wwPDB X-ray Structure Validation Summary Report (i)

Jun 21, 2021 – 10:02 PM EDT

PDB ID	:	1M56
Title	:	Structure of cytochrome c oxidase from Rhodobactor sphaeroides (Wild Type)
Authors	:	Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on	:	2002-07-08
Resolution	:	2.30 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 following versions of software and data (see references (1)) were used in the production of this report:

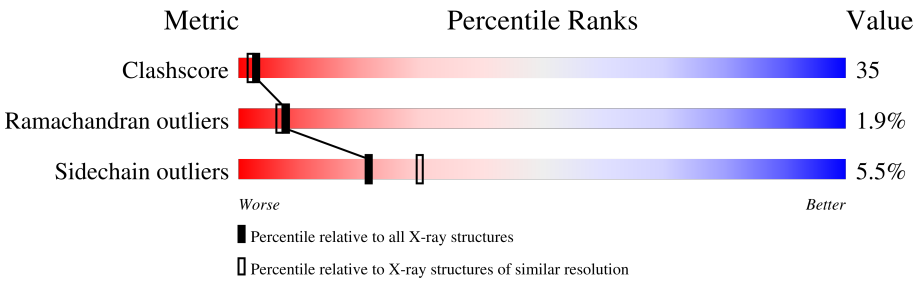
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

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 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	566	41% 43% 11% • •
1	G	566	38% 45% 11% • •
2	B	264	44% 45% 8% • •
2	H	264	45% 44% 8% • •
3	C	266	48% 44% 6% •
3	I	266	44% 49% 6% •
4	D	51	49% 27% • • 18%
4	J	51	39% 33% 8% • 18%

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
8	HEA	A	1001	X	-	-	-
8	HEA	A	1002	X	-	-	-
8	HEA	G	1001	X	-	-	-
8	HEA	G	1002	X	-	-	-
9	3PE	C	2013	-	-	X	-
9	3PE	D	2011	-	-	X	-
9	3PE	I	3010	-	-	X	-
9	3PE	I	3013	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 18934 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4322	2892	684	715	31	0	0	0
1	G	547	4322	2892	684	715	31	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	2046	1334	332	374	6	0	0	0
2	H	260	2046	1334	332	374	6	0	0	0

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	265	2139	1448	342	337	12	0	0	0
3	I	265	2139	1448	342	337	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	42	311	203	52	54	2	0	0	0
4	J	42	311	203	52	54	2	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
5	A	1	1	1	0	0
5	B	2	2	2	0	0
5	G	1	1	1	0	0
5	H	2	2	2	0	0

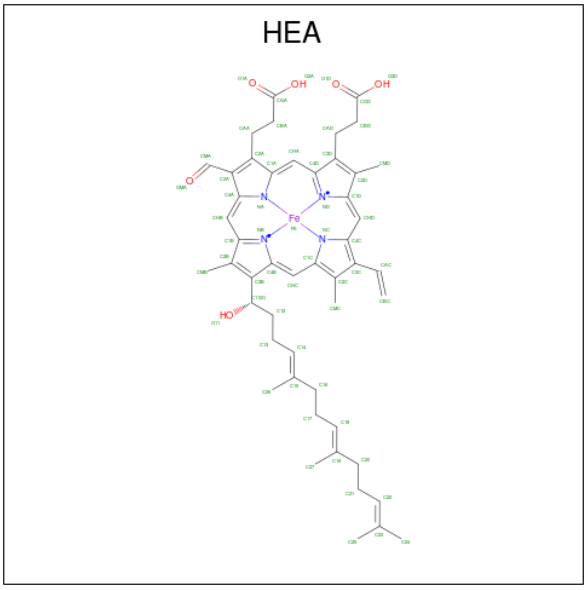
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
6	G	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

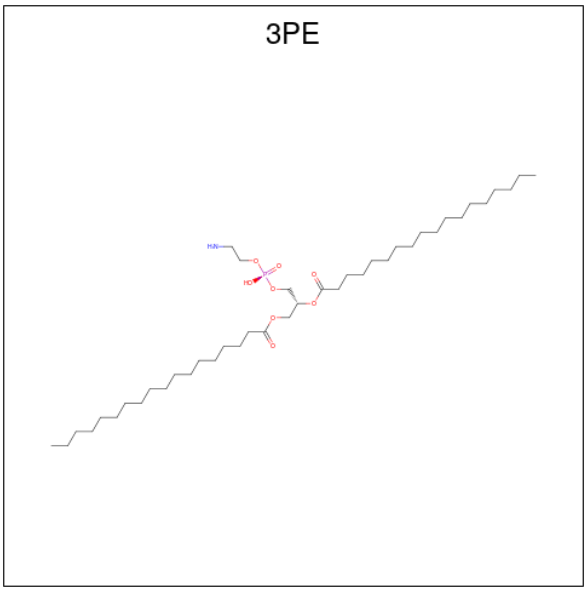
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
7	G	1	1	1	0	0

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	G	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	G	1	60	49	1	4	6	0	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	51	41	1	8	1	0	0
9	A	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	D	1	51	41	1	8	1	0	0
9	G	1	51	41	1	8	1	0	0
9	G	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	J	1	51	41	1	8	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	101	101	101	0	0
			Total	O		
10	B	68	68	68	0	0
			Total	O		
10	C	39	39	39	0	0
			Total	O		
10	D	12	12	12	0	0
			Total	O		
10	G	106	106	106	0	0
			Total	O		
10	H	64	64	64	0	0
			Total	O		
10	I	38	38	38	0	0
			Total	O		
10	J	8	8	8	0	0

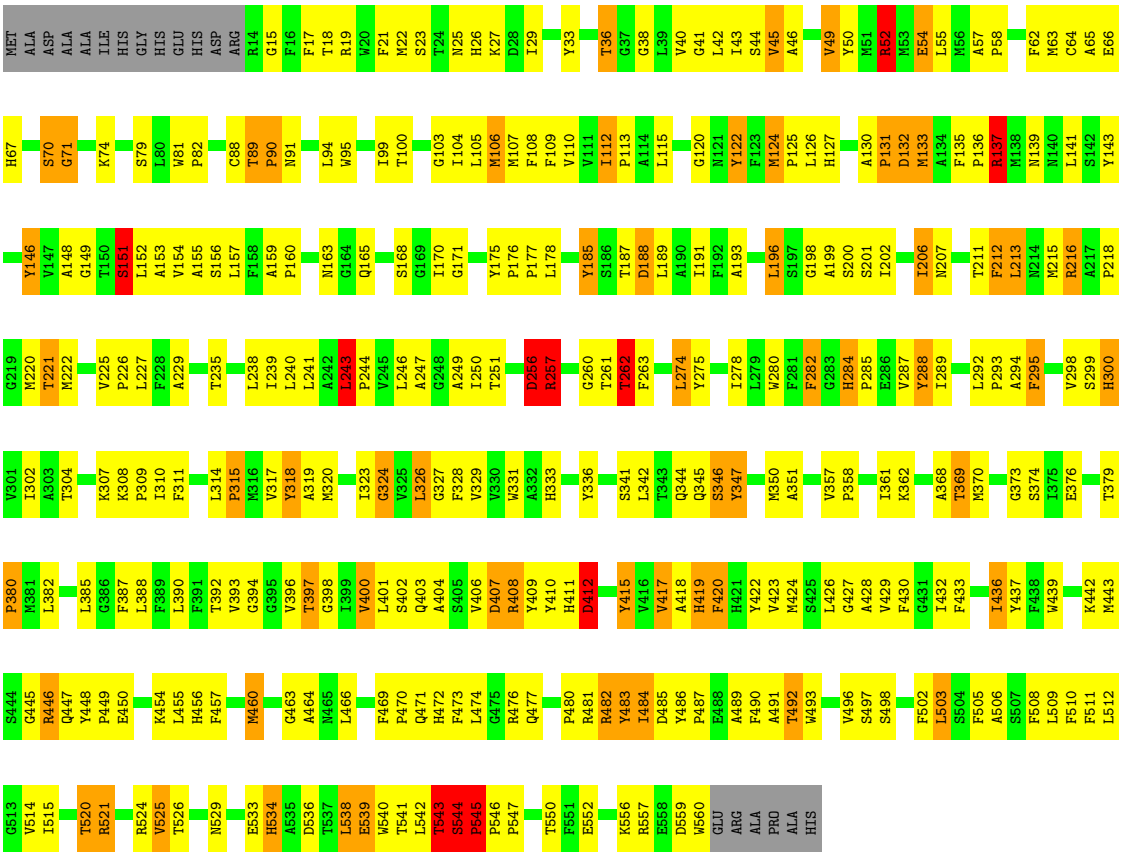
3 Residue-property plots (i)

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.

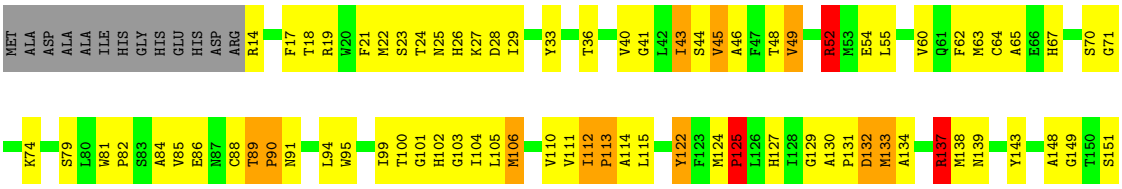
• Molecule 1: CYTOCHROME C OXIDASE

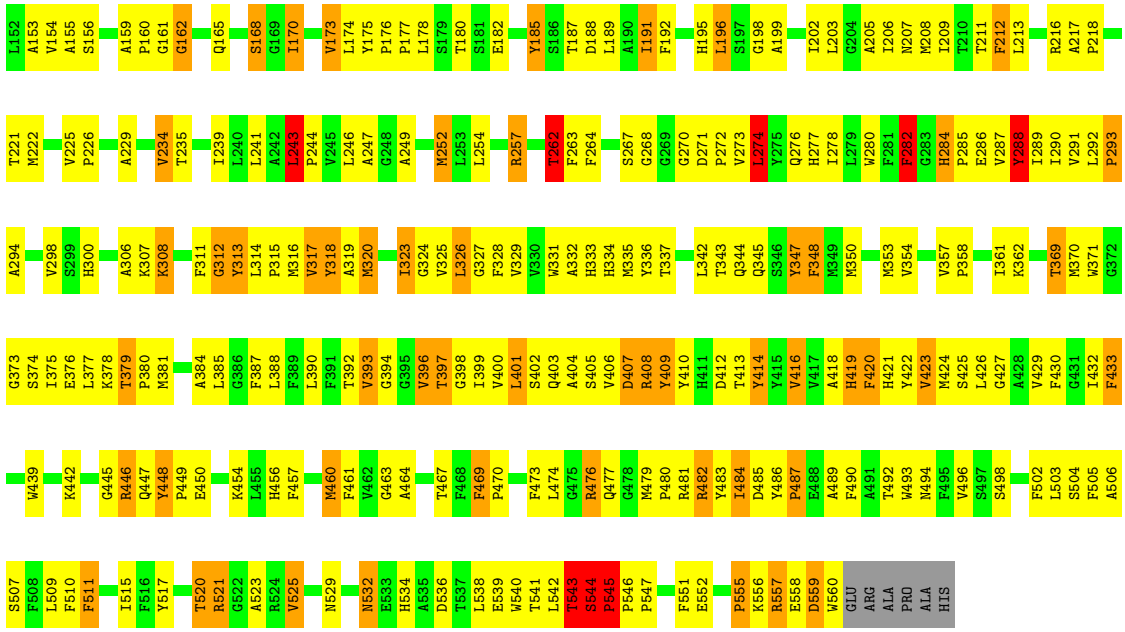
Chain A: 41% 43% 11% • •



• Molecule 1: CYTOCHROME C OXIDASE

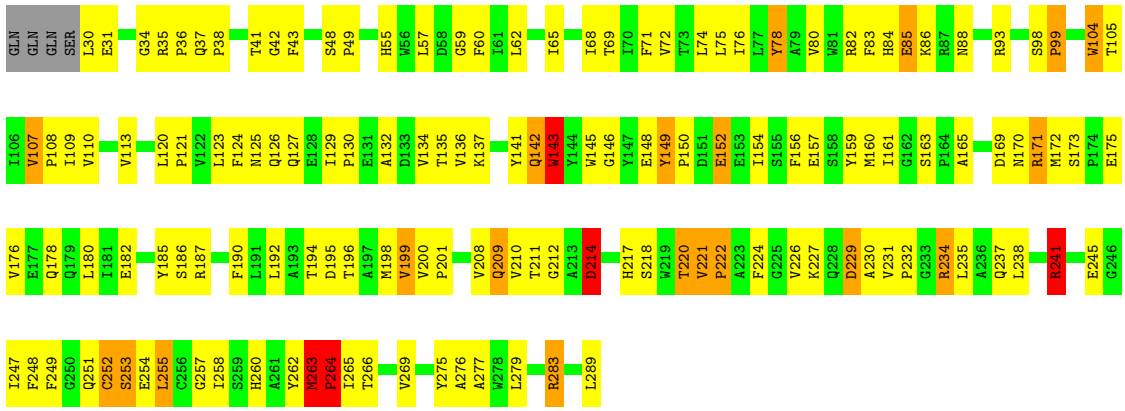
Chain G: 38% 45% 11% • •





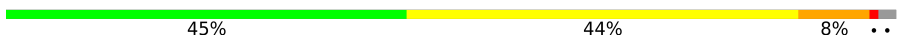
- Molecule 2: CYTOCHROME C OXIDASE

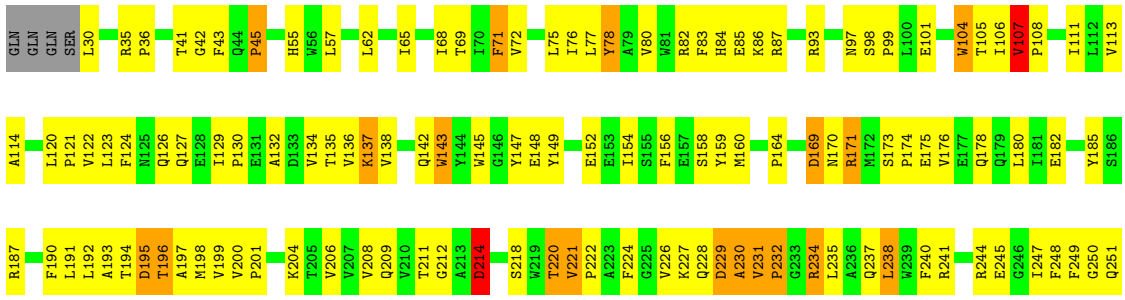
Chain B:



- Molecule 2: CYTOCHROME C OXIDASE

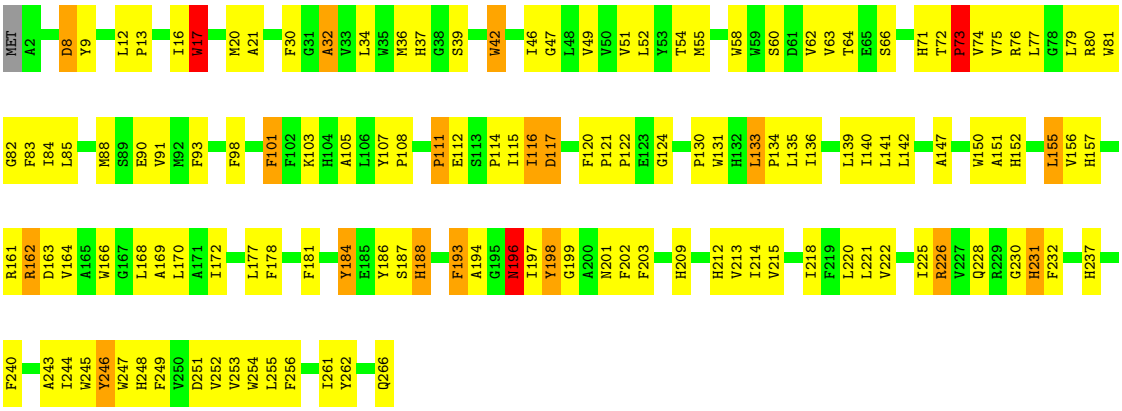
Chain H:





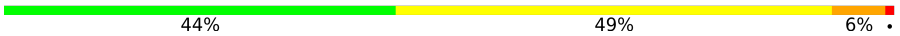
• Molecule 3: CYTOCHROME C OXIDASE

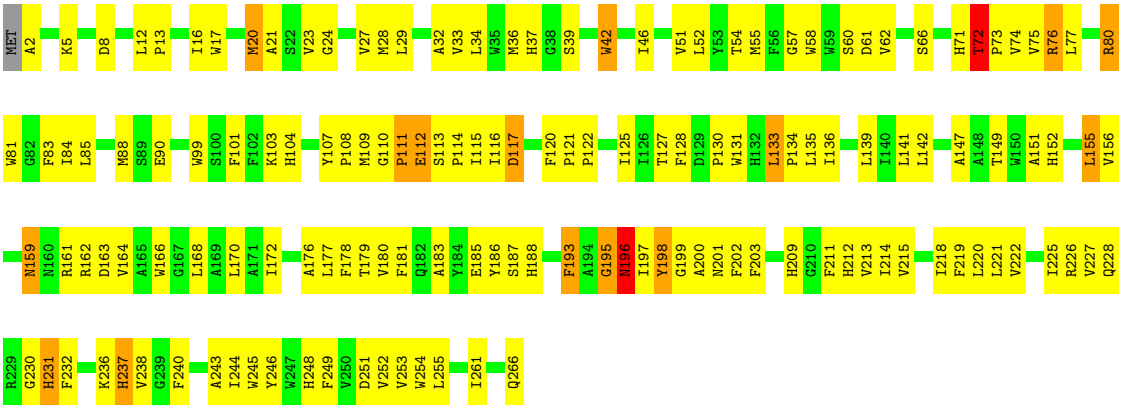
Chain C:



• Molecule 3: CYTOCHROME C OXIDASE

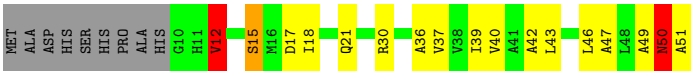
Chain I:





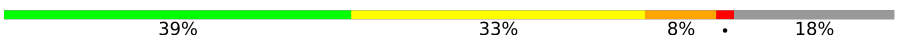
• Molecule 4: CYTOCHROME C OXIDASE

Chain D:



• Molecule 4: CYTOCHROME C OXIDASE

Chain J:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	340.36Å 340.36Å 89.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms ($Å^2$)	29.0	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: MG, CU, CA, HEA, 3PE

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	0.70	2/4482 (0.0%)	1.91	106/6114 (1.7%)
1	G	0.71	1/4482 (0.0%)	1.86	97/6114 (1.6%)
2	B	0.57	0/2105	1.73	38/2879 (1.3%)
2	H	0.58	0/2105	1.67	36/2879 (1.3%)
3	C	0.53	0/2232	1.43	22/3054 (0.7%)
3	I	0.55	0/2232	1.49	22/3054 (0.7%)
4	D	0.52	0/316	1.66	6/428 (1.4%)
4	J	0.53	0/316	1.61	6/428 (1.4%)
All	All	0.63	3/18270 (0.0%)	1.74	333/24950 (1.3%)

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	12
1	G	0	15
2	B	0	6
2	H	0	5
3	C	0	3
3	I	0	2
4	D	0	1
All	All	0	44

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	C-O	5.96	1.34	1.23
1	G	544	SER	N-CA	-5.23	1.35	1.46
1	A	544	SER	N-CA	-5.20	1.35	1.46

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	543	THR	C-N-CA	21.14	174.56	121.70
1	A	257	ARG	NE-CZ-NH1	-20.04	110.28	120.30
2	B	171	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	A	521	ARG	NE-CZ-NH2	-16.71	111.94	120.30
2	B	234	ARG	NE-CZ-NH2	-16.71	111.95	120.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	157	LEU	Mainchain
1	A	202	ILE	Mainchain
1	A	257	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	4322	0	4238	314	0
1	G	4322	0	4238	339	0
2	B	2046	0	2011	126	0
2	H	2046	0	2011	143	0
3	C	2139	0	2056	155	0
3	I	2139	0	2056	153	0
4	D	311	0	319	25	0
4	J	311	0	319	42	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	120	0	108	26	0
8	G	120	0	108	18	0
9	A	102	0	164	34	0
9	C	153	0	246	48	0
9	D	51	0	82	21	0
9	G	102	0	164	29	0
9	I	153	0	246	51	0
9	J	51	0	82	16	0
10	A	101	0	0	7	0
10	B	68	0	0	3	0
10	C	39	0	0	5	0
10	D	12	0	0	0	0
10	G	106	0	0	9	0
10	H	64	0	0	6	0
10	I	38	0	0	4	0
10	J	8	0	0	2	0
All	All	18934	0	18448	1291	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 35.

The worst 5 of 1291 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)
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.27	1.12
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.32	1.12
9:I:3013:3PE:O14	9:I:3013:3PE:H121	1.51	1.11
9:I:3013:3PE:C3H	9:I:3013:3PE:H2D2	1.78	1.11
9:C:2013:3PE:O14	9:C:2013:3PE:H121	1.48	1.06

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	545/566 (96%)	479 (88%)	54 (10%)	12 (2%)	6	5
1	G	545/566 (96%)	466 (86%)	67 (12%)	12 (2%)	6	5
2	B	258/264 (98%)	222 (86%)	32 (12%)	4 (2%)	9	9
2	H	258/264 (98%)	220 (85%)	33 (13%)	5 (2%)	8	7
3	C	263/266 (99%)	229 (87%)	30 (11%)	4 (2%)	10	10
3	I	263/266 (99%)	234 (89%)	25 (10%)	4 (2%)	10	10
4	D	40/51 (78%)	37 (92%)	2 (5%)	1 (2%)	5	4
4	J	40/51 (78%)	32 (80%)	7 (18%)	1 (2%)	5	4
All	All	2212/2294 (96%)	1919 (87%)	250 (11%)	43 (2%)	8	7

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	SER
3	C	111	PRO
1	G	327	GLY
1	G	544	SER
2	H	264	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	446/459 (97%)	422 (95%)	24 (5%)	22	30
1	G	446/459 (97%)	410 (92%)	36 (8%)	11	15
2	B	216/220 (98%)	204 (94%)	12 (6%)	21	29
2	H	216/220 (98%)	209 (97%)	7 (3%)	39	54
3	C	215/216 (100%)	207 (96%)	8 (4%)	34	48
3	I	215/216 (100%)	206 (96%)	9 (4%)	30	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	30/37 (81%)	28 (93%)	2 (7%)	16	21
4	J	30/37 (81%)	29 (97%)	1 (3%)	38	53
All	All	1814/1864 (97%)	1715 (94%)	99 (6%)	21	30

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	131	PRO
1	G	291	VAL
1	G	137	ARG
1	G	243	LEU
1	G	412	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	159	ASN
3	I	201	ASN
4	J	11	HIS
3	C	153	HIS
2	B	237	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
9	3PE	I	3008	-	50,50,50	1.54	2 (4%)	53,55,55	1.15	4 (7%)
9	3PE	C	2013	-	50,50,50	1.59	3 (6%)	53,55,55	1.11	3 (5%)
8	HEA	G	1002	1	44,67,67	1.98	7 (15%)	37,103,103	2.31	14 (37%)
8	HEA	A	1002	1	44,67,67	1.68	6 (13%)	37,103,103	2.00	12 (32%)
9	3PE	C	2010	-	50,50,50	1.61	2 (4%)	53,55,55	0.99	3 (5%)
8	HEA	A	1001	1	44,67,67	1.68	7 (15%)	37,103,103	2.48	15 (40%)
9	3PE	G	3009	-	50,50,50	1.55	2 (4%)	53,55,55	1.02	1 (1%)
9	3PE	C	2008	-	50,50,50	1.58	2 (4%)	53,55,55	1.17	5 (9%)
9	3PE	A	2012	-	50,50,50	1.59	3 (6%)	53,55,55	1.07	5 (9%)
9	3PE	A	2009	-	50,50,50	1.52	2 (4%)	53,55,55	1.01	3 (5%)
9	3PE	G	3012	-	50,50,50	1.58	3 (6%)	53,55,55	1.11	4 (7%)
8	HEA	G	1001	1	44,67,67	1.60	9 (20%)	37,103,103	2.49	18 (48%)
9	3PE	I	3013	-	50,50,50	1.55	4 (8%)	53,55,55	1.08	4 (7%)
9	3PE	J	3011	-	50,50,50	1.54	2 (4%)	53,55,55	1.30	4 (7%)
9	3PE	I	3010	-	50,50,50	1.61	2 (4%)	53,55,55	0.97	3 (5%)
9	3PE	D	2011	-	50,50,50	1.54	2 (4%)	53,55,55	1.28	4 (7%)

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
9	3PE	I	3008	-	-	35/54/54/54	-
9	3PE	C	2013	-	-	27/54/54/54	-
8	HEA	G	1002	1	3/3/7/16	2/24/76/76	-
8	HEA	A	1002	1	3/3/7/16	4/24/76/76	-
9	3PE	C	2010	-	-	29/54/54/54	-
8	HEA	A	1001	1	3/3/7/16	10/24/76/76	-
9	3PE	G	3009	-	-	27/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	3PE	C	2008	-	-	35/54/54/54	-
9	3PE	A	2012	-	-	23/54/54/54	-
9	3PE	A	2009	-	-	31/54/54/54	-
9	3PE	G	3012	-	-	24/54/54/54	-
8	HEA	G	1001	1	3/3/7/16	8/24/76/76	-
9	3PE	I	3013	-	-	28/54/54/54	-
9	3PE	J	3011	-	-	26/54/54/54	-
9	3PE	I	3010	-	-	25/54/54/54	-
9	3PE	D	2011	-	-	22/54/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2013	3PE	O21-C21	7.70	1.56	1.34
9	C	2010	3PE	O31-C31	7.64	1.55	1.33
9	G	3009	3PE	O21-C21	7.52	1.55	1.34
9	C	2008	3PE	O21-C21	7.50	1.55	1.34
9	J	3011	3PE	O21-C21	7.48	1.55	1.34

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	HEA	C13-C14-C15	-6.96	110.89	127.66
8	G	1001	HEA	CBA-CAA-C2A	5.73	123.03	112.48
9	J	3011	3PE	C2-O21-C21	-5.46	104.36	117.79
8	G	1001	HEA	C13-C14-C15	-5.39	114.68	127.66
8	A	1002	HEA	C17-C18-C19	-5.12	115.34	127.66

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1001	HEA	ND
8	A	1001	HEA	NB
8	A	1001	HEA	NA
8	A	1002	HEA	ND
8	A	1002	HEA	NB

5 of 356 torsion outliers are listed below:

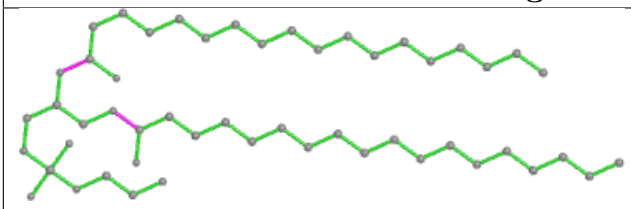
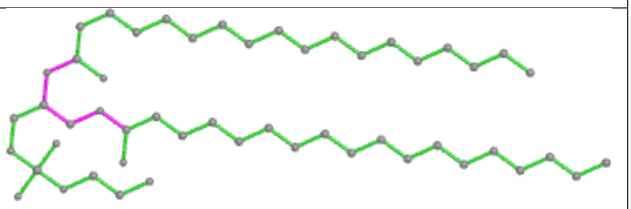
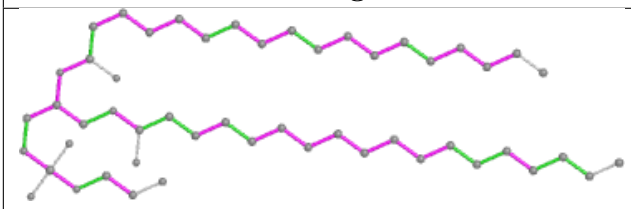
Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C1A-C2A-CAA-CBA
8	A	1001	HEA	C3A-C2A-CAA-CBA
8	A	1001	HEA	C3B-C11-C12-C13
8	A	1001	HEA	O11-C11-C12-C13
8	A	1001	HEA	C11-C12-C13-C14

There are no ring outliers.

16 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	3008	3PE	9	0
9	C	2013	3PE	21	0
8	G	1002	HEA	7	0
8	A	1002	HEA	9	0
9	C	2010	3PE	20	0
8	A	1001	HEA	17	0
9	G	3009	3PE	17	0
9	C	2008	3PE	7	0
9	A	2012	3PE	14	0
9	A	2009	3PE	20	0
9	G	3012	3PE	12	0
8	G	1001	HEA	11	0
9	I	3013	3PE	22	0
9	J	3011	3PE	16	0
9	I	3010	3PE	21	0
9	D	2011	3PE	21	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 3PE I 3008	
 Bond lengths	 Bond angles
 Torsions	Rings

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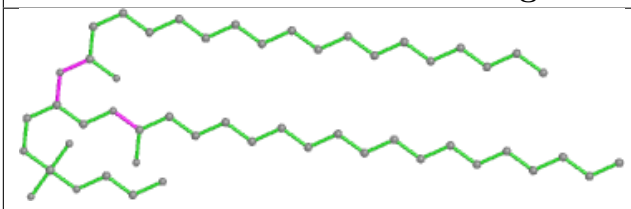
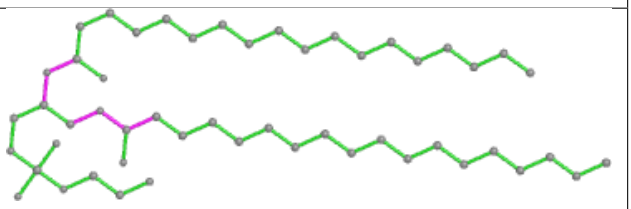
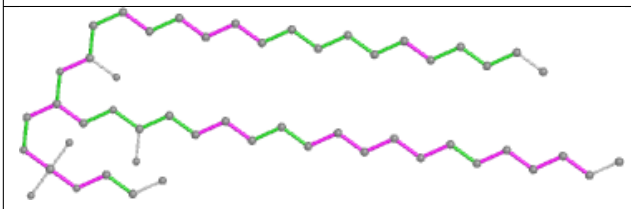
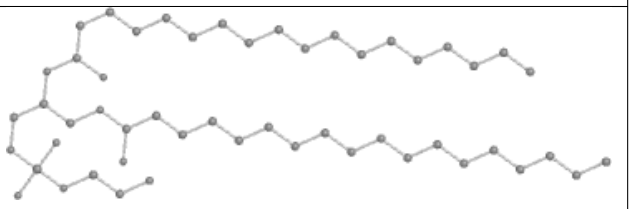
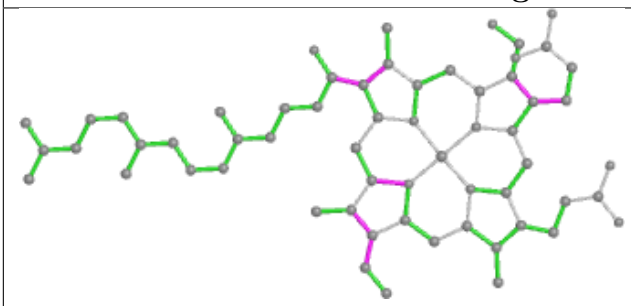
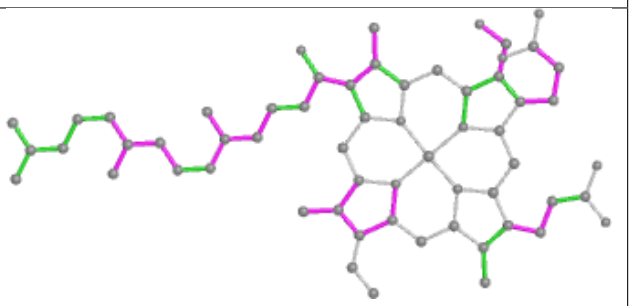
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA G 1002



Bond lengths



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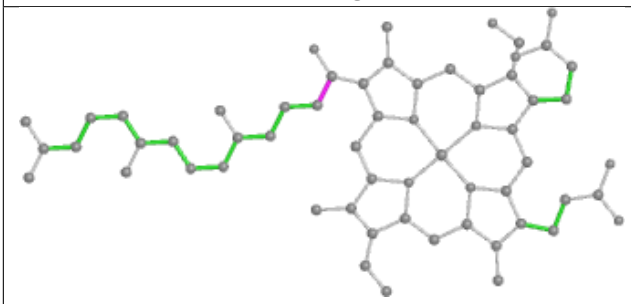

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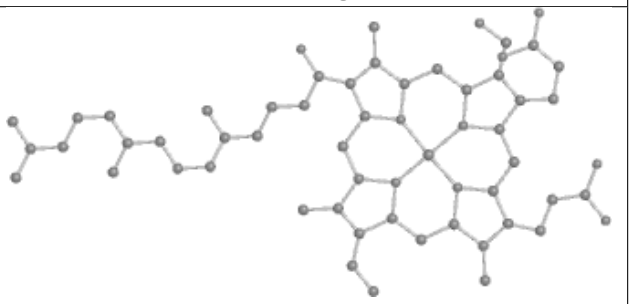
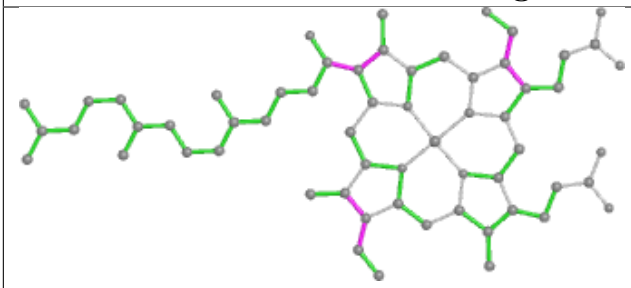


Rings

Ligand HEA A 1002



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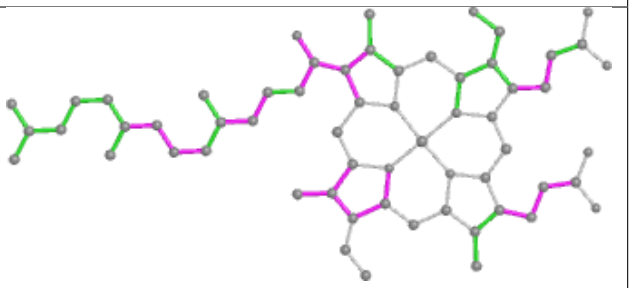

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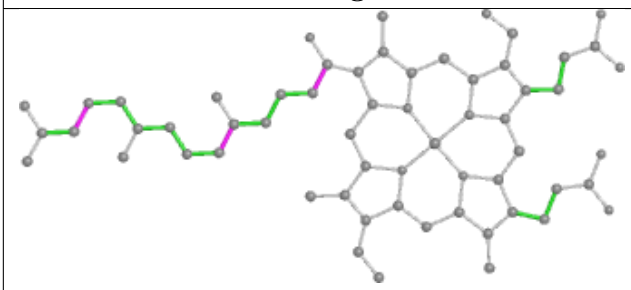

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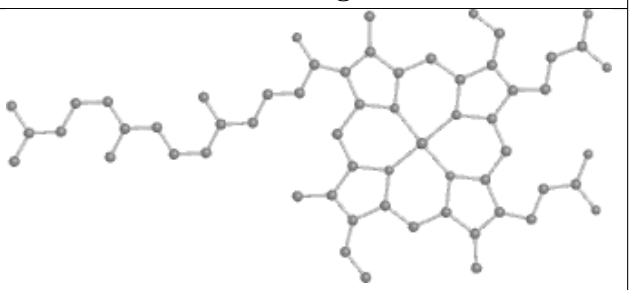
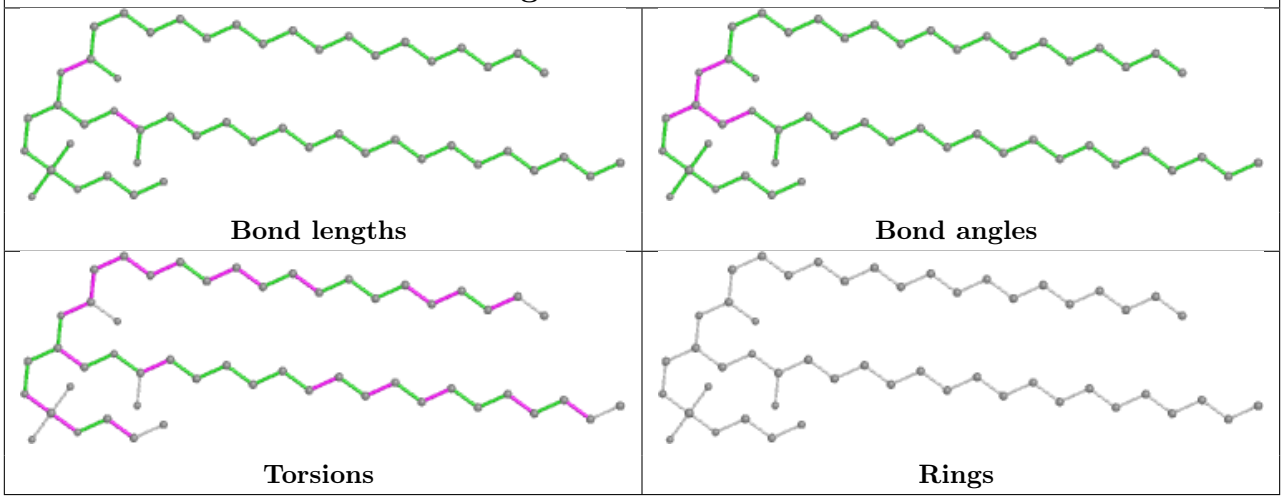


Rings

Ligand 3PE C 2010



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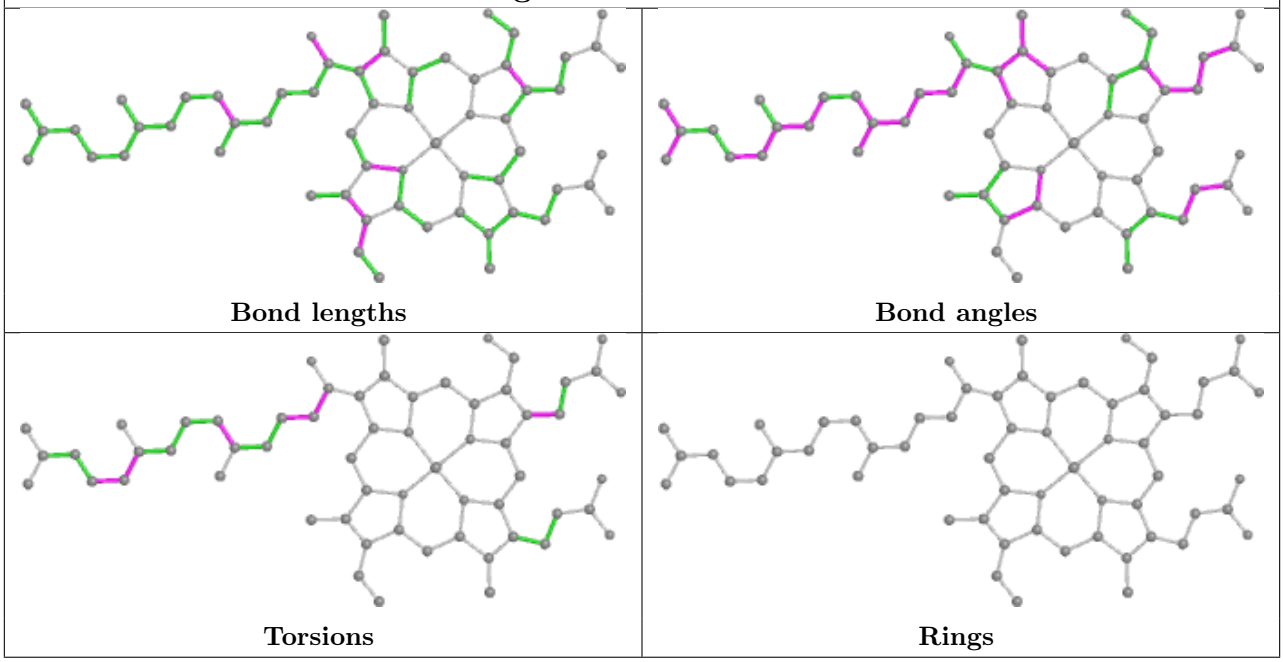
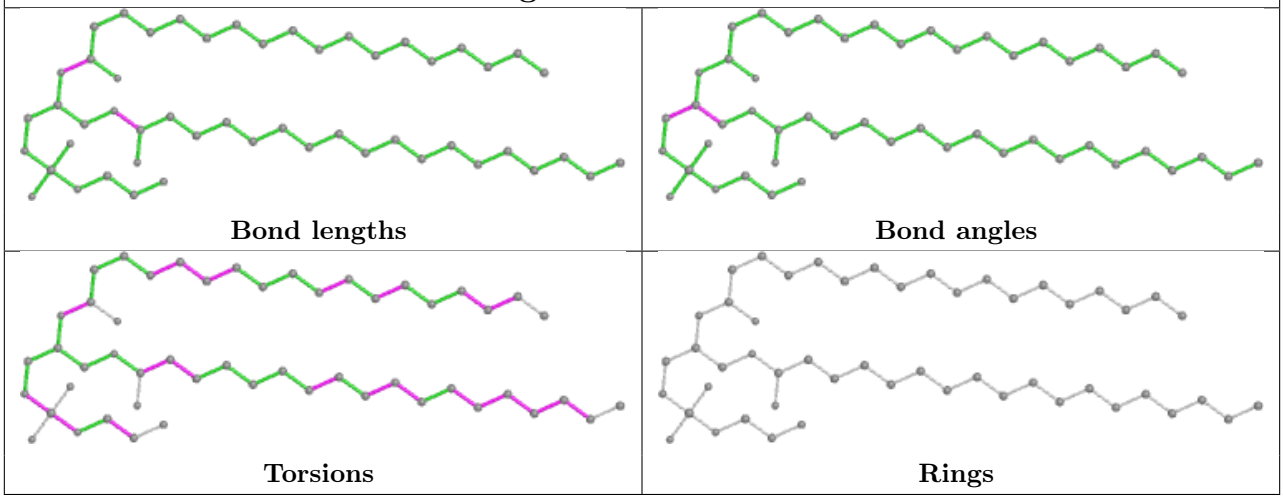
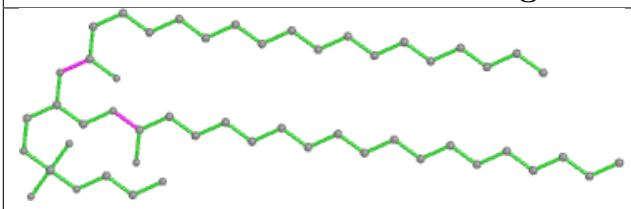


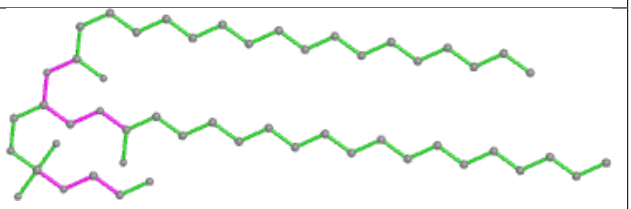
Ligand 3PE G 3009



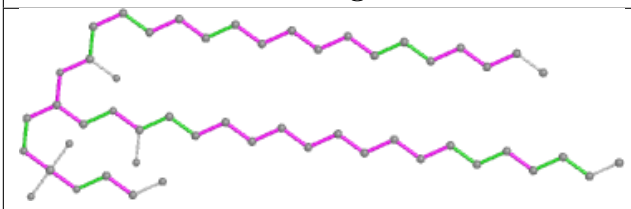
Ligand 3PE C 2008



Bond lengths



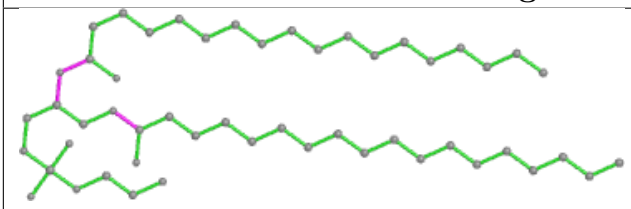
Bond angles



Torsions

Rings

Ligand 3PE A 2012



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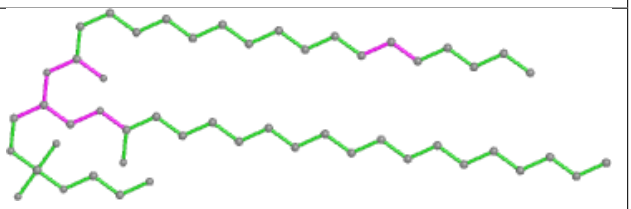

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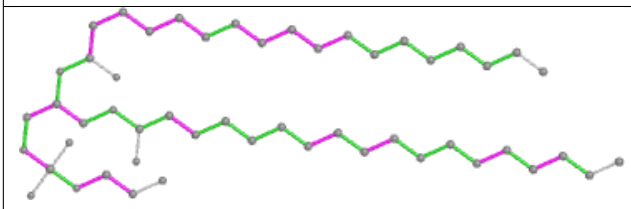
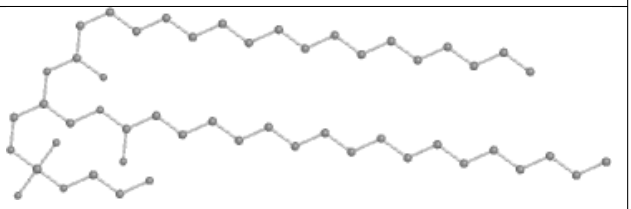


Torsions



Rings

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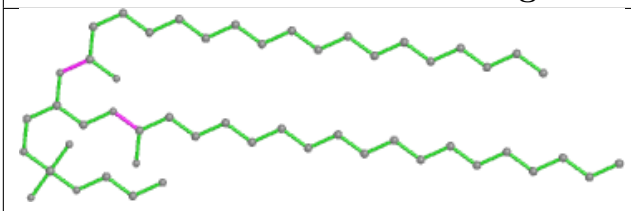

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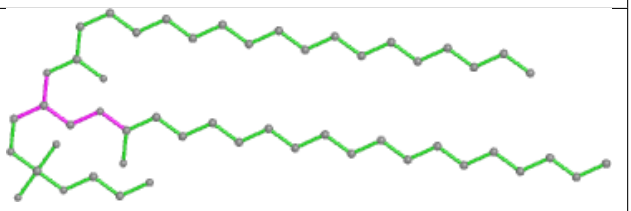
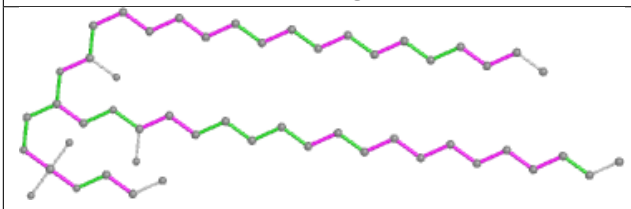


Bond angles



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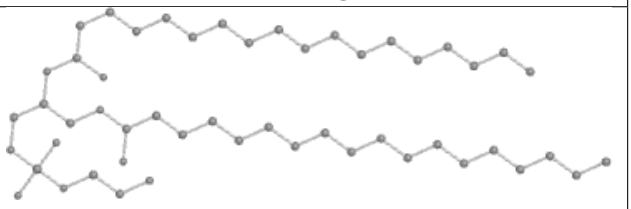
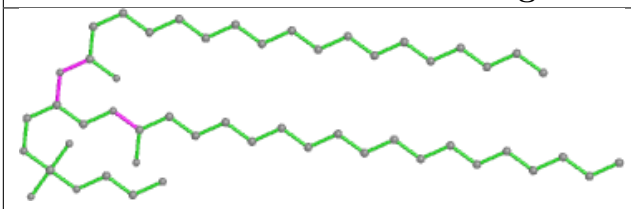
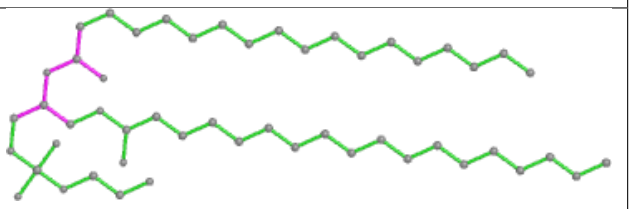


Rings

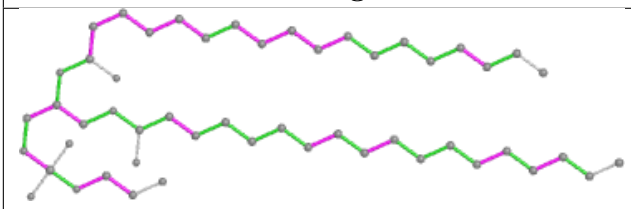
Ligand 3PE G 3012



Bond lengths



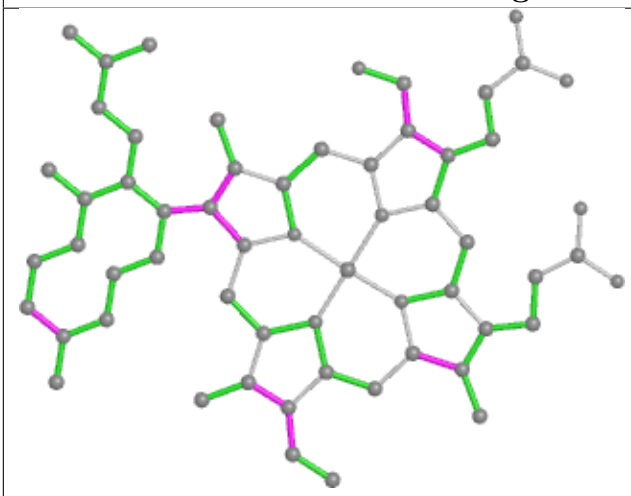
Bond angles



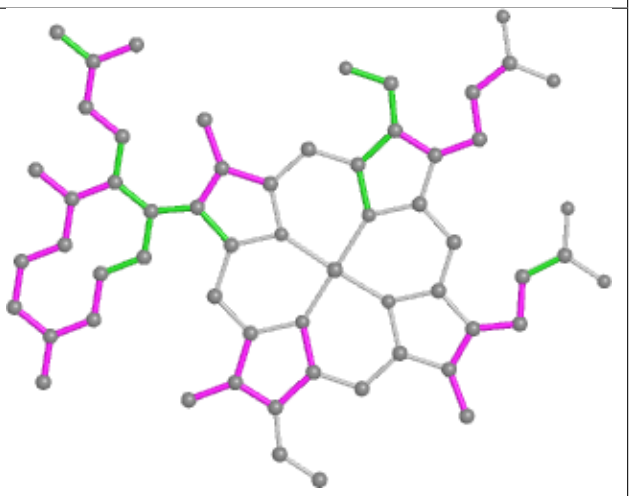
Torsions

Rings

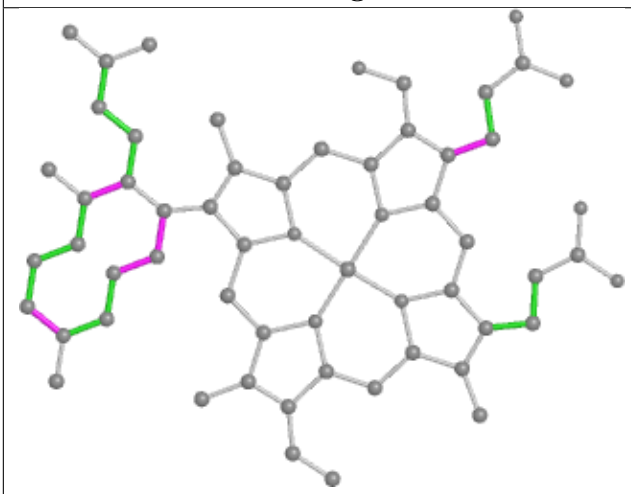
Ligand HEA G 1001



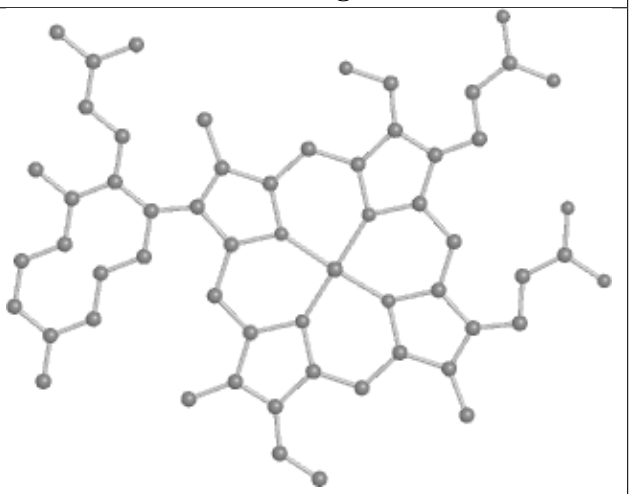
Bond lengths



Bond angles

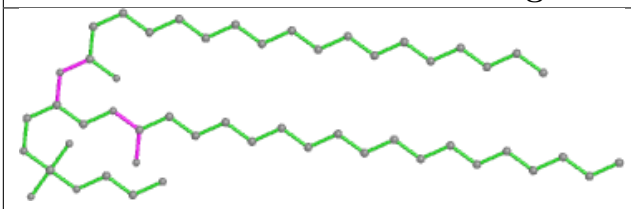


Torsions

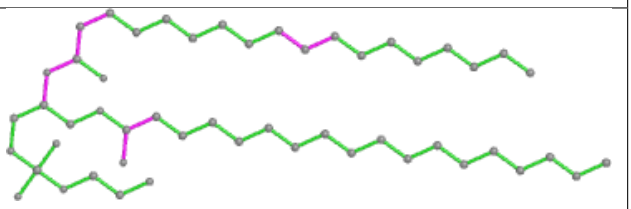


Rings

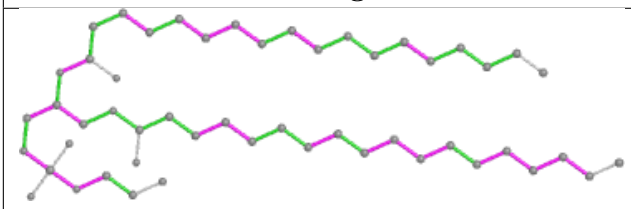
Ligand 3PE I 3013



Bond lengths



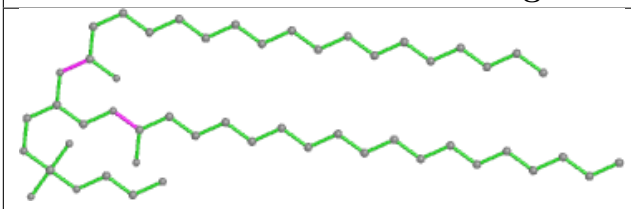
Bond angles



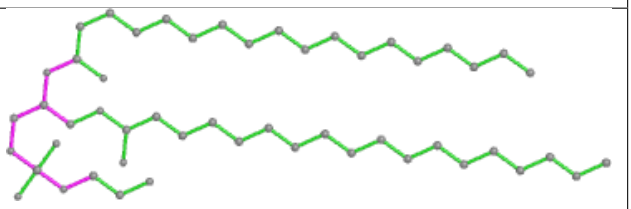
Torsions

Rings

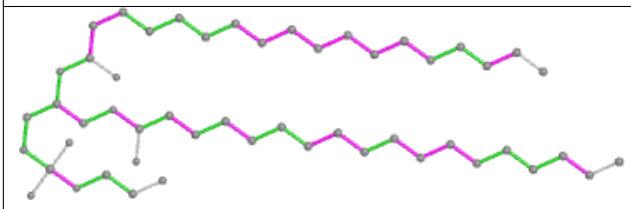
Ligand 3PE J 3011



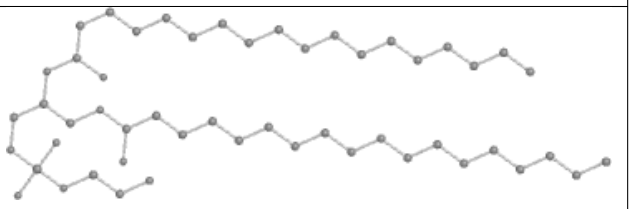
Bond lengths



Bond angles

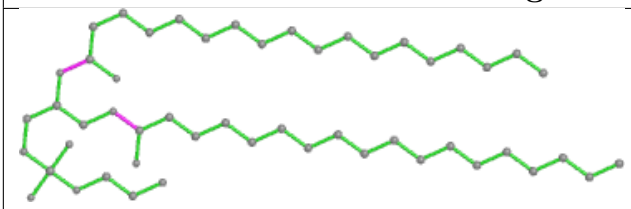


Torsions

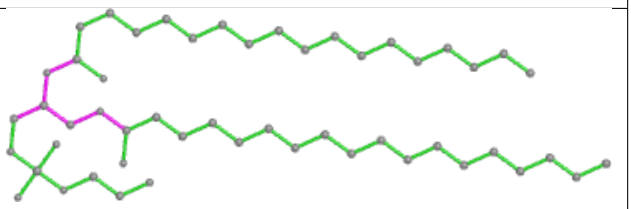


Rings

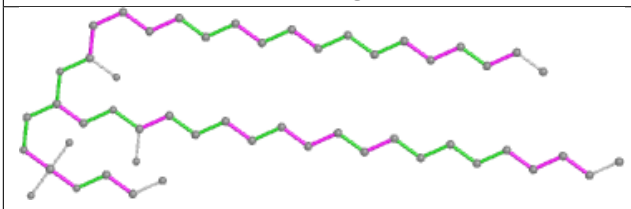
Ligand 3PE I 3010



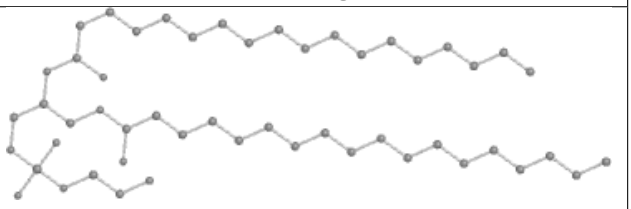
Bond lengths



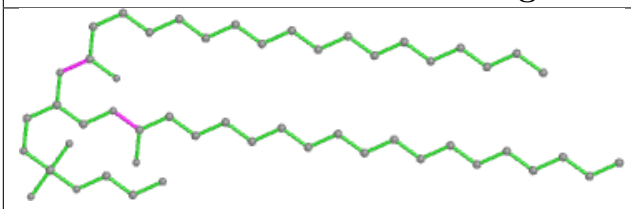
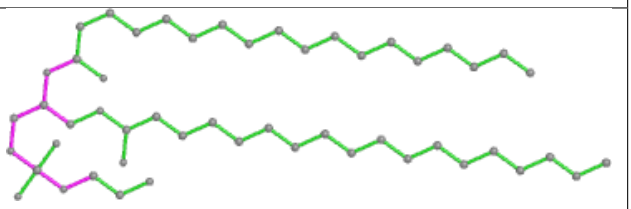
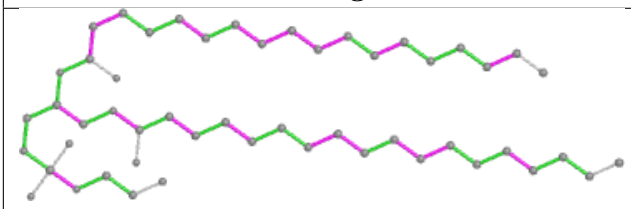
Bond angles



Torsions



Rings

Ligand 3PE D 2011	
 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.