wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 02:56 AM EDT

PDB ID	:	2EIM
Title	:	Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully reduced state
Authors	:	Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2007-03-13
Resolution	:	2.60 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:

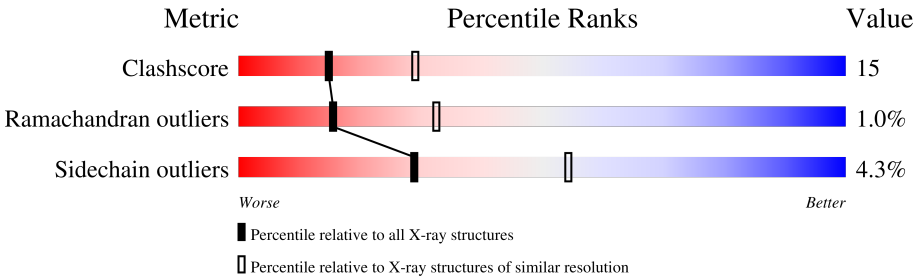
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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	514	71% 27% •
1	N	514	69% 29% •
2	B	227	64% 33% •
2	O	227	62% 34% •
3	C	261	72% 26% ••
3	P	261	68% 30% ••
4	D	147	70% 27% ••
4	Q	147	69% 29% ••

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Mol	Chain	Length	Quality of chain
5	E	109	69% 27%
5	R	109	81% 16%
6	F	98	67% 29%
6	S	98	77% 18%
7	G	85	64% 27% 8%
7	T	85	60% 32% 7%
8	H	85	79% 11% 7%
8	U	85	73% 20% 7%
9	I	73	77% 21%
9	V	73	75% 23%
10	J	59	78% 20%
10	W	59	75% 22%
11	K	56	66% 21% 12%
11	X	56	62% 25% 12%
12	L	47	74% 23%
12	Y	47	68% 28%
13	M	46	63% 26% 7%
13	Z	46	67% 22% 7%

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
20	CHD	C	271	X	-	-	-
20	CHD	J	60	X	-	-	-
20	CHD	W	1060	X	-	-	-
20	CHD	W	1271	X	-	-	-
22	TGL	L	522	-	-	X	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 31961 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 subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Cu	0	0
			1	1		
14	N	1	Total	Cu	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		

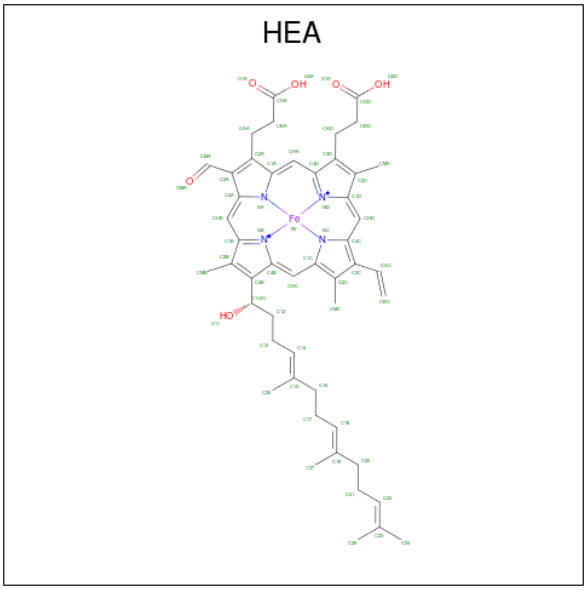
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Zn 1 1	0	0
17	C	1	Total Zn 1 1	0	0
17	F	1	Total Zn 1 1	0	0
17	N	1	Total Zn 1 1	0	0
17	P	1	Total Zn 1 1	0	0
17	S	1	Total Zn 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

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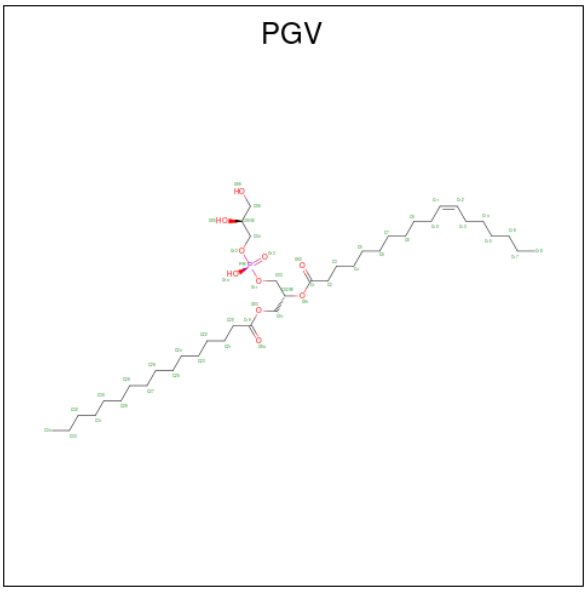
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	O	P		0	0
			51	40	10	1			
19	C	1	Total	C	O	P		0	0
			51	40	10	1			
19	C	1	Total	C	O	P		0	0
			51	40	10	1			
19	C	1	Total	C	O	P		0	0
			51	40	10	1			
19	N	1	Total	C	O	P		0	0
			51	40	10	1			
19	P	1	Total	C	O	P		0	0
			51	40	10	1			
19	P	1	Total	C	O	P		0	0
			51	40	10	1			

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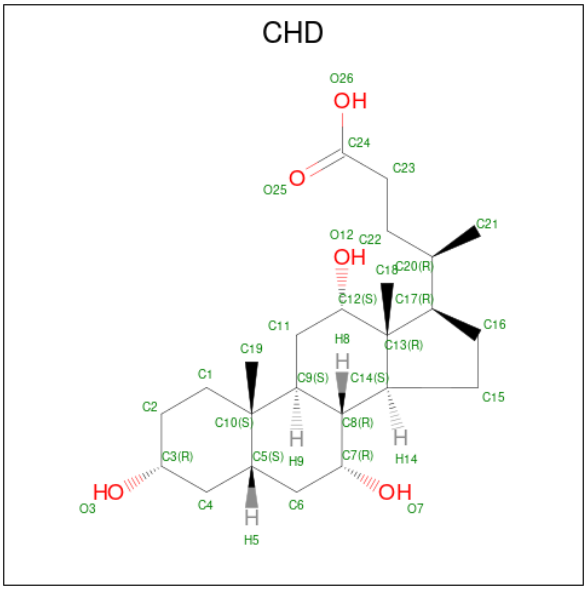
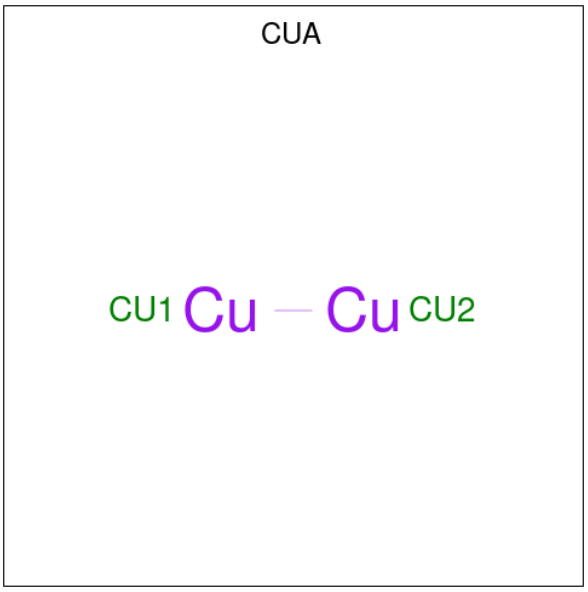
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	P	1	Total C O P 51 40 10 1	0	0

- Molecule 20 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



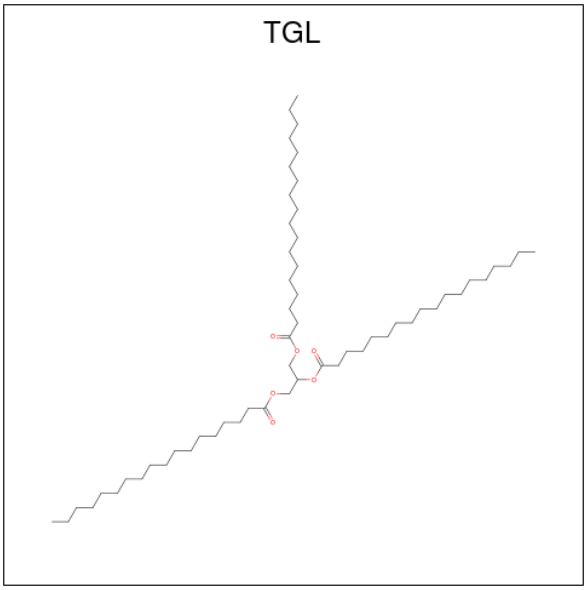
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 29 24 5	0	0
20	B	1	Total C O 29 24 5	0	0
20	C	1	Total C O 29 24 5	0	0
20	J	1	Total C O 29 24 5	0	0
20	N	1	Total C O 29 24 5	0	0
20	P	1	Total C O 29 24 5	0	0
20	W	1	Total C O 29 24 5	0	0
20	W	1	Total C O 29 24 5	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 63 57 6	0	0
22	D	1	Total C O 63 57 6	0	0

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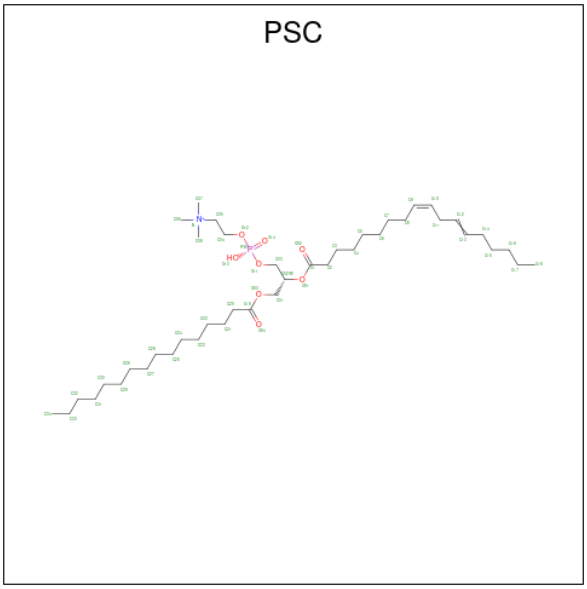
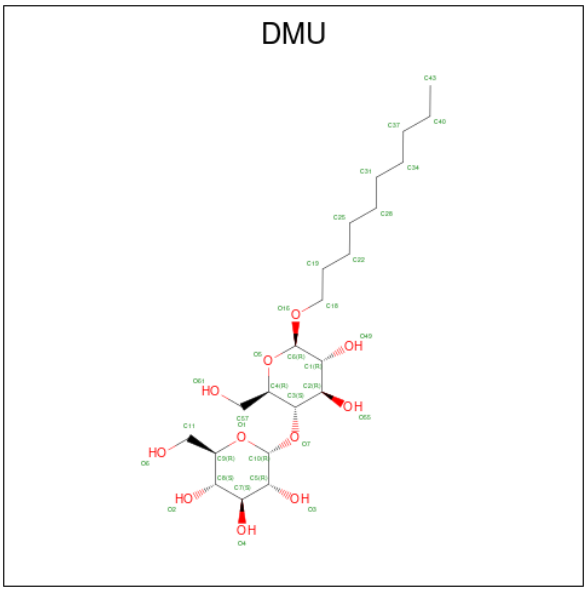
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	L	1	Total C O 63 57 6	0	0
22	N	1	Total C O 63 57 6	0	0
22	N	1	Total C O 63 57 6	0	0
22	O	1	Total C O 63 57 6	0	0

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



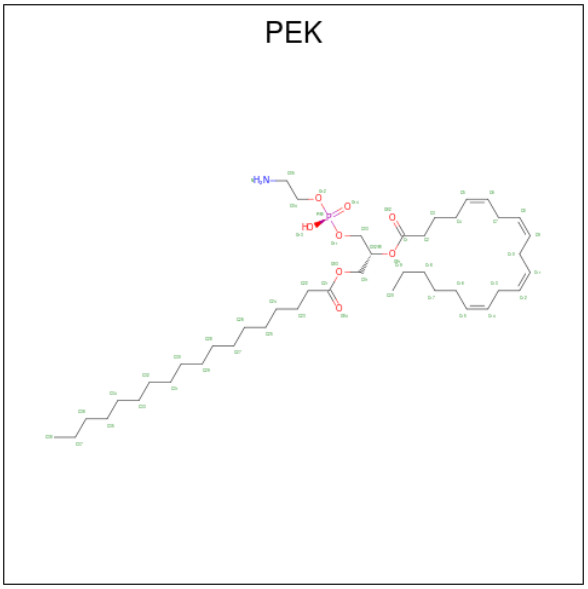
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C N O P 52 42 1 8 1	0	0
23	O	1	Total C N O P 52 42 1 8 1	0	0

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



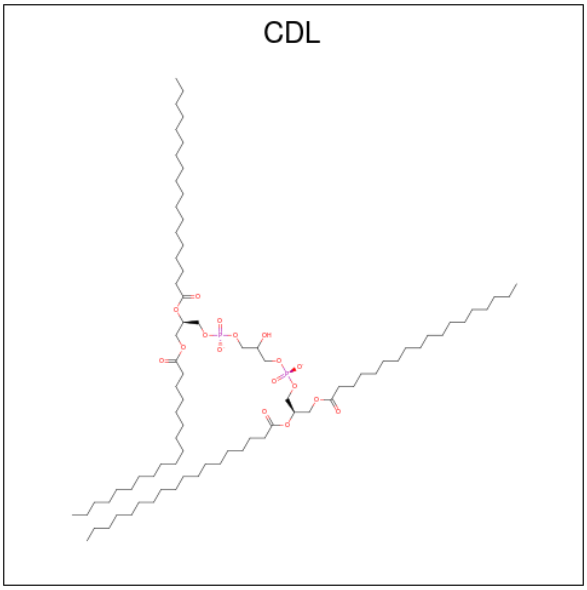
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 33 22 11	0	0
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	182	Total O 182 182	0	0
27	B	96	Total O 96 96	0	0
27	C	82	Total O 82 82	0	0
27	D	61	Total O 61 61	0	0
27	E	43	Total O 43 43	0	0
27	F	52	Total O 52 52	0	0
27	G	37	Total O 37 37	0	0
27	H	35	Total O 35 35	0	0
27	I	22	Total O 22 22	0	0
27	J	12	Total O 12 12	0	0
27	K	12	Total O 12 12	0	0
27	L	13	Total O 13 13	0	0
27	M	13	Total O 13 13	0	0
27	N	171	Total O 171 171	0	0
27	O	79	Total O 79 79	0	0
27	P	73	Total O 73 73	0	0
27	Q	42	Total O 42 42	0	0
27	R	30	Total O 30 30	0	0
27	S	42	Total O 42 42	0	0
27	T	30	Total O 30 30	0	0
27	U	30	Total O 30 30	0	0
27	V	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	W	8	Total O 8 8	0	0
27	X	18	Total O 18 18	0	0
27	Y	14	Total O 14 14	0	0
27	Z	11	Total O 11 11	0	0

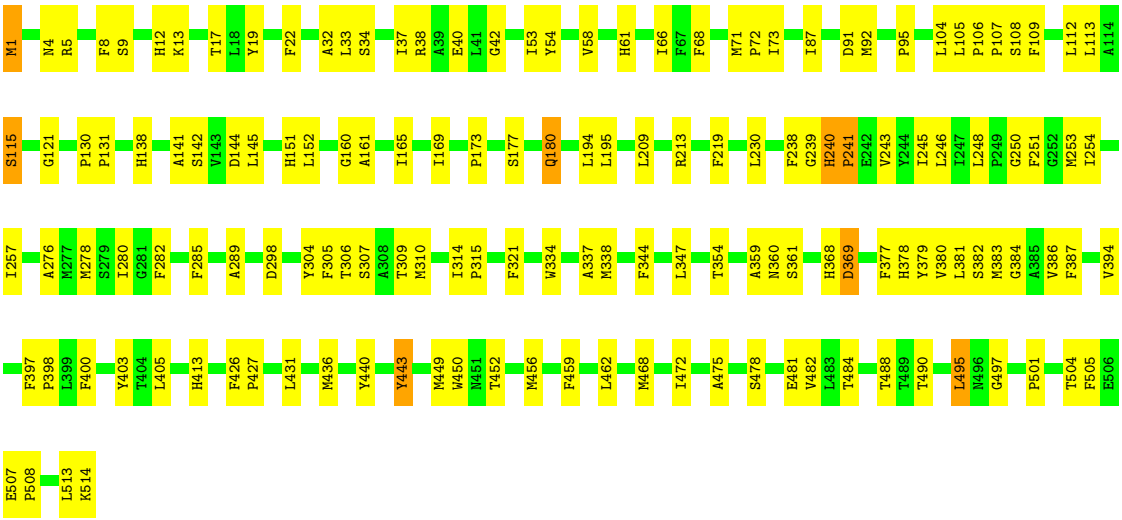
3 Residue-property plots (i)

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.

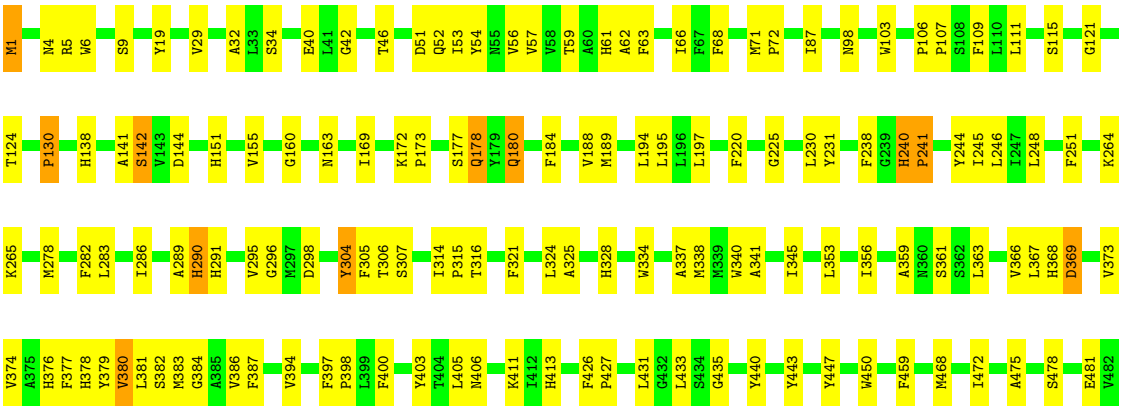
• Molecule 1: Cytochrome c oxidase subunit 1

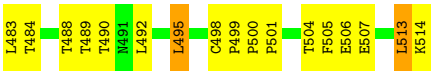
Chain A:



• Molecule 1: Cytochrome c oxidase subunit 1

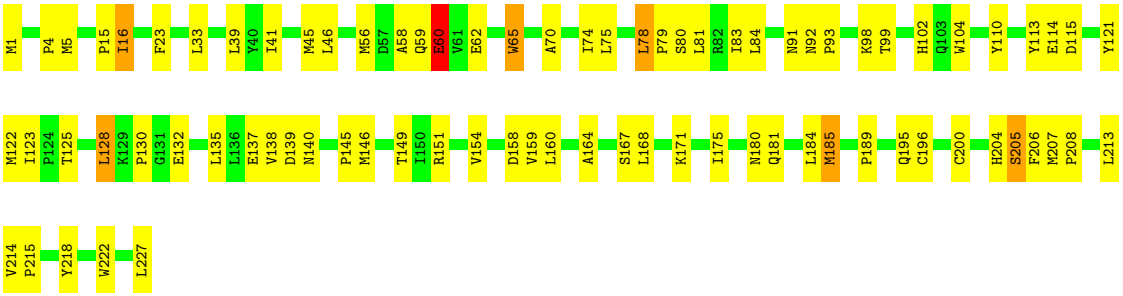
Chain N:





• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

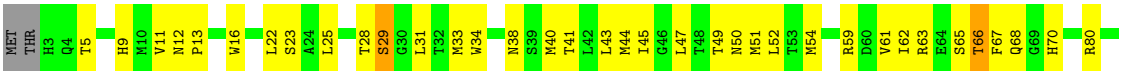
Chain O:

• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

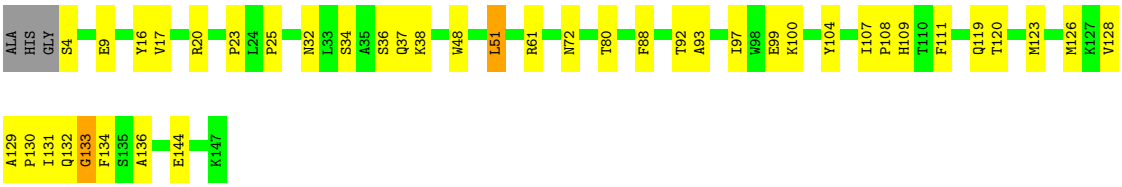
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



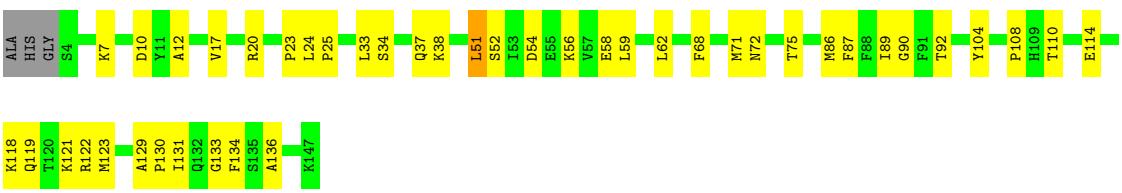
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



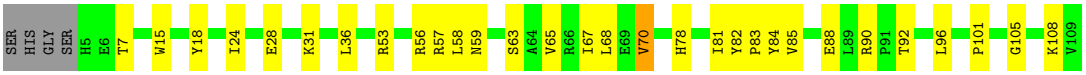
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:

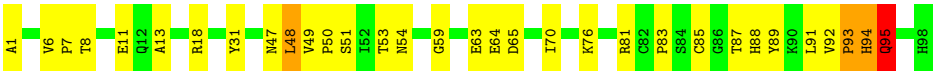


• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:

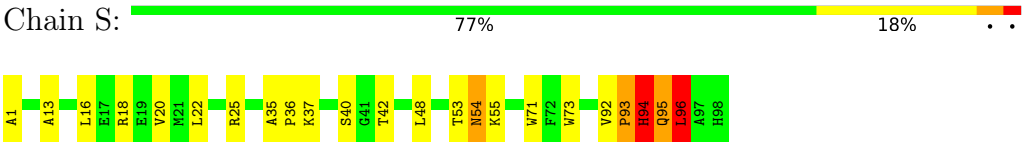
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:



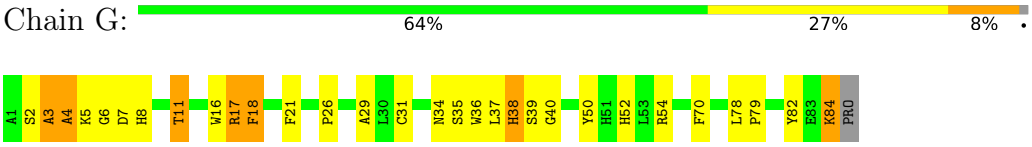
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:



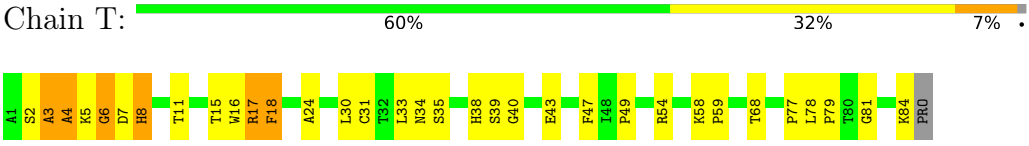
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



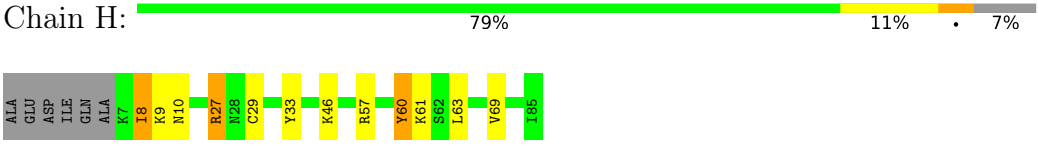
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



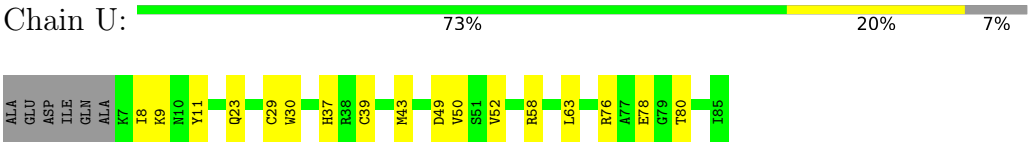
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:



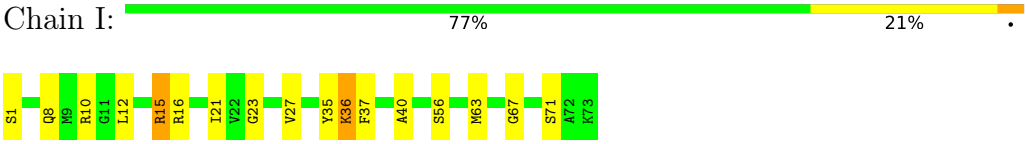
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:



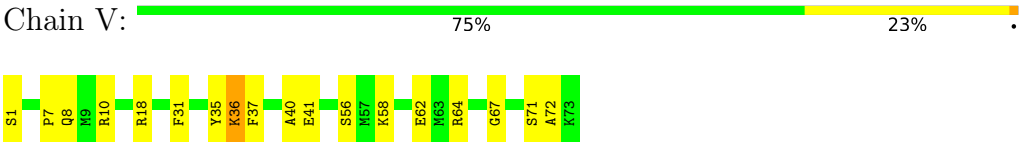
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



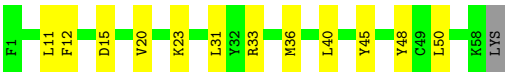
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



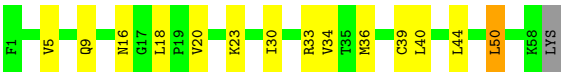
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:



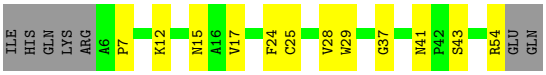
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



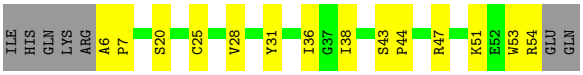
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



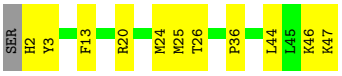
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



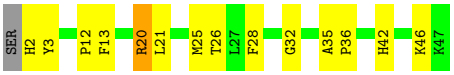
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



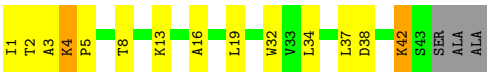
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:


67%
22%
7%


I1
T2
A3
K4
T8
P9
T10
K13
E14
Q15
A16
L19
S25
L34
D38
K42
S43
SER
ALA
ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.91Å 206.72Å 178.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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: TPO, TGL, FME, CHD, CDL, CUA, CU, ZN, PSC, HEA, PGV, MG, PEK, NA, SAC, DMU

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	0/4156	0.78	1/5678 (0.0%)
1	N	0.64	0/4156	0.76	2/5678 (0.0%)
2	B	0.60	0/1860	0.83	1/2534 (0.0%)
2	O	0.59	0/1860	0.83	0/2534
3	C	0.68	0/2197	0.70	0/3005
3	P	0.63	0/2197	0.72	0/3005
4	D	0.60	0/1229	0.73	1/1658 (0.1%)
4	Q	0.64	0/1229	0.71	0/1658
5	E	0.62	0/871	0.73	0/1182
5	R	0.61	0/871	0.75	0/1182
6	F	0.60	0/765	0.86	2/1038 (0.2%)
6	S	0.59	0/765	0.86	2/1038 (0.2%)
7	G	0.61	0/690	0.77	1/937 (0.1%)
7	T	0.63	0/690	0.81	2/937 (0.2%)
8	H	0.64	0/682	0.71	0/921
8	U	0.57	0/682	0.72	0/921
9	I	0.62	0/605	0.70	0/802
9	V	0.60	0/605	0.68	0/802
10	J	0.59	0/471	0.74	0/636
10	W	0.59	0/471	0.73	0/636
11	K	0.71	0/398	0.75	0/546
11	X	0.59	0/398	0.74	0/546
12	L	0.63	0/393	0.69	0/526
12	Y	0.62	0/393	0.67	0/526
13	M	0.57	0/345	0.70	0/470
13	Z	0.60	0/345	0.70	0/470
All	All	0.63	0/29324	0.76	12/39866 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	5
2	B	0	1
2	O	0	1
All	All	0	10

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	94	HIS	N-CA-C	6.74	129.20	111.00
6	F	94	HIS	N-CA-C	6.46	128.43	111.00
2	B	128	LEU	CA-CB-CG	6.03	129.16	115.30
6	S	93	PRO	N-CA-C	5.74	127.02	112.10
7	T	33	LEU	CA-CB-CG	5.72	128.47	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	A	443	TYR	Sidechain
2	B	218	TYR	Sidechain
1	N	19	TYR	Sidechain

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	4027	0	4001	130	0
1	N	4027	0	4001	145	0
2	B	1824	0	1833	66	0
2	O	1824	0	1833	85	0
3	C	2110	0	2027	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2110	0	2027	76	0
4	D	1195	0	1183	34	0
4	Q	1195	0	1183	37	0
5	E	852	0	845	23	0
5	R	852	0	845	11	0
6	F	748	0	728	24	0
6	S	748	0	728	16	0
7	G	675	0	644	35	0
7	T	675	0	644	40	0
8	H	662	0	623	8	0
8	U	662	0	623	14	0
9	I	601	0	613	14	0
9	V	601	0	613	16	0
10	J	460	0	459	12	0
10	W	460	0	459	11	0
11	K	384	0	366	8	0
11	X	384	0	366	9	0
12	L	380	0	380	21	0
12	Y	380	0	380	14	0
13	M	335	0	352	10	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	F	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
17	S	1	0	0	0	0
18	A	120	0	108	9	0
18	N	120	0	108	12	0
19	A	51	0	76	7	0
19	C	153	0	228	12	0
19	N	51	0	76	10	0
19	P	153	0	228	11	0
20	A	29	0	39	1	0
20	B	29	0	39	1	0
20	C	29	0	39	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	29	0	37	5	0
20	N	29	0	39	2	0
20	P	29	0	39	2	0
20	W	58	0	76	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	6	0
22	D	63	0	110	5	0
22	L	63	0	110	27	0
22	N	126	0	220	22	0
22	O	63	0	110	8	0
23	B	52	0	80	19	0
23	O	52	0	80	18	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	37	4	0
24	Z	33	0	38	0	0
25	C	106	0	154	17	0
25	G	53	0	77	9	0
25	P	106	0	154	18	0
25	T	53	0	77	14	0
26	C	100	0	156	19	0
26	G	100	0	156	22	0
26	P	100	0	156	13	0
26	T	100	0	156	23	0
27	A	182	0	0	9	0
27	B	96	0	0	2	0
27	C	82	0	0	5	0
27	D	61	0	0	7	0
27	E	43	0	0	4	0
27	F	52	0	0	5	0
27	G	37	0	0	1	0
27	H	35	0	0	1	0
27	I	22	0	0	2	0
27	J	12	0	0	1	0
27	K	12	0	0	2	0
27	L	13	0	0	0	0
27	M	13	0	0	2	0
27	N	171	0	0	14	0
27	O	79	0	0	4	0
27	P	73	0	0	0	0
27	Q	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	R	30	0	0	2	0
27	S	42	0	0	0	0
27	T	30	0	0	3	0
27	U	30	0	0	0	0
27	V	19	0	0	3	0
27	W	8	0	0	0	0
27	X	18	0	0	1	0
27	Y	14	0	0	0	0
27	Z	11	0	0	2	0
All	All	31961	0	31295	945	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 15.

The worst 5 of 945 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)
10:W:33:ARG:HG2	20:W:1060:CHD:H152	1.29	1.14
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.19	1.07
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.30	0.97
23:O:1230:PSC:H142	23:O:1230:PSC:H343	1.46	0.97
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.49	0.95

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	512/514 (100%)	488 (95%)	24 (5%)	0	100 100
1	N	512/514 (100%)	484 (94%)	27 (5%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	225/227 (99%)	210 (93%)	10 (4%)	5 (2%)	6 12
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	12 24
3	C	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	34 57
3	P	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	34 57
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100 100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100 100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100 100
5	R	103/109 (94%)	94 (91%)	9 (9%)	0	100 100
6	F	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	4 6
6	S	96/98 (98%)	85 (88%)	7 (7%)	4 (4%)	3 3
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1 0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1 1
8	H	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	12 24
8	U	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	12 24
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11 22
9	V	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11 22
10	J	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8 16
10	W	56/59 (95%)	52 (93%)	4 (7%)	0	100 100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100 100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100 100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100 100
All	All	3504/3614 (97%)	3279 (94%)	189 (5%)	36 (1%)	15 32

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
7	G	39	SER
6	S	94	HIS

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	426/426 (100%)	413 (97%)	13 (3%)	40 66
1	N	426/426 (100%)	411 (96%)	15 (4%)	36 62
2	B	210/210 (100%)	196 (93%)	14 (7%)	16 33
2	O	210/210 (100%)	200 (95%)	10 (5%)	25 49
3	C	224/226 (99%)	213 (95%)	11 (5%)	25 48
3	P	224/226 (99%)	216 (96%)	8 (4%)	35 61
4	D	128/129 (99%)	125 (98%)	3 (2%)	50 75
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40 66
5	E	92/95 (97%)	89 (97%)	3 (3%)	38 64
5	R	92/95 (97%)	91 (99%)	1 (1%)	73 88
6	F	81/81 (100%)	78 (96%)	3 (4%)	34 60
6	S	81/81 (100%)	75 (93%)	6 (7%)	13 28
7	G	67/68 (98%)	60 (90%)	7 (10%)	7 13
7	T	67/68 (98%)	62 (92%)	5 (8%)	13 27
8	H	71/75 (95%)	67 (94%)	4 (6%)	21 42
8	U	71/75 (95%)	70 (99%)	1 (1%)	67 85
9	I	57/57 (100%)	55 (96%)	2 (4%)	36 62
9	V	57/57 (100%)	56 (98%)	1 (2%)	59 80
10	J	49/50 (98%)	49 (100%)	0	100 100
10	W	49/50 (98%)	48 (98%)	1 (2%)	55 78
11	K	39/46 (85%)	38 (97%)	1 (3%)	46 72
11	X	39/46 (85%)	36 (92%)	3 (8%)	13 25
12	L	39/40 (98%)	37 (95%)	2 (5%)	24 46
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46 72
13	M	37/38 (97%)	30 (81%)	7 (19%)	1 2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3040/3082 (99%)	2910 (96%)	130 (4%)	29 54

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	18	PHE
8	U	29	CYS
7	G	18	PHE
7	G	17	ARG
10	W	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	512	ASN
3	P	68	GLN
2	O	10	GLN
3	P	3	HIS
3	P	243	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	2.86	2 (28%)	8,9,11	3.22	5 (62%)
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	2.28	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	TPO	G	11	7	8,10,11	1.68	2 (25%)	10,14,16	0.95	0
2	FME	B	1	2	8,9,10	1.01	0	7,9,11	1.66	2 (28%)
1	FME	A	1	1	8,9,10	0.76	0	7,9,11	1.25	1 (14%)
1	FME	N	1	1	8,9,10	0.87	0	7,9,11	1.26	1 (14%)
7	TPO	T	11	7	8,10,11	1.39	1 (12%)	10,14,16	1.03	0
9	SAC	I	1	9	7,8,9	2.53	2 (28%)	8,9,11	2.92	3 (37%)

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	SAC	V	1	9	-	3/7/8/10	-
2	FME	O	1	2	-	2/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	3/7/8/10	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.46	1.35	1.23
9	I	1	SAC	OAC-C1A	5.21	1.35	1.23
9	V	1	SAC	CA-N	4.51	1.52	1.46
9	I	1	SAC	CA-N	3.85	1.51	1.46
7	G	11	TPO	CB-CA	3.04	1.60	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	CA-N-C1A	-7.18	109.91	123.15
9	I	1	SAC	CA-N-C1A	-6.40	111.34	123.15
2	O	1	FME	C-CA-N	4.73	118.27	109.73
2	O	1	FME	CA-N-CN	-3.50	117.45	122.82
9	I	1	SAC	CB-CA-N	3.19	117.71	110.55

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
1	A	1	FME	2	0
1	N	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
22	TGL	N	1522	-	62,62,62	1.49	6 (9%)	65,65,65	1.64	10 (15%)
19	PGV	P	1266	-	50,50,50	1.36	6 (12%)	53,56,56	1.04	4 (7%)
20	CHD	J	60	-	32,32,32	1.90	10 (31%)	51,51,51	3.97	28 (54%)
22	TGL	L	522	-	62,62,62	1.35	5 (8%)	65,65,65	1.68	12 (18%)
24	DMU	Z	1526	-	34,34,34	3.25	8 (23%)	45,45,45	3.95	20 (44%)
19	PGV	C	268	-	50,50,50	1.45	7 (14%)	53,56,56	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	A	524	-	50,50,50	1.26	5 (10%)	53,56,56	0.82	1 (1%)
19	PGV	C	267	-	50,50,50	1.04	3 (6%)	53,56,56	1.05	5 (9%)
20	CHD	W	1271	-	32,32,32	1.31	4 (12%)	51,51,51	3.53	25 (49%)
22	TGL	N	1523	-	62,62,62	0.96	3 (4%)	65,65,65	1.25	7 (10%)
22	TGL	D	523	-	62,62,62	1.01	3 (4%)	65,65,65	1.30	9 (13%)
20	CHD	W	1060	-	32,32,32	2.04	8 (25%)	51,51,51	4.02	28 (54%)
25	PEK	C	265	-	52,52,52	1.75	11 (21%)	55,57,57	1.21	7 (12%)
25	PEK	P	1265	-	52,52,52	1.78	11 (21%)	55,57,57	1.19	7 (12%)
19	PGV	N	1524	-	50,50,50	1.23	5 (10%)	53,56,56	0.89	1 (1%)
20	CHD	P	1525	-	32,32,32	1.03	2 (6%)	51,51,51	2.59	23 (45%)
18	HEA	A	515	1	57,67,67	1.47	7 (12%)	61,103,103	1.64	14 (22%)
18	HEA	N	515	1	57,67,67	1.33	7 (12%)	61,103,103	1.76	15 (24%)
23	PSC	O	1230	-	51,51,51	1.52	7 (13%)	57,59,59	0.98	1 (1%)
24	DMU	P	1272	-	34,34,34	2.70	15 (44%)	45,45,45	3.95	17 (37%)
25	PEK	P	1264	-	52,52,52	1.65	8 (15%)	55,57,57	1.37	7 (12%)
26	CDL	T	1269	-	99,99,99	1.25	11 (11%)	105,111,111	0.99	7 (6%)
24	DMU	M	526	-	34,34,34	3.36	9 (26%)	45,45,45	3.94	21 (46%)
18	HEA	N	516	1	57,67,67	1.30	8 (14%)	61,103,103	1.43	10 (16%)
21	CUA	O	228	2	0,1,1	-	-	-		
20	CHD	B	1086	-	32,32,32	0.85	0	51,51,51	2.46	20 (39%)
22	TGL	O	1521	-	62,62,62	1.11	5 (8%)	65,65,65	1.46	8 (12%)
18	HEA	A	516	1	57,67,67	1.39	7 (12%)	61,103,103	1.38	9 (14%)
25	PEK	G	1263	-	52,52,52	2.08	11 (21%)	55,57,57	1.29	4 (7%)
22	TGL	B	521	-	62,62,62	1.08	3 (4%)	65,65,65	1.46	8 (12%)
20	CHD	N	1604	-	32,32,32	0.97	2 (6%)	51,51,51	2.41	17 (33%)
26	CDL	C	270	-	99,99,99	1.07	8 (8%)	105,111,111	1.09	9 (8%)
25	PEK	T	263	-	52,52,52	2.12	12 (23%)	55,57,57	1.32	4 (7%)
20	CHD	A	525	-	32,32,32	0.99	1 (3%)	51,51,51	2.48	18 (35%)
19	PGV	C	266	-	50,50,50	1.17	5 (10%)	53,56,56	0.95	2 (3%)
26	CDL	P	1270	-	99,99,99	1.21	9 (9%)	105,111,111	1.09	5 (4%)
23	PSC	B	230	-	51,51,51	1.40	6 (11%)	57,59,59	1.00	2 (3%)
21	CUA	B	228	2	0,1,1	-	-	-		
19	PGV	P	1267	-	50,50,50	0.96	3 (6%)	53,56,56	1.02	4 (7%)
20	CHD	C	271	-	32,32,32	1.36	3 (9%)	51,51,51	3.62	24 (47%)
25	PEK	C	264	-	52,52,52	1.45	6 (11%)	55,57,57	1.24	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	P	1268	-	50,50,50	1.43	5 (10%)	53,56,56	0.87	1 (1%)
24	DMU	C	272	-	34,34,34	2.64	16 (47%)	45,45,45	3.99	18 (40%)
26	CDL	G	269	-	99,99,99	1.25	9 (9%)	105,111,111	0.98	8 (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
22	TGL	N	1522	-	-	19/65/65/65	-
19	PGV	P	1266	-	-	15/55/55/55	-
20	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
22	TGL	L	522	-	-	19/65/65/65	-
24	DMU	Z	1526	-	5/5/10/10	8/19/59/59	0/2/2/2
19	PGV	C	268	-	-	34/55/55/55	-
20	CHD	W	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	A	524	-	-	35/55/55/55	-
19	PGV	C	267	-	-	17/55/55/55	-
22	TGL	N	1523	-	-	15/65/65/65	-
22	TGL	D	523	-	-	15/65/65/65	-
20	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	C	265	-	-	21/56/56/56	-
25	PEK	P	1265	-	-	20/56/56/56	-
19	PGV	N	1524	-	-	35/55/55/55	-
20	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
18	HEA	A	515	1	-	7/32/76/76	-
18	HEA	N	515	1	-	7/32/76/76	-
23	PSC	O	1230	-	-	37/55/55/55	-
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
25	PEK	P	1264	-	-	24/56/56/56	-
26	CDL	T	1269	-	-	62/110/110/110	-
24	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
18	HEA	N	516	1	-	5/32/76/76	-
25	PEK	G	1263	-	-	29/56/56/56	-
20	CHD	B	1086	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	TGL	O	1521	-	-	14/65/65/65	-
18	HEA	A	516	1	-	5/32/76/76	-
22	TGL	B	521	-	-	14/65/65/65	-
20	CHD	N	1604	-	-	3/9/74/74	0/4/4/4
26	CDL	C	270	-	-	68/110/110/110	-
25	PEK	T	263	-	-	29/56/56/56	-
20	CHD	A	525	-	-	2/9/74/74	0/4/4/4
19	PGV	C	266	-	-	16/55/55/55	-
26	CDL	P	1270	-	-	69/110/110/110	-
23	PSC	B	230	-	-	37/55/55/55	-
19	PGV	P	1267	-	-	17/55/55/55	-
20	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	C	264	-	-	23/56/56/56	-
19	PGV	P	1268	-	-	35/55/55/55	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
26	CDL	G	269	-	-	62/110/110/110	-

The worst 5 of 280 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.58	1.21	1.43
24	M	526	DMU	O16-C6	-7.92	1.26	1.40
24	Z	1526	DMU	O7-C3	-7.78	1.23	1.43
24	Z	1526	DMU	O1-C9	-7.52	1.26	1.44
24	M	526	DMU	O1-C9	-7.50	1.26	1.44

The worst 5 of 443 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	1272	DMU	O16-C6-C1	11.86	126.82	108.30
24	C	272	DMU	O16-C6-C1	10.72	125.04	108.30
24	M	526	DMU	C1-C2-C3	9.86	132.19	109.68
24	Z	1526	DMU	C1-C2-C3	9.75	131.95	109.68
20	C	271	CHD	C10-C9-C8	9.68	122.21	111.82

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	C	271	CHD	C14
20	C	271	CHD	C3
20	C	271	CHD	C12
20	C	271	CHD	C9
20	C	271	CHD	C8

5 of 883 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C14-C15-C16-C17
18	A	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C14-C15-C16-C17
18	N	515	HEA	C26-C15-C16-C17
19	A	524	PGV	C04-O12-P-O11

There are no ring outliers.

41 monomers are involved in 312 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	1522	TGL	15	0
19	P	1266	PGV	2	0
20	J	60	CHD	5	0
22	L	522	TGL	27	0
19	C	268	PGV	2	0
19	A	524	PGV	7	0
19	C	267	PGV	7	0
20	W	1271	CHD	2	0
22	N	1523	TGL	7	0
22	D	523	TGL	5	0
20	W	1060	CHD	3	0
25	C	265	PEK	11	0
25	P	1265	PEK	9	0
19	N	1524	PGV	10	0
20	P	1525	CHD	2	0
18	A	515	HEA	4	0
18	N	515	HEA	4	0
23	O	1230	PSC	18	0
24	P	1272	DMU	4	0
25	P	1264	PEK	9	0
26	T	1269	CDL	23	0
24	M	526	DMU	1	0
18	N	516	HEA	8	0
20	B	1086	CHD	1	0

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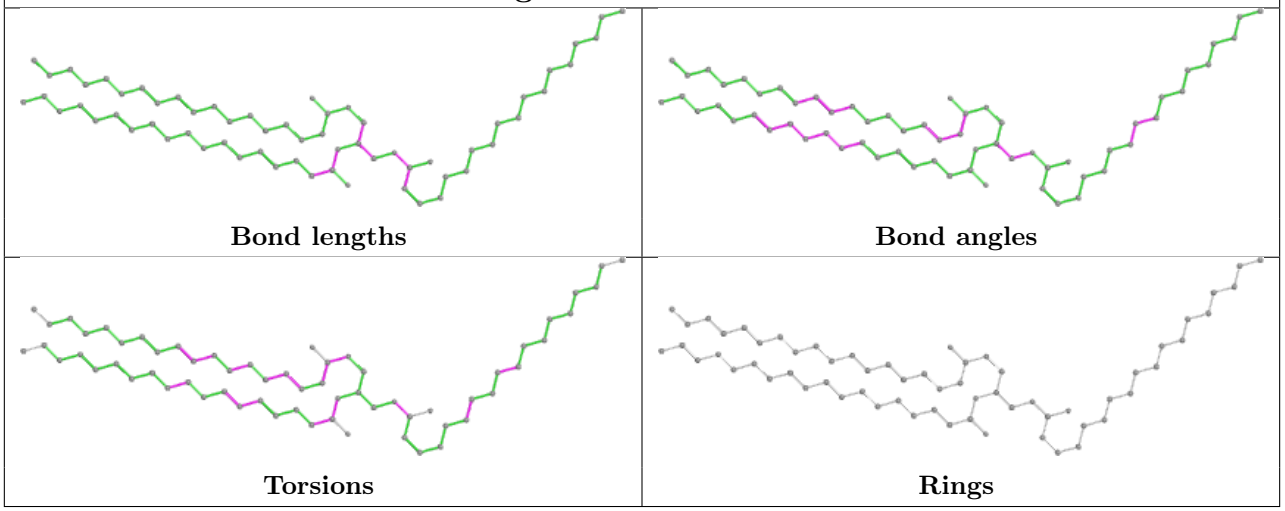
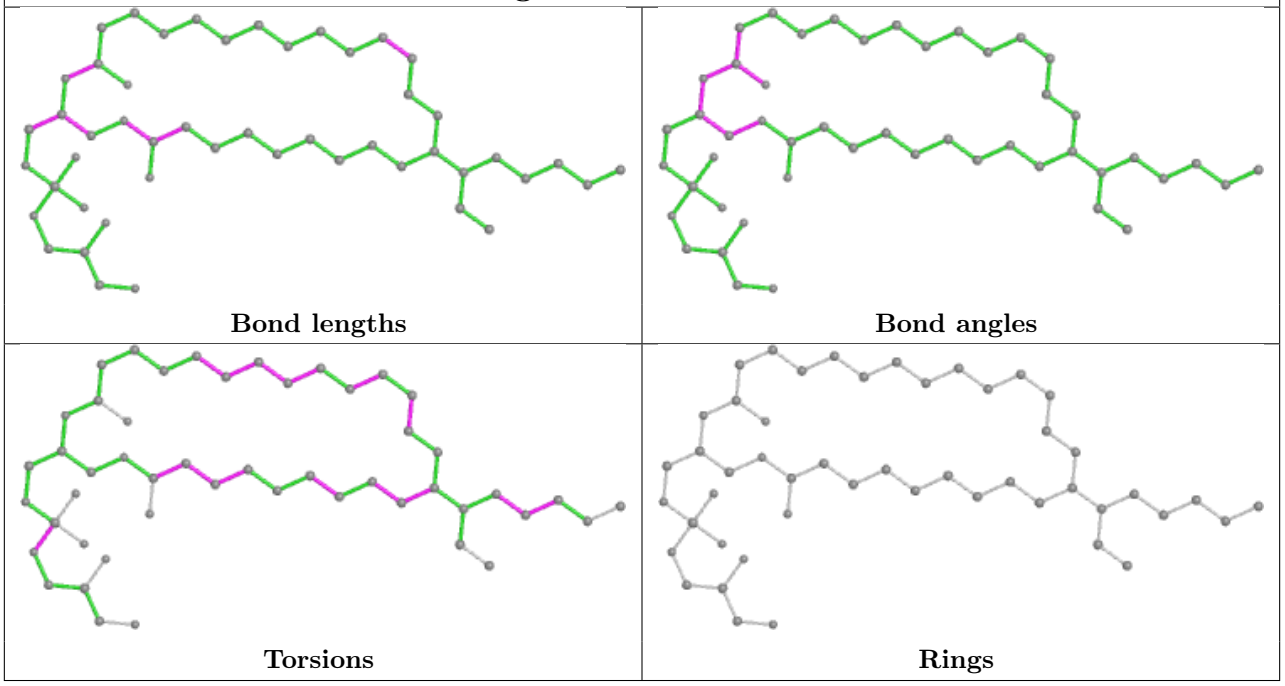
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	1521	TGL	8	0
18	A	516	HEA	5	0
25	G	1263	PEK	9	0
22	B	521	TGL	6	0
20	N	1604	CHD	2	0
26	C	270	CDL	19	0
25	T	263	PEK	14	0
20	A	525	CHD	1	0
19	C	266	PGV	3	0
26	P	1270	CDL	13	0
23	B	230	PSC	19	0
19	P	1267	PGV	8	0
20	C	271	CHD	2	0
25	C	264	PEK	6	0
19	P	1268	PGV	1	0
24	C	272	DMU	3	0
26	G	269	CDL	22	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.

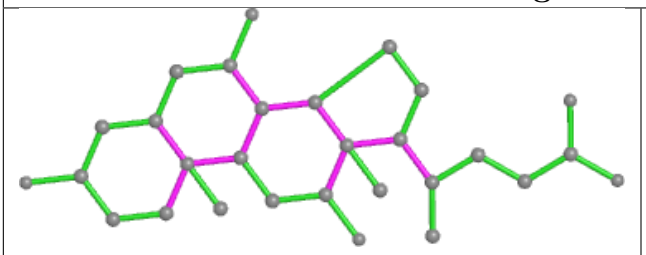
Ligand TGL N 1522



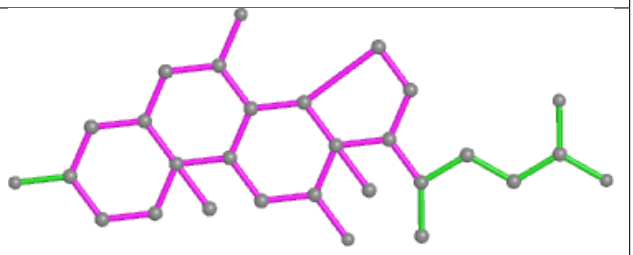
Ligand PGV P 1266



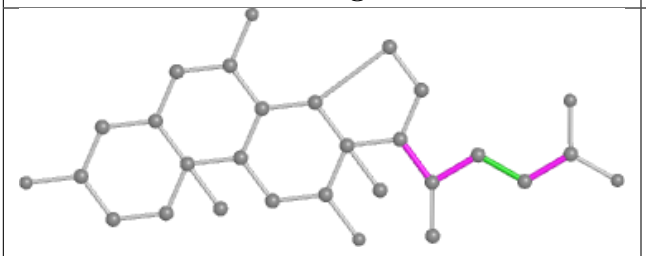
Ligand CHD J 60



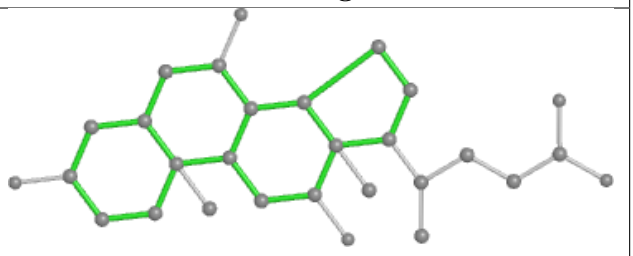
Bond lengths



Bond angles

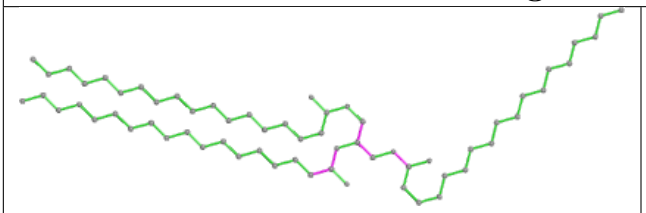


Torsions

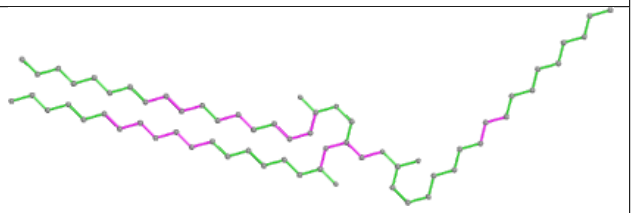


Rings

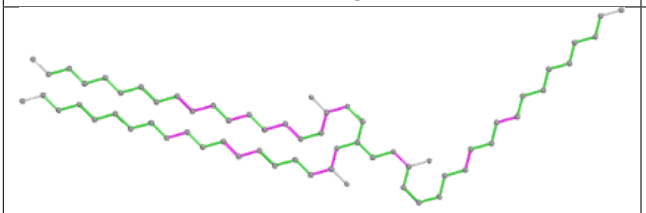
Ligand TGL L 522



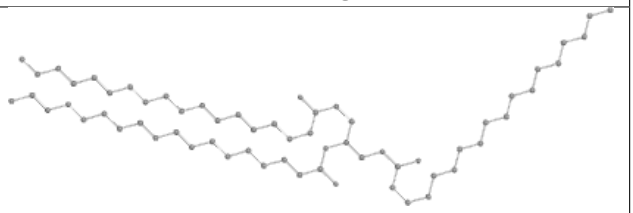
Bond lengths



Bond angles

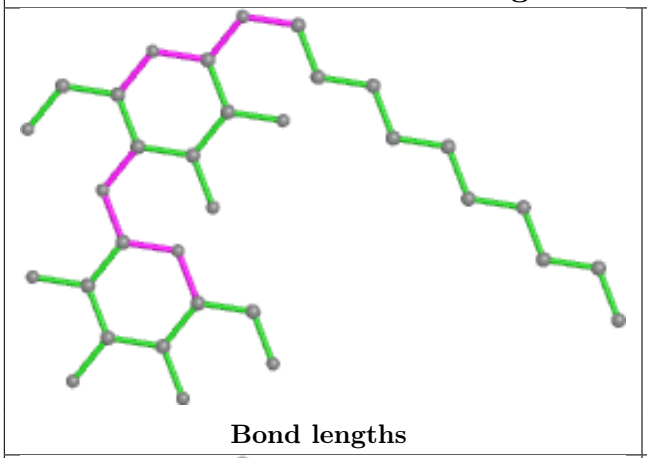


Torsions

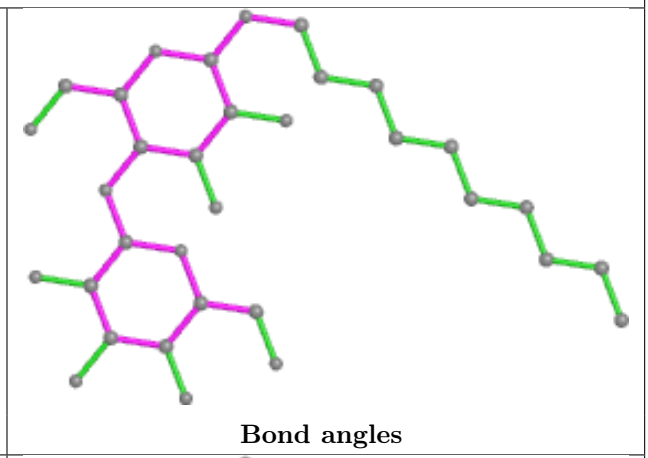


Rings

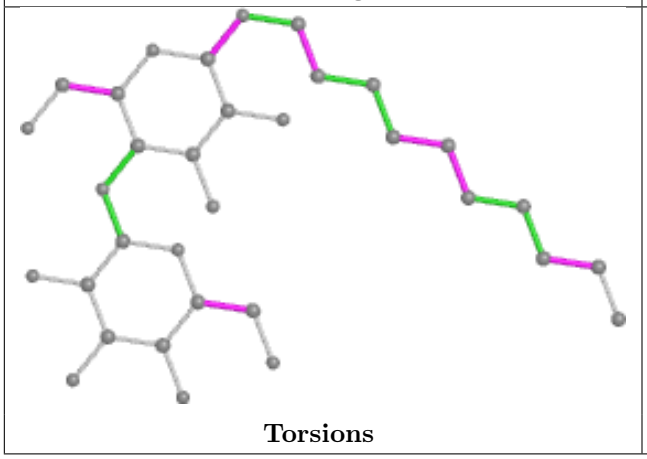
Ligand DMU Z 1526



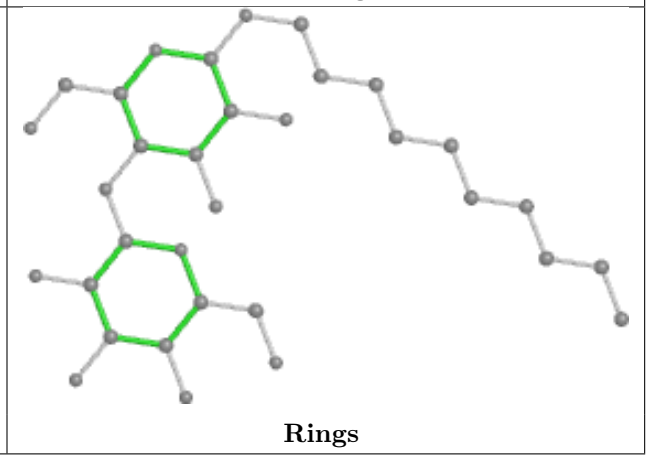
Bond lengths



Bond angles

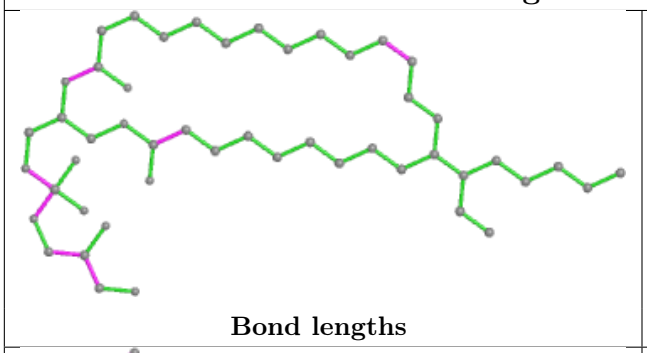


Torsions



Rings

Ligand PGV C 268



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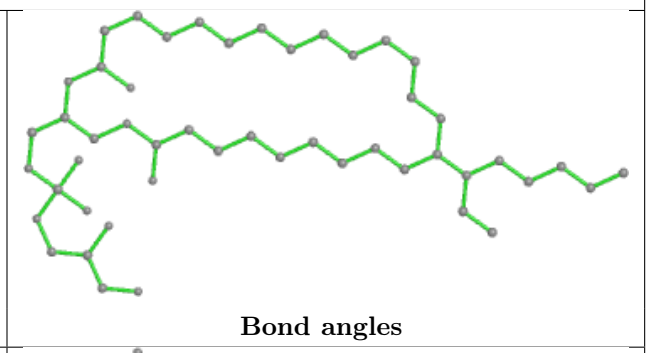
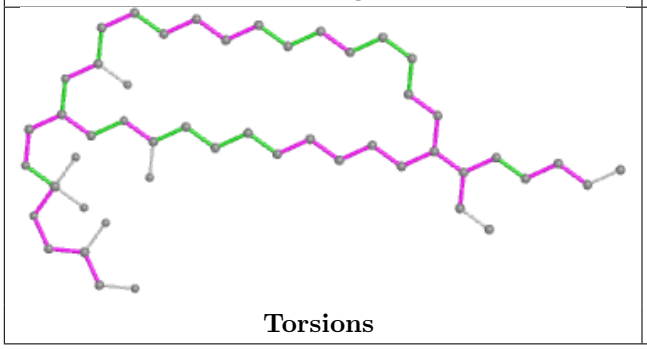
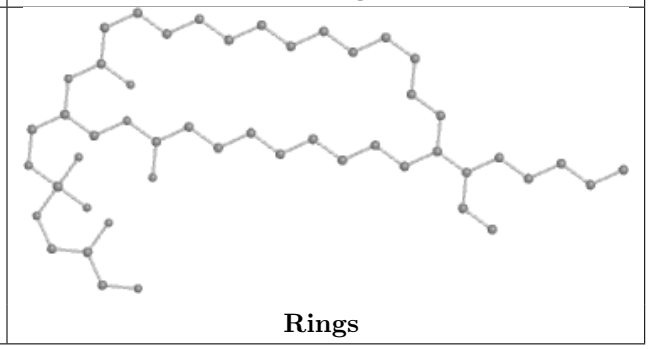


Bond angles

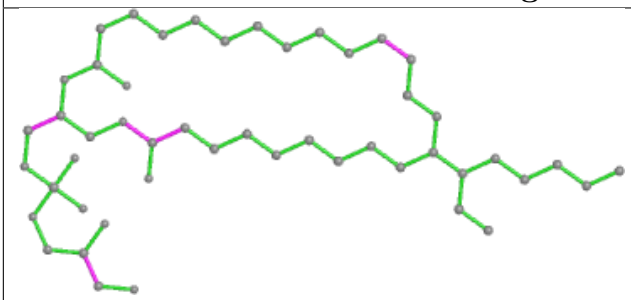


Torsions



Rings

Ligand PGV A 524



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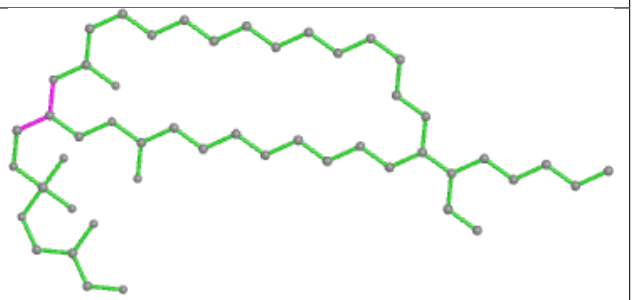
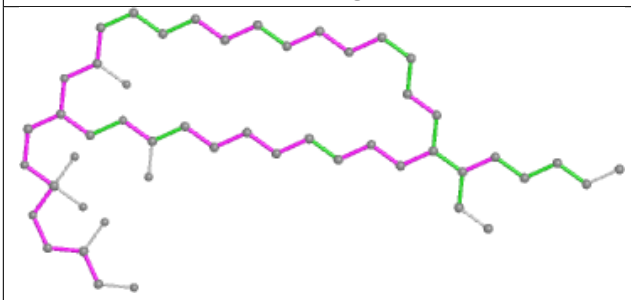
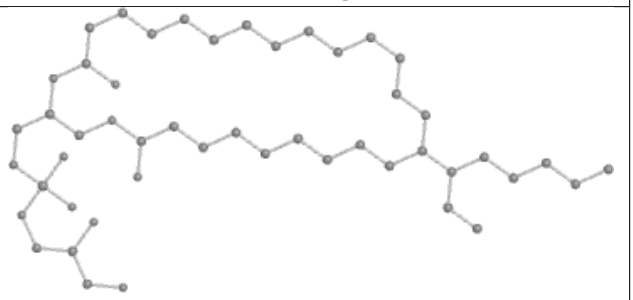


Bond angles

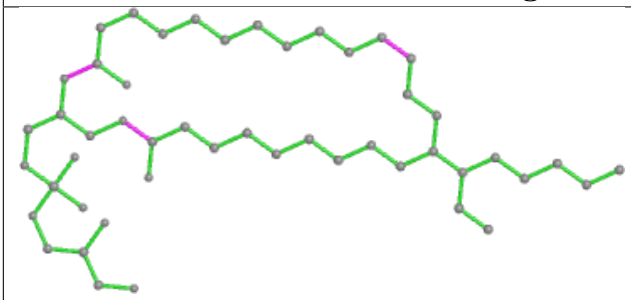


Torsions



Rings

Ligand PGV C 267



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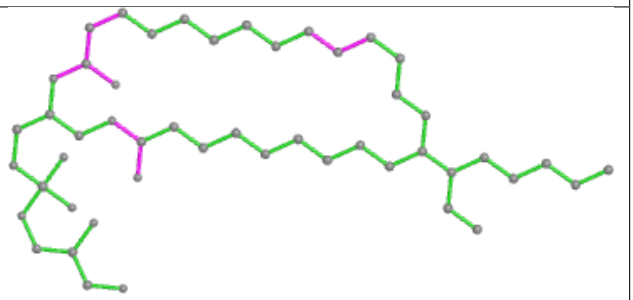
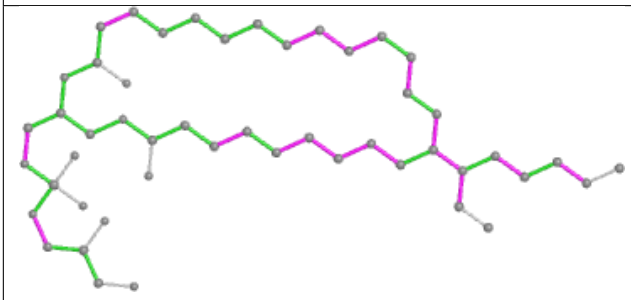
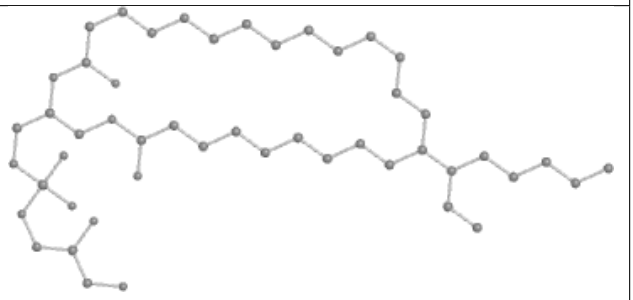


Bond angles

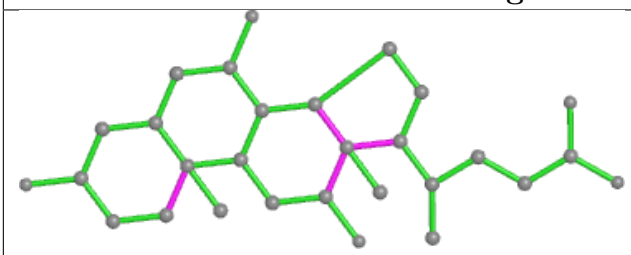


Torsions



Rings

Ligand CHD W 1271



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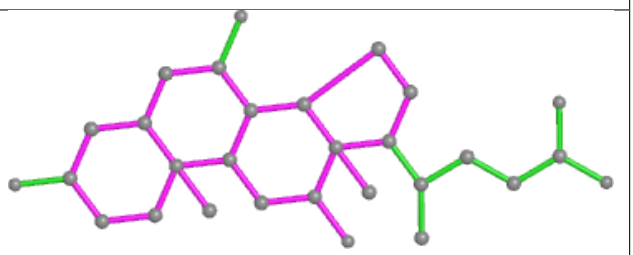
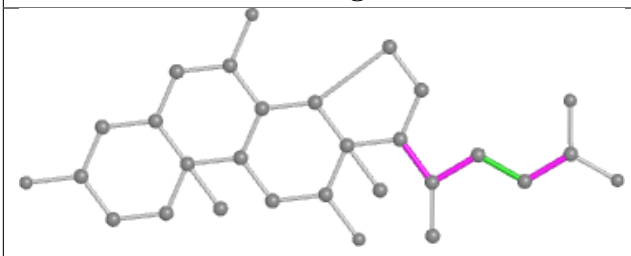
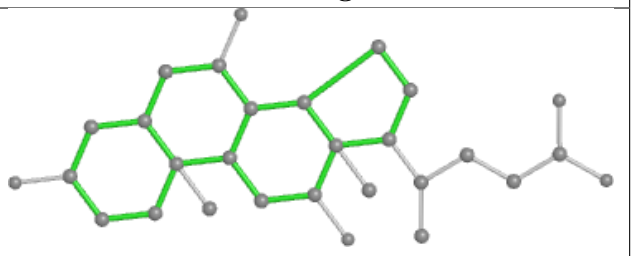


Bond angles

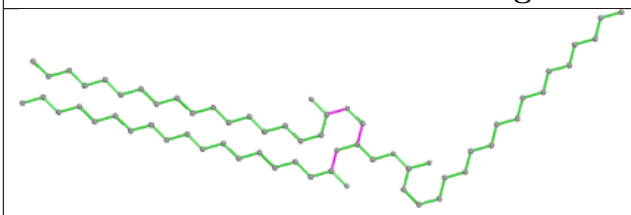


Torsions



Rings

Ligand TGL N 1523



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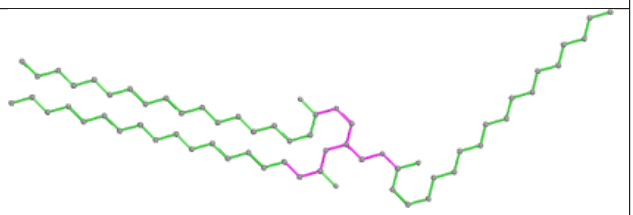
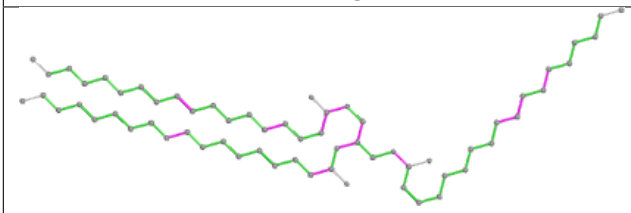
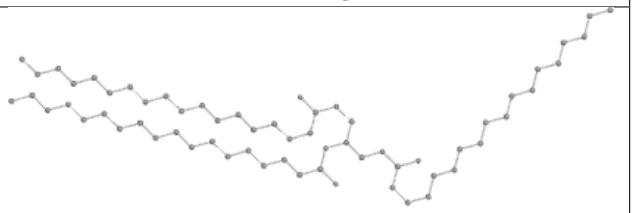


Bond angles

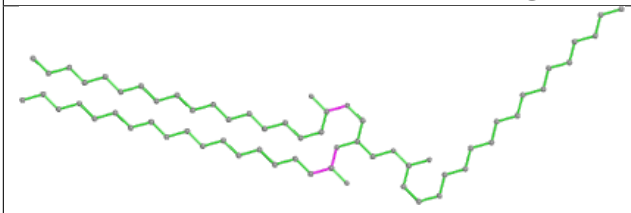


Torsions



Rings

Ligand TGL D 523



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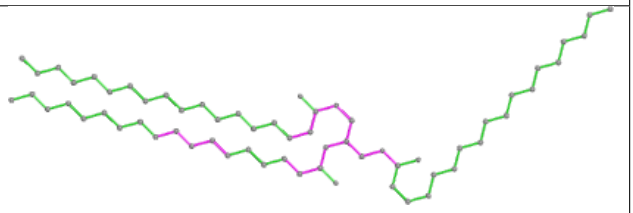
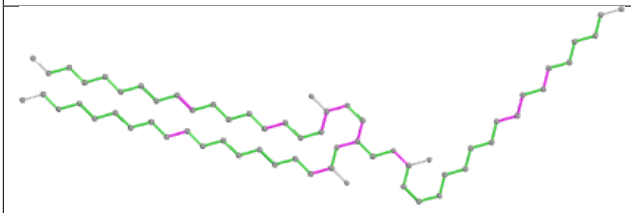
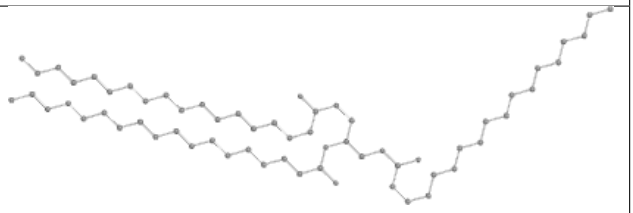


Bond angles

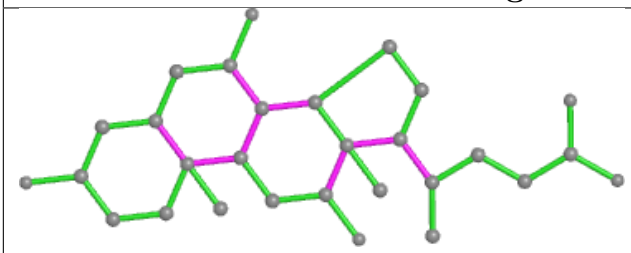


Torsions

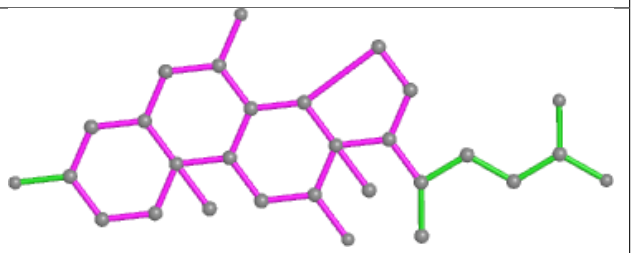


Rings

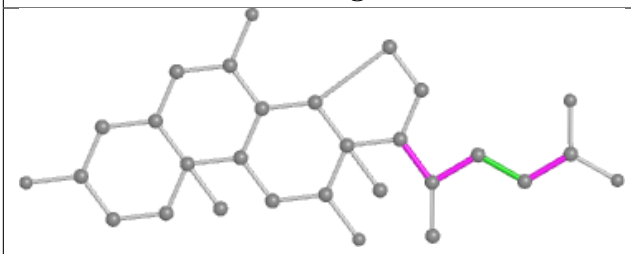
Ligand CHD W 1060



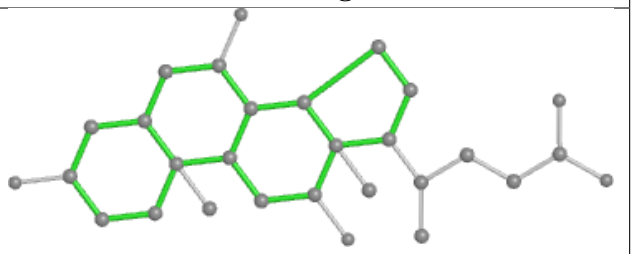
Bond lengths



Bond angles

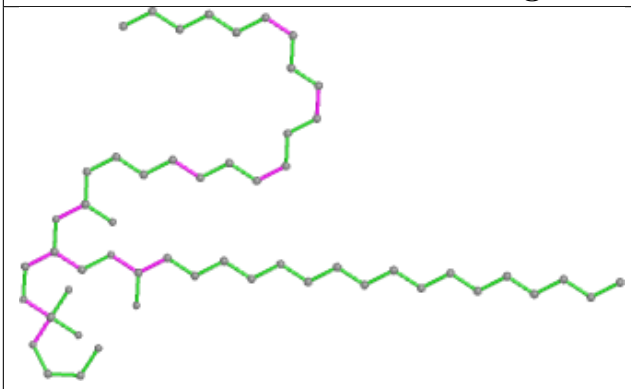


Torsions



Rings

Ligand PEK C 265



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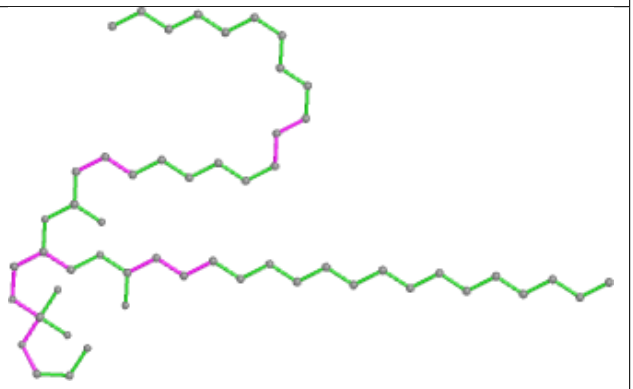
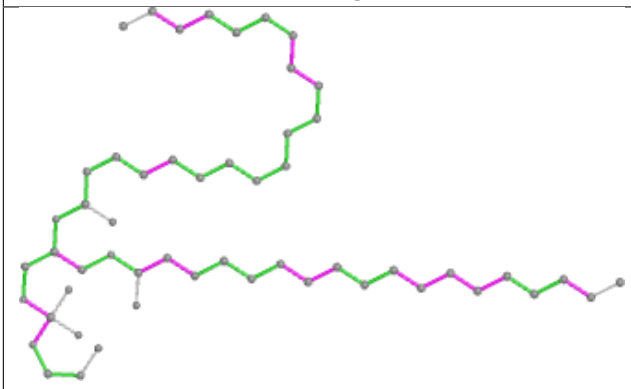
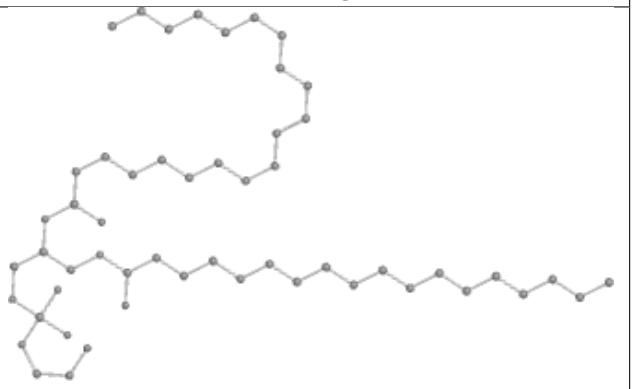


Bond angles

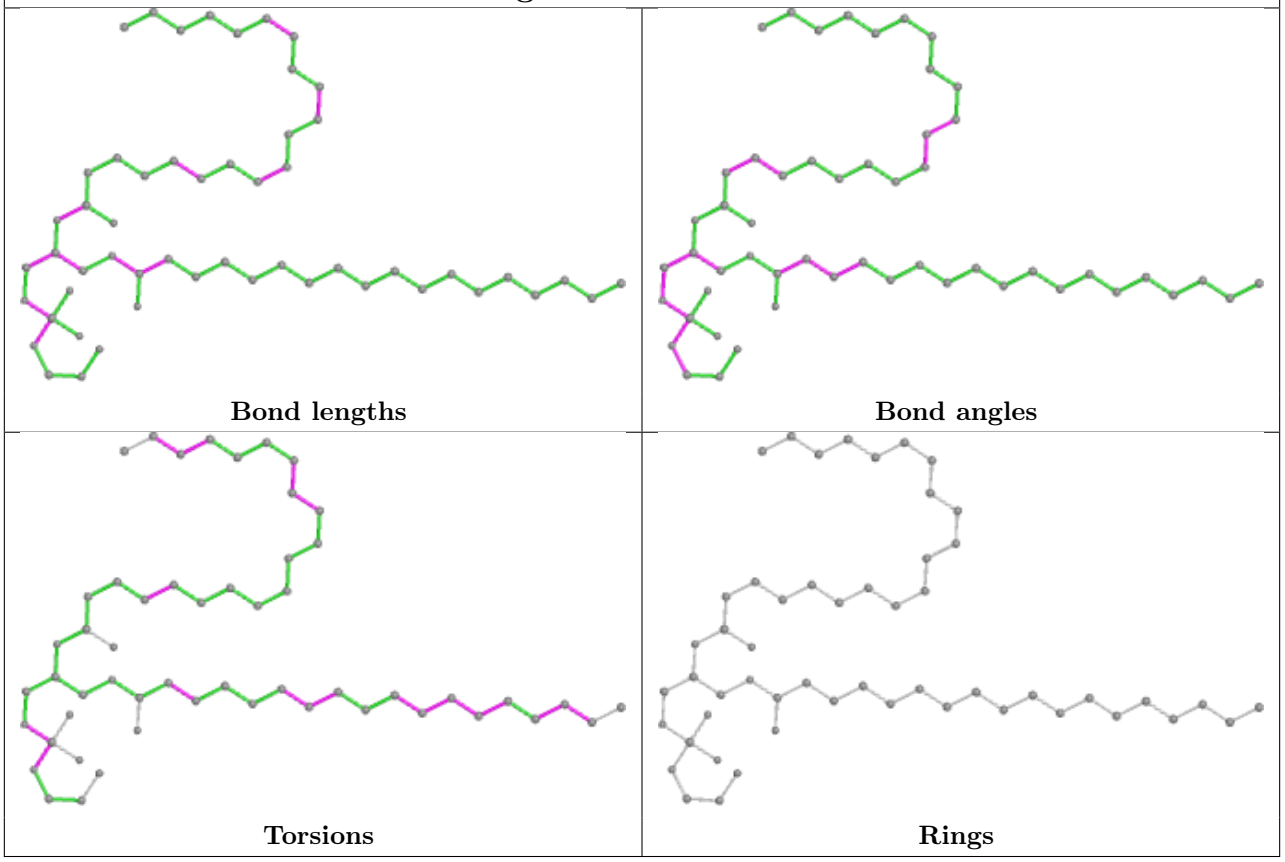


Torsions

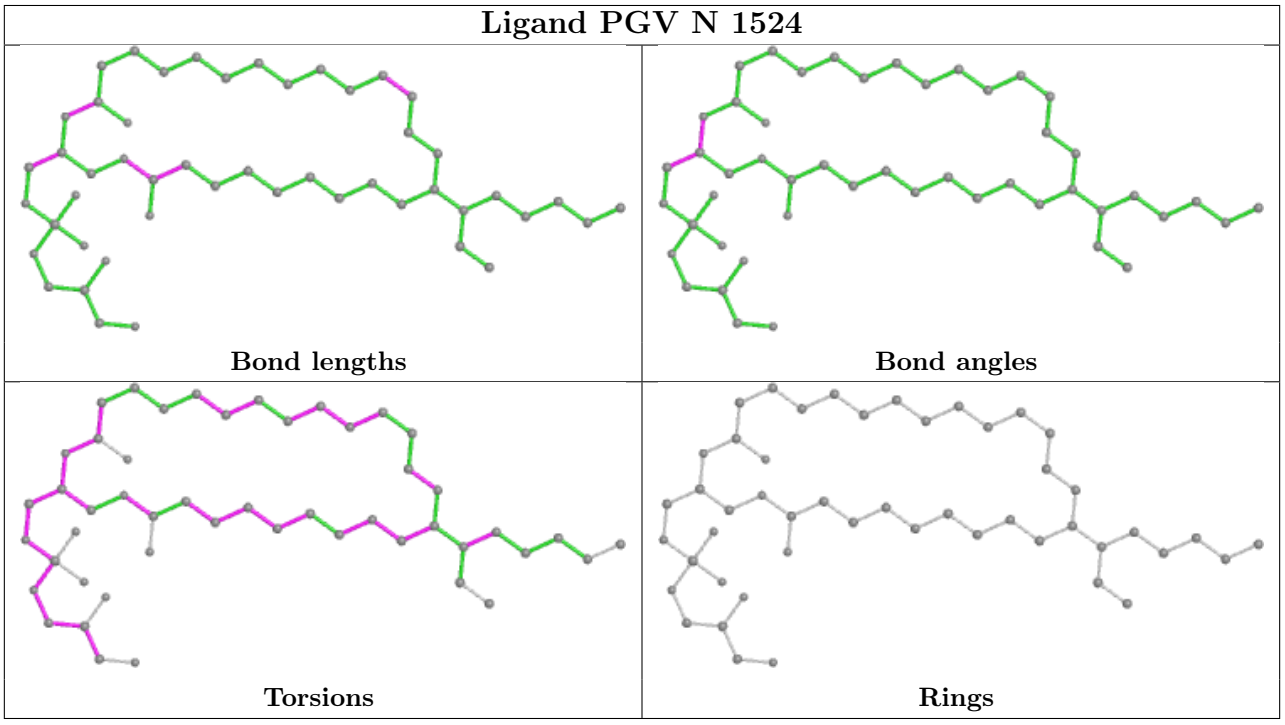


Rings

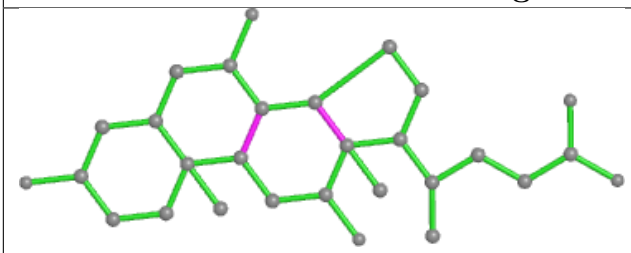
Ligand PEK P 1265



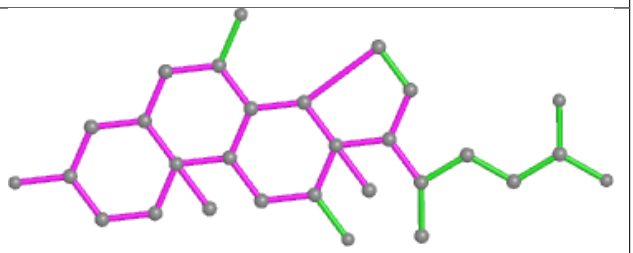
Ligand PGV N 1524



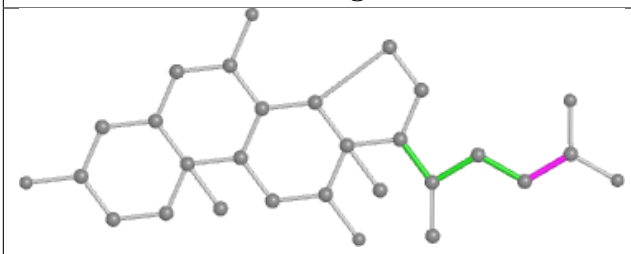
Ligand CHD P 1525



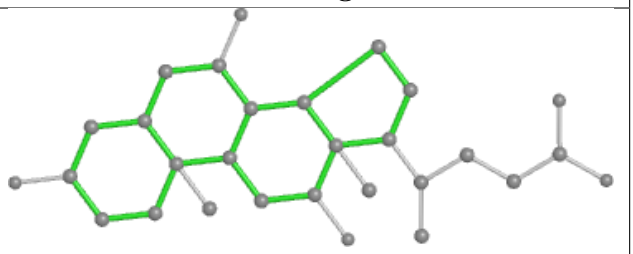
Bond lengths



Bond angles

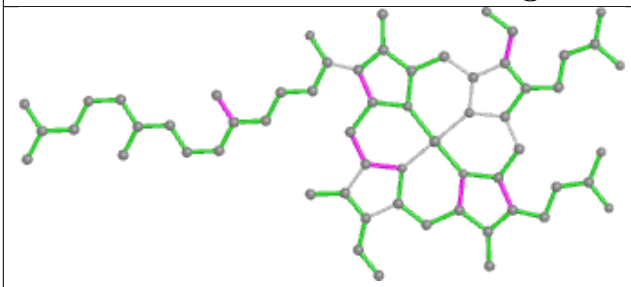


Torsions

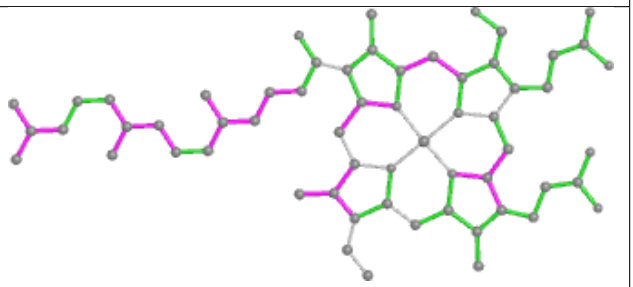


Rings

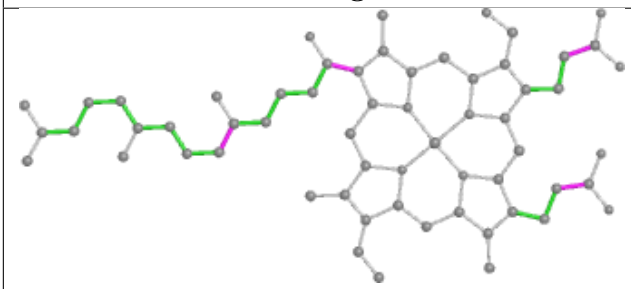
Ligand HEA A 515



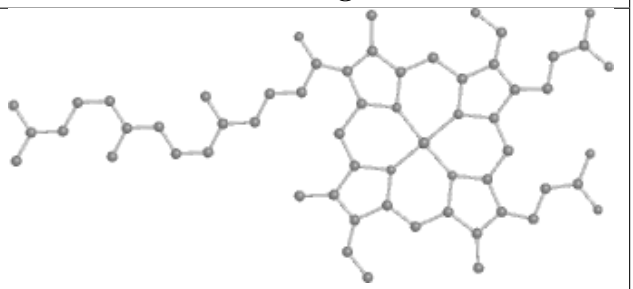
Bond lengths



Bond angles

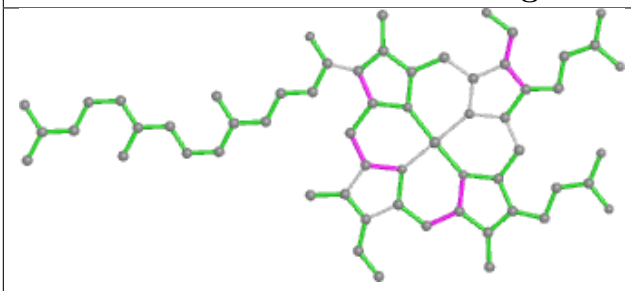


Torsions

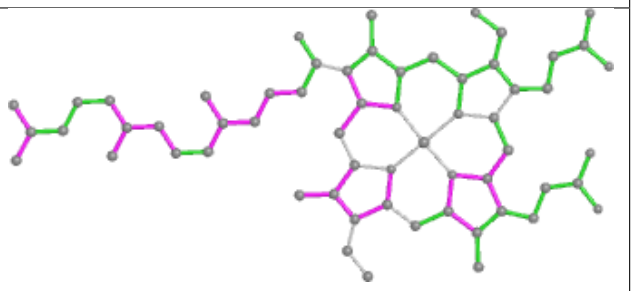


Rings

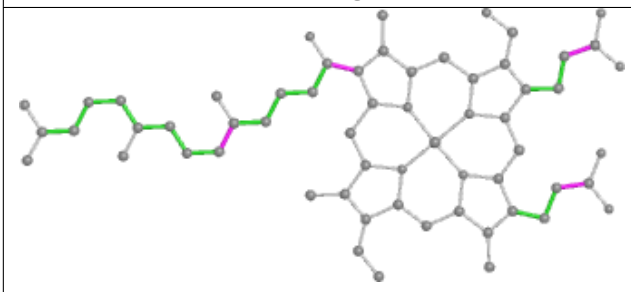
Ligand HEA N 515



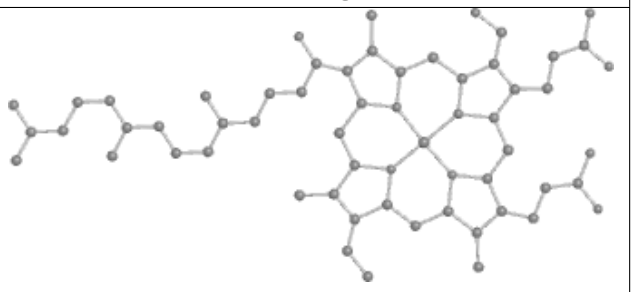
Bond lengths



Bond angles

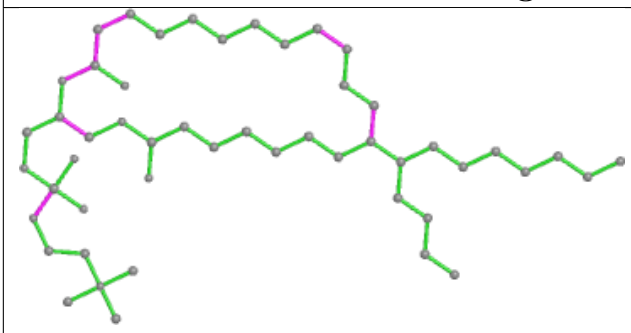


Torsions

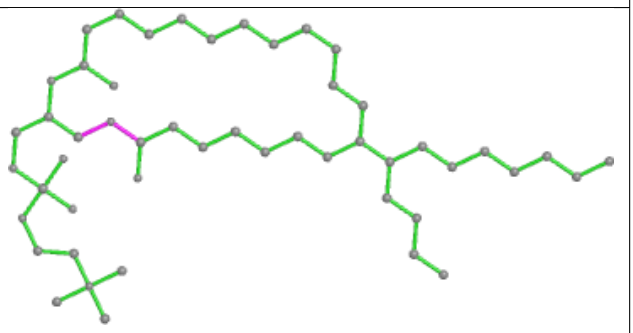


Rings

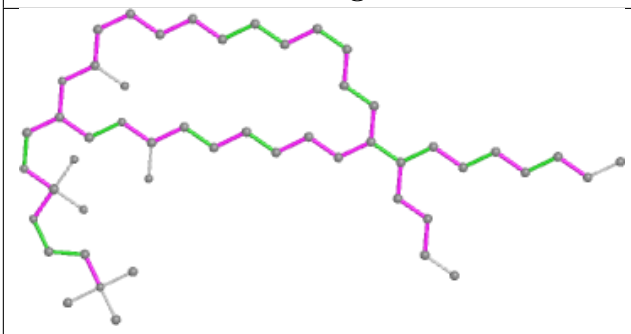
Ligand PSC O 1230



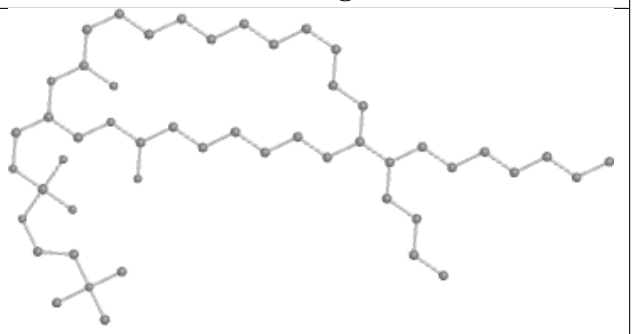
Bond lengths



Bond angles

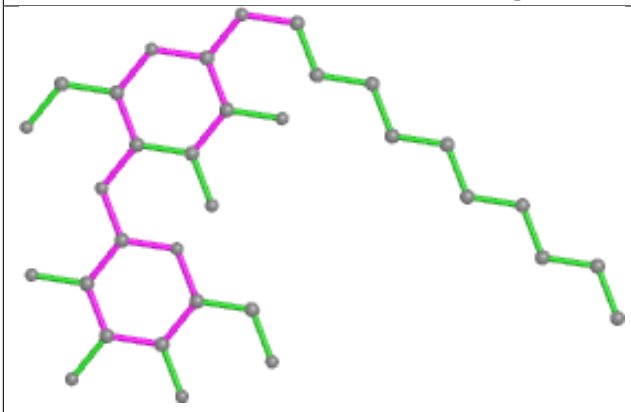


Torsions

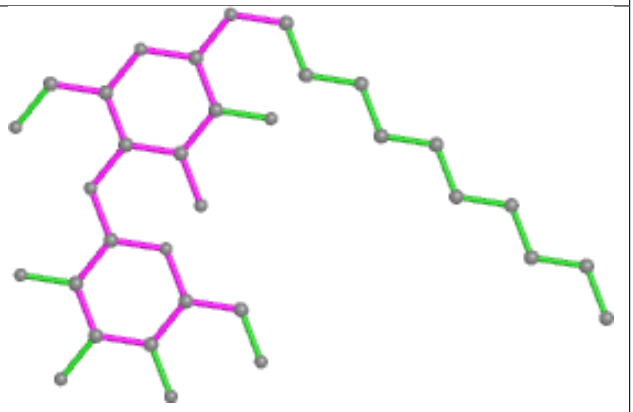


Rings

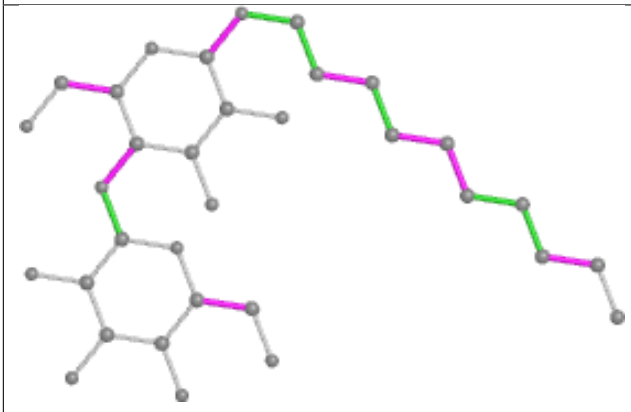
Ligand DMU P 1272



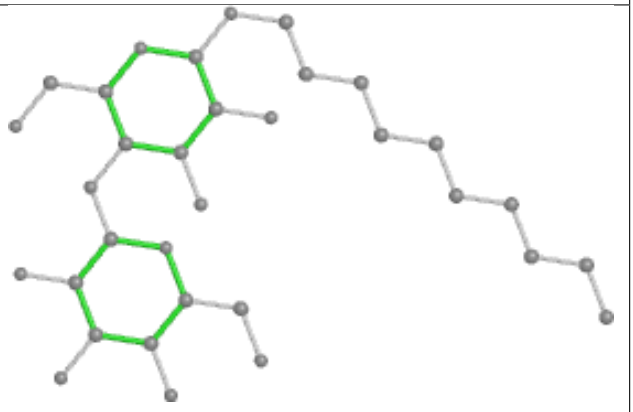
Bond lengths



Bond angles

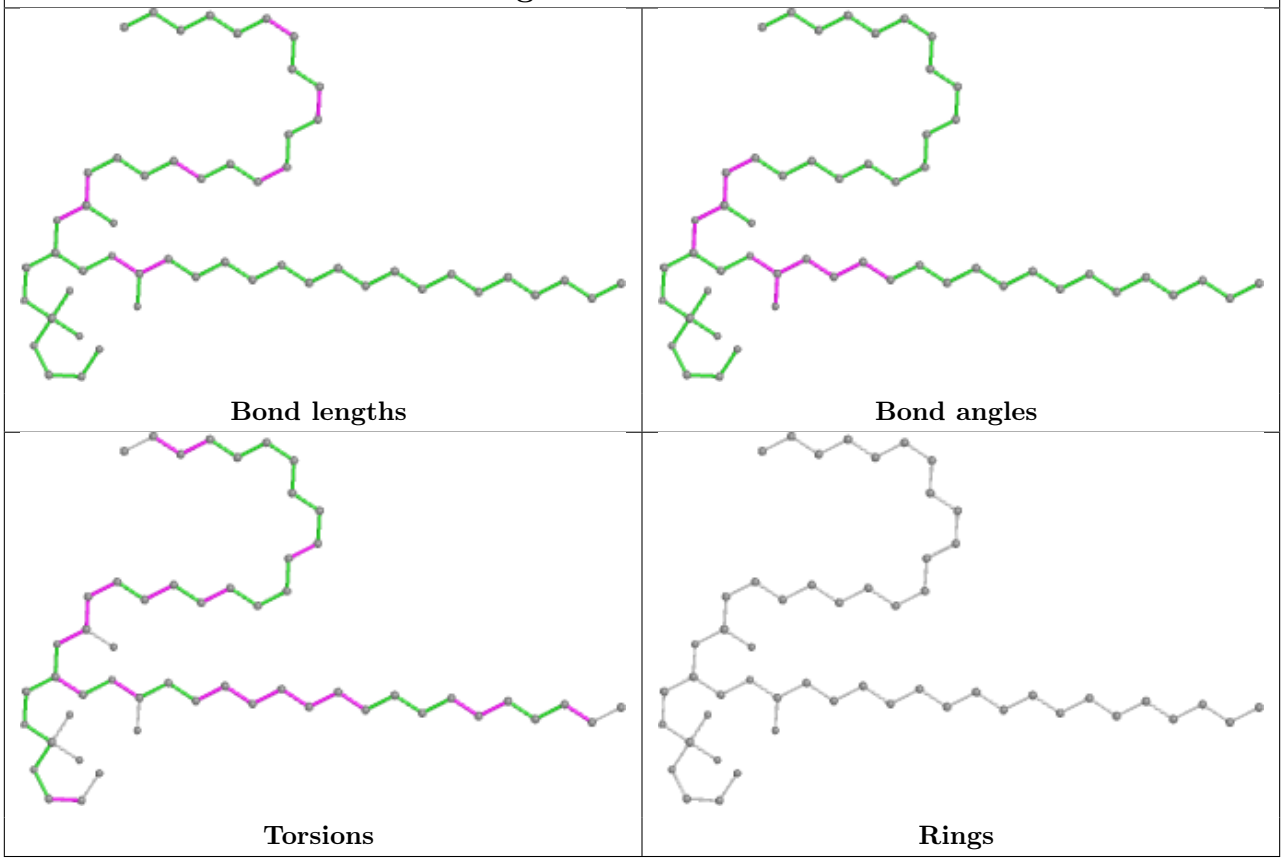


Torsions

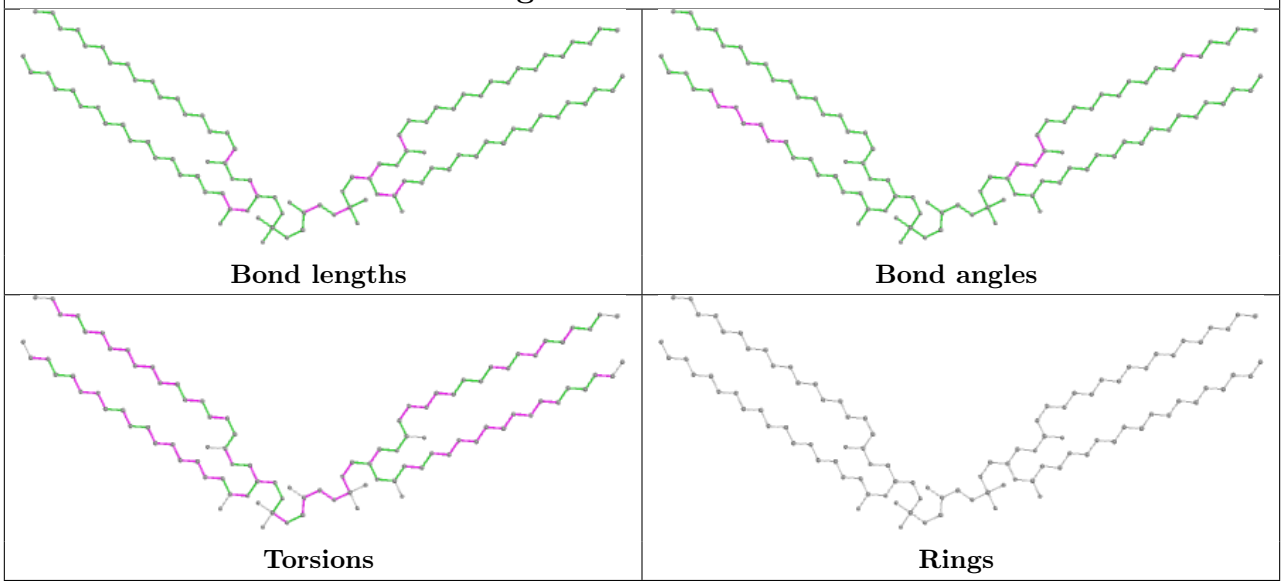


Rings

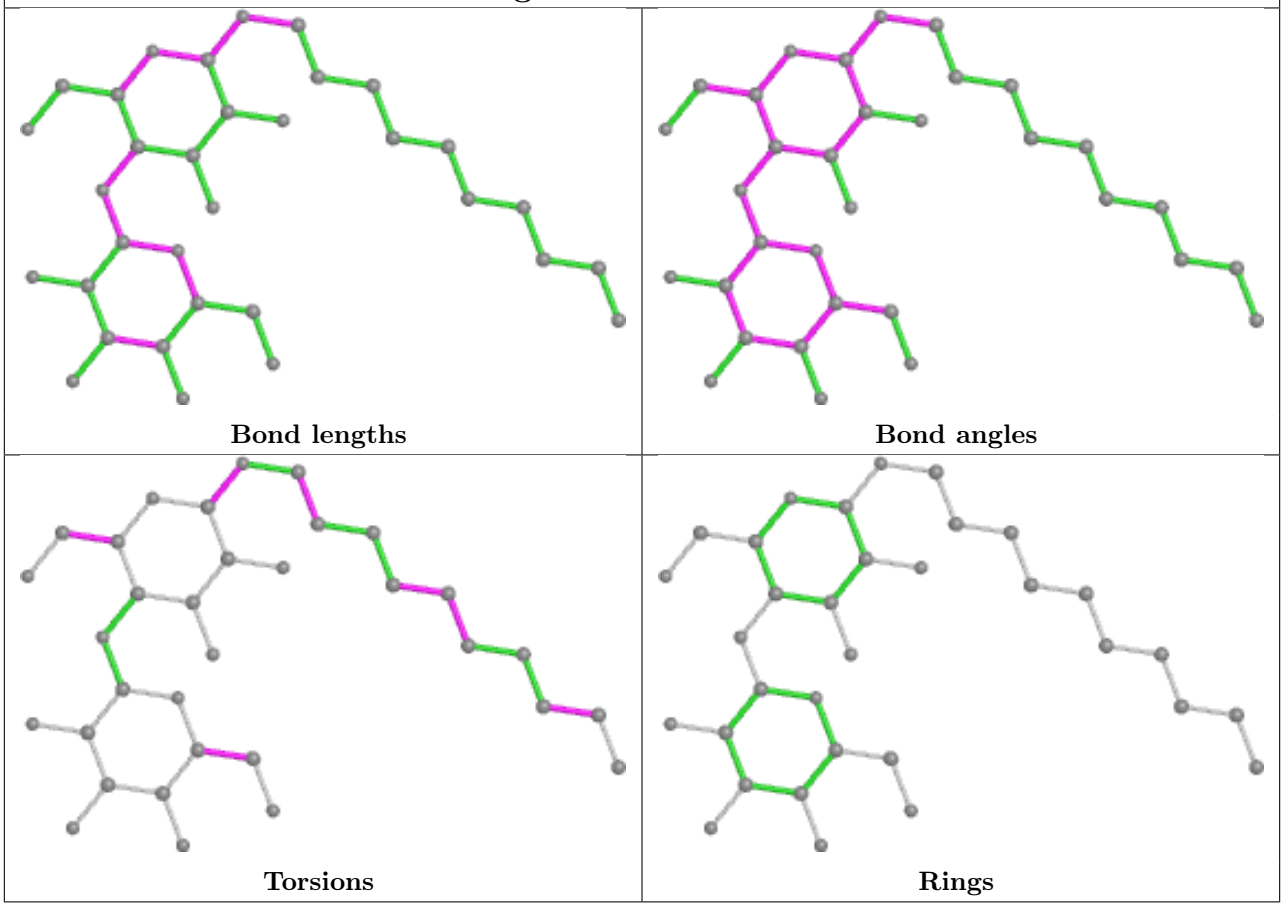
Ligand PEK P 1264



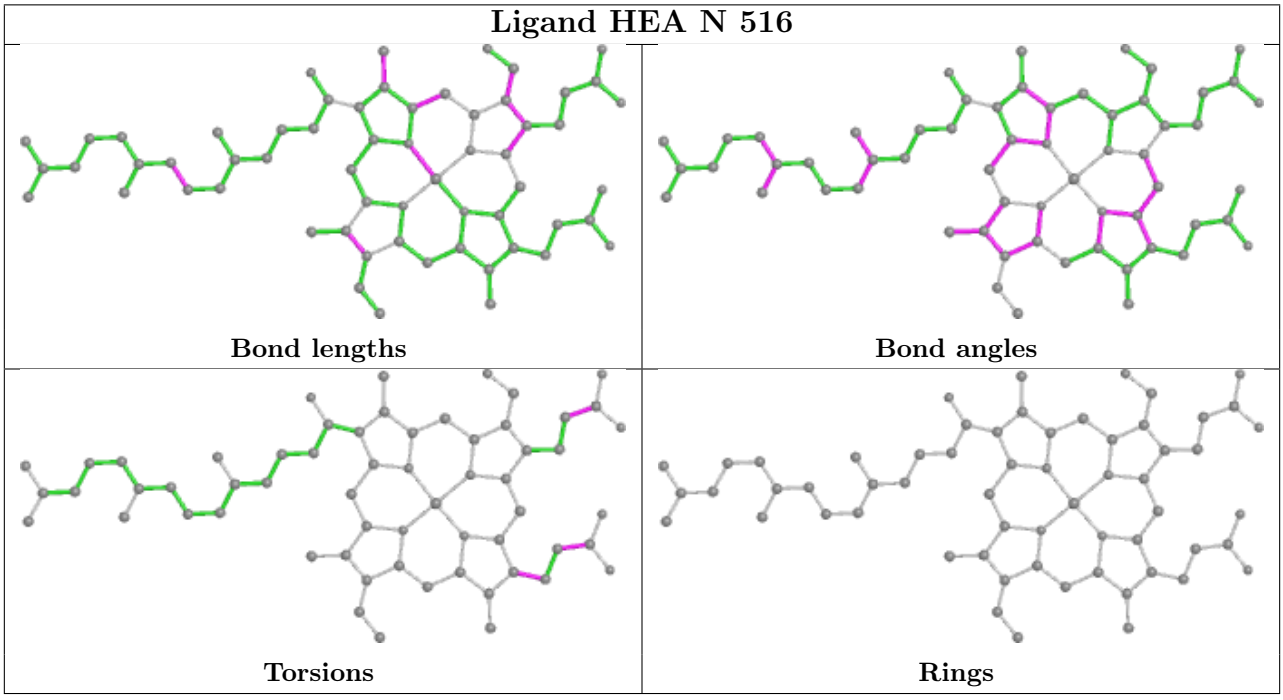
Ligand CDL T 1269



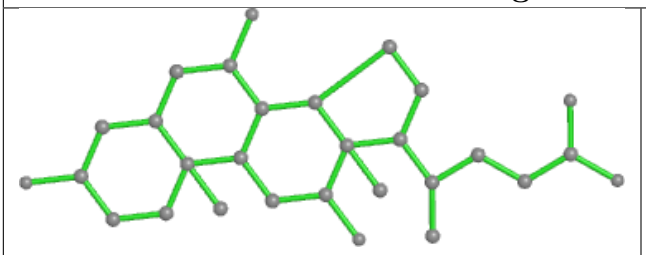
Ligand DMU M 526



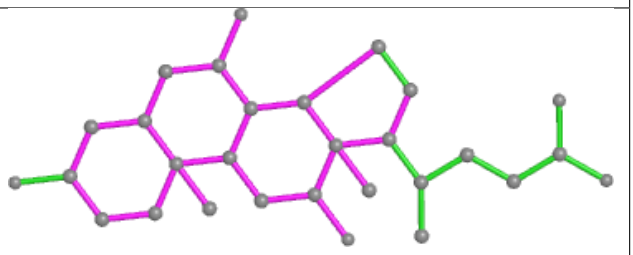
Ligand HEA N 516



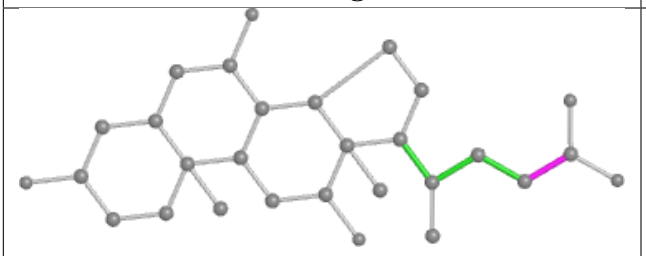
Ligand CHD B 1086



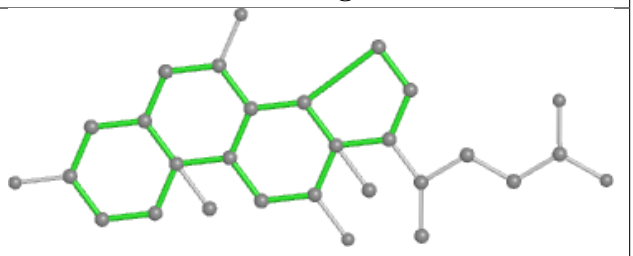
Bond lengths



Bond angles

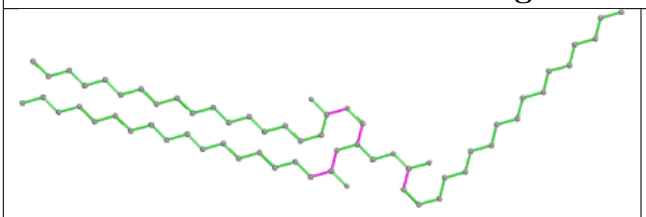


Torsions

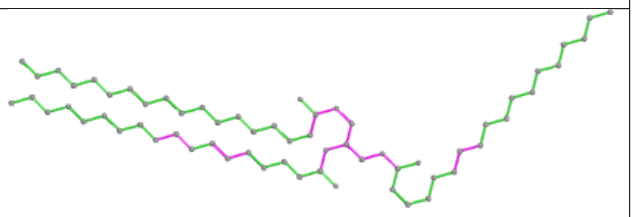


Rings

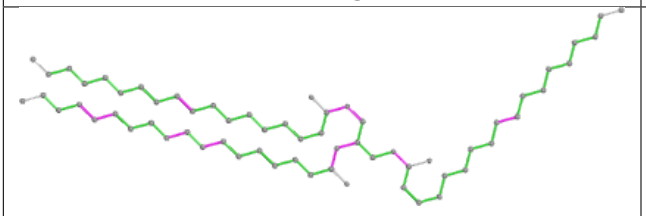
Ligand TGL O 1521



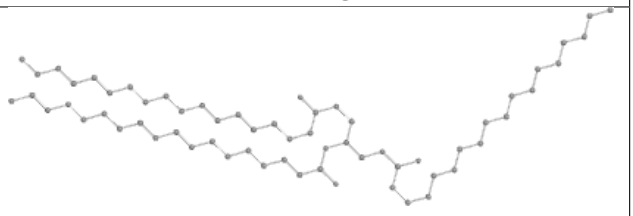
Bond lengths



Bond angles

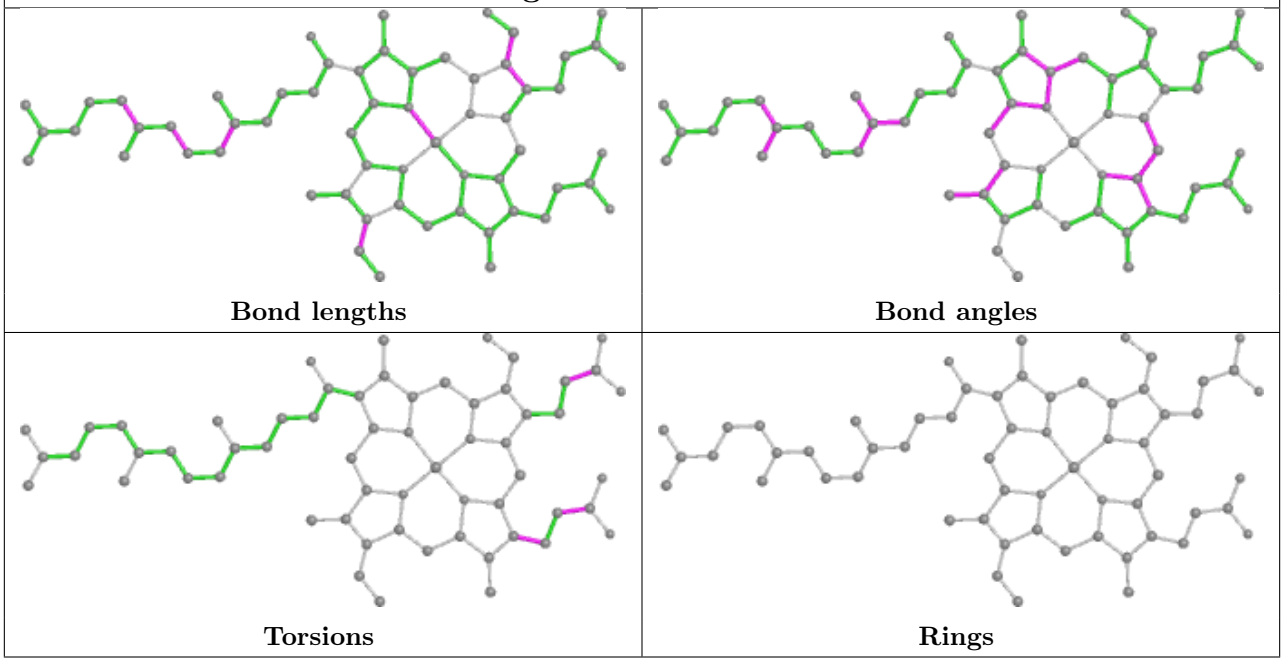


Torsions

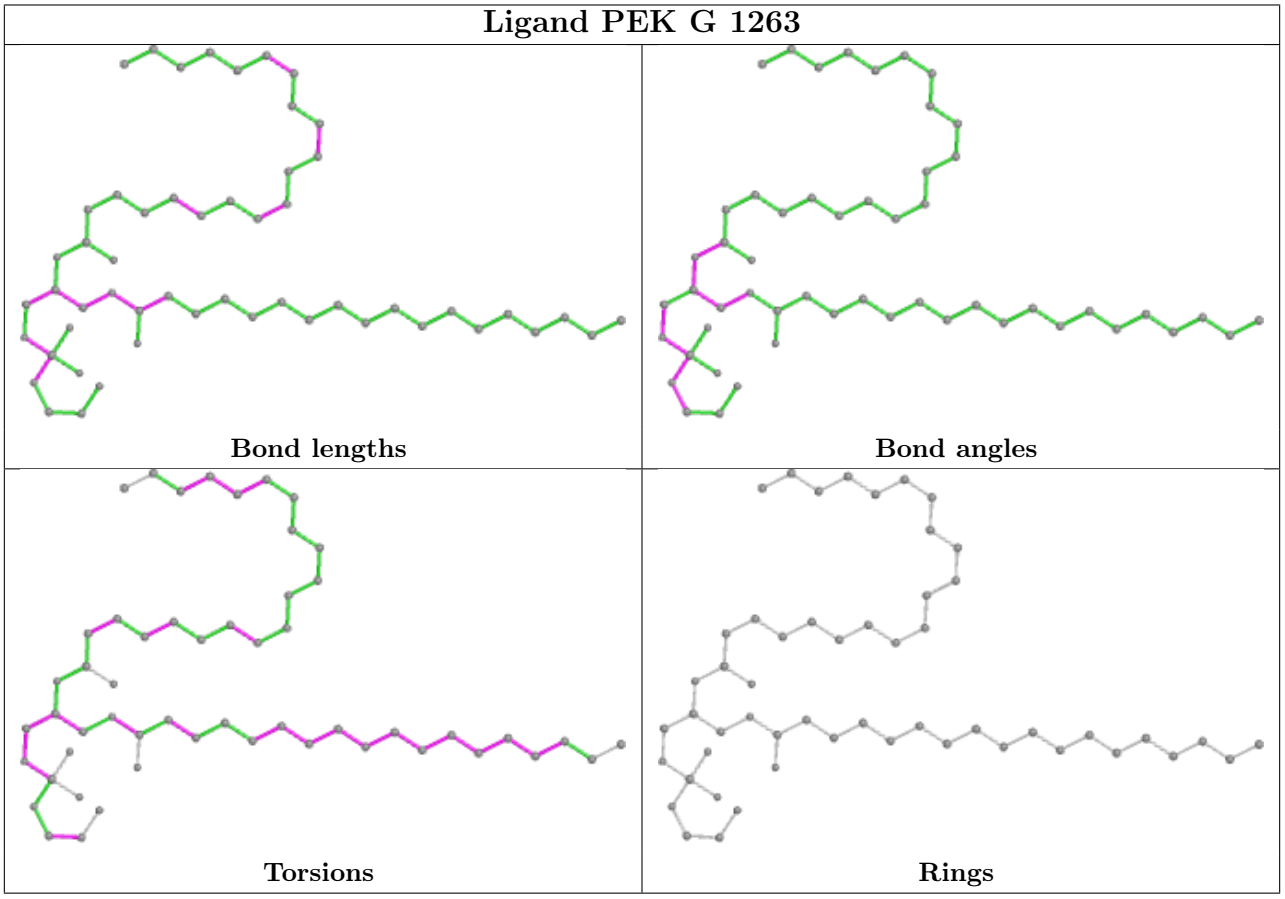


Rings

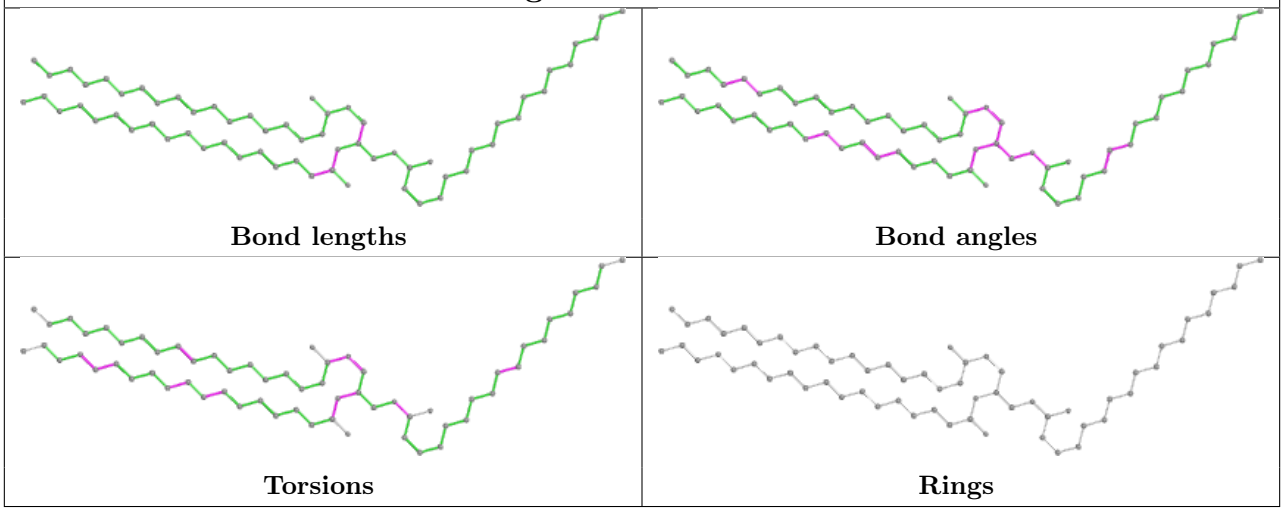
Ligand HEA A 516



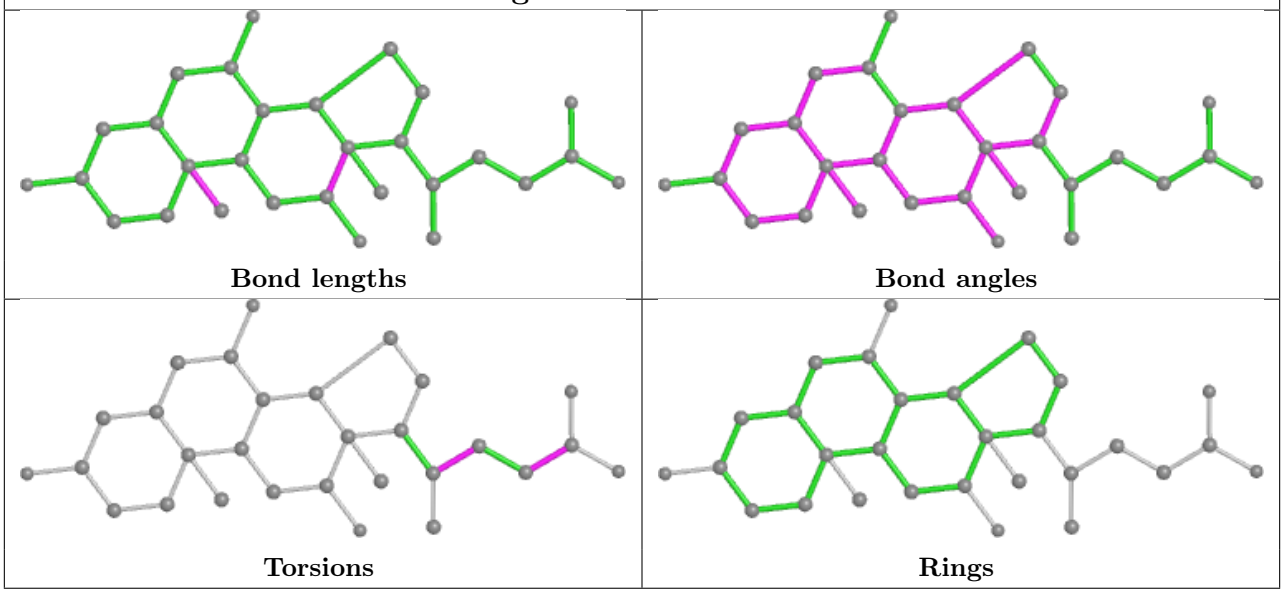
Ligand PEK G 1263



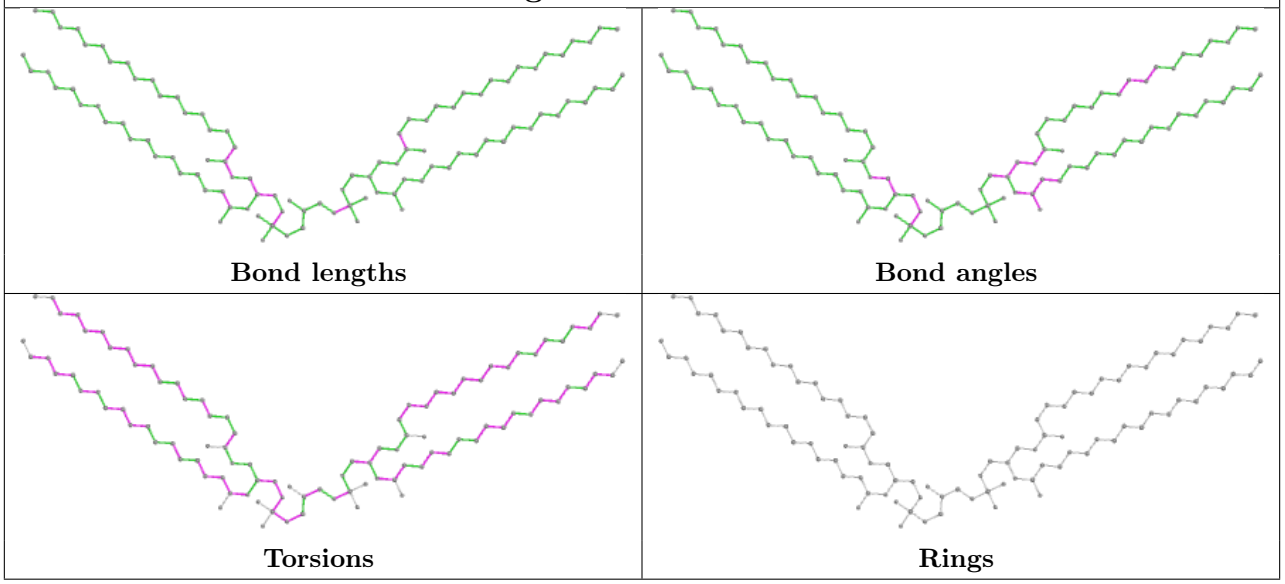
Ligand TGL B 521



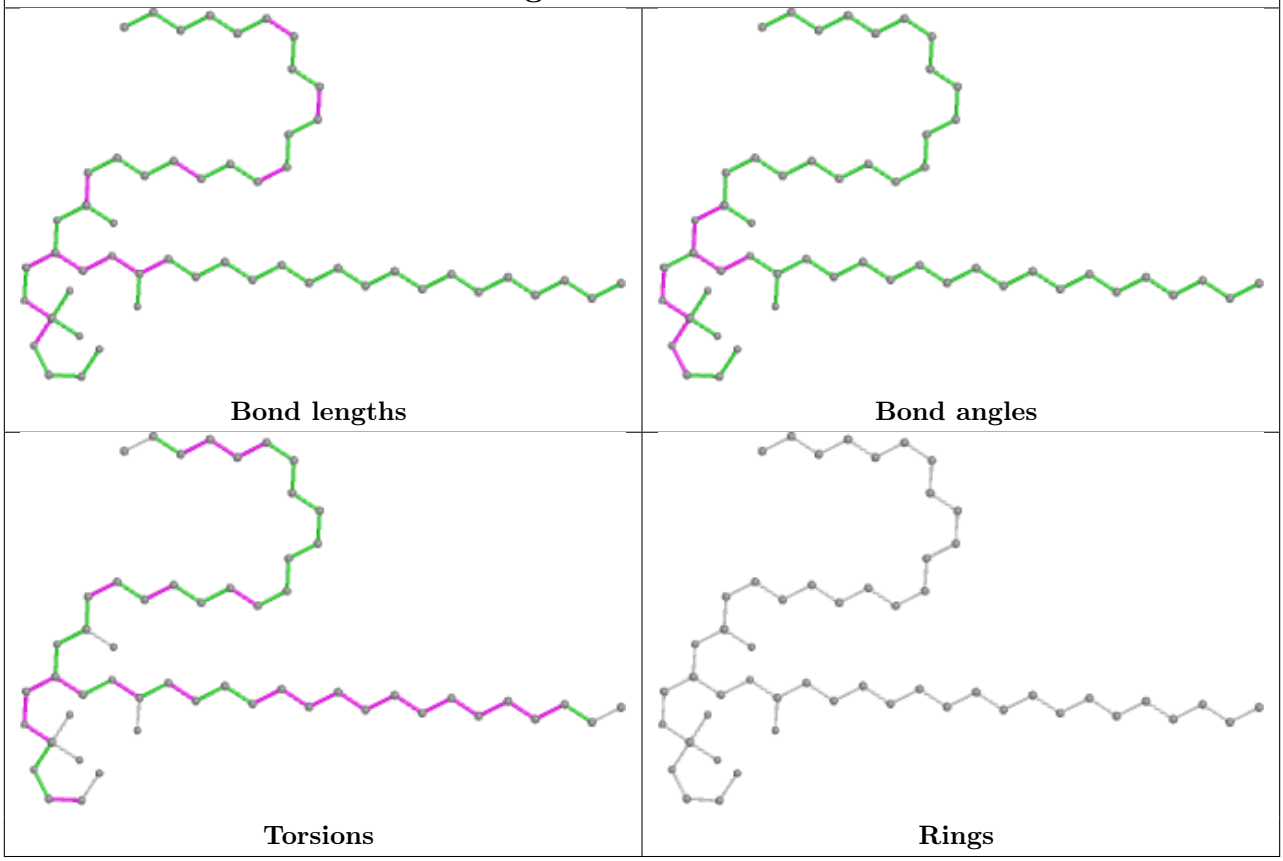
Ligand CHD N 1604



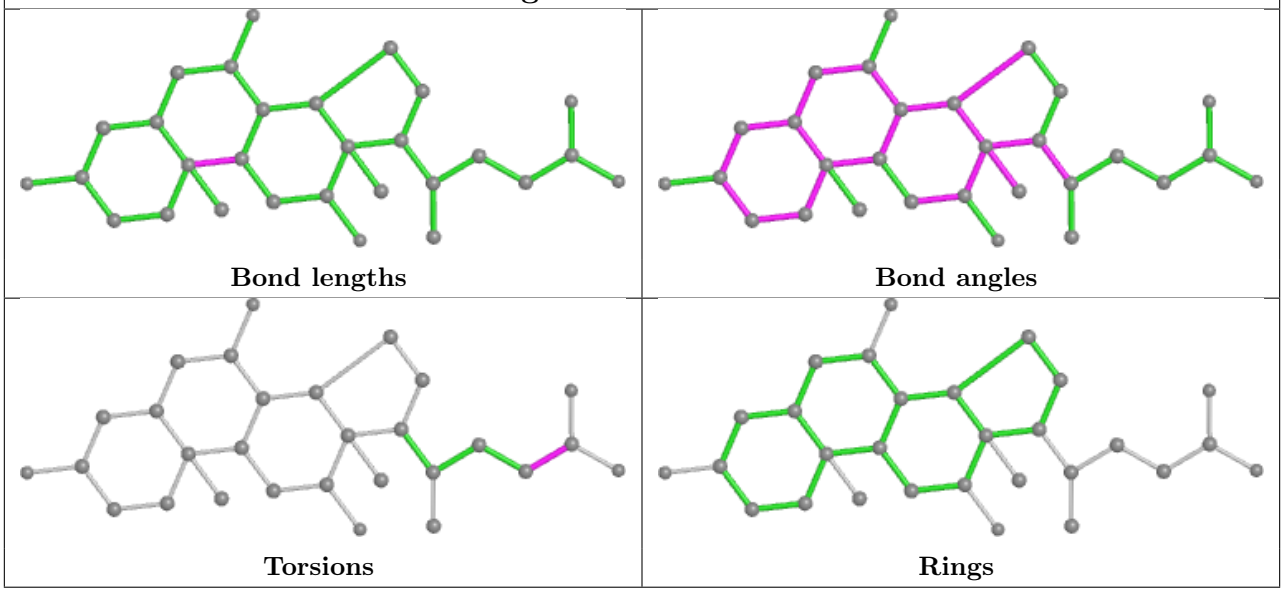
Ligand CDL C 270



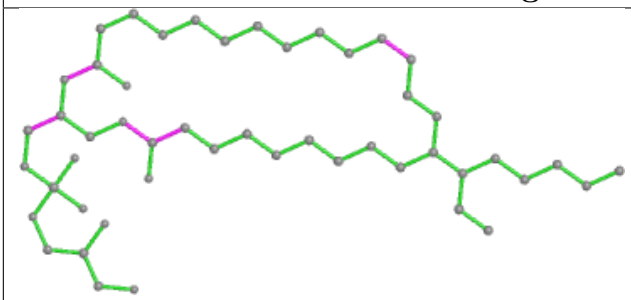
Ligand PEK T 263



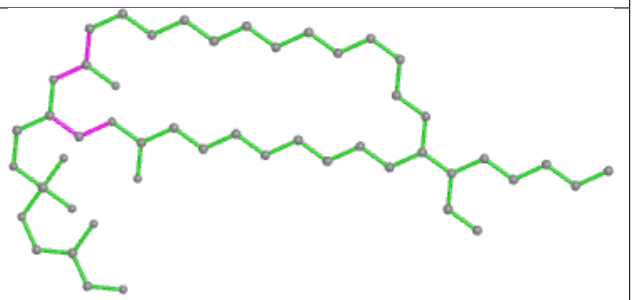
Ligand CHD A 525



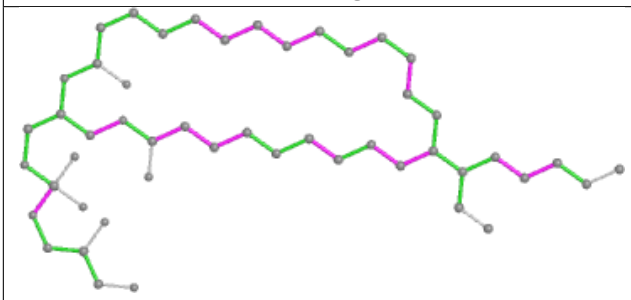
Ligand PGV C 266



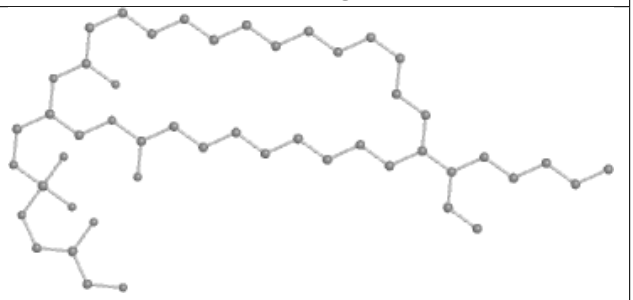
Bond lengths



Bond angles

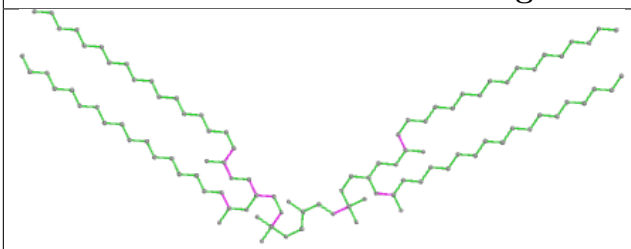


Torsions

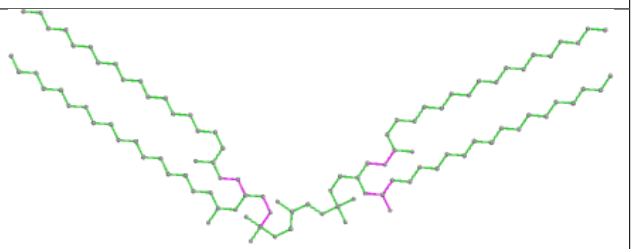


Rings

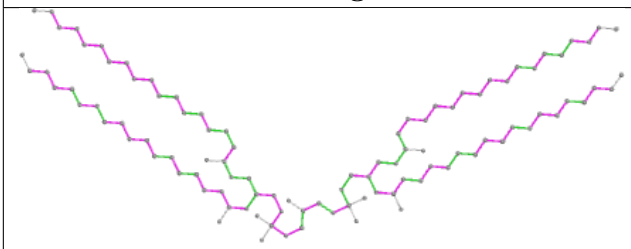
Ligand CDL P 1270



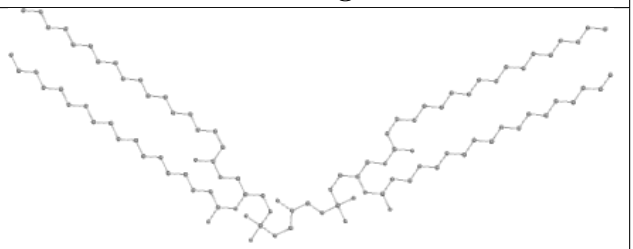
Bond lengths



Bond angles

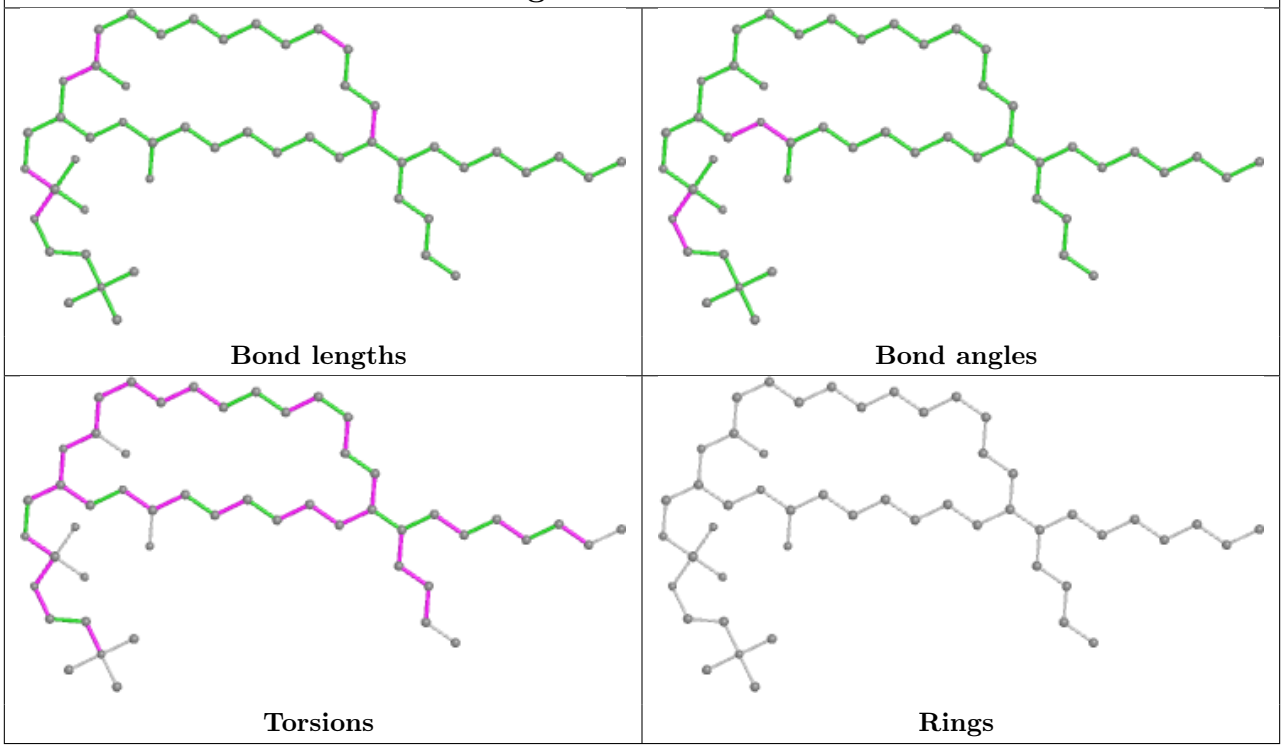


Torsions

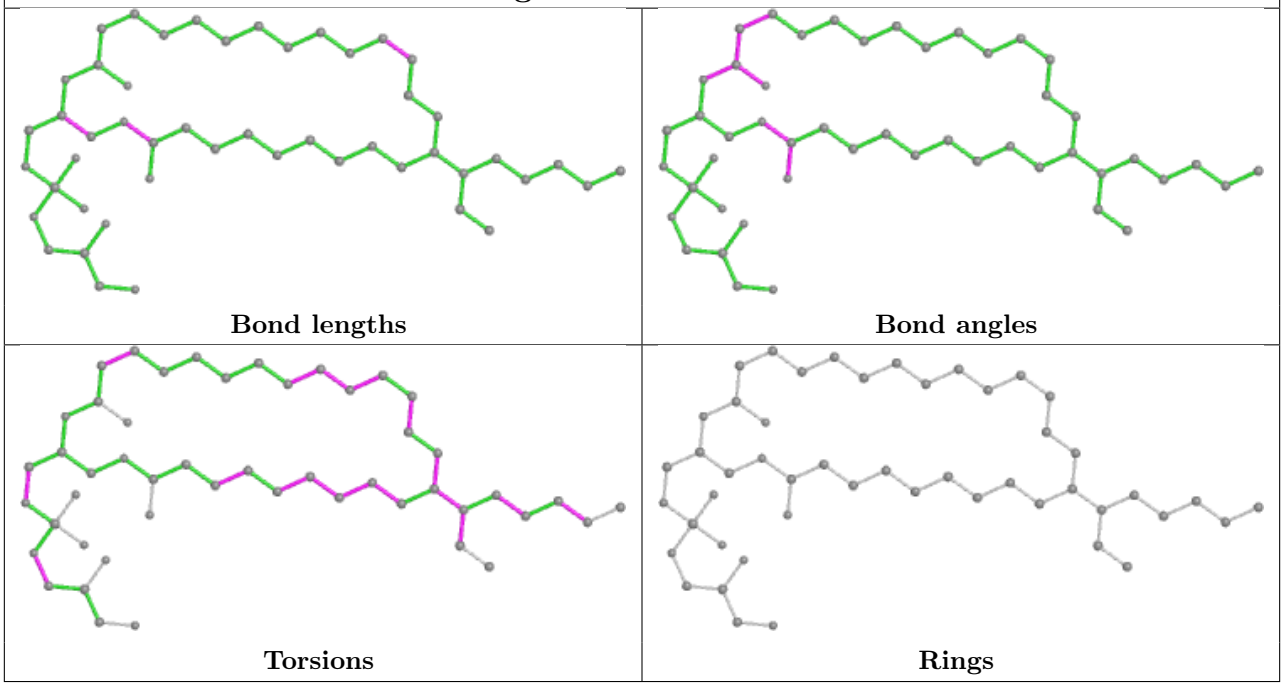


Rings

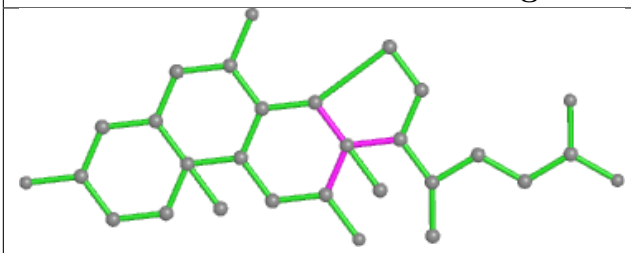
Ligand PSC B 230



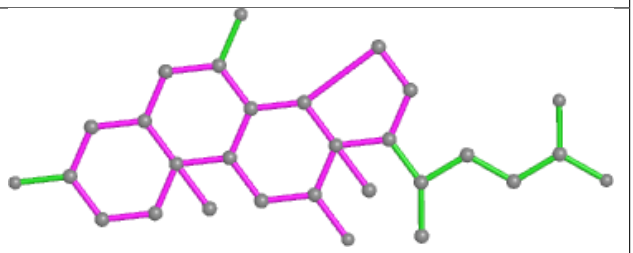
Ligand PGV P 1267



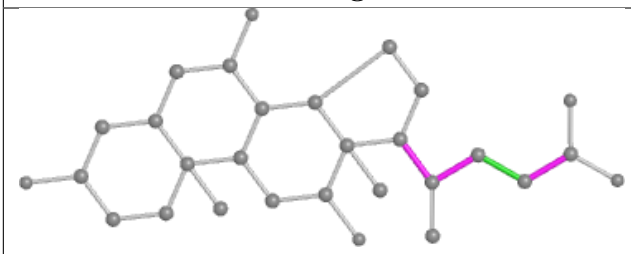
Ligand CHD C 271



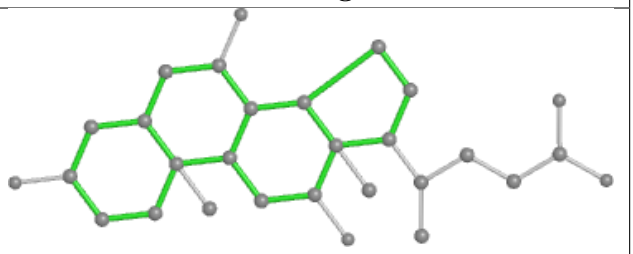
Bond lengths



Bond angles

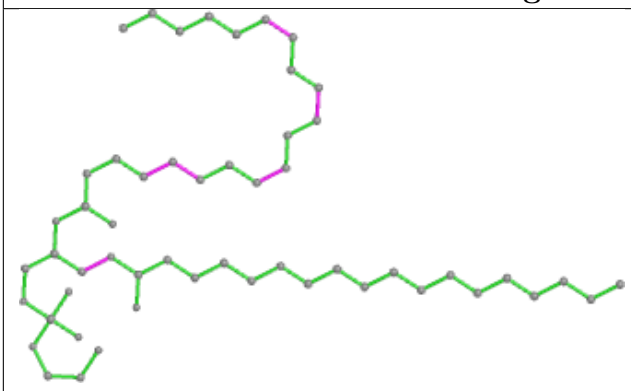


Torsions

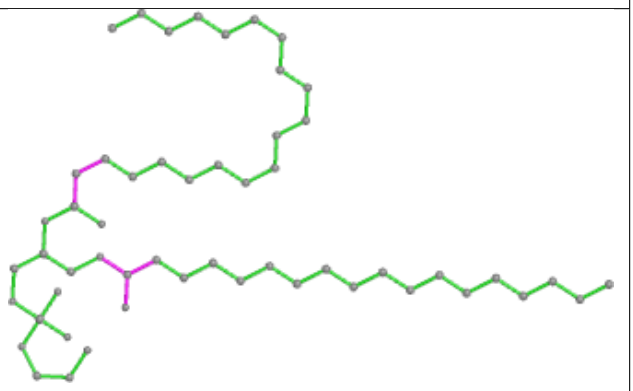


Rings

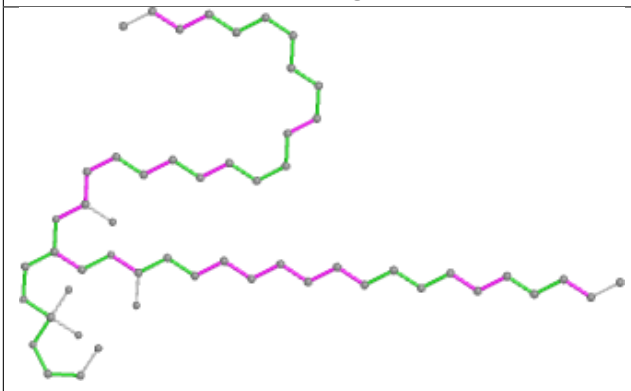
Ligand PEK C 264



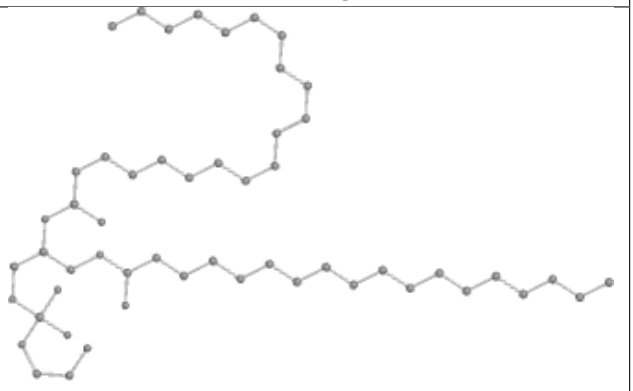
Bond lengths



Bond angles

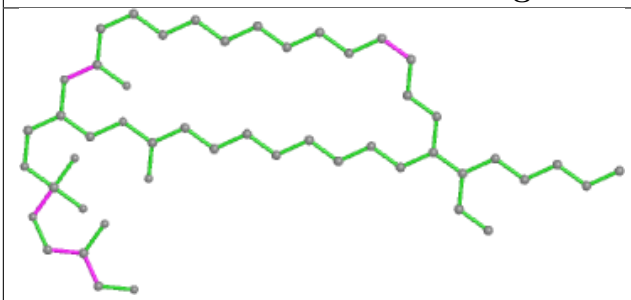


Torsions

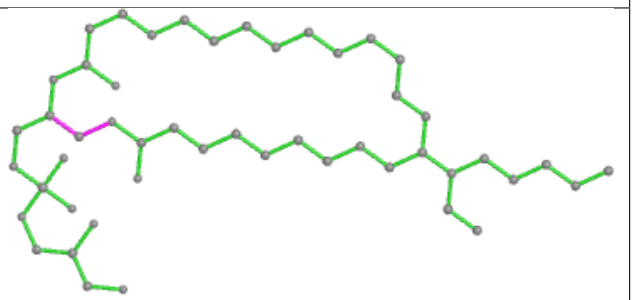


Rings

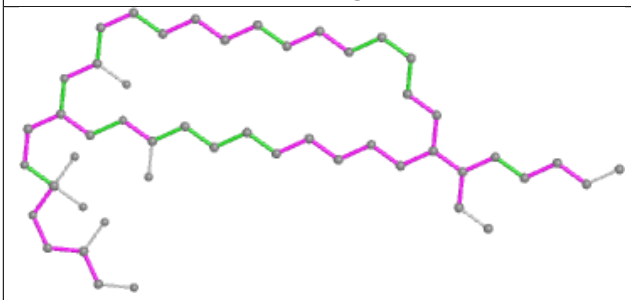
Ligand PGV P 1268



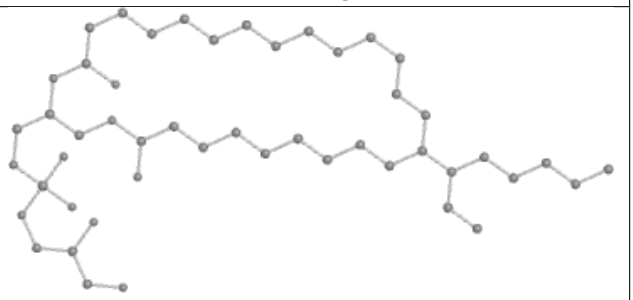
Bond lengths



Bond angles

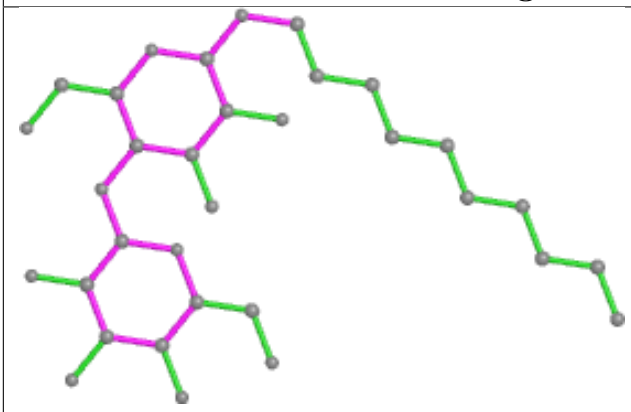


Torsions

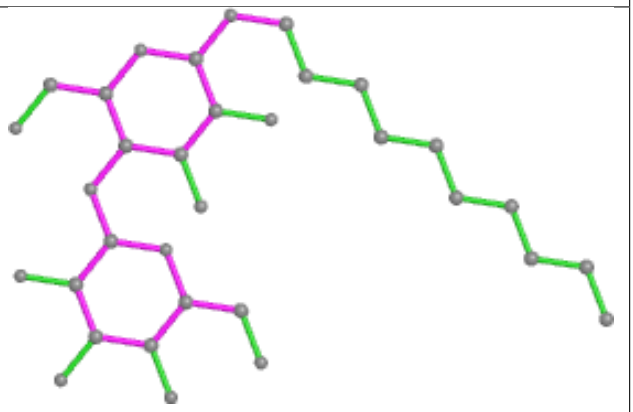


Rings

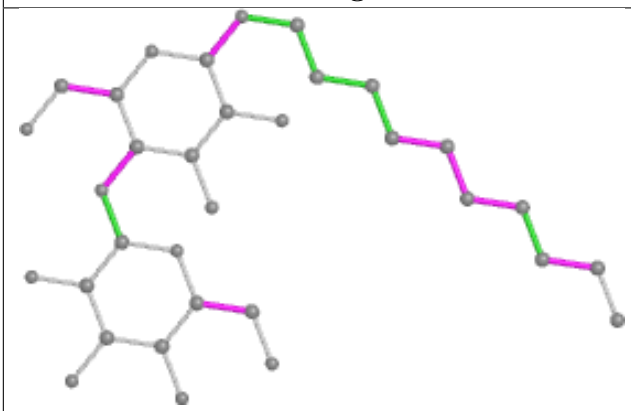
Ligand DMU C 272



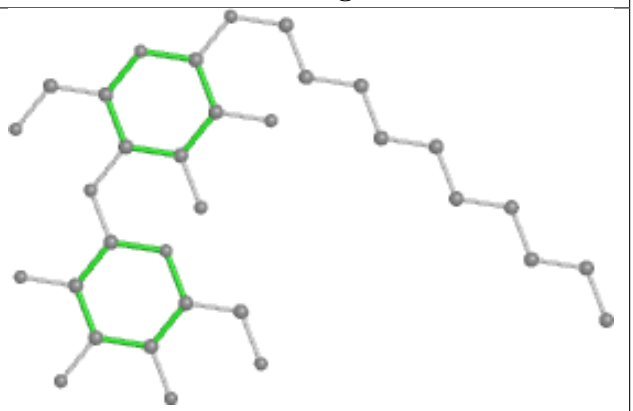
Bond lengths



Bond angles

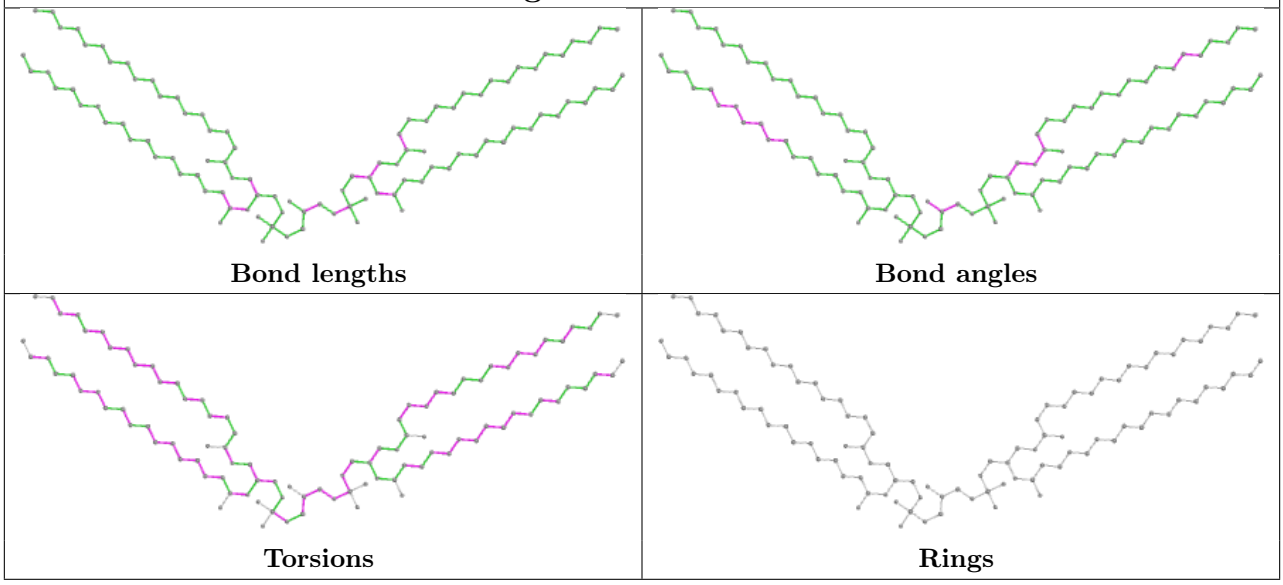


Torsions



Rings

Ligand CDL G 269



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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.