Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 06:05 pm BST

PDB ID	:	6ZKB / pdb_00006zkb
EMDB ID	:	EMD-11243
Title	:	Membrane domain of closed complex I during turnover
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	2.90 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:

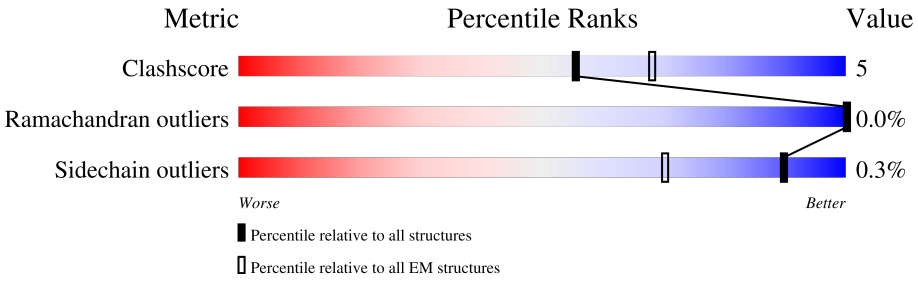
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	4	457	8% · 91%
2	L	606	86% 14%
3	M	459	85% 15%
4	N	347	87% 13%
5	V	141	85% 13% ··
6	W	189	66% 7% 26%
7	X	157	55% · 45%
8	Y	172	91% 9% ·
9	Z	175	90% 7% ·

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Mol	Chain	Length	Quality of chain
10	k	355	90% 10%
11	l	106	99%
12	m	84	94% 5%
13	n	98	81% 19%
14	o	122	98%
15	p	130	98%
16	q	144	81% 19%
17	r	128	77% 23%
18	s	137	88% 11%
19	t	179	98%
20	u	108	60% 40%
21	v	186	83% 17%
22	w	154	66% 34%
23	x	76	64% 36%
24	y	58	86% 14%
25	z	70	100%
26	A	115	92% 7%
27	H	318	83% 17%
28	J	175	84% 16%
29	K	98	76% 23%

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
32	CDL	L	1003	X	-	-	-
32	CDL	M	503	X	-	-	-
32	CDL	N	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CDL	V	203	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 39924 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 Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	40	Total	C	N	O	S	0	0
			334	217	56	60	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	606	Total	C	N	O	S	0	0
			4807	3188	746	829	44		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 5 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 6 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 7 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		

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

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

- Molecule 9 is a protein called Mitochondrial complex I, PDSW subunit.

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

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

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

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 12 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 16 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	117	Total	C	N	O	S	0	0
			967	621	168	170	8		

- Molecule 17 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

8, mitochondrial.

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

- Molecule 22 is a protein called Mitochondrial complex I, ESSS subunit.

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

- Molecule 23 is a protein called Mitochondrial complex I, KFYI subunit.

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

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

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

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

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

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

- Molecule 27 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

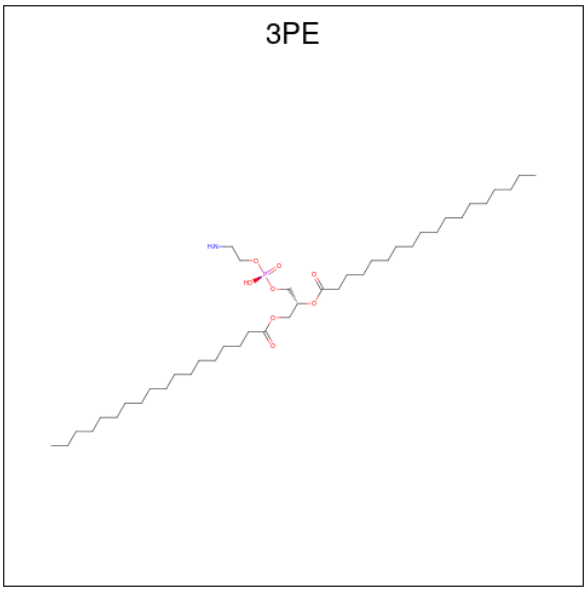
- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 30 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
30	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
30	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
30	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
30	o	1	Total	C	N	O	P	0
			31	21	1	8	1	

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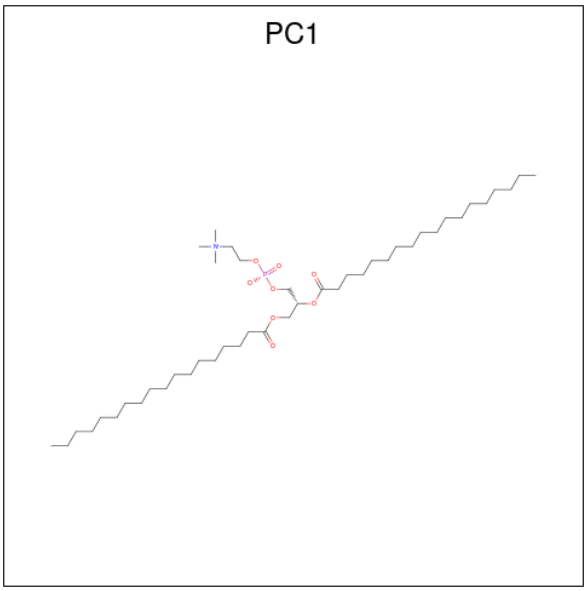
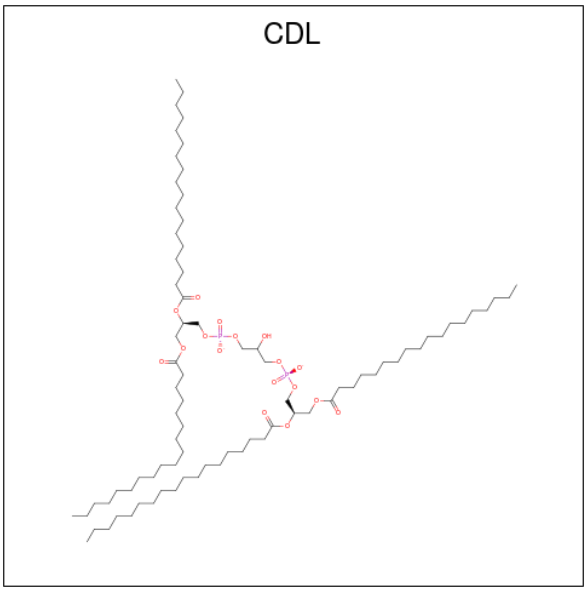
Mol	Chain	Residues	Atoms	AltConf
30	p	1	Total C O P 27 18 8 1	0
30	A	1	Total C N O P 51 41 1 8 1	0
30	J	1	Total C N O P 51 41 1 8 1	0
30	J	1	Total C N O P 40 30 1 8 1	0

- Molecule 31 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



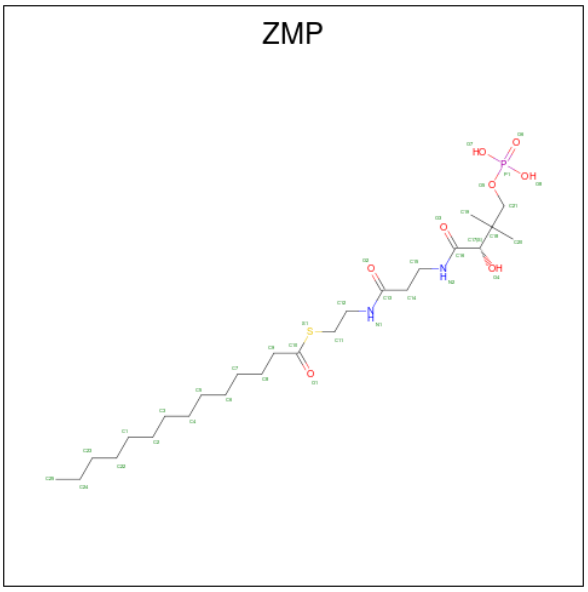
Mol	Chain	Residues	Atoms	AltConf
31	L	1	Total C N O P 54 44 1 8 1	0
31	M	1	Total C N O P 54 44 1 8 1	0
31	w	1	Total C N O P 54 44 1 8 1	0
31	H	1	Total C N O P 54 44 1 8 1	0

- Molecule 32 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



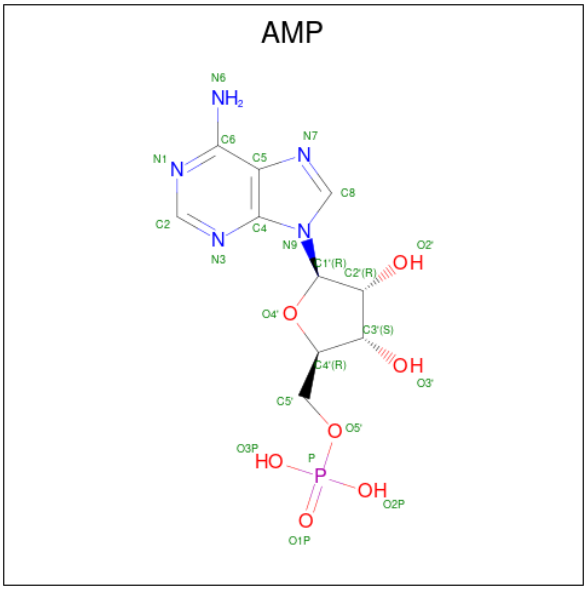
Mol	Chain	Residues	Atoms				AltConf
32	L	1	Total	C	O	P	0
			100	81	17	2	
32	M	1	Total	C	O	P	0
			100	81	17	2	
32	M	1	Total	C	O	P	0
			90	71	17	2	
32	N	1	Total	C	O	P	0
			75	56	17	2	
32	V	1	Total	C	O	P	0
			94	75	17	2	
32	V	1	Total	C	O	P	0
			85	66	17	2	
32	W	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 33 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



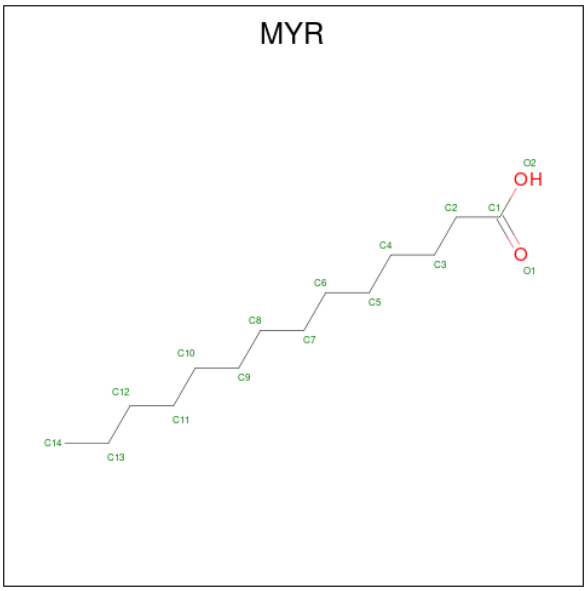
Mol	Chain	Residues	Atoms						AltConf
33	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 34 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 35 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	4	10	Total O 10 10	0
36	L	47	Total O 47 47	0
36	M	58	Total O 58 58	0
36	N	37	Total O 37 37	0
36	V	10	Total O 10 10	0
36	W	26	Total O 26 26	0
36	X	6	Total O 6 6	0
36	Y	13	Total O 13 13	0
36	Z	15	Total O 15 15	0
36	k	28	Total O 28 28	0
36	l	12	Total O 12 12	0

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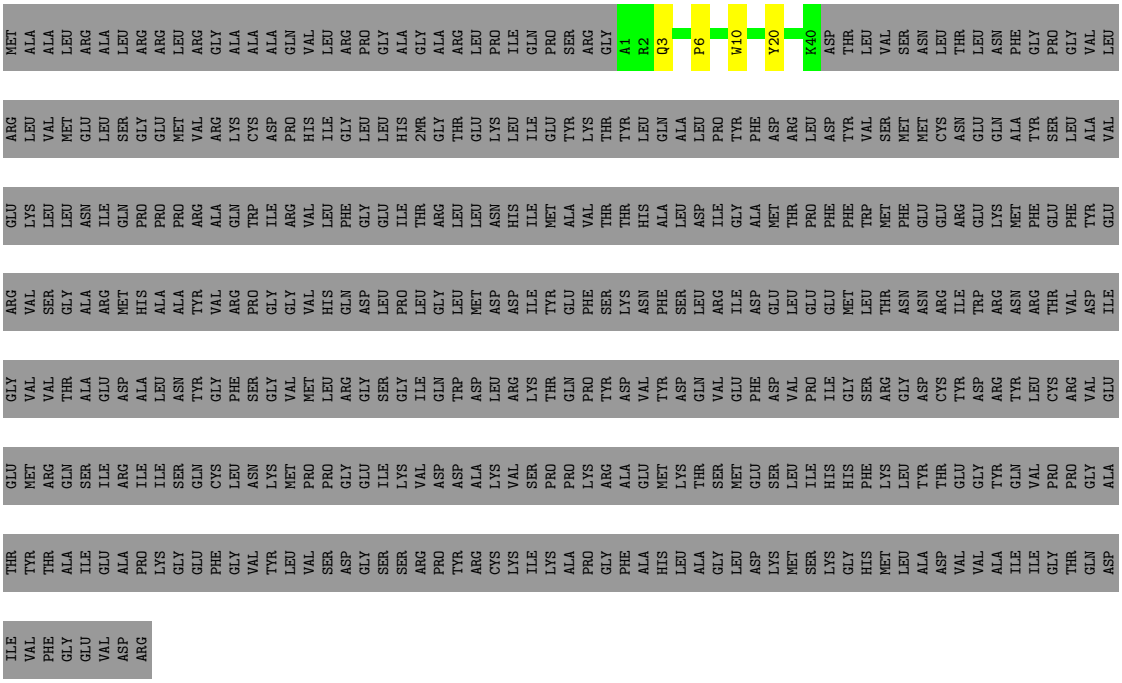
Mol	Chain	Residues	Atoms	AltConf
36	m	2	Total O 2 2	0
36	n	4	Total O 4 4	0
36	o	17	Total O 17 17	0
36	p	15	Total O 15 15	0
36	q	16	Total O 16 16	0
36	r	8	Total O 8 8	0
36	s	2	Total O 2 2	0
36	t	17	Total O 17 17	0
36	u	3	Total O 3 3	0
36	v	15	Total O 15 15	0
36	w	9	Total O 9 9	0
36	x	6	Total O 6 6	0
36	y	7	Total O 7 7	0
36	z	6	Total O 6 6	0
36	A	13	Total O 13 13	0
36	H	21	Total O 21 21	0
36	J	13	Total O 13 13	0
36	K	10	Total O 10 10	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.

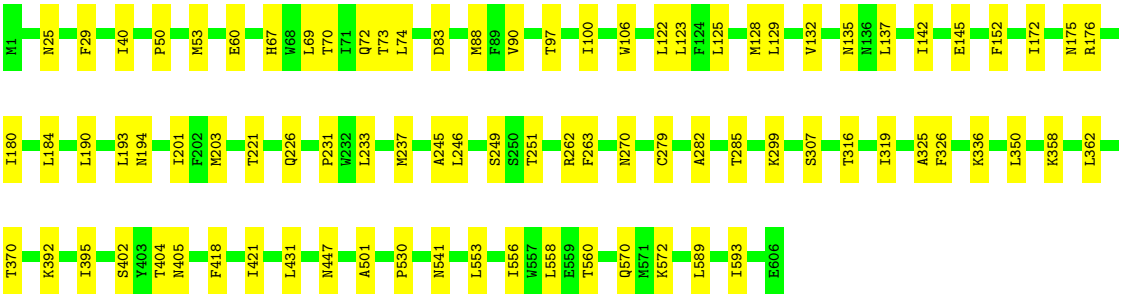
• Molecule 1: Mitochondrial complex I, 49 kDa subunit

Chain 4:



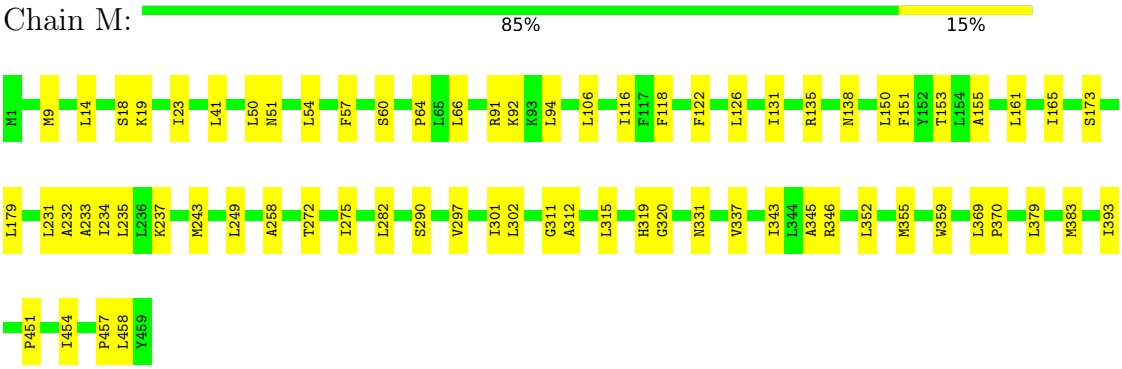
• Molecule 2: NADH-ubiquinone oxidoreductase chain 5

Chain L:



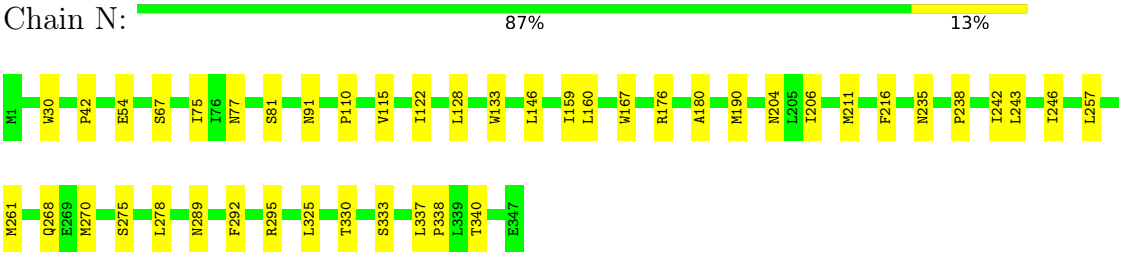
• Molecule 3: NADH-ubiquinone oxidoreductase chain 4

Chain M:



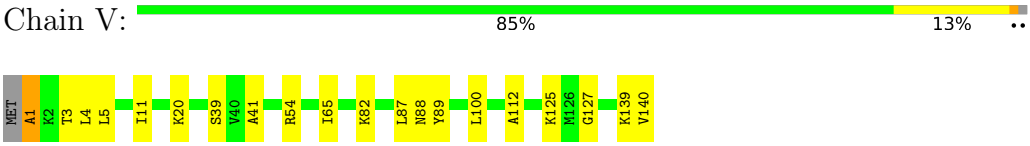
• Molecule 4: NADH-ubiquinone oxidoreductase chain 2

Chain N:



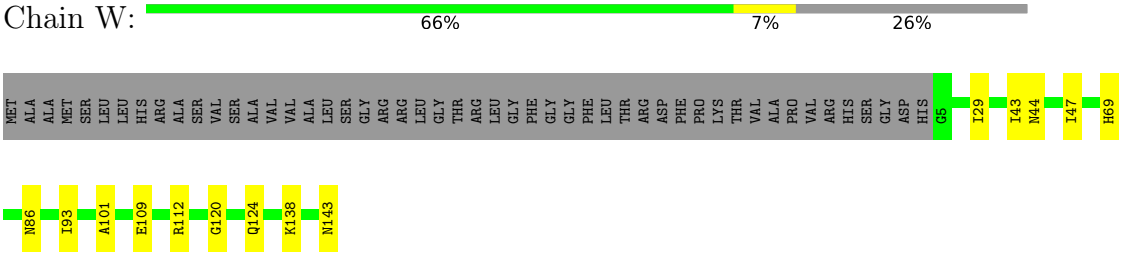
• Molecule 5: Mitochondrial complex I, B14.7 subunit

Chain V:



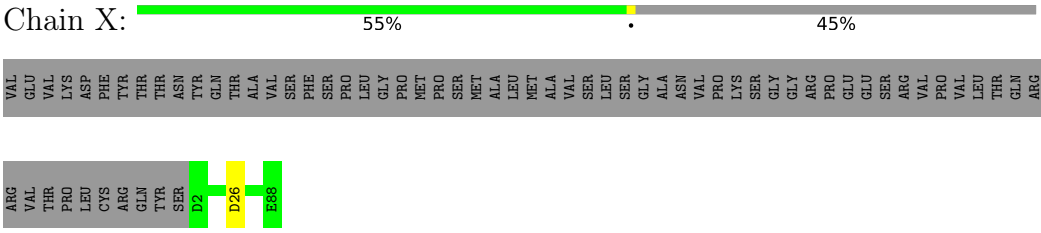
• Molecule 6: NADH:ubiquinone oxidoreductase subunit B5

Chain W:



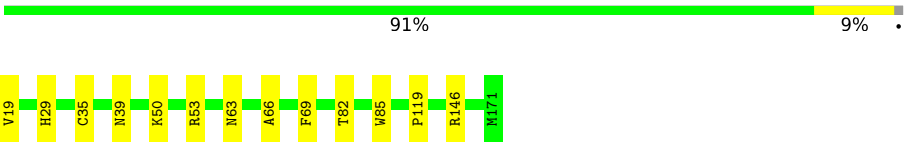
• Molecule 7: Acyl carrier protein

Chain X:



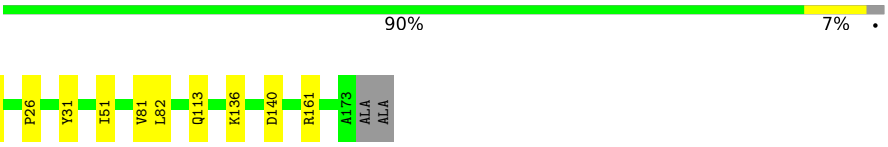
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:



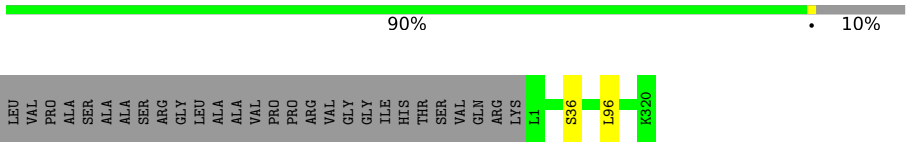
• Molecule 9: Mitochondrial complex I, PDSW subunit

Chain Z:



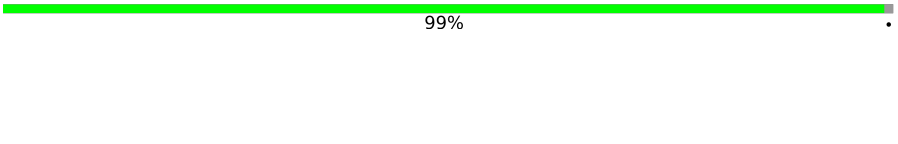
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:



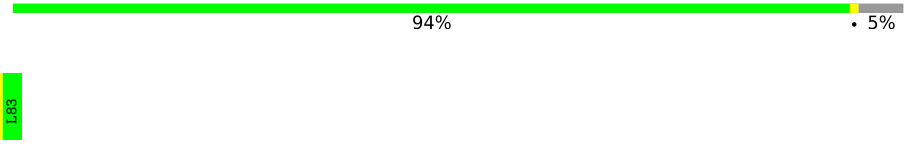
• Molecule 11: NADH:ubiquinone oxidoreductase subunit S5

Chain l:



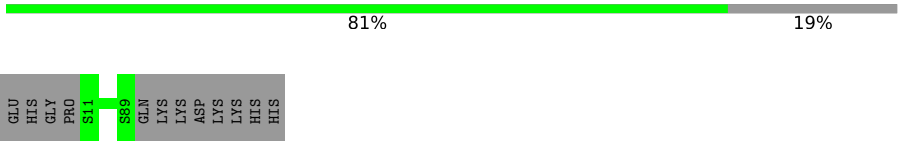
• Molecule 12: NADH:ubiquinone oxidoreductase subunit A3

Chain m:



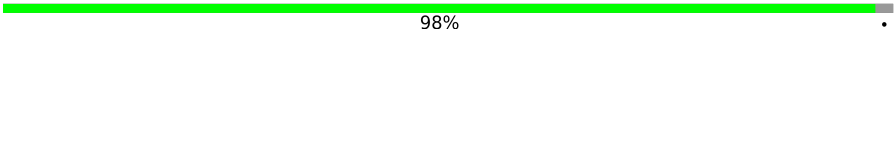
• Molecule 13: NADH:ubiquinone oxidoreductase subunit B3

Chain n:



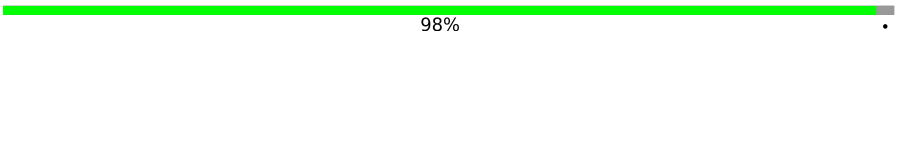
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:



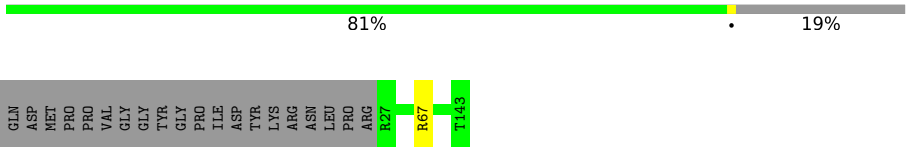
• Molecule 15: NADH:ubiquinone oxidoreductase subunit B4

Chain p:



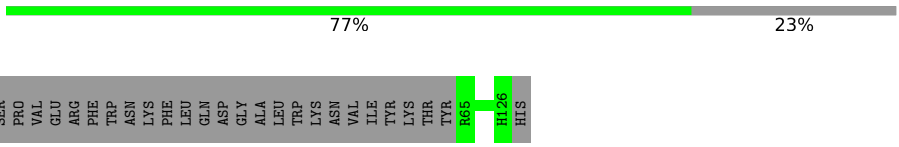
• Molecule 16: Mitochondrial complex I, B16.6 subunit

Chain q:



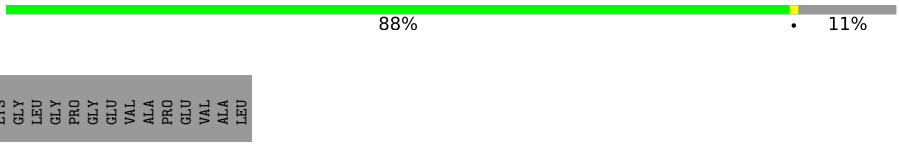
• Molecule 17: Mitochondrial complex I, B17 subunit

Chain r:



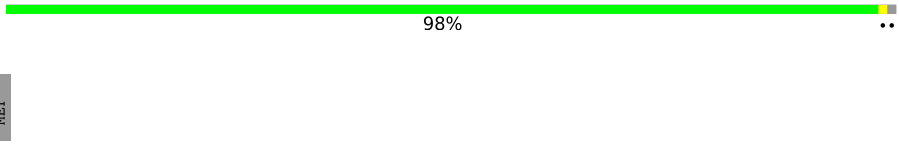
• Molecule 18: NADH:ubiquinone oxidoreductase subunit B7

Chain s:



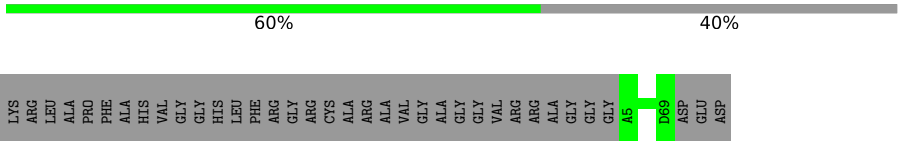
• Molecule 19: NADH:ubiquinone oxidoreductase subunit B9

Chain t:



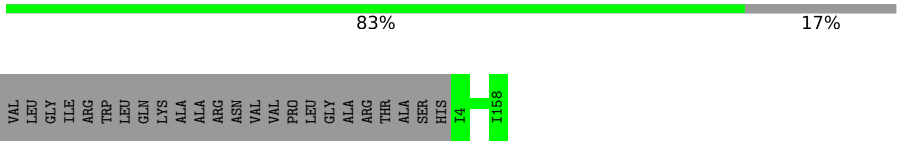
• Molecule 20: NADH:ubiquinone oxidoreductase subunit B2

Chain u:



• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:

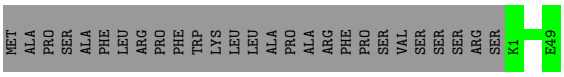


• Molecule 22: Mitochondrial complex I, ESSS subunit

Chain w:

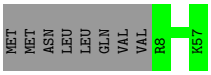
• Molecule 23: Mitochondrial complex I, KFYI subunit

Chain x:



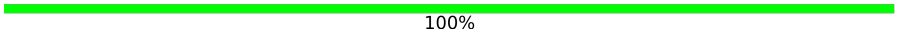
• Molecule 24: Mitochondrial complex I, MNLL subunit

Chain y:



• Molecule 25: Mitochondrial complex I, MWFE subunit

Chain z:



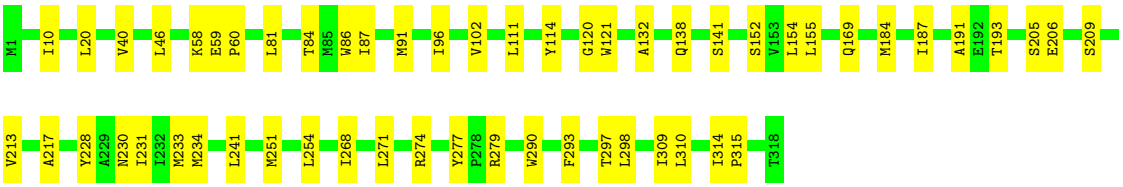
There are no outlier residues recorded for this chain.

• Molecule 26: NADH-ubiquinone oxidoreductase chain 3

Chain A:

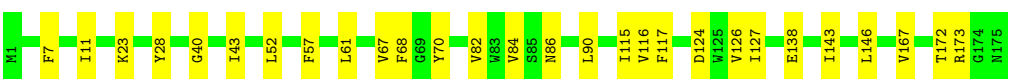
• Molecule 27: NADH-ubiquinone oxidoreductase chain 1

Chain H:



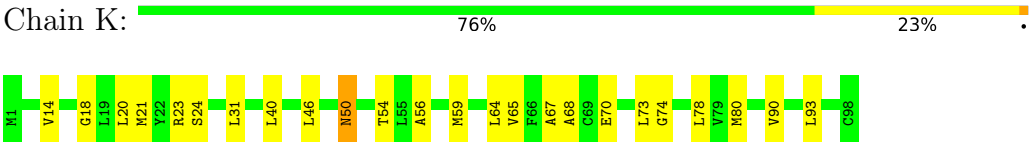
• Molecule 28: NADH-ubiquinone oxidoreductase chain 6

Chain J:



• Molecule 29: NADH-ubiquinone oxidoreductase chain 4L

Chain K:


76%
23%
M1
V14
G18
L19
L20
M21
Y22
R23
S24
L31
L40
L46
N50
T54
L55
A56
M59
L64
V65
F66
A67
A68
C69
E70
L73
G74
L78
V79
M80
V90
L93
C98

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29057	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: ZMP, AYA, SEP, 3PE, AMP, CDL, FME, PC1, MYR

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	4	0.34	0/351	0.47	0/485
2	L	0.36	0/4925	0.57	0/6700
3	M	0.39	0/3731	0.62	1/5085 (0.0%)
4	N	0.40	0/2787	0.60	1/3795 (0.0%)
5	V	0.28	0/1041	0.50	1/1412 (0.1%)
6	W	0.35	0/1188	0.50	0/1607
7	X	0.33	0/713	0.48	0/963
8	Y	0.34	0/1440	0.52	0/1942
9	Z	0.35	0/1475	0.48	0/1989
10	k	0.35	0/2646	0.49	1/3579 (0.0%)
11	l	0.35	0/896	0.53	0/1200
12	m	0.29	0/647	0.45	0/890
13	n	0.29	0/653	0.44	0/882
14	o	0.38	0/1035	0.50	0/1398
15	p	0.31	0/1085	0.49	0/1467
16	q	0.33	0/990	0.48	0/1333
17	r	0.35	0/874	0.53	0/1188
18	s	0.33	0/1072	0.47	0/1436
19	t	0.34	0/1573	0.50	0/2130
20	u	0.31	0/590	0.45	0/810
21	v	0.34	0/1361	0.51	0/1861
22	w	0.37	0/872	0.53	0/1185
23	x	0.28	0/425	0.40	0/576
24	y	0.32	0/449	0.49	0/605
25	z	0.37	0/591	0.54	0/795
26	A	0.36	0/947	0.63	2/1296 (0.2%)
27	H	0.37	0/2603	0.64	2/3561 (0.1%)
28	J	0.42	0/1378	0.64	1/1868 (0.1%)
29	K	0.37	0/749	0.67	1/1014 (0.1%)
All	All	0.36	0/39087	0.55	10/53052 (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
28	J	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	146	LEU	CA-CB-CG	6.03	129.18	115.30
29	K	20	LEU	CA-CB-CG	6.00	129.10	115.30
3	M	458	LEU	CA-CB-CG	5.53	128.02	115.30
26	A	13	LEU	CA-CB-CG	5.40	127.72	115.30
27	H	91	MET	C-N-CD	-5.39	108.74	120.60
5	V	87	LEU	CA-CB-CG	5.35	127.61	115.30
4	N	146	LEU	CA-CB-CG	5.27	127.41	115.30
27	H	310	LEU	CA-CB-CG	5.23	127.33	115.30
10	k	96	LEU	CA-CB-CG	5.23	127.32	115.30
26	A	3	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	J	115	ILE	Peptide

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	4	334	0	304	3	0
2	L	4807	0	4949	51	0
3	M	3647	0	3849	45	0
4	N	2723	0	2930	32	0
5	V	1028	0	1036	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	1155	0	1177	9	0
7	X	701	0	692	1	0
8	Y	1403	0	1392	8	0
9	Z	1441	0	1419	8	0
10	k	2596	0	2559	0	0
11	l	874	0	869	0	0
12	m	626	0	635	0	0
13	n	634	0	616	0	0
14	o	1004	0	995	0	0
15	p	1059	0	1062	0	0
16	q	967	0	959	0	0
17	r	846	0	864	0	0
18	s	1047	0	1013	0	0
19	t	1520	0	1477	0	0
20	u	563	0	509	0	0
21	v	1307	0	1207	0	0
22	w	846	0	792	0	0
23	x	412	0	411	0	0
24	y	436	0	437	0	0
25	z	576	0	570	0	0
26	A	922	0	953	8	0
27	H	2528	0	2641	32	0
28	J	1344	0	1364	18	0
29	K	749	0	793	17	0
30	A	51	0	82	1	0
30	J	91	0	136	4	0
30	L	82	0	118	2	0
30	M	44	0	65	2	0
30	N	91	0	136	6	0
30	V	37	0	48	2	0
30	o	31	0	36	0	0
30	p	27	0	27	0	0
31	H	54	0	88	2	0
31	L	54	0	88	2	0
31	M	54	0	88	3	0
31	w	54	0	88	0	0
32	L	100	0	156	6	0
32	M	190	0	289	16	0
32	N	75	0	97	2	0
32	V	179	0	261	8	0
32	W	100	0	156	4	0
33	X	31	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	k	23	0	12	0	0
35	s	15	0	27	0	0
36	4	10	0	0	0	0
36	A	13	0	0	0	0
36	H	21	0	0	0	0
36	J	13	0	0	1	0
36	K	10	0	0	0	0
36	L	47	0	0	3	0
36	M	58	0	0	2	0
36	N	37	0	0	0	0
36	V	10	0	0	1	0
36	W	26	0	0	1	0
36	X	6	0	0	0	0
36	Y	13	0	0	1	0
36	Z	15	0	0	0	0
36	k	28	0	0	0	0
36	l	12	0	0	0	0
36	m	2	0	0	0	0
36	n	4	0	0	0	0
36	o	17	0	0	0	0
36	p	15	0	0	0	0
36	q	16	0	0	0	0
36	r	8	0	0	0	0
36	s	2	0	0	0	0
36	t	17	0	0	0	0
36	u	3	0	0	0	0
36	v	15	0	0	0	0
36	w	9	0	0	0	0
36	x	6	0	0	0	0
36	y	7	0	0	0	0
36	z	6	0	0	0	0
All	All	39924	0	40506	244	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 5.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:243:LEU:HD22	4:N:330:THR:HG21	1.77	0.66
29:K:64:LEU:O	29:K:67:ALA:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:J:201:3PE:H2F2	30:J:201:3PE:H371	1.79	0.65
28:J:67:VAL:HG11	29:K:31:LEU:HD21	1.80	0.63
3:M:126:LEU:HD21	3:M:153:THR:HG21	1.81	0.63
27:H:169:GLN:NE2	27:H:241:LEU:O	2.31	0.62
32:L:1003:CDL:H642	32:L:1003:CDL:H562	1.81	0.62
2:L:100:ILE:HG21	2:L:246:LEU:HB2	1.82	0.61
30:N:402:3PE:H251	30:N:402:3PE:H351	1.81	0.61
28:J:84:VAL:HG12	28:J:90:LEU:HD13	1.83	0.60
3:M:94:LEU:HD21	32:M:504:CDL:H541	1.82	0.60
2:L:370:THR:HG23	2:L:431:LEU:HD13	1.84	0.59
27:H:81:LEU:HA	27:H:84:THR:HG22	1.84	0.59
26:A:67:LEU:HD11	29:K:68:ALA:HB3	1.84	0.59
26:A:67:LEU:HD22	29:K:65:VAL:HA	1.85	0.59
2:L:106:TRP:HD1	2:L:447:ASN:HD22	1.50	0.59
2:L:279:CYS:SG	2:L:405:ASN:ND2	2.76	0.59
3:M:231:LEU:HA	3:M:235:LEU:HB2	1.83	0.59
4:N:160:LEU:HD21	32:V:202:CDL:H191	1.84	0.58
2:L:249:SER:HB2	2:L:336:LYS:HG3	1.85	0.58
8:Y:35:CYS:O	8:Y:39:ASN:ND2	2.37	0.57
1:4:20:TYR:OH	4:N:295:ARG:NH2	2.38	0.57
30:J:202:3PE:H11	29:K:23:ARG:HG2	1.87	0.57
3:M:243:MET:HB3	3:M:301:ILE:HG21	1.86	0.57
4:N:91:ASN:HD21	28:J:117:PHE:HE1	1.53	0.57
2:L:90:VAL:HG22	2:L:129:LEU:HD22	1.87	0.56
32:M:503:CDL:H872	32:M:503:CDL:H652	1.87	0.56
32:M:503:CDL:H852	32:M:504:CDL:H673	1.87	0.56
4:N:159:ILE:HG21	4:N:278:LEU:HD11	1.87	0.56
5:V:39:SER:OG	5:V:54:ARG:NH2	2.39	0.56
27:H:20:LEU:HD21	27:H:231:ILE:HD11	1.89	0.55
1:4:3:GLN:NE2	3:M:135:ARG:O	2.38	0.55
2:L:570:GLN:OE1	4:N:167:TRP:NE1	2.36	0.55
2:L:72:GLN:NE2	36:L:1104:HOH:O	2.40	0.55
32:M:504:CDL:H591	4:N:246:ILE:HG21	1.88	0.55
32:M:504:CDL:H873	4:N:246:ILE:HA	1.87	0.55
2:L:123:LEU:HD13	32:L:1003:CDL:H712	1.89	0.54
8:Y:66:ALA:O	8:Y:69:PHE:HB3	2.07	0.54
2:L:233:LEU:HD23	2:L:307:SER:HB3	1.89	0.54
4:N:211:MET:HG2	4:N:333:SER:HB2	1.89	0.54
2:L:73:THR:HB	2:L:194:ASN:HD21	1.73	0.54
2:L:221:THR:HG23	2:L:226:GLN:HB2	1.87	0.54
2:L:97:THR:HG21	2:L:125:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:122:ILE:O	4:N:176:ARG:NH1	2.40	0.54
27:H:141:SER:HA	27:H:290:TRP:HE1	1.72	0.54
3:M:19:LYS:NZ	36:M:607:HOH:O	2.40	0.54
28:J:173:ARG:NH2	36:J:304:HOH:O	2.41	0.53
9:Z:140:ASP:O	9:Z:161:ARG:NH1	2.42	0.53
29:K:46:LEU:O	29:K:50:ASN:HB2	2.08	0.53
2:L:316:THR:HA	2:L:319:ILE:HG12	1.89	0.53
4:N:206:ILE:HG23	30:N:402:3PE:H2H2	1.91	0.53
2:L:67:HIS:NE2	2:L:70:THR:OG1	2.39	0.53
4:N:30:TRP:NE1	4:N:67:SER:OG	2.42	0.53
28:J:23:LYS:NZ	29:K:18:GLY:O	2.42	0.53
2:L:40:ILE:HD11	2:L:122:LEU:HD13	1.90	0.52
3:M:64:PRO:HB3	3:M:454:ILE:HG22	1.90	0.52
32:L:1003:CDL:H532	32:L:1003:CDL:H362	1.90	0.52
3:M:232:ALA:O	3:M:237:LYS:NZ	2.43	0.52
27:H:111:LEU:HD22	28:J:57:PHE:HZ	1.75	0.52
3:M:343:ILE:O	3:M:346:ARG:NH1	2.43	0.51
26:A:88:LEU:HD13	27:H:309:ILE:HD12	1.92	0.51
32:M:503:CDL:H792	4:N:338:PRO:HG3	1.91	0.51
2:L:358:LYS:NZ	36:L:1106:HOH:O	2.44	0.51
3:M:116:ILE:HD11	3:M:161:LEU:HD12	1.92	0.51
32:N:403:CDL:H131	32:N:403:CDL:H522	1.91	0.51
6:W:44:ASN:OD1	6:W:69:HIS:NE2	2.42	0.51
29:K:24:SER:HA	29:K:90:VAL:HG22	1.93	0.51
27:H:114:TYR:OH	28:J:61:LEU:O	2.22	0.51
30:J:202:3PE:H292	29:K:14:VAL:HG22	1.93	0.50
3:M:331:ASN:ND2	36:M:611:HOH:O	2.44	0.50
29:K:70:GLU:O	29:K:73:LEU:HB3	2.12	0.50
2:L:74:LEU:HD13	2:L:190:LEU:HD13	1.94	0.50
27:H:20:LEU:HD23	27:H:228:TYR:HB3	1.91	0.50
28:J:126:VAL:HG23	28:J:127:ILE:HG23	1.94	0.50
2:L:231:PRO:HB3	2:L:530:PRO:HG3	1.94	0.50
32:L:1003:CDL:H391	32:L:1003:CDL:H171	1.93	0.50
32:M:504:CDL:HB4	4:N:238:PRO:HB2	1.92	0.49
2:L:69:LEU:HD13	3:M:451:PRO:HG2	1.94	0.49
2:L:142:ILE:HG12	3:M:370:PRO:HB2	1.93	0.49
3:M:54:LEU:HD23	6:W:93:ILE:HG23	1.93	0.49
3:M:18:SER:HB2	3:M:23:ILE:HG22	1.94	0.49
36:W:302:HOH:O	8:Y:50:LYS:NZ	2.45	0.49
5:V:127:GLY:HA3	30:V:201:3PE:H342	1.93	0.49
5:V:112:ALA:HB1	32:V:203:CDL:H531	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:237:MET:HB3	2:L:299:LYS:HE2	1.95	0.49
3:M:50:LEU:HA	6:W:86:ASN:HD21	1.77	0.49
2:L:145:GLU:OE2	2:L:176:ARG:NH1	2.45	0.49
2:L:245:ALA:O	2:L:249:SER:OG	2.30	0.48
6:W:120:GLY:O	6:W:124:GLN:NE2	2.45	0.48
9:Z:5:ASP:HB3	9:Z:8:VAL:HG12	1.95	0.48
2:L:175:ASN:ND2	36:L:1107:HOH:O	2.44	0.48
4:N:42:PRO:HG2	28:J:167:VAL:HG22	1.95	0.48
5:V:139:LYS:NZ	36:V:602:HOH:O	2.43	0.48
27:H:120:GLY:HA3	27:H:132:ALA:HB2	1.96	0.48
3:M:369:LEU:HD12	3:M:370:PRO:HD2	1.95	0.48
2:L:593:ILE:HD12	5:V:41:ALA:HB2	1.96	0.48
5:V:65:ILE:HD11	5:V:100:LEU:HD23	1.96	0.48
31:L:1002:PC1:H372	32:W:201:CDL:H512	1.95	0.47
30:A:201:3PE:H2H1	30:A:201:3PE:H292	1.96	0.47
2:L:421:ILE:HG12	2:L:501:ALA:HB2	1.94	0.47
27:H:138:GLN:NE2	27:H:191:ALA:O	2.47	0.47
32:L:1003:CDL:H741	3:M:369:LEU:HD21	1.97	0.47
6:W:43:ILE:HG12	6:W:47:ILE:HD12	1.96	0.47
30:J:201:3PE:H2A2	30:J:201:3PE:H341	1.95	0.47
2:L:350:LEU:HD11	2:L:362:LEU:HD11	1.97	0.47
3:M:155:ALA:HB1	31:M:502:PC1:H2H2	1.96	0.47
29:K:56:ALA:O	29:K:59:MET:HB3	2.14	0.47
2:L:83:ASP:OD2	2:L:262:ARG:NH1	2.47	0.47
3:M:41:LEU:HD13	3:M:66:LEU:HD13	1.97	0.47
2:L:88:MET:HB2	2:L:326:PHE:HE2	1.79	0.47
2:L:129:LEU:HA	2:L:132:VAL:HG22	1.96	0.47
5:V:1:AYA:HA	5:V:4:LEU:HD23	1.97	0.47
26:A:80:GLN:NE2	27:H:315:PRO:O	2.46	0.47
27:H:293:PHE:O	27:H:297:THR:OG1	2.28	0.47
6:W:138:LYS:HB2	6:W:143:ASN:HD21	1.80	0.47
27:H:87:ILE:HD12	27:H:96:ILE:HD12	1.96	0.47
2:L:203:MET:HB2	9:Z:113:GLN:HG3	1.95	0.47
8:Y:146:ARG:NH2	36:Y:205:HOH:O	2.47	0.46
3:M:290:SER:HA	3:M:319:HIS:HE2	1.80	0.46
2:L:316:THR:HG23	2:L:325:ALA:HB2	1.97	0.46
8:Y:29:HIS:HB3	8:Y:119:PRO:HD2	1.97	0.46
27:H:187:ILE:HD12	31:H:401:PC1:H351	1.96	0.46
27:H:206:GLU:OE1	27:H:279:ARG:NH2	2.48	0.46
32:M:503:CDL:HA61	32:M:503:CDL:HA21	1.98	0.46
2:L:572:LYS:HG2	32:V:203:CDL:H311	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:352:LEU:HB3	3:M:355:MET:HB3	1.98	0.46
27:H:184:MET:SD	27:H:297:THR:OG1	2.73	0.46
27:H:251:MET:HB3	27:H:254:LEU:HD13	1.97	0.46
2:L:137:LEU:HD21	2:L:263:PHE:HZ	1.81	0.46
5:V:11:ILE:HB	5:V:20:LYS:HD3	1.97	0.45
3:M:9:MET:HB3	32:M:503:CDL:H232	1.98	0.45
3:M:179:LEU:HD13	3:M:249:LEU:HD11	1.98	0.45
33:X:101:ZMP:H17	33:X:101:ZMP:H15	1.62	0.45
27:H:102:VAL:HG11	27:H:154:LEU:HD11	1.98	0.45
2:L:152:PHE:HB2	2:L:172:ILE:HD11	1.97	0.45
26:A:13:LEU:HD11	27:H:10:ILE:HD12	1.98	0.45
3:M:337:VAL:HG11	3:M:345:ALA:HB2	1.97	0.45
4:N:75:ILE:HD12	29:K:40:LEU:HD22	1.98	0.45
3:M:91:ARG:HD3	3:M:135:ARG:HH21	1.81	0.45
4:N:337:LEU:O	4:N:340:THR:OG1	2.27	0.45
32:W:201:CDL:H112	9:Z:51:ILE:HD11	1.99	0.45
27:H:277:TYR:HE2	31:H:401:PC1:H382	1.82	0.45
28:J:52:LEU:HD22	28:J:143:ILE:HD11	1.98	0.45
26:A:55:PHE:HB3	26:A:113:TRP:CE2	2.52	0.45
2:L:128:MET:HG2	2:L:251:THR:HG22	1.98	0.45
32:M:504:CDL:H861	4:N:257:LEU:HD21	1.98	0.45
4:N:115:VAL:HG12	4:N:180:ALA:HB1	1.99	0.45
4:N:261:MET:HG3	4:N:340:THR:HG23	1.99	0.44
26:A:56:PHE:O	28:J:70:TYR:OH	2.35	0.44
31:M:502:PC1:H2C2	31:M:502:PC1:H392	1.99	0.44
3:M:165:ILE:HG21	4:N:268:GLN:HA	1.99	0.44
27:H:58:LYS:HB3	27:H:217:ALA:HB3	1.99	0.44
2:L:50:PRO:HA	2:L:53:MET:HG2	1.99	0.44
9:Z:26:PRO:HB2	9:Z:31:TYR:HE2	1.82	0.44
3:M:23:ILE:HD11	3:M:92:LYS:HD2	1.99	0.44
3:M:173:SER:HB2	6:W:101:ALA:HB2	1.98	0.44
4:N:110:PRO:HD3	4:N:160:LEU:HD23	2.00	0.44
3:M:272:THR:HA	3:M:275:ILE:HD12	2.00	0.44
3:M:282:LEU:HD21	3:M:359:TRP:HH2	1.83	0.44
32:V:202:CDL:H712	32:V:203:CDL:H152	2.00	0.44
32:M:504:CDL:H791	4:N:242:ILE:HG23	2.00	0.44
27:H:59:GLU:HA	27:H:60:PRO:HD3	1.86	0.44
5:V:5:LEU:HD23	30:V:201:3PE:H231	2.00	0.43
4:N:128:LEU:HD13	4:N:216:PHE:HB2	2.00	0.43
27:H:209:SER:HB3	27:H:213:VAL:HA	2.00	0.43
2:L:589:LEU:HD23	29:K:21:MET:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:556:ILE:O	2:L:560:THR:N	2.51	0.43
27:H:121:TRP:HB2	28:J:68:PHE:HZ	1.83	0.43
27:H:152:SER:HA	27:H:155:LEU:HD12	2.01	0.43
2:L:184:LEU:HD13	3:M:393:ILE:HG21	2.00	0.43
2:L:392:LYS:HA	2:L:395:ILE:HD12	1.99	0.43
32:M:504:CDL:H532	4:N:242:ILE:HD13	2.00	0.43
6:W:109:GLU:OE2	6:W:112:ARG:NH2	2.37	0.43
28:J:124:ASP:N	28:J:124:ASP:OD1	2.52	0.43
2:L:402:SER:OG	2:L:404:THR:OG1	2.32	0.43
8:Y:17:VAL:HG12	8:Y:19:VAL:HG22	2.00	0.43
2:L:25:ASN:HD22	2:L:29:PHE:HE2	1.67	0.43
3:M:106:LEU:HD13	3:M:234:ILE:HG21	2.01	0.43
2:L:60:GLU:HG2	2:L:83:ASP:HA	2.00	0.43
7:X:26:ASP:OD1	7:X:26:ASP:N	2.51	0.43
9:Z:3:SER:OG	9:Z:4:TRP:N	2.52	0.43
26:A:98:LEU:HD22	27:H:298:LEU:HD11	2.01	0.43
5:V:1:AYA:HM2	5:V:3:THR:HG22	2.00	0.42
32:V:202:CDL:H541	32:V:203:CDL:H162	2.01	0.42
32:V:202:CDL:H322	32:V:202:CDL:H351	1.82	0.42
27:H:40:VAL:HG12	27:H:46:LEU:HB3	2.01	0.42
27:H:205:SER:H	27:H:279:ARG:HH22	1.67	0.42
28:J:7:PHE:O	28:J:11:ILE:HG12	2.20	0.42
3:M:311:GLY:O	3:M:315:LEU:HB2	2.20	0.42
32:M:503:CDL:H152	32:M:503:CDL:H571	2.01	0.42
32:N:403:CDL:H582	32:N:403:CDL:H781	2.02	0.42
8:Y:82:THR:HA	8:Y:85:TRP:CD1	2.54	0.42
4:N:77:ASN:O	4:N:81:SER:OG	2.30	0.42
1:4:6:PRO:HB3	1:4:10:TRP:CD1	2.55	0.42
3:M:14:LEU:O	3:M:18:SER:OG	2.31	0.42
3:M:60:SER:HB2	3:M:457:PRO:HA	2.02	0.42
3:M:118:PHE:O	3:M:122:PHE:CB	2.67	0.42
3:M:126:LEU:HD13	3:M:150:LEU:HD12	2.02	0.42
5:V:82:LYS:O	5:V:88:ASN:ND2	2.53	0.42
28:J:138:GLU:O	29:K:54:THR:OG1	2.35	0.42
3:M:379:LEU:O	3:M:383:MET:HG2	2.19	0.42
32:W:201:CDL:H862	32:W:201:CDL:H832	1.87	0.42
30:M:501:3PE:H361	30:M:501:3PE:H391	1.92	0.41
5:V:139:LYS:HG3	5:V:140:VAL:HG13	2.01	0.41
27:H:309:ILE:HG12	27:H:314:ILE:HD11	2.02	0.41
3:M:233:ALA:HA	3:M:320:GLY:HA2	2.01	0.41
32:M:503:CDL:H841	32:M:503:CDL:H662	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:190:MET:HG2	4:N:204:ASN:HB3	2.02	0.41
28:J:40:GLY:HA2	28:J:43:ILE:HD12	2.02	0.41
2:L:193:LEU:HD23	2:L:201:ILE:HA	2.03	0.41
29:K:74:GLY:O	29:K:78:LEU:N	2.53	0.41
9:Z:81:VAL:HG23	9:Z:82:LEU:HD22	2.02	0.41
28:J:172:THR:HA	29:K:80:MET:HE3	2.01	0.41
3:M:258:ALA:HB1	3:M:302:LEU:HB3	2.02	0.41
3:M:151:PHE:HB3	30:N:401:3PE:H382	2.02	0.41
2:L:180:ILE:HD13	30:L:1001:3PE:H2H2	2.02	0.41
30:L:1001:3PE:H231	30:L:1001:3PE:H262	1.94	0.41
31:L:1002:PC1:H3H2	32:W:201:CDL:H872	2.03	0.41
32:L:1003:CDL:H181	6:W:29:ILE:HD13	2.03	0.41
3:M:131:ILE:O	3:M:135:ARG:HB3	2.20	0.41
3:M:297:VAL:HG13	3:M:312:ALA:HB1	2.02	0.41
32:M:503:CDL:H632	32:M:503:CDL:H601	1.92	0.41
4:N:133:TRP:HE3	30:N:402:3PE:H382	1.85	0.41
4:N:270:MET:O	4:N:275:SER:OG	2.35	0.41
4:N:289:ASN:HA	4:N:292:PHE:CE1	2.56	0.41
30:N:402:3PE:H272	30:N:402:3PE:H2A1	1.81	0.41
32:V:203:CDL:H332	32:V:203:CDL:H542	2.03	0.41
28:J:28:TYR:CZ	28:J:82:VAL:HG13	2.56	0.41
4:N:54:GLU:HG3	29:K:93:LEU:HB3	2.02	0.41
9:Z:136:LYS:NZ	9:Z:140:ASP:OD2	2.51	0.41
27:H:268:ILE:HD13	27:H:271:LEU:HD12	2.02	0.41
31:M:502:PC1:H2D1	31:M:502:PC1:H3F2	2.02	0.40
5:V:89:TYR:CD2	5:V:125:LYS:HB2	2.56	0.40
27:H:230:ASN:O	27:H:234:MET:HB2	2.22	0.40
2:L:418:PHE:HD1	2:L:421:ILE:HD12	1.86	0.40
2:L:553:LEU:HB3	2:L:558:LEU:HD23	2.02	0.40
3:M:51:ASN:HA	3:M:57:PHE:HB2	2.02	0.40
30:M:501:3PE:H3E2	32:V:203:CDL:H841	2.03	0.40
8:Y:5:GLU:O	8:Y:53:ARG:NH1	2.52	0.40
27:H:86:TRP:CE2	27:H:233:MET:HB2	2.57	0.40
2:L:282:ALA:HA	2:L:285:THR:HG22	2.03	0.40
2:L:316:THR:HB	2:L:395:ILE:HG23	2.03	0.40
4:N:325:LEU:HD12	30:N:402:3PE:H271	2.03	0.40
32:M:503:CDL:H311	32:M:503:CDL:H562	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	38/457 (8%)	34 (90%)	4 (10%)	0	100	100
2	L	604/606 (100%)	576 (95%)	28 (5%)	0	100	100
3	M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
4	N	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
5	V	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
6	W	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
7	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100
8	Y	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
9	Z	169/175 (97%)	167 (99%)	2 (1%)	0	100	100
10	k	317/355 (89%)	300 (95%)	17 (5%)	0	100	100
11	l	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
12	m	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
13	n	77/98 (79%)	74 (96%)	3 (4%)	0	100	100
14	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
15	p	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
16	q	115/144 (80%)	115 (100%)	0	0	100	100
17	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
18	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
19	t	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
20	u	63/108 (58%)	60 (95%)	3 (5%)	0	100	100
21	v	153/186 (82%)	146 (95%)	7 (5%)	0	100	100
22	w	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
23	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
24	y	48/58 (83%)	48 (100%)	0	0	100	100
25	z	68/70 (97%)	68 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
27	H	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
28	J	173/175 (99%)	166 (96%)	6 (4%)	1 (1%)	22	52
29	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
All	All	4642/5544 (84%)	4482 (97%)	159 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	J	116	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	34/387 (9%)	34 (100%)	0	100	100
2	L	538/538 (100%)	535 (99%)	3 (1%)	84	95
3	M	411/411 (100%)	410 (100%)	1 (0%)	92	98
4	N	315/315 (100%)	314 (100%)	1 (0%)	91	97
5	V	101/102 (99%)	101 (100%)	0	100	100
6	W	122/160 (76%)	122 (100%)	0	100	100
7	X	80/141 (57%)	80 (100%)	0	100	100
8	Y	154/155 (99%)	153 (99%)	1 (1%)	84	95
9	Z	155/157 (99%)	155 (100%)	0	100	100
10	k	283/309 (92%)	283 (100%)	0	100	100
11	l	94/95 (99%)	94 (100%)	0	100	100
12	m	69/72 (96%)	68 (99%)	1 (1%)	62	86
13	n	61/76 (80%)	61 (100%)	0	100	100
14	o	107/109 (98%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	p	114/116 (98%)	114 (100%)	0	100	100
16	q	100/122 (82%)	99 (99%)	1 (1%)	73	91
17	r	95/122 (78%)	95 (100%)	0	100	100
18	s	110/120 (92%)	109 (99%)	1 (1%)	75	92
19	t	159/161 (99%)	158 (99%)	1 (1%)	84	95
20	u	59/84 (70%)	59 (100%)	0	100	100
21	v	140/160 (88%)	140 (100%)	0	100	100
22	w	92/130 (71%)	92 (100%)	0	100	100
23	x	44/67 (66%)	44 (100%)	0	100	100
24	y	46/54 (85%)	46 (100%)	0	100	100
25	z	59/59 (100%)	59 (100%)	0	100	100
26	A	103/103 (100%)	103 (100%)	0	100	100
27	H	278/278 (100%)	276 (99%)	2 (1%)	81	94
28	J	144/144 (100%)	143 (99%)	1 (1%)	81	94
29	K	86/86 (100%)	85 (99%)	1 (1%)	67	89
All	All	4153/4833 (86%)	4139 (100%)	14 (0%)	90	97

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	135	ASN
2	L	270	ASN
2	L	541	ASN
3	M	138	ASN
4	N	235	ASN
8	Y	63	ASN
12	m	82	ARG
16	q	67	ARG
18	s	103	ARG
19	t	128	ARG
27	H	193	THR
27	H	274	ARG
28	J	86	ASN
29	K	50	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	405	ASN
6	W	143	ASN
11	l	6	GLN
14	o	61	GLN
16	q	53	ASN
27	H	230	ASN
27	H	235	ASN
29	K	83	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)

5 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	$\#\|Z\| > 2$
2	FME	L	1	2	8,9,10	0.92	0	7,9,11	0.92	0
29	FME	K	1	29	8,9,10	0.95	0	7,9,11	0.86	0
3	FME	M	1	3	8,9,10	0.96	0	7,9,11	0.74	0
5	AYA	V	1	5	6,7,8	1.26	1 (16%)	5,8,10	1.69	1 (20%)
10	SEP	k	36	10	8,9,10	1.53	1 (12%)	8,12,14	1.65	2 (25%)

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
2	FME	L	1	2	-	2/7/9/11	-
29	FME	K	1	29	-	1/7/9/11	-
3	FME	M	1	3	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AYA	V	1	5	-	2/4/6/8	-
10	SEP	k	36	10	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	k	36	SEP	P-O1P	3.32	1.61	1.50
5	V	1	AYA	CA-N	-2.50	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	36	SEP	OG-CB-CA	3.01	111.07	108.14
10	k	36	SEP	P-OG-CB	-2.96	110.13	118.30
5	V	1	AYA	CB-CA-N	2.55	112.45	109.61

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	FME	CA-CB-CG-SD
3	M	1	FME	C-CA-CB-CG
3	M	1	FME	O-C-CA-CB
10	k	36	SEP	CB-OG-P-O2P
10	k	36	SEP	CB-OG-P-O3P
5	V	1	AYA	OT-CT-N-CA
5	V	1	AYA	CM-CT-N-CA
29	K	1	FME	CA-CB-CG-SD
10	k	36	SEP	CB-OG-P-O1P
10	k	36	SEP	CA-CB-OG-P
3	M	1	FME	CB-CG-SD-CE
2	L	1	FME	N-CA-CB-CG
3	M	1	FME	N-CA-CB-CG
3	M	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	1	AYA	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.38	0
32	CDL	M	503	-	99,99,99	0.27	0	105,111,111	0.33	0
34	AMP	k	501	-	22,25,25	0.88	1 (4%)	25,38,38	1.20	2 (8%)
30	3PE	V	201	-	36,36,50	0.35	0	39,41,55	0.32	0
32	CDL	M	504	-	89,89,99	0.28	0	95,101,111	0.41	0
30	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.43	0
30	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.72	1 (3%)
30	3PE	p	201	-	26,26,50	0.48	0	30,31,55	0.53	1 (3%)
32	CDL	L	1003	-	99,99,99	0.25	0	105,111,111	0.32	0
31	PC1	H	401	-	53,53,53	0.30	0	59,61,61	0.48	0
30	3PE	N	401	-	39,39,50	0.33	0	42,44,55	0.33	0
33	ZMP	X	101	7	24,30,36	0.80	1 (4%)	29,37,45	1.02	1 (3%)
30	3PE	J	202	-	39,39,50	0.36	0	42,44,55	0.38	0
30	3PE	L	1001	-	50,50,50	0.31	0	53,55,55	0.37	0
32	CDL	V	203	-	84,84,99	0.29	0	90,96,111	0.25	0
31	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.63	2 (3%)
30	3PE	J	201	-	50,50,50	0.32	0	53,55,55	0.40	0
30	3PE	A	201	-	50,50,50	0.30	0	53,55,55	0.31	0
31	PC1	M	502	-	53,53,53	0.31	0	59,61,61	0.39	0
32	CDL	W	201	-	99,99,99	0.27	0	105,111,111	0.30	0
35	MYR	s	201	18	14,14,15	0.19	0	13,13,15	0.20	0
32	CDL	V	202	-	93,93,99	0.27	0	99,105,111	0.25	0
32	CDL	N	403	-	74,74,99	0.31	0	80,86,111	0.46	1 (1%)
30	3PE	N	402	-	50,50,50	0.33	0	53,55,55	0.54	2 (3%)
30	3PE	M	501	-	43,43,50	0.33	0	46,48,55	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PC1	w	801	-	-	12/57/57/57	-
32	CDL	M	503	-	1/1/9/9	28/110/110/110	-
34	AMP	k	501	-	-	4/6/26/26	0/3/3/3
30	3PE	V	201	-	-	12/40/40/54	-
30	3PE	o	501	-	-	7/34/34/54	-
32	CDL	M	504	-	-	33/100/100/110	-
30	3PE	L	1004	-	-	7/34/34/54	-
30	3PE	p	201	-	-	3/27/27/54	-
32	CDL	L	1003	-	1/1/9/9	38/110/110/110	-
31	PC1	H	401	-	-	17/57/57/57	-
30	3PE	N	401	-	-	8/43/43/54	-
33	ZMP	X	101	7	-	17/35/37/43	-
30	3PE	J	202	-	-	11/43/43/54	-
30	3PE	L	1001	-	-	14/54/54/54	-
32	CDL	V	203	-	1/1/9/9	33/95/95/110	-
31	PC1	L	1002	-	-	20/57/57/57	-
30	3PE	J	201	-	-	14/54/54/54	-
30	3PE	A	201	-	-	13/54/54/54	-
31	PC1	M	502	-	-	23/57/57/57	-
32	CDL	W	201	-	-	21/110/110/110	-
35	MYR	s	201	18	-	1/11/12/13	-
32	CDL	V	202	-	-	24/104/104/110	-
32	CDL	N	403	-	2/2/9/9	19/85/85/110	-
30	3PE	N	402	-	-	17/54/54/54	-
30	3PE	M	501	-	-	8/47/47/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	101	ZMP	C9-C10	2.43	1.53	1.50
34	k	501	AMP	C5-C4	2.39	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	k	501	AMP	N3-C2-N1	-3.16	123.73	128.68
34	k	501	AMP	C4-C5-N7	-2.66	106.63	109.40
33	X	101	ZMP	O1-C10-C9	-2.62	120.90	123.99
31	L	1002	PC1	C2-O21-C21	2.46	123.85	117.79
30	L	1004	3PE	C2-O21-C21	2.38	123.66	117.79
31	L	1002	PC1	O21-C2-C1	2.21	116.39	108.40
30	N	402	3PE	C2-O21-C21	2.18	123.15	117.79
30	p	201	3PE	O12-P-O14	2.13	119.02	110.68
32	N	403	CDL	CB4-OB6-CB5	2.08	122.92	117.79
30	N	402	3PE	O21-C2-C3	2.03	115.74	108.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	L	1003	CDL	CB4
32	M	503	CDL	CB4
32	N	403	CDL	CB4
32	N	403	CDL	CA4
32	V	203	CDL	CB4

All (404) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	L	1004	3PE	C1-O11-P-O13
30	L	1004	3PE	C2-C1-O11-P
30	L	1004	3PE	O13-C11-C12-N
30	M	501	3PE	C11-O13-P-O12
30	M	501	3PE	C11-O13-P-O14
30	N	401	3PE	C1-O11-P-O12
30	N	401	3PE	C1-O11-P-O13
30	N	401	3PE	C1-O11-P-O14
30	N	402	3PE	C1-O11-P-O12
30	N	402	3PE	C1-O11-P-O14
30	V	201	3PE	O13-C11-C12-N
30	o	501	3PE	C11-O13-P-O11
30	o	501	3PE	C11-O13-P-O12
30	o	501	3PE	C11-O13-P-O14
30	o	501	3PE	O13-C11-C12-N
30	A	201	3PE	C1-O11-P-O12
30	J	201	3PE	C1-O11-P-O14
30	J	201	3PE	C11-O13-P-O12
30	J	201	3PE	O13-C11-C12-N
30	J	202	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
31	L	1002	PC1	C11-O13-P-O14
31	L	1002	PC1	C1-O11-P-O12
31	L	1002	PC1	C2-C1-O11-P
31	M	502	PC1	C11-O13-P-O14
31	M	502	PC1	C1-O11-P-O12
31	M	502	PC1	C1-O11-P-O14
31	H	401	PC1	C11-O13-P-O14
31	H	401	PC1	C11-O13-P-O11
31	H	401	PC1	C1-O11-P-O14
32	L	1003	CDL	CA2-OA2-PA1-OA4
32	L	1003	CDL	CA3-OA5-PA1-OA2
32	L	1003	CDL	CA3-OA5-PA1-OA4
32	L	1003	CDL	CB3-OB5-PB2-OB3
32	M	503	CDL	CB2-OB2-PB2-OB3
32	M	504	CDL	CA2-OA2-PA1-OA4
32	M	504	CDL	CB2-OB2-PB2-OB3
32	M	504	CDL	CB3-OB5-PB2-OB3
32	N	403	CDL	CA2-OA2-PA1-OA3
32	N	403	CDL	CA2-OA2-PA1-OA4
32	N	403	CDL	CB2-OB2-PB2-OB4
32	V	203	CDL	CA2-OA2-PA1-OA3
32	V	203	CDL	CA2-OA2-PA1-OA4
32	V	203	CDL	CB3-OB5-PB2-OB3
32	W	201	CDL	CA2-OA2-PA1-OA3
32	W	201	CDL	CA2-OA2-PA1-OA4
32	W	201	CDL	CB3-OB5-PB2-OB3
33	X	101	ZMP	C17-C18-C21-O5
33	X	101	ZMP	O4-C17-C18-C21
33	X	101	ZMP	C16-C17-C18-C21
33	X	101	ZMP	O4-C17-C18-C19
33	X	101	ZMP	C16-C17-C18-C20
33	X	101	ZMP	C17-C16-N2-C15
34	k	501	AMP	C5'-O5'-P-O1P
34	k	501	AMP	C5'-O5'-P-O2P
34	k	501	AMP	C5'-O5'-P-O3P
32	M	503	CDL	O1-C1-CB2-OB2
32	M	504	CDL	O1-C1-CB2-OB2
32	V	203	CDL	O1-C1-CA2-OA2
33	X	101	ZMP	O3-C16-N2-C15
32	M	504	CDL	CA2-C1-CB2-OB2
32	V	203	CDL	CB2-C1-CA2-OA2
32	L	1003	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
32	M	504	CDL	CB5-C51-C52-C53
30	p	201	3PE	C21-C22-C23-C24
32	M	503	CDL	CB5-C51-C52-C53
30	L	1001	3PE	C11-O13-P-O11
30	M	501	3PE	C11-O13-P-O11
30	N	401	3PE	C11-O13-P-O11
30	N	402	3PE	C1-O11-P-O13
30	V	201	3PE	C1-O11-P-O13
30	V	201	3PE	C11-O13-P-O11
30	A	201	3PE	C1-O11-P-O13
30	A	201	3PE	C11-O13-P-O11
30	J	202	3PE	C1-O11-P-O13
31	L	1002	PC1	C11-O13-P-O11
31	M	502	PC1	C1-O11-P-O13
32	L	1003	CDL	CA2-OA2-PA1-OA5
32	L	1003	CDL	CB3-OB5-PB2-OB2
32	M	504	CDL	CA2-OA2-PA1-OA5
32	M	504	CDL	CB2-OB2-PB2-OB5
32	N	403	CDL	CA2-OA2-PA1-OA5
32	N	403	CDL	CA3-OA5-PA1-OA2
32	N	403	CDL	CB2-OB2-PB2-OB5
32	N	403	CDL	CB3-OB5-PB2-OB2
32	V	203	CDL	CA3-OA5-PA1-OA2
32	V	203	CDL	CB2-OB2-PB2-OB5
32	V	203	CDL	CB3-OB5-PB2-OB2
32	W	201	CDL	CA2-OA2-PA1-OA5
32	W	201	CDL	CB3-OB5-PB2-OB2
32	L	1003	CDL	C21-C22-C23-C24
31	H	401	PC1	C3B-C3C-C3D-C3E
32	L	1003	CDL	C82-C83-C84-C85
32	M	503	CDL	C81-C82-C83-C84
32	M	504	CDL	C78-C79-C80-C81
32	W	201	CDL	C82-C83-C84-C85
30	L	1001	3PE	C34-C35-C36-C37
30	N	402	3PE	C37-C38-C39-C3A
32	W	201	CDL	C35-C36-C37-C38
32	N	403	CDL	CA4-CA3-OA5-PA1
32	L	1003	CDL	C22-C23-C24-C25
32	V	202	CDL	C79-C80-C81-C82
32	M	504	CDL	C81-C82-C83-C84
32	L	1003	CDL	C56-C57-C58-C59
32	V	203	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	L	1001	3PE	C3B-C3C-C3D-C3E
31	H	401	PC1	C3C-C3D-C3E-C3F
30	J	202	3PE	C21-C22-C23-C24
32	W	201	CDL	CB5-C51-C52-C53
32	M	503	CDL	C12-C13-C14-C15
32	M	503	CDL	C63-C64-C65-C66
31	L	1002	PC1	C38-C39-C3A-C3B
32	L	1003	CDL	C41-C42-C43-C44
30	A	201	3PE	C38-C39-C3A-C3B
31	M	502	PC1	C3A-C3B-C3C-C3D
32	L	1003	CDL	C77-C78-C79-C80
31	M	502	PC1	C11-C12-N-C14
32	M	503	CDL	C52-C53-C54-C55
30	M	501	3PE	O13-C11-C12-N
30	N	402	3PE	O13-C11-C12-N
30	N	402	3PE	C2B-C2C-C2D-C2E
32	V	203	CDL	C78-C79-C80-C81
33	X	101	ZMP	C3-C4-C5-C6
33	X	101	ZMP	C6-C7-C8-C9
31	L	1002	PC1	C36-C37-C38-C39
32	V	202	CDL	C40-C41-C42-C43
32	W	201	CDL	C31-C32-C33-C34
30	J	202	3PE	C32-C33-C34-C35
30	N	402	3PE	C24-C25-C26-C27
31	H	401	PC1	C2C-C2D-C2E-C2F
32	V	203	CDL	O1-C1-CB2-OB2
30	J	201	3PE	C21-C22-C23-C24
30	J	202	3PE	C33-C34-C35-C36
30	N	401	3PE	C31-C32-C33-C34
30	A	201	3PE	C2C-C2D-C2E-C2F
32	M	503	CDL	C14-C15-C16-C17
30	N	402	3PE	C28-C29-C2A-C2B
30	A	201	3PE	C2E-C2F-C2G-C2H
30	L	1004	3PE	C21-C22-C23-C24
32	W	201	CDL	OB5-CB3-CB4-OB6
31	H	401	PC1	C22-C23-C24-C25
30	N	402	3PE	O21-C2-C3-O31
30	J	201	3PE	O21-C2-C3-O31
30	J	202	3PE	C26-C27-C28-C29
31	M	502	PC1	C11-C12-N-C15
32	M	503	CDL	C11-C12-C13-C14
30	M	501	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	J	201	3PE	C11-O13-P-O11
31	H	401	PC1	C1-O11-P-O13
32	M	504	CDL	CB3-OB5-PB2-OB2
32	V	202	CDL	CA2-OA2-PA1-OA5
32	V	203	CDL	CA2-OA2-PA1-OA5
30	V	201	3PE	C2-C1-O11-P
31	L	1002	PC1	O11-C1-C2-C3
32	V	202	CDL	OA5-CA3-CA4-CA6
31	M	502	PC1	C2D-C2E-C2F-C2G
32	L	1003	CDL	C17-C18-C19-C20
30	J	201	3PE	C27-C28-C29-C2A
31	M	502	PC1	C11-C12-N-C13
30	J	202	3PE	C1-C2-C3-O31
32	L	1003	CDL	CA3-CA4-CA6-OA8
32	M	503	CDL	CA3-CA4-CA6-OA8
32	V	203	CDL	CB3-CB4-CB6-OB8
32	N	403	CDL	C34-C35-C36-C37
31	L	1002	PC1	C21-C22-C23-C24
32	V	202	CDL	OB5-CB3-CB4-OB6
32	M	503	CDL	C35-C36-C37-C38
30	J	202	3PE	C34-C35-C36-C37
33	X	101	ZMP	O4-C17-C18-C20
32	W	201	CDL	OB5-CB3-CB4-CB6
32	V	202	CDL	CA7-C31-C32-C33
30	A	201	3PE	C35-C36-C37-C38
32	V	203	CDL	C72-C73-C74-C75
31	w	801	PC1	C3E-C3F-C3G-C3H
31	H	401	PC1	C22-C21-O21-C2
32	M	504	CDL	C1-CA2-OA2-PA1
32	V	203	CDL	C1-CA2-OA2-PA1
32	V	203	CDL	C33-C34-C35-C36
32	L	1003	CDL	C34-C35-C36-C37
30	L	1001	3PE	C1-C2-C3-O31
30	N	402	3PE	C1-C2-C3-O31
30	J	201	3PE	C1-C2-C3-O31
35	s	201	MYR	C11-C10-C9-C8
30	L	1001	3PE	O11-C1-C2-O21
31	M	502	PC1	O11-C1-C2-O21
32	V	202	CDL	OA5-CA3-CA4-OA6
32	V	203	CDL	C73-C74-C75-C76
30	o	501	3PE	C25-C26-C27-C28
32	L	1003	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
32	V	203	CDL	OA6-CA4-CA6-OA8
32	M	503	CDL	C36-C37-C38-C39
32	M	503	CDL	CA2-C1-CB2-OB2
32	M	503	CDL	C58-C59-C60-C61
30	M	501	3PE	C2-C1-O11-P
32	M	504	CDL	CB4-CB3-OB5-PB2
32	V	202	CDL	CA4-CA3-OA5-PA1
32	V	202	CDL	C71-C72-C73-C74
32	L	1003	CDL	C58-C59-C60-C61
32	M	503	CDL	C59-C60-C61-C62
33	X	101	ZMP	C5-C6-C7-C8
30	L	1001	3PE	O11-C1-C2-C3
31	M	502	PC1	O11-C1-C2-C3
32	V	202	CDL	OB5-CB3-CB4-CB6
32	M	504	CDL	C54-C55-C56-C57
32	M	503	CDL	C57-C58-C59-C60
31	H	401	PC1	O22-C21-O21-C2
32	N	403	CDL	C52-C51-CB5-OB6
31	L	1002	PC1	C33-C34-C35-C36
31	M	502	PC1	C2-C1-O11-P
32	M	504	CDL	CB3-CB4-CB6-OB8
32	V	202	CDL	CB3-CB4-CB6-OB8
32	V	203	CDL	C1-CB2-OB2-PB2
31	L	1002	PC1	O11-C1-C2-O21
33	X	101	ZMP	C16-C17-C18-C19
32	L	1003	CDL	C37-C38-C39-C40
32	V	203	CDL	OB6-CB4-CB6-OB8
32	M	504	CDL	C62-C63-C64-C65
31	w	801	PC1	C39-C3A-C3B-C3C
32	V	203	CDL	C71-C72-C73-C74
30	N	402	3PE	C23-C24-C25-C26
30	N	402	3PE	C11-O13-P-O11
30	J	201	3PE	C1-O11-P-O13
31	L	1002	PC1	C1-O11-P-O13
31	M	502	PC1	C11-O13-P-O11
31	w	801	PC1	C11-O13-P-O11
32	L	1003	CDL	CB2-OB2-PB2-OB5
32	L	1003	CDL	C1-CB2-OB2-PB2
32	M	504	CDL	C53-C54-C55-C56
30	L	1001	3PE	C11-O13-P-O14
30	L	1004	3PE	C1-O11-P-O14
30	N	401	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
30	V	201	3PE	C1-O11-P-O12
30	V	201	3PE	C1-O11-P-O14
30	V	201	3PE	C11-O13-P-O14
30	A	201	3PE	C11-O13-P-O14
30	J	201	3PE	C11-O13-P-O14
31	L	1002	PC1	C11-O13-P-O12
31	L	1002	PC1	C1-O11-P-O14
31	H	401	PC1	C1-O11-P-O12
32	L	1003	CDL	CA2-OA2-PA1-OA3
32	L	1003	CDL	CA3-OA5-PA1-OA3
32	L	1003	CDL	CB3-OB5-PB2-OB4
32	M	504	CDL	CA2-OA2-PA1-OA3
32	M	504	CDL	CB2-OB2-PB2-OB4
32	M	504	CDL	CB3-OB5-PB2-OB4
32	N	403	CDL	CA3-OA5-PA1-OA3
32	N	403	CDL	CA3-OA5-PA1-OA4
32	N	403	CDL	CB3-OB5-PB2-OB3
32	N	403	CDL	CB3-OB5-PB2-OB4
32	V	202	CDL	CA2-OA2-PA1-OA4
32	V	203	CDL	CA3-OA5-PA1-OA3
32	V	203	CDL	CB2-OB2-PB2-OB3
32	V	203	CDL	CB2-OB2-PB2-OB4
32	V	203	CDL	CB3-OB5-PB2-OB4
32	W	201	CDL	CB3-OB5-PB2-OB4
31	w	801	PC1	C31-C32-C33-C34
32	V	203	CDL	OA5-CA3-CA4-CA6
30	M	501	3PE	C37-C38-C39-C3A
31	H	401	PC1	C3A-C3B-C3C-C3D
31	L	1002	PC1	C37-C38-C39-C3A
31	M	502	PC1	C23-C24-C25-C26
32	V	203	CDL	OA5-CA3-CA4-OA6
32	L	1003	CDL	C32-C33-C34-C35
32	V	202	CDL	C77-C78-C79-C80
31	L	1002	PC1	O13-C11-C12-N
31	H	401	PC1	O13-C11-C12-N
32	V	202	CDL	C31-C32-C33-C34
30	N	402	3PE	C27-C28-C29-C2A
32	W	201	CDL	C15-C16-C17-C18
33	X	101	ZMP	O3-C16-C17-O4
30	J	202	3PE	C25-C26-C27-C28
32	W	201	CDL	CA7-C31-C32-C33
32	M	504	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
33	X	101	ZMP	C19-C18-C21-O5
33	X	101	ZMP	C20-C18-C21-O5
31	L	1002	PC1	C23-C24-C25-C26
32	M	504	CDL	C52-C53-C54-C55
33	X	101	ZMP	C2-C3-C4-C5
31	H	401	PC1	C2D-C2E-C2F-C2G
30	N	402	3PE	C36-C37-C38-C39
32	L	1003	CDL	C1-CA2-OA2-PA1
30	A	201	3PE	C3C-C3D-C3E-C3F
32	M	504	CDL	CA5-C11-C12-C13
31	w	801	PC1	C27-C28-C29-C2A
30	J	202	3PE	O21-C2-C3-O31
32	M	503	CDL	OA6-CA4-CA6-OA8
32	V	202	CDL	OB6-CB4-CB6-OB8
32	M	503	CDL	CB3-OB5-PB2-OB2
32	M	504	CDL	CA3-OA5-PA1-OA2
30	o	501	3PE	C22-C23-C24-C25
31	L	1002	PC1	C3E-C3F-C3G-C3H
32	L	1003	CDL	C39-C40-C41-C42
32	V	202	CDL	C13-C14-C15-C16
32	W	201	CDL	CA5-C11-C12-C13
32	M	503	CDL	C84-C85-C86-C87
32	N	403	CDL	C16-C17-C18-C19
32	L	1003	CDL	C38-C39-C40-C41
30	L	1001	3PE	C24-C25-C26-C27
32	L	1003	CDL	C76-C77-C78-C79
30	A	201	3PE	C2D-C2E-C2F-C2G
31	w	801	PC1	C2B-C2C-C2D-C2E
32	M	504	CDL	OA6-CA4-CA6-OA8
30	o	501	3PE	C2-C1-O11-P
32	M	503	CDL	CA7-C31-C32-C33
31	M	502	PC1	C39-C3A-C3B-C3C
32	N	403	CDL	CB7-C71-C72-C73
32	M	504	CDL	CA3-CA4-CA6-OA8
32	L	1003	CDL	C55-C56-C57-C58
31	w	801	PC1	C3A-C3B-C3C-C3D
31	L	1002	PC1	C1-C2-O21-C21
31	H	401	PC1	C3-C2-O21-C21
32	V	203	CDL	C72-C71-CB7-OB8
32	L	1003	CDL	C81-C82-C83-C84
32	V	202	CDL	CA5-C11-C12-C13
31	L	1002	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	M	502	PC1	O21-C21-C22-C23
32	M	504	CDL	C72-C73-C74-C75
32	M	504	CDL	OB5-CB3-CB4-CB6
32	M	503	CDL	C15-C16-C17-C18
32	V	203	CDL	C18-C19-C20-C21
30	L	1001	3PE	C38-C39-C3A-C3B
32	V	203	CDL	CB7-C71-C72-C73
31	H	401	PC1	C34-C35-C36-C37
33	X	101	ZMP	C12-C11-S1-C10
32	V	203	CDL	CA2-C1-CB2-OB2
31	M	502	PC1	C36-C37-C38-C39
30	p	201	3PE	C22-C23-C24-C25
30	A	201	3PE	C39-C3A-C3B-C3C
32	L	1003	CDL	C33-C34-C35-C36
31	L	1002	PC1	C39-C3A-C3B-C3C
31	w	801	PC1	C24-C25-C26-C27
32	V	202	CDL	C38-C39-C40-C41
30	J	202	3PE	C29-C2A-C2B-C2C
32	V	203	CDL	C52-C53-C54-C55
30	L	1001	3PE	O13-C11-C12-N
30	V	201	3PE	C27-C28-C29-C2A
32	M	503	CDL	C12-C11-CA5-OA6
30	V	201	3PE	O31-C31-C32-C33
30	A	201	3PE	O21-C21-C22-C23
32	N	403	CDL	CB6-CB4-OB6-CB5
32	M	503	CDL	C52-C51-CB5-OB6
32	M	503	CDL	C72-C71-CB7-OB8
32	L	1003	CDL	CA4-CA3-OA5-PA1
32	V	203	CDL	CA3-CA4-CA6-OA8
32	M	504	CDL	C61-C62-C63-C64
32	L	1003	CDL	C32-C31-CA7-OA8
31	w	801	PC1	C11-C12-N-C14
31	M	502	PC1	C25-C26-C27-C28
30	M	501	3PE	C32-C31-O31-C3
30	p	201	3PE	C26-C27-C28-C29
32	M	504	CDL	C73-C74-C75-C76
32	V	202	CDL	C11-C12-C13-C14
30	V	201	3PE	C32-C33-C34-C35
32	W	201	CDL	C53-C54-C55-C56
34	k	501	AMP	O4'-C4'-C5'-O5'
32	W	201	CDL	C19-C20-C21-C22
30	L	1001	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
30	L	1001	3PE	O31-C31-C32-C33
32	M	504	CDL	C72-C71-CB7-OB8
30	J	201	3PE	C37-C38-C39-C3A
32	M	503	CDL	C12-C11-CA5-OA7
32	M	503	CDL	C52-C51-CB5-OB7
31	M	502	PC1	C3B-C3C-C3D-C3E
32	L	1003	CDL	C32-C31-CA7-OA9
32	M	503	CDL	C72-C71-CB7-OB9
30	A	201	3PE	O22-C21-C22-C23
32	M	504	CDL	C31-C32-C33-C34
30	V	201	3PE	O32-C31-C32-C33
32	W	201	CDL	C83-C84-C85-C86
30	N	401	3PE	O21-C21-C22-C23
31	M	502	PC1	C2B-C2C-C2D-C2E
30	L	1004	3PE	C1-O11-P-O12
32	V	202	CDL	CA2-OA2-PA1-OA3
32	M	504	CDL	C72-C71-CB7-OB9
30	L	1001	3PE	O21-C21-C22-C23
30	N	402	3PE	O21-C21-C22-C23
30	J	201	3PE	O11-C1-C2-C3
32	W	201	CDL	C14-C15-C16-C17
31	M	502	PC1	C28-C29-C2A-C2B
32	M	503	CDL	C82-C83-C84-C85
32	N	403	CDL	C72-C71-CB7-OB8
32	V	202	CDL	C19-C20-C21-C22
31	w	801	PC1	C28-C29-C2A-C2B
30	L	1004	3PE	C1-C2-O21-C21
30	N	402	3PE	C1-C2-O21-C21
30	V	201	3PE	C12-C11-O13-P
31	w	801	PC1	C12-C11-O13-P
31	M	502	PC1	C2F-C2G-C2H-C2I
30	L	1001	3PE	O32-C31-C32-C33
31	w	801	PC1	C11-C12-N-C15
30	J	201	3PE	O21-C21-C22-C23
32	L	1003	CDL	C72-C71-CB7-OB8
31	M	502	PC1	C32-C33-C34-C35
32	N	403	CDL	C52-C51-CB5-OB7
32	W	201	CDL	C72-C73-C74-C75
32	W	201	CDL	C12-C11-CA5-OA6
31	H	401	PC1	C31-C32-C33-C34
32	V	202	CDL	C32-C33-C34-C35
30	N	401	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
30	N	402	3PE	O22-C21-C22-C23
32	L	1003	CDL	C72-C71-CB7-OB9
32	V	202	CDL	C32-C31-CA7-OA8
32	V	202	CDL	C32-C31-CA7-OA9
32	L	1003	CDL	C73-C74-C75-C76
30	J	201	3PE	O22-C21-C22-C23

There are no ring outliers.

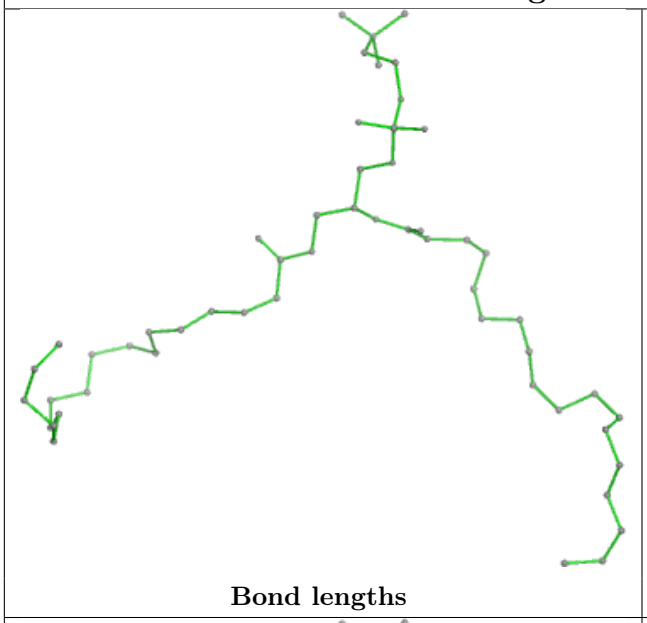
19 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	M	503	CDL	9	0
30	V	201	3PE	2	0
32	M	504	CDL	8	0
32	L	1003	CDL	6	0
31	H	401	PC1	2	0
30	N	401	3PE	1	0
33	X	101	ZMP	1	0
30	J	202	3PE	2	0
30	L	1001	3PE	2	0
32	V	203	CDL	6	0
31	L	1002	PC1	2	0
30	J	201	3PE	2	0
30	A	201	3PE	1	0
31	M	502	PC1	3	0
32	W	201	CDL	4	0
32	V	202	CDL	4	0
32	N	403	CDL	2	0
30	N	402	3PE	5	0
30	M	501	3PE	2	0

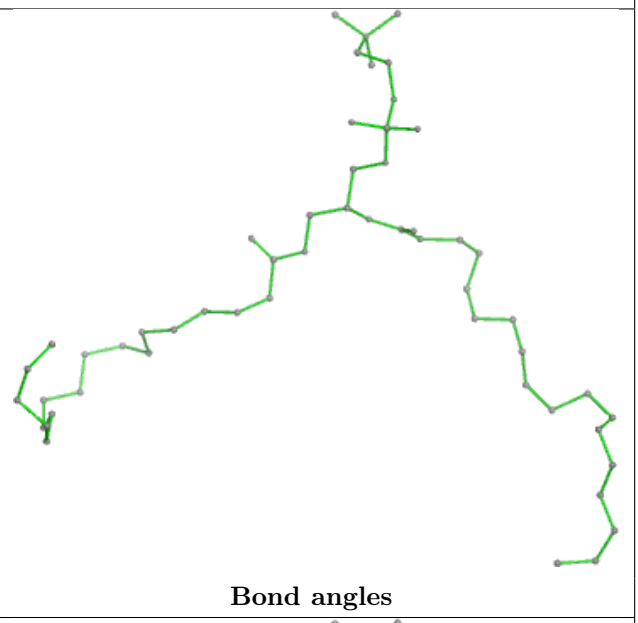
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

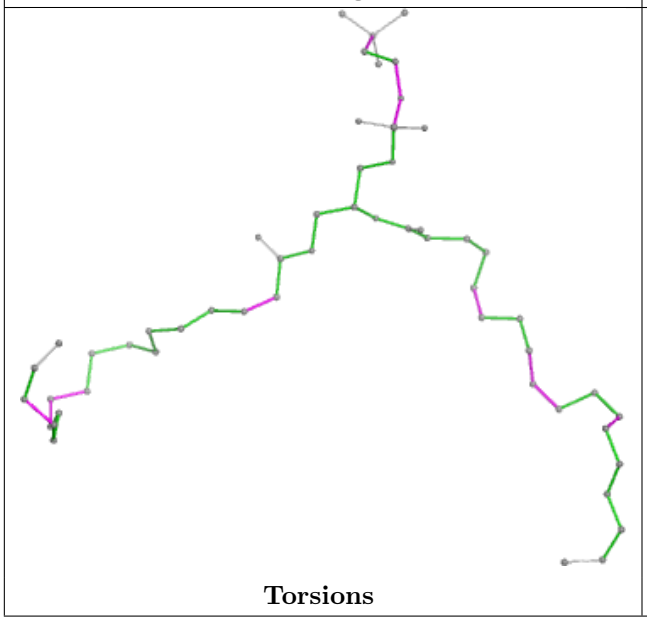
Ligand PC1 w 801



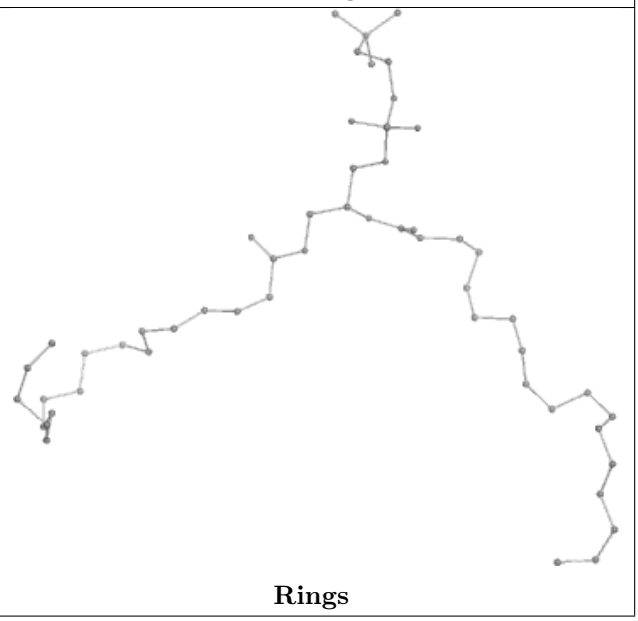
Bond lengths



Bond angles



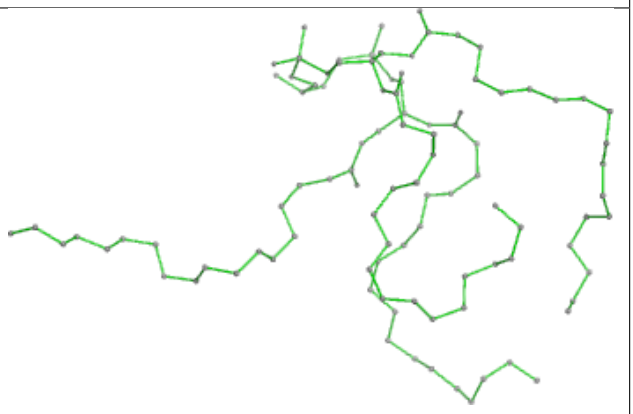
Torsions



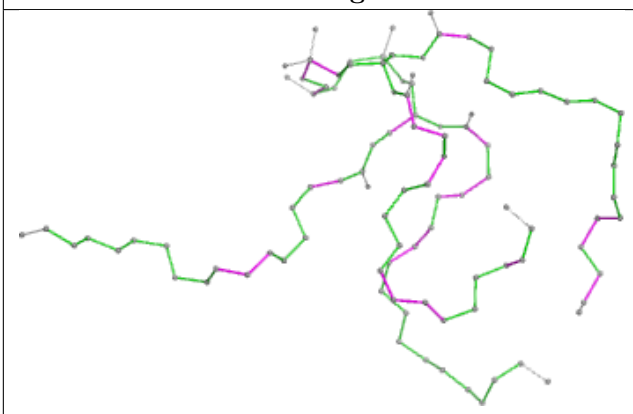
Rings

Ligand CDL M 503

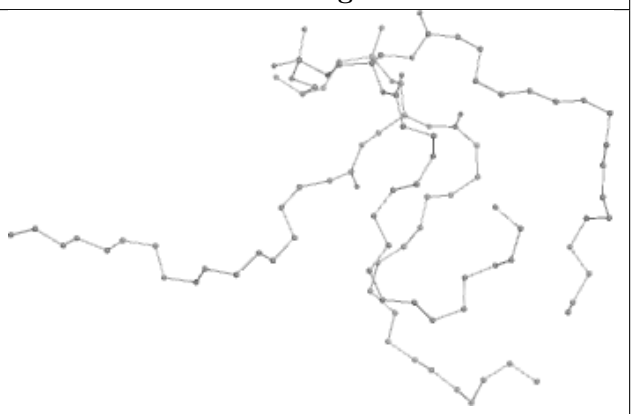
Bond lengths



Bond angles

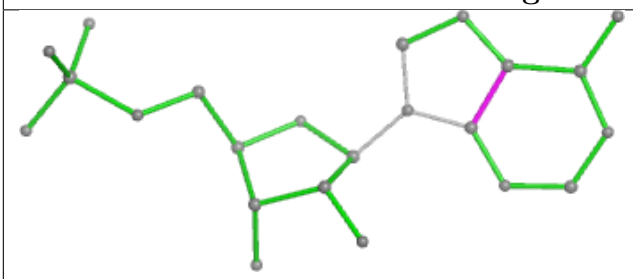


Torsions

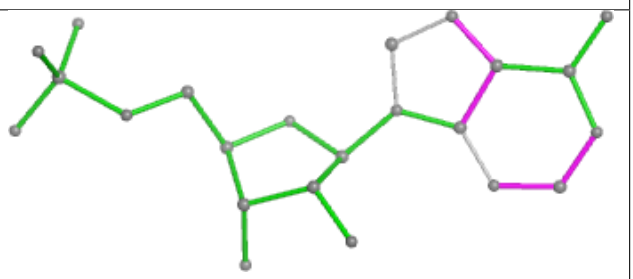


Rings

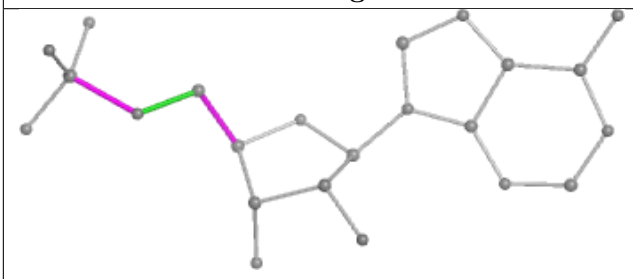
Ligand AMP k 501



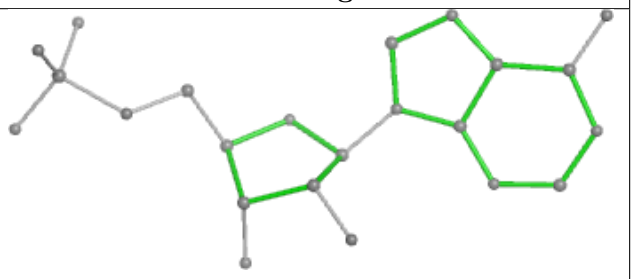
Bond lengths



Bond angles

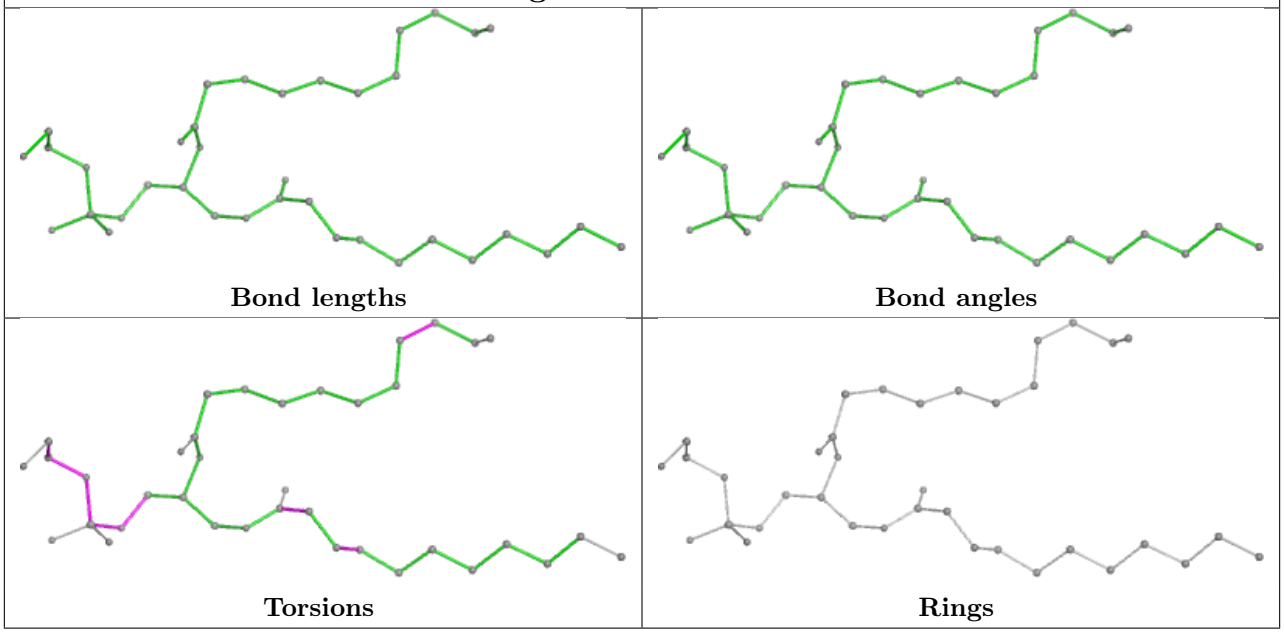


Torsions

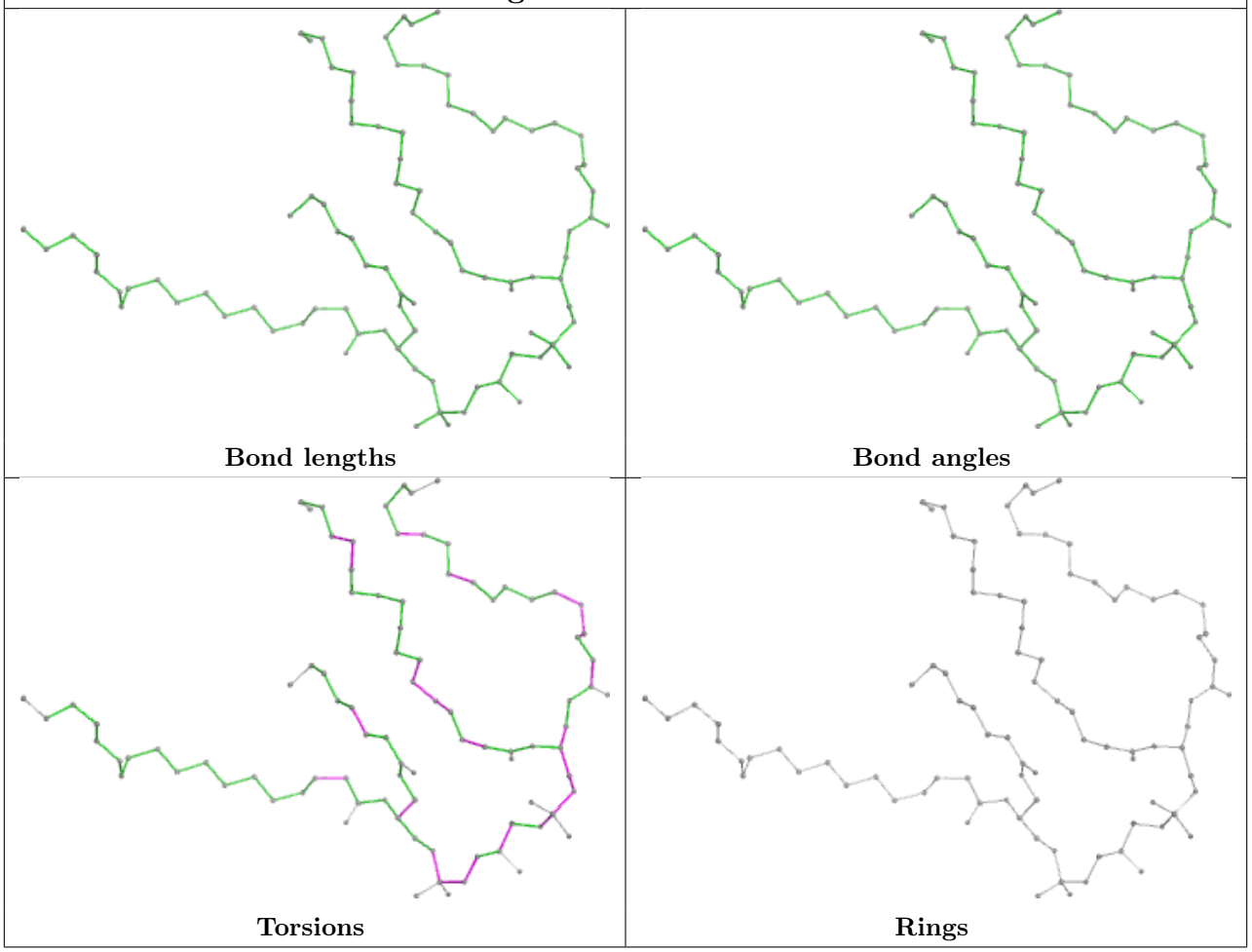


Rings

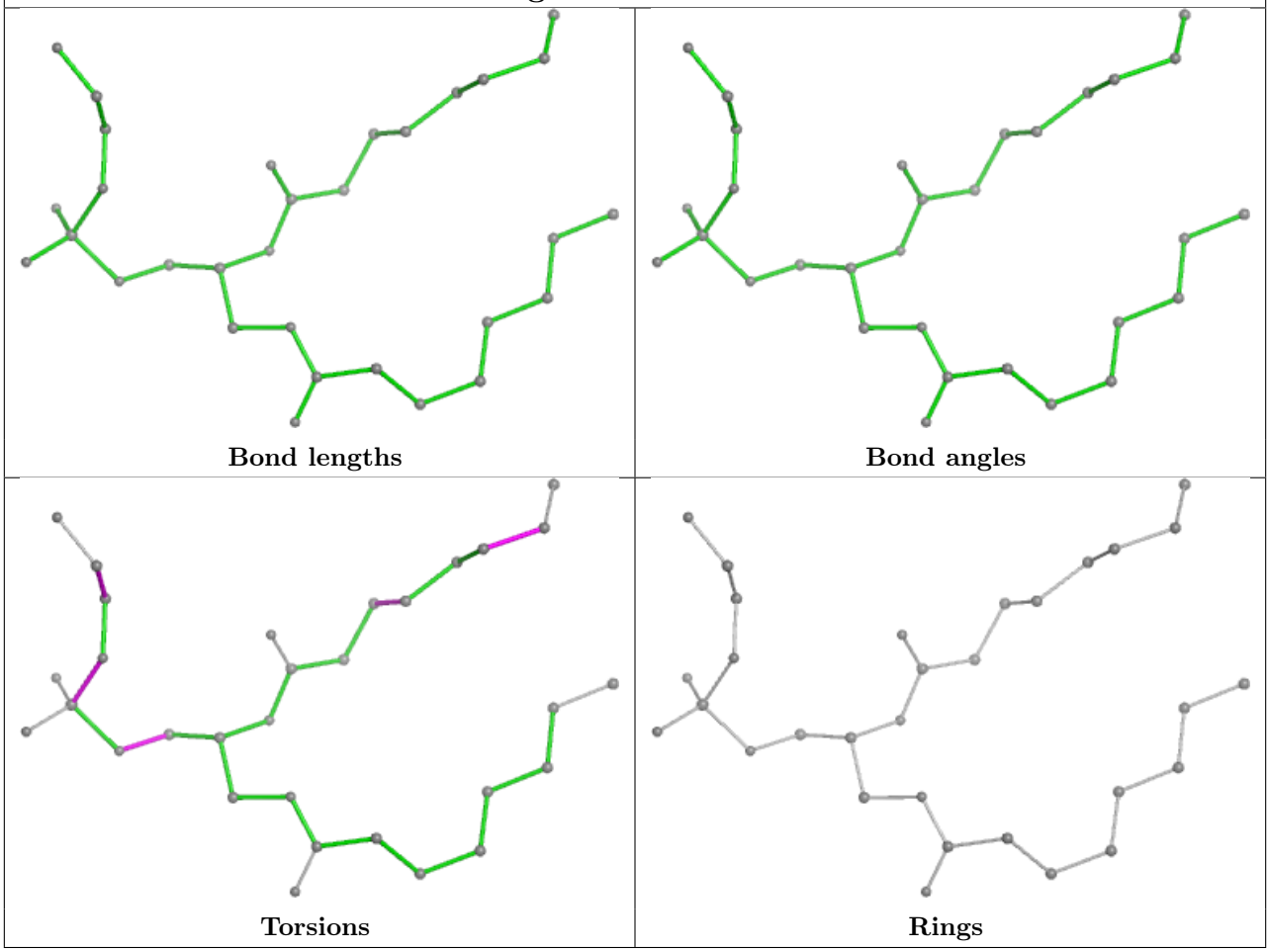
Ligand 3PE V 201



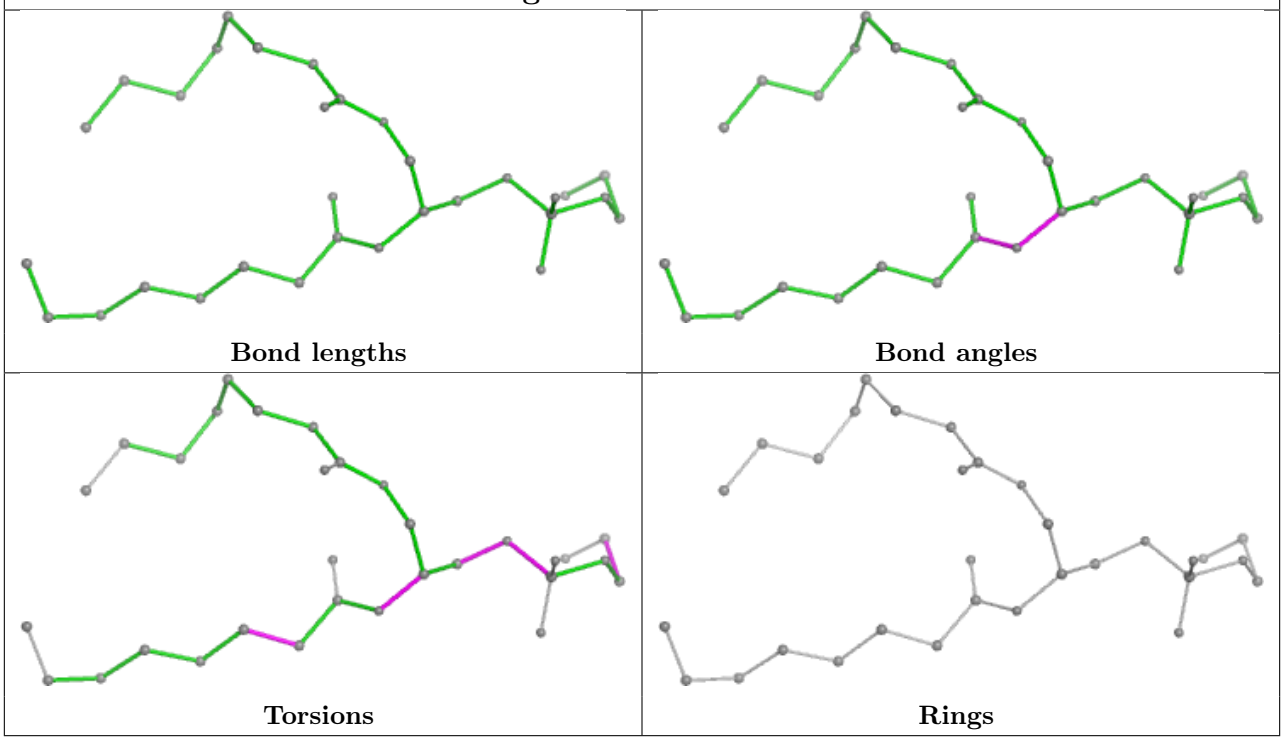
Ligand CDL M 504



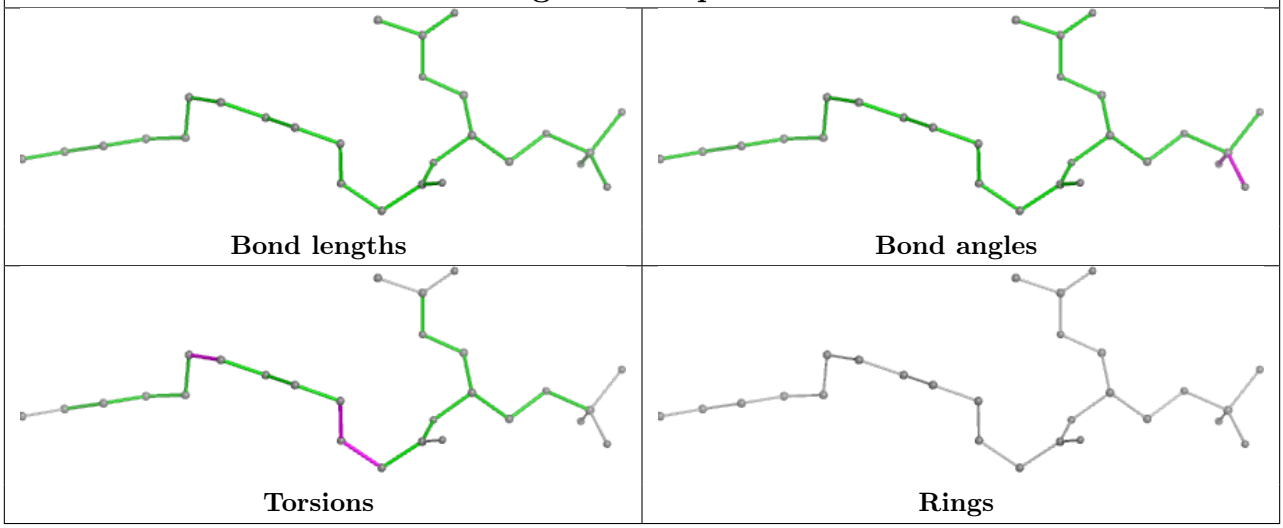
Ligand 3PE o 501



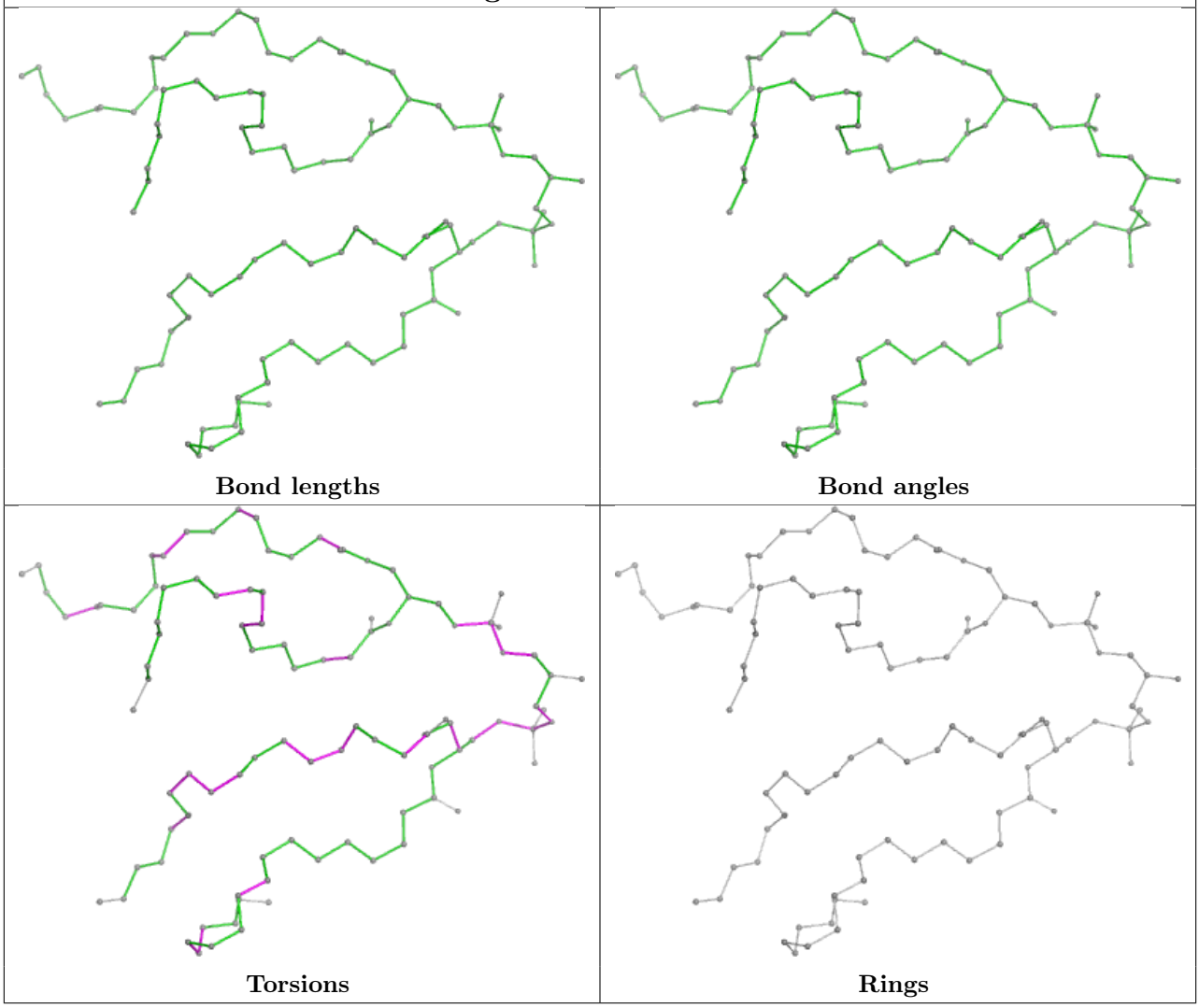
Ligand 3PE L 1004



Ligand 3PE p 201



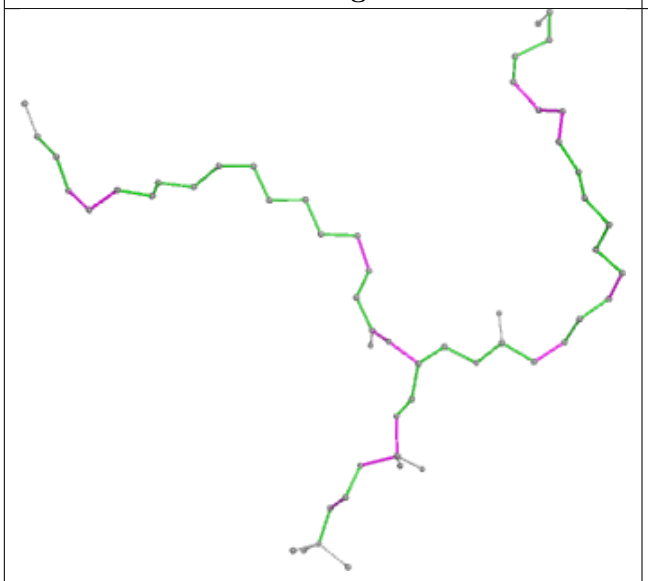
Ligand CDL L 1003



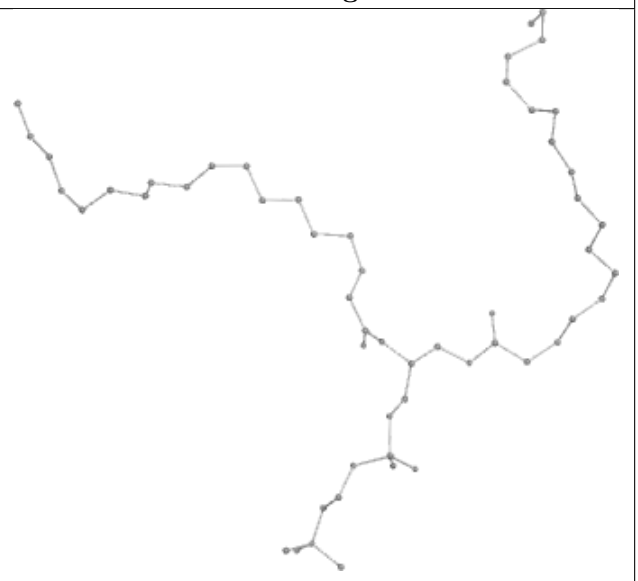
Ligand PC1 H 401

Bond lengths

Bond angles

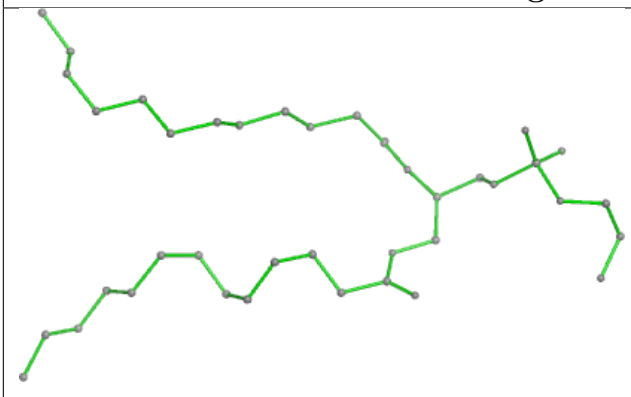


Torsions

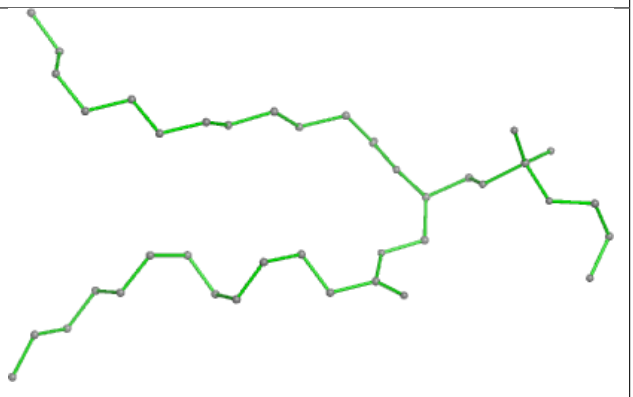


Rings

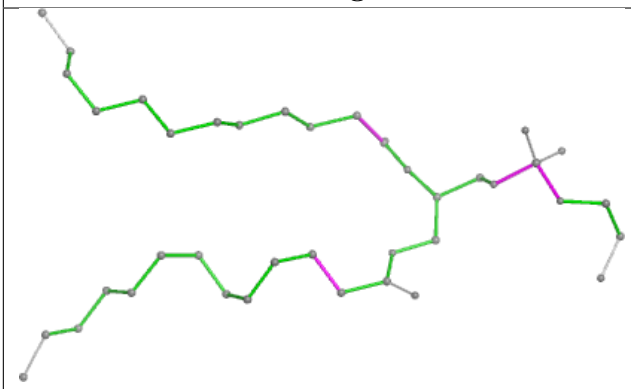
Ligand 3PE N 401



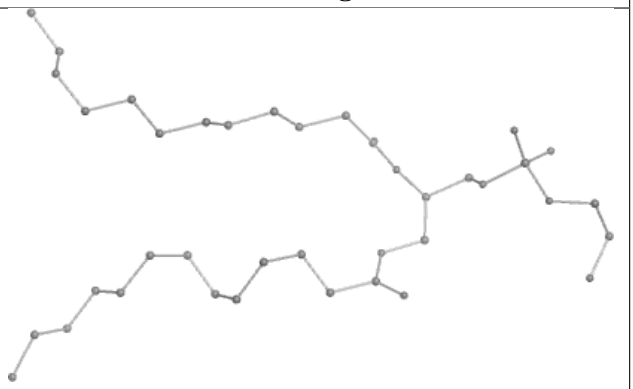
Bond lengths



Bond angles

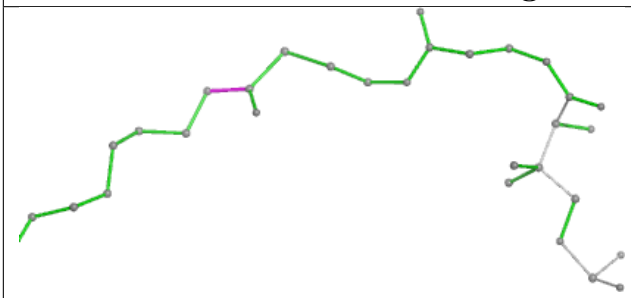


Torsions

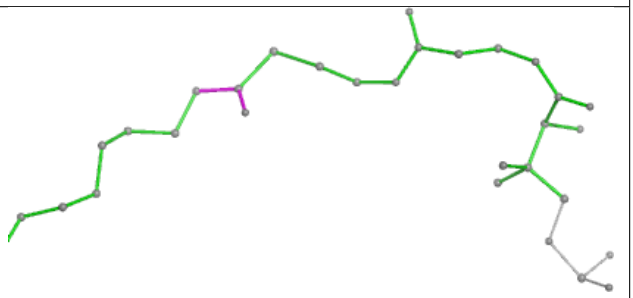


Rings

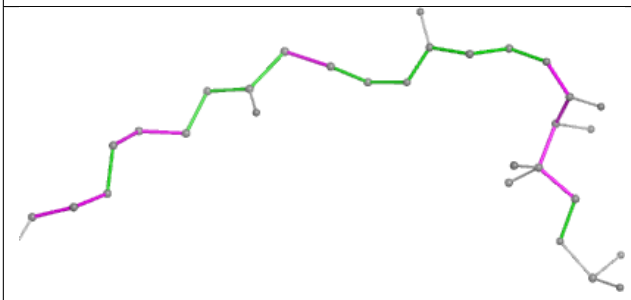
Ligand ZMP X 101



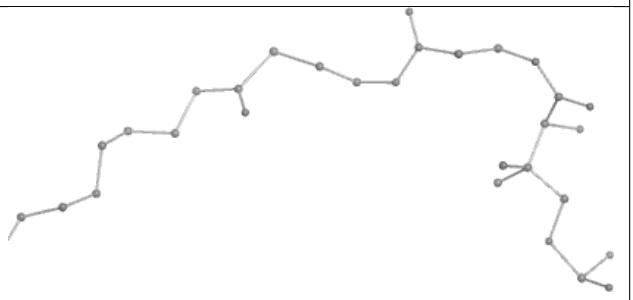
Bond lengths



Bond angles

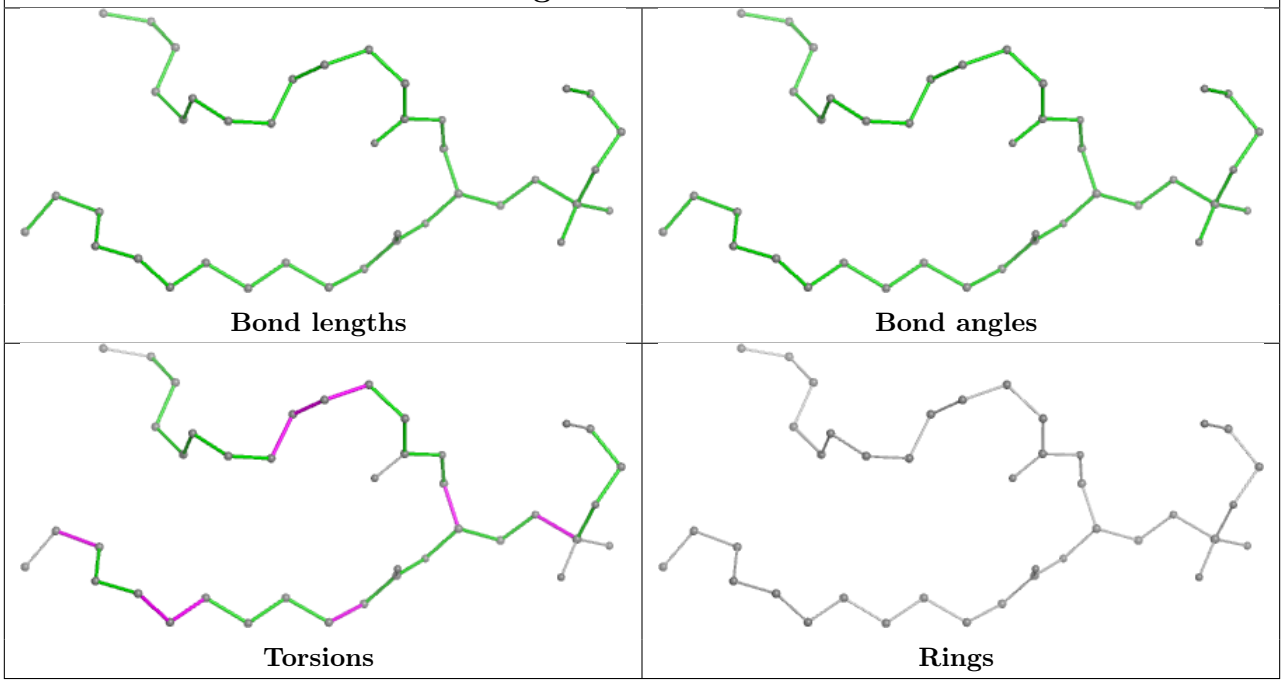


Torsions

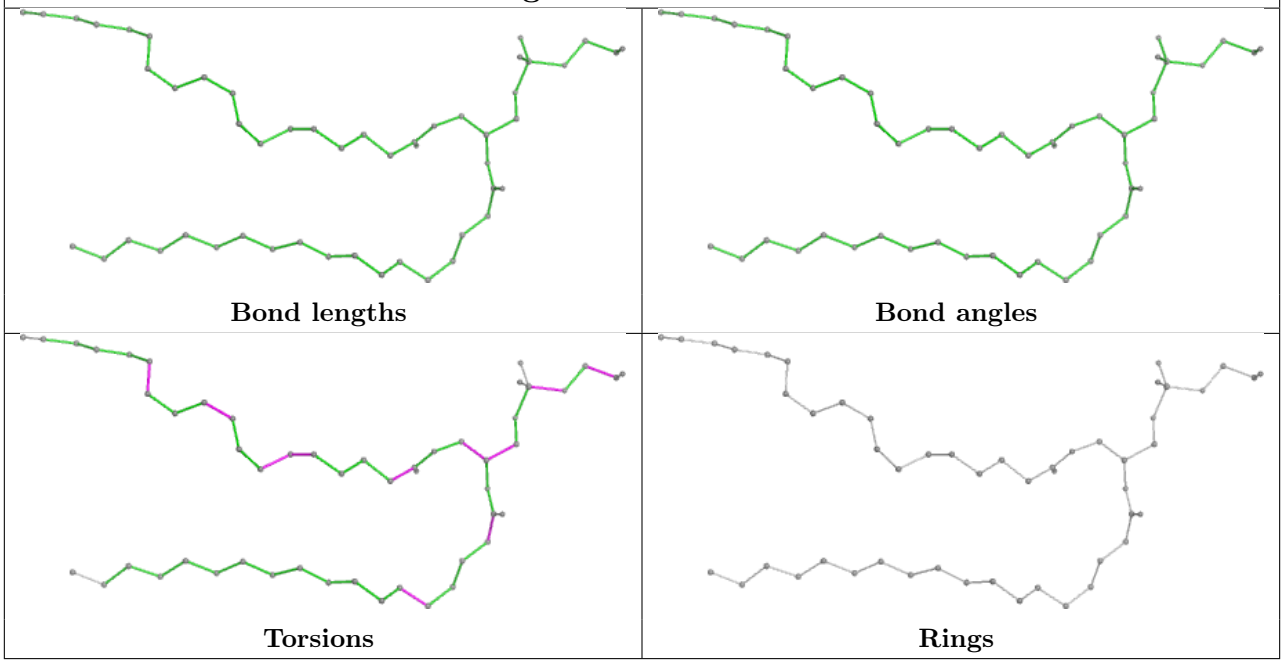


Rings

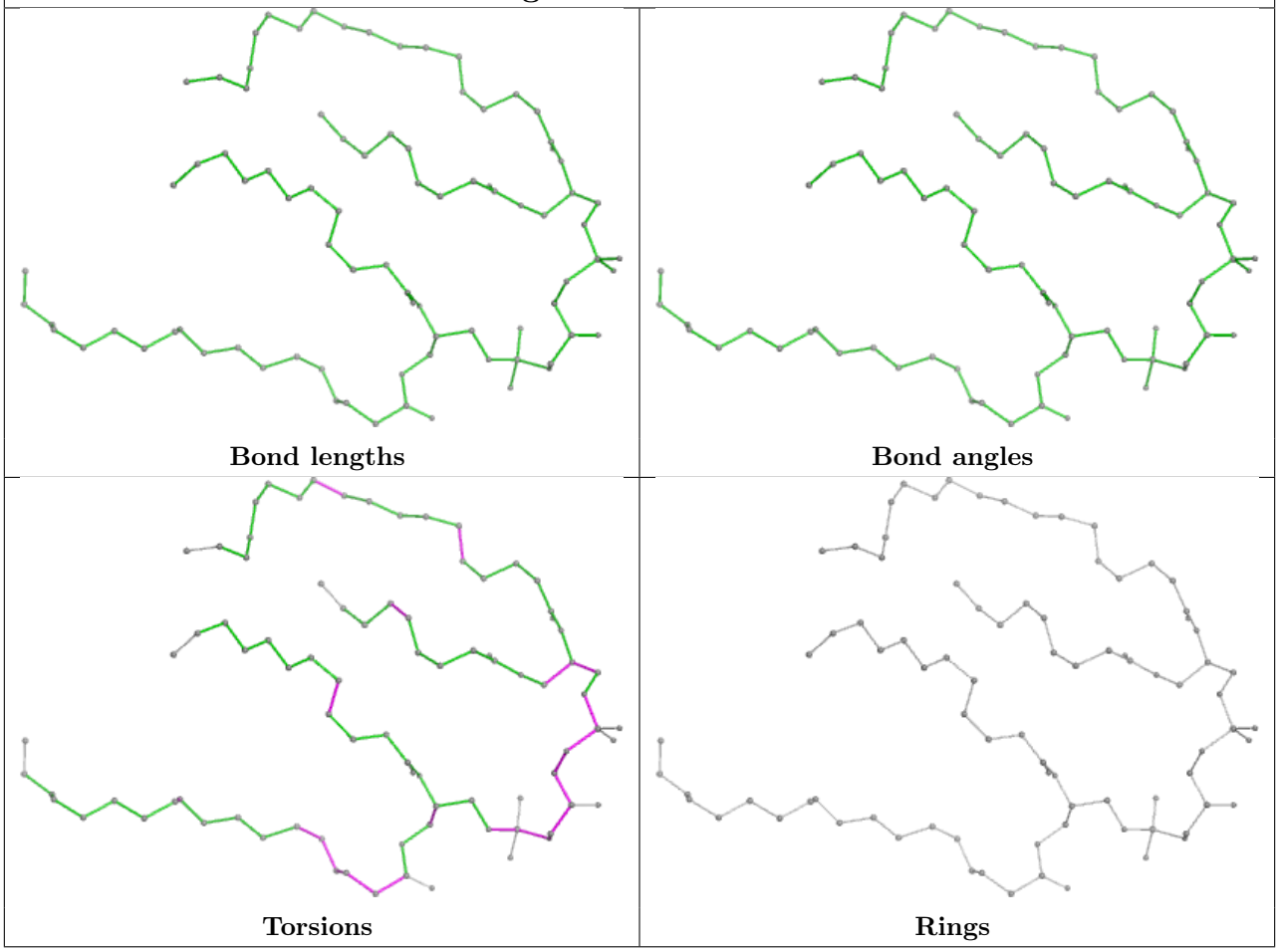
Ligand 3PE J 202



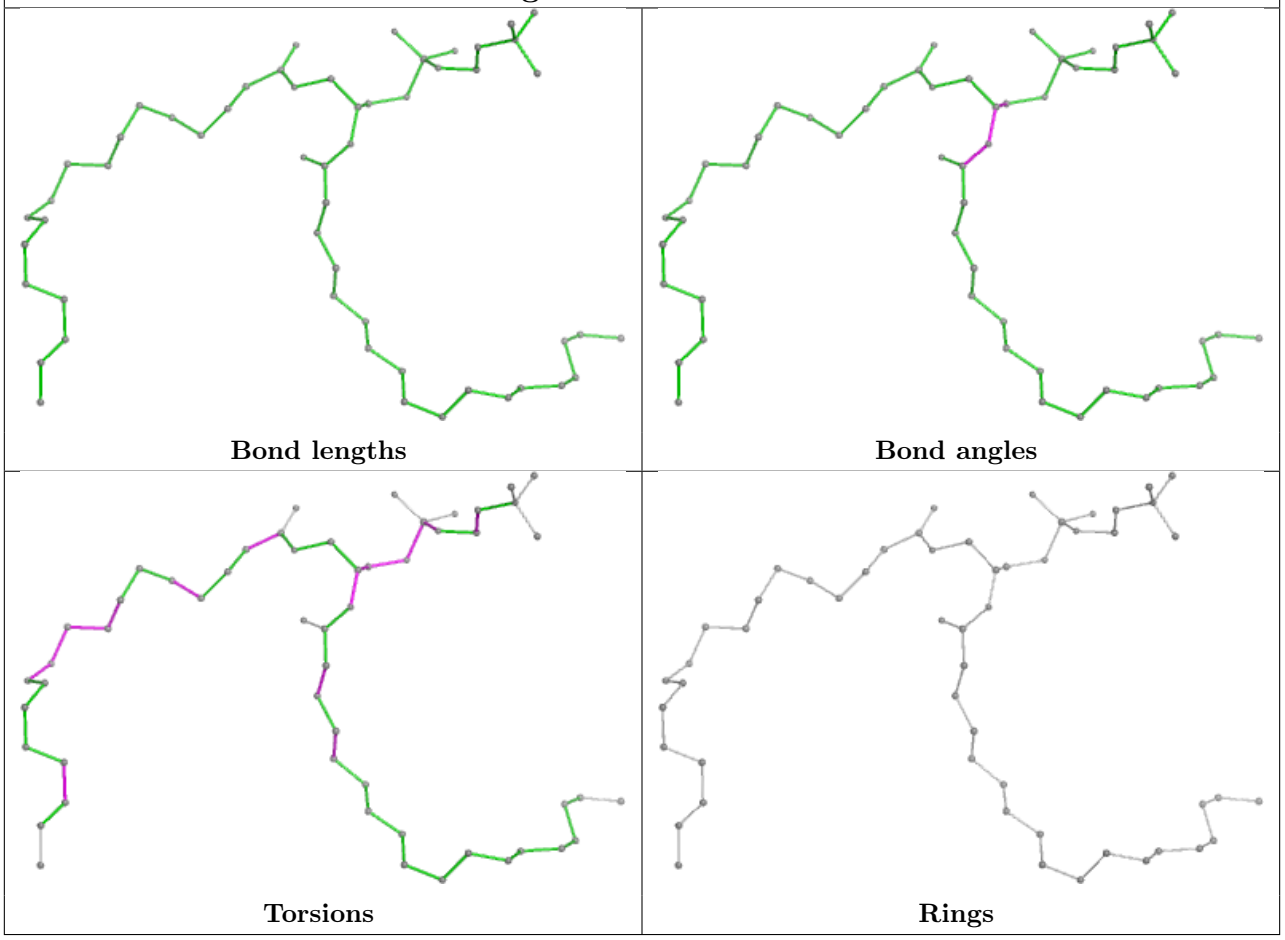
Ligand 3PE L 1001



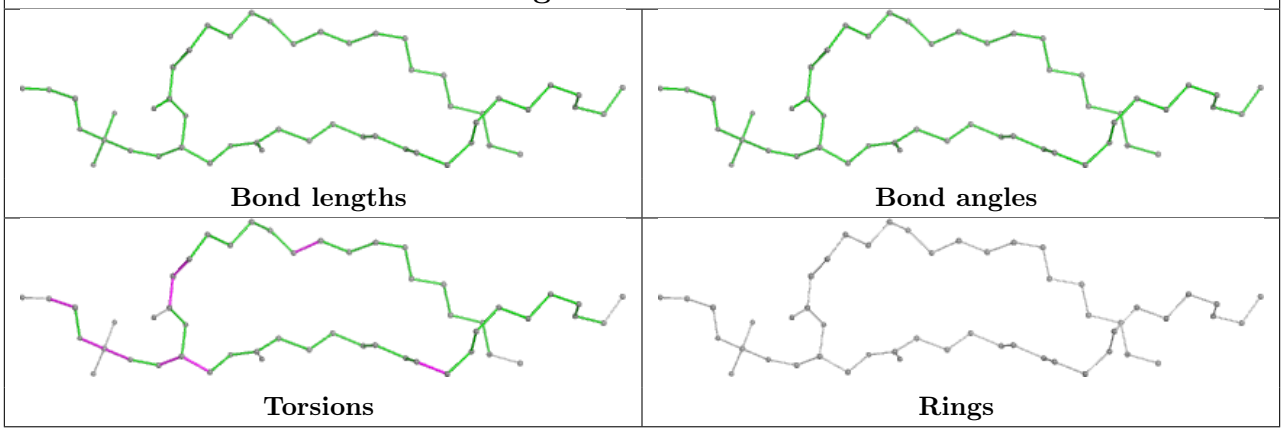
Ligand CDL V 203



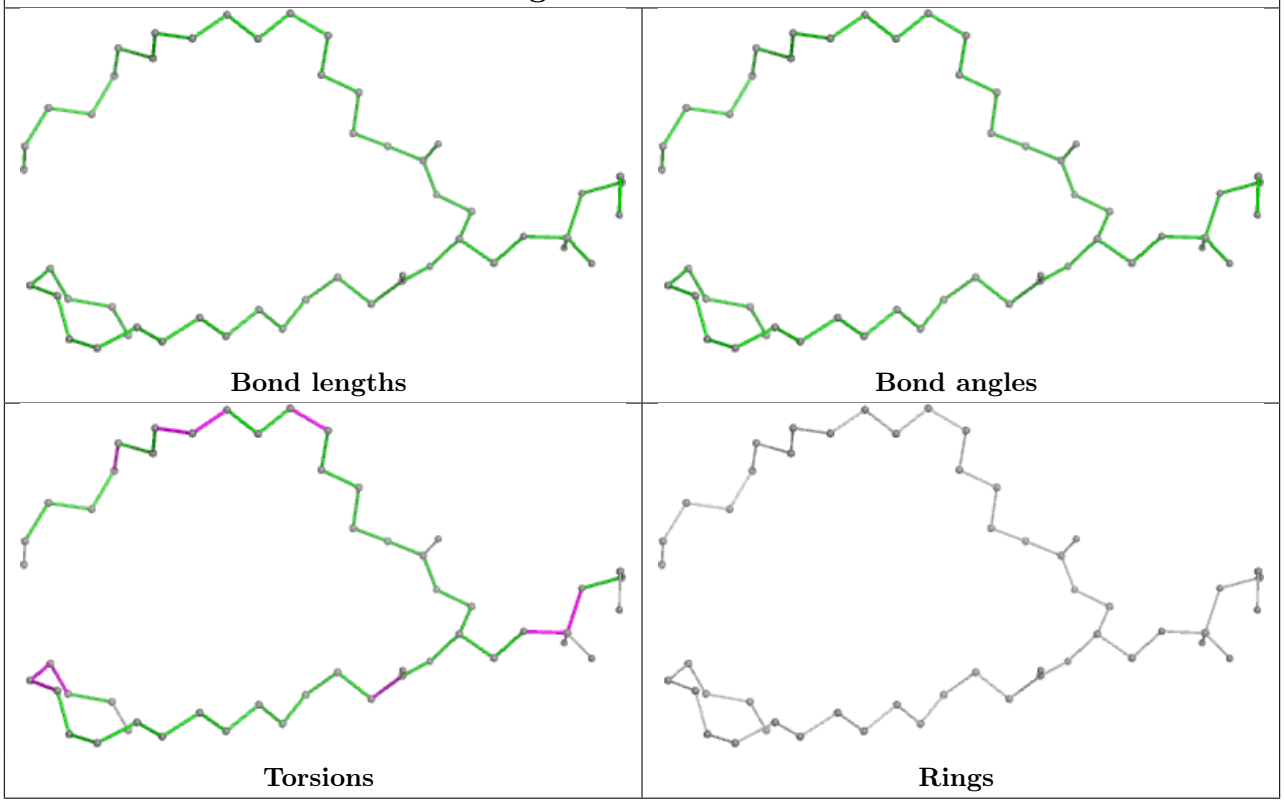
Ligand PC1 L 1002



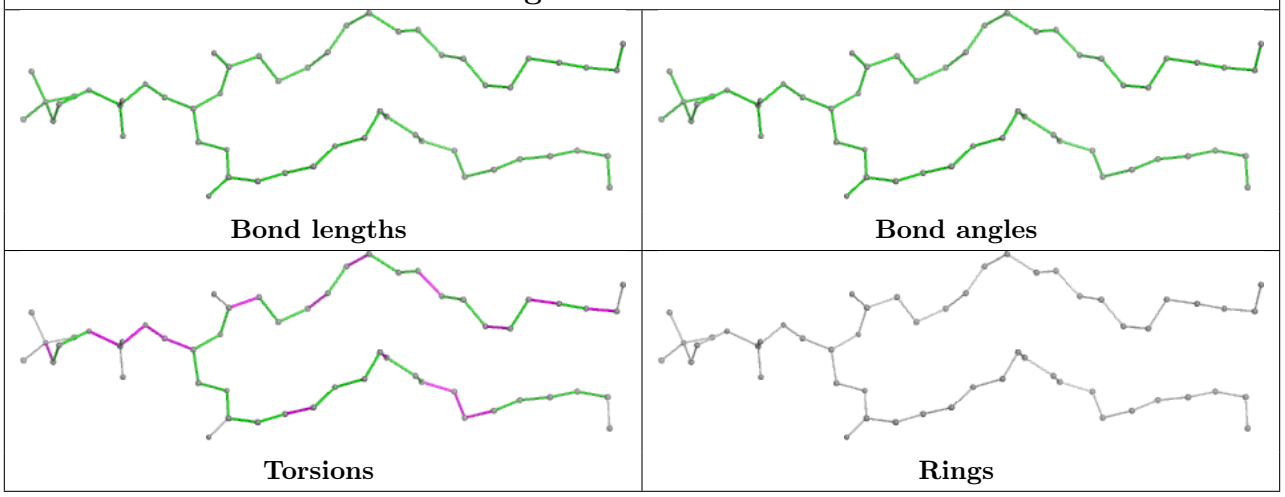
Ligand 3PE J 201



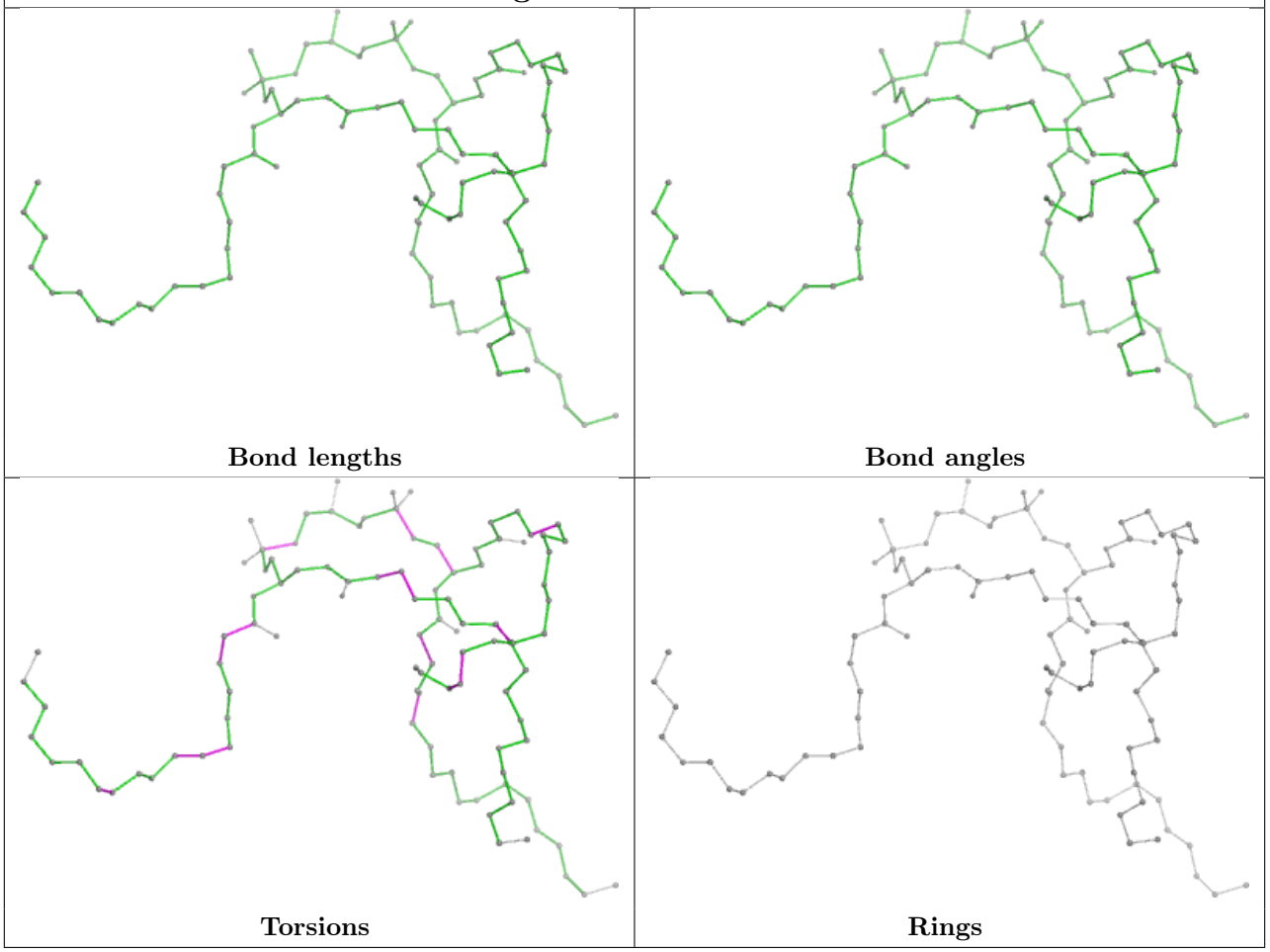
Ligand 3PE A 201



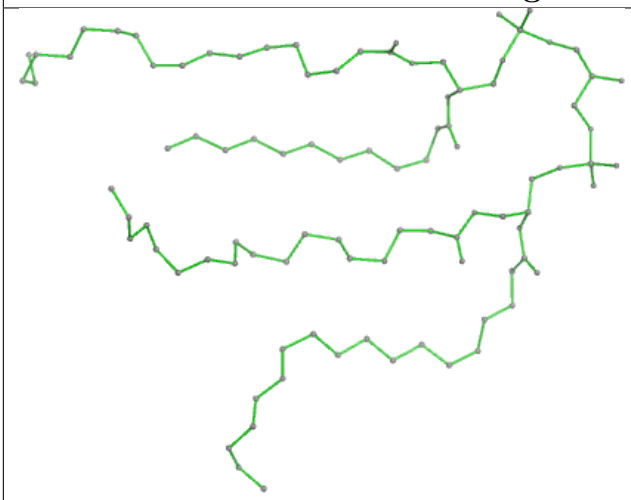
Ligand PC1 M 502



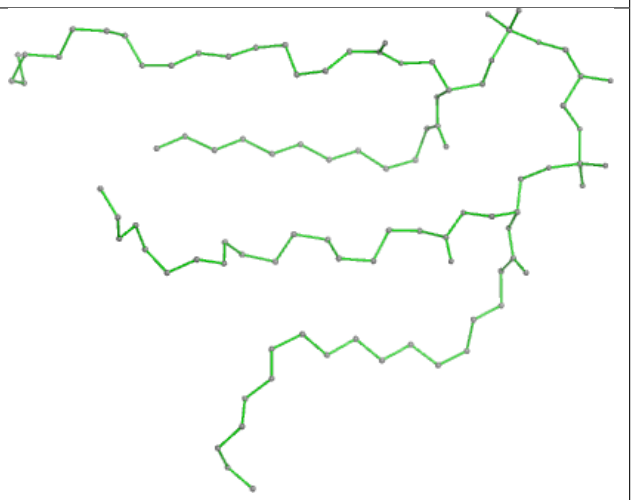
Ligand CDL W 201



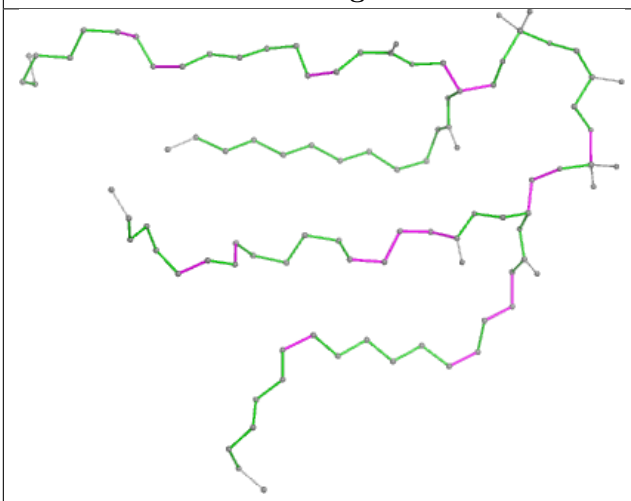
Ligand CDL V 202



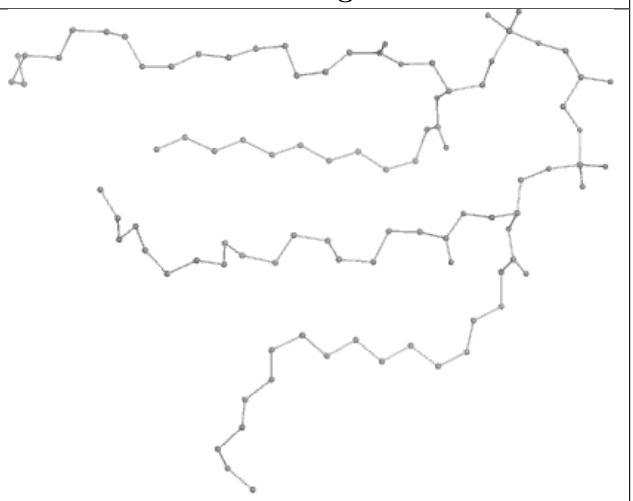
Bond lengths



Bond angles

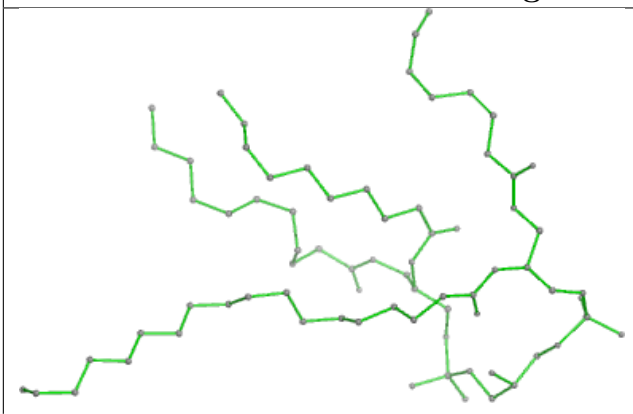


Torsions

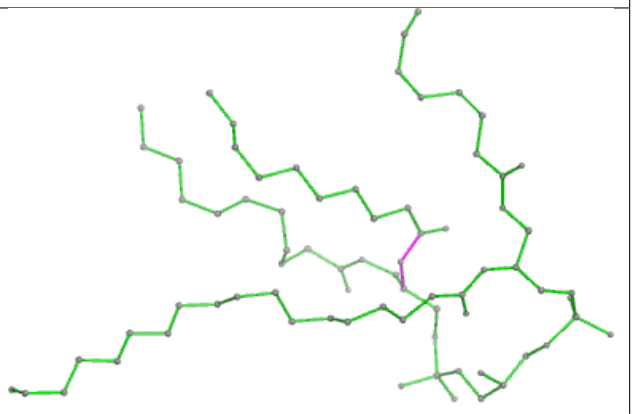


Rings

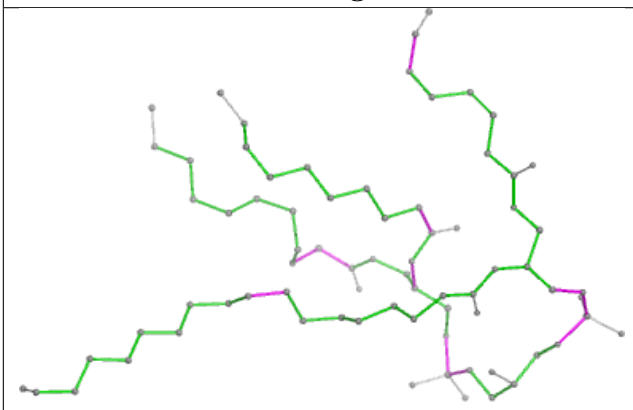
Ligand CDL N 403



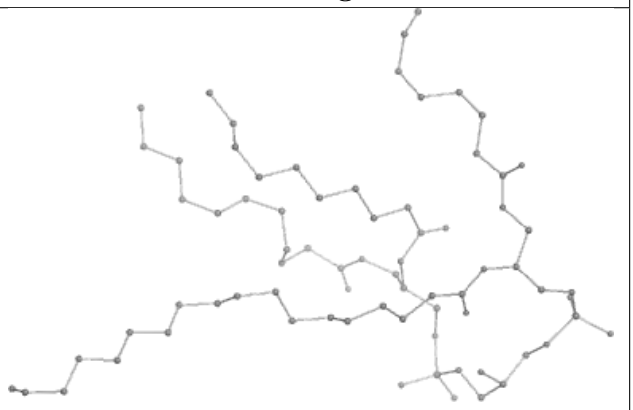
Bond lengths



Bond angles

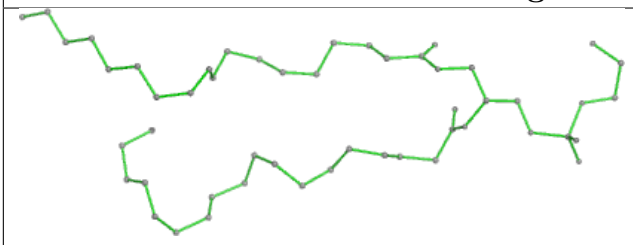


Torsions

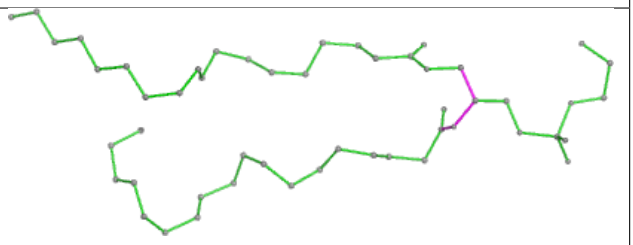


Rings

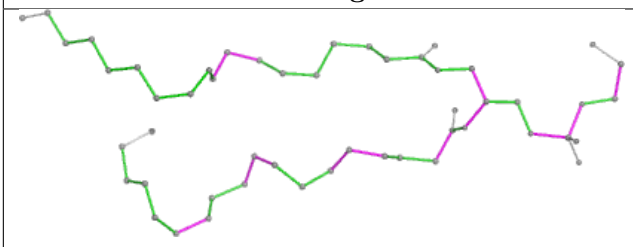
Ligand 3PE N 402



Bond lengths



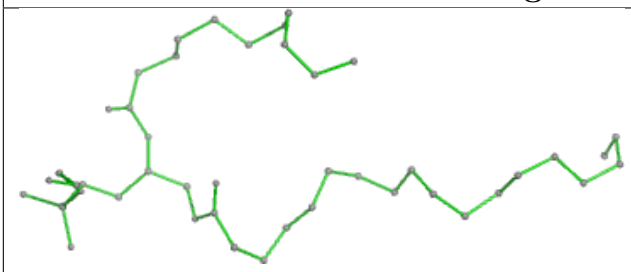
Bond angles



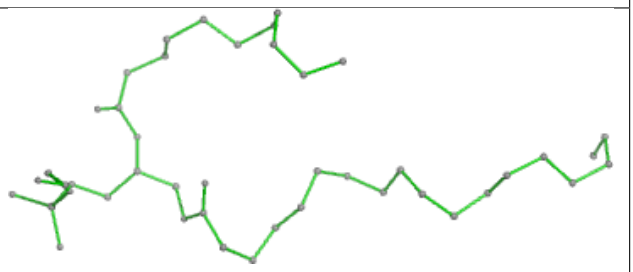
Torsions

Rings

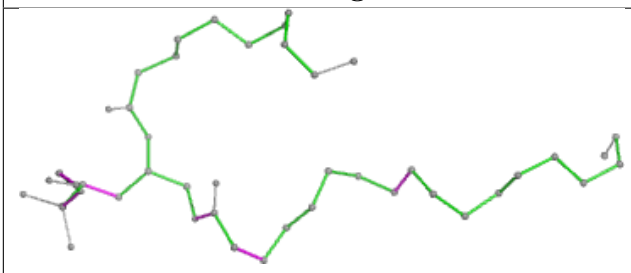
Ligand 3PE M 501



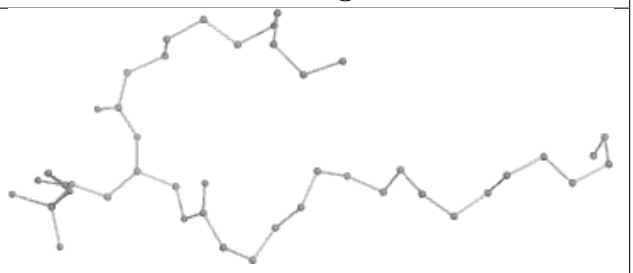
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11243. 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.