wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 06:42 PM EDT

PDB ID	:	1SQP / pdb_00001sqp
Title	:	Crystal Structure Analysis of Bovine Bc1 with Myxothiazol
Authors	:	Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on	:	2004-03-19
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

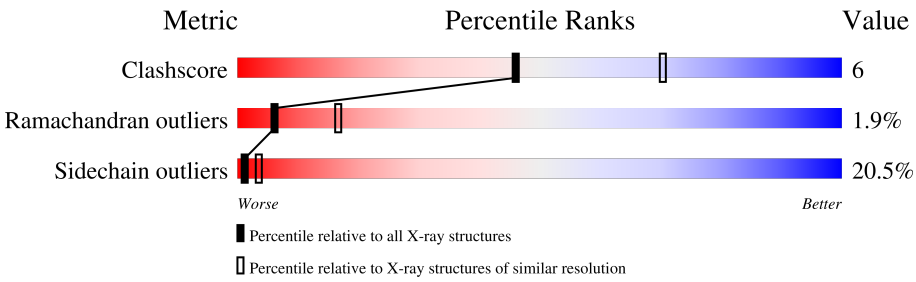
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	480	69% 22% • 7%
2	B	453	72% 17% • • 7%
3	C	379	69% 25% 5% •
4	D	241	64% 29% 5% •
5	E	196	64% 32% •
6	F	110	82% 13% • 5%
7	G	81	62% 28% • 7%
8	H	78	46% 33% 5% • 14%

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Mol	Chain	Length	Quality of chain
9	I	78	27% 27% 17% • 27%
10	J	62	53% 37% 8% •
11	K	56	59% 29% 7% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CDL	A	447	X	-	-	-
12	CDL	D	242	X	-	-	-
12	CDL	G	82	X	-	-	-
14	HEC	C	382	X	-	-	-
14	HEC	D	243	X	-	-	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 17274 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	3172	1993	562	610	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	378	3003	2013	471	501	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1519	957	263	291	8	0	0	0

- Molecule 6 is a protein called sub6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	105	911	576	165	168	2	0	0	0

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	75	628	410	118	99	1	0	0	0

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	67	548	332	99	112	5	0	0	0

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	57	406	253	77	74	2	0	0	0

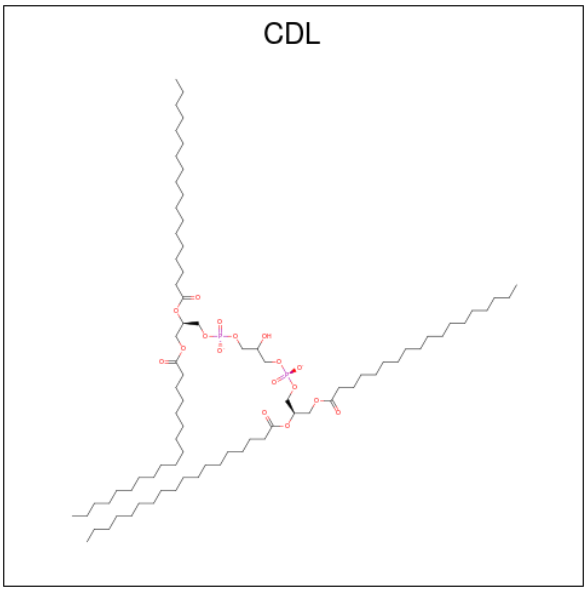
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

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

- Molecule 11 is a protein called Ubiquinol-cytochrome c reductase complex 6.4 kDa protein.

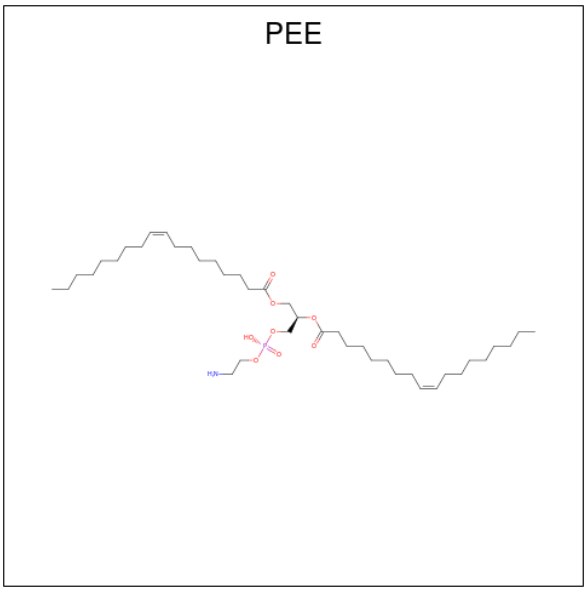
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	53	436	292	78	65	1	0	0	0

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



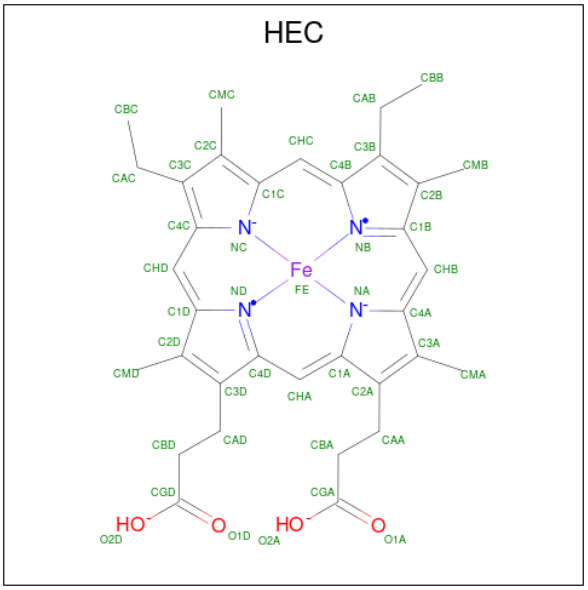
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
12	A	1	64	45	17	2	0	0
			Total	C	O	P		
12	D	1	64	45	17	2	0	0
			Total	C	O	P		
12	G	1	64	45	17	2	0	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



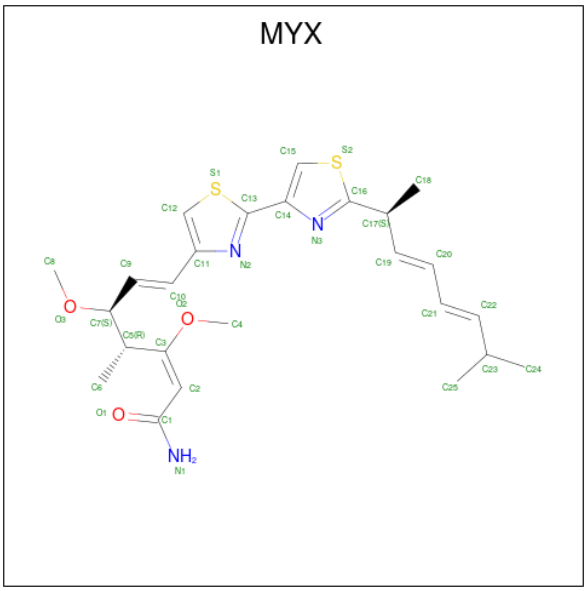
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	A	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
13	C	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
13	E	1	49	39	1	8	1	0	0

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



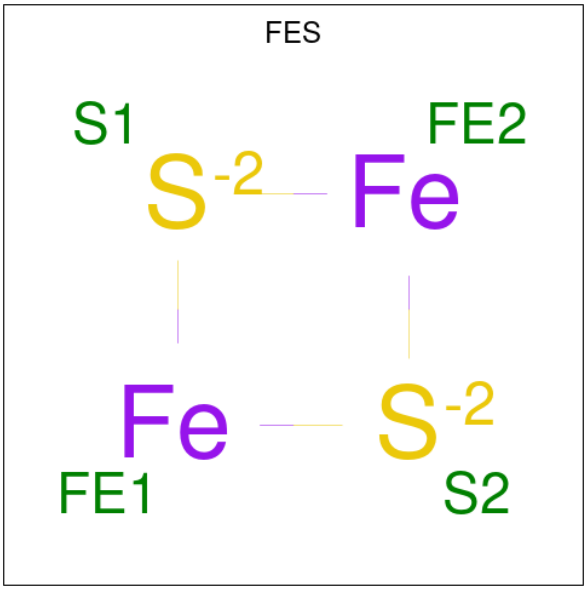
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
14	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
14	D	1	43	34	1	4	4	0	0

- Molecule 15 is (2Z,6E)-7-{2'-[(2E,4E)-1,6-DIMETHYLHEPTA-2,4-DIENYL]-2,4'-BI-1,3-THIAZOL-4-YL}-3,5-DIMETHOXY-4-METHYLHEPTA-2,6-DIENAMID E (CCD ID: MYX) (formula: $C_{25}H_{33}N_3O_3S_2$).



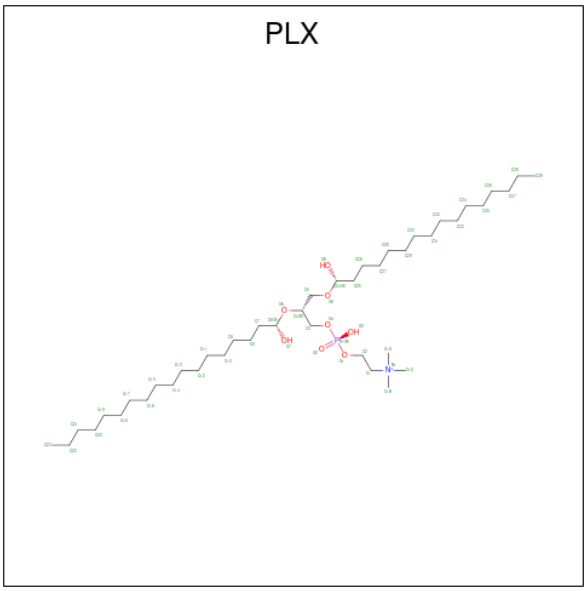
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
15	C	1	33	25	3	3	2	0	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 17 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	51	51	51	0	0
18	B	84	84	84	0	0
18	C	36	36	36	0	0
18	D	11	11	11	0	0
18	E	2	2	2	0	0
18	F	15	15	15	0	0
18	G	11	11	11	0	0
18	I	2	2	2	0	0
18	K	3	3	3	0	0

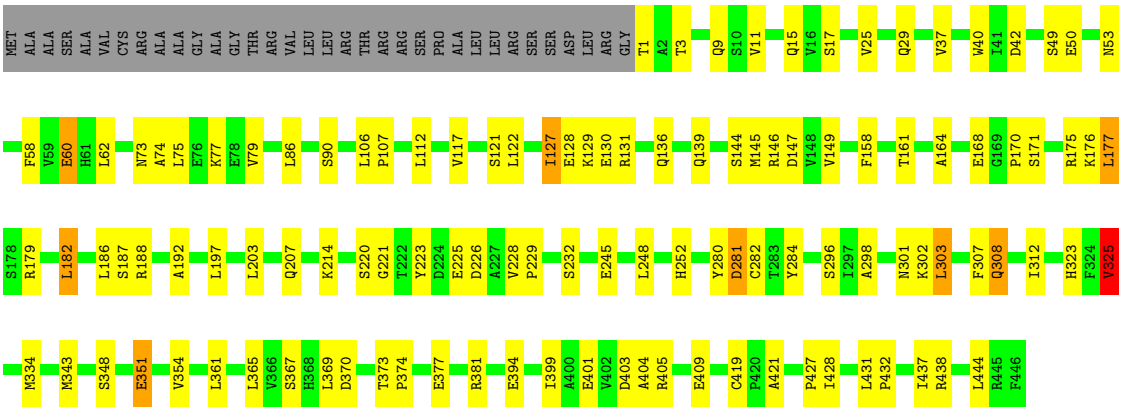
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

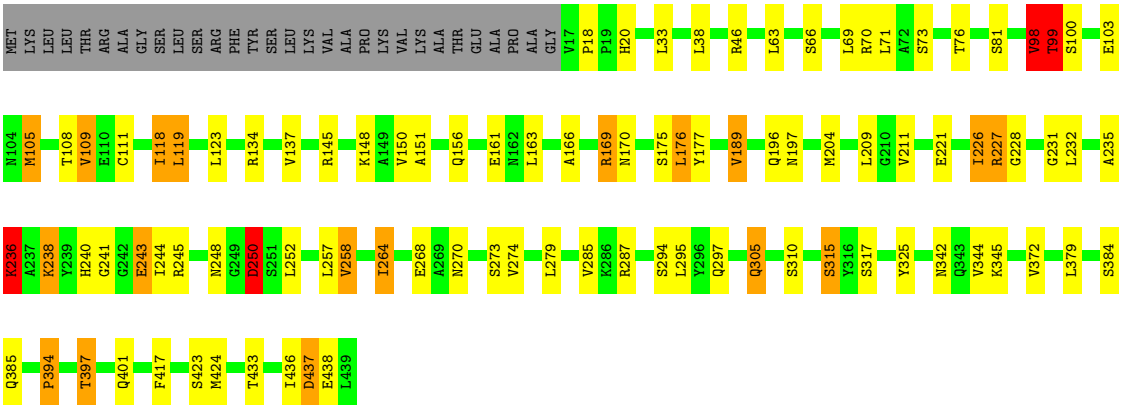
• Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor

Chain A: 69% 22% • 7%



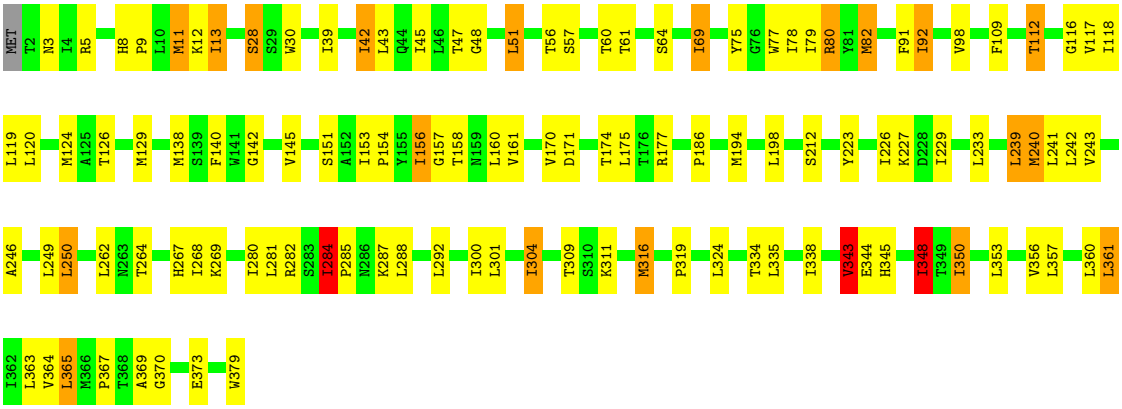
• Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor

Chain B: 72% 17% • • 7%



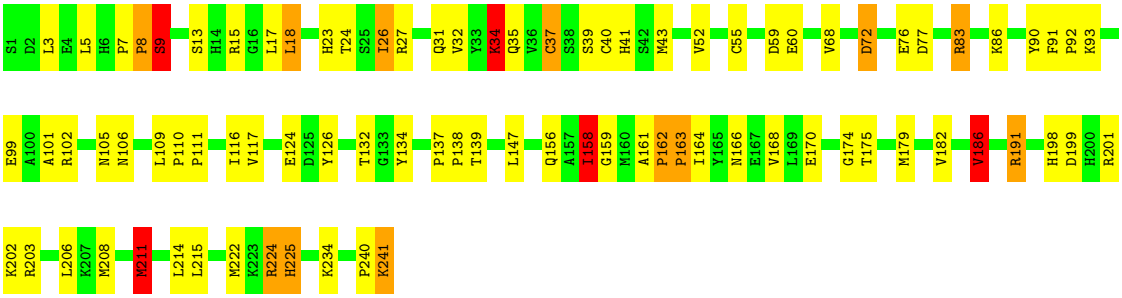
• Molecule 3: Cytochrome b

Chain C: 69% 25% 5% •



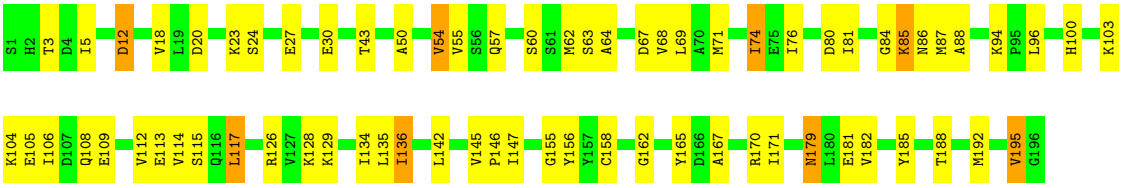
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



• Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]

Chain E:

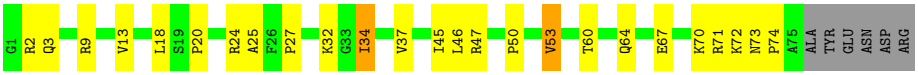


• Molecule 6: sub6

Chain F:

• Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain G:

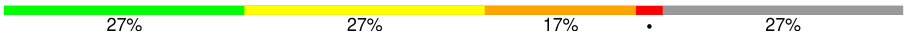


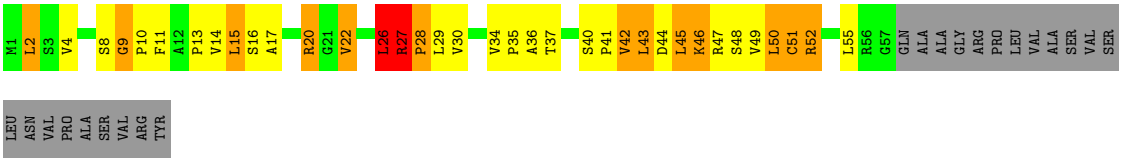
• Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

Chain H:

• Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]

Chain I:





• Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain J:

• Molecule 11: Ubiquinol-cytochrome c reductase complex 6.4 kDa protein

Chain K:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.70Å 153.70Å 596.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (40.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.263 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17274	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

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: MYX, HEC, CDL, FES, PEE, PLX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.05	8/3531 (0.2%)	1.10	3/4792 (0.1%)
2	B	1.23	12/3232 (0.4%)	1.13	3/4386 (0.1%)
3	C	1.22	16/3100 (0.5%)	1.20	4/4242 (0.1%)
4	D	1.16	6/1978 (0.3%)	1.21	8/2684 (0.3%)
5	E	1.32	10/1553 (0.6%)	1.10	2/2100 (0.1%)
6	F	1.14	1/930 (0.1%)	1.12	1/1246 (0.1%)
7	G	1.33	3/649 (0.5%)	1.16	2/878 (0.2%)
8	H	1.20	5/553 (0.9%)	1.19	0/741
9	I	1.87	8/411 (1.9%)	1.43	3/558 (0.5%)
10	J	1.18	2/515 (0.4%)	1.16	0/696
11	K	1.35	1/452 (0.2%)	1.23	2/618 (0.3%)
All	All	1.21	72/16904 (0.4%)	1.16	28/22941 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
6	F	0	1
All	All	0	3

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	34	ILE	CA-CB	12.18	1.60	1.54
2	B	105	MET	SD-CE	-9.31	1.56	1.79
1	A	334	MET	SD-CE	-9.06	1.56	1.79
3	C	11	MET	SD-CE	9.02	2.02	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	26	LEU	CA-C	8.83	1.62	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	35	GLN	OE1-CD-NE2	-9.59	113.01	122.60
7	G	50	PRO	N-CA-C	7.36	119.68	110.70
9	I	26	LEU	N-CA-C	6.91	119.50	107.49
4	D	34	LYS	N-CA-C	6.74	118.28	111.07
3	C	345	HIS	N-CA-C	6.42	124.00	109.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	LEU	Peptide
2	B	169	ARG	Mainchain
6	F	99	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	31	0
2	B	3172	0	3152	45	0
3	C	3003	0	3065	40	0
4	D	1919	0	1869	37	0
5	E	1519	0	1504	14	0
6	F	911	0	902	3	0
7	G	628	0	636	8	0
8	H	548	0	530	3	0
9	I	406	0	437	27	0
10	J	502	0	505	5	0
11	K	436	0	445	12	0
12	A	64	0	72	1	0
12	D	64	0	72	0	0
12	G	64	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	49	0	75	1	0
13	C	49	0	75	1	0
13	E	49	0	75	3	0
14	C	86	0	64	10	0
14	D	43	0	31	11	0
15	C	33	0	33	1	0
16	E	4	0	0	0	0
17	J	52	0	88	4	0
18	A	51	0	0	0	0
18	B	84	0	0	2	0
18	C	36	0	0	0	0
18	D	11	0	0	0	0
18	E	2	0	0	1	0
18	F	15	0	0	0	0
18	G	11	0	0	1	0
18	I	2	0	0	0	0
18	K	3	0	0	0	0
All	All	17274	0	17058	198	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 6.

The worst 5 of 198 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)
4:D:40:CYS:SG	14:D:243:HEC:HAC	1.33	1.68
3:C:11:MET:CE	3:C:11:MET:SD	2.02	1.48
11:K:38:TRP:HE3	11:K:41:ILE:CD1	1.25	1.48
4:D:37:CYS:SG	14:D:243:HEC:CAB	2.06	1.42
11:K:38:TRP:CE3	11:K:41:ILE:CD1	2.04	1.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/480 (92%)	418 (94%)	20 (4%)	6 (1%)	9	23
2	B	421/453 (93%)	390 (93%)	27 (6%)	4 (1%)	12	32
3	C	376/379 (99%)	353 (94%)	19 (5%)	4 (1%)	11	29
4	D	239/241 (99%)	211 (88%)	21 (9%)	7 (3%)	3	9
5	E	194/196 (99%)	162 (84%)	29 (15%)	3 (2%)	8	22
6	F	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	4	10
8	H	65/78 (83%)	58 (89%)	5 (8%)	2 (3%)	3	8
9	I	55/78 (70%)	31 (56%)	16 (29%)	8 (14%)	0	0
10	J	59/62 (95%)	50 (85%)	7 (12%)	2 (3%)	3	7
11	K	51/56 (91%)	43 (84%)	7 (14%)	1 (2%)	6	16
All	All	2080/2214 (94%)	1880 (90%)	161 (8%)	39 (2%)	6	17

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	ASP
3	C	154	PRO
4	D	8	PRO
7	G	73	ASN
9	I	29	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/394 (94%)	312 (84%)	58 (16%)	2	7
2	B	332/355 (94%)	288 (87%)	44 (13%)	4	10
3	C	326/327 (100%)	256 (78%)	70 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	206/206 (100%)	155 (75%)	51 (25%)	1 2
5	E	168/168 (100%)	127 (76%)	41 (24%)	1 2
6	F	96/99 (97%)	87 (91%)	9 (9%)	8 21
7	G	66/71 (93%)	54 (82%)	12 (18%)	2 5
8	H	64/74 (86%)	36 (56%)	28 (44%)	0 0
9	I	44/60 (73%)	30 (68%)	14 (32%)	0 1
10	J	51/52 (98%)	29 (57%)	22 (43%)	0 0
11	K	42/45 (93%)	29 (69%)	13 (31%)	0 1
All	All	1765/1851 (95%)	1403 (80%)	362 (20%)	1 3

5 of 362 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	62	MET
8	H	14	VAL
5	E	76	ILE
5	E	179	ASN
8	H	43	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	97	ASN
7	G	3	GLN
4	D	105	ASN
5	E	57	GLN
11	K	12	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CDL	D	242	-	63,63,99	1.73	9 (14%)	69,75,111	1.61	7 (10%)
13	PEE	E	197	-	48,48,50	1.57	6 (12%)	51,53,55	1.40	4 (7%)
14	HEC	C	381	3	50,50,50	1.27	5 (10%)	68,82,82	1.97	20 (29%)
15	MYX	C	383	-	30,34,34	2.38	5 (16%)	32,45,45	1.92	9 (28%)
14	HEC	C	382	3	50,50,50	1.40	7 (14%)	68,82,82	1.81	13 (19%)
12	CDL	A	447	-	63,63,99	1.70	8 (12%)	69,75,111	1.65	8 (11%)
13	PEE	C	380	-	48,48,50	1.56	6 (12%)	51,53,55	1.42	6 (11%)
16	FES	E	198	5	0,4,4	-	-	-		
13	PEE	A	448	-	48,48,50	1.63	6 (12%)	51,53,55	1.52	5 (9%)
14	HEC	D	243	4	50,50,50	1.45	7 (14%)	68,82,82	1.92	16 (23%)
12	CDL	G	82	-	63,63,99	1.78	8 (12%)	69,75,111	1.74	10 (14%)
17	PLX	J	63	-	51,51,51	0.77	2 (3%)	53,59,59	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	D	242	-	1/1/9/9	44/74/74/110	-
13	PEE	E	197	-	-	19/52/52/54	-
14	HEC	C	381	3	-	4/14/54/54	-
15	MYX	C	383	-	-	0/34/36/36	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEC	C	382	3	1/1/3/7	8/14/54/54	-
12	CDL	A	447	-	1/1/9/9	39/74/74/110	-
13	PEE	C	380	-	-	24/52/52/54	-
16	FES	E	198	5	-	-	0/1/1/1
13	PEE	A	448	-	-	29/52/52/54	-
14	HEC	D	243	4	1/1/3/7	8/14/54/54	-
12	CDL	G	82	-	1/1/9/9	42/74/74/110	-
17	PLX	J	63	-	-	36/55/55/55	-

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	383	MYX	C16-N3	6.80	1.45	1.30
15	C	383	MYX	C13-N2	6.41	1.44	1.31
15	C	383	MYX	O2-C3	6.15	1.47	1.35
12	G	82	CDL	PB2-OB3	5.86	1.71	1.50
12	D	242	CDL	PB2-OB3	5.68	1.70	1.50

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	447	CDL	OB6-CB5-OB7	-6.87	107.64	123.70
12	G	82	CDL	OB8-CB7-OB9	-6.55	107.25	123.63
12	G	82	CDL	OA6-CA5-OA7	-6.10	109.44	123.70
12	D	242	CDL	OB6-CB5-OB7	-6.03	109.60	123.70
14	D	243	HEC	CHA-C1A-NA	6.03	131.02	124.45

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	447	CDL	CA4
12	D	242	CDL	CA4
12	G	82	CDL	CA4
14	C	382	HEC	NA
14	D	243	HEC	NA

5 of 253 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	447	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
12	A	447	CDL	CA3-OA5-PA1-OA3
12	A	447	CDL	CA3-OA5-PA1-OA4
12	A	447	CDL	CB3-OB5-PB2-OB2
12	A	447	CDL	CB3-OB5-PB2-OB3

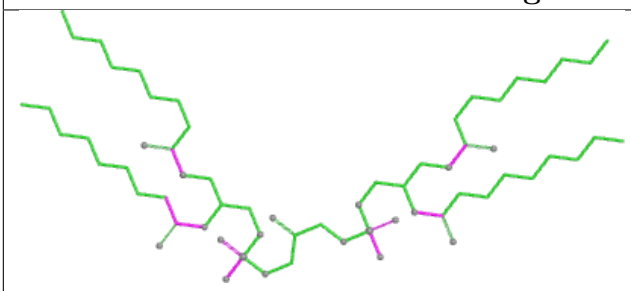
There are no ring outliers.

10 monomers are involved in 32 short contacts:

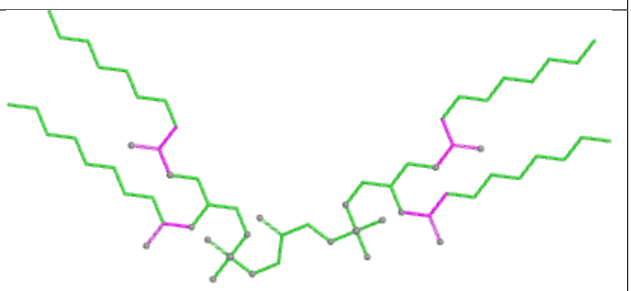
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	197	PEE	3	0
14	C	381	HEC	6	0
15	C	383	MYX	1	0
14	C	382	HEC	4	0
12	A	447	CDL	1	0
13	C	380	PEE	1	0
13	A	448	PEE	1	0
14	D	243	HEC	11	0
12	G	82	CDL	2	0
17	J	63	PLX	4	0

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

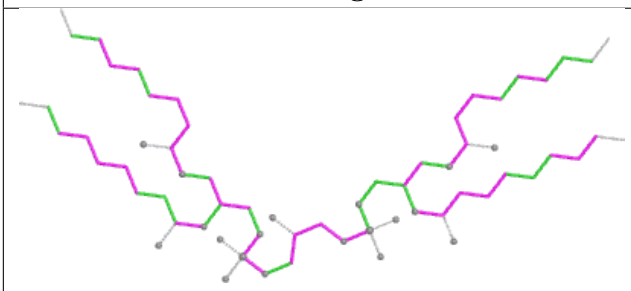
Ligand CDL D 242



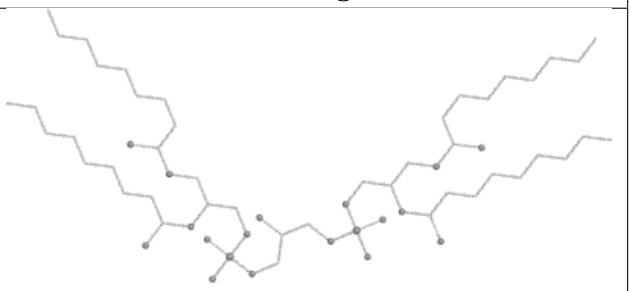
Bond lengths



Bond angles

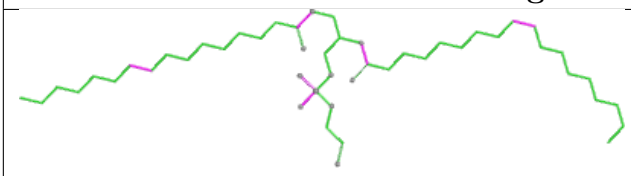


Torsions



Rings

Ligand PEE E 197



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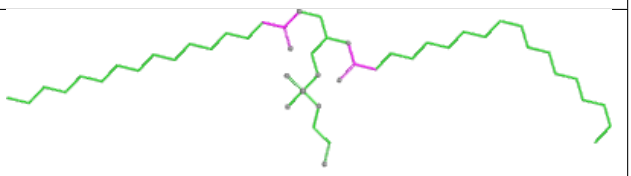

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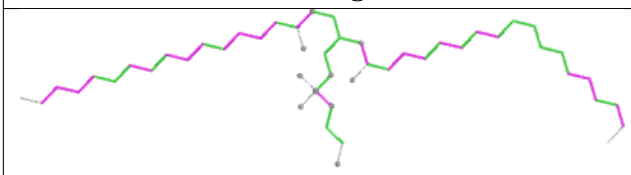

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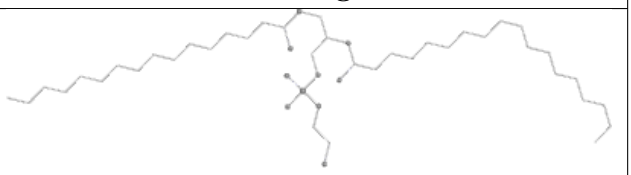
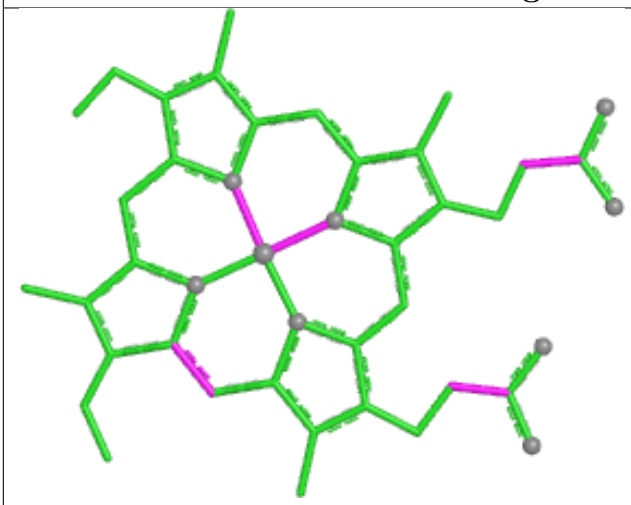
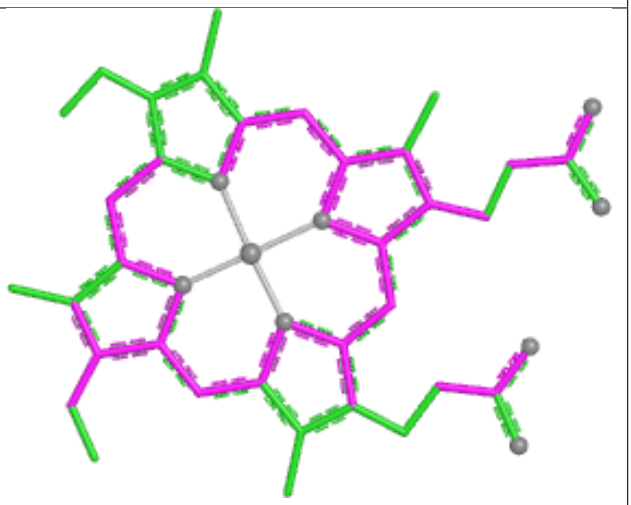


Rings

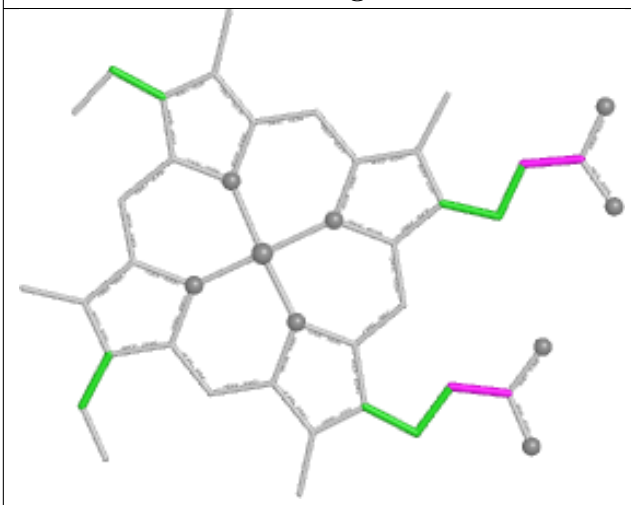
Ligand HEC C 381



Bond lengths



Bond angles



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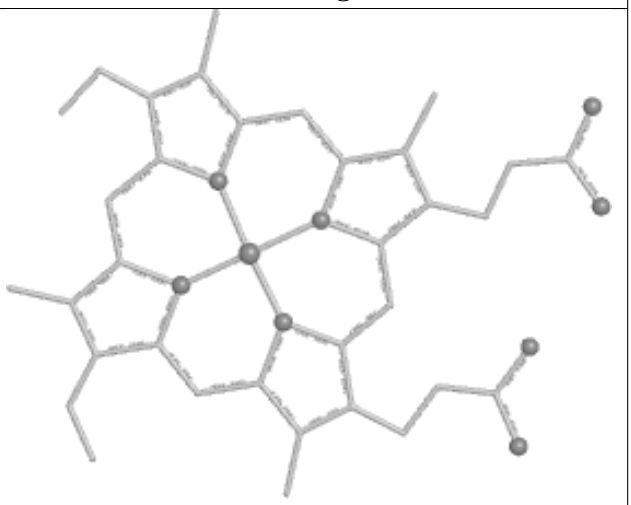
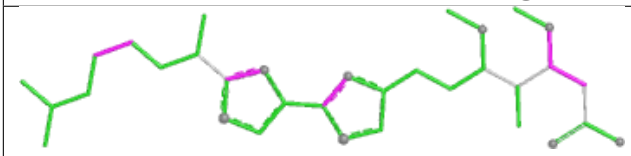


Rings

Ligand MYX C 383



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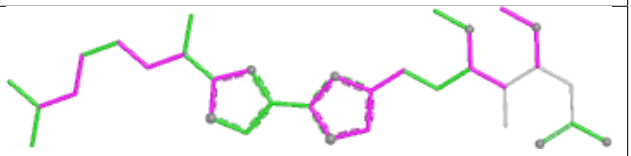

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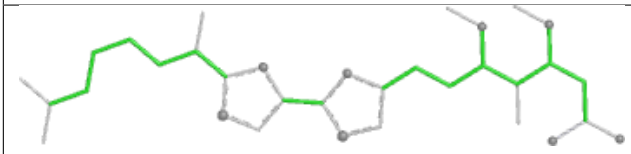
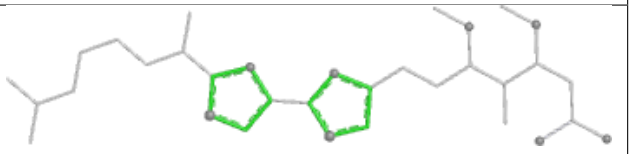
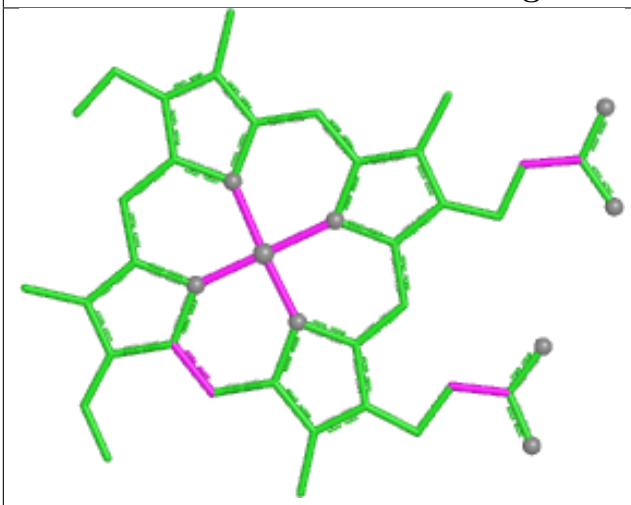


Torsions

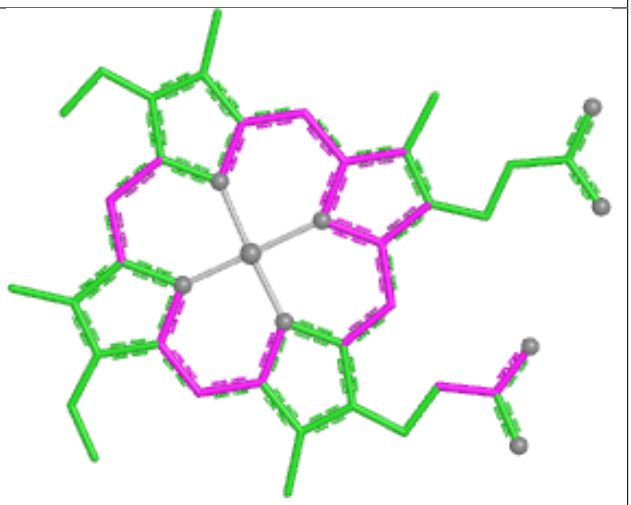


Rings

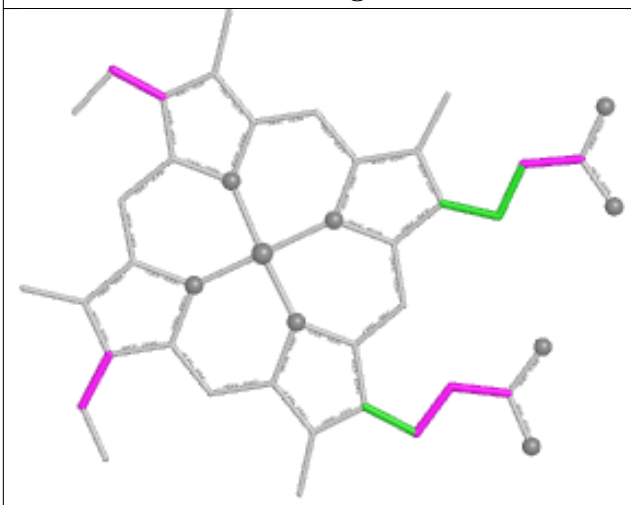
Ligand HEC C 382



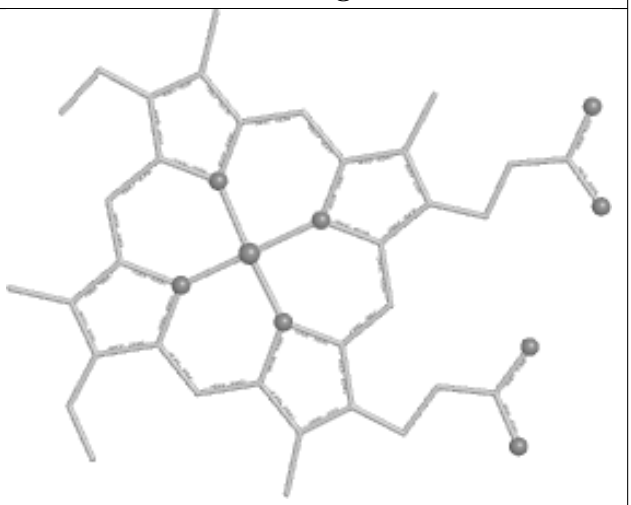
Bond lengths



Bond angles

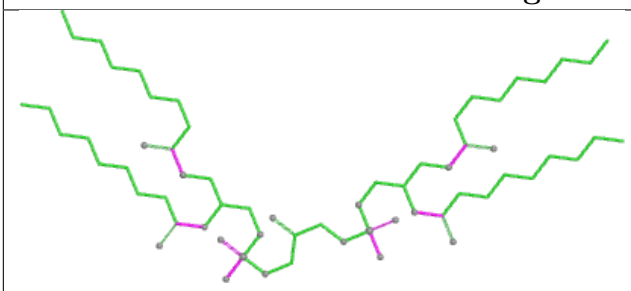


Torsions

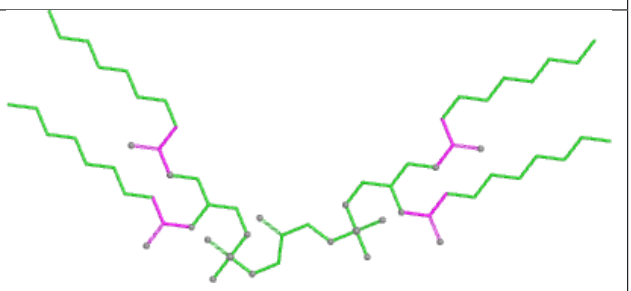


Rings

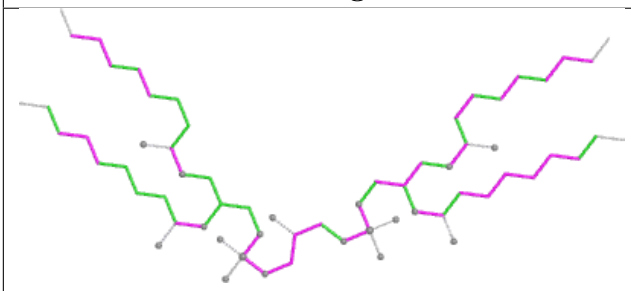
Ligand CDL A 447



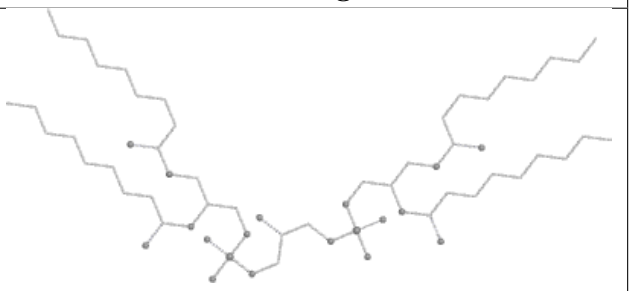
Bond lengths



Bond angles

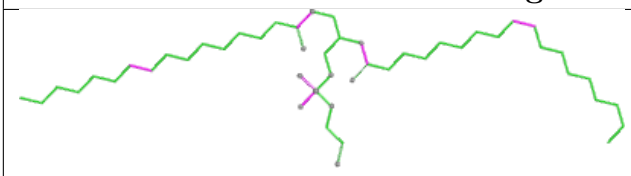


Torsions

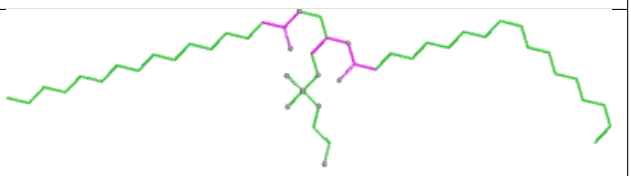


Rings

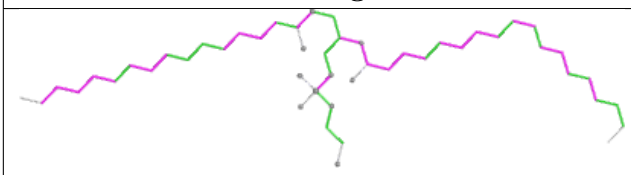
Ligand PEE C 380



Bond lengths



Bond angles



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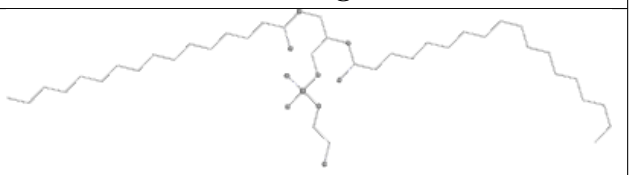
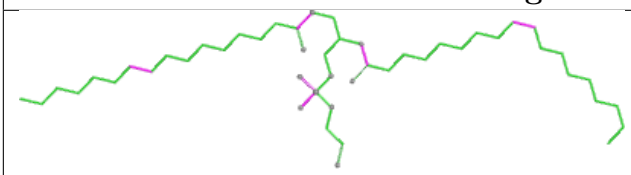


Rings

Ligand PEE A 448



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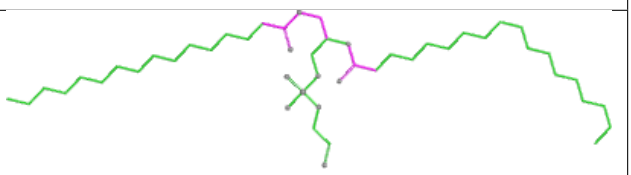
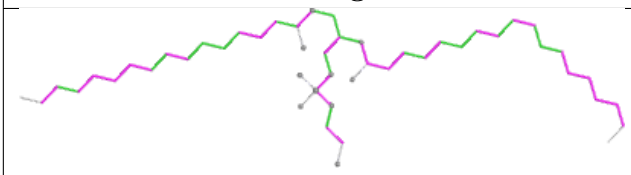
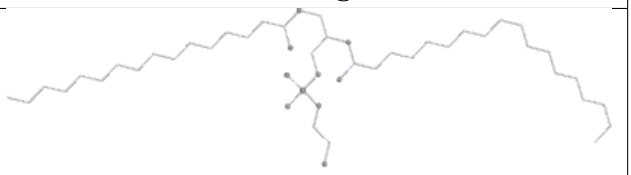


Bond angles

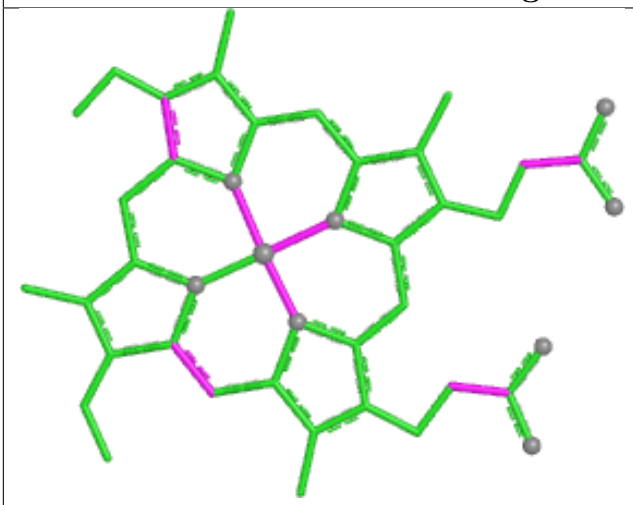


Torsions

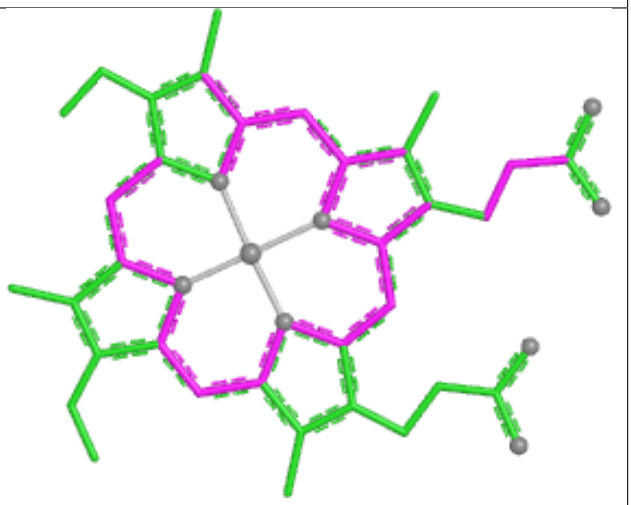


Rings

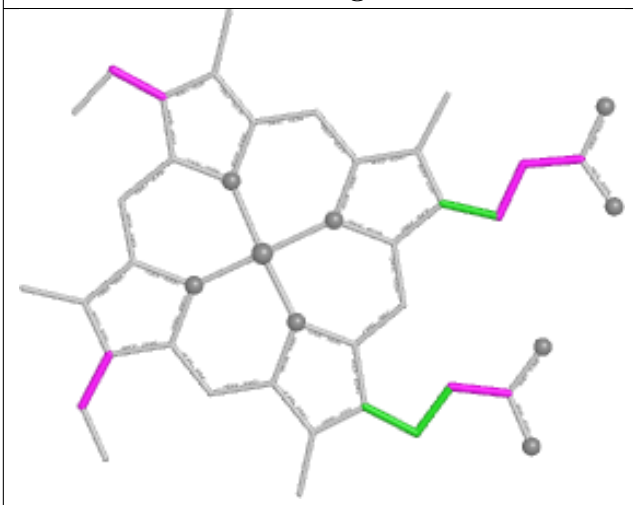
Ligand HEC D 243



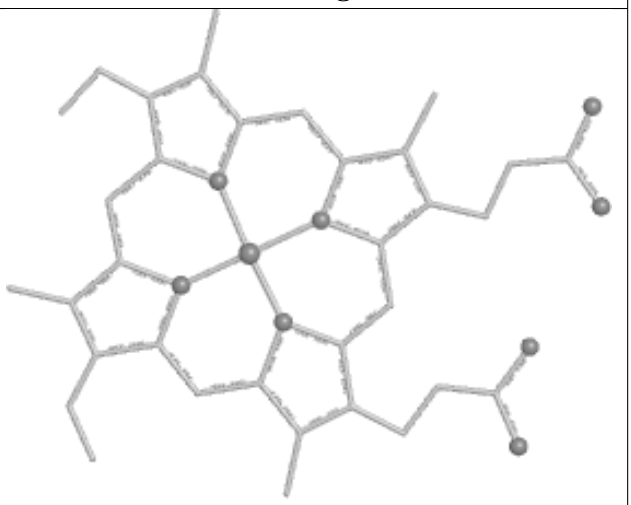
Bond lengths



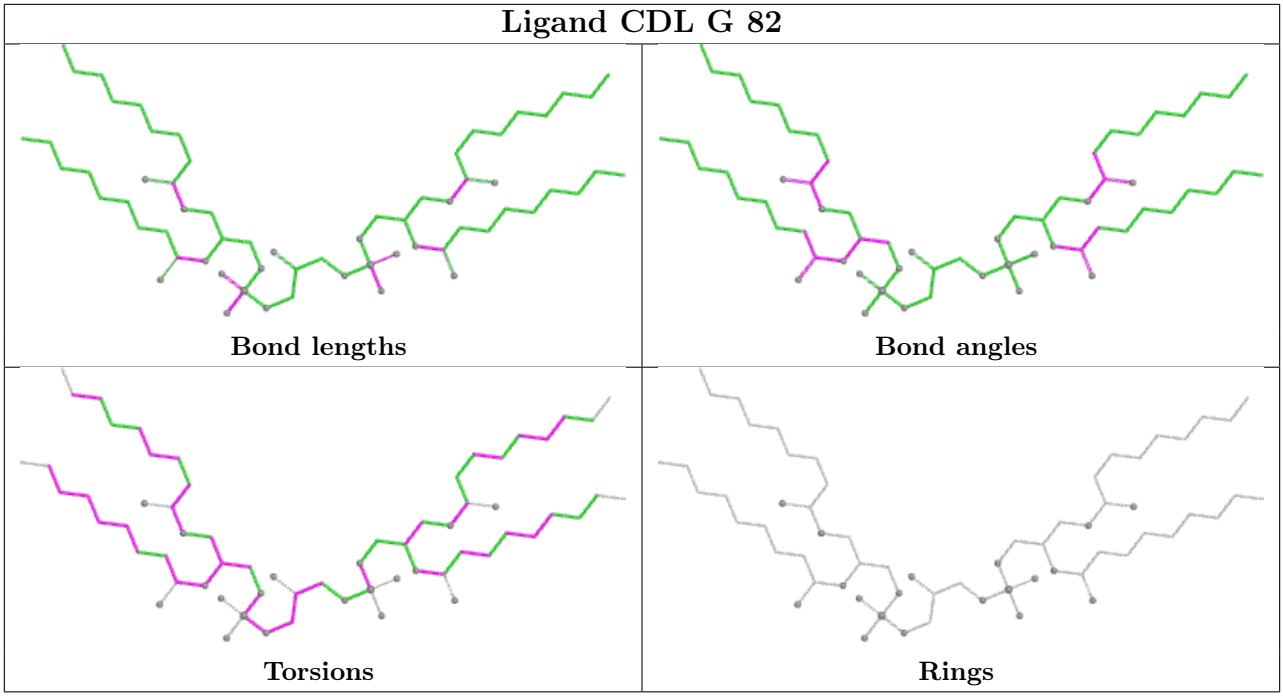
Bond angles

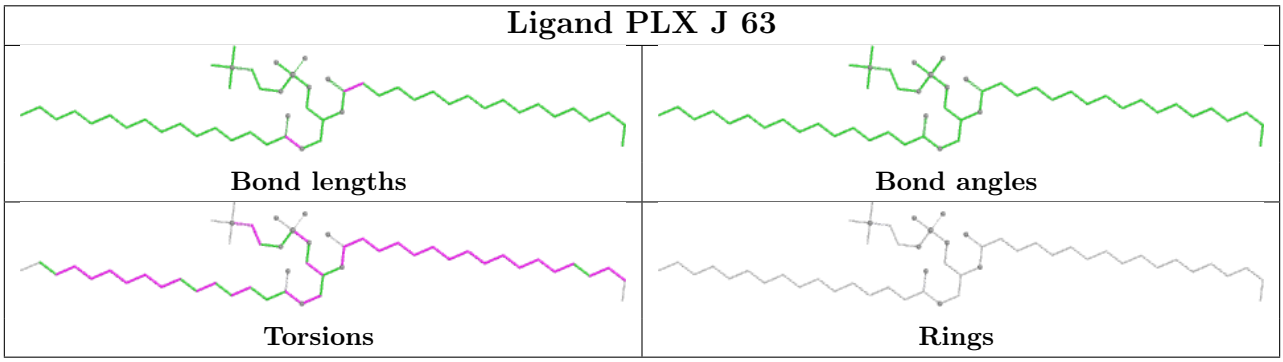


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.