Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 12:44 am BST

PDB ID	:	6ZKU / pdb_00006zku
EMDB ID	:	EMD-11262
Title	:	Deactive complex I, open3
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	3.00 Å(reported)
Based on initial model	:	5LNK

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

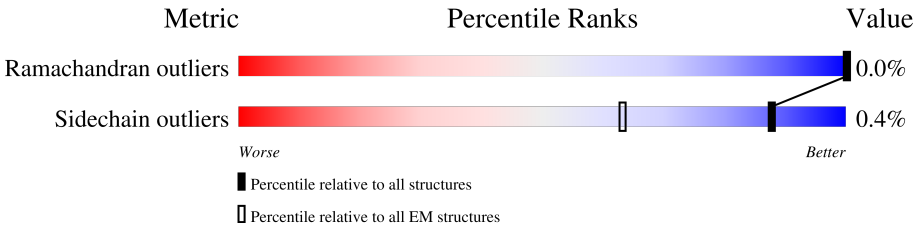
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	464	92% 7%
2	2	246	86% 13%
3	3	727	94% • 5%
4	4	463	88% • 11%
5	5	266	78% 22%
6	6	223	69% • 30%
7	9	217	81% 19%
8	A	115	95% • •
9	H	318	97% • •
10	J	175	98% •

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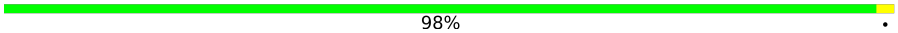
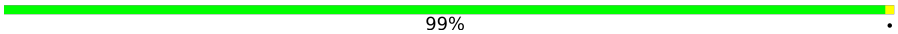
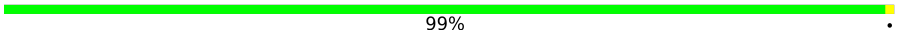
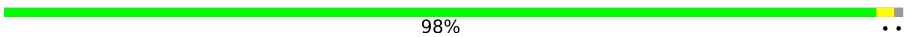
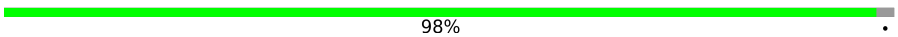
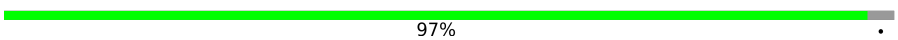
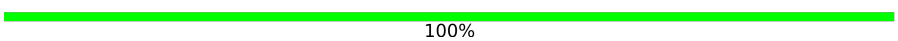
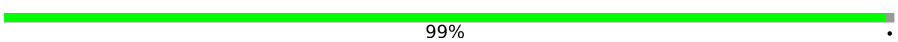
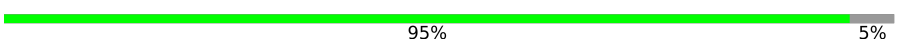
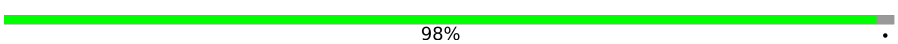
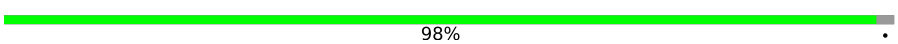
Mol	Chain	Length	Quality of chain
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	
29	k	355	
30	l	106	
31	m	84	
32	n	98	
33	o	122	
34	p	130	

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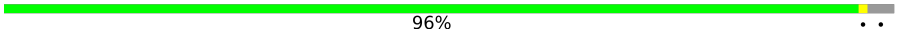
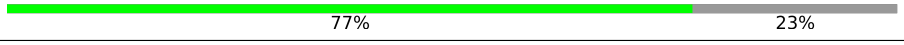
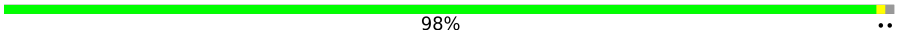
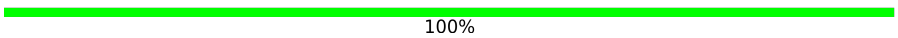
Mol	Chain	Length	Quality of chain
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

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
51	CDL	M	501	X	-	-	-
51	CDL	Y	201	X	-	-	-
51	CDL	x	101	X	-	-	-

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 65505 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	213	1655	1058	278	309	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	411	3301	2106	566	604	25	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	156	1247	795	225	213	14	0	0

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	311	Total	C	N	O	S	0	0
			2479	1675	377	408	19		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1344	904	192	235	13		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	540	Total	C	N	O	S	0	0
			4285	2845	667	732	41		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	19	Total	C	N	O	S	0	0
			149	100	24	24	1		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	x	49	Total	C	N	O	0	0
			412	271	70	71		

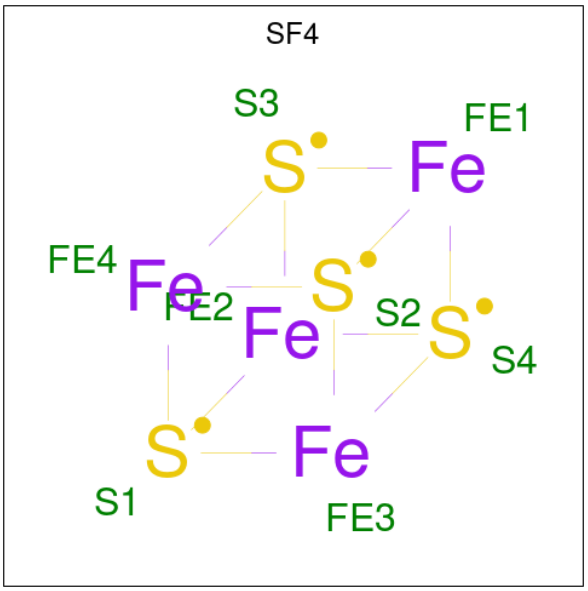
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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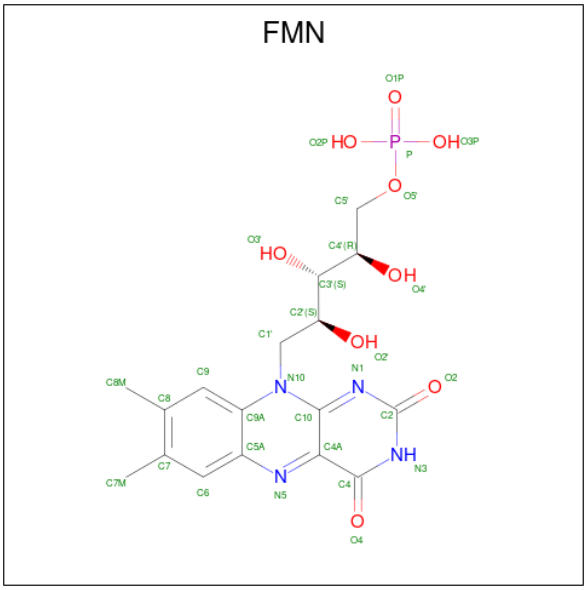
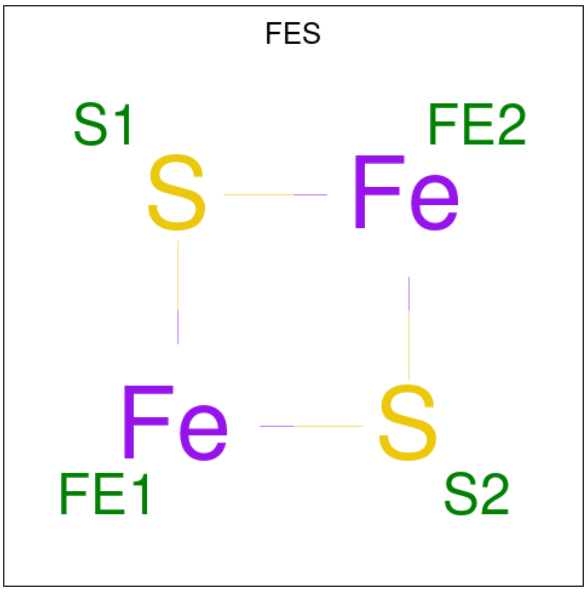
Mol	Chain	Residues	Atoms	AltConf
45	9	1	Total Fe S 8 4 4	0
45	9	1	Total Fe S 8 4 4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms	AltConf
46	1	1	Total C N O P 31 17 4 9 1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

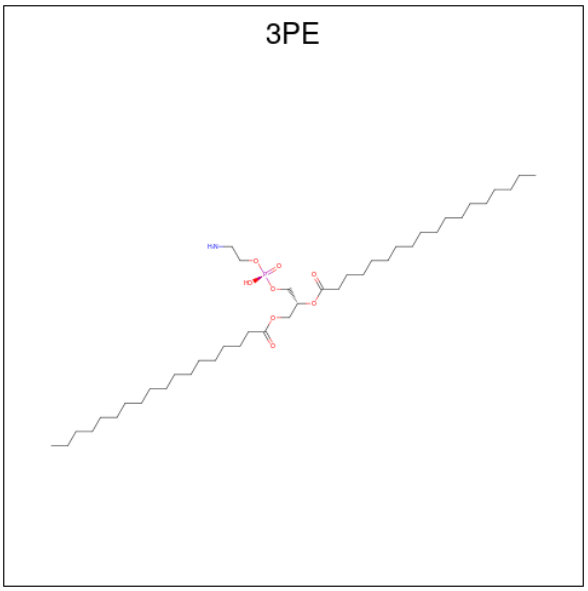


Mol	Chain	Residues	Atoms	AltConf
47	2	1	Total Fe S 4 2 2	0
47	3	1	Total Fe S 4 2 2	0

- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

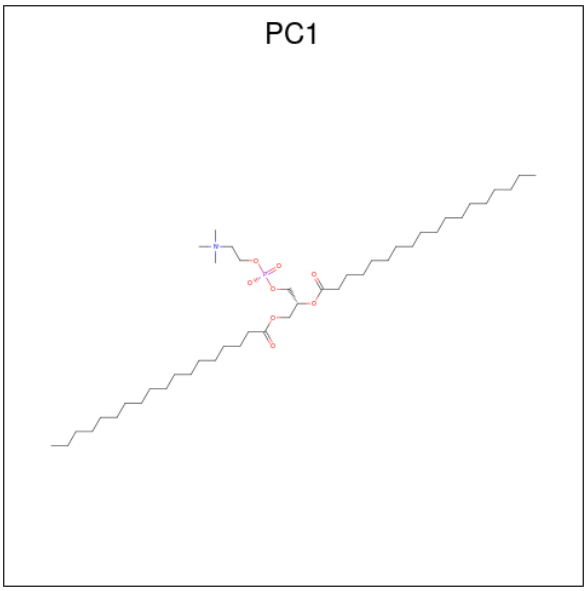
Mol	Chain	Residues	Atoms	AltConf
48	3	1	Total K 1 1	0

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



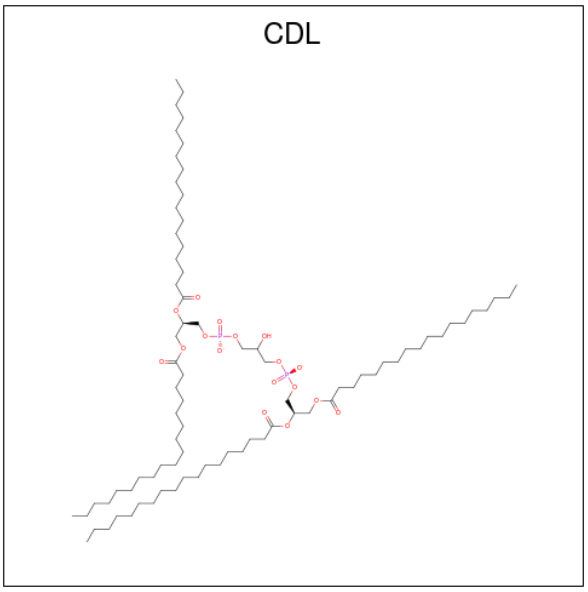
Mol	Chain	Residues	Atoms					AltConf
49	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
49	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	N	1	Total	C	N	O	P	0
			31	21	1	8	1	
49	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
50	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
50	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	V	1	Total	C	N	O	P	0
			36	26	1	8	1	
50	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	M	1	Total	C	O	P	0
			100	81	17	2	
51	W	1	Total	C	O	P	0
			100	81	17	2	
51	Y	1	Total	C	O	P	0
			100	81	17	2	
51	o	1	Total	C	O	P	0
			90	71	17	2	
51	x	1	Total	C	O	P	0
			75	56	17	2	
51	z	1	Total	C	O	P	0
			58	39	17	2	

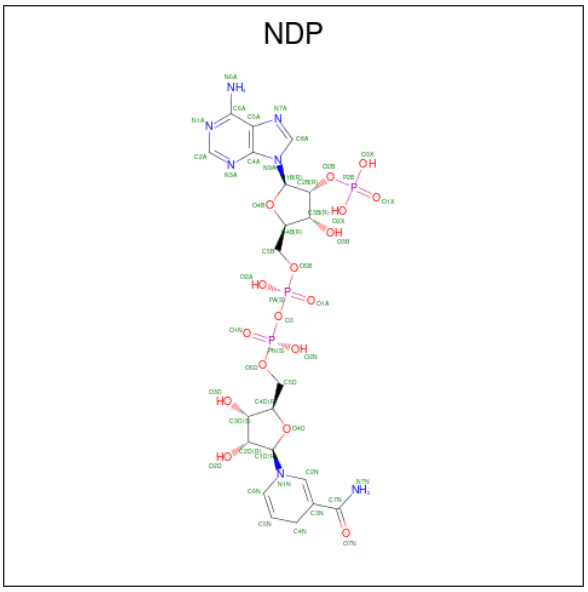
- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

Mol	Chain	Residues	Atoms						AltConf
52	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
52	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

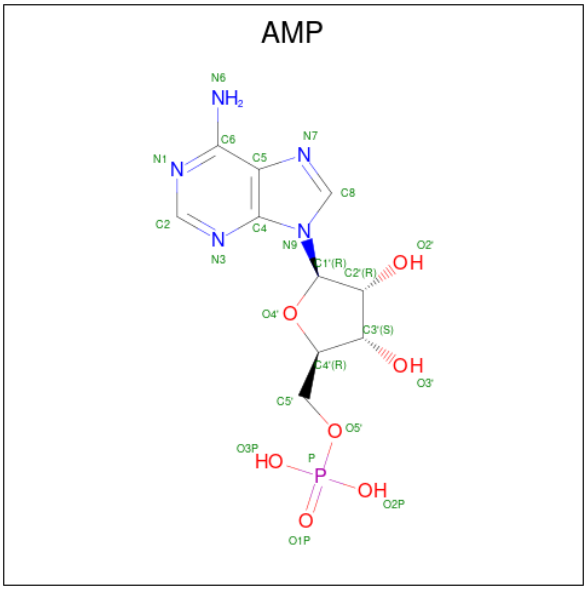
Mol	Chain	Residues	Atoms		AltConf
53	b	1	Total	Zn	0
			1	1	

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



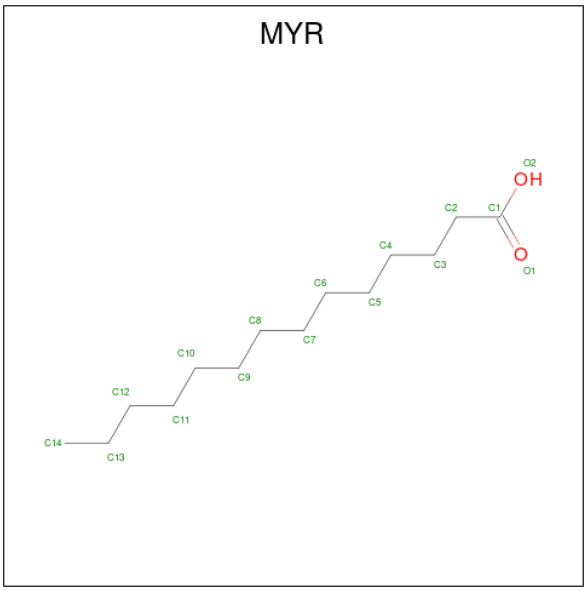
Mol	Chain	Residues	Atoms					AltConf
54	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
55	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 56 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



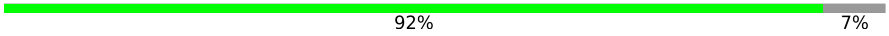
Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			15	14	1	

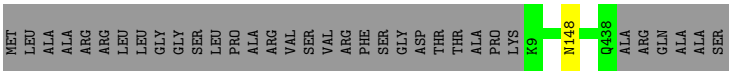
3 Residue-property plots (i)

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

• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



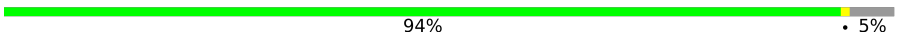


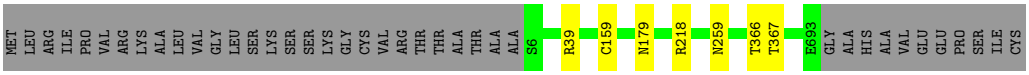
• Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:

• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

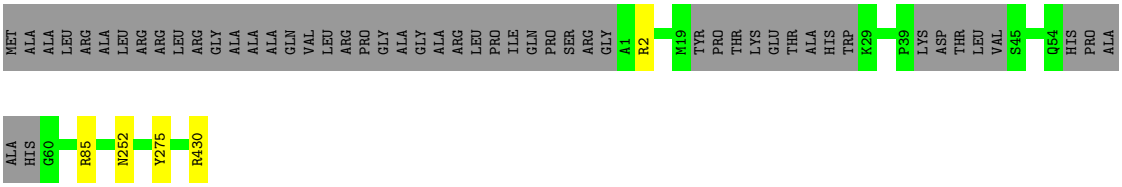
Chain 3:





• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:

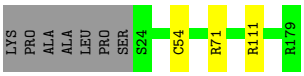


• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:

• Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:

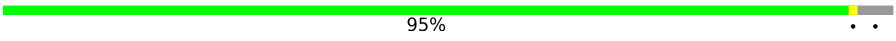


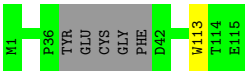
• Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:

• Molecule 8: NADH-ubiquinone oxidoreductase chain 3

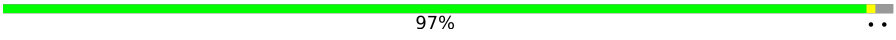
Chain A:

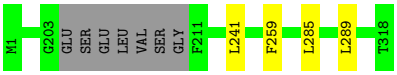




• Molecule 9: NADH-ubiquinone oxidoreductase chain 1

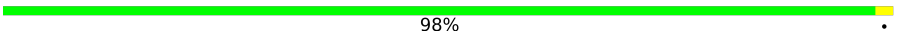
Chain H:

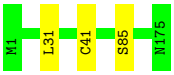




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

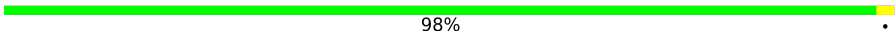
Chain J:





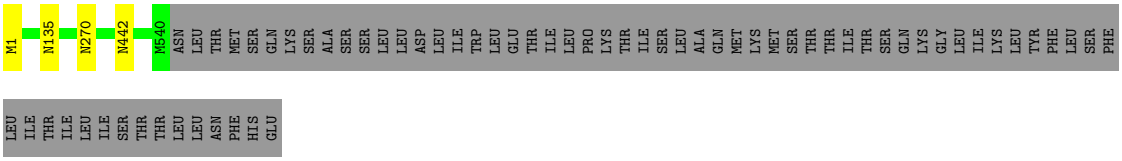
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



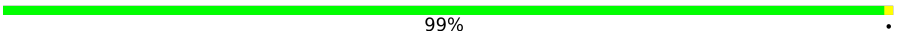
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



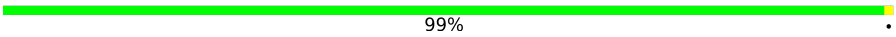
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



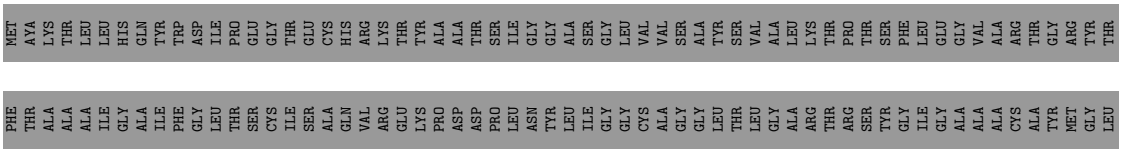
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



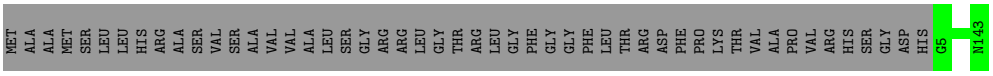
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V:



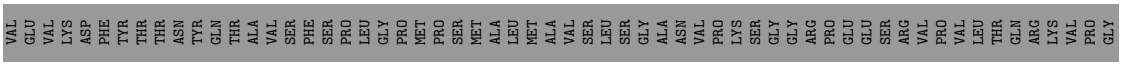
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

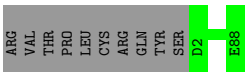
Chain W:



• Molecule 17: Acyl carrier protein

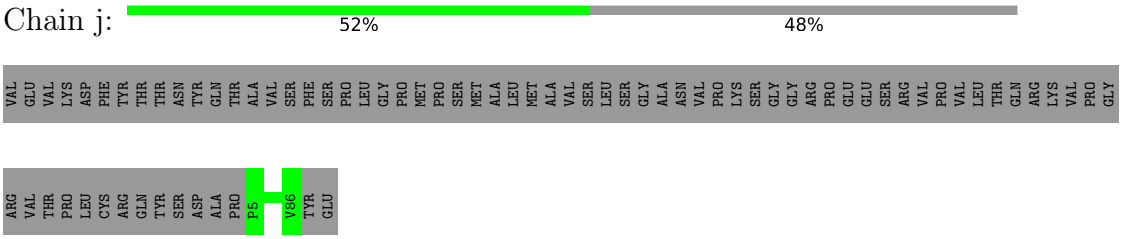
Chain X:





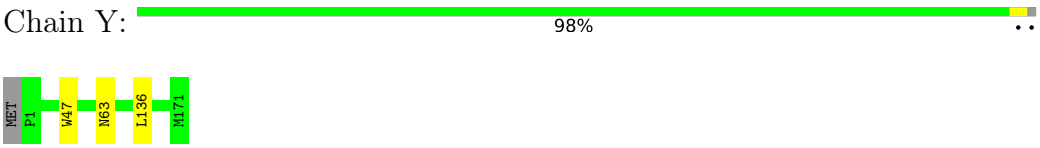
• Molecule 17: Acyl carrier protein

Chain j:



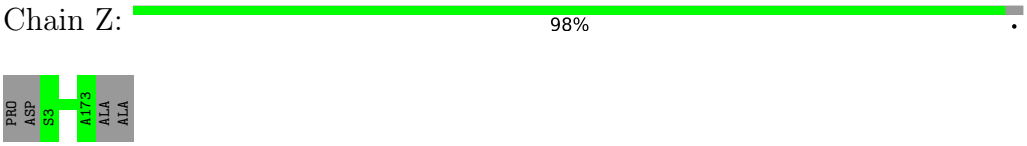
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:



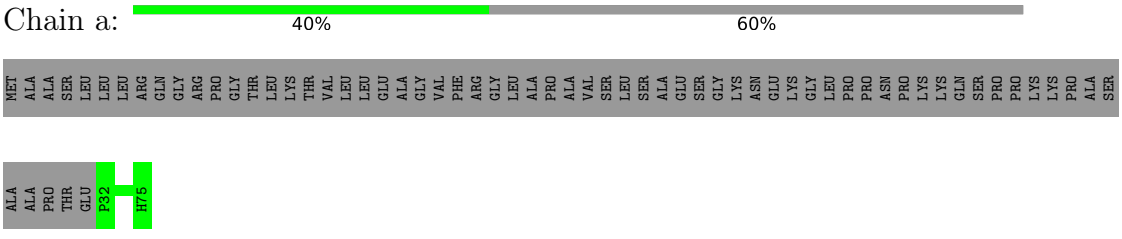
• Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:



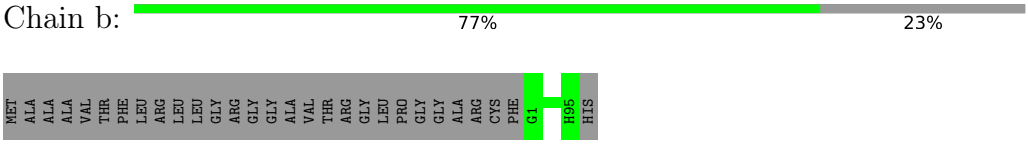
• Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:



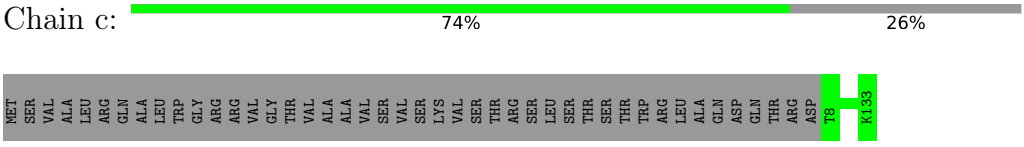
• Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:



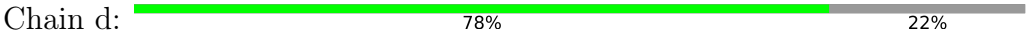
• Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

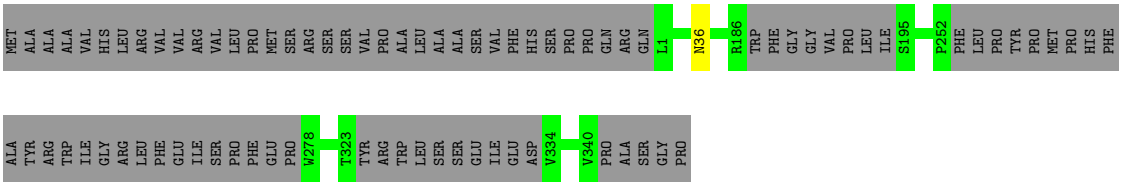
Chain c:



• Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:



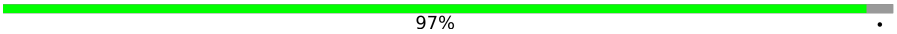


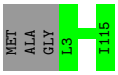
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:

• Molecule 25: Mitochondrial complex I, B13 subunit

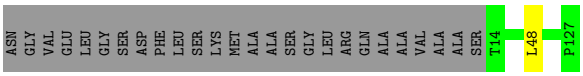
Chain f:





• Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:

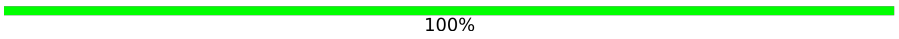


• Molecule 27: Mitochondrial complex I, B14.5a subunit

Chain h:

• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

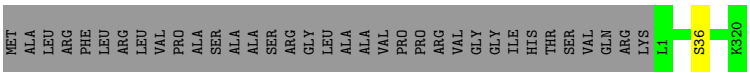
Chain i:



There are no outlier residues recorded for this chain.

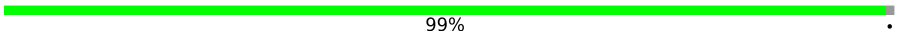
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:



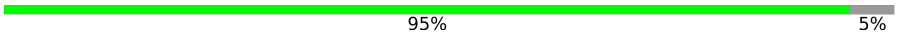
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

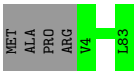
Chain l:



• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

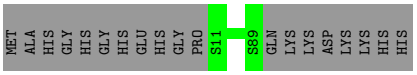
Chain m:





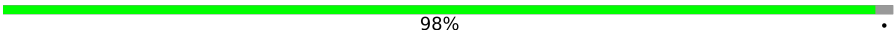
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n:



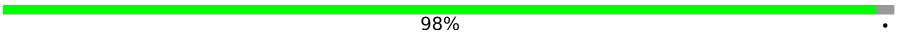
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:



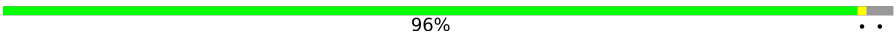
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

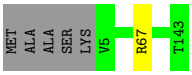
Chain p:



• Molecule 35: Mitochondrial complex I, B16.6 subunit

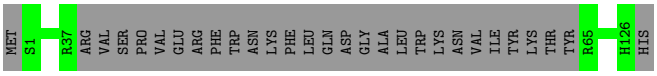
Chain q:





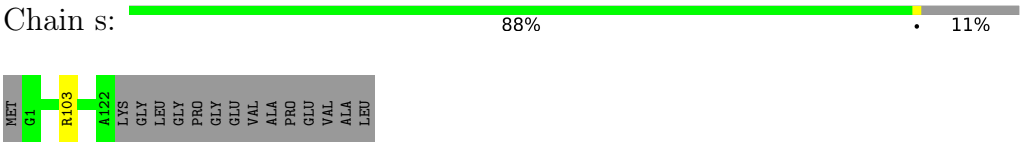
• Molecule 36: Mitochondrial complex I, B17 subunit

Chain r:



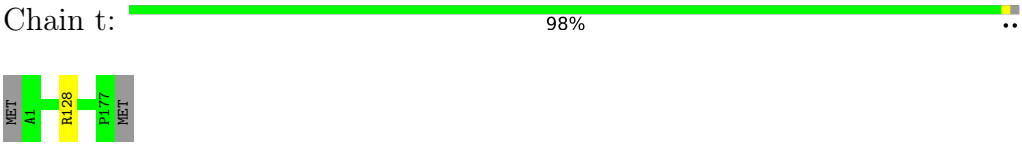
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain s:



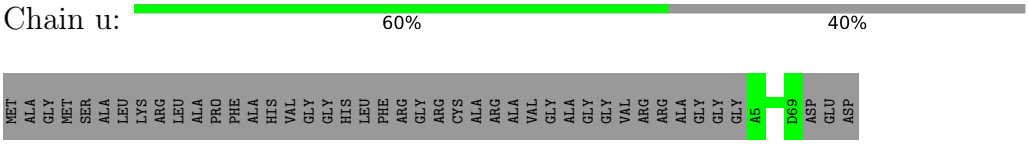
• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain t:



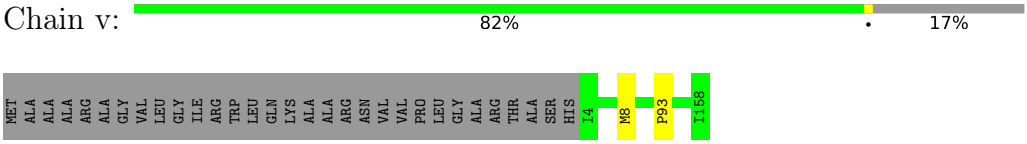
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u:



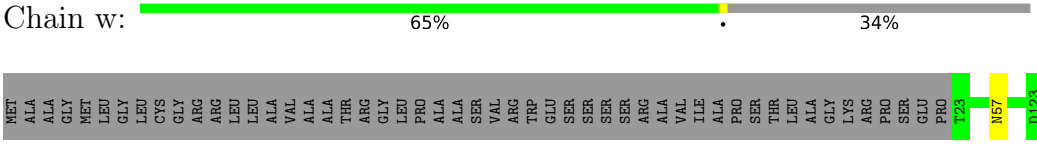
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:



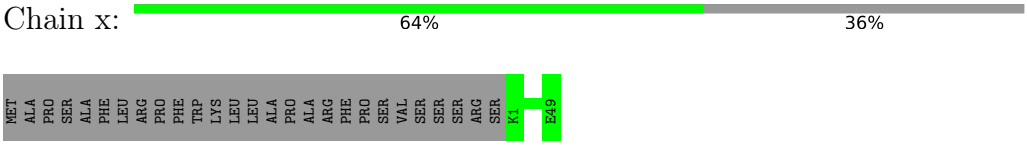
• Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w:



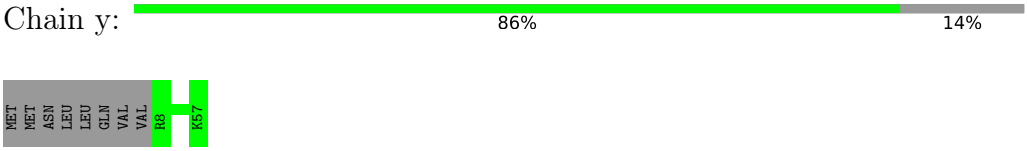
• Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x:



• Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y:



• Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, FES, AMP, ZMP, AYA, 2MR, 3PE, MYR, FME, NDP, SF4, K, FMN, SEP, ZN, PC1

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	1	0.45	0/3386	0.59	0/4575
2	2	0.43	0/1695	0.59	0/2306
3	3	0.47	1/5362 (0.0%)	0.60	0/7266
4	4	0.50	0/3368	0.62	0/4555
5	5	0.48	0/1776	0.57	0/2417
6	6	0.54	0/1278	0.58	0/1728
7	9	0.55	0/1445	0.63	1/1956 (0.1%)
8	A	0.37	0/902	0.62	0/1234
9	H	0.45	0/2553	0.67	2/3492 (0.1%)
10	J	0.44	1/1378 (0.1%)	0.67	1/1868 (0.1%)
11	K	0.38	0/749	0.68	1/1014 (0.1%)
12	L	0.34	0/4395	0.56	0/5983
13	M	0.37	0/3731	0.62	1/5085 (0.0%)
14	N	0.40	0/2787	0.64	2/3795 (0.1%)
15	V	0.26	0/152	0.48	0/203
16	W	0.36	0/1188	0.52	0/1607
17	X	0.31	0/713	0.52	0/963
17	j	0.32	0/670	0.54	0/902
18	Y	0.39	0/1440	0.54	1/1942 (0.1%)
19	Z	0.35	0/1475	0.49	0/1989
20	a	0.36	0/383	0.53	0/518
21	b	0.44	0/749	0.52	0/1009
22	c	0.43	0/1047	0.52	0/1415
23	d	0.39	0/2424	0.55	0/3276
24	e	0.35	0/702	0.52	0/945
25	f	0.37	0/937	0.55	0/1271
26	g	0.41	0/993	0.55	1/1336 (0.1%)
27	h	0.43	0/779	0.56	0/1053
28	i	0.44	0/1250	0.52	0/1698
29	k	0.30	0/2646	0.48	0/3579
30	l	0.40	0/896	0.57	0/1200
31	m	0.36	0/647	0.52	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	n	0.28	0/653	0.47	0/882
33	o	0.39	0/1035	0.51	0/1398
34	p	0.30	0/1085	0.49	0/1467
35	q	0.37	0/1171	0.54	0/1579
36	r	0.32	0/874	0.53	0/1188
37	s	0.28	0/1072	0.47	0/1436
38	t	0.31	0/1573	0.53	0/2130
39	u	0.31	0/590	0.46	0/810
40	v	0.29	0/1361	0.55	2/1861 (0.1%)
41	w	0.36	0/872	0.52	0/1185
42	x	0.28	0/425	0.40	0/576
43	y	0.31	0/449	0.51	0/605
44	z	0.45	0/591	0.59	0/795
All	All	0.40	2/65647 (0.0%)	0.57	12/88982 (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
3	3	0	3
4	4	0	1
8	A	0	1
10	J	0	1
14	N	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	159	CYS	CB-SG	-8.47	1.67	1.82
10	J	41	CYS	CB-SG	-5.71	1.72	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	241	LEU	CB-CG-CD1	-6.05	100.71	111.00
7	9	40	TYR	CB-CG-CD2	-6.00	117.40	121.00
11	K	19	LEU	CA-CB-CG	5.76	128.54	115.30
40	v	8	MET	C-N-CA	5.66	135.84	121.70
14	N	146	LEU	CA-CB-CG	5.57	128.12	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	v	93	PRO	C-N-CA	5.50	135.44	121.70
14	N	170	LEU	CA-CB-CG	5.47	127.89	115.30
10	J	31	LEU	CA-CB-CG	5.31	127.50	115.30
13	M	458	LEU	CA-CB-CG	5.13	127.09	115.30
9	H	289	LEU	CA-CB-CG	-5.12	103.52	115.30
18	Y	136	LEU	CA-CB-CG	5.10	127.02	115.30
26	g	48	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	218	ARG	Peptide
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide
8	A	113	TRP	Peptide
10	J	85	SER	Peptide
14	N	302	LEU	Peptide
14	N	305	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	411 (96%)	17 (4%)	0	100	100
2	2	211/246 (86%)	195 (92%)	16 (8%)	0	100	100
3	3	686/727 (94%)	657 (96%)	28 (4%)	1 (0%)	48	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	402/463 (87%)	388 (96%)	14 (4%)	0	100	100
5	5	206/266 (77%)	197 (96%)	9 (4%)	0	100	100
6	6	154/223 (69%)	147 (96%)	7 (4%)	0	100	100
7	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
8	A	106/115 (92%)	96 (91%)	10 (9%)	0	100	100
9	H	307/318 (96%)	299 (97%)	8 (3%)	0	100	100
10	J	173/175 (99%)	155 (90%)	18 (10%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	538/606 (89%)	513 (95%)	25 (5%)	0	100	100
13	M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	N	345/347 (99%)	330 (96%)	15 (4%)	0	100	100
15	V	17/141 (12%)	16 (94%)	1 (6%)	0	100	100
16	W	137/189 (72%)	135 (98%)	2 (2%)	0	100	100
17	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100
17	j	80/157 (51%)	74 (92%)	6 (8%)	0	100	100
18	Y	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
21	b	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
22	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
23	d	289/380 (76%)	283 (98%)	6 (2%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
25	f	111/116 (96%)	107 (96%)	4 (4%)	0	100	100
26	g	112/140 (80%)	106 (95%)	6 (5%)	0	100	100
27	h	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
28	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
29	k	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
30	l	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
31	m	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
32	n	77/98 (79%)	74 (96%)	3 (4%)	0	100	100
33	o	118/122 (97%)	114 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	p	126/130 (97%)	119 (94%)	7 (6%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	88 (93%)	7 (7%)	0	100	100
37	s	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
38	t	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
39	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
40	v	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
41	w	99/154 (64%)	92 (93%)	7 (7%)	0	100	100
42	x	47/76 (62%)	47 (100%)	0	0	100	100
43	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
44	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
All	All	7854/9247 (85%)	7532 (96%)	321 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	367	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	343 (100%)	1 (0%)	91	96
2	2	183/210 (87%)	182 (100%)	1 (0%)	86	94
3	3	578/608 (95%)	576 (100%)	2 (0%)	91	96
4	4	354/391 (90%)	351 (99%)	3 (1%)	79	90
5	5	189/230 (82%)	188 (100%)	1 (0%)	86	94
6	6	132/181 (73%)	129 (98%)	3 (2%)	45	75
7	9	151/179 (84%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	A	99/103 (96%)	99 (100%)	0	100 100
9	H	272/278 (98%)	270 (99%)	2 (1%)	81 91
10	J	144/144 (100%)	144 (100%)	0	100 100
11	K	86/86 (100%)	85 (99%)	1 (1%)	67 86
12	L	475/538 (88%)	472 (99%)	3 (1%)	84 93
13	M	411/411 (100%)	410 (100%)	1 (0%)	92 97
14	N	315/315 (100%)	314 (100%)	1 (0%)	91 96
15	V	15/102 (15%)	15 (100%)	0	100 100
16	W	122/160 (76%)	122 (100%)	0	100 100
17	X	80/141 (57%)	80 (100%)	0	100 100
17	j	76/141 (54%)	76 (100%)	0	100 100
18	Y	154/155 (99%)	152 (99%)	2 (1%)	65 85
19	Z	155/157 (99%)	155 (100%)	0	100 100
20	a	43/93 (46%)	43 (100%)	0	100 100
21	b	79/97 (81%)	79 (100%)	0	100 100
22	c	113/150 (75%)	113 (100%)	0	100 100
23	d	255/326 (78%)	254 (100%)	1 (0%)	89 95
24	e	76/82 (93%)	76 (100%)	0	100 100
25	f	101/102 (99%)	101 (100%)	0	100 100
26	g	107/124 (86%)	107 (100%)	0	100 100
27	h	84/96 (88%)	84 (100%)	0	100 100
28	i	131/131 (100%)	131 (100%)	0	100 100
29	k	283/309 (92%)	283 (100%)	0	100 100
30	l	94/95 (99%)	94 (100%)	0	100 100
31	m	69/72 (96%)	69 (100%)	0	100 100
32	n	61/76 (80%)	61 (100%)	0	100 100
33	o	107/109 (98%)	107 (100%)	0	100 100
34	p	114/116 (98%)	114 (100%)	0	100 100
35	q	119/122 (98%)	118 (99%)	1 (1%)	79 90
36	r	95/122 (78%)	95 (100%)	0	100 100
37	s	110/120 (92%)	109 (99%)	1 (1%)	75 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	t	159/161 (99%)	158 (99%)	1 (1%)	84 93
39	u	59/84 (70%)	59 (100%)	0	100 100
40	v	140/160 (88%)	140 (100%)	0	100 100
41	w	92/130 (71%)	91 (99%)	1 (1%)	70 87
42	x	44/67 (66%)	44 (100%)	0	100 100
43	y	46/54 (85%)	46 (100%)	0	100 100
44	z	59/59 (100%)	59 (100%)	0	100 100
All	All	6975/7955 (88%)	6949 (100%)	26 (0%)	88 95

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
2	2	122	LYS
3	3	39	ARG
3	3	179	ASN
4	4	2	ARG
4	4	252	ASN
4	4	430	ARG
5	5	195	ARG
6	6	54	CYS
6	6	71	ARG
6	6	111	ARG
9	H	259	PHE
9	H	285	LEU
11	K	50	ASN
12	L	135	ASN
12	L	270	ASN
12	L	442	ASN
13	M	144	ASN
14	N	240	MET
18	Y	47	TRP
18	Y	63	ASN
23	d	36	ASN
35	q	67	ARG
37	s	103	ARG
38	t	128	ARG
41	w	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	257	ASN
1	1	373	ASN
1	1	437	HIS
2	2	121	GLN
2	2	157	ASN
3	3	277	GLN
4	4	5	GLN
4	4	149	ASN
4	4	252	ASN
5	5	87	GLN
9	H	124	ASN
9	H	292	ASN
11	K	50	ASN
11	K	92	ASN
12	L	135	ASN
12	L	199	GLN
12	L	210	ASN
12	L	248	HIS
12	L	270	ASN
12	L	274	GLN
12	L	446	ASN
13	M	81	GLN
13	M	139	GLN
13	M	144	ASN
14	N	235	ASN
16	W	143	ASN
19	Z	114	GLN
23	d	36	ASN
23	d	87	HIS
25	f	49	GLN
26	g	125	HIS
27	h	24	GLN
29	k	107	GLN
29	k	180	GLN
29	k	204	ASN
29	k	287	HIS
34	p	47	GLN
35	q	53	ASN
38	t	25	HIS
38	t	138	GLN
41	w	57	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	$\#\|Z\| > 2$
12	FME	L	1	12	8,9,10	0.85	0	7,9,11	1.61	2 (28%)
11	FME	K	1	11	8,9,10	0.95	0	7,9,11	0.91	0
4	2MR	4	85	4	10,12,13	2.41	3 (30%)	5,13,15	1.01	0
13	FME	M	1	13	8,9,10	0.96	1 (12%)	7,9,11	1.01	0
29	SEP	k	36	29	8,9,10	1.55	1 (12%)	8,12,14	1.53	2 (25%)
27	AYA	h	1	27	6,7,8	1.27	1 (16%)	5,8,10	1.43	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L	1	12	-	3/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
4	2MR	4	85	4	-	3/10/13/15	-
13	FME	M	1	13	-	1/7/9/11	-
29	SEP	k	36	29	-	4/5/8/10	-
27	AYA	h	1	27	-	0/4/6/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	4.87	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.75	1.43	1.33
29	k	36	SEP	P-O1P	3.32	1.61	1.50
27	h	1	AYA	CA-N	-2.64	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.25	1.41	1.46
13	M	1	FME	CA-N	-2.00	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	1	FME	C-CA-N	3.29	115.66	109.73
27	h	1	AYA	CB-CA-N	2.92	112.86	109.61
29	k	36	SEP	P-OG-CB	-2.86	110.41	118.30
29	k	36	SEP	OG-CB-CA	2.64	110.72	108.14
12	L	1	FME	CA-N-CN	2.28	126.33	122.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	C-CA-CB-CG
29	k	36	SEP	CB-OG-P-O1P
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
4	4	85	2MR	C-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
4	4	85	2MR	CA-CB-CG-CD
4	4	85	2MR	NE-CD-CG-CB
12	L	1	FME	N-CA-CB-CG
29	k	36	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
49	3PE	6	202	-	50,50,50	0.31	0	53,55,55	0.32	0
46	FMN	1	501	-	33,33,33	1.24	2 (6%)	48,50,50	1.28	6 (12%)
50	PC1	A	402	-	36,36,53	0.36	0	42,44,61	0.58	1 (2%)
56	MYR	s	201	37	14,14,15	0.22	0	13,13,15	0.19	0
49	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.51	2 (3%)
52	ZMP	g	201	-	27,33,36	0.69	1 (3%)	32,40,45	1.52	6 (18%)
51	CDL	M	501	-	99,99,99	0.25	0	105,111,111	0.31	0
45	SF4	1	500	1	0,12,12	-	-	-		
45	SF4	9	402	7	0,12,12	-	-	-		
45	SF4	3	802	3	0,12,12	-	-	-		
45	SF4	6	201	6	0,12,12	-	-	-		
51	CDL	Y	201	-	99,99,99	0.27	0	105,111,111	0.33	0
55	AMP	k	501	-	22,25,25	0.93	1 (4%)	25,38,38	1.31	3 (12%)
50	PC1	V	201	-	35,35,53	0.36	0	41,43,61	0.29	0
49	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.29	0
51	CDL	x	101	-	74,74,99	0.32	0	80,86,111	0.44	1 (1%)
51	CDL	W	201	-	99,99,99	0.29	0	105,111,111	0.30	0
51	CDL	z	101	-	57,57,99	0.36	0	63,69,111	0.34	0
49	3PE	N	402	-	30,30,50	0.38	0	33,35,55	0.40	0
49	3PE	L	1003	-	30,30,50	0.42	0	33,35,55	0.72	1 (3%)
45	SF4	9	403	7	0,12,12	-	-	-		
49	3PE	L	1001	-	50,50,50	0.31	0	53,55,55	0.39	0
49	3PE	A	403	-	50,50,50	0.30	0	53,55,55	0.29	0
47	FES	3	803	3	0,4,4	-	-	-		
50	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.61	1 (1%)
49	3PE	H	401	-	50,50,50	0.32	0	53,55,55	0.44	1 (1%)
50	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.49	0
51	CDL	o	201	-	89,89,99	0.30	0	95,101,111	0.41	0
50	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.38	0
52	ZMP	X	101	17	24,30,36	0.82	1 (4%)	29,37,45	0.97	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	PC1	A	401	-	45,45,53	0.32	0	51,53,61	0.36	0
47	FES	2	300	2	0,4,4	-	-	-		
45	SF4	3	801	3	0,12,12	-	-	-		
54	NDP	d	401	-	45,52,52	0.64	0	53,80,80	0.59	1 (1%)

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
49	3PE	6	202	-	-	11/54/54/54	-
46	FMN	1	501	-	-	9/18/18/18	0/3/3/3
50	PC1	A	402	-	-	6/40/40/57	-
56	MYR	s	201	37	-	3/11/12/13	-
49	3PE	N	401	-	-	20/54/54/54	-
52	ZMP	g	201	-	-	5/38/40/43	-
51	CDL	M	501	-	1/1/9/9	36/110/110/110	-
45	SF4	1	500	1	-	-	0/6/5/5
45	SF4	9	402	7	-	-	0/6/5/5
51	CDL	Y	201	-	1/1/9/9	32/110/110/110	-
55	AMP	k	501	-	-	5/6/26/26	0/3/3/3
45	SF4	3	802	3	-	-	0/6/5/5
45	SF4	6	201	6	-	-	0/6/5/5
51	CDL	x	101	-	2/2/9/9	21/85/85/110	-
49	3PE	i	201	-	-	5/54/54/54	-
50	PC1	V	201	-	-	11/39/39/57	-
51	CDL	z	101	-	-	20/68/68/110	-
49	3PE	N	402	-	-	4/34/34/54	-
49	3PE	L	1003	-	-	13/34/34/54	-
49	3PE	L	1001	-	-	12/54/54/54	-
45	SF4	9	403	7	-	-	0/6/5/5
49	3PE	A	403	-	-	15/54/54/54	-
47	FES	3	803	3	-	-	0/1/1/1
50	PC1	L	1002	-	-	13/57/57/57	-
49	3PE	H	401	-	-	14/54/54/54	-
45	SF4	3	801	3	-	-	0/6/5/5
50	PC1	9	401	-	-	17/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	o	201	-	-	29/100/100/110	-
50	PC1	w	801	-	-	11/57/57/57	-
52	ZMP	X	101	17	-	14/35/37/43	-
50	PC1	A	401	-	-	8/49/49/57	-
47	FES	2	300	2	-	-	0/1/1/1
51	CDL	W	201	-	-	27/110/110/110	-
54	NDP	d	401	-	-	4/30/77/77	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	501	FMN	C4A-N5	3.11	1.36	1.30
52	X	101	ZMP	C9-C10	2.95	1.53	1.50
55	k	501	AMP	C5-C4	2.87	1.48	1.40
52	g	201	ZMP	C10-S1	-2.11	1.71	1.76
46	1	501	FMN	C4A-C10	-2.07	1.38	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	g	201	ZMP	C14-C15-N2	-3.65	104.53	111.90
46	1	501	FMN	C4-N3-C2	-3.54	119.10	125.64
52	g	201	ZMP	C15-C14-C13	-3.50	106.52	112.36
52	g	201	ZMP	O1-C10-C9	-3.20	120.22	123.99
55	k	501	AMP	C1'-N9-C4	3.07	132.04	126.64
46	1	501	FMN	C4A-C10-N10	2.94	120.78	116.48
46	1	501	FMN	O4-C4-C4A	-2.85	119.04	126.60
55	k	501	AMP	N3-C2-N1	-2.85	124.23	128.68
52	g	201	ZMP	C9-C10-S1	2.76	116.67	113.46
46	1	501	FMN	C4A-C4-N3	2.69	120.01	113.19
52	g	201	ZMP	C20-C18-C17	2.55	113.25	108.82
46	1	501	FMN	C4A-C10-N1	-2.49	118.95	124.73
49	L	1003	3PE	C2-O21-C21	2.48	123.90	117.79
50	L	1002	PC1	C2-O21-C21	2.37	123.64	117.79
46	1	501	FMN	C4-C4A-C10	2.31	120.67	116.79
55	k	501	AMP	C4-C5-N7	-2.28	107.02	109.40
52	X	101	ZMP	O1-C10-C9	-2.25	121.34	123.99
50	A	402	PC1	C2-O21-C21	2.19	123.17	117.79
54	d	401	NDP	C5A-C6A-N6A	2.14	123.61	120.35
49	N	401	3PE	C2-O21-C21	2.14	123.05	117.79
49	H	401	3PE	O31-C3-C2	2.08	114.49	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	N	401	3PE	O21-C2-C1	2.07	115.89	108.40
51	x	101	CDL	CB4-OB6-CB5	2.02	122.76	117.79
52	g	201	ZMP	C8-C9-C10	-2.01	107.88	112.33

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
51	M	501	CDL	CB4
51	Y	201	CDL	CB4
51	x	101	CDL	CA4
51	x	101	CDL	CB4

All (365) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	501	FMN	N10-C1'-C2'-O2'
46	1	501	FMN	C5'-O5'-P-O2P
46	1	501	FMN	C5'-O5'-P-O3P
49	6	202	3PE	C11-O13-P-O14
49	6	202	3PE	O13-C11-C12-N
49	A	403	3PE	C11-O13-P-O12
49	A	403	3PE	C11-O13-P-O14
49	A	403	3PE	O13-C11-C12-N
49	H	401	3PE	C11-O13-P-O11
49	H	401	3PE	C11-O13-P-O12
49	H	401	3PE	C11-O13-P-O14
49	H	401	3PE	O13-C11-C12-N
49	L	1001	3PE	C1-O11-P-O14
49	L	1003	3PE	C1-O11-P-O12
49	L	1003	3PE	C1-O11-P-O14
49	L	1003	3PE	C11-O13-P-O12
49	L	1003	3PE	C11-O13-P-O14
49	L	1003	3PE	O13-C11-C12-N
49	N	401	3PE	C11-O13-P-O12
49	N	401	3PE	C11-O13-P-O14
49	N	402	3PE	C11-O13-P-O11
49	i	201	3PE	C11-O13-P-O11
49	i	201	3PE	C11-O13-P-O14
50	9	401	PC1	C11-O13-P-O14
50	L	1002	PC1	C1-O11-P-O12
50	V	201	PC1	C11-O13-P-O12
50	V	201	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
50	V	201	PC1	C1-O11-P-O14
50	w	801	PC1	O13-C11-C12-N
51	M	501	CDL	CA3-OA5-PA1-OA2
51	M	501	CDL	CA3-OA5-PA1-OA3
51	M	501	CDL	CA3-OA5-PA1-OA4
51	W	201	CDL	CA2-OA2-PA1-OA3
51	W	201	CDL	CA2-OA2-PA1-OA4
51	W	201	CDL	CB3-OB5-PB2-OB3
51	Y	201	CDL	O1-C1-CB2-OB2
51	Y	201	CDL	CB3-OB5-PB2-OB2
51	Y	201	CDL	CB3-OB5-PB2-OB3
51	o	201	CDL	CA2-OA2-PA1-OA3
51	o	201	CDL	CA2-OA2-PA1-OA4
51	o	201	CDL	CB2-OB2-PB2-OB3
51	o	201	CDL	CB2-OB2-PB2-OB4
51	o	201	CDL	CB2-OB2-PB2-OB5
51	x	101	CDL	CA2-OA2-PA1-OA3
51	x	101	CDL	CA2-OA2-PA1-OA4
51	x	101	CDL	CA2-OA2-PA1-OA5
51	x	101	CDL	CB3-OB5-PB2-OB4
51	z	101	CDL	CA2-C1-CB2-OB2
51	z	101	CDL	CB3-OB5-PB2-OB2
51	z	101	CDL	CB3-OB5-PB2-OB3
51	z	101	CDL	CB3-OB5-PB2-OB4
52	X	101	ZMP	O4-C17-C18-C21
52	X	101	ZMP	C16-C17-C18-C21
52	X	101	ZMP	O3-C16-C17-O4
52	X	101	ZMP	C17-C16-N2-C15
52	X	101	ZMP	C7-C8-C9-C10
52	g	201	ZMP	S1-C11-C12-N1
55	k	501	AMP	C5'-O5'-P-O1P
55	k	501	AMP	C5'-O5'-P-O2P
55	k	501	AMP	C5'-O5'-P-O3P
51	z	101	CDL	O1-C1-CB2-OB2
52	X	101	ZMP	O3-C16-N2-C15
51	M	501	CDL	CA2-C1-CB2-OB2
51	x	101	CDL	CB7-C71-C72-C73
51	M	501	CDL	CB7-C71-C72-C73
50	A	401	PC1	C11-C12-N-C14
51	x	101	CDL	CA7-C31-C32-C33
49	6	202	3PE	C11-O13-P-O11
49	A	403	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
49	L	1001	3PE	C1-O11-P-O13
49	L	1003	3PE	C1-O11-P-O13
49	L	1003	3PE	C11-O13-P-O11
49	N	401	3PE	C11-O13-P-O11
50	V	201	PC1	C11-O13-P-O11
50	V	201	PC1	C1-O11-P-O13
51	M	501	CDL	CB2-OB2-PB2-OB5
51	W	201	CDL	CA2-OA2-PA1-OA5
51	W	201	CDL	CA3-OA5-PA1-OA2
51	o	201	CDL	CA2-OA2-PA1-OA5
51	o	201	CDL	CB3-OB5-PB2-OB2
51	x	101	CDL	CA3-OA5-PA1-OA2
51	x	101	CDL	CB2-OB2-PB2-OB5
51	x	101	CDL	CB3-OB5-PB2-OB2
51	z	101	CDL	CA3-OA5-PA1-OA2
51	z	101	CDL	CB2-OB2-PB2-OB5
50	A	401	PC1	C11-C12-N-C15
49	A	403	3PE	C2D-C2E-C2F-C2G
49	N	401	3PE	C32-C33-C34-C35
51	M	501	CDL	C82-C83-C84-C85
51	W	201	CDL	C35-C36-C37-C38
49	6	202	3PE	C36-C37-C38-C39
51	o	201	CDL	C81-C82-C83-C84
51	Y	201	CDL	CA5-C11-C12-C13
51	Y	201	CDL	C52-C53-C54-C55
51	o	201	CDL	C71-C72-C73-C74
50	L	1002	PC1	C3D-C3E-C3F-C3G
51	Y	201	CDL	C81-C82-C83-C84
51	M	501	CDL	O1-C1-CB2-OB2
51	o	201	CDL	C78-C79-C80-C81
52	X	101	ZMP	C3-C4-C5-C6
51	M	501	CDL	C21-C22-C23-C24
49	i	201	3PE	C29-C2A-C2B-C2C
50	L	1002	PC1	C39-C3A-C3B-C3C
51	o	201	CDL	CB5-C51-C52-C53
50	w	801	PC1	C2D-C2E-C2F-C2G
51	M	501	CDL	C77-C78-C79-C80
51	M	501	CDL	C41-C42-C43-C44
51	W	201	CDL	C72-C73-C74-C75
50	w	801	PC1	C31-C32-C33-C34
51	W	201	CDL	CB5-C51-C52-C53
51	M	501	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
50	w	801	PC1	C25-C26-C27-C28
51	M	501	CDL	C22-C23-C24-C25
51	Y	201	CDL	C59-C60-C61-C62
51	M	501	CDL	C53-C54-C55-C56
49	L	1001	3PE	C35-C36-C37-C38
49	A	403	3PE	C38-C39-C3A-C3B
50	9	401	PC1	C22-C21-O21-C2
50	9	401	PC1	C2C-C2D-C2E-C2F
50	w	801	PC1	C3E-C3F-C3G-C3H
51	M	501	CDL	C17-C18-C19-C20
51	W	201	CDL	C19-C20-C21-C22
51	M	501	CDL	C34-C35-C36-C37
51	Y	201	CDL	CB5-C51-C52-C53
49	6	202	3PE	C38-C39-C3A-C3B
51	Y	201	CDL	C12-C13-C14-C15
51	Y	201	CDL	CB7-C71-C72-C73
51	M	501	CDL	C37-C38-C39-C40
50	9	401	PC1	O22-C21-O21-C2
51	M	501	CDL	C56-C57-C58-C59
50	A	401	PC1	C11-C12-N-C13
51	x	101	CDL	C75-C76-C77-C78
50	9	401	PC1	C11-O13-P-O11
51	M	501	CDL	CA2-OA2-PA1-OA5
51	Y	201	CDL	C15-C16-C17-C18
50	L	1002	PC1	C2-C1-O11-P
50	V	201	PC1	C22-C23-C24-C25
49	H	401	3PE	O11-C1-C2-C3
50	L	1002	PC1	O11-C1-C2-C3
51	W	201	CDL	OA5-CA3-CA4-CA6
50	A	401	PC1	C3B-C3C-C3D-C3E
49	N	401	3PE	C2C-C2D-C2E-C2F
51	Y	201	CDL	CA2-C1-CB2-OB2
52	X	101	ZMP	C6-C7-C8-C9
49	N	401	3PE	C1-C2-C3-O31
51	o	201	CDL	CA3-CA4-CA6-OA8
51	z	101	CDL	CA3-CA4-CA6-OA8
51	Y	201	CDL	C13-C14-C15-C16
51	M	501	CDL	C81-C82-C83-C84
49	N	401	3PE	C23-C24-C25-C26
50	9	401	PC1	C39-C3A-C3B-C3C
50	9	401	PC1	C3B-C3C-C3D-C3E
55	k	501	AMP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
46	1	501	FMN	C5'-O5'-P-O1P
50	9	401	PC1	C22-C23-C24-C25
51	W	201	CDL	OB5-CB3-CB4-OB6
49	6	202	3PE	C3D-C3E-C3F-C3G
49	H	401	3PE	C26-C27-C28-C29
51	W	201	CDL	C14-C15-C16-C17
49	N	401	3PE	O13-C11-C12-N
49	N	402	3PE	O13-C11-C12-N
50	w	801	PC1	C21-C22-C23-C24
50	9	401	PC1	C2-C1-O11-P
51	Y	201	CDL	C58-C59-C60-C61
51	M	501	CDL	CA3-CA4-CA6-OA8
51	z	101	CDL	CB3-CB4-CB6-OB8
50	w	801	PC1	C39-C3A-C3B-C3C
51	M	501	CDL	C35-C36-C37-C38
51	Y	201	CDL	C37-C38-C39-C40
51	Y	201	CDL	C54-C55-C56-C57
51	W	201	CDL	CB3-OB5-PB2-OB2
49	L	1001	3PE	C3B-C3C-C3D-C3E
49	L	1001	3PE	O11-C1-C2-O21
52	g	201	ZMP	C12-C11-S1-C10
49	N	401	3PE	O21-C2-C3-O31
51	M	501	CDL	OA6-CA4-CA6-OA8
51	Y	201	CDL	OA6-CA4-CA6-OA8
51	o	201	CDL	OA6-CA4-CA6-OA8
50	A	401	PC1	C23-C24-C25-C26
49	L	1003	3PE	C2-C1-O11-P
51	M	501	CDL	CA4-CA3-OA5-PA1
51	o	201	CDL	C1-CB2-OB2-PB2
51	z	101	CDL	CB4-CB3-OB5-PB2
52	g	201	ZMP	O1-C10-S1-C11
49	N	401	3PE	C28-C29-C2A-C2B
51	W	201	CDL	C31-C32-C33-C34
51	x	101	CDL	C71-C72-C73-C74
49	L	1001	3PE	O11-C1-C2-C3
51	W	201	CDL	OB5-CB3-CB4-CB6
49	L	1001	3PE	C34-C35-C36-C37
51	Y	201	CDL	C23-C24-C25-C26
51	Y	201	CDL	C11-C12-C13-C14
52	g	201	ZMP	C9-C10-S1-C11
51	Y	201	CDL	CA3-CA4-CA6-OA8
50	w	801	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
52	X	101	ZMP	C16-C17-C18-C19
52	X	101	ZMP	C16-C17-C18-C20
51	W	201	CDL	OB6-CB4-CB6-OB8
51	z	101	CDL	OA6-CA4-CA6-OA8
54	d	401	NDP	C5D-O5D-PN-O3
51	W	201	CDL	C83-C84-C85-C86
56	s	201	MYR	C11-C10-C9-C8
50	A	402	PC1	C11-O13-P-O11
50	L	1002	PC1	C1-O11-P-O13
46	1	501	FMN	C4'-C5'-O5'-P
49	H	401	3PE	C2-C1-O11-P
51	z	101	CDL	C1-CB2-OB2-PB2
49	6	202	3PE	C11-O13-P-O12
49	L	1001	3PE	C1-O11-P-O12
49	N	402	3PE	C11-O13-P-O12
50	9	401	PC1	C11-O13-P-O12
50	L	1002	PC1	C1-O11-P-O14
51	M	501	CDL	CA2-OA2-PA1-OA3
51	M	501	CDL	CA2-OA2-PA1-OA4
51	M	501	CDL	CB2-OB2-PB2-OB3
51	W	201	CDL	CA3-OA5-PA1-OA3
51	W	201	CDL	CB3-OB5-PB2-OB4
51	o	201	CDL	CB3-OB5-PB2-OB3
51	o	201	CDL	CB3-OB5-PB2-OB4
51	x	101	CDL	CA3-OA5-PA1-OA3
51	x	101	CDL	CA3-OA5-PA1-OA4
51	x	101	CDL	CB2-OB2-PB2-OB3
51	x	101	CDL	CB3-OB5-PB2-OB3
51	z	101	CDL	CA3-OA5-PA1-OA3
51	z	101	CDL	CA3-OA5-PA1-OA4
51	z	101	CDL	CB2-OB2-PB2-OB3
54	d	401	NDP	C5D-O5D-PN-O2N
50	w	801	PC1	O11-C1-C2-C3
49	H	401	3PE	C12-C11-O13-P
50	V	201	PC1	C12-C11-O13-P
50	w	801	PC1	C26-C27-C28-C29
46	1	501	FMN	N10-C1'-C2'-C3'
49	L	1003	3PE	O11-C1-C2-O21
50	A	402	PC1	O11-C1-C2-O21
51	W	201	CDL	CA7-C31-C32-C33
54	d	401	NDP	O4D-C1D-N1N-C6N
50	9	401	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
50	9	401	PC1	O13-C11-C12-N
50	L	1002	PC1	O13-C11-C12-N
56	s	201	MYR	C1-C2-C3-C4
51	Y	201	CDL	C57-C58-C59-C60
51	o	201	CDL	C31-C32-C33-C34
50	V	201	PC1	C23-C24-C25-C26
51	x	101	CDL	C22-C23-C24-C25
51	o	201	CDL	C12-C13-C14-C15
49	6	202	3PE	C33-C34-C35-C36
49	N	401	3PE	C22-C23-C24-C25
51	W	201	CDL	CA5-C11-C12-C13
50	A	402	PC1	O31-C31-C32-C33
50	9	401	PC1	C3-C2-O21-C21
46	1	501	FMN	O3'-C3'-C4'-C5'
51	o	201	CDL	CB4-CB3-OB5-PB2
49	H	401	3PE	O11-C1-C2-O21
51	W	201	CDL	OA5-CA3-CA4-OA6
51	Y	201	CDL	OB5-CB3-CB4-OB6
49	A	403	3PE	C1-O11-P-O13
49	L	1001	3PE	C11-O13-P-O11
50	9	401	PC1	C1-O11-P-O13
51	o	201	CDL	CA3-OA5-PA1-OA2
51	z	101	CDL	CA2-OA2-PA1-OA5
52	X	101	ZMP	O4-C17-C18-C19
51	o	201	CDL	C53-C54-C55-C56
50	9	401	PC1	C3C-C3D-C3E-C3F
50	L	1002	PC1	C29-C2A-C2B-C2C
51	Y	201	CDL	C62-C63-C64-C65
50	A	401	PC1	C3A-C3B-C3C-C3D
51	z	101	CDL	OB6-CB4-CB6-OB8
50	V	201	PC1	O31-C31-C32-C33
49	L	1001	3PE	C26-C27-C28-C29
55	k	501	AMP	O4'-C4'-C5'-O5'
51	W	201	CDL	CB3-CB4-CB6-OB8
52	X	101	ZMP	C19-C18-C21-O5
51	o	201	CDL	C63-C64-C65-C66
49	L	1003	3PE	C1-C2-O21-C21
49	N	401	3PE	C3-C2-O21-C21
50	L	1002	PC1	C1-C2-O21-C21
49	H	401	3PE	C3F-C3G-C3H-C3I
51	o	201	CDL	C57-C58-C59-C60
51	Y	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
51	z	101	CDL	O1-C1-CA2-OA2
50	A	401	PC1	C26-C27-C28-C29
51	W	201	CDL	C53-C54-C55-C56
49	A	403	3PE	C3C-C3D-C3E-C3F
51	o	201	CDL	C80-C81-C82-C83
49	N	402	3PE	C25-C26-C27-C28
52	X	101	ZMP	C2-C3-C4-C5
50	V	201	PC1	C35-C36-C37-C38
49	H	401	3PE	C29-C2A-C2B-C2C
51	x	101	CDL	C52-C51-CB5-OB6
49	A	403	3PE	C3A-C3B-C3C-C3D
54	d	401	NDP	O4B-C4B-C5B-O5B
50	L	1002	PC1	O11-C1-C2-O21
51	x	101	CDL	OA5-CA3-CA4-OA6
49	L	1001	3PE	C36-C37-C38-C39
51	x	101	CDL	OA5-CA3-CA4-CA6
46	1	501	FMN	C2'-C3'-C4'-O4'
49	N	401	3PE	C33-C34-C35-C36
50	L	1002	PC1	C32-C33-C34-C35
52	X	101	ZMP	N2-C16-C17-O4
52	g	201	ZMP	N2-C16-C17-O4
49	6	202	3PE	C2D-C2E-C2F-C2G
51	M	501	CDL	C39-C40-C41-C42
49	N	401	3PE	C38-C39-C3A-C3B
49	i	201	3PE	O21-C21-C22-C23
51	Y	201	CDL	C31-C32-C33-C34
51	M	501	CDL	C58-C59-C60-C61
51	o	201	CDL	C34-C35-C36-C37
51	M	501	CDL	C32-C31-CA7-OA8
46	1	501	FMN	O3'-C3'-C4'-O4'
49	H	401	3PE	C3C-C3D-C3E-C3F
49	L	1003	3PE	O21-C21-C22-C23
51	x	101	CDL	C72-C71-CB7-OB8
49	A	403	3PE	C35-C36-C37-C38
49	A	403	3PE	O21-C2-C3-O31
50	A	402	PC1	O21-C21-C22-C23
51	z	101	CDL	C52-C51-CB5-OB6
49	A	403	3PE	O21-C21-C22-C23
51	Y	201	CDL	C82-C83-C84-C85
49	6	202	3PE	C23-C24-C25-C26
51	M	501	CDL	C72-C73-C74-C75
51	W	201	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
49	i	201	3PE	O22-C21-C22-C23
49	6	202	3PE	C25-C26-C27-C28
51	M	501	CDL	C32-C31-CA7-OA9
49	N	401	3PE	C3B-C3C-C3D-C3E
51	M	501	CDL	C79-C80-C81-C82
49	L	1003	3PE	O22-C21-C22-C23
51	W	201	CDL	CA3-CA4-CA6-OA8
51	Y	201	CDL	C14-C15-C16-C17
50	V	201	PC1	C27-C28-C29-C2A
49	A	403	3PE	C2-C1-O11-P
51	M	501	CDL	C84-C85-C86-C87
49	N	401	3PE	C1-O11-P-O12
49	N	401	3PE	C1-O11-P-O14
50	A	402	PC1	C11-O13-P-O12
50	w	801	PC1	C1-O11-P-O14
51	Y	201	CDL	CB2-OB2-PB2-OB3
49	A	403	3PE	O22-C21-C22-C23
50	9	401	PC1	C3D-C3E-C3F-C3G
51	Y	201	CDL	C12-C11-CA5-OA6
56	s	201	MYR	C9-C10-C11-C12
51	W	201	CDL	C58-C59-C60-C61
51	M	501	CDL	C52-C51-CB5-OB6
49	N	401	3PE	C21-C22-C23-C24
49	L	1003	3PE	C12-C11-O13-P
49	N	401	3PE	C12-C11-O13-P
50	9	401	PC1	C12-C11-O13-P
50	A	402	PC1	C1-C2-O21-C21
51	o	201	CDL	CB3-CB4-OB6-CB5
51	x	101	CDL	C72-C71-CB7-OB9
51	Y	201	CDL	C32-C31-CA7-OA8
49	N	401	3PE	C31-C32-C33-C34
51	z	101	CDL	C52-C51-CB5-OB7
49	H	401	3PE	O31-C31-C32-C33
50	A	401	PC1	O31-C31-C32-C33
50	L	1002	PC1	O31-C31-C32-C33
51	Y	201	CDL	C76-C77-C78-C79
49	A	403	3PE	C24-C25-C26-C27
51	o	201	CDL	C54-C55-C56-C57
49	L	1001	3PE	O21-C21-C22-C23
49	H	401	3PE	O32-C31-C32-C33
51	M	501	CDL	C52-C51-CB5-OB7
51	Y	201	CDL	C32-C31-CA7-OA9

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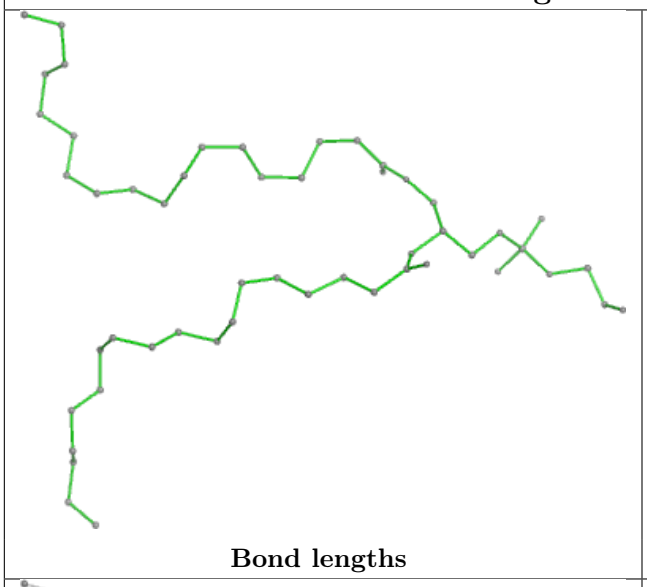
Mol	Chain	Res	Type	Atoms
51	o	201	CDL	C15-C16-C17-C18
51	o	201	CDL	C58-C59-C60-C61

There are no ring outliers.

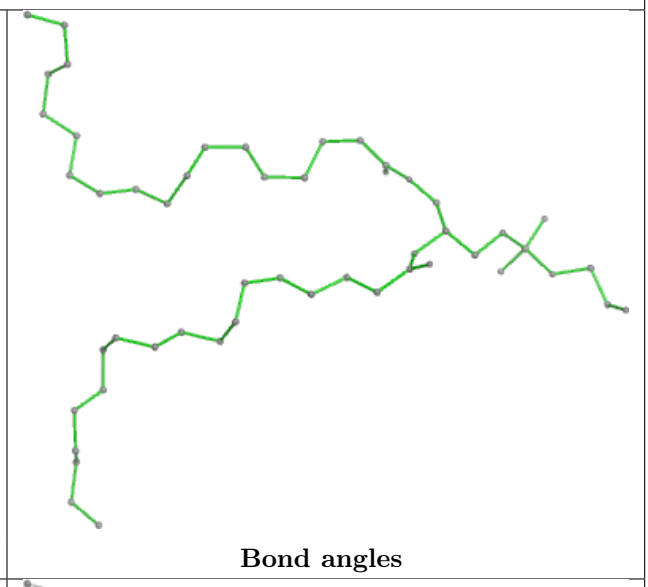
No monomer is involved in short contacts.

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.

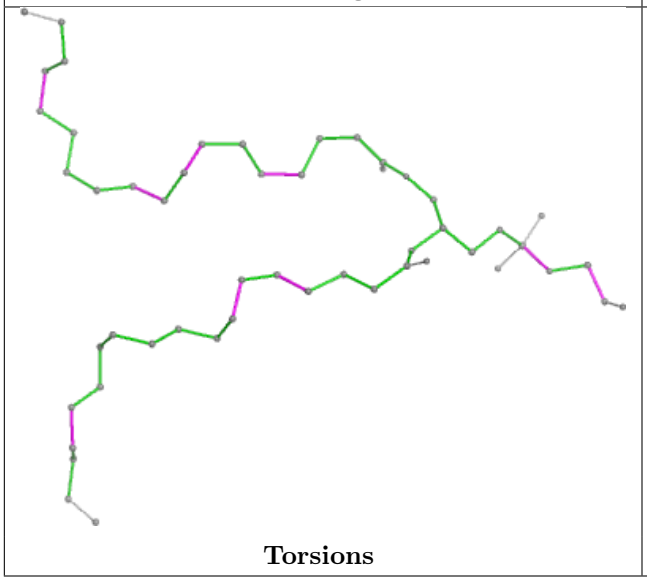
Ligand 3PE 6 202



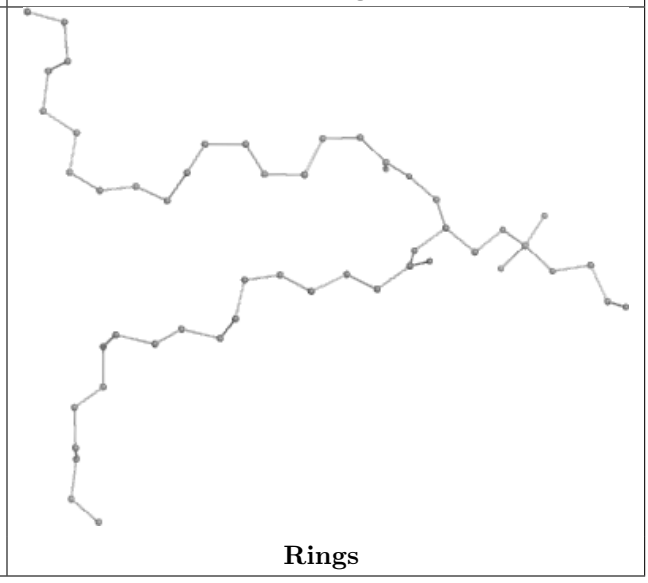
Bond lengths



Bond angles

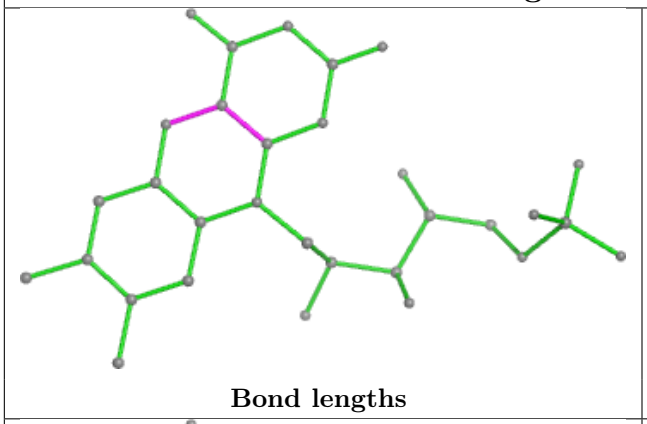


Torsions

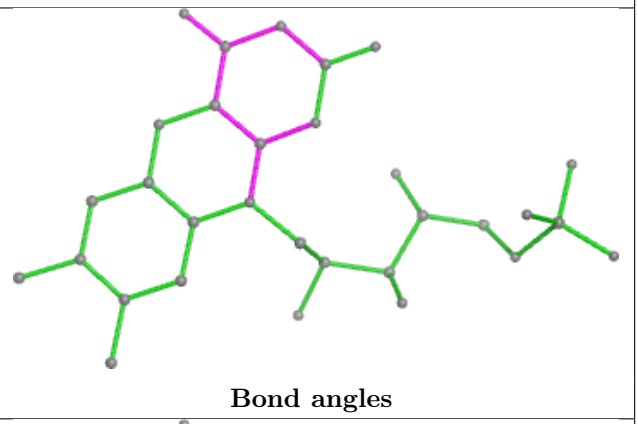


Rings

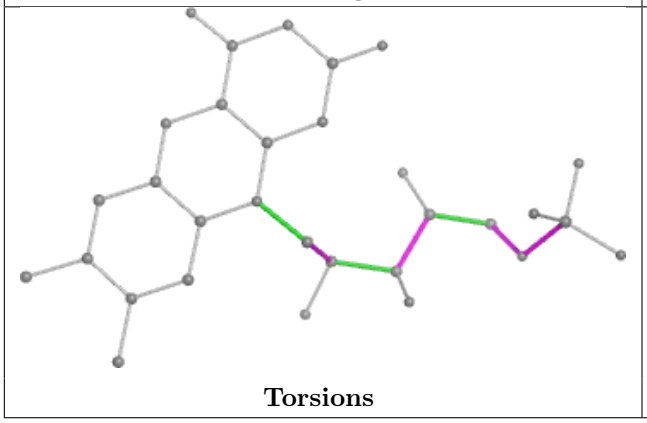
Ligand FMN 1 501



Bond lengths



Bond angles



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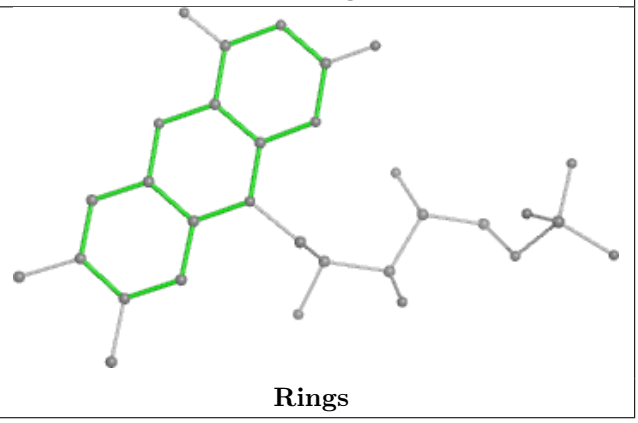
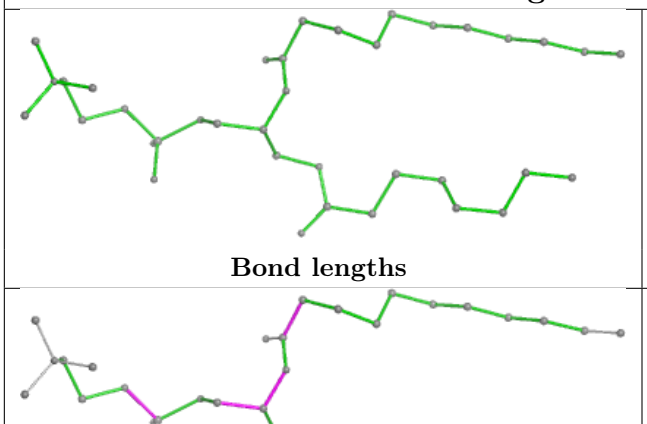
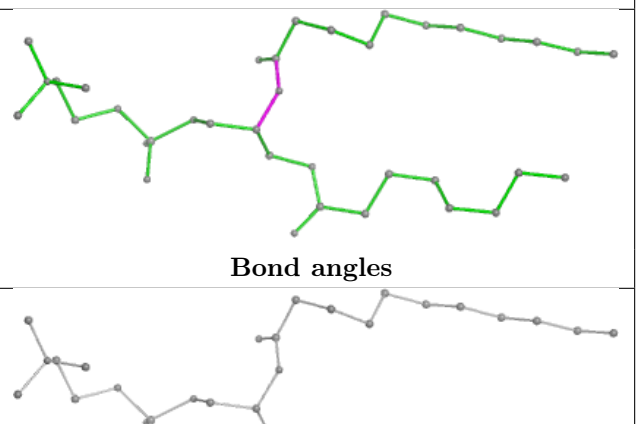


Rings

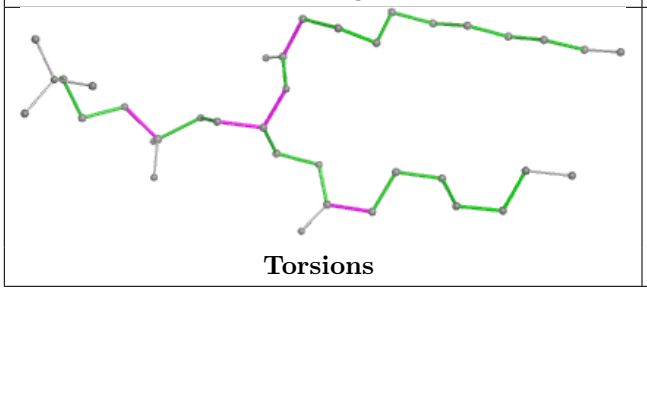
Ligand PC1 A 402



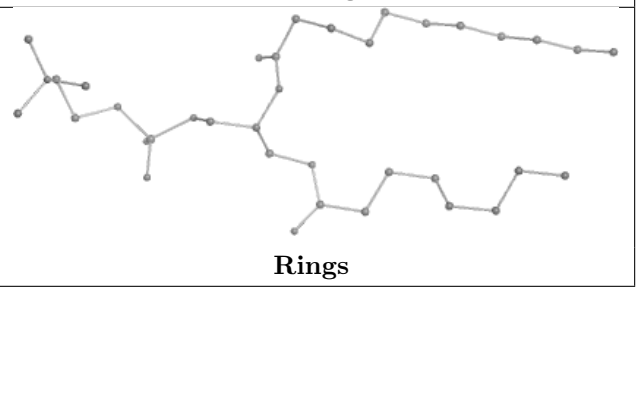
Bond lengths



Bond angles

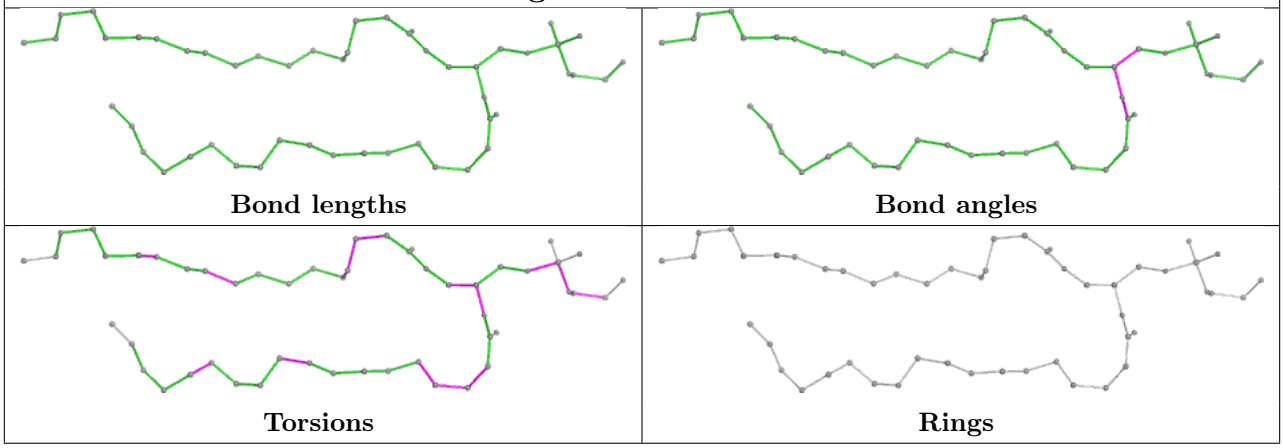


Torsions

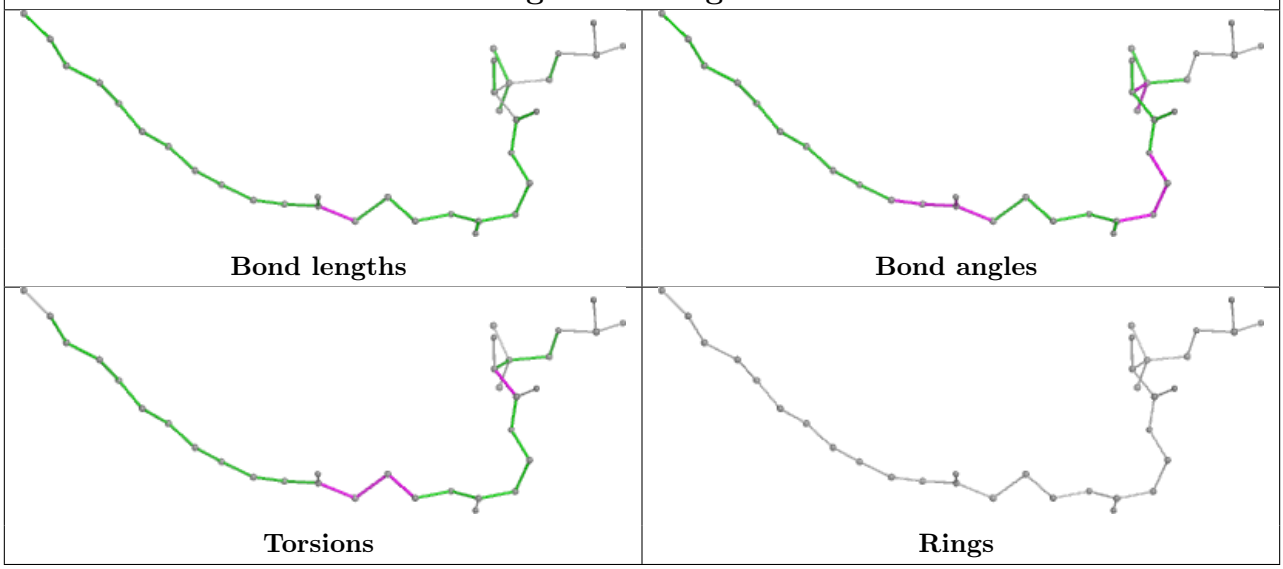


Rings

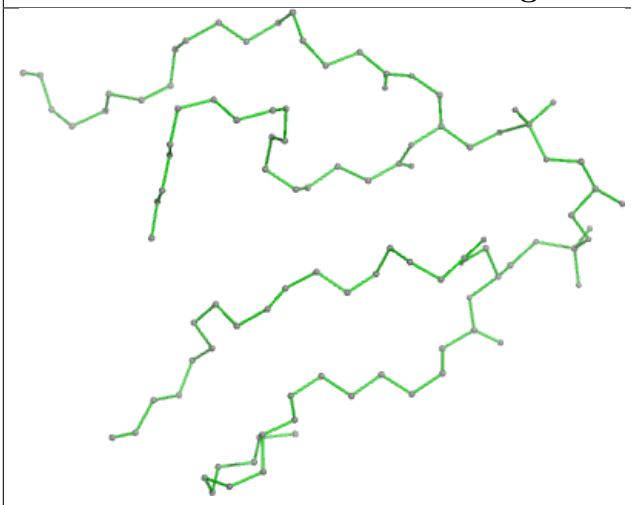
Ligand 3PE N 401



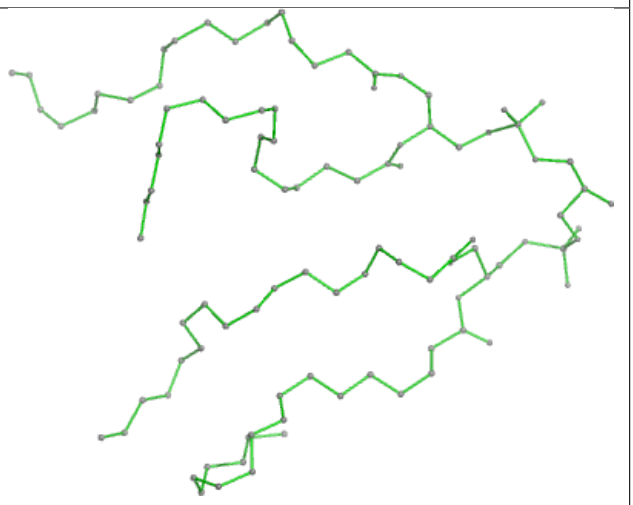
Ligand ZMP g 201



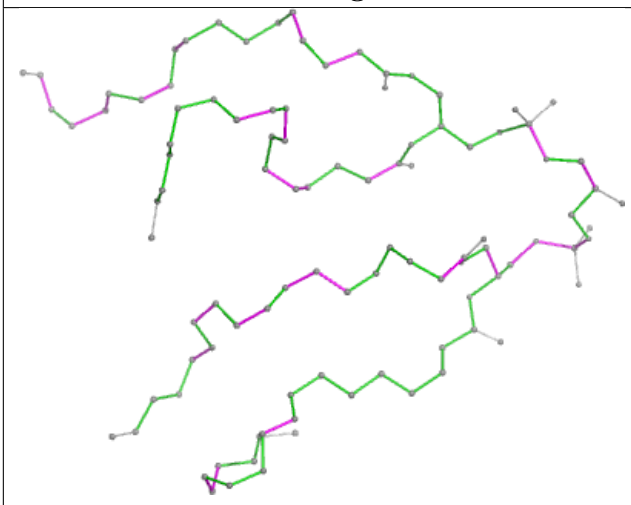
Ligand CDL M 501



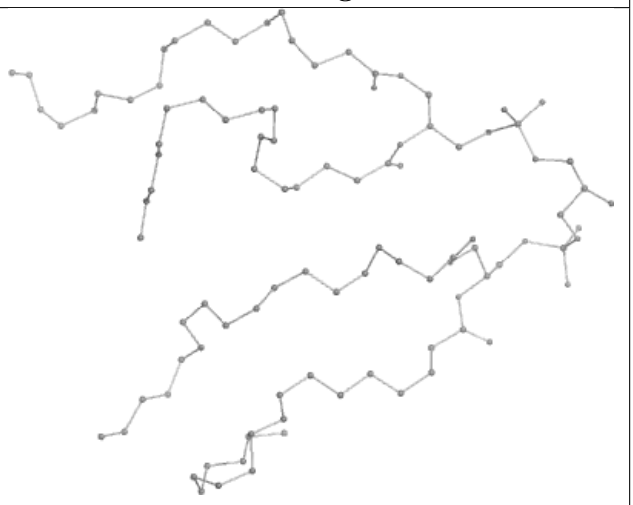
Bond lengths



Bond angles

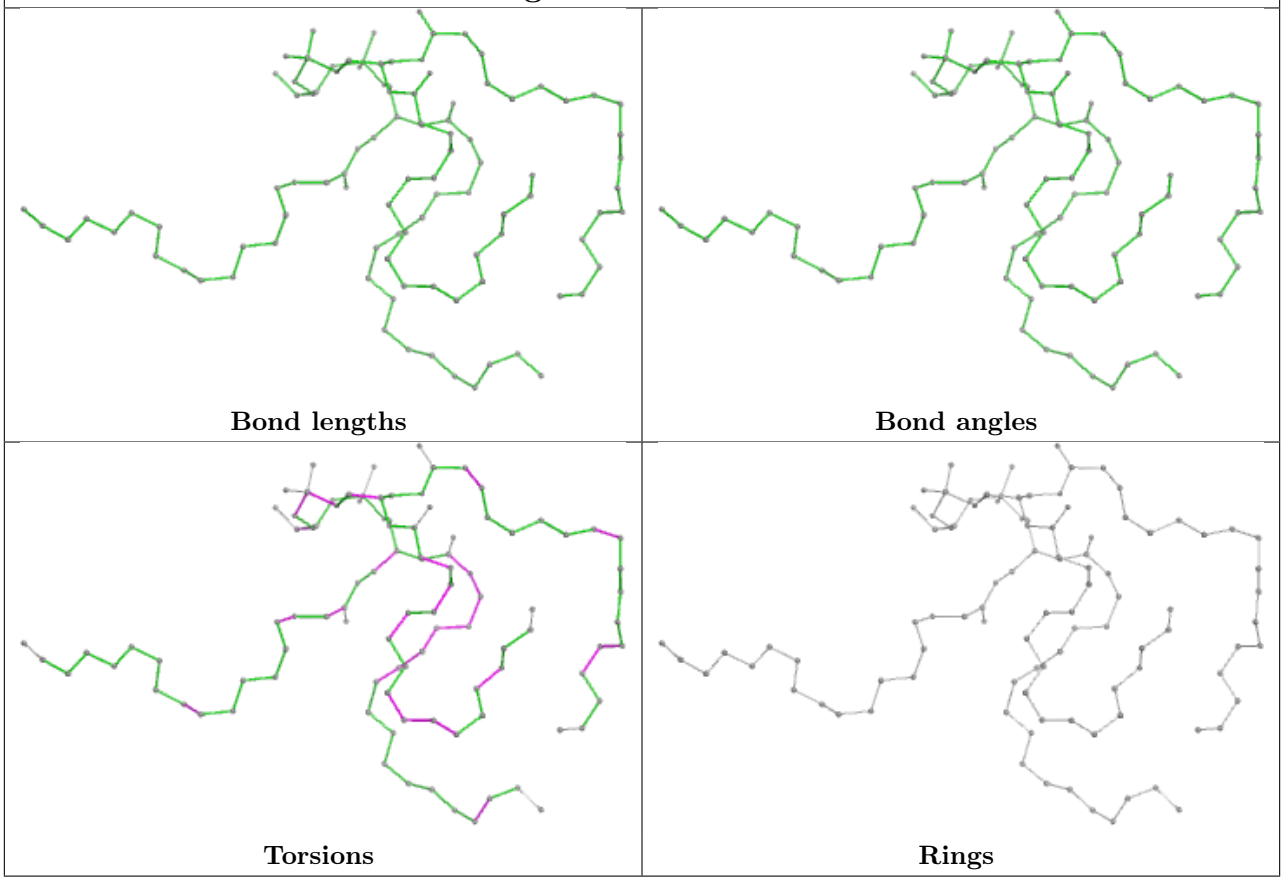


Torsions

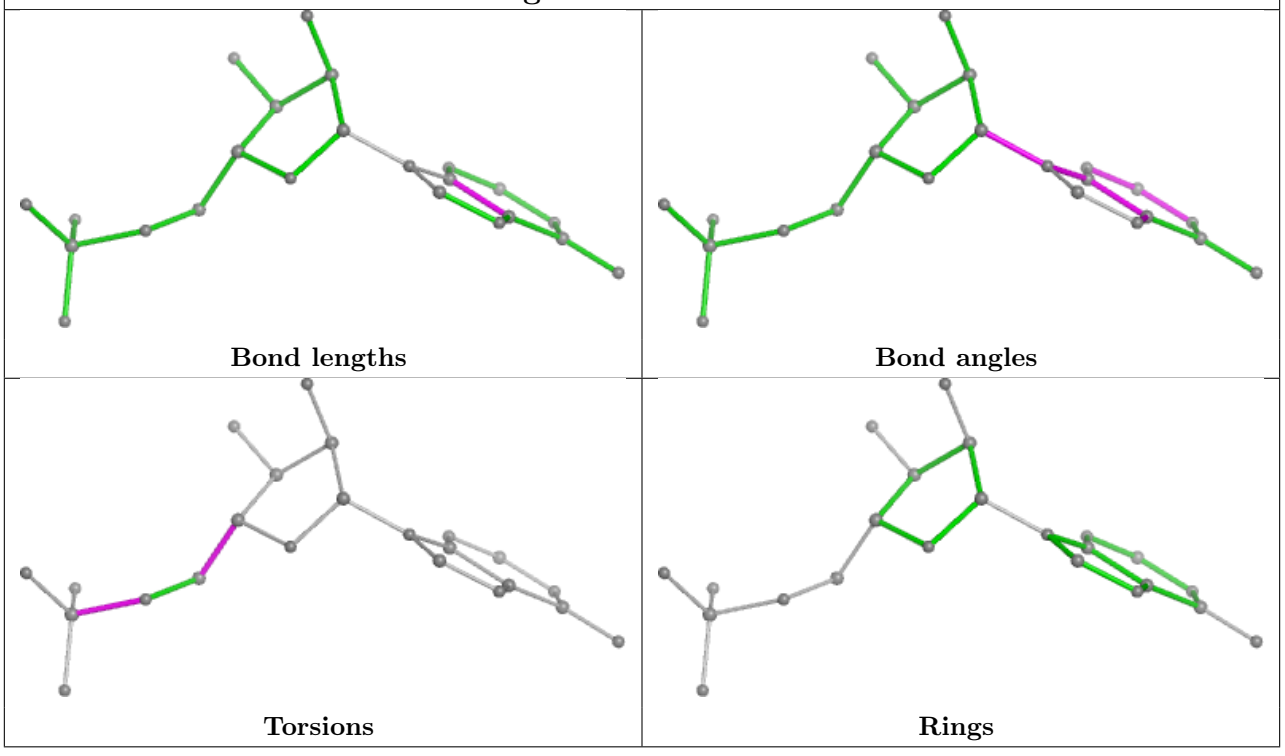


Rings

Ligand CDL Y 201



Ligand AMP k 501



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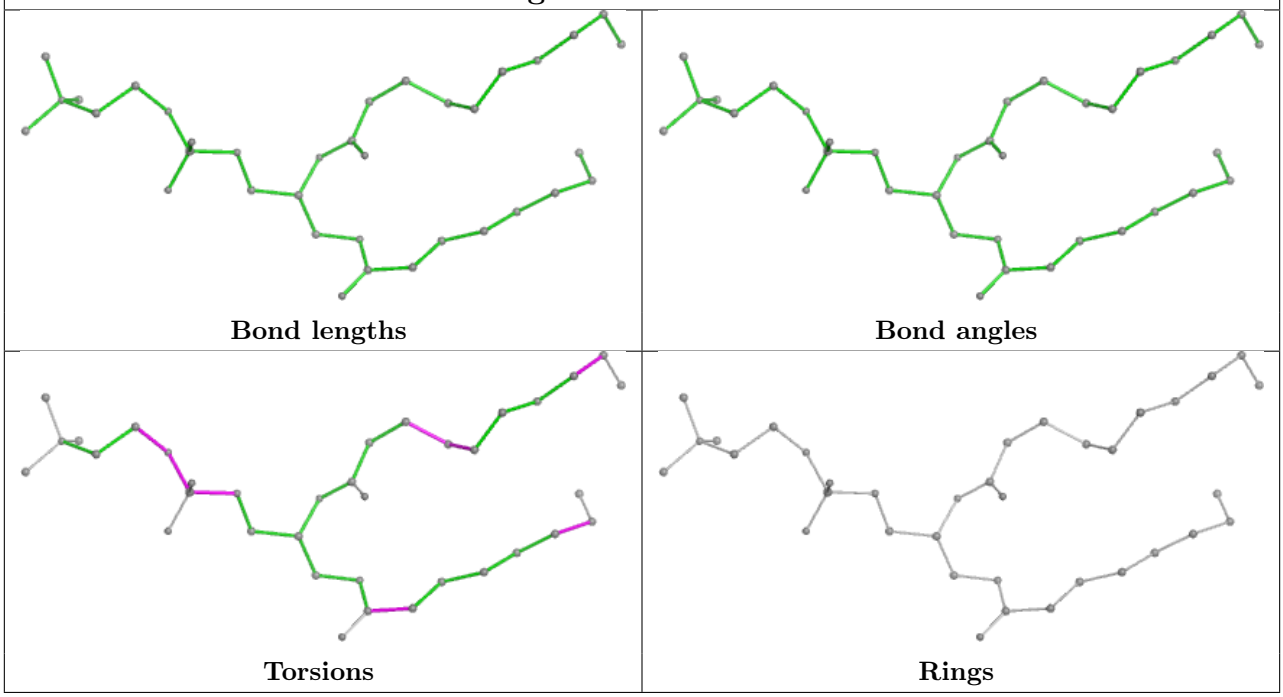

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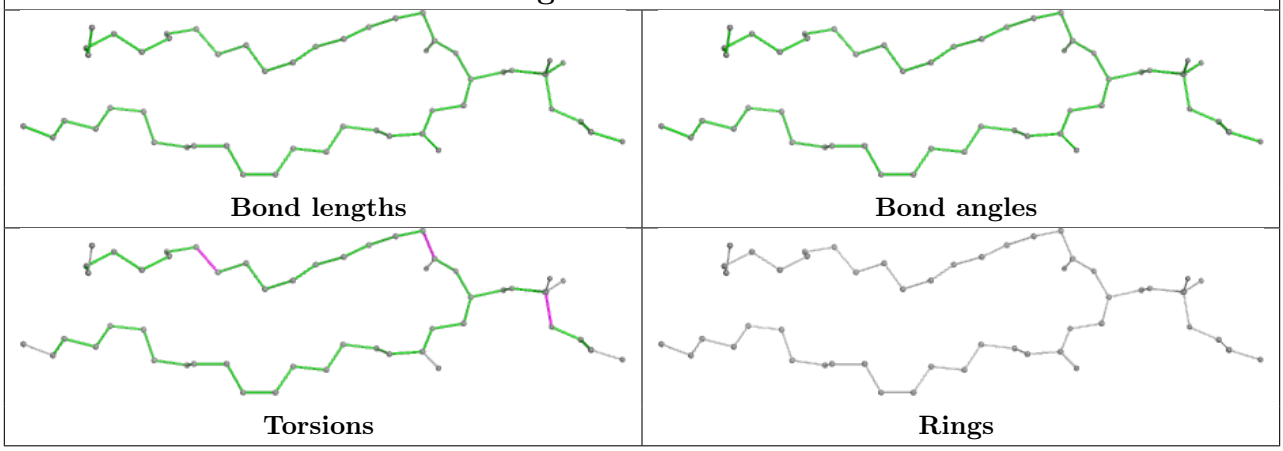
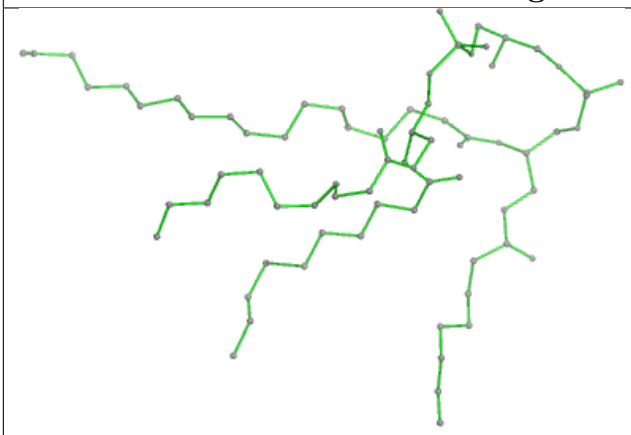
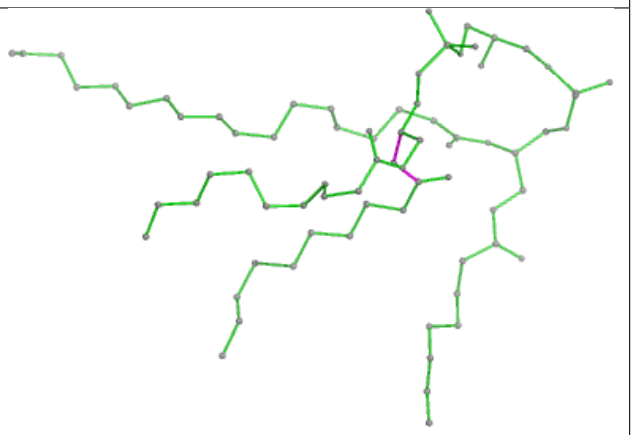


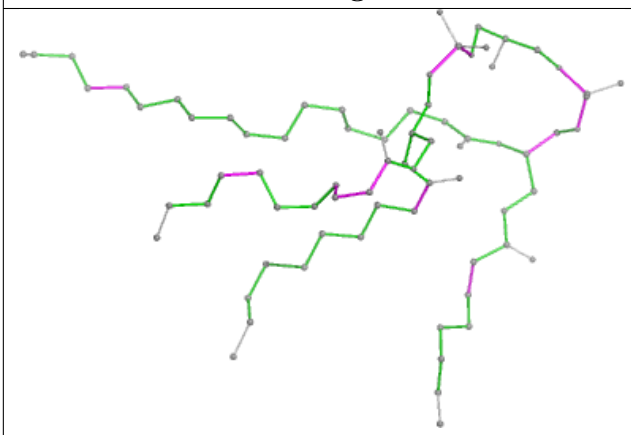
Ligand CDL x 101



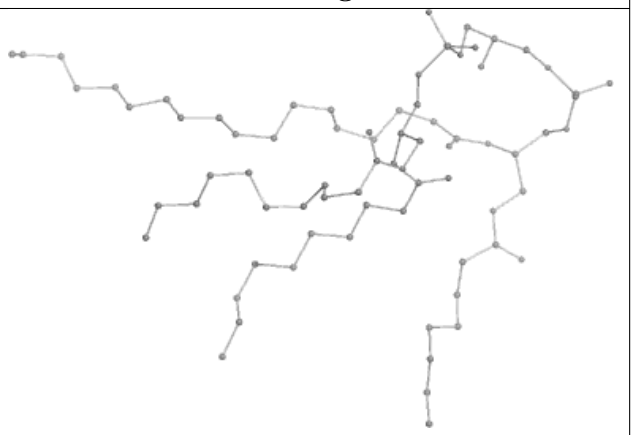
Bond lengths



Bond angles

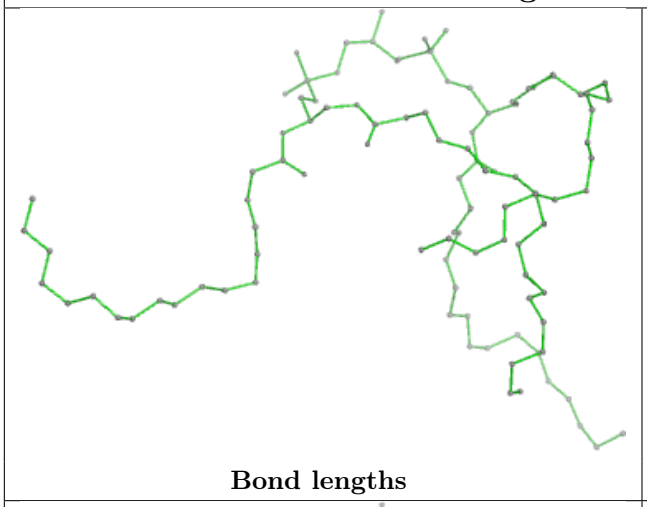


Torsions

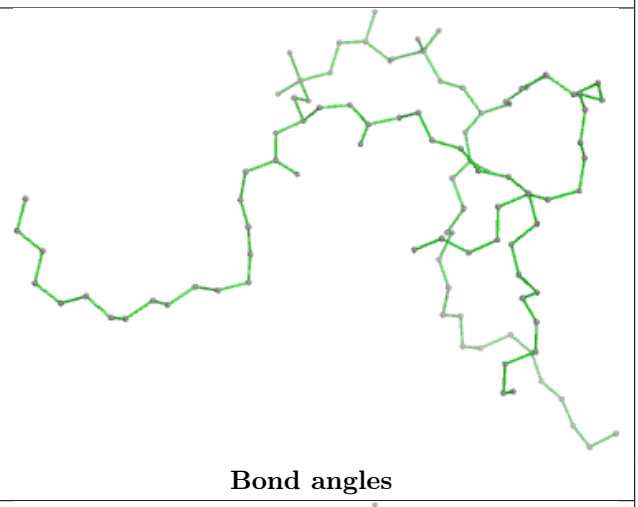


Rings

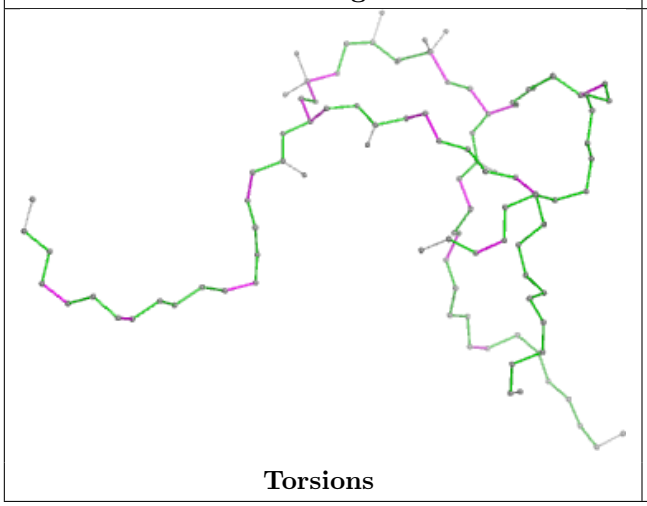
Ligand CDL W 201



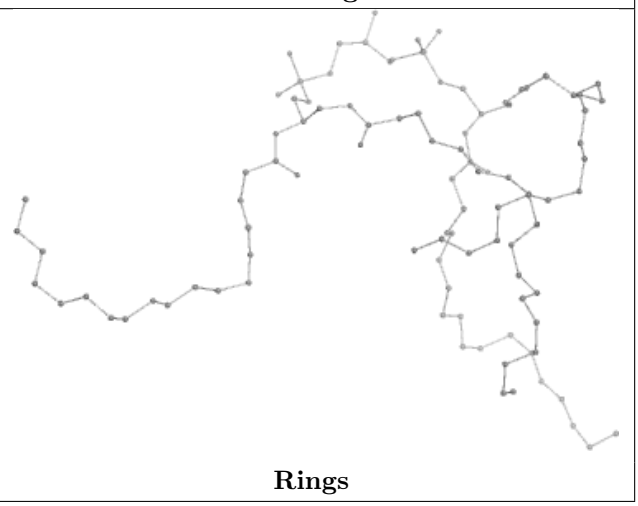
Bond lengths



Bond angles

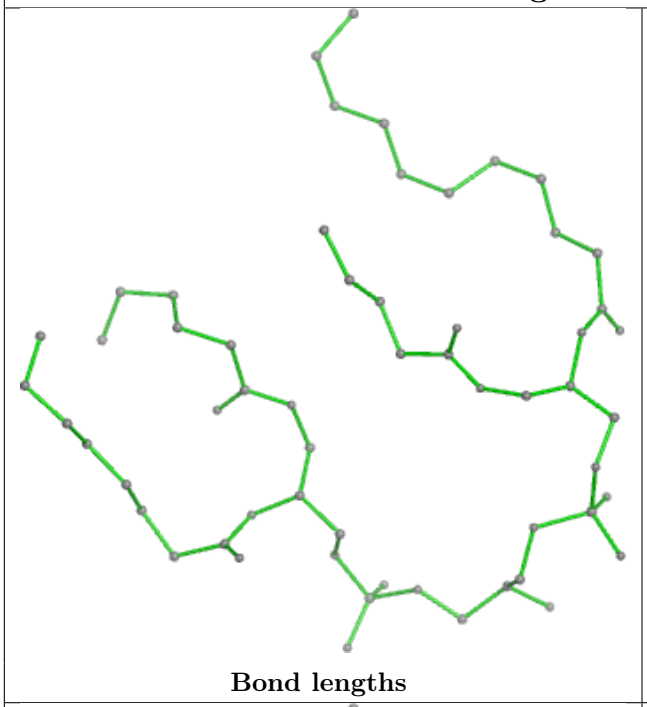


Torsions

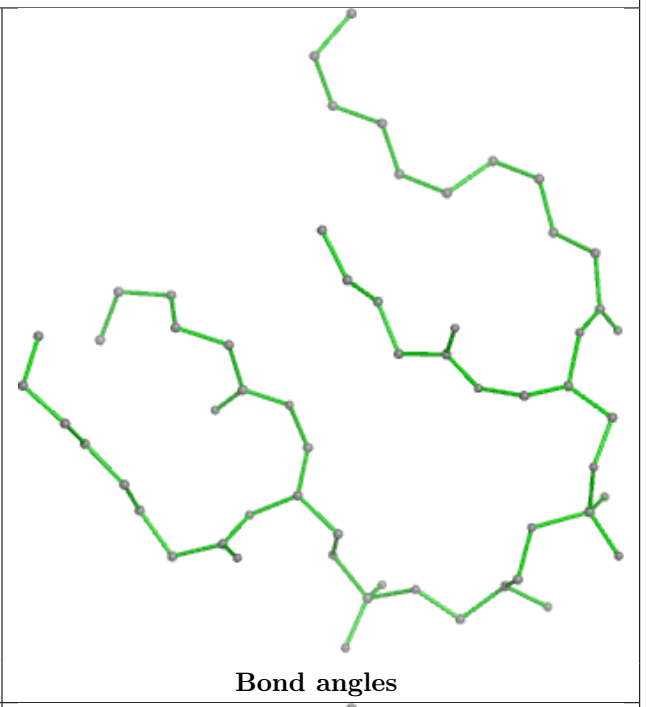


Rings

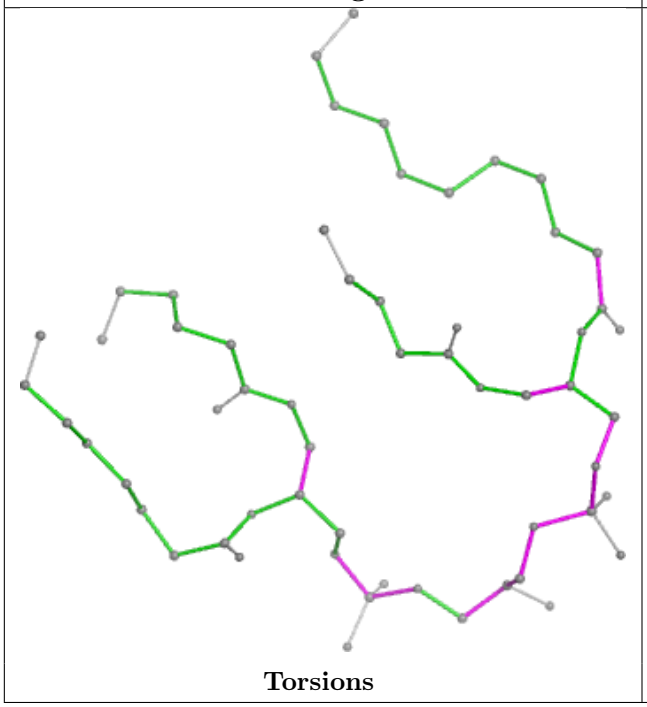
Ligand CDL z 101



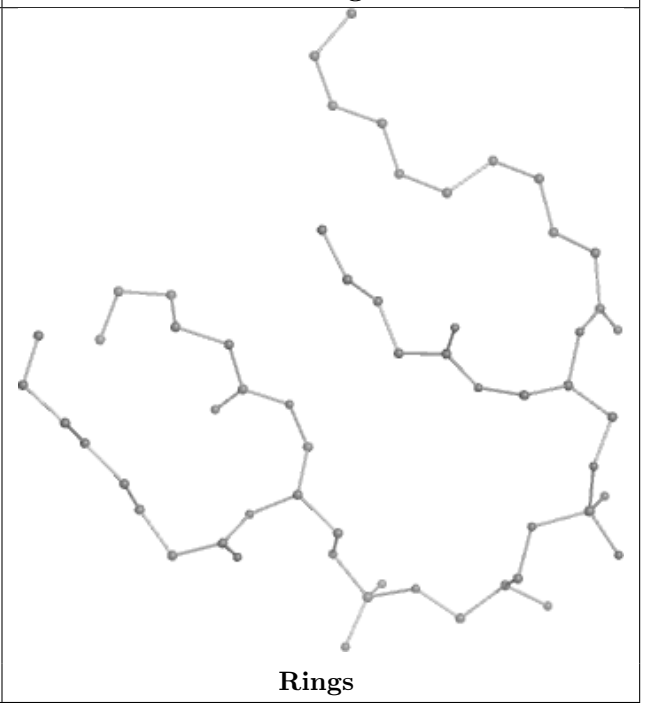
Bond lengths



Bond angles

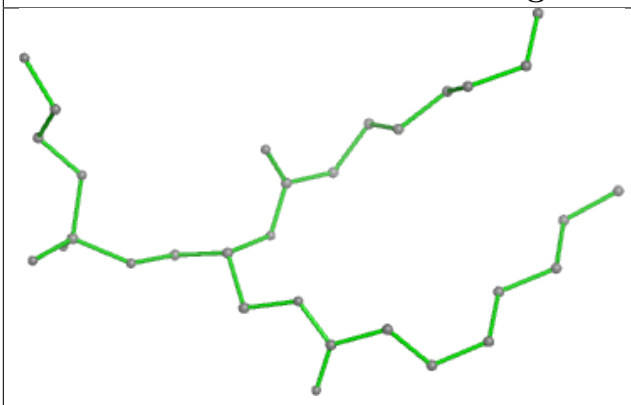


Torsions



Rings

Ligand 3PE N 402



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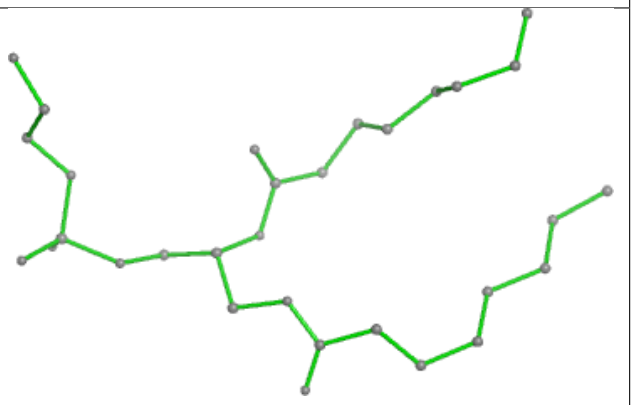
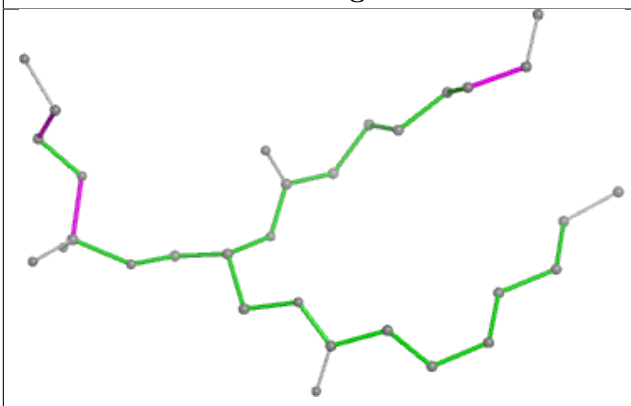
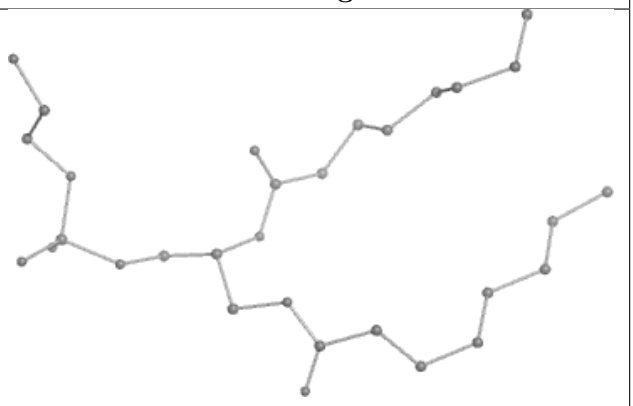


Bond angles

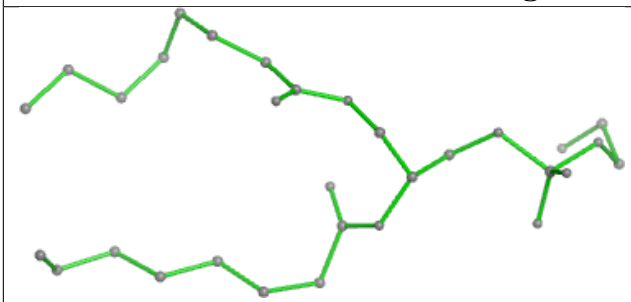


Torsions

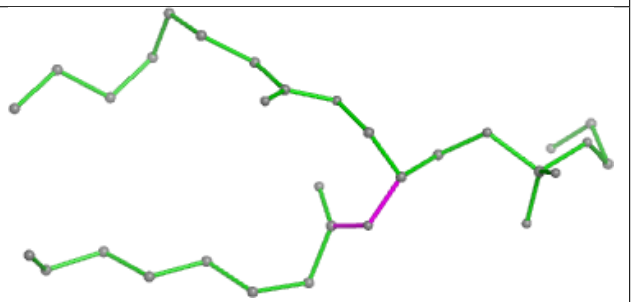


Rings

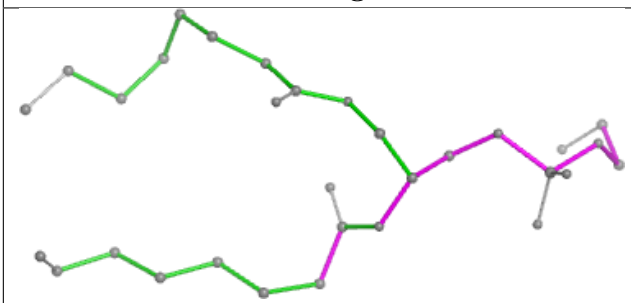
Ligand 3PE L 1003



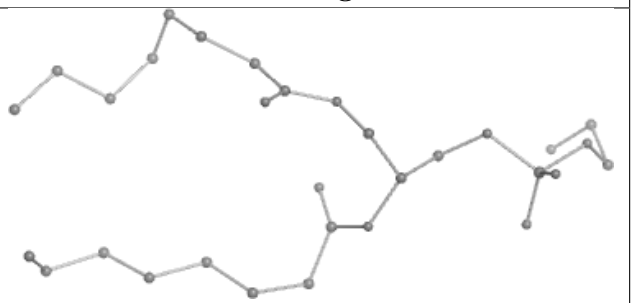
Bond lengths



Bond angles

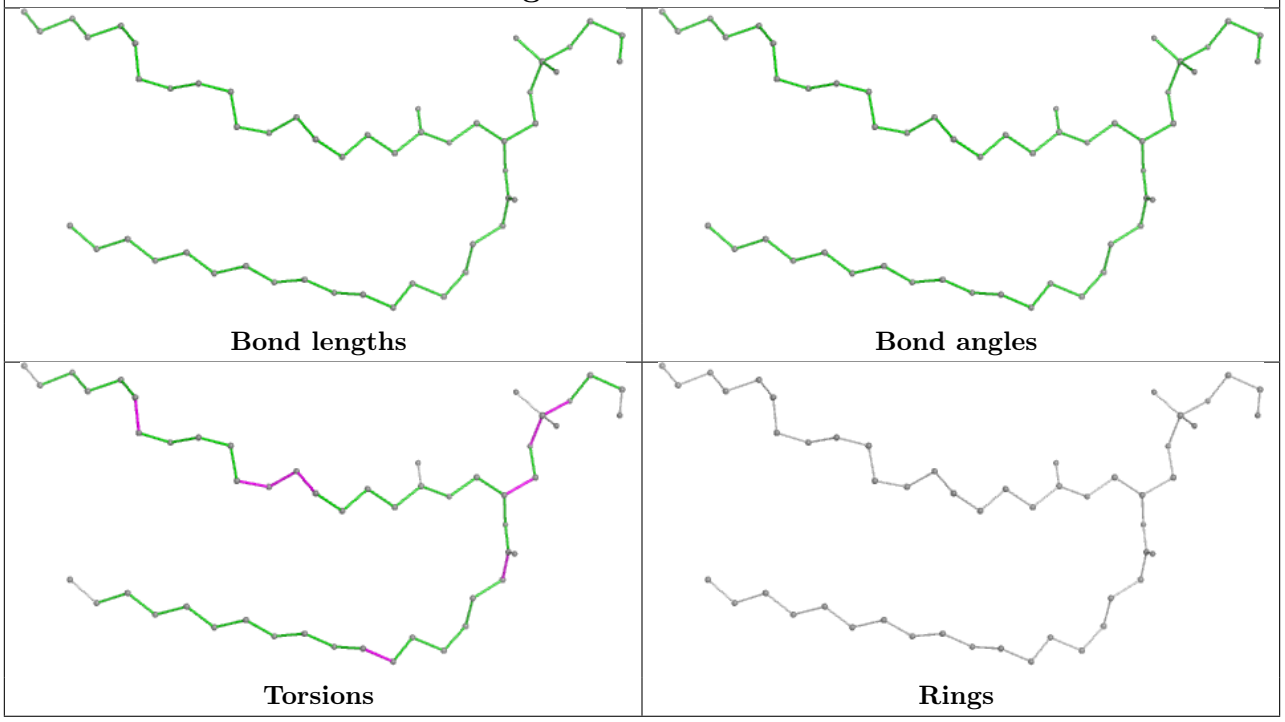


Torsions

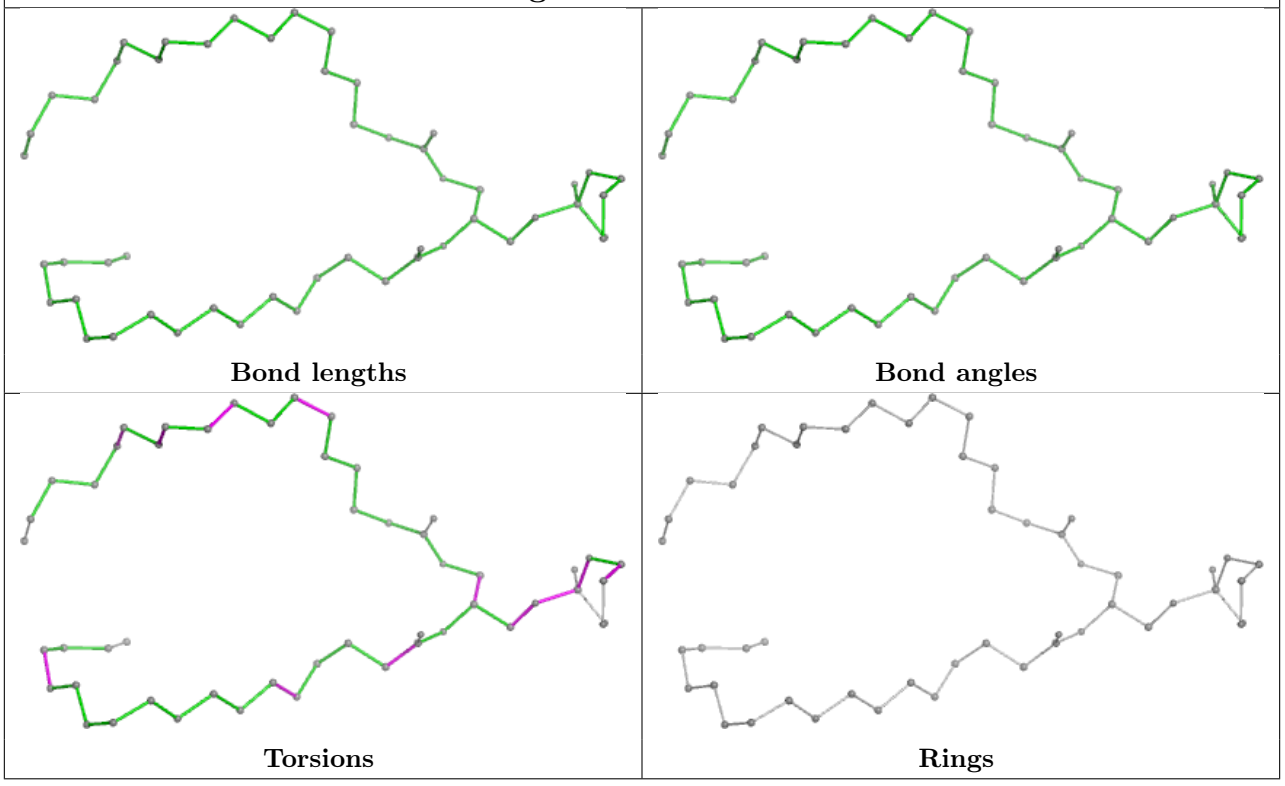


Rings

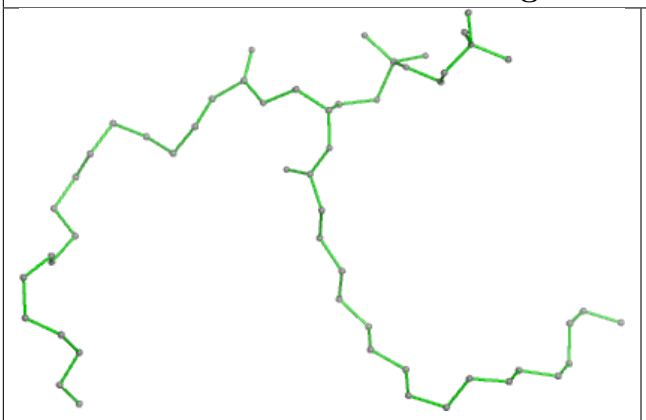
Ligand 3PE L 1001



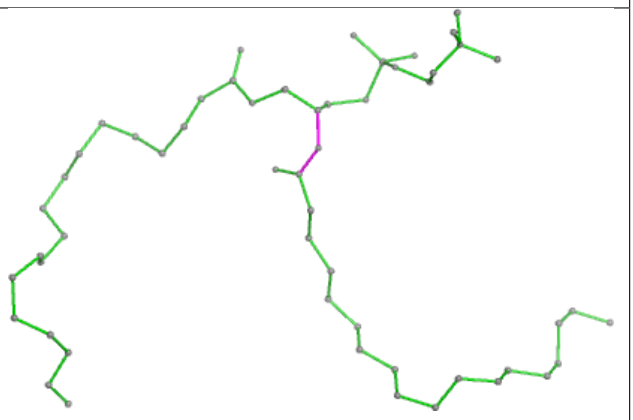
Ligand 3PE A 403



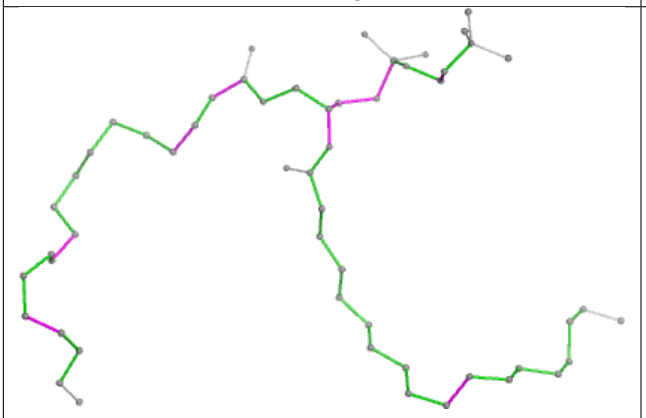
Ligand PC1 L 1002



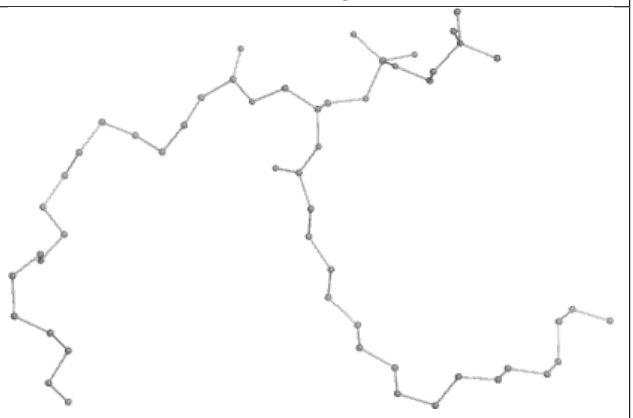
Bond lengths



Bond angles

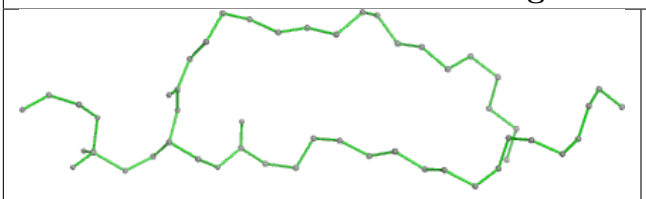


Torsions



Rings

Ligand 3PE H 401



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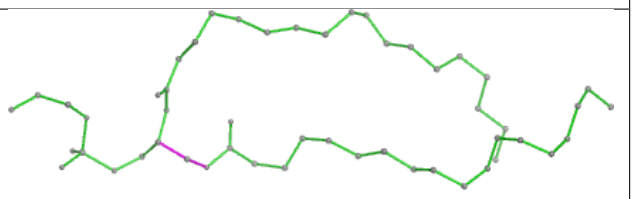
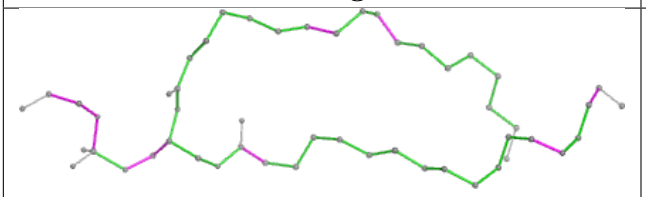


Bond angles

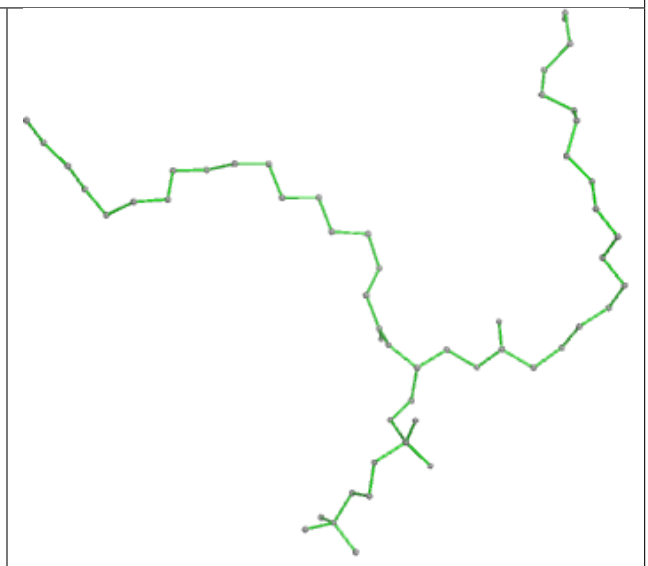


Torsions

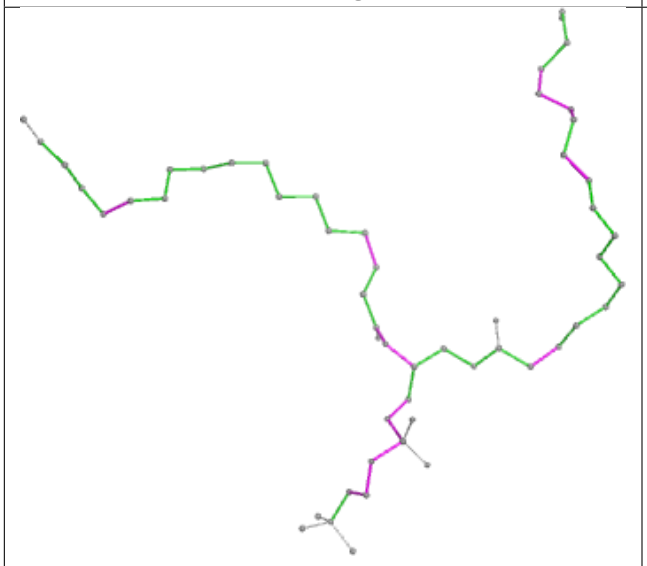
Rings

Ligand PC1 9 401

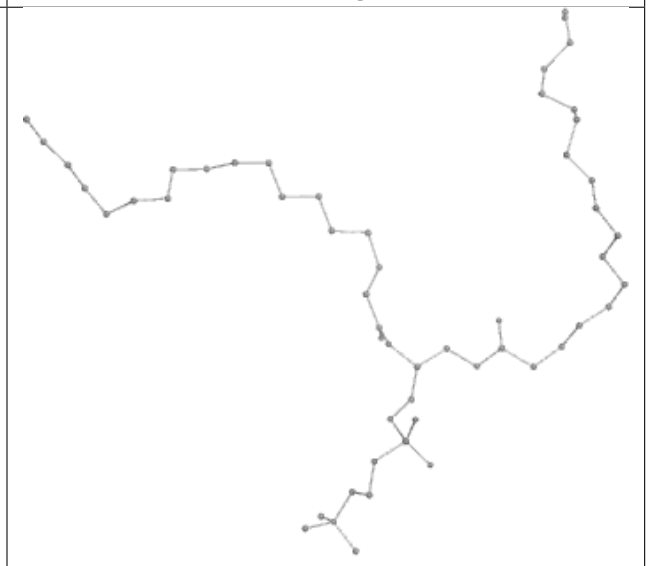
Bond lengths



Bond angles

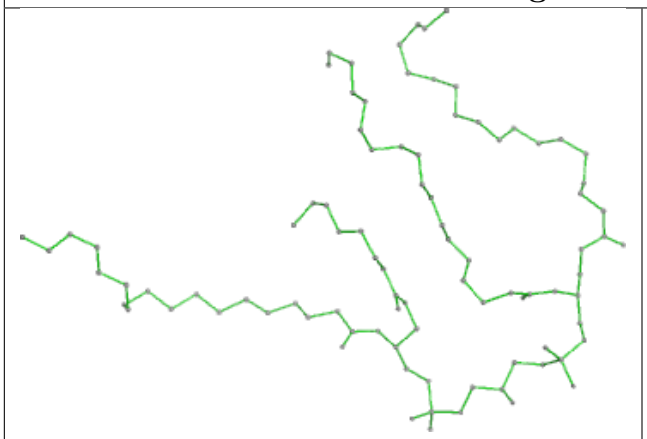


Torsions



Rings

Ligand CDL o 201



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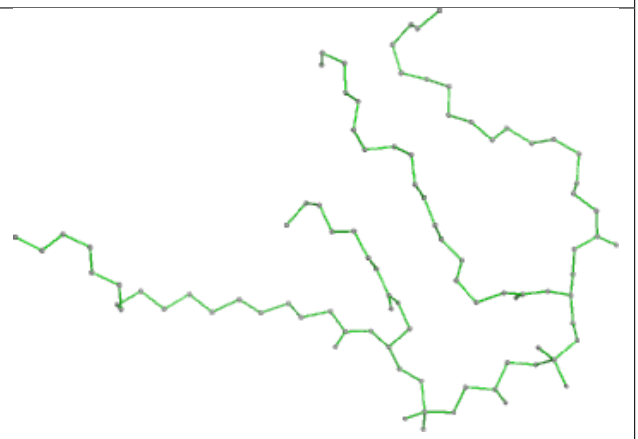
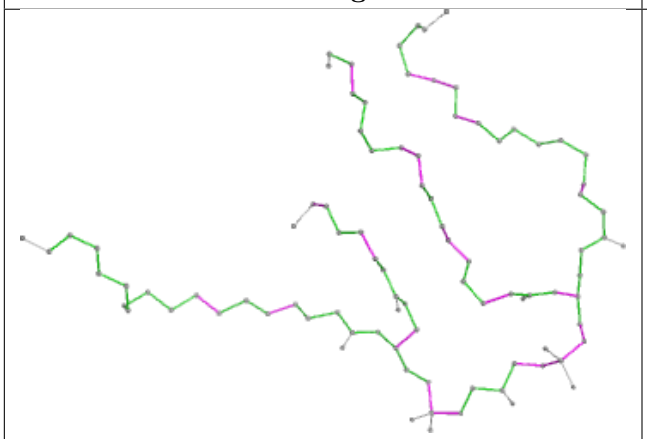
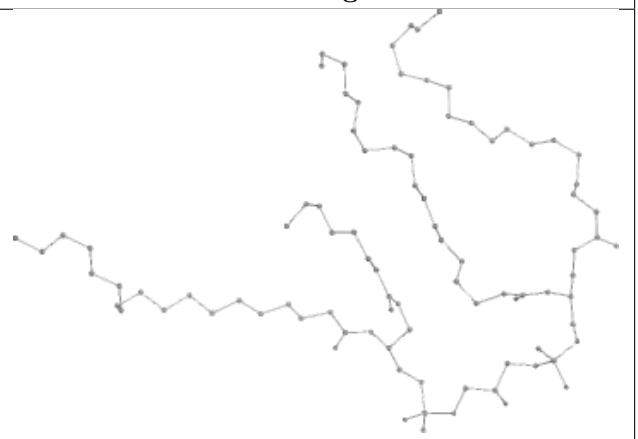


Bond angles

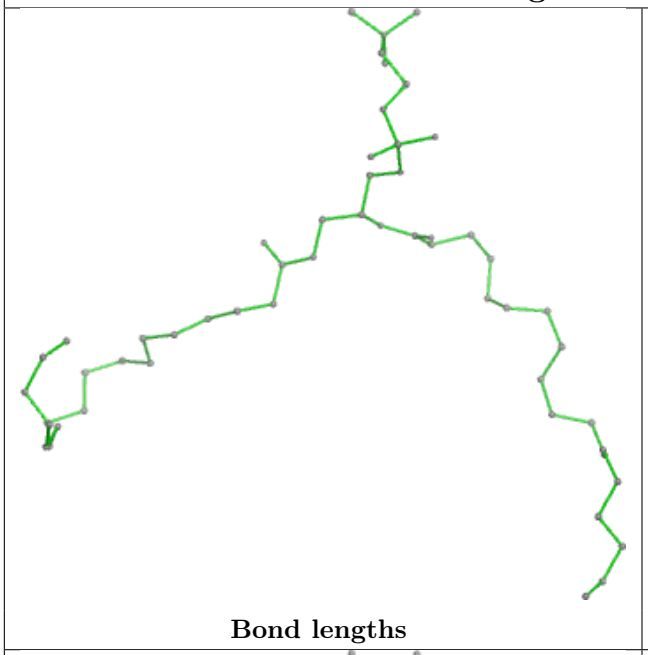


Torsions

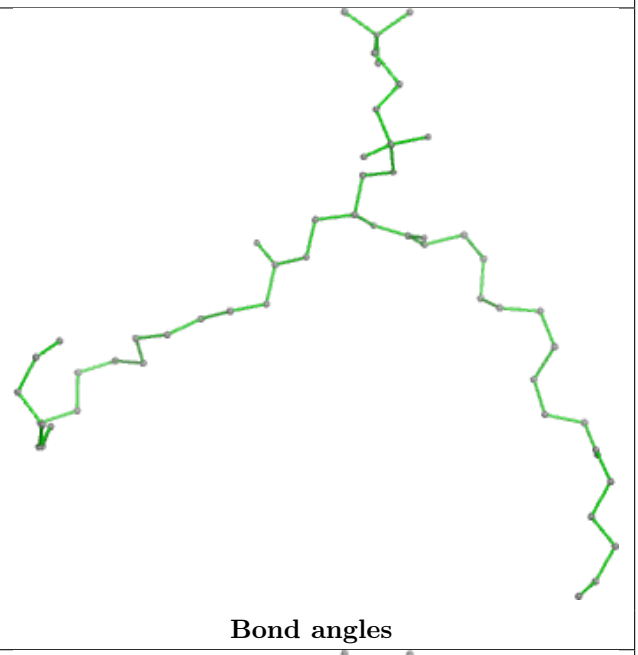


Rings

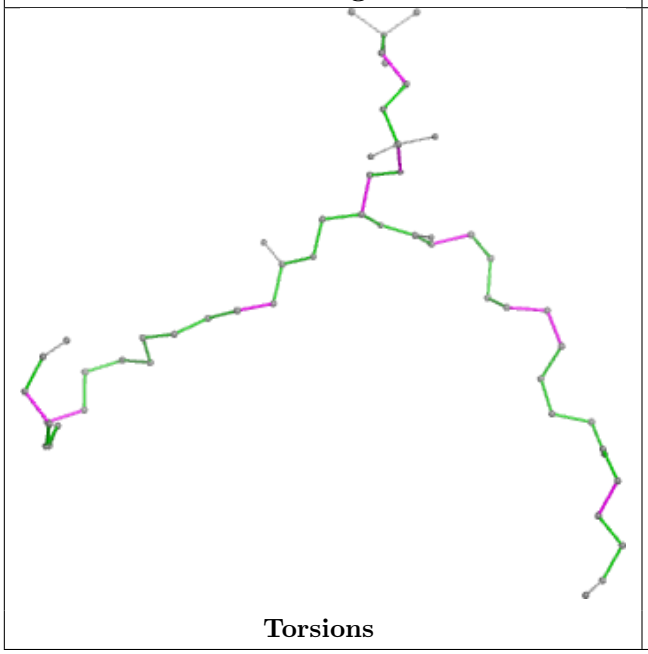
Ligand PC1 w 801



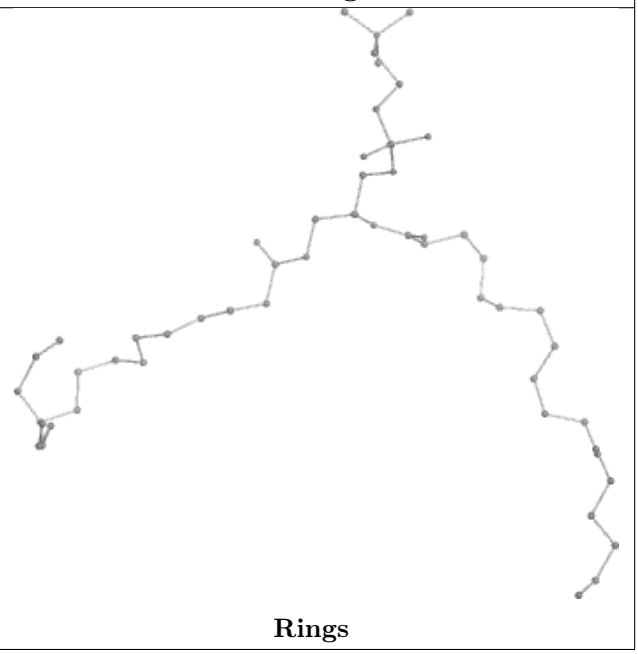
Bond lengths



Bond angles

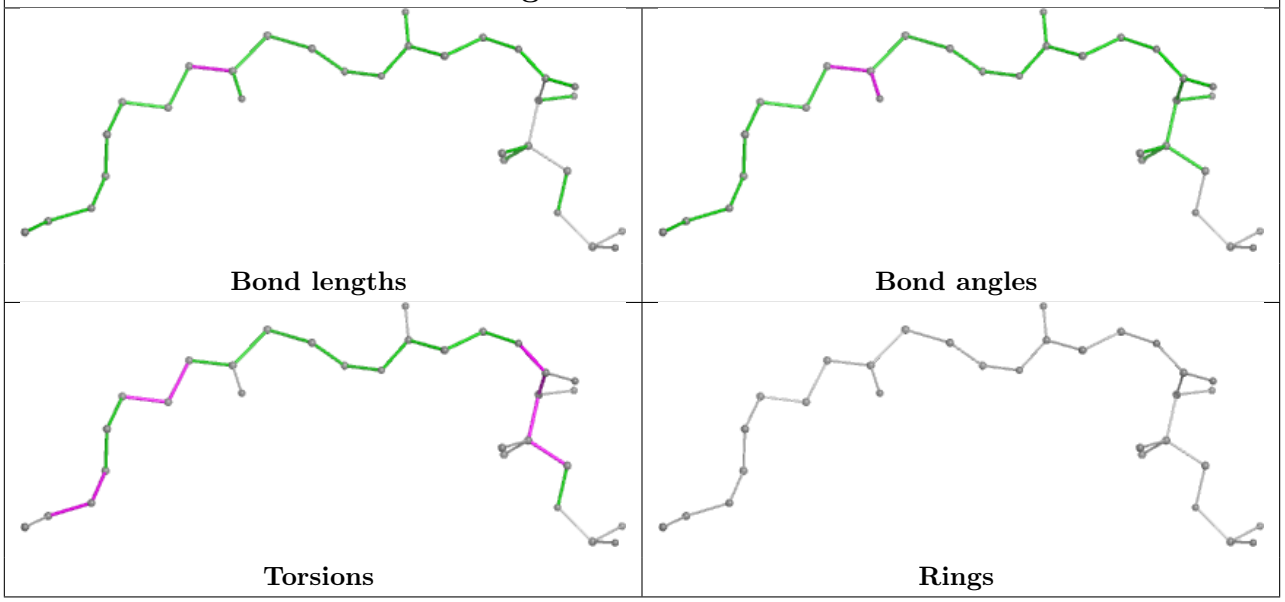


Torsions

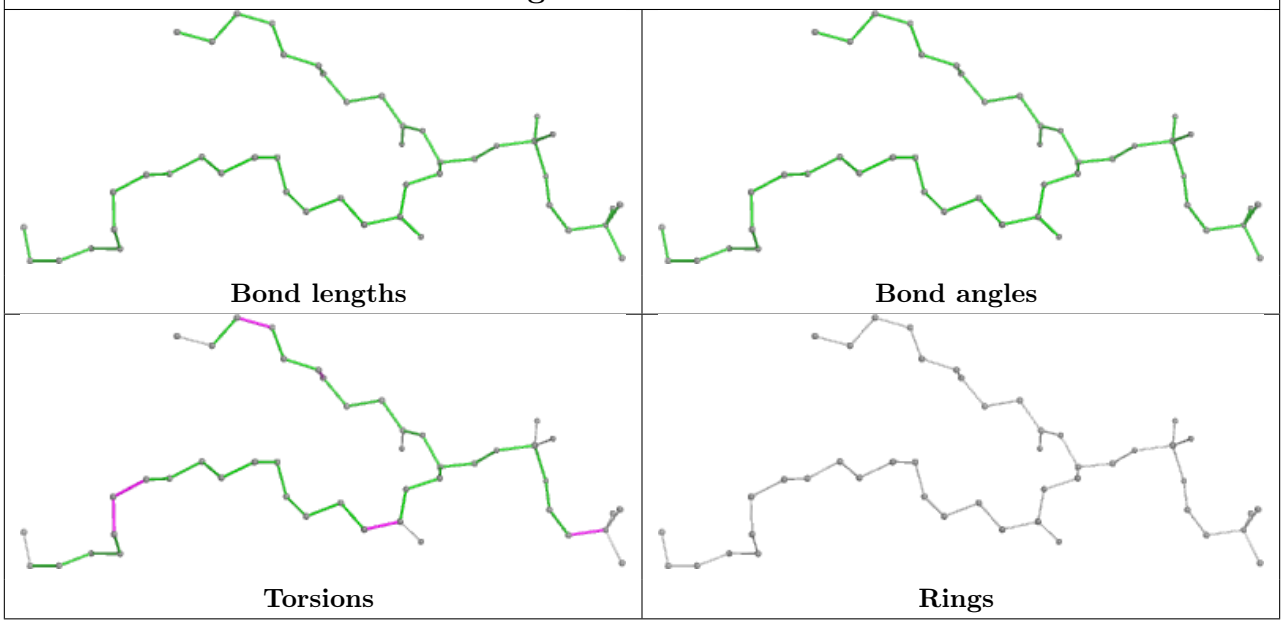


Rings

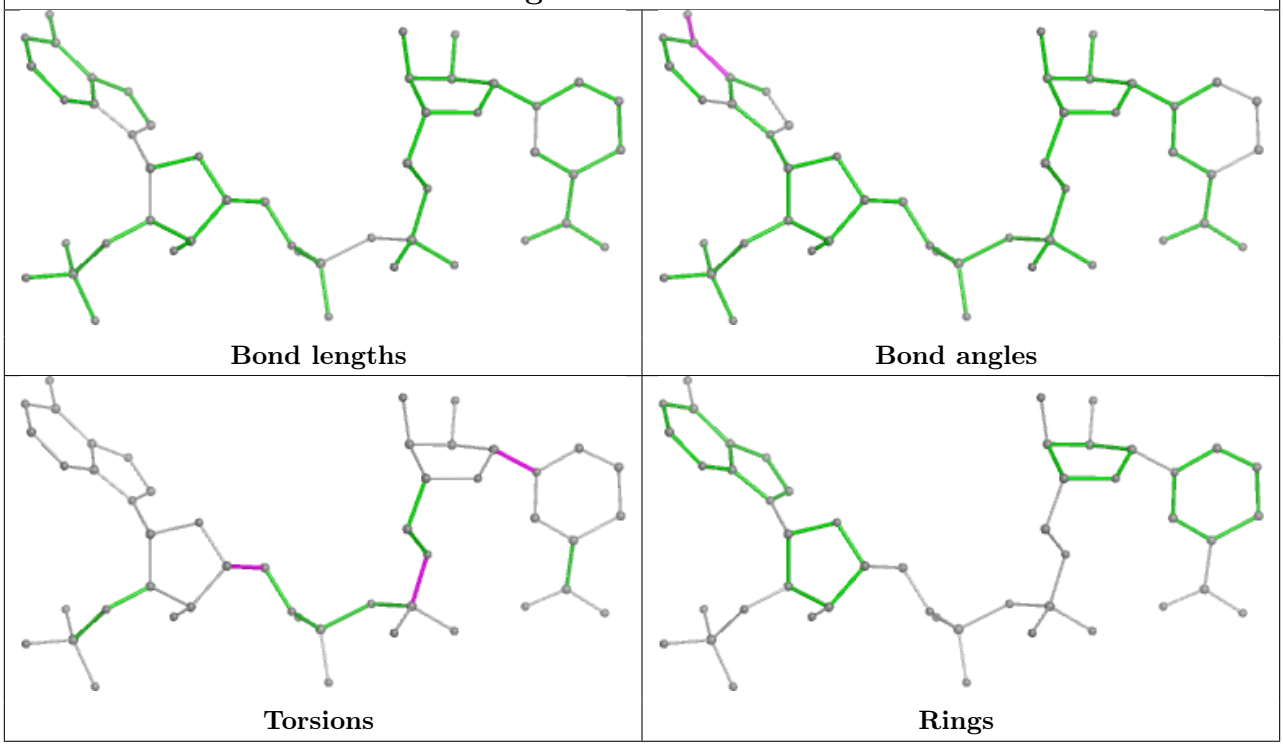
Ligand ZMP X 101



Ligand PC1 A 401



Ligand NDP d 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11262. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.