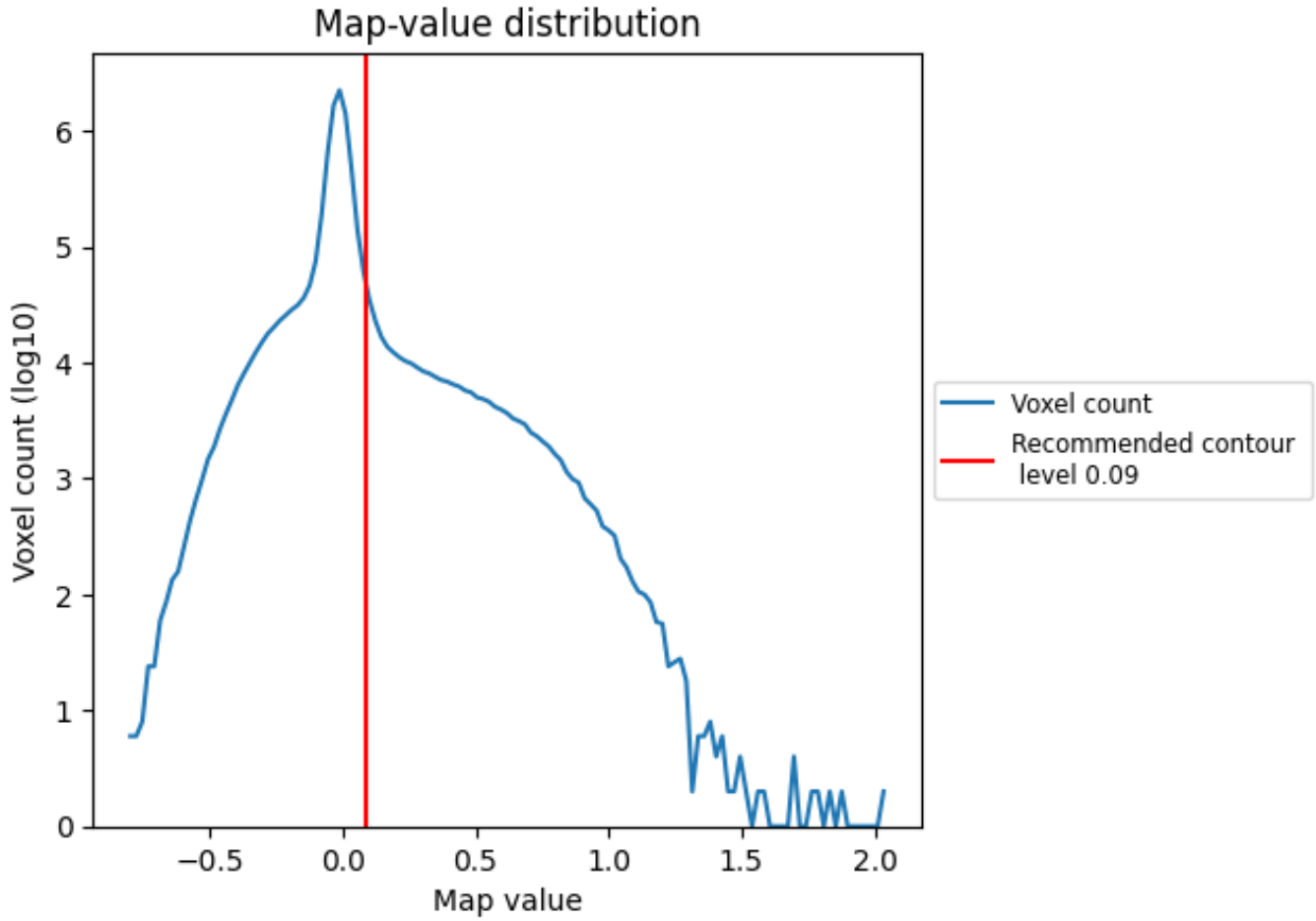
6.6 Mask visualisation (i)

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

7 Map analysis

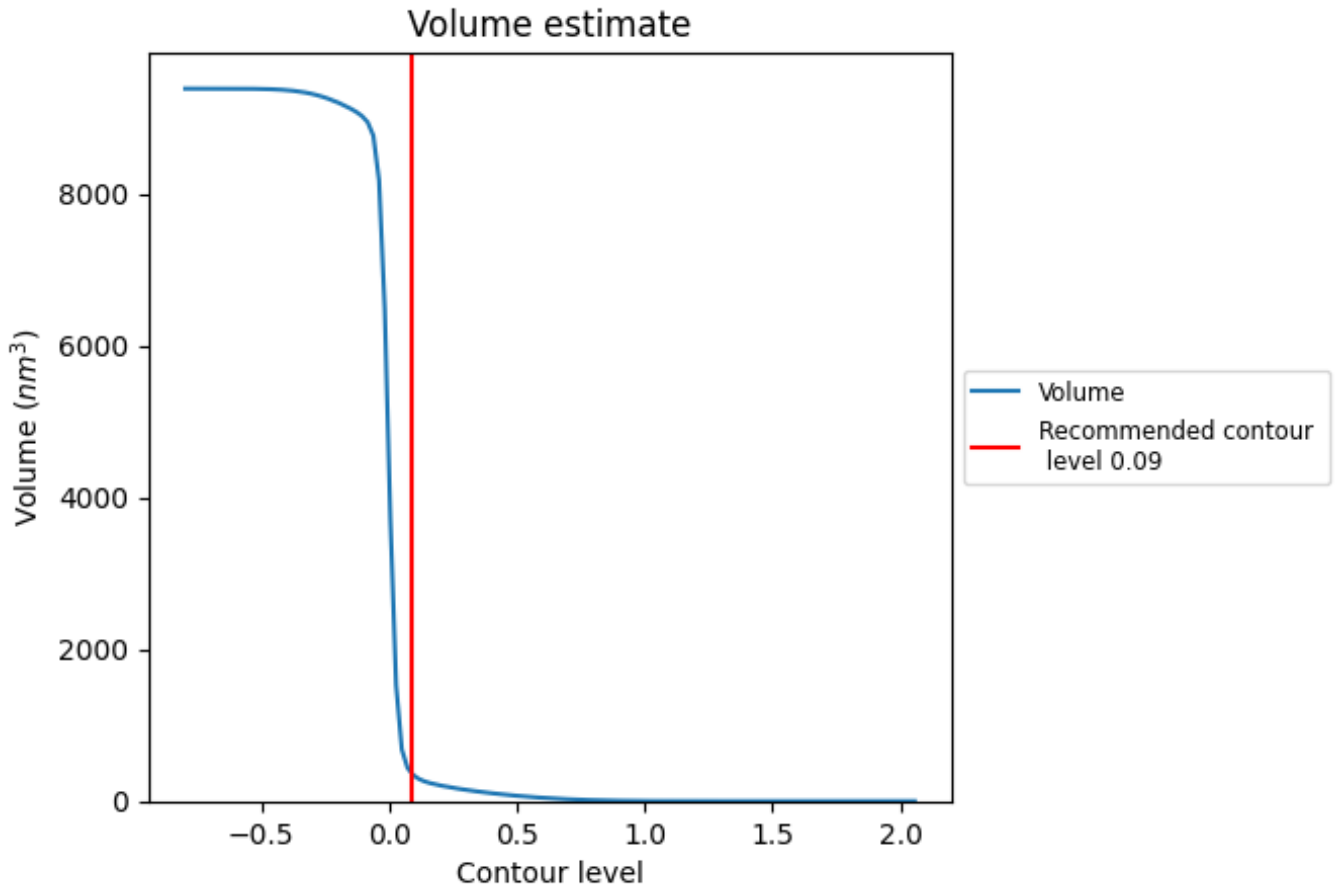
This section contains the results of statistical analysis of the map.

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



The volume at the recommended contour level is 359 nm^3; this corresponds to an approximate mass of 325 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

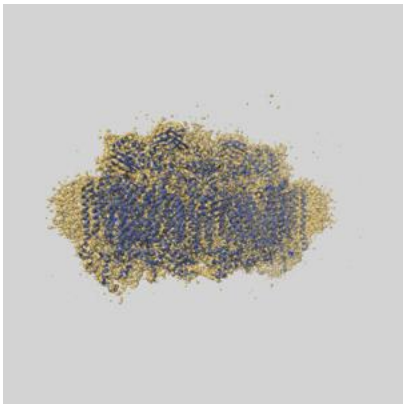
8 Fourier-Shell correlation (i)

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

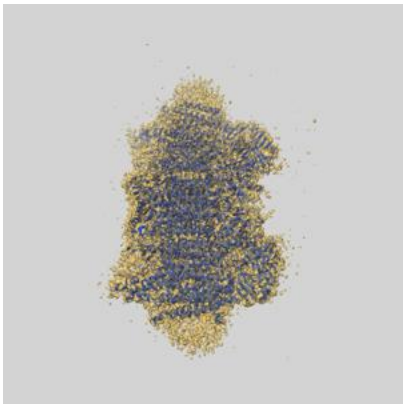
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13977 and PDB model 7QHO. Per-residue inclusion information can be found in section 3 on page 20.

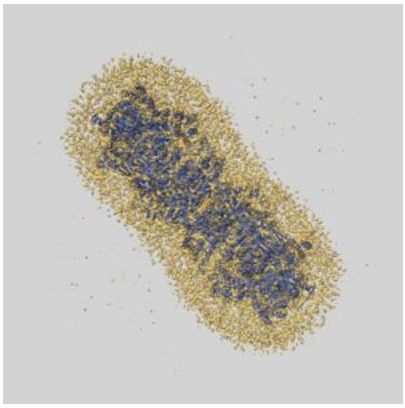
9.1 Map-model overlay



X



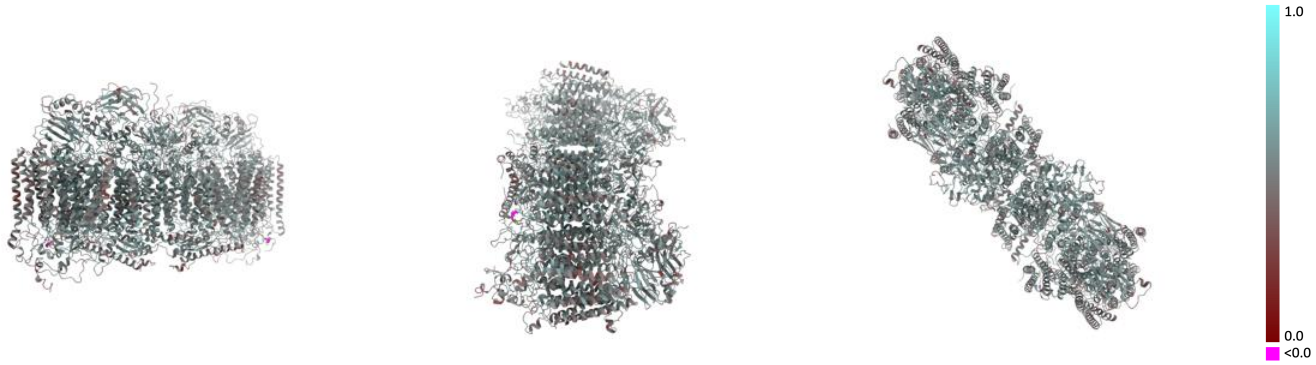
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

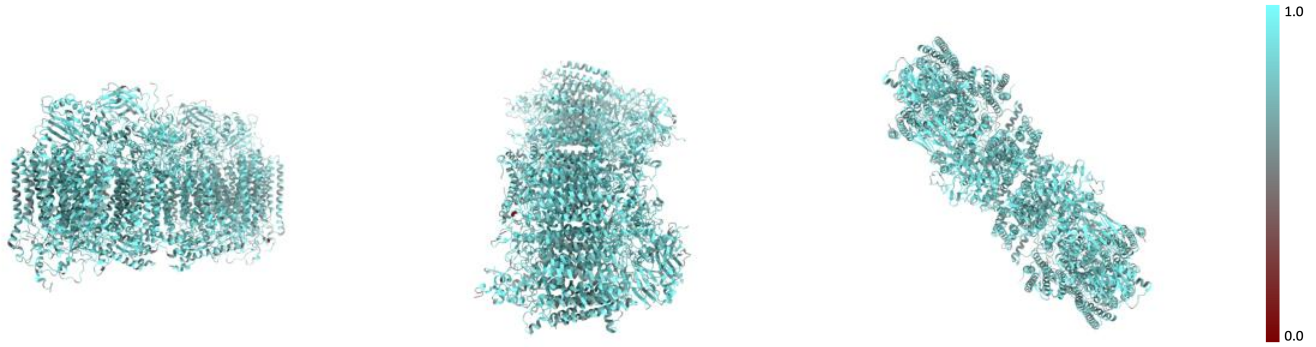
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

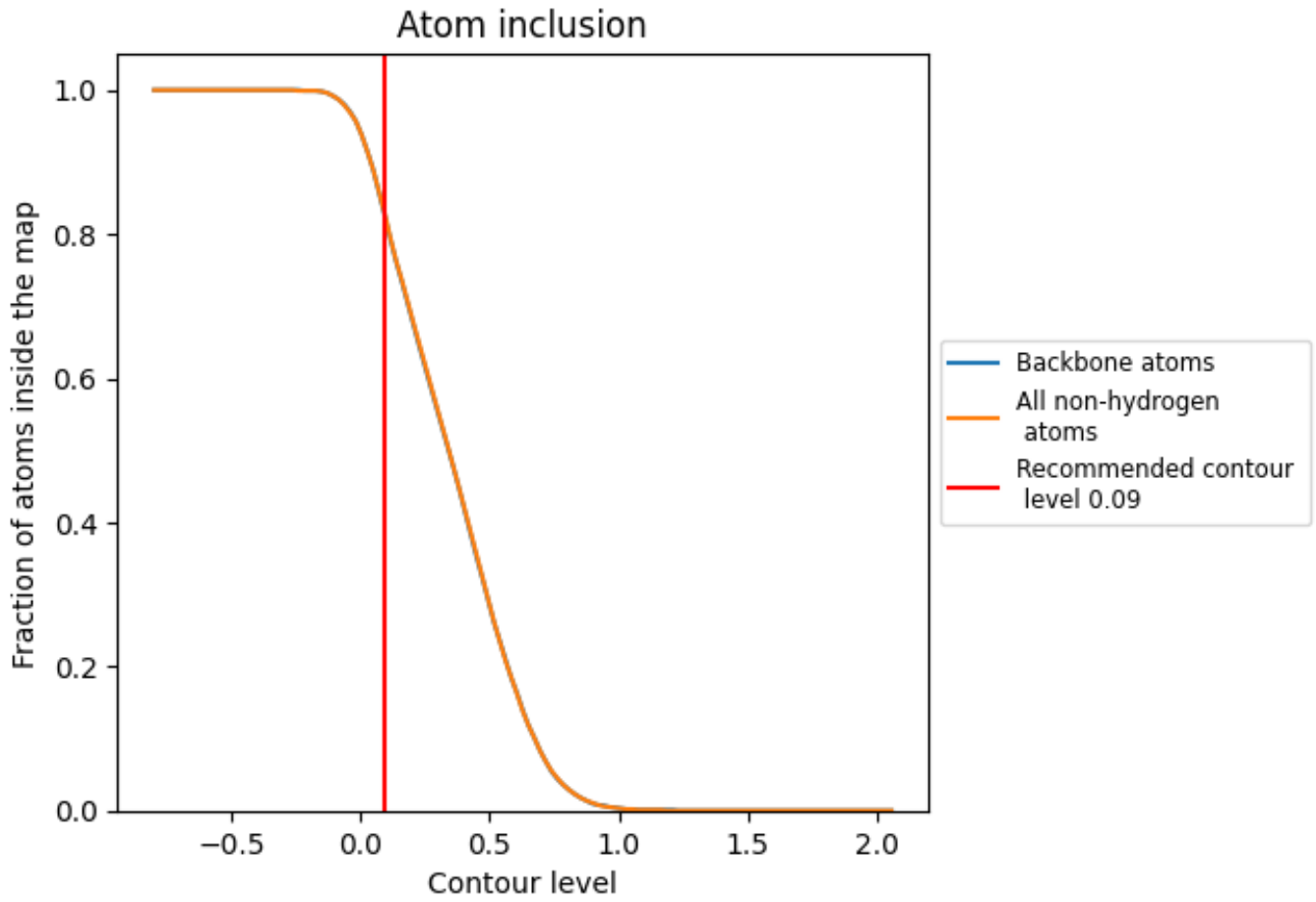
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5160
A	0.8510	0.5230
B	0.8770	0.5420
C	0.8580	0.5370
D	0.8600	0.5360
E	0.8160	0.5020
F	0.8270	0.5120
G	0.8110	0.5000
H	0.7850	0.4870
I	0.7920	0.4870
J	0.7520	0.4580
K	0.8060	0.4840
L	0.7480	0.4400
M	0.7340	0.4390
N	0.8450	0.5200
O	0.8750	0.5390
P	0.8520	0.5340
Q	0.8610	0.5350
R	0.8120	0.5010
S	0.8300	0.5090
T	0.8120	0.5000
U	0.7900	0.4860
V	0.7950	0.4850
W	0.7560	0.4590
X	0.7920	0.4770
Y	0.7460	0.4370
Z	0.7250	0.4350