Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:09 pm BST

PDB ID	:	6ZKG / pdb_00006zkg
EMDB ID	:	EMD-11248
Title	:	Complex I with NADH, closed
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	3.40 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:

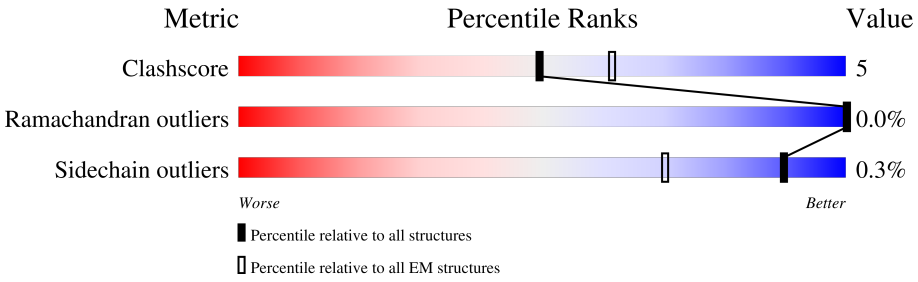
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1	464	79% 14% 7%
2	2	246	73% 13% 13%
3	3	727	78% 17% 5%
4	4	463	75% 18% 7%
5	5	266	65% 13% 22%
6	6	223	56% 14% 30%
7	9	217	69% 12% 19%
8	A	115	78% 20% .
9	H	318	86% 14%

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Mol	Chain	Length	Quality of chain
10	J	175	82% 18%
11	K	98	74% 24%
12	L	606	86% 14%
13	M	459	84% 16%
14	N	347	84% 16%
15	V	141	83% 16%
16	W	189	68% 6% 26%
17	X	157	52% 45%
17	j	157	52% 48%
18	Y	172	92% 8%
19	Z	175	92% 6%
20	a	109	40% 60%
21	b	124	77% 23%
22	c	170	74% 26%
23	d	380	89% 11%
24	e	99	87% 13%
25	f	116	97%
26	g	140	81% 19%
27	h	114	83% 16%
28	i	145	99%
29	k	355	90% 10%
30	l	106	98%
31	m	84	94% 5%
32	n	98	81% 19%
33	o	122	98%

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Mol	Chain	Length	Quality of chain
34	p	130	98%
35	q	144	96%
36	r	128	77% 23%
37	s	137	88% 11%
38	t	179	98%
39	u	108	60% 40%
40	v	186	83% 17%
41	w	154	66% 34%
42	x	76	64% 36%
43	y	58	86% 14%
44	z	70	100%

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
45	SF4	3	801	-	-	X	-
52	CDL	L	705	X	-	-	-
52	CDL	L	706	X	-	-	-
52	CDL	M	503	X	-	-	-
52	CDL	x	101	X	-	-	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 67921 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	430	3457	2207	594	631	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	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	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	606	Total	C	N	O	S	0	0
			4807	3188	746	829	44		

- 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	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- 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	340	Total	C	N	O	S	0	0
			2748	1775	489	478	6		

- 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		

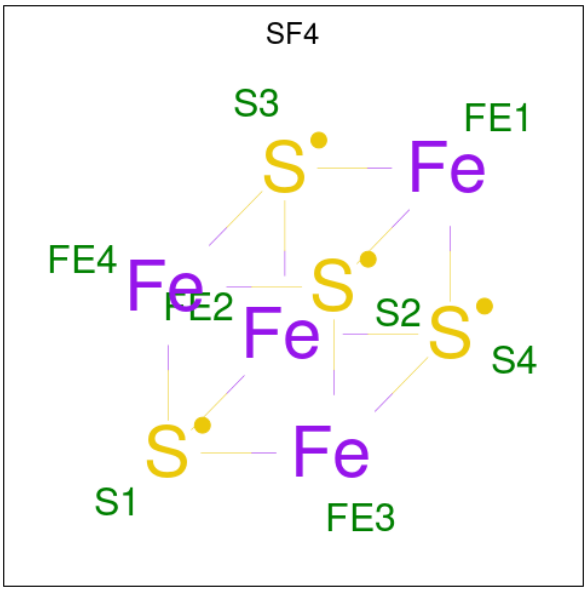
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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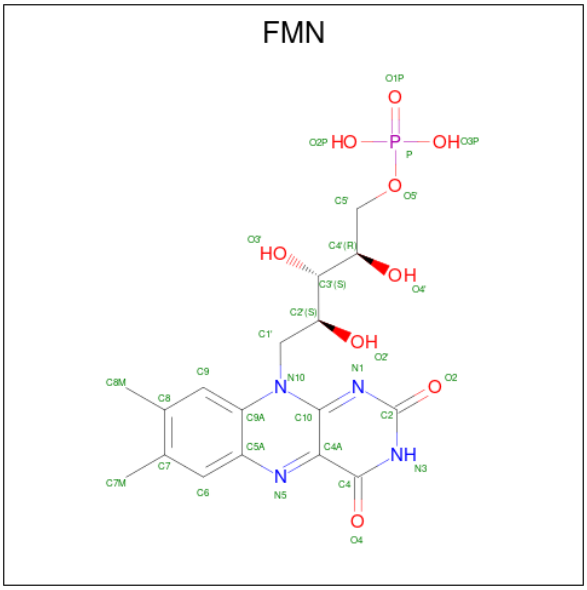
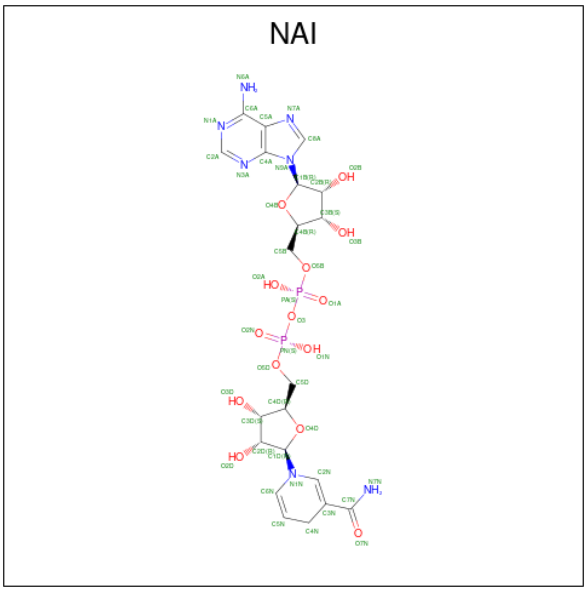
Mol	Chain	Residues	Atoms	AltConf
45	9	1	Total Fe S 8 4 4	0
45	9	1	Total Fe S 8 4 4	0

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



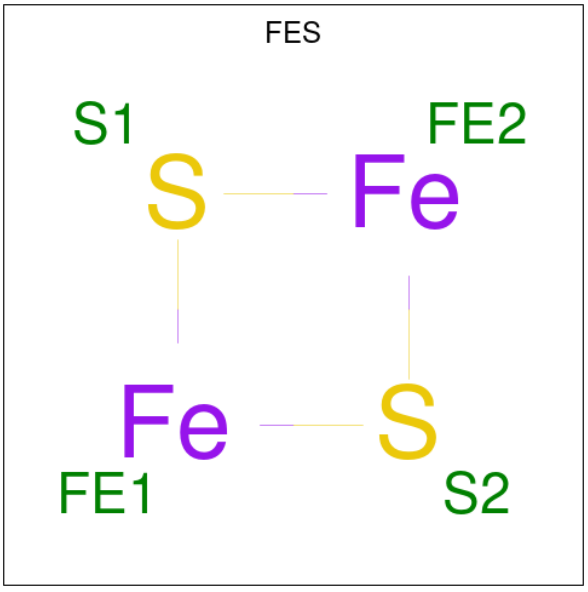
Mol	Chain	Residues	Atoms	AltConf
46	1	1	Total C N O P 31 17 4 9 1	0

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
47	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

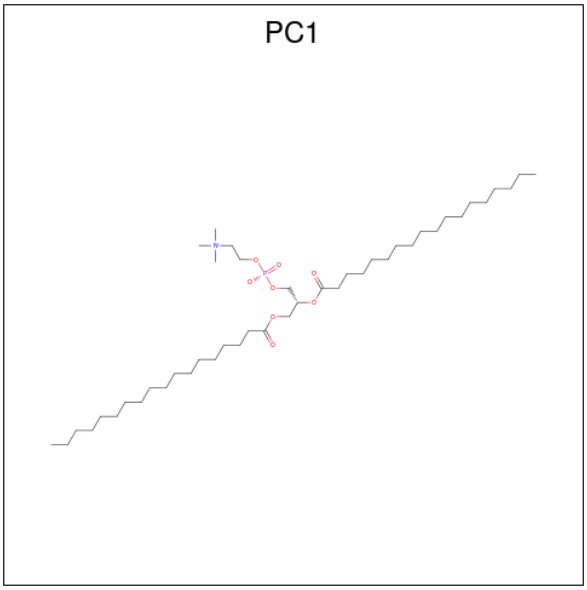


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

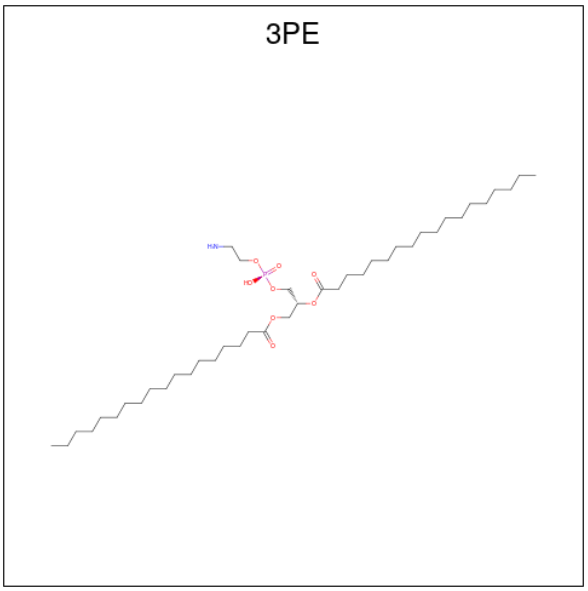
Mol	Chain	Residues	Atoms	AltConf
49	3	1	Total K 1 1	0

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



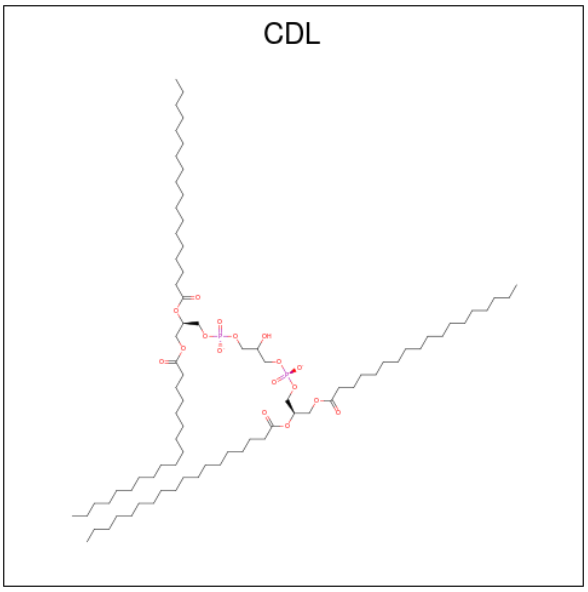
Mol	Chain	Residues	Atoms	AltConf
50	6	1	Total C N O P 46 36 1 8 1	0
50	9	1	Total C N O P 54 44 1 8 1	0
50	L	1	Total C N O P 54 44 1 8 1	0
50	M	1	Total C N O P 54 44 1 8 1	0
50	w	1	Total C N O P 54 44 1 8 1	0

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
51	6	1	Total C N O P 51 41 1 8 1	0
51	A	1	Total C N O P 51 41 1 8 1	0
51	J	1	Total C N O P 51 41 1 8 1	0
51	J	1	Total C N O P 40 30 1 8 1	0
51	L	1	Total C N O P 40 30 1 8 1	0
51	L	1	Total C N O P 51 41 1 8 1	0
51	L	1	Total C N O P 31 21 1 8 1	0
51	M	1	Total C N O P 44 34 1 8 1	0
51	N	1	Total C N O P 51 41 1 8 1	0
51	V	1	Total C O P 27 18 8 1	0
51	V	1	Total C N O P 37 27 1 8 1	0
51	i	1	Total C N O P 51 41 1 8 1	0
51	o	1	Total C N O P 31 21 1 8 1	0

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	L	1	Total	C	O	P	0
			85	66	17	2	
52	L	1	Total	C	O	P	0
			100	81	17	2	
52	M	1	Total	C	O	P	0
			100	81	17	2	
52	M	1	Total	C	O	P	0
			90	71	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	W	1	Total	C	O	P	0
			100	81	17	2	
52	x	1	Total	C	O	P	0
			75	56	17	2	
52	z	1	Total	C	O	P	0
			58	39	17	2	

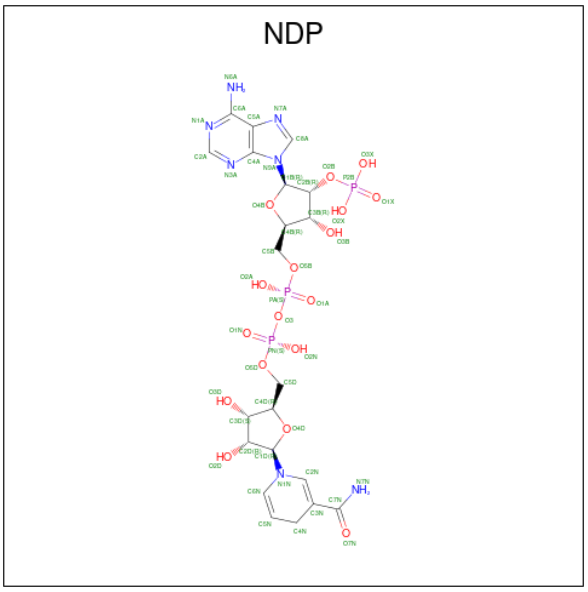
- Molecule 53 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

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

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

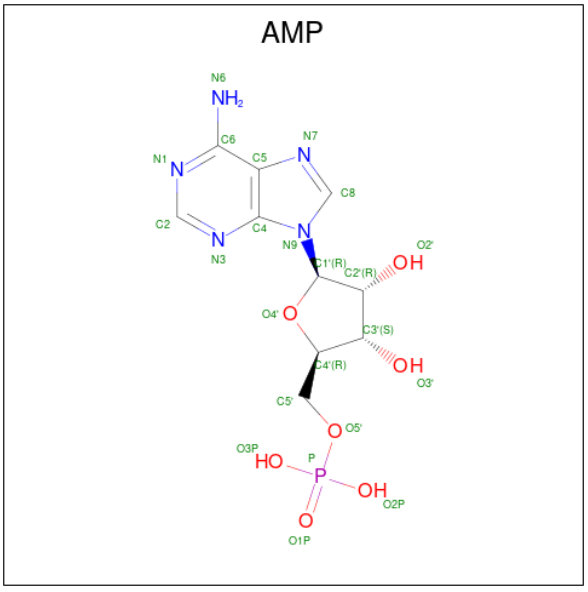
Mol	Chain	Residues	Atoms		AltConf
54	b	1	Total	Zn	0
			1	1	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



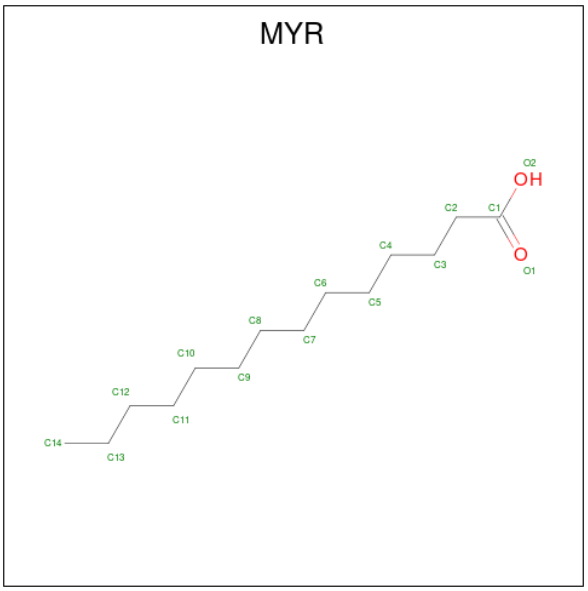
Mol	Chain	Residues	Atoms					AltConf
55	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 57 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



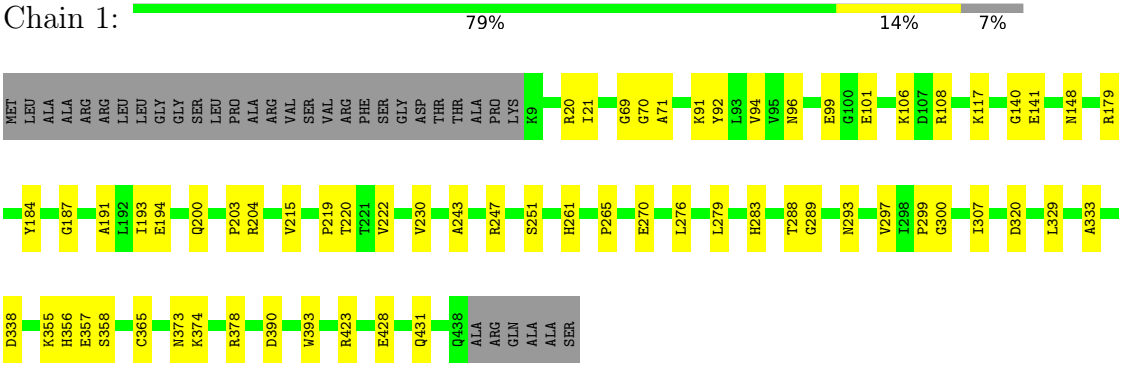
Mol	Chain	Residues	Atoms			AltConf
57	s	1	Total	C	O	0
			15	14	1	

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.

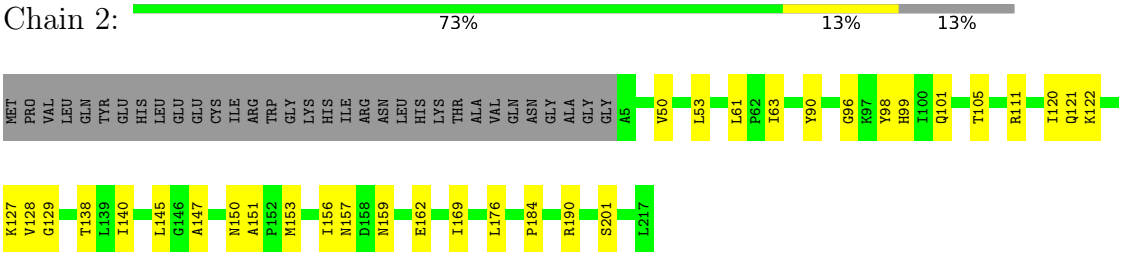
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



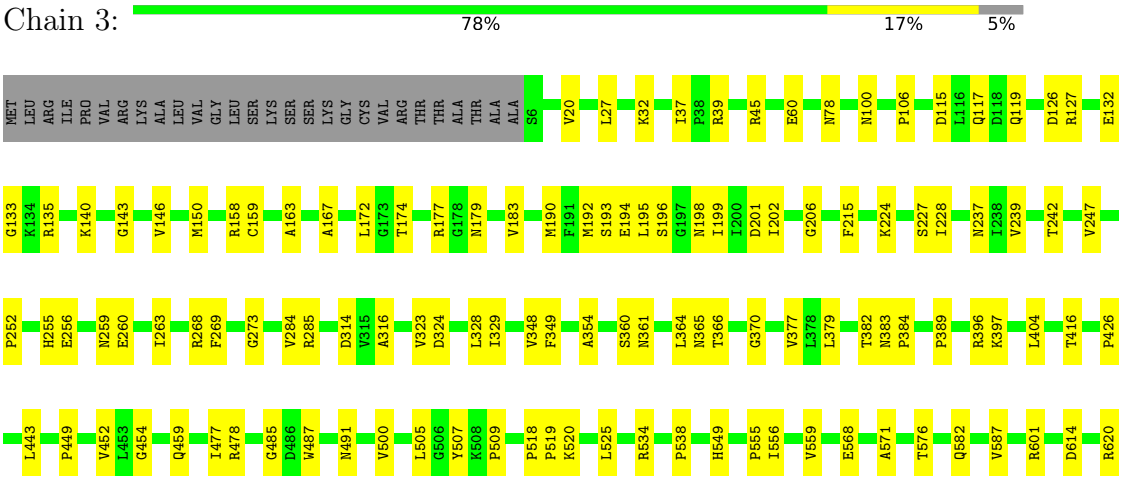
• Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:



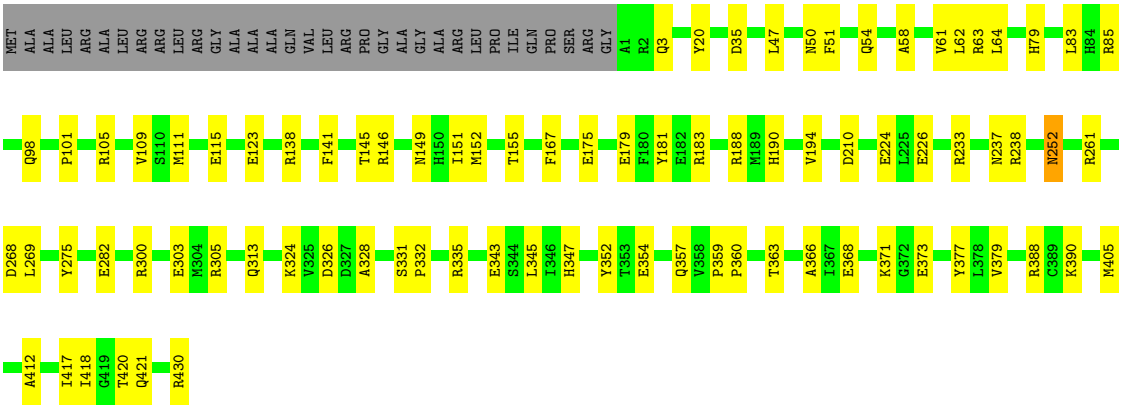
• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain 3:



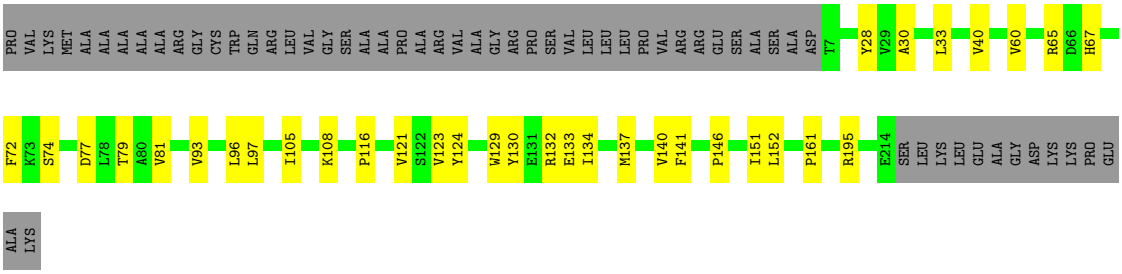
• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:



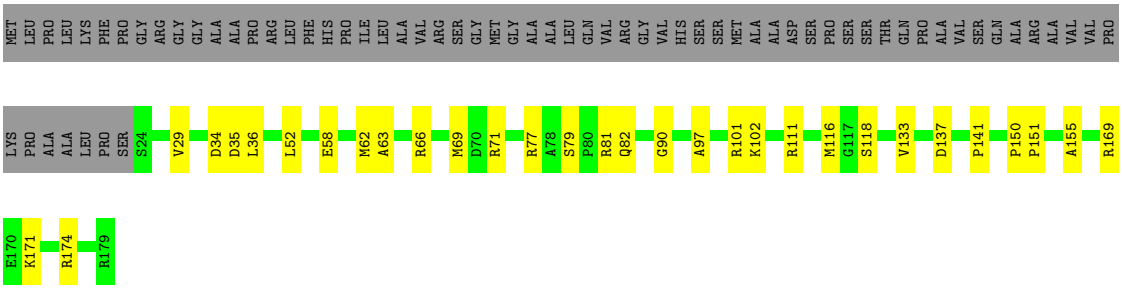
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:



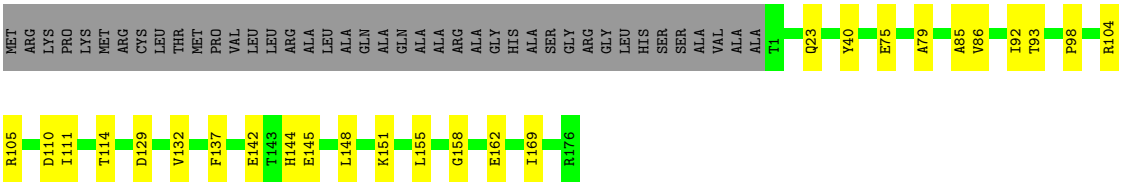
• Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:



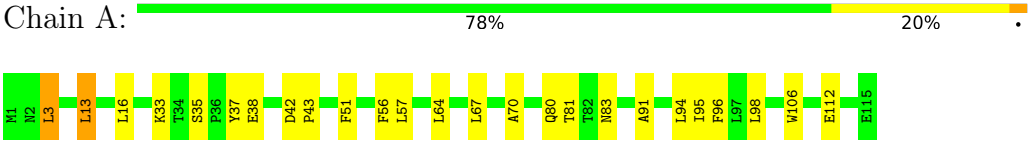
• Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:



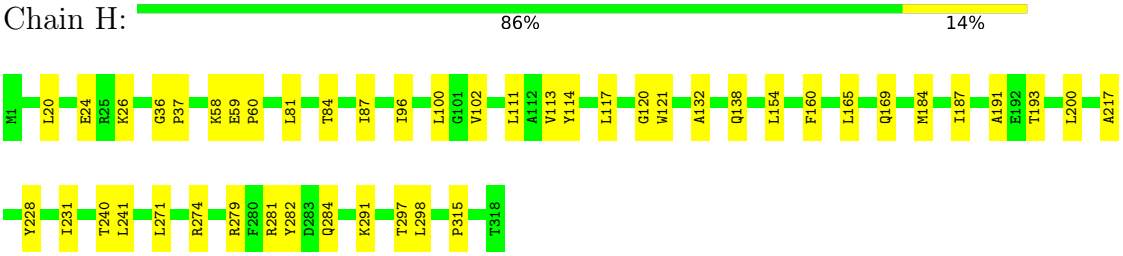
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A:



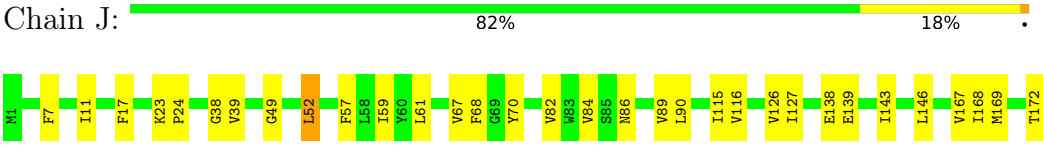
• Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H:



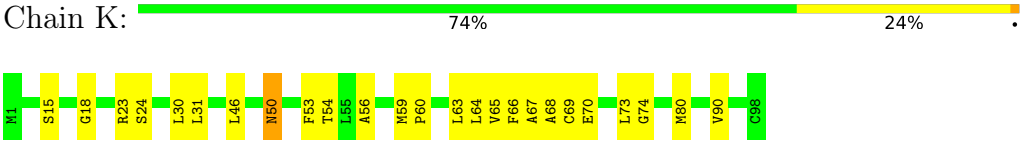
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



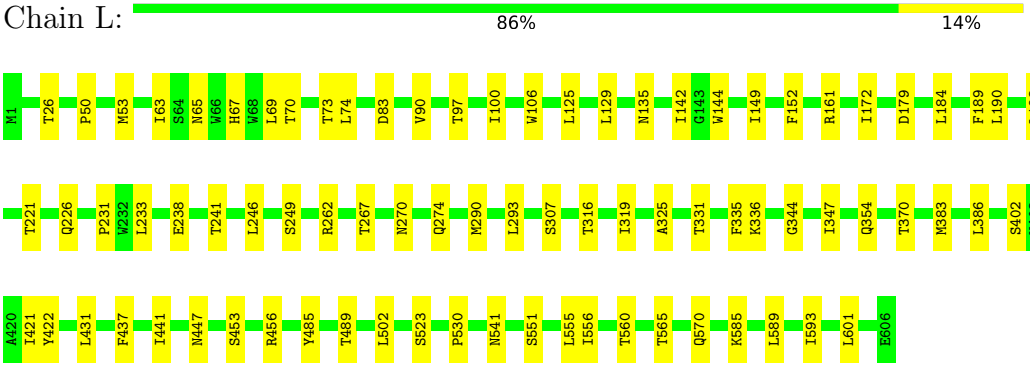
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



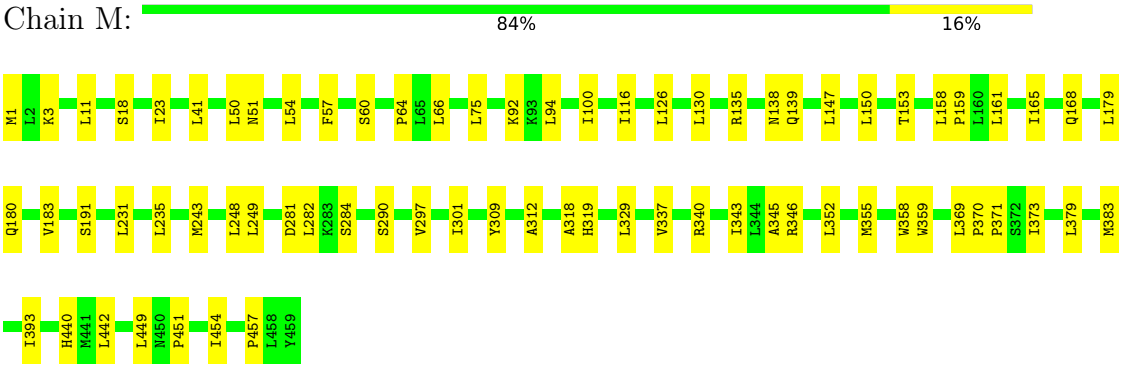
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



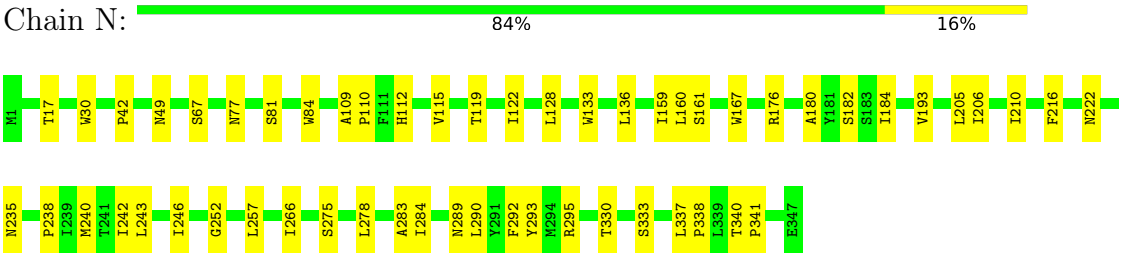
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



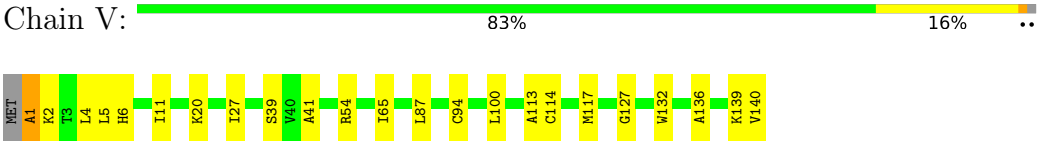
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



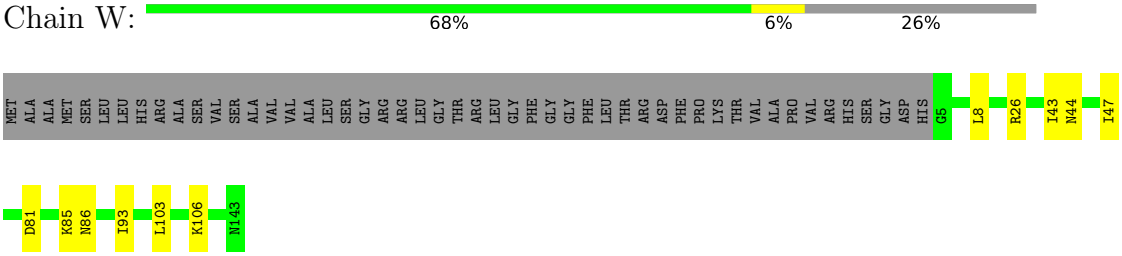
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V:



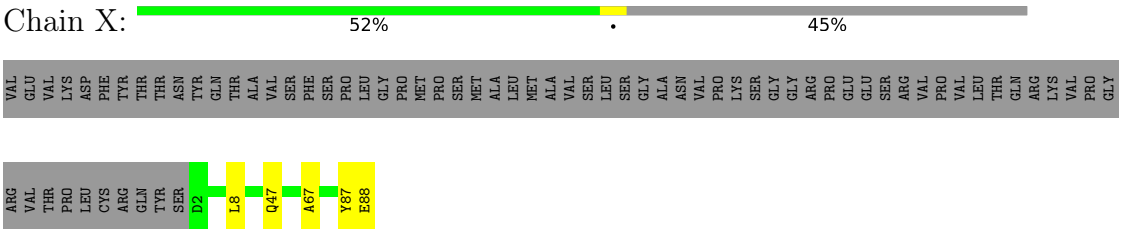
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W:



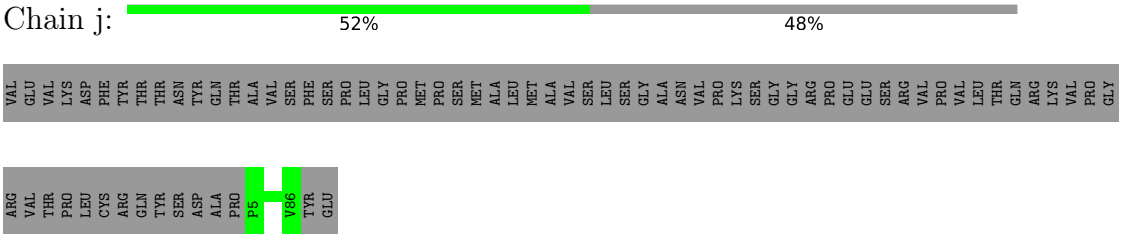
• Molecule 17: Acyl carrier protein

Chain X:



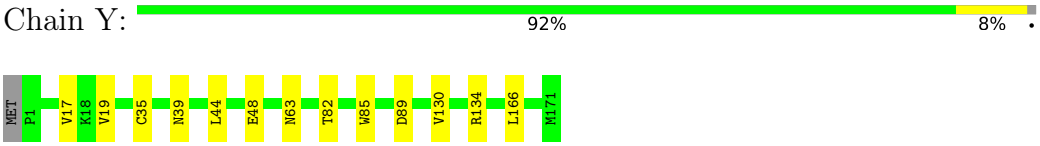
• Molecule 17: Acyl carrier protein

Chain j:



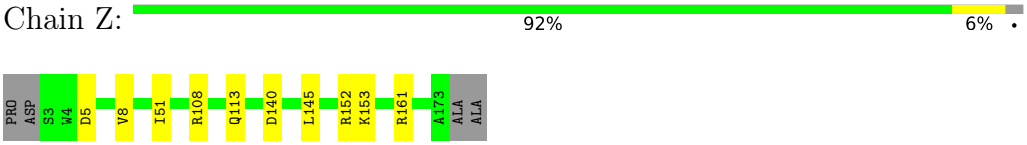
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:



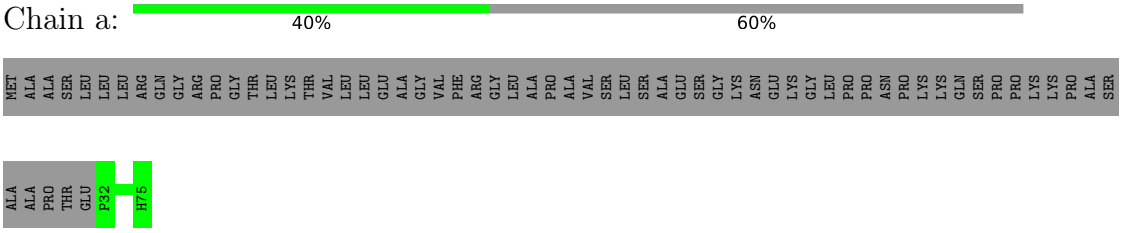
• Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:



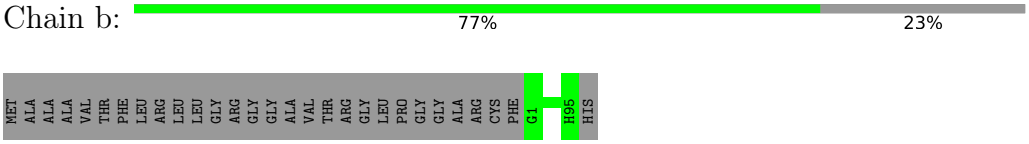
• Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:



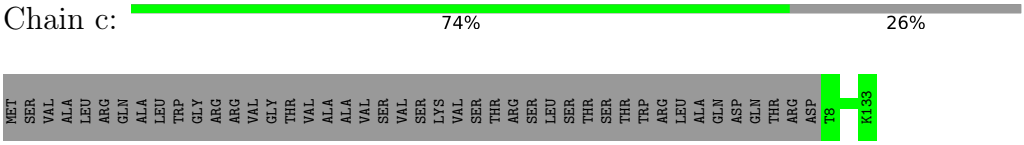
• Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:



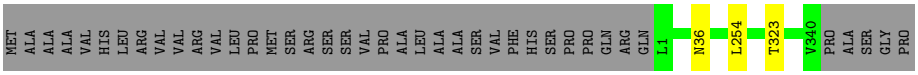
• Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:



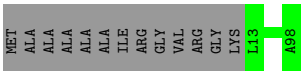
• Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:



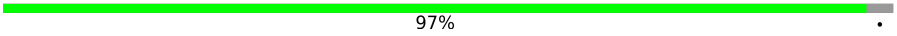
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

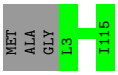
Chain e:



• Molecule 25: Mitochondrial complex I, B13 subunit

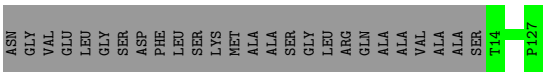
Chain f:





• Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:

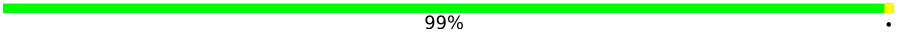


• Molecule 27: Mitochondrial complex I, B14.5a subunit

Chain h:

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

Chain i:

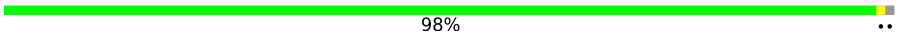


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:

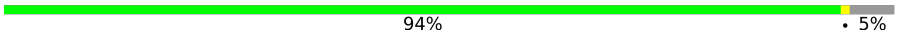
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

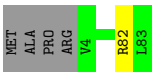
Chain l:



• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

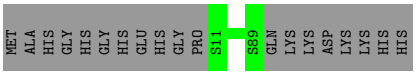
Chain m:





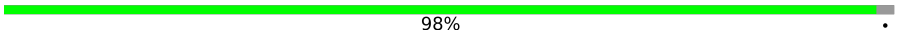
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n:



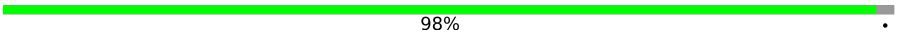
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:



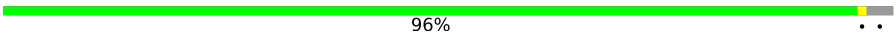
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

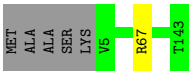
Chain p:



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

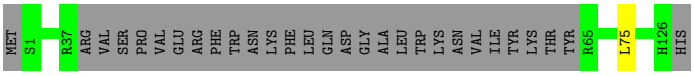
Chain q:





• Molecule 36: Mitochondrial complex I, B17 subunit

Chain r:

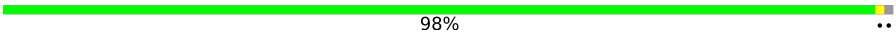


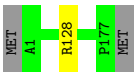
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

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

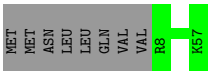
Chain w:

• 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, Not provided	
Number of particles used	14451	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 (i)

5.1 Standard geometry (i)

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

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	0.36	0/3386	0.55	0/4575
2	2	0.33	0/1695	0.55	0/2306
3	3	0.36	0/5362	0.55	0/7266
4	4	0.40	0/3535	0.57	0/4791
5	5	0.37	0/1776	0.54	0/2417
6	6	0.43	0/1278	0.55	0/1728
7	9	0.45	0/1445	0.57	0/1956
8	A	0.35	0/947	0.64	2/1296 (0.2%)
9	H	0.38	0/2603	0.65	0/3561
10	J	0.39	0/1378	0.65	2/1868 (0.1%)
11	K	0.33	0/749	0.62	0/1014
12	L	0.34	0/4925	0.57	0/6700
13	M	0.34	0/3731	0.60	0/5085
14	N	0.36	0/2787	0.58	0/3795
15	V	0.28	0/1041	0.51	1/1412 (0.1%)
16	W	0.32	0/1188	0.50	0/1607
17	X	0.29	0/713	0.51	0/963
17	j	0.29	0/670	0.50	0/902
18	Y	0.31	0/1440	0.53	0/1942
19	Z	0.31	0/1475	0.48	0/1989
20	a	0.29	0/383	0.47	0/518
21	b	0.33	0/749	0.46	0/1009
22	c	0.32	0/1047	0.50	0/1415
23	d	0.33	0/2824	0.54	1/3830 (0.0%)
24	e	0.29	0/702	0.51	0/945
25	f	0.31	0/937	0.49	0/1271
26	g	0.33	0/993	0.51	0/1336
27	h	0.34	0/779	0.53	0/1053
28	i	0.37	0/1250	0.51	0/1698
29	k	0.33	0/2646	0.51	1/3579 (0.0%)
30	l	0.32	0/896	0.54	1/1200 (0.1%)
31	m	0.29	0/647	0.48	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	n	0.29	0/653	0.46	0/882
33	o	0.34	0/1035	0.49	0/1398
34	p	0.29	0/1085	0.48	0/1467
35	q	0.32	0/1171	0.50	0/1579
36	r	0.30	0/874	0.53	1/1188 (0.1%)
37	s	0.29	0/1072	0.48	0/1436
38	t	0.31	0/1573	0.49	0/2130
39	u	0.30	0/590	0.47	0/810
40	v	0.31	0/1361	0.49	0/1861
41	w	0.32	0/872	0.51	0/1185
42	x	0.27	0/425	0.41	0/576
43	y	0.29	0/449	0.49	0/605
44	z	0.38	0/591	0.54	0/795
All	All	0.34	0/67728	0.54	9/91829 (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
2	2	0	1
3	3	0	1
4	4	0	1
10	J	0	2
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	146	LEU	CA-CB-CG	6.31	129.82	115.30
8	A	13	LEU	CA-CB-CG	5.61	128.21	115.30
29	k	96	LEU	CA-CB-CG	5.59	128.17	115.30
15	V	87	LEU	CA-CB-CG	5.45	127.82	115.30
8	A	3	LEU	CA-CB-CG	5.42	127.78	115.30
23	d	254	LEU	CA-CB-CG	5.29	127.46	115.30
10	J	52	LEU	CA-CB-CG	5.14	127.12	115.30
30	l	103	LEU	CA-CB-CG	5.06	126.94	115.30
36	r	75	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	63	ILE	Peptide
3	3	259	ASN	Peptide
4	4	275	TYR	Peptide
10	J	115	ILE	Peptide
10	J	82	VAL	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	1	3312	0	3269	43	0
2	2	1655	0	1668	19	0
3	3	5275	0	5300	70	0
4	4	3457	0	3397	58	0
5	5	1726	0	1676	20	0
6	6	1247	0	1259	26	0
7	9	1414	0	1371	19	0
8	A	922	0	953	23	0
9	H	2528	0	2641	29	0
10	J	1344	0	1364	22	0
11	K	749	0	793	18	0
12	L	4807	0	4949	50	0
13	M	3647	0	3849	48	0
14	N	2723	0	2930	37	0
15	V	1028	0	1036	16	0
16	W	1155	0	1177	8	0
17	X	701	0	692	3	0
17	j	660	0	663	0	0
18	Y	1403	0	1392	8	0
19	Z	1441	0	1419	7	0
20	a	371	0	344	0	0
21	b	737	0	710	0	0
22	c	1024	0	1023	0	0
23	d	2748	0	2763	0	0
24	e	691	0	706	0	0
25	f	917	0	958	0	0
26	g	969	0	980	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	h	769	0	780	0	0
28	i	1209	0	1182	0	0
29	k	2596	0	2559	0	0
30	l	874	0	869	0	0
31	m	626	0	635	0	0
32	n	634	0	616	0	0
33	o	1004	0	995	0	0
34	p	1059	0	1062	0	0
35	q	1142	0	1137	0	0
36	r	846	0	864	0	0
37	s	1047	0	1013	0	0
38	t	1520	0	1477	0	0
39	u	563	0	509	0	0
40	v	1307	0	1207	0	0
41	w	846	0	792	0	0
42	x	412	0	411	0	0
43	y	436	0	437	0	0
44	z	576	0	570	0	0
45	1	8	0	0	1	0
45	3	16	0	0	2	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	1	0
47	1	44	0	27	5	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	6	46	0	69	1	0
50	9	54	0	88	1	0
50	L	54	0	88	2	0
50	M	54	0	88	2	0
50	w	54	0	88	0	0
51	6	51	0	82	4	0
51	A	51	0	82	4	0
51	J	91	0	136	6	0
51	L	122	0	172	1	0
51	M	44	0	65	1	0
51	N	51	0	82	2	0
51	V	64	0	75	3	0
51	i	51	0	82	0	0
51	o	31	0	36	0	0
52	L	185	0	276	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	M	190	0	289	13	0
52	V	94	0	141	9	0
52	W	100	0	156	3	0
52	x	75	0	97	0	0
52	z	58	0	60	0	0
53	X	31	0	34	0	0
53	g	34	0	40	0	0
54	b	1	0	0	0	0
55	d	48	0	26	0	0
56	k	23	0	12	0	0
57	s	15	0	27	0	0
All	All	67921	0	68834	474	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 (474) 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)
5:5:28:TYR:HH	5:5:67:HIS:HE2	1.22	0.87
5:5:129:TRP:O	5:5:132:ARG:HB3	1.90	0.72
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.57	0.69
52:L:706:CDL:H562	52:L:706:CDL:H642	1.77	0.65
52:L:706:CDL:H362	52:L:706:CDL:H532	1.79	0.64
11:K:70:GLU:O	11:K:73:LEU:HB3	1.99	0.63
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.81	0.63
3:3:518:PRO:HB2	3:3:538:PRO:HD3	1.81	0.63
52:L:705:CDL:H542	52:L:705:CDL:H362	1.78	0.63
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.80	0.63
4:4:51:PHE:HB3	4:4:64:LEU:HB2	1.82	0.62
4:4:3:GLN:NE2	13:M:135:ARG:O	2.33	0.61
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.82	0.61
51:J:202:3PE:H11	11:K:23:ARG:HG2	1.83	0.61
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.34	0.60
1:1:300:GLY:HA2	1:1:333:ALA:H	1.67	0.60
6:6:77:ARG:HB3	6:6:82:GLN:HG3	1.84	0.60
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.84	0.60
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.84	0.60
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.84	0.59
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.83	0.59
12:L:73:THR:HB	12:L:194:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:64:LEU:O	11:K:67:ALA:HB3	2.03	0.59
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.33	0.59
6:6:169:ARG:NH2	7:9:142:GLU:OE2	2.35	0.59
3:3:158:ARG:HB3	3:3:202:ILE:HD12	1.85	0.59
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.35	0.59
52:M:503:CDL:H852	52:M:504:CDL:H673	1.85	0.59
3:3:45:ARG:NH2	3:3:256:GLU:OE2	2.32	0.58
6:6:102:LYS:NZ	8:A:42:ASP:OD1	2.35	0.58
9:H:169:GLN:NE2	9:H:241:LEU:O	2.34	0.58
52:V:203:CDL:H362	52:V:203:CDL:H571	1.86	0.58
4:4:146:ARG:NH2	4:4:368:GLU:O	2.36	0.58
4:4:175:GLU:OE2	4:4:188:ARG:NH1	2.37	0.58
52:M:504:CDL:HB4	14:N:238:PRO:HB2	1.86	0.58
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.86	0.57
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.69	0.57
2:2:105:THR:OG1	48:2:300:FES:S2	2.61	0.57
51:J:201:3PE:H2F2	51:J:201:3PE:H371	1.85	0.57
4:4:109:VAL:HG11	4:4:152:MET:HG2	1.86	0.57
14:N:30:TRP:NE1	14:N:67:SER:OG	2.38	0.57
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.86	0.57
19:Z:5:ASP:HB3	19:Z:8:VAL:HG12	1.87	0.57
3:3:348:VAL:H	3:3:459:GLN:HE22	1.53	0.57
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.38	0.57
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.37	0.57
13:M:158:LEU:HD23	14:N:283:ALA:HB1	1.87	0.57
12:L:565:THR:HB	52:L:705:CDL:H521	1.87	0.56
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.37	0.56
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.87	0.56
8:A:67:LEU:HD22	11:K:65:VAL:HA	1.87	0.56
14:N:160:LEU:HD21	52:V:203:CDL:H191	1.88	0.56
15:V:5:LEU:HD23	51:V:202:3PE:H231	1.87	0.56
5:5:79:THR:HB	5:5:93:VAL:HB	1.87	0.56
9:H:81:LEU:HA	9:H:84:THR:HG22	1.87	0.56
52:L:706:CDL:H611	13:M:369:LEU:HD23	1.87	0.56
51:A:201:3PE:H3I2	51:A:201:3PE:H2F2	1.86	0.56
11:K:24:SER:HA	11:K:90:VAL:HG22	1.87	0.56
4:4:145:THR:HG1	4:4:181:TYR:HH	1.53	0.56
13:M:50:LEU:HA	16:W:86:ASN:HD21	1.70	0.56
18:Y:48:GLU:OE1	18:Y:134:ARG:NH2	2.39	0.56
1:1:358:SER:OG	1:1:365:CYS:SG	2.62	0.56
8:A:98:LEU:HD22	9:H:298:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:156:ILE:HD13	2:2:176:LEU:HD11	1.89	0.55
1:1:21:ILE:O	1:1:117:LYS:NZ	2.33	0.55
6:6:36:LEU:HD13	51:6:203:3PE:H392	1.88	0.55
52:M:503:CDL:H792	14:N:338:PRO:HG3	1.89	0.55
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.69	0.55
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.88	0.55
3:3:127:ARG:NH2	4:4:326:ASP:O	2.39	0.55
4:4:237:ASN:O	9:H:284:GLN:NE2	2.35	0.55
13:M:179:LEU:HD13	13:M:249:LEU:HD11	1.87	0.55
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.25	0.55
12:L:161:ARG:NE	12:L:238:GLU:OE2	2.39	0.55
9:H:200:LEU:HD22	9:H:282:TYR:HB3	1.88	0.55
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.89	0.55
8:A:56:PHE:O	10:J:70:TYR:OH	2.25	0.55
1:1:108:ARG:NH2	2:2:162:GLU:OE2	2.40	0.55
13:M:1:FME:O1	13:M:3:LYS:NZ	2.40	0.55
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.89	0.55
15:V:39:SER:OG	15:V:54:ARG:NH2	2.39	0.55
6:6:118:SER:N	45:6:201:SF4:S4	2.80	0.54
52:M:503:CDL:H152	52:M:503:CDL:H571	1.88	0.54
17:X:47:GLN:NE2	17:X:67:ALA:O	2.39	0.54
1:1:96:ASN:ND2	1:1:187:GLY:O	2.36	0.54
1:1:390:ASP:OD1	1:1:423:ARG:NH2	2.39	0.54
1:1:94:VAL:O	1:1:222:VAL:HA	2.08	0.54
12:L:316:THR:HA	12:L:319:ILE:HG12	1.88	0.54
8:A:67:LEU:HD11	11:K:68:ALA:HB3	1.90	0.54
3:3:159:CYS:HB3	3:3:172:LEU:HD13	1.88	0.54
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.41	0.54
9:H:20:LEU:HD21	9:H:231:ILE:HD11	1.88	0.54
10:J:84:VAL:HG12	10:J:90:LEU:HD13	1.90	0.54
12:L:203:MET:HB2	19:Z:113:GLN:HG3	1.89	0.54
13:M:352:LEU:HB3	13:M:355:MET:HB3	1.89	0.54
52:M:503:CDL:HA61	52:M:503:CDL:HA21	1.90	0.54
52:M:504:CDL:H873	14:N:246:ILE:HA	1.90	0.54
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.89	0.54
3:3:140:LYS:HD3	3:3:150:MET:HG3	1.89	0.54
52:L:705:CDL:H152	52:V:203:CDL:H712	1.90	0.54
9:H:114:TYR:OH	10:J:61:LEU:O	2.23	0.53
3:3:382:THR:HB	3:3:454:GLY:HA3	1.90	0.53
1:1:365:CYS:HB3	45:1:501:SF4:S3	2.47	0.53
9:H:102:VAL:HG11	9:H:154:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.42	0.53
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.90	0.53
4:4:35:ASP:O	14:N:49:ASN:ND2	2.41	0.53
6:6:81:ARG:NH1	8:A:33:LYS:O	2.39	0.53
4:4:377:TYR:HB3	4:4:390:LYS:HB3	1.88	0.53
14:N:252:GLY:HA3	14:N:290:LEU:HD13	1.90	0.53
4:4:101:PRO:O	4:4:105:ARG:NH1	2.41	0.53
11:K:56:ALA:O	11:K:59:MET:HB3	2.08	0.53
52:M:504:CDL:H861	14:N:257:LEU:HD21	1.91	0.53
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.39	0.52
4:4:405:MET:SD	4:4:421:GLN:NE2	2.73	0.52
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.90	0.52
5:5:65:ARG:NH1	5:5:123:VAL:O	2.42	0.52
10:J:23:LYS:O	11:K:23:ARG:NH1	2.42	0.52
3:3:360:SER:O	3:3:365:ASN:ND2	2.41	0.52
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.35	0.52
4:4:226:GLU:OE1	4:4:305:ARG:NH2	2.36	0.52
10:J:52:LEU:HD22	10:J:143:ILE:HD11	1.90	0.52
1:1:261:HIS:ND1	1:1:338:ASP:OD1	2.42	0.52
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.92	0.52
16:W:43:ILE:HG12	16:W:47:ILE:HD12	1.92	0.52
3:3:285:ARG:NH2	3:3:555:PRO:O	2.42	0.52
8:A:57:LEU:HD21	10:J:169:MET:HG2	1.92	0.52
5:5:93:VAL:HG22	5:5:108:LYS:HG2	1.92	0.51
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.91	0.51
4:4:58:ALA:HB1	4:4:62:LEU:HB3	1.91	0.51
11:K:60:PRO:O	11:K:63:LEU:HB3	2.09	0.51
14:N:17:THR:HG1	14:N:133:TRP:HE1	1.58	0.51
12:L:142:ILE:HG12	13:M:370:PRO:HB2	1.92	0.51
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.76	0.51
4:4:50:ASN:HB3	8:A:38:GLU:HG3	1.93	0.51
13:M:23:ILE:HD11	13:M:92:LYS:HD2	1.91	0.51
4:4:64:LEU:HD11	4:4:418:ILE:HD11	1.91	0.51
1:1:91:LYS:HG2	1:1:219:PRO:HB2	1.92	0.51
1:1:200:GLN:NE2	3:3:174:THR:O	2.42	0.51
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.42	0.51
6:6:137:ASP:OD2	7:9:144:HIS:ND1	2.44	0.51
50:9:401:PC1:H351	9:H:187:ILE:HD12	1.92	0.51
50:L:704:PC1:H381	52:W:201:CDL:H512	1.93	0.51
1:1:356:HIS:O	3:3:177:ARG:NH2	2.41	0.51
4:4:238:ARG:NH1	9:H:279:ARG:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.75	0.51
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.92	0.51
50:M:502:PC1:H2C2	50:M:502:PC1:H3B1	1.93	0.51
19:Z:145:LEU:HD22	19:Z:153:LYS:HB3	1.92	0.51
10:J:23:LYS:NZ	11:K:18:GLY:O	2.41	0.50
6:6:79:SER:H	6:6:82:GLN:HE21	1.59	0.50
13:M:165:ILE:O	13:M:168:GLN:HB3	2.11	0.50
51:V:202:3PE:H292	52:V:203:CDL:H861	1.93	0.50
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.93	0.50
1:1:374:LYS:NZ	3:3:133:GLY:O	2.44	0.50
52:L:705:CDL:H112	52:V:203:CDL:HB31	1.93	0.50
1:1:243:ALA:HA	1:1:251:SER:HB3	1.94	0.50
3:3:354:ALA:HB3	3:3:361:ASN:HD21	1.76	0.50
13:M:297:VAL:HG13	13:M:312:ALA:HB1	1.94	0.50
6:6:36:LEU:HD22	51:6:203:3PE:H3A1	1.94	0.50
13:M:343:ILE:O	13:M:346:ARG:NH1	2.44	0.50
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.93	0.50
6:6:71:ARG:HA	9:H:37:PRO:HA	1.94	0.50
9:H:111:LEU:HD22	10:J:57:PHE:HZ	1.77	0.50
10:J:67:VAL:HG11	11:K:31:LEU:HD21	1.94	0.50
12:L:106:TRP:HD1	12:L:447:ASN:HD22	1.59	0.50
52:L:705:CDL:H511	52:L:705:CDL:H332	1.94	0.50
13:M:301:ILE:HA	13:M:309:TYR:HE1	1.76	0.50
13:M:337:VAL:HG11	13:M:345:ALA:HB2	1.93	0.50
13:M:41:LEU:HD13	13:M:66:LEU:HD13	1.94	0.49
4:4:98:GLN:NE2	7:9:85:ALA:O	2.46	0.49
12:L:601:LEU:O	15:V:1:AYA:N	2.41	0.49
1:1:20:ARG:HH12	2:2:201:SER:HB2	1.77	0.49
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.94	0.49
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.94	0.49
4:4:141:PHE:O	4:4:145:THR:OG1	2.30	0.49
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.94	0.49
3:3:324:ASP:N	3:3:324:ASP:OD1	2.43	0.49
4:4:47:LEU:HD13	8:A:51:PHE:HD1	1.78	0.49
11:K:66:PHE:HA	11:K:69:CYS:HB3	1.95	0.49
2:2:96:GLY:H	2:2:138:THR:HG1	1.57	0.49
7:9:158:GLY:O	7:9:162:GLU:HB2	2.12	0.49
12:L:402:SER:OG	12:L:404:THR:OG1	2.31	0.49
13:M:159:PRO:HD3	14:N:284:ILE:HD11	1.94	0.49
8:A:3:LEU:HD12	51:J:201:3PE:H252	1.95	0.49
52:W:201:CDL:H112	19:Z:51:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:8:LEU:H	17:X:87:TYR:HE2	1.61	0.49
10:J:126:VAL:HG23	10:J:127:ILE:HG23	1.95	0.49
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.94	0.49
10:J:167:VAL:HG22	14:N:42:PRO:HG2	1.94	0.48
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.95	0.48
4:4:61:VAL:HG21	4:4:83:LEU:HB2	1.94	0.48
6:6:35:ASP:HB3	51:6:203:3PE:H331	1.95	0.48
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.94	0.48
13:M:180:GLN:HA	13:M:248:LEU:HD21	1.94	0.48
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.46	0.48
1:1:194:GLU:OE2	1:1:204:ARG:NE	2.38	0.48
4:4:155:THR:HB	4:4:167:PHE:HA	1.94	0.48
9:H:184:MET:SD	9:H:297:THR:OG1	2.71	0.48
3:3:60:GLU:HG2	3:3:78:ASN:HB3	1.94	0.48
3:3:377:VAL:HG23	3:3:404:LEU:HD11	1.96	0.48
4:4:300:ARG:NH2	4:4:420:THR:O	2.45	0.48
13:M:191:SER:HG	15:V:132:TRP:HE1	1.58	0.48
18:Y:85:TRP:O	18:Y:89:ASP:HB2	2.14	0.48
4:4:417:ILE:HA	4:4:420:THR:HG22	1.94	0.48
3:3:396:ARG:NH1	3:3:416:THR:O	2.47	0.48
4:4:324:LYS:HD3	4:4:331:SER:HB3	1.95	0.48
10:J:24:PRO:HB3	10:J:89:VAL:HG11	1.94	0.48
1:1:247:ARG:HH22	1:1:320:ASP:HB2	1.78	0.48
52:M:504:CDL:H791	14:N:242:ILE:HG23	1.94	0.48
2:2:147:ALA:HB3	2:2:153:MET:HG2	1.96	0.48
4:4:261:ARG:NH2	4:4:303:GLU:OE2	2.45	0.48
16:W:103:LEU:HD23	16:W:106:LYS:HD2	1.96	0.48
3:3:194:GLU:HG2	3:3:195:LEU:HG	1.94	0.47
6:6:97:ALA:HB2	6:6:133:VAL:HG21	1.95	0.47
3:3:215:PHE:HB2	7:9:98:PRO:HD3	1.95	0.47
4:4:324:LYS:HE2	4:4:332:PRO:HG2	1.95	0.47
8:A:80:GLN:NE2	9:H:315:PRO:O	2.46	0.47
14:N:110:PRO:HD3	14:N:160:LEU:HD23	1.96	0.47
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.78	0.47
4:4:111:MET:SD	4:4:111:MET:N	2.87	0.47
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.50	0.47
9:H:120:GLY:HA3	9:H:132:ALA:HB2	1.97	0.47
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.96	0.47
15:V:1:AYA:HA	15:V:4:LEU:HD23	1.97	0.47
5:5:137:MET:HA	5:5:161:PRO:HD2	1.95	0.47
12:L:241:THR:HG21	12:L:344:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:L:706:CDL:H182	13:M:442:LEU:HD22	1.96	0.47
13:M:191:SER:HB3	50:M:502:PC1:H31	1.96	0.47
14:N:77:ASN:O	14:N:81:SER:OG	2.31	0.47
4:4:261:ARG:NH1	4:4:268:ASP:OD1	2.47	0.47
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.80	0.47
4:4:412:ALA:HB3	9:H:281:ARG:HG3	1.97	0.47
3:3:146:VAL:HG21	3:3:199:ILE:HD11	1.96	0.47
3:3:323:VAL:HG11	3:3:525:LEU:HD13	1.96	0.47
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.96	0.47
1:1:71:ALA:HB2	47:1:503:NAI:H4D	1.97	0.46
3:3:190:MET:HG2	3:3:192:MET:HG2	1.97	0.46
1:1:288:THR:O	1:1:293:ASN:ND2	2.49	0.46
3:3:100:ASN:HB3	3:3:135:ARG:HG2	1.97	0.46
9:H:24:GLU:HA	9:H:271:LEU:HD13	1.96	0.46
10:J:138:GLU:O	11:K:54:THR:OG1	2.30	0.46
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.49	0.46
9:H:26:LYS:HA	9:H:36:GLY:HA3	1.97	0.46
13:M:54:LEU:HD23	16:W:93:ILE:HG23	1.96	0.46
12:L:50:PRO:HA	12:L:53:MET:HG2	1.98	0.46
16:W:44:ASN:HB3	52:W:201:CDL:HA31	1.98	0.46
2:2:99:HIS:CE1	2:2:101:GLN:HE21	2.33	0.46
3:3:242:THR:HG22	3:3:247:VAL:HA	1.98	0.46
51:L:701:3PE:H342	13:M:147:LEU:HB3	1.98	0.46
3:3:383:ASN:ND2	3:3:665:GLN:O	2.44	0.46
4:4:145:THR:OG1	4:4:181:TYR:OH	2.26	0.46
4:4:343:GLU:O	4:4:347:HIS:ND1	2.37	0.46
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.96	0.46
13:M:116:ILE:HD11	13:M:161:LEU:HD12	1.97	0.46
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.96	0.46
3:3:426:PRO:HG3	3:3:661:LEU:HG	1.98	0.46
5:5:134:ILE:HG22	5:5:140:VAL:HB	1.98	0.46
12:L:249:SER:HB2	12:L:336:LYS:HG3	1.97	0.46
12:L:485:TYR:O	12:L:489:THR:OG1	2.34	0.46
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.97	0.46
15:V:11:ILE:HB	15:V:20:LYS:HD3	1.97	0.46
1:1:191:ALA:HB2	1:1:203:PRO:HG3	1.98	0.46
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.50	0.46
4:4:238:ARG:NH2	4:4:412:ALA:O	2.46	0.46
7:9:132:VAL:HG11	7:9:169:ILE:HD11	1.98	0.46
3:3:284:VAL:HG12	3:3:559:VAL:HG22	1.98	0.45
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:63:ALA:HA	6:6:69:MET:HG2	1.98	0.45
7:9:151:LYS:HE2	7:9:155:LEU:HD11	1.98	0.45
16:W:81:ASP:HB3	16:W:85:LYS:HD3	1.98	0.45
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.98	0.45
15:V:2:LYS:O	15:V:6:HIS:ND1	2.37	0.45
15:V:27:ILE:HG23	52:V:203:CDL:H473	1.99	0.45
3:3:534:ARG:NH2	3:3:556:ILE:O	2.45	0.45
2:2:111:ARG:HD3	2:2:151:ALA:HB3	1.99	0.45
3:3:328:LEU:HD22	3:3:507:TYR:HE2	1.81	0.45
3:3:193:SER:H	3:3:196:SER:HB3	1.81	0.45
3:3:273:GLY:O	3:3:549:HIS:NE2	2.41	0.45
8:A:112:GLU:OE2	9:H:291:LYS:NZ	2.49	0.45
52:L:705:CDL:H151	52:V:203:CDL:H511	1.97	0.45
52:L:706:CDL:H641	13:M:371:PRO:HD2	1.98	0.45
14:N:112:HIS:HB2	14:N:184:ILE:HD13	1.98	0.45
1:1:69:GLY:O	47:1:503:NAI:H2N	2.15	0.45
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.39	0.45
3:3:117:GLN:NE2	45:3:801:SF4:S3	2.89	0.45
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.81	0.45
1:1:390:ASP:O	1:1:393:TRP:HB3	2.17	0.45
9:H:165:LEU:HD23	9:H:240:THR:HG22	1.98	0.45
12:L:74:LEU:HD13	12:L:190:LEU:HD13	1.99	0.45
50:L:704:PC1:H2B1	13:M:449:LEU:HD23	1.99	0.45
52:L:705:CDL:H862	51:M:501:3PE:H392	1.99	0.45
4:4:123:GLU:OE2	4:4:138:ARG:NH2	2.49	0.45
3:3:158:ARG:NH1	3:3:202:ILE:O	2.50	0.44
52:L:705:CDL:H352	52:L:705:CDL:H142	1.98	0.44
3:3:316:ALA:HB3	3:3:519:PRO:HG3	1.99	0.44
3:3:366:THR:HG22	3:3:370:GLY:HA3	1.99	0.44
5:5:30:ALA:HB2	5:5:40:VAL:HG21	1.98	0.44
5:5:195:ARG:HH12	7:9:93:THR:HA	1.82	0.44
1:1:276:LEU:HD21	1:1:297:VAL:HG11	1.99	0.44
3:3:227:SER:OG	3:3:228:ILE:N	2.50	0.44
3:3:568:GLU:HG2	3:3:587:VAL:HG23	1.98	0.44
2:2:129:GLY:HA2	2:2:140:ILE:HG22	1.99	0.44
9:H:138:GLN:NE2	9:H:191:ALA:O	2.50	0.44
12:L:347:ILE:HD13	12:L:354:GLN:HG2	1.99	0.44
14:N:193:VAL:HB	14:N:266:ILE:HG23	2.00	0.44
14:N:206:ILE:HG23	51:N:401:3PE:H2H2	1.98	0.44
3:3:206:GLY:N	45:3:801:SF4:S2	2.80	0.44
3:3:449:PRO:O	3:3:487:TRP:NE1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:159:ASN:HB3	2:2:184:PRO:HB3	2.00	0.44
5:5:121:VAL:HG21	5:5:146:PRO:HD3	2.00	0.44
8:A:38:GLU:HB2	8:A:43:PRO:HG3	1.98	0.44
12:L:290:MET:O	12:L:523:SER:OG	2.32	0.44
13:M:60:SER:HB2	13:M:457:PRO:HA	2.00	0.44
52:V:203:CDL:H351	52:V:203:CDL:H322	1.78	0.44
52:M:503:CDL:H632	52:M:503:CDL:H601	1.87	0.44
3:3:500:VAL:HG21	3:3:576:THR:HA	2.00	0.44
9:H:113:VAL:O	9:H:117:LEU:HB2	2.18	0.44
4:4:224:GLU:OE2	7:9:40:TYR:OH	2.31	0.43
12:L:144:TRP:NE1	12:L:179:ASP:OD1	2.50	0.43
12:L:453:SER:HA	12:L:456:ARG:HH21	1.83	0.43
12:L:556:ILE:O	12:L:560:THR:N	2.52	0.43
8:A:81:THR:HG23	8:A:83:ASN:H	1.83	0.43
1:1:193:ILE:HG23	1:1:215:VAL:HA	2.00	0.43
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.84	0.43
4:4:63:ARG:HB3	4:4:79:HIS:HB2	2.00	0.43
11:K:46:LEU:O	11:K:50:ASN:HB2	2.17	0.43
13:M:183:VAL:O	19:Z:152:ARG:NH1	2.39	0.43
1:1:279:LEU:HD12	1:1:283:HIS:HD2	1.83	0.43
7:9:75:GLU:O	7:9:105:ARG:NH1	2.51	0.43
13:M:369:LEU:HD12	13:M:370:PRO:HD2	2.00	0.43
10:J:172:THR:HA	11:K:80:MET:HE3	1.99	0.43
3:3:260:GLU:OE2	3:3:397:LYS:NZ	2.36	0.43
6:6:81:ARG:NH2	8:A:35:SER:O	2.51	0.43
14:N:119:THR:HG22	14:N:176:ARG:HB3	2.01	0.43
14:N:182:SER:OG	14:N:293:TYR:OH	2.32	0.43
1:1:96:ASN:ND2	46:1:502:FMN:O4'	2.47	0.43
3:3:314:ASP:HB3	3:3:520:LYS:HE2	2.00	0.43
4:4:379:VAL:HB	4:4:388:ARG:HB3	2.01	0.43
7:9:92:ILE:HA	7:9:110:ASP:O	2.19	0.43
3:3:379:LEU:HD23	3:3:452:VAL:HB	2.00	0.43
12:L:589:LEU:HD12	15:V:41:ALA:HA	2.01	0.43
4:4:388:ARG:HG2	5:5:81:VAL:HG22	2.00	0.43
6:6:101:ARG:HH12	6:6:141:PRO:HD3	1.83	0.43
12:L:267:THR:O	12:L:274:GLN:NE2	2.50	0.43
5:5:116:PRO:HB3	5:5:141:PHE:HD2	1.83	0.43
9:H:59:GLU:HA	9:H:60:PRO:HD3	1.90	0.43
3:3:329:ILE:HD13	3:3:505:LEU:HD22	2.01	0.42
9:H:121:TRP:HB2	10:J:68:PHE:HZ	1.84	0.42
13:M:329:LEU:HB3	13:M:359:TRP:CZ2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:128:LEU:HD13	14:N:216:PHE:HB2	2.01	0.42
4:4:252:ASN:HD21	5:5:124:TYR:HA	1.84	0.42
12:L:90:VAL:HG22	12:L:129:LEU:HD22	2.01	0.42
14:N:109:ALA:HB3	14:N:161:SER:HA	2.01	0.42
1:1:99:GLU:OE2	1:1:106:LYS:N	2.52	0.42
2:2:120:ILE:HD11	2:2:169:ILE:HG12	2.00	0.42
3:3:237:ASN:HD22	3:3:255:HIS:HB2	1.83	0.42
8:A:106:TRP:HE1	51:A:201:3PE:H32	1.85	0.42
12:L:63:ILE:HG22	12:L:65:ASN:HB3	2.01	0.42
13:M:139:GLN:HG3	13:M:340:ARG:HH22	1.85	0.42
1:1:21:ILE:HG21	1:1:230:VAL:HG12	2.01	0.42
4:4:363:THR:O	4:4:377:TYR:HA	2.19	0.42
5:5:130:TYR:O	5:5:133:GLU:HB3	2.19	0.42
13:M:130:LEU:HD22	13:M:150:LEU:HD13	2.01	0.42
3:3:115:ASP:O	3:3:119:GLN:HG2	2.19	0.42
50:6:202:PC1:H391	50:6:202:PC1:H291	2.01	0.42
12:L:184:LEU:HD13	13:M:393:ILE:HG21	2.02	0.42
12:L:437:PHE:HE2	12:L:441:ILE:HG13	1.85	0.42
3:3:224:LYS:HG3	3:3:239:VAL:HG11	2.00	0.42
12:L:331:THR:HG22	12:L:335:PHE:HE1	1.84	0.42
13:M:94:LEU:HD21	52:M:504:CDL:H541	2.01	0.42
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.54	0.42
16:W:8:LEU:HD11	17:X:88:GLU:HG3	2.01	0.42
3:3:20:VAL:HG12	3:3:32:LYS:HD3	2.01	0.42
9:H:24:GLU:HG2	9:H:271:LEU:HD22	2.02	0.42
11:K:30:LEU:HD11	11:K:74:GLY:HA3	2.01	0.42
12:L:316:THR:HG23	12:L:325:ALA:HB2	2.02	0.42
15:V:94:CYS:HA	15:V:114:CYS:HA	2.02	0.42
52:V:203:CDL:H202	52:V:203:CDL:H372	2.02	0.42
1:1:69:GLY:O	47:1:503:NAI:N7N	2.41	0.42
1:1:265:PRO:O	2:2:190:ARG:NH1	2.37	0.42
1:1:299:PRO:HG3	1:1:307:ILE:HG12	2.02	0.42
1:1:300:GLY:HA3	1:1:329:LEU:O	2.19	0.42
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.84	0.42
13:M:379:LEU:O	13:M:383:MET:HG2	2.20	0.42
15:V:127:GLY:HA3	51:V:202:3PE:H342	2.02	0.42
19:Z:8:VAL:HA	19:Z:108:ARG:HH21	1.85	0.42
1:1:140:GLY:O	1:1:179:ARG:NH2	2.50	0.42
3:3:269:PHE:HB3	3:3:683:THR:HG21	2.02	0.42
6:6:29:VAL:HG22	51:6:203:3PE:H3I3	2.02	0.42
6:6:155:ALA:HB2	7:9:137:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:64:LEU:HD11	10:J:168:ILE:HD12	2.01	0.42
10:J:38:GLY:HA3	51:J:201:3PE:H2F1	2.02	0.42
11:K:53:PHE:HE2	14:N:84:TRP:HE1	1.68	0.42
4:4:54:GLN:OE1	8:A:37:TYR:OH	2.26	0.41
12:L:231:PRO:HB3	12:L:530:PRO:HG3	2.02	0.41
2:2:121:GLN:HG2	2:2:127:LYS:HA	2.01	0.41
3:3:348:VAL:H	3:3:459:GLN:NE2	2.18	0.41
5:5:72:PHE:O	5:5:124:TYR:OH	2.32	0.41
6:6:171:LYS:HG2	6:6:174:ARG:HE	1.86	0.41
12:L:26:THR:OG1	16:W:26:ARG:NH1	2.39	0.41
3:3:163:ALA:HA	3:3:167:ALA:HB3	2.03	0.41
3:3:174:THR:HG22	3:3:183:VAL:HG22	2.02	0.41
12:L:189:PHE:HD1	12:L:193:LEU:HD22	1.86	0.41
3:3:478:ARG:NH2	3:3:485:GLY:O	2.54	0.41
9:H:87:ILE:HD12	9:H:96:ILE:HD12	2.02	0.41
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.55	0.41
52:M:504:CDL:H532	14:N:242:ILE:HD13	2.01	0.41
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	2.02	0.41
18:Y:44:LEU:HD22	18:Y:130:VAL:HB	2.03	0.41
1:1:70:GLY:HA3	47:1:503:NAI:H1D	2.03	0.41
3:3:27:LEU:HA	3:3:37:ILE:HD12	2.03	0.41
4:4:366:ALA:HB1	4:4:373:GLU:HG3	2.02	0.41
51:A:201:3PE:H292	51:A:201:3PE:H2H1	2.02	0.41
12:L:152:PHE:HB2	12:L:172:ILE:HD11	2.01	0.41
13:M:290:SER:HA	13:M:319:HIS:HE2	1.86	0.41
14:N:337:LEU:O	14:N:340:THR:OG1	2.28	0.41
9:H:20:LEU:HD23	9:H:228:TYR:HB3	2.01	0.41
9:H:100:LEU:HD23	9:H:160:PHE:HB2	2.03	0.41
10:J:7:PHE:O	10:J:11:ILE:HG12	2.21	0.41
12:L:383:MET:HB3	12:L:386:LEU:HD12	2.03	0.41
12:L:551:SER:HA	12:L:555:LEU:HD12	2.03	0.41
14:N:341:PRO:HG3	18:Y:166:LEU:HD23	2.01	0.41
1:1:92:TYR:O	1:1:220:THR:HA	2.20	0.41
5:5:74:SER:HB3	5:5:97:LEU:HB3	2.02	0.41
6:6:58:GLU:HB3	6:6:116:MET:HE1	2.02	0.41
6:6:58:GLU:HG2	6:6:151:PRO:O	2.20	0.41
7:9:79:ALA:O	7:9:104:ARG:NH2	2.53	0.41
12:L:418:PHE:HD1	12:L:421:ILE:HD12	1.85	0.41
2:2:50:VAL:O	2:2:53:LEU:HB3	2.20	0.41
2:2:61:LEU:HD12	2:2:90:TYR:HB3	2.02	0.41
3:3:106:PRO:HD3	4:4:345:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:349:PHE:H	3:3:509:PRO:HB2	1.85	0.41
4:4:20:TYR:OH	14:N:295:ARG:NH2	2.54	0.41
8:A:13:LEU:HA	8:A:16:LEU:HB2	2.03	0.41
13:M:11:LEU:HB3	13:M:100:ILE:HD13	2.02	0.41
13:M:51:ASN:HA	13:M:57:PHE:HB2	2.02	0.41
13:M:281:ASP:OD2	13:M:284:SER:N	2.46	0.41
14:N:136:LEU:HD23	14:N:205:LEU:HD21	2.02	0.41
14:N:275:SER:HB3	15:V:136:ALA:HB3	2.03	0.41
15:V:139:LYS:HG3	15:V:140:VAL:HG13	2.03	0.41
3:3:324:ASP:HB3	3:3:571:ALA:HB1	2.03	0.41
9:H:58:LYS:HB3	9:H:217:ALA:HB3	2.02	0.41
12:L:290:MET:HA	12:L:293:LEU:HG	2.03	0.41
13:M:355:MET:HA	13:M:358:TRP:HD1	1.86	0.41
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.56	0.41
3:3:143:GLY:HA2	3:3:190:MET:HG3	2.02	0.40
4:4:151:ILE:O	4:4:155:THR:OG1	2.32	0.40
4:4:233:ARG:NH2	7:9:23:GLN:O	2.47	0.40
6:6:34:ASP:OD2	6:6:174:ARG:N	2.54	0.40
8:A:70:ALA:HB2	10:J:59:ILE:HD11	2.03	0.40
8:A:96:PHE:HE1	51:A:201:3PE:H3E2	1.87	0.40
10:J:39:VAL:HG12	51:J:201:3PE:H2C2	2.02	0.40
13:M:318:ALA:HB2	13:M:373:ILE:HG13	2.03	0.40
52:M:504:CDL:H311	52:M:504:CDL:H531	2.02	0.40
1:1:141:GLU:HG2	2:2:145:LEU:HD22	2.03	0.40
6:6:62:MET:SD	6:6:69:MET:HB3	2.62	0.40
8:A:94:LEU:HD23	8:A:94:LEU:HA	1.95	0.40
10:J:17:PHE:CD1	11:K:15:SER:HB3	2.57	0.40
10:J:49:GLY:HA2	10:J:139:GLU:HG2	2.03	0.40
12:L:502:LEU:HD23	12:L:502:LEU:HA	1.94	0.40
52:M:504:CDL:H832	52:M:504:CDL:H862	1.94	0.40
14:N:122:ILE:O	14:N:176:ARG:NH1	2.55	0.40
8:A:91:ALA:O	8:A:95:ILE:HD12	2.21	0.40
51:J:202:3PE:O14	12:L:585:LYS:NZ	2.48	0.40
12:L:149:ILE:HD13	12:L:149:ILE:HA	1.91	0.40
51:N:401:3PE:H352	51:N:401:3PE:H251	2.02	0.40
18:Y:166:LEU:HD12	18:Y:166:LEU:HA	1.93	0.40
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.47	0.40
4:4:115:GLU:HB3	4:4:194:VAL:HB	2.03	0.40
4:4:359:PRO:HA	4:4:360:PRO:HD3	1.89	0.40
12:L:193:LEU:HB3	12:L:195:THR:HG22	2.03	0.40
12:L:419:THR:HA	12:L:422:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:113:ALA:O	15:V:117:MET:HB2	2.21	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	1	428/464 (92%)	407 (95%)	21 (5%)	0	100	100
2	2	211/246 (86%)	194 (92%)	17 (8%)	0	100	100
3	3	686/727 (94%)	656 (96%)	30 (4%)	0	100	100
4	4	427/463 (92%)	402 (94%)	25 (6%)	0	100	100
5	5	206/266 (77%)	190 (92%)	16 (8%)	0	100	100
6	6	154/223 (69%)	145 (94%)	9 (6%)	0	100	100
7	9	174/217 (80%)	163 (94%)	11 (6%)	0	100	100
8	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
9	H	316/318 (99%)	301 (95%)	15 (5%)	0	100	100
10	J	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	22	50
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	575 (95%)	29 (5%)	0	100	100
13	M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
16	W	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
17	X	85/157 (54%)	80 (94%)	5 (6%)	0	100	100
17	j	80/157 (51%)	75 (94%)	5 (6%)	0	100	100
18	Y	169/172 (98%)	161 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	93 (100%)	0	0	100	100
22	c	124/170 (73%)	120 (97%)	4 (3%)	0	100	100
23	d	338/380 (89%)	319 (94%)	18 (5%)	1 (0%)	37	66
24	e	84/99 (85%)	80 (95%)	4 (5%)	0	100	100
25	f	111/116 (96%)	105 (95%)	6 (5%)	0	100	100
26	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
27	h	92/114 (81%)	86 (94%)	6 (6%)	0	100	100
28	i	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
29	k	317/355 (89%)	301 (95%)	16 (5%)	0	100	100
30	l	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
31	m	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
32	n	77/98 (79%)	72 (94%)	5 (6%)	0	100	100
33	o	118/122 (97%)	115 (98%)	3 (2%)	0	100	100
34	p	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
35	q	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
36	r	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
37	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
38	t	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
39	u	63/108 (58%)	60 (95%)	3 (5%)	0	100	100
40	v	153/186 (82%)	146 (95%)	7 (5%)	0	100	100
41	w	99/154 (64%)	92 (93%)	7 (7%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	45 (94%)	3 (6%)	0	100	100
44	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	8131/9247 (88%)	7761 (95%)	368 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	116	VAL
23	d	323	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 95
2	2	183/210 (87%)	182 (100%)	1 (0%)	86 91
3	3	578/608 (95%)	576 (100%)	2 (0%)	91 95
4	4	370/391 (95%)	368 (100%)	2 (0%)	86 91
5	5	189/230 (82%)	189 (100%)	0	100 100
6	6	132/181 (73%)	131 (99%)	1 (1%)	79 87
7	9	151/179 (84%)	151 (100%)	0	100 100
8	A	103/103 (100%)	103 (100%)	0	100 100
9	H	278/278 (100%)	276 (99%)	2 (1%)	81 88
10	J	144/144 (100%)	143 (99%)	1 (1%)	81 88
11	K	86/86 (100%)	85 (99%)	1 (1%)	67 80
12	L	538/538 (100%)	535 (99%)	3 (1%)	84 90
13	M	411/411 (100%)	410 (100%)	1 (0%)	92 96
14	N	315/315 (100%)	314 (100%)	1 (0%)	91 95
15	V	101/102 (99%)	101 (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%)	153 (99%)	1 (1%)	84 90
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	294/326 (90%)	293 (100%)	1 (0%)	91 95
24	e	76/82 (93%)	76 (100%)	0	100 100
25	f	101/102 (99%)	101 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	130 (99%)	1 (1%)	79	87
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%)	68 (99%)	1 (1%)	62	77
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	87
36	r	95/122 (78%)	95 (100%)	0	100	100
37	s	110/120 (92%)	109 (99%)	1 (1%)	75	86
38	t	159/161 (99%)	158 (99%)	1 (1%)	84	90
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%)	92 (100%)	0	100	100
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	7189/7955 (90%)	7166 (100%)	23 (0%)	90	95

All (23) 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	252	ASN
4	4	430	ARG
6	6	111	ARG
9	H	193	THR
9	H	274	ARG
10	J	86	ASN
11	K	50	ASN

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Mol	Chain	Res	Type
12	L	135	ASN
12	L	270	ASN
12	L	541	ASN
13	M	138	ASN
14	N	235	ASN
18	Y	63	ASN
23	d	36	ASN
28	i	133	LYS
31	m	82	ARG
35	q	67	ARG
37	s	103	ARG
38	t	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	257	ASN
1	1	356	HIS
1	1	373	ASN
2	2	9	HIS
2	2	99	HIS
3	3	237	ASN
4	4	149	ASN
4	4	252	ASN
6	6	82	GLN
8	A	108	GLN
9	H	230	ASN
10	J	86	ASN
11	K	83	ASN
12	L	405	ASN
12	L	546	GLN
13	M	26	ASN
19	Z	55	HIS
23	d	87	HIS
23	d	180	ASN
23	d	184	ASN
23	d	288	HIS
26	g	125	HIS
29	k	107	GLN
31	m	70	GLN
33	o	61	GLN

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Mol	Chain	Res	Type
34	p	74	ASN
38	t	138	GLN
39	u	21	GLN
43	y	13	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

7 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	$\#\|Z\|>2$
11	FME	K	1	11	8,9,10	0.96	0	7,9,11	0.76	0
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.86	0
13	FME	M	1	13	8,9,10	0.92	0	7,9,11	0.97	0
15	AYA	V	1	15	6,7,8	1.18	1 (16%)	5,8,10	2.01	2 (40%)
27	AYA	h	1	27	6,7,8	1.28	1 (16%)	5,8,10	1.43	1 (20%)
4	2MR	4	85	4	10,12,13	2.34	3 (30%)	5,13,15	1.33	0
29	SEP	k	36	29	8,9,10	1.53	1 (12%)	8,12,14	1.62	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
11	FME	K	1	11	-	2/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
13	FME	M	1	13	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	AYA	V	1	15	-	2/4/6/8	-
27	AYA	h	1	27	-	0/4/6/8	-
4	2MR	4	85	4	-	0/10/13/15	-
29	SEP	k	36	29	-	4/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	4.76	1.44	1.34
4	4	85	2MR	CZ-NH2	4.68	1.43	1.33
29	k	36	SEP	P-O1P	3.36	1.61	1.50
27	h	1	AYA	CA-N	-2.55	1.43	1.46
15	V	1	AYA	CA-N	-2.19	1.44	1.46
4	4	85	2MR	CQ1-NH1	-2.15	1.42	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	k	36	SEP	P-OG-CB	-3.17	109.57	118.30
27	h	1	AYA	CB-CA-N	3.09	113.04	109.61
15	V	1	AYA	CB-CA-N	2.99	112.93	109.61
29	k	36	SEP	OG-CB-CA	2.81	110.88	108.14
15	V	1	AYA	CA-N-CT	2.75	125.51	121.52

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	C-CA-CB-CG
13	M	1	FME	O-C-CA-CB
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
15	V	1	AYA	OT-CT-N-CA
15	V	1	AYA	CM-CT-N-CA
11	K	1	FME	CA-CB-CG-SD
29	k	36	SEP	CB-OG-P-O1P
12	L	1	FME	N-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
29	k	36	SEP	CA-CB-OG-P
13	M	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
13	M	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
15	V	1	AYA	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 2 are monoatomic - leaving 41 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	$\#\|Z\| > 2$
51	3PE	N	401	-	50,50,50	0.33	0	53,55,55	0.58	2 (3%)
52	CDL	z	101	-	57,57,99	0.34	0	63,69,111	0.28	0
55	NDP	d	401	-	45,52,52	0.55	0	53,80,80	0.57	1 (1%)
51	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.36	0
51	3PE	J	201	-	50,50,50	0.31	0	53,55,55	0.32	0
52	CDL	L	706	-	99,99,99	0.26	0	105,111,111	0.31	0
51	3PE	A	201	-	50,50,50	0.30	0	53,55,55	0.34	0
52	CDL	L	705	-	84,84,99	0.28	0	90,96,111	0.31	0
51	3PE	o	501	-	30,30,50	0.37	0	33,35,55	0.37	0
51	3PE	L	701	-	39,39,50	0.33	0	42,44,55	0.30	0
45	SF4	9	403	7	0,12,12	-	-	-		
51	3PE	i	201	-	50,50,50	0.29	0	53,55,55	0.31	0
56	AMP	k	501	-	22,25,25	0.91	1 (4%)	25,38,38	1.21	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	3PE	L	703	-	30,30,50	0.41	0	33,35,55	0.70	1 (3%)
50	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.36	0
50	PC1	9	401	-	53,53,53	0.30	0	59,61,61	0.50	1 (1%)
51	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.34	0
52	CDL	x	101	-	74,74,99	0.31	0	80,86,111	0.41	1 (1%)
52	CDL	V	203	-	93,93,99	0.27	0	99,105,111	0.23	0
45	SF4	9	402	7	0,12,12	-	-	-		
53	ZMP	X	101	17	24,30,36	0.81	1 (4%)	29,37,45	1.01	2 (6%)
57	MYR	s	201	37	14,14,15	0.23	0	13,13,15	0.20	0
45	SF4	1	501	1	0,12,12	-	-	-		
50	PC1	L	704	-	53,53,53	0.31	0	59,61,61	0.59	2 (3%)
53	ZMP	g	201	-	27,33,36	0.67	1 (3%)	32,40,45	1.12	3 (9%)
52	CDL	W	201	-	99,99,99	0.26	0	105,111,111	0.30	0
48	FES	3	803	3	0,4,4	-	-	-		
52	CDL	M	503	-	99,99,99	0.26	0	105,111,111	0.33	0
50	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.33	0
48	FES	2	300	2	0,4,4	-	-	-		
51	3PE	M	501	-	43,43,50	0.33	0	46,48,55	0.36	0
51	3PE	6	203	-	50,50,50	0.31	0	53,55,55	0.32	0
50	PC1	M	502	-	53,53,53	0.30	0	59,61,61	0.35	0
51	3PE	V	201	-	26,26,50	0.47	0	30,31,55	0.56	1 (3%)
47	NAI	1	503	-	42,48,48	0.56	0	47,73,73	2.02	4 (8%)
45	SF4	3	801	3	0,12,12	-	-	-		
51	3PE	J	202	-	39,39,50	0.36	0	42,44,55	0.35	0
52	CDL	M	504	-	89,89,99	0.29	0	95,101,111	0.41	0
45	SF4	6	201	6	0,12,12	-	-	-		
45	SF4	3	802	3	0,12,12	-	-	-		
46	FMN	1	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.23	7 (14%)

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
51	3PE	N	401	-	-	19/54/54/54	-
52	CDL	z	101	-	-	14/68/68/110	-
55	NDP	d	401	-	-	8/30/77/77	0/5/5/5
51	3PE	L	702	-	-	11/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	J	201	-	-	13/54/54/54	-
52	CDL	L	706	-	1/1/9/9	36/110/110/110	-
51	3PE	A	201	-	-	12/54/54/54	-
52	CDL	L	705	-	1/1/9/9	24/95/95/110	-
51	3PE	o	501	-	-	8/34/34/54	-
51	3PE	L	701	-	-	8/43/43/54	-
51	3PE	i	201	-	-	9/54/54/54	-
56	AMP	k	501	-	-	2/6/26/26	0/3/3/3
45	SF4	9	403	7	-	-	0/6/5/5
51	3PE	L	703	-	-	9/34/34/54	-
50	PC1	w	801	-	-	12/57/57/57	-
50	PC1	9	401	-	-	15/57/57/57	-
52	CDL	x	101	-	2/2/9/9	22/85/85/110	-
51	3PE	V	202	-	-	16/40/40/54	-
52	CDL	V	203	-	-	20/104/104/110	-
57	MYR	s	201	37	-	2/11/12/13	-
53	ZMP	X	101	17	-	9/35/37/43	-
45	SF4	9	402	7	-	-	0/6/5/5
50	PC1	L	704	-	-	16/57/57/57	-
45	SF4	1	501	1	-	-	0/6/5/5
53	ZMP	g	201	-	-	9/38/40/43	-
52	CDL	W	201	-	-	31/110/110/110	-
48	FES	3	803	3	-	-	0/1/1/1
52	CDL	M	503	-	1/1/9/9	28/110/110/110	-
50	PC1	6	202	-	-	13/49/49/57	-
48	FES	2	300	2	-	-	0/1/1/1
51	3PE	M	501	-	-	8/47/47/54	-
51	3PE	6	203	-	-	13/54/54/54	-
50	PC1	M	502	-	-	23/57/57/57	-
51	3PE	V	201	-	-	5/27/27/54	-
47	NAI	1	503	-	-	9/25/72/72	0/5/5/5
51	3PE	J	202	-	-	14/43/43/54	-
45	SF4	3	801	3	-	-	0/6/5/5
52	CDL	M	504	-	-	31/100/100/110	-
45	SF4	6	201	6	-	-	0/6/5/5
45	SF4	3	802	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	1	502	-	-	10/18/18/18	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	502	FMN	C4A-N5	3.23	1.37	1.30
53	X	101	ZMP	C9-C10	2.81	1.53	1.50
56	k	501	AMP	C5-C4	2.39	1.47	1.40
46	1	502	FMN	C10-N1	2.28	1.37	1.33
53	g	201	ZMP	C9-C10	2.03	1.52	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	1	503	NAI	O5B-PA-O1A	-10.02	69.91	109.07
47	1	503	NAI	O2A-PA-O1A	-8.26	71.42	112.24
56	k	501	AMP	N3-C2-N1	-3.39	123.37	128.68
46	1	502	FMN	C4-N3-C2	-3.20	119.72	125.64
47	1	503	NAI	O2A-PA-O5B	2.79	120.72	107.75
53	g	201	ZMP	C15-C14-C13	-2.79	107.70	112.36
46	1	502	FMN	C4A-C10-N10	2.78	120.55	116.48
46	1	502	FMN	O4-C4-C4A	-2.73	119.36	126.60
53	X	101	ZMP	O1-C10-C9	-2.72	120.78	123.99
53	g	201	ZMP	O1-C10-C9	-2.71	120.79	123.99
46	1	502	FMN	C4A-C4-N3	2.69	120.02	113.19
50	L	704	PC1	C2-O21-C21	2.64	124.29	117.79
46	1	502	FMN	C4A-C10-N1	-2.41	119.13	124.73
53	g	201	ZMP	C14-C15-N2	-2.37	107.12	111.90
51	N	401	3PE	C2-O21-C21	2.36	123.60	117.79
51	L	703	3PE	C2-O21-C21	2.31	123.48	117.79
47	1	503	NAI	C5A-C6A-N6A	2.30	123.85	120.35
55	d	401	NDP	C5A-C6A-N6A	2.25	123.78	120.35
51	V	201	3PE	O12-P-O14	2.17	119.17	110.68
53	X	101	ZMP	C9-C10-S1	2.16	115.97	113.46
50	L	704	PC1	O21-C2-C1	2.14	116.15	108.40
56	k	501	AMP	C4-C5-N7	-2.12	107.19	109.40
52	x	101	CDL	CB4-OB6-CB5	2.10	122.95	117.79
46	1	502	FMN	C4-C4A-C10	2.07	120.28	116.79
46	1	502	FMN	C10-C4A-N5	-2.05	120.51	124.86
50	9	401	PC1	O21-C2-C1	2.03	115.75	108.40
51	N	401	3PE	O21-C2-C3	2.02	115.72	108.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	L	705	CDL	CB4
52	L	706	CDL	CB4
52	M	503	CDL	CB4
52	x	101	CDL	CA4
52	x	101	CDL	CB4

All (479) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
47	1	503	NAI	C5B-O5B-PA-O2A
50	6	202	PC1	C11-O13-P-O12
50	6	202	PC1	C1-O11-P-O14
50	9	401	PC1	C11-O13-P-O12
50	9	401	PC1	C11-O13-P-O14
50	L	704	PC1	C11-O13-P-O14
50	L	704	PC1	C1-O11-P-O12
50	L	704	PC1	O13-C11-C12-N
50	M	502	PC1	C11-O13-P-O12
50	M	502	PC1	C11-O13-P-O14
50	M	502	PC1	C11-O13-P-O11
50	M	502	PC1	C1-O11-P-O12
50	w	801	PC1	C11-O13-P-O11
51	6	203	3PE	C1-O11-P-O12
51	6	203	3PE	O13-C11-C12-N
51	A	201	3PE	C1-O11-P-O12
51	A	201	3PE	C11-O13-P-O11
51	A	201	3PE	C11-O13-P-O14
51	J	202	3PE	C1-O11-P-O13
51	J	202	3PE	C1-O11-P-O14
51	L	701	3PE	C11-O13-P-O11
51	L	701	3PE	C11-O13-P-O14
51	L	701	3PE	O13-C11-C12-N
51	L	702	3PE	O13-C11-C12-N
51	L	703	3PE	C11-O13-P-O12
51	L	703	3PE	C2-C1-O11-P
51	L	703	3PE	O13-C11-C12-N
51	N	401	3PE	C1-O11-P-O12
51	N	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
51	N	401	3PE	C1-O11-P-O14
51	N	401	3PE	C11-O13-P-O11
51	N	401	3PE	C11-O13-P-O14
51	N	401	3PE	O13-C11-C12-N
51	V	201	3PE	C1-O11-P-O14
51	V	202	3PE	C11-O13-P-O11
51	V	202	3PE	C11-O13-P-O12
51	V	202	3PE	C11-O13-P-O14
51	V	202	3PE	C2-C1-O11-P
51	V	202	3PE	O13-C11-C12-N
51	i	201	3PE	C11-O13-P-O14
51	o	501	3PE	C11-O13-P-O11
51	o	501	3PE	C11-O13-P-O12
51	o	501	3PE	C11-O13-P-O14
51	o	501	3PE	O13-C11-C12-N
52	L	705	CDL	CA2-C1-CB2-OB2
52	L	706	CDL	CA3-OA5-PA1-OA2
52	L	706	CDL	CA3-OA5-PA1-OA3
52	L	706	CDL	CA3-OA5-PA1-OA4
52	L	706	CDL	CB2-OB2-PB2-OB4
52	L	706	CDL	CB2-OB2-PB2-OB5
52	M	503	CDL	CA3-OA5-PA1-OA3
52	M	503	CDL	CA3-OA5-PA1-OA4
52	M	504	CDL	CA2-OA2-PA1-OA3
52	M	504	CDL	CA2-OA2-PA1-OA4
52	M	504	CDL	CA2-OA2-PA1-OA5
52	M	504	CDL	CA3-OA5-PA1-OA3
52	M	504	CDL	CB2-OB2-PB2-OB3
52	M	504	CDL	CB2-OB2-PB2-OB4
52	M	504	CDL	CB2-OB2-PB2-OB5
52	V	203	CDL	CA3-OA5-PA1-OA3
52	W	201	CDL	CA3-OA5-PA1-OA3
52	W	201	CDL	CA3-OA5-PA1-OA4
52	W	201	CDL	CB2-OB2-PB2-OB3
52	W	201	CDL	CB2-OB2-PB2-OB4
52	W	201	CDL	CB2-OB2-PB2-OB5
52	W	201	CDL	CB3-OB5-PB2-OB4
52	W	201	CDL	OB5-CB3-CB4-OB6
52	x	101	CDL	CA3-OA5-PA1-OA3
52	z	101	CDL	CA2-C1-CB2-OB2
52	z	101	CDL	CB3-OB5-PB2-OB2
52	z	101	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
52	z	101	CDL	CB3-OB5-PB2-OB4
53	X	101	ZMP	C16-C17-C18-C21
53	X	101	ZMP	C17-C16-N2-C15
53	g	201	ZMP	S1-C11-C12-N1
53	g	201	ZMP	C7-C8-C9-C10
52	L	705	CDL	O1-C1-CB2-OB2
52	M	504	CDL	O1-C1-CB2-OB2
52	z	101	CDL	O1-C1-CB2-OB2
53	X	101	ZMP	O3-C16-N2-C15
50	L	704	PC1	C2-C1-O11-P
52	x	101	CDL	CA4-CA3-OA5-PA1
52	L	706	CDL	CA2-C1-CB2-OB2
50	M	502	PC1	C11-C12-N-C14
52	x	101	CDL	O1-C1-CA2-OA2
52	M	504	CDL	CB5-C51-C52-C53
50	M	502	PC1	C11-C12-N-C15
50	L	704	PC1	C31-C32-C33-C34
52	L	706	CDL	O1-C1-CB2-OB2
46	1	502	FMN	O3'-C3'-C4'-C5'
52	M	503	CDL	CB5-C51-C52-C53
50	6	202	PC1	C1-O11-P-O13
50	9	401	PC1	C11-O13-P-O11
51	A	201	3PE	C1-O11-P-O13
51	J	201	3PE	C1-O11-P-O13
51	J	201	3PE	C11-O13-P-O11
51	L	703	3PE	C1-O11-P-O13
51	M	501	3PE	C11-O13-P-O11
51	V	202	3PE	C1-O11-P-O13
52	L	705	CDL	CA3-OA5-PA1-OA2
52	M	503	CDL	CA2-OA2-PA1-OA5
52	M	503	CDL	CA3-OA5-PA1-OA2
52	M	504	CDL	CA3-OA5-PA1-OA2
52	M	504	CDL	CB3-OB5-PB2-OB2
52	V	203	CDL	CA3-OA5-PA1-OA2
52	W	201	CDL	CA3-OA5-PA1-OA2
52	W	201	CDL	CB3-OB5-PB2-OB2
52	x	101	CDL	CB3-OB5-PB2-OB2
47	1	503	NAI	C2D-C1D-N1N-C2N
50	L	704	PC1	C23-C24-C25-C26
52	L	706	CDL	C22-C23-C24-C25
52	M	503	CDL	C52-C53-C54-C55
52	M	504	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
52	M	504	CDL	C81-C82-C83-C84
52	L	706	CDL	C82-C83-C84-C85
52	W	201	CDL	C35-C36-C37-C38
52	L	706	CDL	C77-C78-C79-C80
51	A	201	3PE	C39-C3A-C3B-C3C
51	J	201	3PE	C38-C39-C3A-C3B
52	L	706	CDL	C56-C57-C58-C59
52	M	503	CDL	C63-C64-C65-C66
52	V	203	CDL	O1-C1-CB2-OB2
52	W	201	CDL	O1-C1-CA2-OA2
52	L	706	CDL	CB5-C51-C52-C53
51	6	203	3PE	C3C-C3D-C3E-C3F
52	M	503	CDL	C12-C13-C14-C15
52	V	203	CDL	C11-C12-C13-C14
50	6	202	PC1	C23-C24-C25-C26
52	W	201	CDL	CB5-C51-C52-C53
47	1	503	NAI	C2D-C1D-N1N-C6N
51	N	401	3PE	C37-C38-C39-C3A
52	L	706	CDL	C41-C42-C43-C44
50	9	401	PC1	C3C-C3D-C3E-C3F
50	L	704	PC1	C38-C39-C3A-C3B
51	A	201	3PE	C2C-C2D-C2E-C2F
51	i	201	3PE	C29-C2A-C2B-C2C
52	V	203	CDL	C39-C40-C41-C42
52	V	203	CDL	C79-C80-C81-C82
52	M	503	CDL	C35-C36-C37-C38
52	W	201	CDL	C82-C83-C84-C85
51	6	203	3PE	C36-C37-C38-C39
51	L	702	3PE	C3B-C3C-C3D-C3E
50	9	401	PC1	C2C-C2D-C2E-C2F
51	J	202	3PE	C26-C27-C28-C29
51	J	201	3PE	C31-C32-C33-C34
52	x	101	CDL	O1-C1-CB2-OB2
51	J	202	3PE	C33-C34-C35-C36
52	V	203	CDL	CA2-C1-CB2-OB2
51	J	202	3PE	C32-C33-C34-C35
52	M	503	CDL	C81-C82-C83-C84
52	L	705	CDL	CB7-C71-C72-C73
51	L	702	3PE	C35-C36-C37-C38
51	V	201	3PE	C21-C22-C23-C24
52	M	504	CDL	C53-C54-C55-C56
52	L	705	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
51	V	202	3PE	C21-C22-C23-C24
50	w	801	PC1	C2D-C2E-C2F-C2G
51	M	501	3PE	C39-C3A-C3B-C3C
52	L	706	CDL	C21-C22-C23-C24
50	6	202	PC1	C3B-C3C-C3D-C3E
52	W	201	CDL	CA5-C11-C12-C13
50	M	502	PC1	C25-C26-C27-C28
51	N	401	3PE	O21-C2-C3-O31
50	M	502	PC1	C11-C12-N-C13
51	A	201	3PE	C35-C36-C37-C38
51	L	702	3PE	C34-C35-C36-C37
52	M	504	CDL	C62-C63-C64-C65
46	1	502	FMN	C2'-C3'-C4'-O4'
50	6	202	PC1	C11-O13-P-O11
52	V	203	CDL	CA2-OA2-PA1-OA5
52	x	101	CDL	CA3-OA5-PA1-OA2
50	L	704	PC1	O11-C1-C2-C3
52	L	706	CDL	OB5-CB3-CB4-CB6
52	W	201	CDL	OA5-CA3-CA4-CA6
52	M	503	CDL	C11-C12-C13-C14
52	M	504	CDL	C71-C72-C73-C74
52	W	201	CDL	CB2-C1-CA2-OA2
51	N	401	3PE	C24-C25-C26-C27
51	N	401	3PE	C2B-C2C-C2D-C2E
51	6	203	3PE	C25-C26-C27-C28
51	J	202	3PE	C1-C2-C3-O31
52	L	706	CDL	CA3-CA4-CA6-OA8
52	M	504	CDL	CB3-CB4-CB6-OB8
52	V	203	CDL	CB3-CB4-CB6-OB8
52	x	101	CDL	C52-C51-CB5-OB6
52	x	101	CDL	C34-C35-C36-C37
46	1	502	FMN	O3'-C3'-C4'-O4'
52	L	705	CDL	C13-C14-C15-C16
46	1	502	FMN	C5'-O5'-P-O1P
51	A	201	3PE	C2D-C2E-C2F-C2G
52	M	503	CDL	C14-C15-C16-C17
51	V	202	3PE	O11-C1-C2-O21
51	V	202	3PE	C31-C32-C33-C34
52	M	503	CDL	C57-C58-C59-C60
53	g	201	ZMP	O4-C17-C18-C20
51	J	201	3PE	C24-C25-C26-C27
52	W	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
51	A	201	3PE	C2E-C2F-C2G-C2H
50	6	202	PC1	C22-C23-C24-C25
52	M	504	CDL	CA2-C1-CB2-OB2
57	s	201	MYR	C11-C10-C9-C8
50	M	502	PC1	C28-C29-C2A-C2B
52	M	504	CDL	OB5-CB3-CB4-CB6
52	W	201	CDL	OB5-CB3-CB4-CB6
52	L	705	CDL	C72-C71-CB7-OB8
50	M	502	PC1	C31-C32-C33-C34
51	J	202	3PE	C34-C35-C36-C37
52	V	203	CDL	CA5-C11-C12-C13
51	N	401	3PE	C1-C2-C3-O31
52	M	504	CDL	CA3-CA4-CA6-OA8
51	N	401	3PE	C27-C28-C29-C2A
50	L	704	PC1	O11-C1-C2-O21
52	z	101	CDL	OB5-CB3-CB4-OB6
50	9	401	PC1	C3B-C3C-C3D-C3E
50	6	202	PC1	C36-C37-C38-C39
51	J	201	3PE	O21-C2-C3-O31
52	L	706	CDL	OA6-CA4-CA6-OA8
52	M	503	CDL	OA6-CA4-CA6-OA8
52	M	504	CDL	OA6-CA4-CA6-OA8
52	V	203	CDL	OB6-CB4-CB6-OB8
50	M	502	PC1	O31-C31-C32-C33
52	x	101	CDL	C11-C12-C13-C14
52	L	705	CDL	C78-C79-C80-C81
52	L	705	CDL	C1-CA2-OA2-PA1
52	L	706	CDL	C1-CA2-OA2-PA1
52	M	504	CDL	C1-CA2-OA2-PA1
52	M	504	CDL	CA4-CA3-OA5-PA1
52	V	203	CDL	CA4-CA3-OA5-PA1
50	M	502	PC1	C2C-C2D-C2E-C2F
51	M	501	3PE	C31-C32-C33-C34
52	V	203	CDL	CA7-C31-C32-C33
50	M	502	PC1	C2B-C2C-C2D-C2E
47	1	503	NAI	PN-O3-PA-O5B
51	V	202	3PE	O11-C1-C2-C3
46	1	502	FMN	C2'-C3'-C4'-C5'
52	M	503	CDL	CA3-CA4-CA6-OA8
52	z	101	CDL	C1-CB2-OB2-PB2
50	M	502	PC1	O11-C1-C2-O21
52	L	705	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
53	X	101	ZMP	C16-C17-C18-C20
51	N	401	3PE	C28-C29-C2A-C2B
51	J	202	3PE	O21-C2-C3-O31
47	1	503	NAI	C5B-O5B-PA-O3
55	d	401	NDP	C5D-O5D-PN-O3
52	W	201	CDL	CA7-C31-C32-C33
47	1	503	NAI	PA-O3-PN-O2N
50	w	801	PC1	C3E-C3F-C3G-C3H
47	1	503	NAI	O4D-C1D-N1N-C2N
47	1	503	NAI	O4D-C1D-N1N-C6N
50	L	704	PC1	C11-O13-P-O11
50	L	704	PC1	C1-O11-P-O13
51	6	203	3PE	C1-O11-P-O13
51	6	203	3PE	C11-O13-P-O11
51	i	201	3PE	C11-O13-P-O11
52	x	101	CDL	CA2-OA2-PA1-OA5
52	W	201	CDL	O1-C1-CB2-OB2
51	M	501	3PE	C2-C1-O11-P
52	L	706	CDL	CA4-CA3-OA5-PA1
52	z	101	CDL	CB4-CB3-OB5-PB2
50	6	202	PC1	C11-O13-P-O14
50	6	202	PC1	C1-O11-P-O12
50	L	704	PC1	C1-O11-P-O14
50	w	801	PC1	C11-O13-P-O12
51	6	203	3PE	C1-O11-P-O14
51	J	201	3PE	C1-O11-P-O14
51	J	201	3PE	C11-O13-P-O14
51	J	202	3PE	C11-O13-P-O14
51	L	703	3PE	C1-O11-P-O14
51	M	501	3PE	C11-O13-P-O14
51	V	202	3PE	C1-O11-P-O12
51	V	202	3PE	C1-O11-P-O14
51	i	201	3PE	C1-O11-P-O12
52	L	705	CDL	CA3-OA5-PA1-OA3
52	L	706	CDL	CB2-OB2-PB2-OB3
52	M	503	CDL	CA2-OA2-PA1-OA3
52	M	503	CDL	CA2-OA2-PA1-OA4
52	M	504	CDL	CB3-OB5-PB2-OB3
52	M	504	CDL	CB3-OB5-PB2-OB4
52	V	203	CDL	CA3-OA5-PA1-OA4
52	x	101	CDL	CA3-OA5-PA1-OA4
52	x	101	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
55	d	401	NDP	C5D-O5D-PN-O2N
50	M	502	PC1	O11-C1-C2-C3
51	L	702	3PE	O11-C1-C2-C3
52	z	101	CDL	OB5-CB3-CB4-CB6
53	X	101	ZMP	C2-C3-C4-C5
51	L	701	3PE	C31-C32-C33-C34
51	V	201	3PE	C22-C23-C24-C25
53	g	201	ZMP	C3-C4-C5-C6
51	o	501	3PE	C22-C23-C24-C25
50	M	502	PC1	C3A-C3B-C3C-C3D
51	6	203	3PE	O21-C21-C22-C23
51	V	202	3PE	C32-C33-C34-C35
52	V	203	CDL	C31-C32-C33-C34
50	w	801	PC1	O11-C1-C2-O21
50	w	801	PC1	C31-C32-C33-C34
51	L	702	3PE	O11-C1-C2-O21
52	L	705	CDL	OB5-CB3-CB4-OB6
52	L	706	CDL	OB5-CB3-CB4-OB6
52	V	203	CDL	OA5-CA3-CA4-OA6
52	W	201	CDL	OA5-CA3-CA4-OA6
51	J	202	3PE	C25-C26-C27-C28
50	9	401	PC1	C22-C21-O21-C2
50	9	401	PC1	O13-C11-C12-N
53	g	201	ZMP	O4-C17-C18-C21
50	M	502	PC1	C2-C1-O11-P
52	L	705	CDL	C34-C35-C36-C37
53	X	101	ZMP	O3-C16-C17-O4
50	M	502	PC1	C27-C28-C29-C2A
52	L	705	CDL	C73-C74-C75-C76
51	L	701	3PE	C21-C22-C23-C24
51	L	701	3PE	O31-C31-C32-C33
50	9	401	PC1	C3-C2-O21-C21
51	J	201	3PE	O11-C1-C2-C3
52	V	203	CDL	OA5-CA3-CA4-CA6
50	9	401	PC1	O22-C21-O21-C2
51	J	202	3PE	C21-C22-C23-C24
52	L	706	CDL	CB7-C71-C72-C73
52	W	201	CDL	C54-C55-C56-C57
51	V	201	3PE	C23-C24-C25-C26
52	L	705	CDL	OA6-CA4-CA6-OA8
51	o	501	3PE	C25-C26-C27-C28
52	M	503	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
52	x	101	CDL	CB2-OB2-PB2-OB5
52	z	101	CDL	CB2-OB2-PB2-OB5
53	g	201	ZMP	O4-C17-C18-C19
52	L	705	CDL	C71-C72-C73-C74
55	d	401	NDP	O4D-C1D-N1N-C6N
52	M	503	CDL	C59-C60-C61-C62
52	L	705	CDL	C51-C52-C53-C54
46	1	502	FMN	C4'-C5'-O5'-P
51	J	201	3PE	C2-C1-O11-P
50	M	502	PC1	C3B-C3C-C3D-C3E
51	A	201	3PE	C36-C37-C38-C39
52	W	201	CDL	CA2-C1-CB2-OB2
51	L	702	3PE	C26-C27-C28-C29
53	g	201	ZMP	C22-C1-C2-C3
52	z	101	CDL	C51-C52-C53-C54
52	L	706	CDL	C79-C80-C81-C82
52	L	705	CDL	C52-C53-C54-C55
52	M	504	CDL	C20-C21-C22-C23
52	M	504	CDL	CB4-CB3-OB5-PB2
52	x	101	CDL	C52-C51-CB5-OB7
52	M	504	CDL	C55-C56-C57-C58
52	V	203	CDL	C71-C72-C73-C74
52	W	201	CDL	C40-C41-C42-C43
50	L	704	PC1	C1-C2-O21-C21
50	6	202	PC1	C11-C12-N-C14
51	L	702	3PE	C23-C24-C25-C26
51	i	201	3PE	C2C-C2D-C2E-C2F
52	L	706	CDL	CB4-CB3-OB5-PB2
50	w	801	PC1	O11-C1-C2-C3
52	L	705	CDL	OA5-CA3-CA4-CA6
50	9	401	PC1	C37-C38-C39-C3A
51	6	203	3PE	C27-C28-C29-C2A
55	d	401	NDP	O4B-C4B-C5B-O5B
52	x	101	CDL	C33-C34-C35-C36
53	g	201	ZMP	C12-C11-S1-C10
52	L	706	CDL	C37-C38-C39-C40
52	x	101	CDL	CB2-C1-CA2-OA2
50	w	801	PC1	C26-C27-C28-C29
50	L	704	PC1	O31-C31-C32-C33
52	L	706	CDL	C32-C33-C34-C35
52	L	705	CDL	C72-C71-CB7-OB9
51	M	501	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
51	N	401	3PE	C23-C24-C25-C26
50	w	801	PC1	C39-C3A-C3B-C3C
52	M	503	CDL	C82-C83-C84-C85
52	M	503	CDL	C72-C71-CB7-OB8
52	L	706	CDL	C55-C56-C57-C58
55	d	401	NDP	C2B-O2B-P2B-O1X
51	A	201	3PE	O21-C21-C22-C23
51	i	201	3PE	O21-C21-C22-C23
52	x	101	CDL	C72-C71-CB7-OB8
55	d	401	NDP	C2D-C1D-N1N-C6N
52	V	203	CDL	C32-C33-C34-C35
53	X	101	ZMP	C5-C6-C7-C8
51	6	203	3PE	C33-C34-C35-C36
52	x	101	CDL	CB6-CB4-OB6-CB5
52	z	101	CDL	C52-C51-CB5-OB6
50	M	502	PC1	C3F-C3G-C3H-C3I
52	L	706	CDL	C72-C71-CB7-OB8
52	M	503	CDL	C12-C11-CA5-OA6
52	L	705	CDL	CA3-CA4-CA6-OA8
52	W	201	CDL	C15-C16-C17-C18
53	g	201	ZMP	C16-C17-C18-C20
51	N	401	3PE	O21-C21-C22-C23
52	L	705	CDL	OB5-CB3-CB4-CB6
51	V	202	3PE	C25-C26-C27-C28
52	W	201	CDL	C78-C79-C80-C81
50	w	801	PC1	O31-C31-C32-C33
51	N	401	3PE	C29-C2A-C2B-C2C
50	6	202	PC1	C11-C12-N-C15
55	d	401	NDP	C5B-O5B-PA-O3
55	d	401	NDP	C2B-O2B-P2B-O3X
52	M	503	CDL	C33-C34-C35-C36
52	L	706	CDL	C32-C31-CA7-OA8
52	L	705	CDL	C72-C73-C74-C75
51	L	702	3PE	C33-C34-C35-C36
50	L	704	PC1	C36-C37-C38-C39
52	L	706	CDL	C20-C21-C22-C23
51	i	201	3PE	O22-C21-C22-C23
56	k	501	AMP	O4'-C4'-C5'-O5'
51	M	501	3PE	O21-C21-C22-C23
51	A	201	3PE	O22-C21-C22-C23
52	x	101	CDL	C72-C71-CB7-OB9
52	x	101	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
52	L	706	CDL	C72-C71-CB7-OB9
51	N	401	3PE	C2D-C2E-C2F-C2G
52	M	503	CDL	C58-C59-C60-C61
52	M	504	CDL	C84-C85-C86-C87
51	J	201	3PE	C27-C28-C29-C2A
52	M	503	CDL	C12-C11-CA5-OA7
51	J	201	3PE	C1-C2-C3-O31
52	W	201	CDL	CA3-CA4-CA6-OA8
52	M	503	CDL	C62-C63-C64-C65
52	M	503	CDL	C72-C71-CB7-OB9
50	M	502	PC1	C36-C37-C38-C39
52	W	201	CDL	C22-C23-C24-C25
56	k	501	AMP	C4'-C5'-O5'-P
57	s	201	MYR	C3-C4-C5-C6
47	1	503	NAI	C2N-C3N-C7N-N7N
50	6	202	PC1	C11-C12-N-C13
50	L	704	PC1	C11-O13-P-O12
50	M	502	PC1	C1-O11-P-O14
51	6	203	3PE	C11-O13-P-O12
51	L	701	3PE	C1-O11-P-O14
51	L	703	3PE	C11-O13-P-O14
51	i	201	3PE	C1-O11-P-O14
52	L	706	CDL	CA2-OA2-PA1-OA3
52	W	201	CDL	CA2-OA2-PA1-OA3
52	x	101	CDL	CB3-OB5-PB2-OB3
52	z	101	CDL	CB2-OB2-PB2-OB3
50	M	502	PC1	O32-C31-C32-C33
50	w	801	PC1	O32-C31-C32-C33
51	J	202	3PE	O11-C1-C2-C3
52	L	706	CDL	C35-C36-C37-C38
51	J	202	3PE	O31-C31-C32-C33
52	M	503	CDL	C32-C31-CA7-OA8
52	L	706	CDL	C39-C40-C41-C42
53	X	101	ZMP	C6-C7-C8-C9
51	N	401	3PE	O22-C21-C22-C23
51	V	202	3PE	C27-C28-C29-C2A
52	W	201	CDL	C53-C54-C55-C56
52	V	203	CDL	C19-C20-C21-C22
51	J	201	3PE	C12-C11-O13-P
51	J	202	3PE	C12-C11-O13-P
51	L	703	3PE	C12-C11-O13-P
51	N	401	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
52	z	101	CDL	C52-C51-CB5-OB7
50	9	401	PC1	C34-C35-C36-C37
51	L	703	3PE	O21-C21-C22-C23
51	V	201	3PE	O21-C21-C22-C23
51	L	701	3PE	C23-C24-C25-C26
50	w	801	PC1	C11-C12-N-C14
50	9	401	PC1	O31-C31-C32-C33
51	L	702	3PE	O21-C21-C22-C23
51	o	501	3PE	O31-C31-C32-C33
52	M	504	CDL	C32-C31-CA7-OA8
51	V	202	3PE	O21-C21-C22-C23
52	x	101	CDL	CA2-C1-CB2-OB2
51	6	203	3PE	C2D-C2E-C2F-C2G
52	L	706	CDL	C32-C31-CA7-OA9
52	L	706	CDL	C11-C12-C13-C14
50	9	401	PC1	C2D-C2E-C2F-C2G
51	L	703	3PE	O22-C21-C22-C23
51	i	201	3PE	O31-C31-C32-C33
51	M	501	3PE	O22-C21-C22-C23
52	L	705	CDL	C32-C31-CA7-OA8
52	W	201	CDL	C12-C11-CA5-OA6
53	X	101	ZMP	C3-C4-C5-C6
51	L	702	3PE	O22-C21-C22-C23
50	9	401	PC1	O32-C31-C32-C33
51	o	501	3PE	O32-C31-C32-C33
52	M	504	CDL	C32-C31-CA7-OA9

There are no ring outliers.

24 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	N	401	3PE	2	0
51	J	201	3PE	4	0
52	L	706	CDL	5	0
51	A	201	3PE	4	0
52	L	705	CDL	8	0
51	L	701	3PE	1	0
50	9	401	PC1	1	0
51	V	202	3PE	3	0
52	V	203	CDL	9	0
45	1	501	SF4	1	0
50	L	704	PC1	2	0

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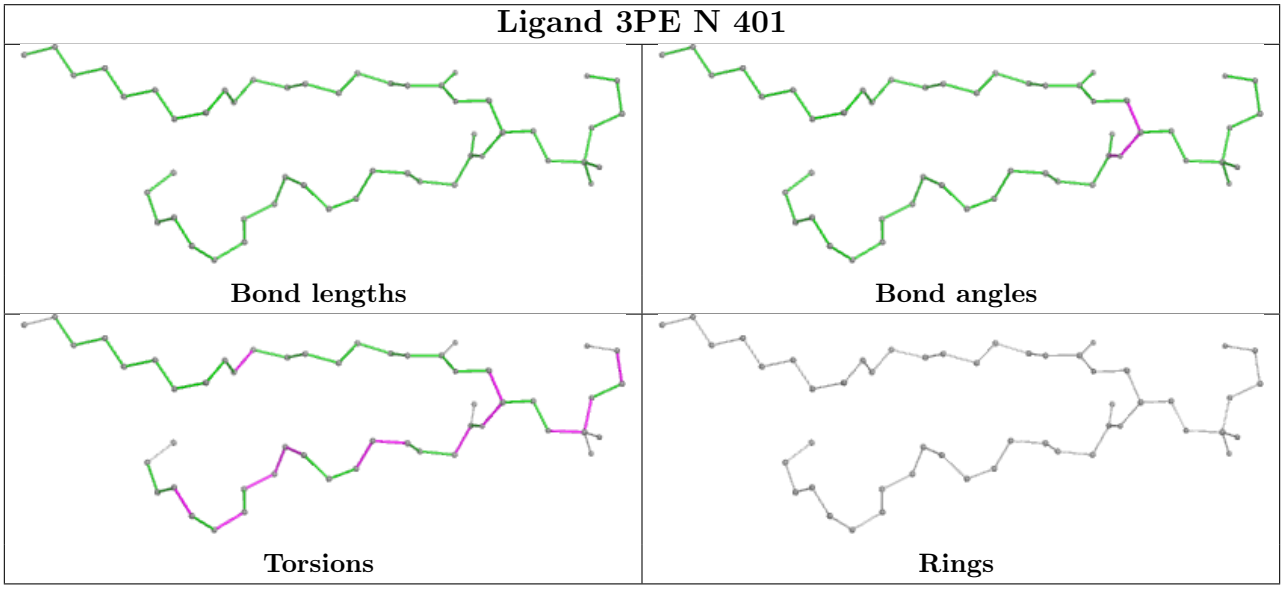
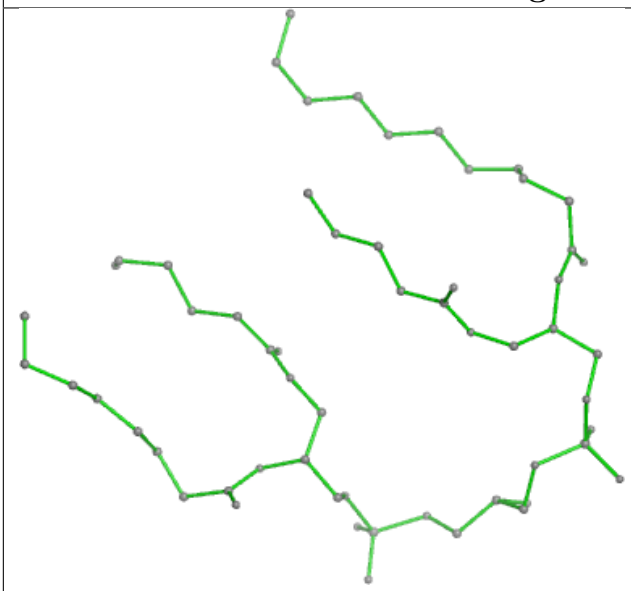
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	W	201	CDL	3	0
52	M	503	CDL	5	0
50	6	202	PC1	1	0
48	2	300	FES	1	0
51	M	501	3PE	1	0
51	6	203	3PE	4	0
50	M	502	PC1	2	0
47	1	503	NAI	5	0
45	3	801	SF4	2	0
51	J	202	3PE	2	0
52	M	504	CDL	9	0
45	6	201	SF4	1	0
46	1	502	FMN	1	0

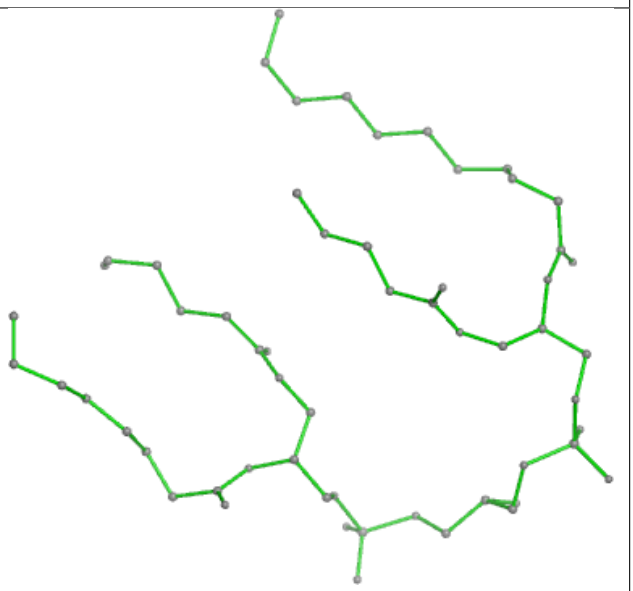
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



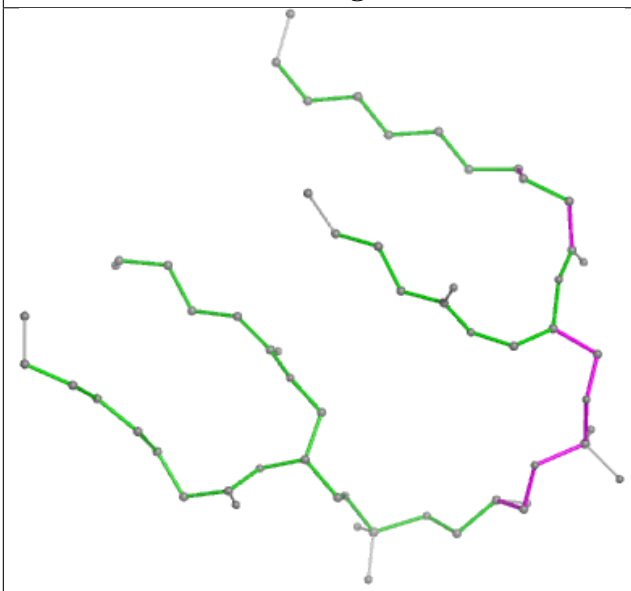
Ligand CDL z 101



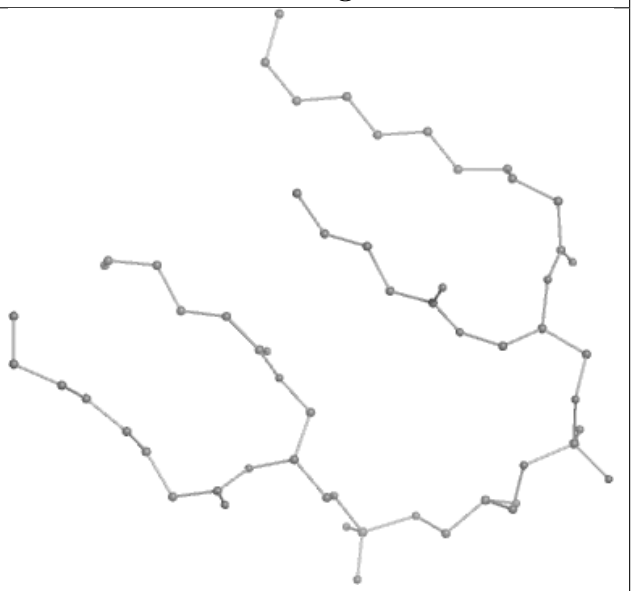
Bond lengths



Bond angles

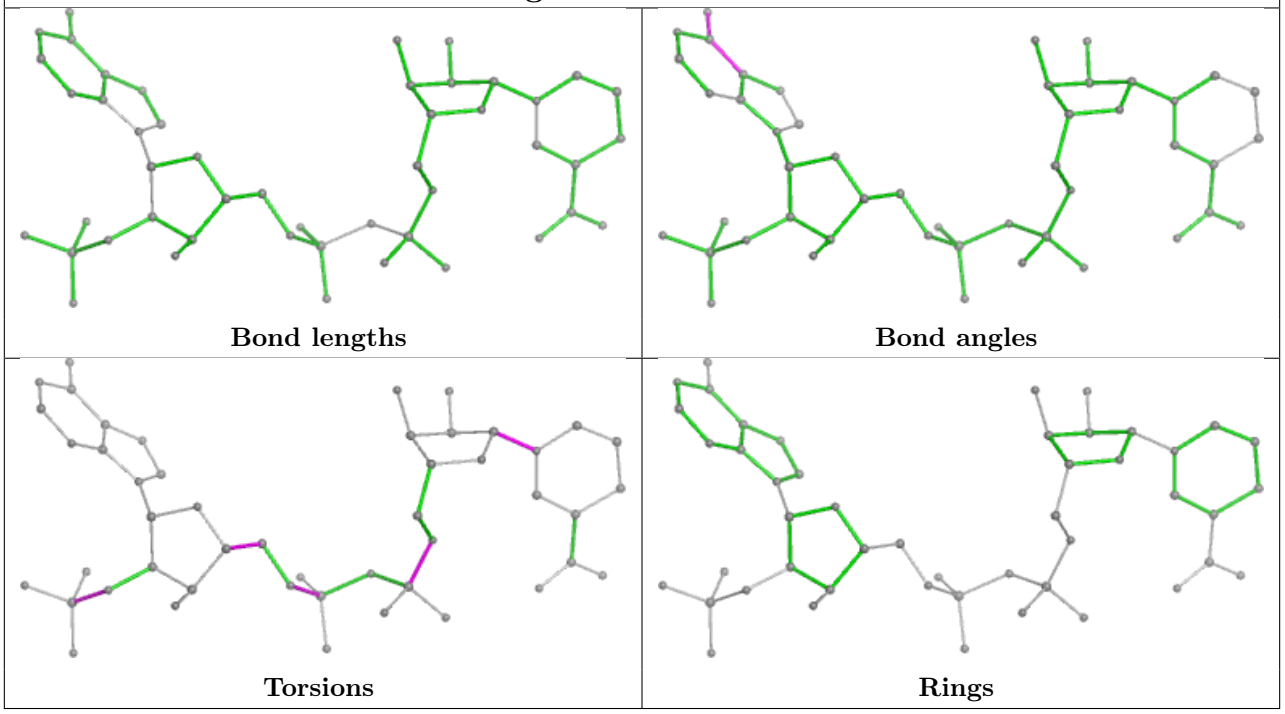


Torsions

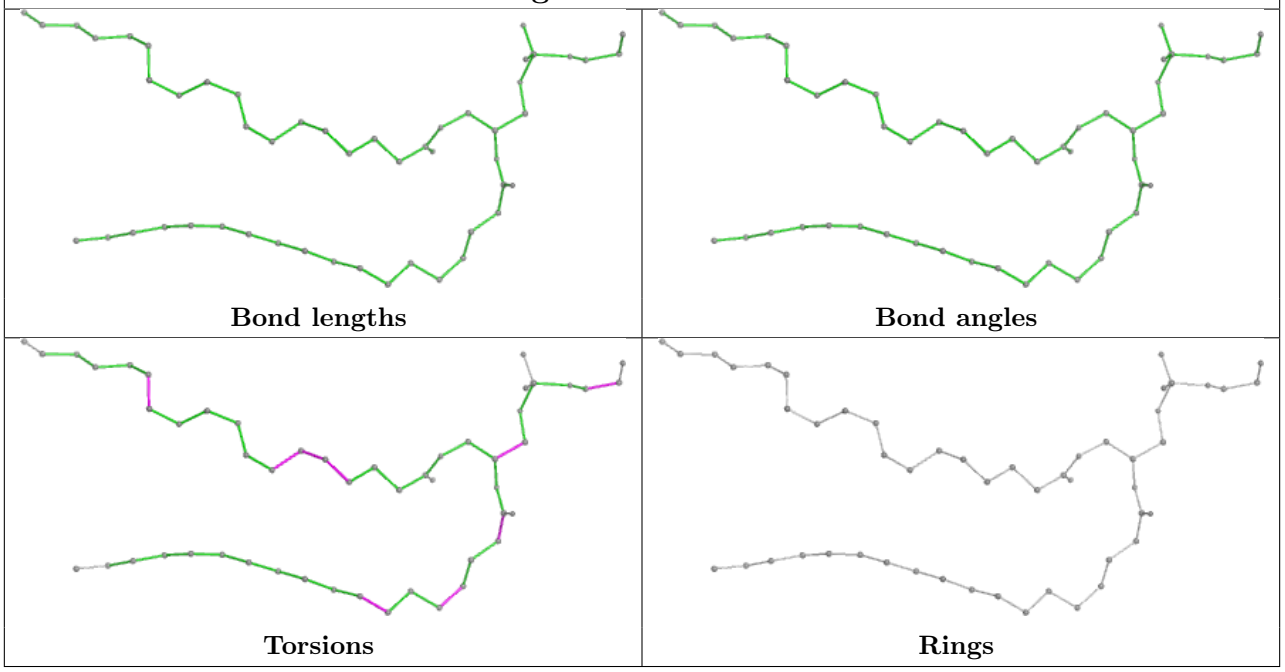


Rings

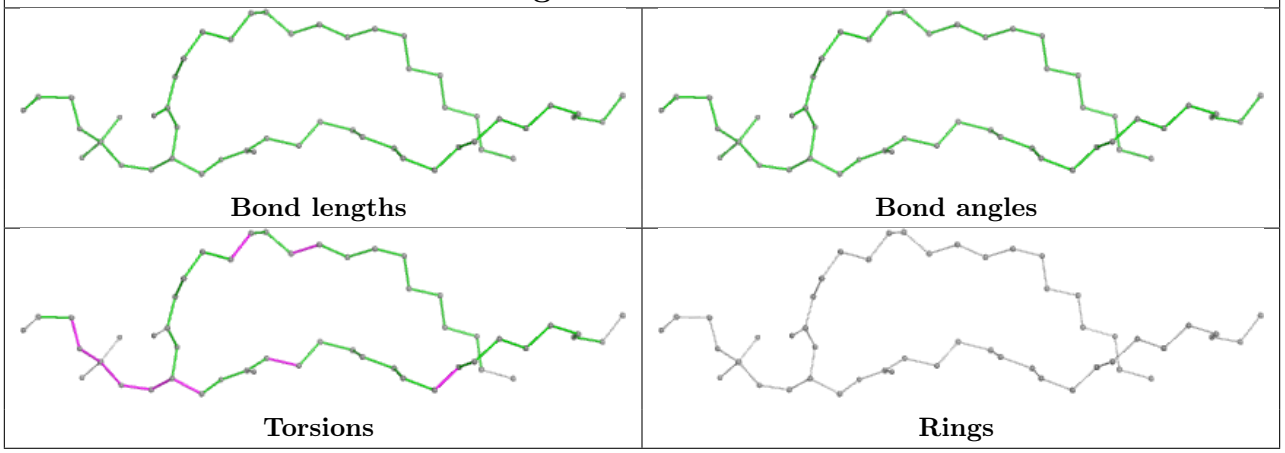
Ligand NDP d 401



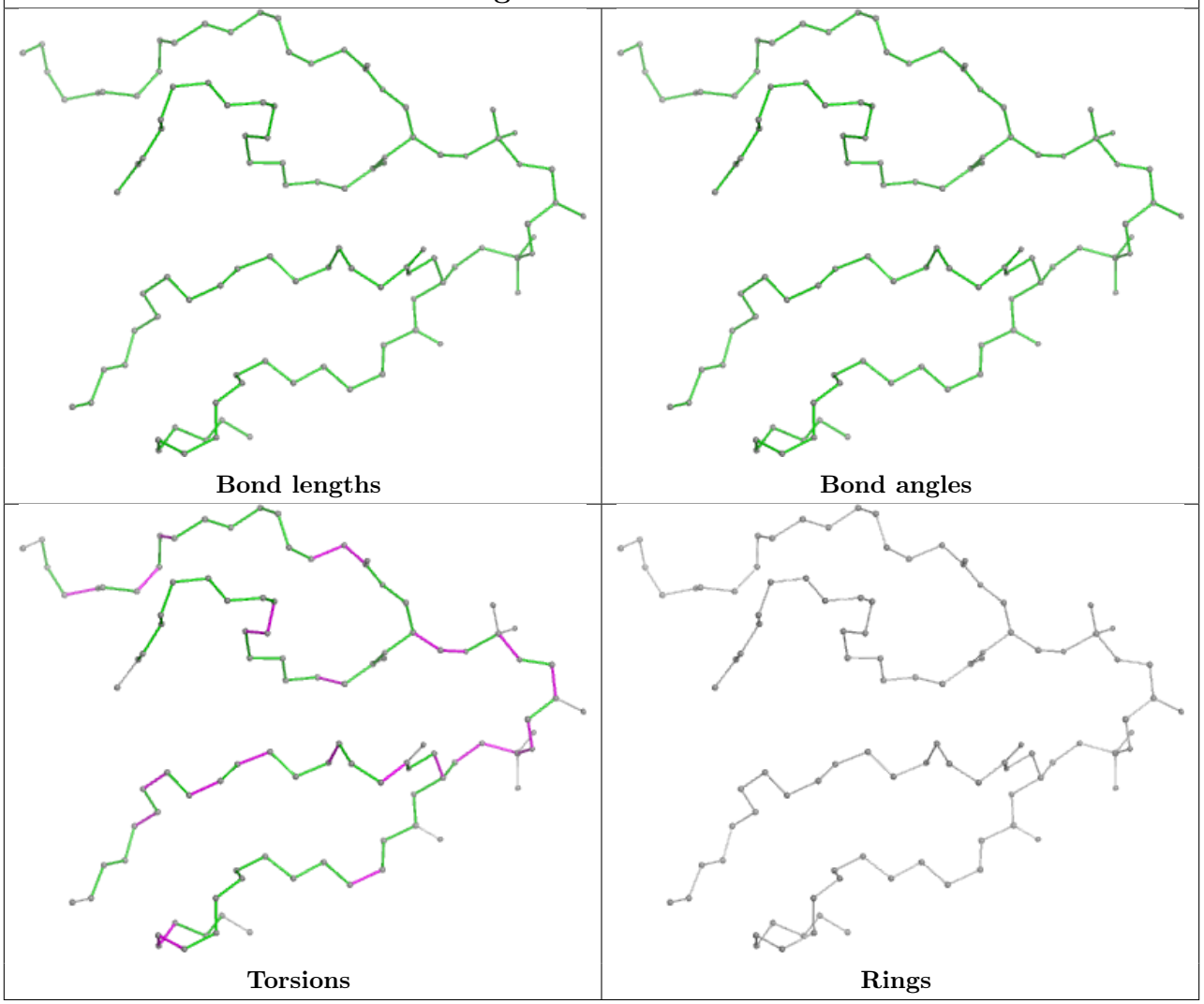
Ligand 3PE L 702



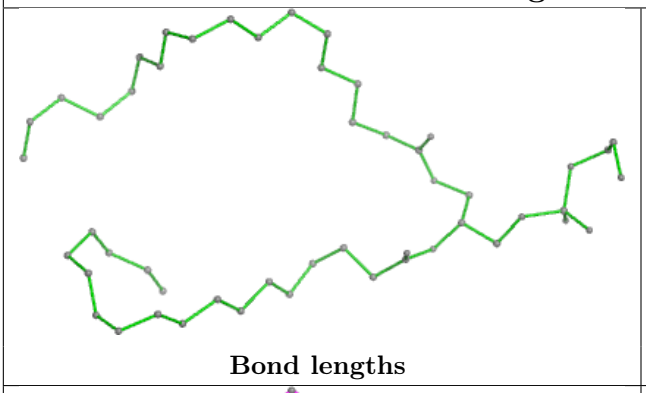
Ligand 3PE J 201



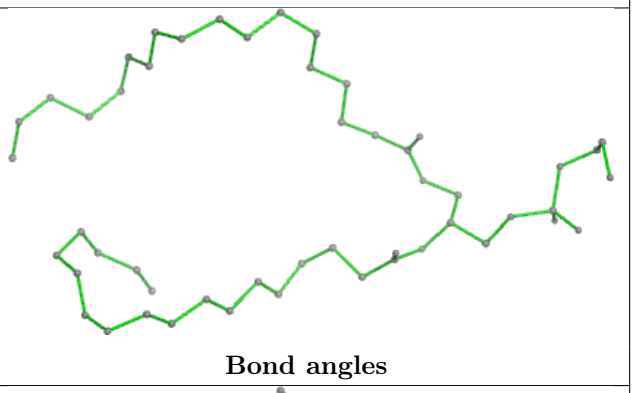
Ligand CDL L 706



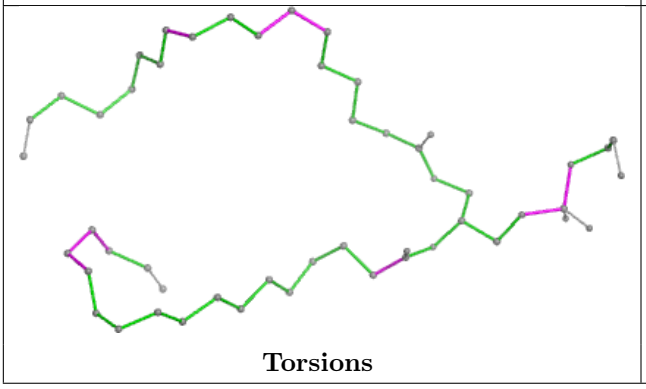
Ligand 3PE A 201



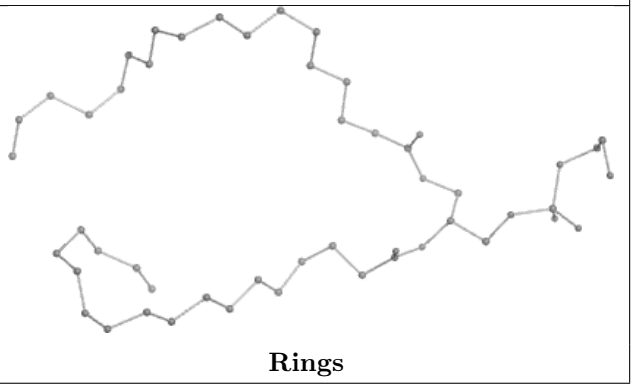
Bond lengths



Bond angles

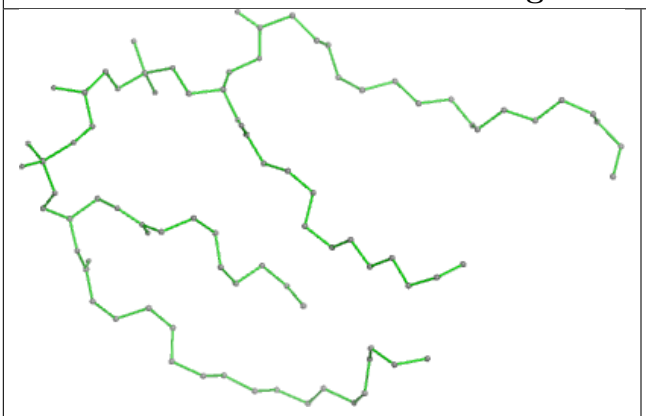


Torsions

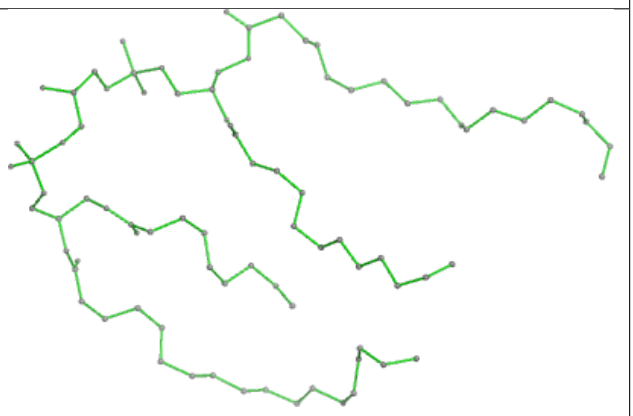


Rings

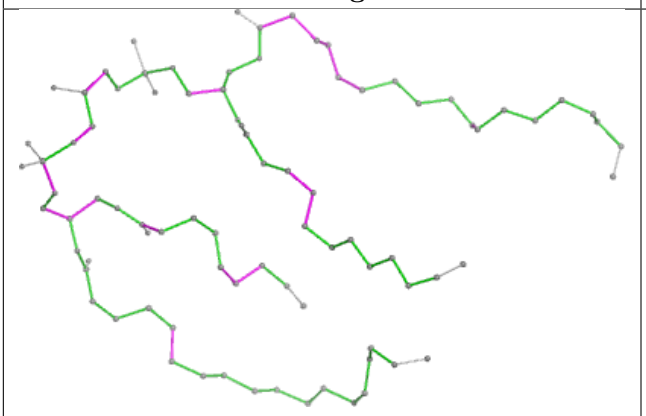
Ligand CDL L 705



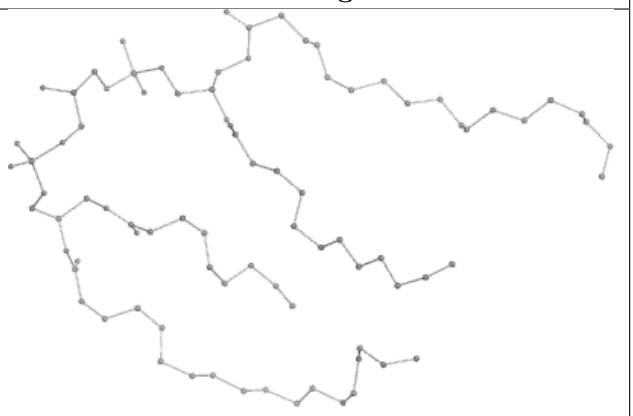
Bond lengths



Bond angles

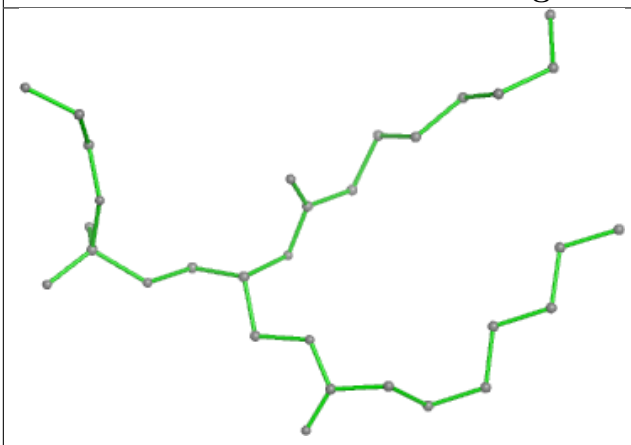


Torsions



Rings

Ligand 3PE o 501



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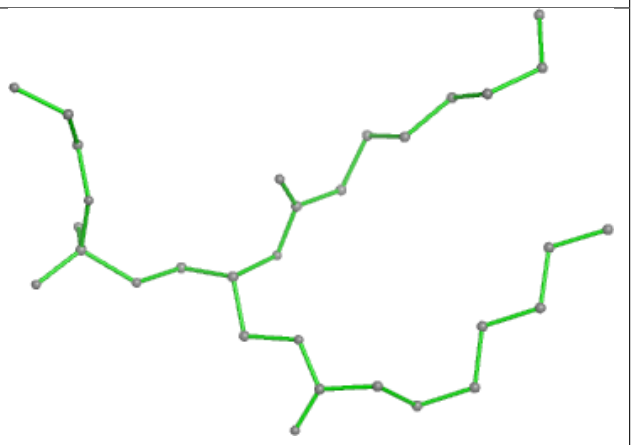

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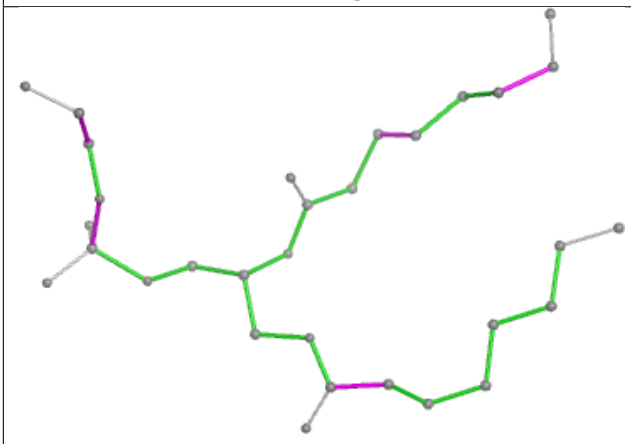

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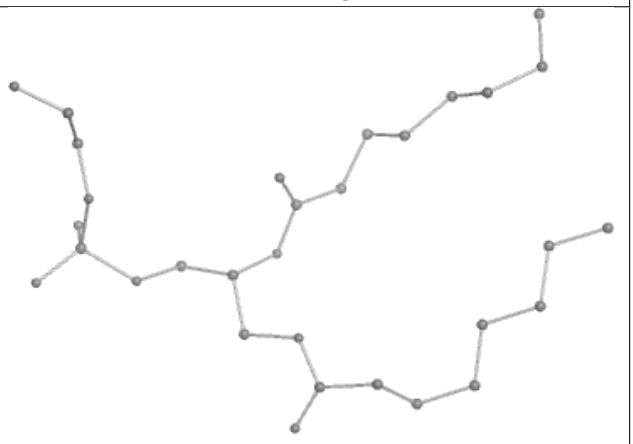
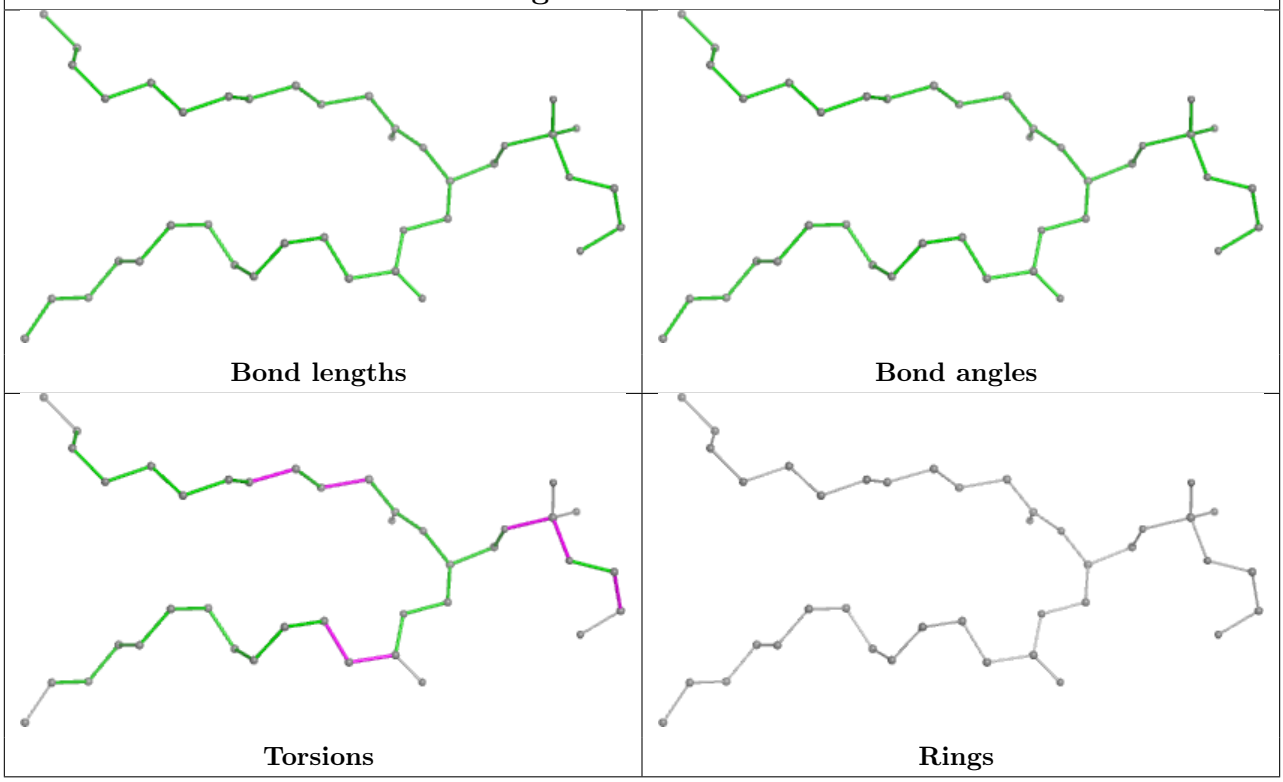
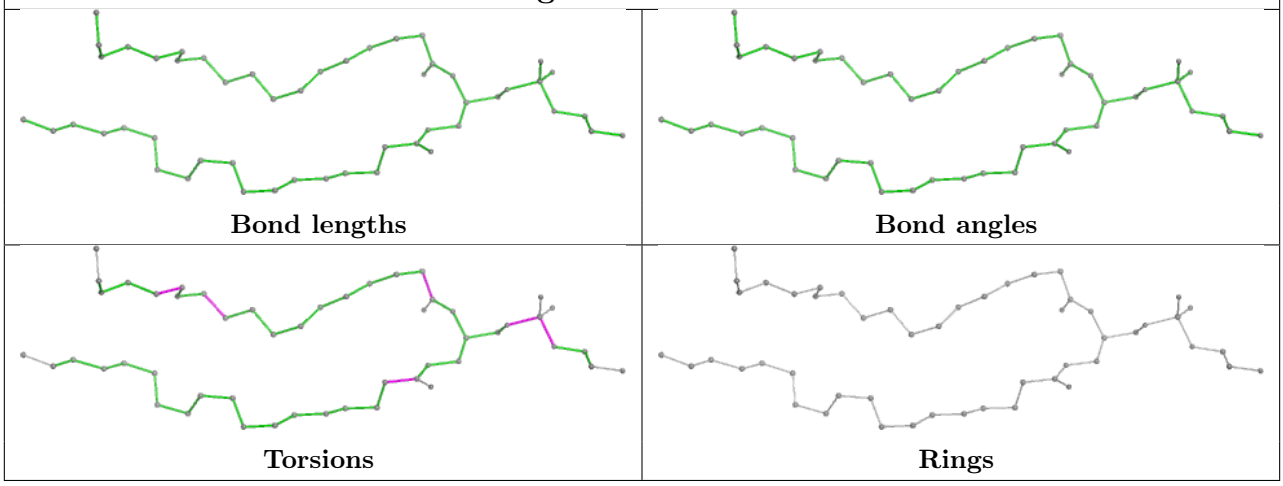


Rings

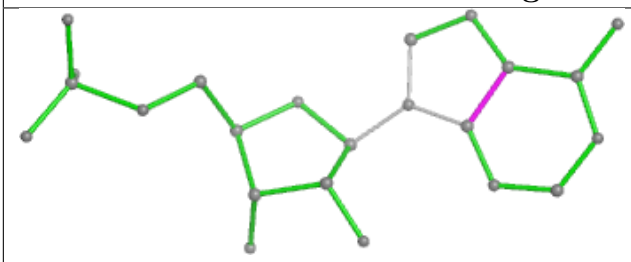
Ligand 3PE L 701



Ligand 3PE i 201



Ligand AMP k 501



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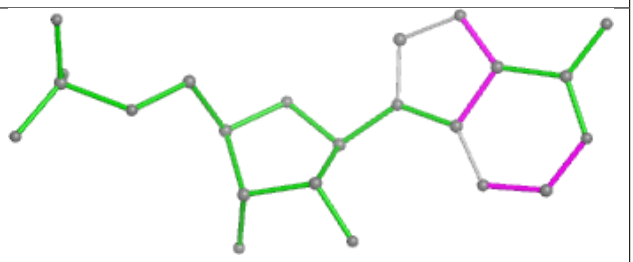
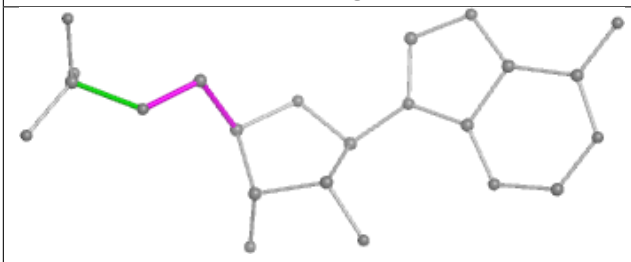


Bond angles



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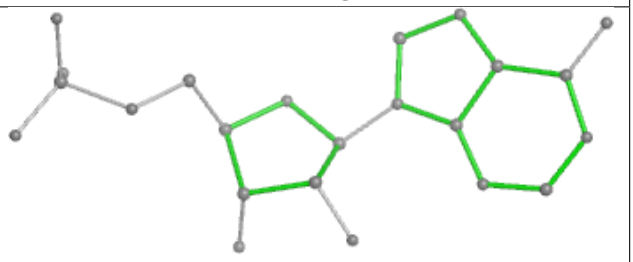

Rings

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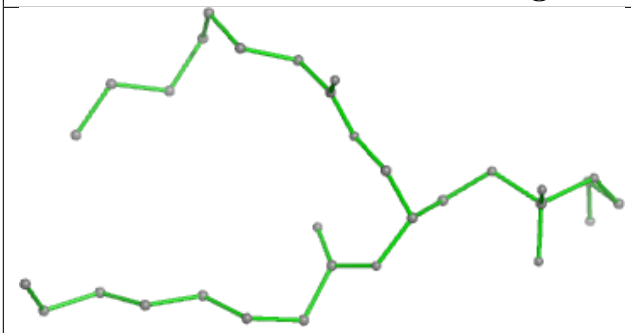

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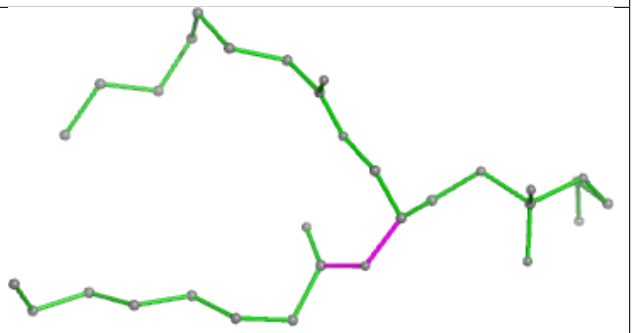

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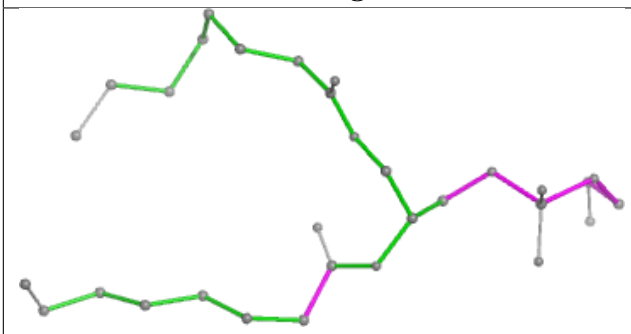

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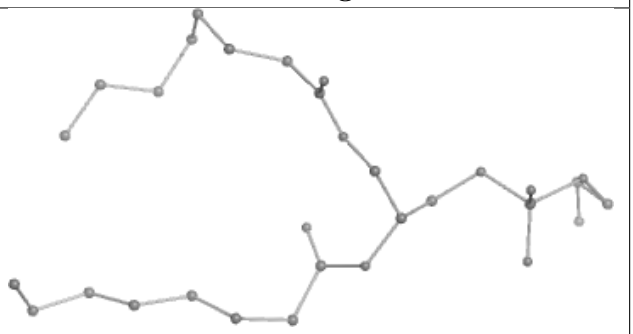
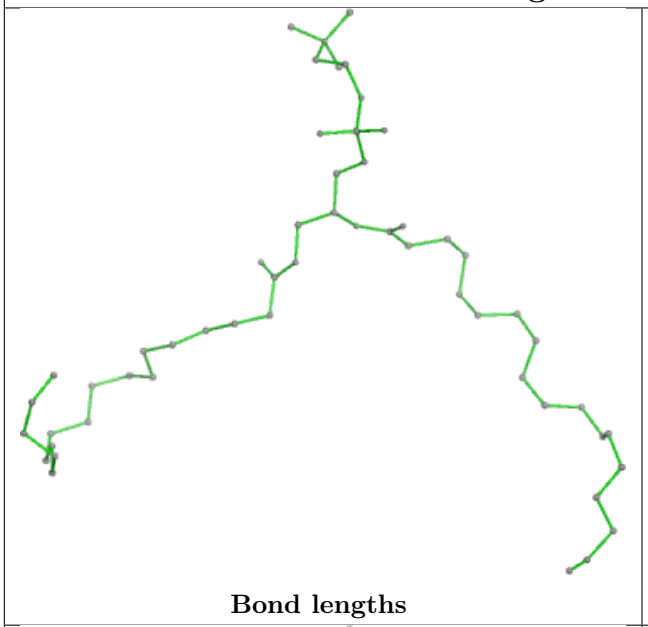


Rings

Ligand PC1 w 801



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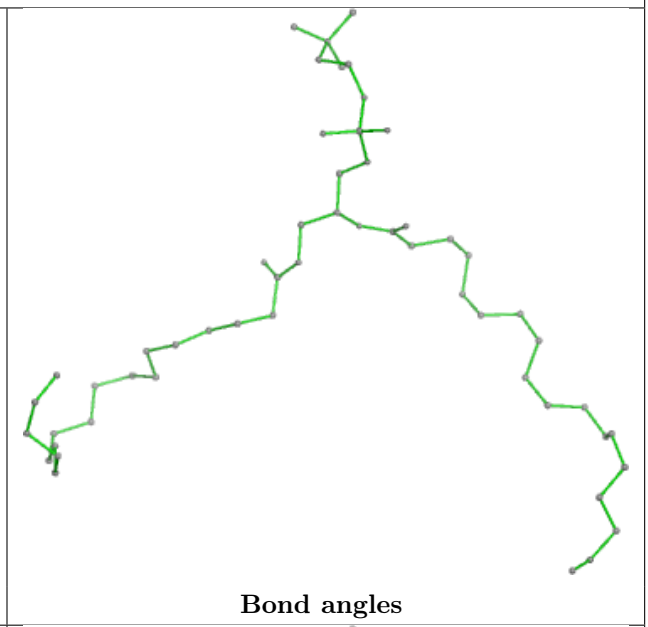
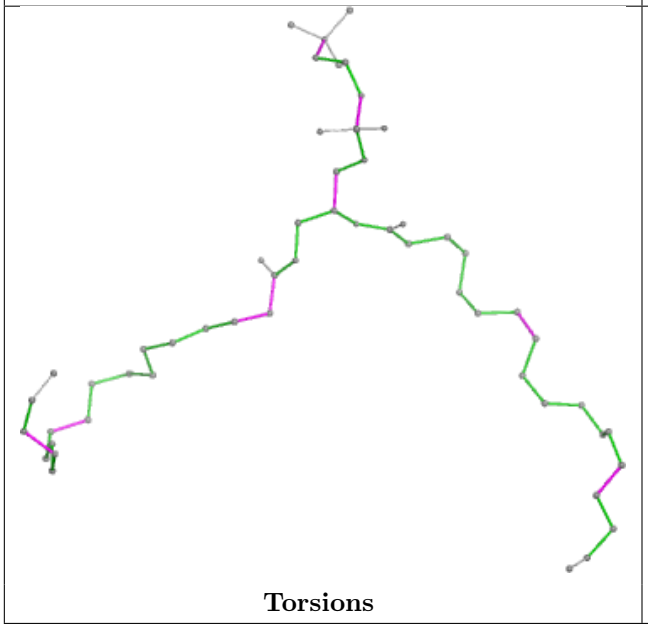


Bond angles



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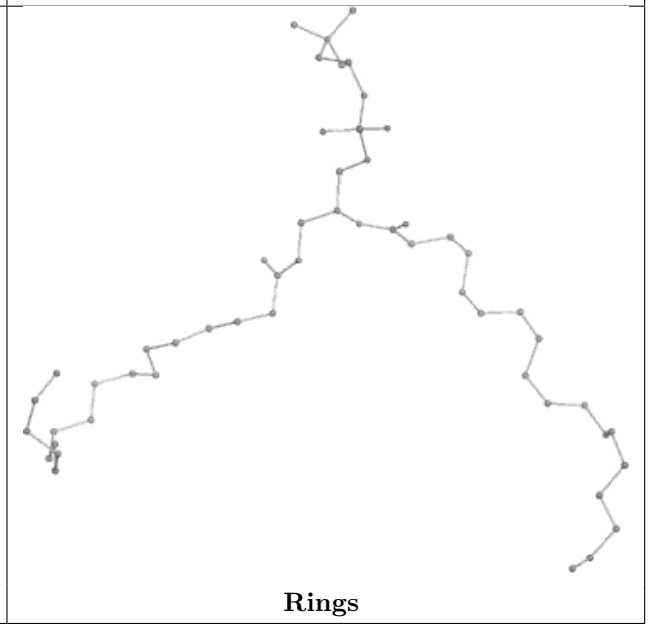

Rings

Ligand PC1 9 401

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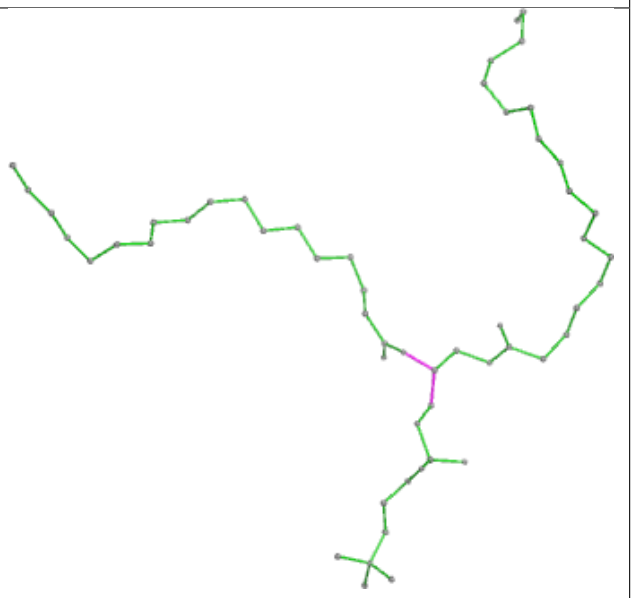
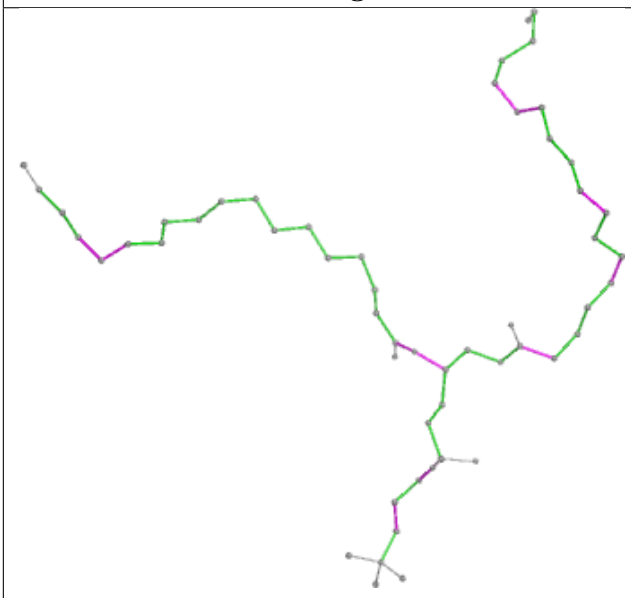


Bond angles



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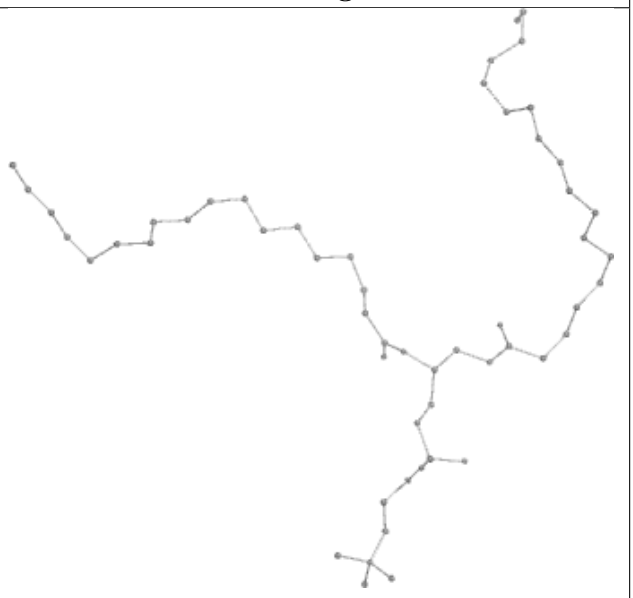
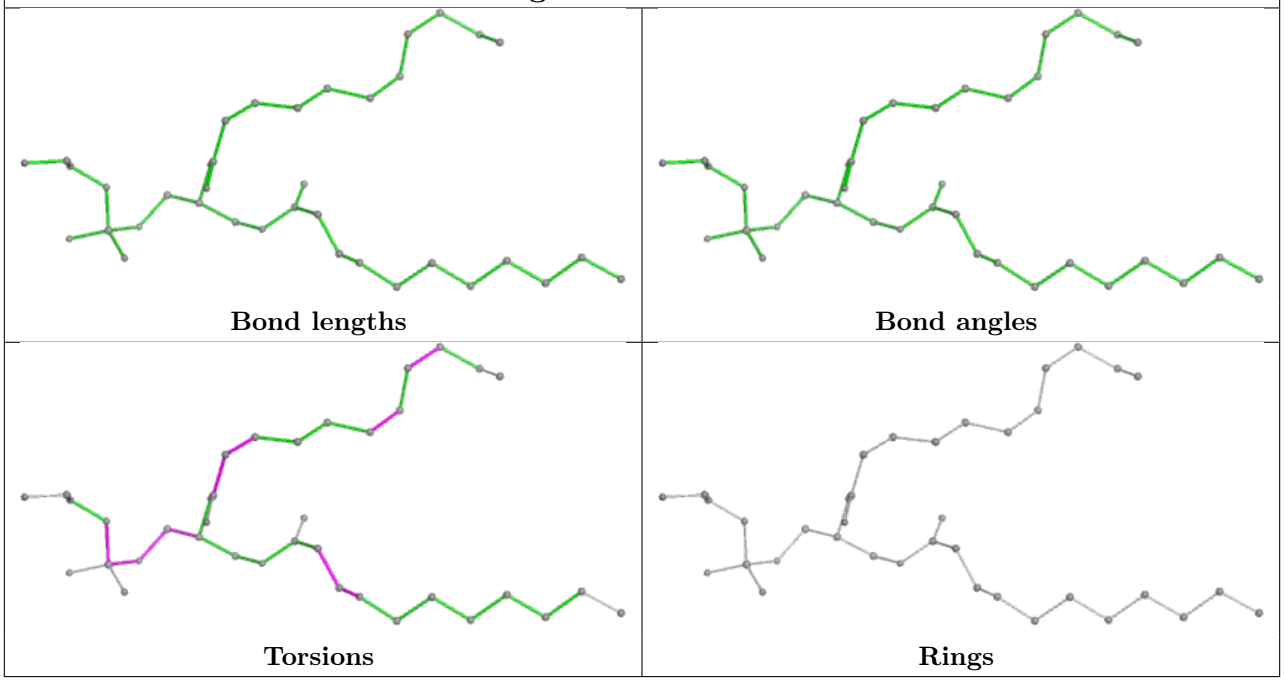
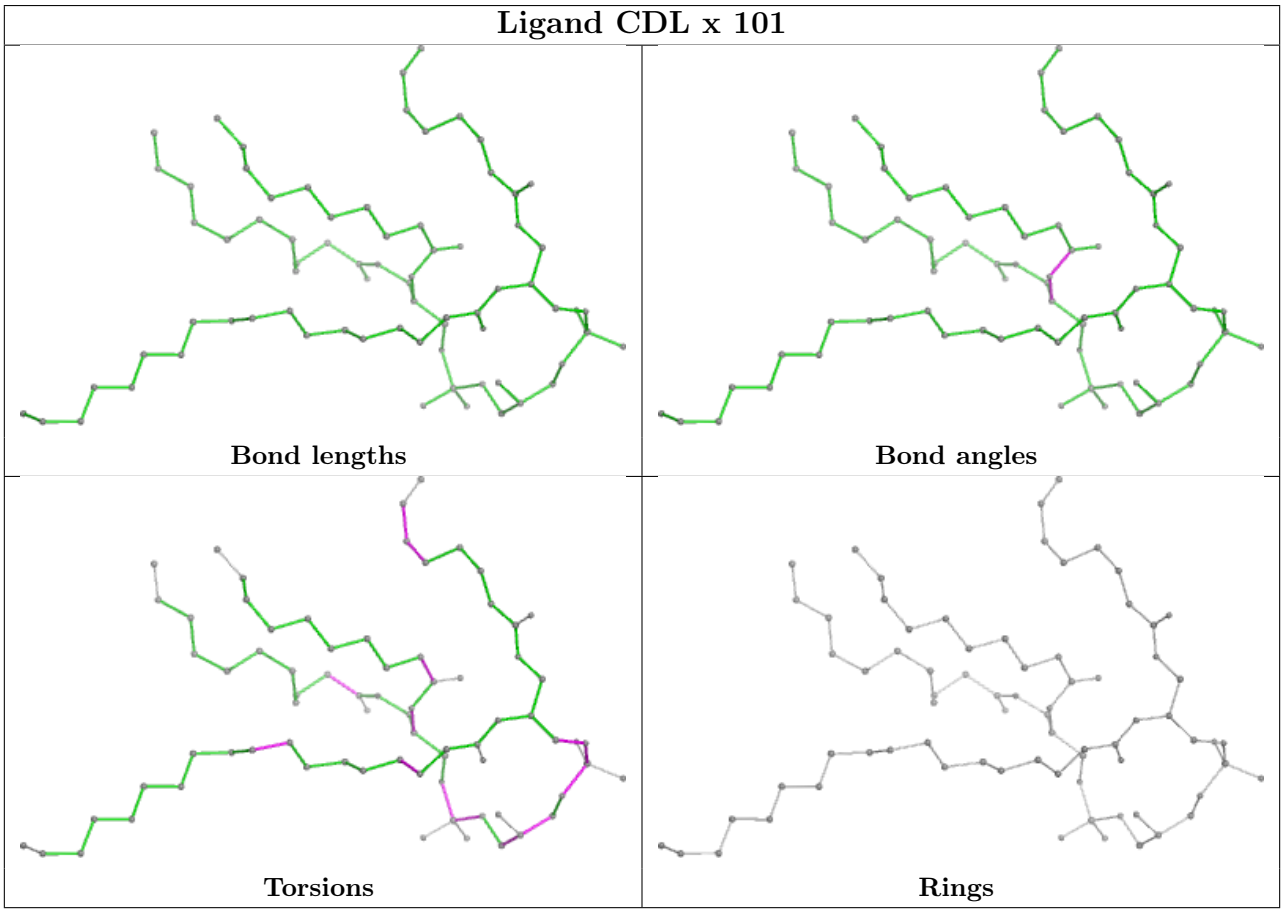


Rings

Ligand 3PE V 202



Ligand CDL x 101



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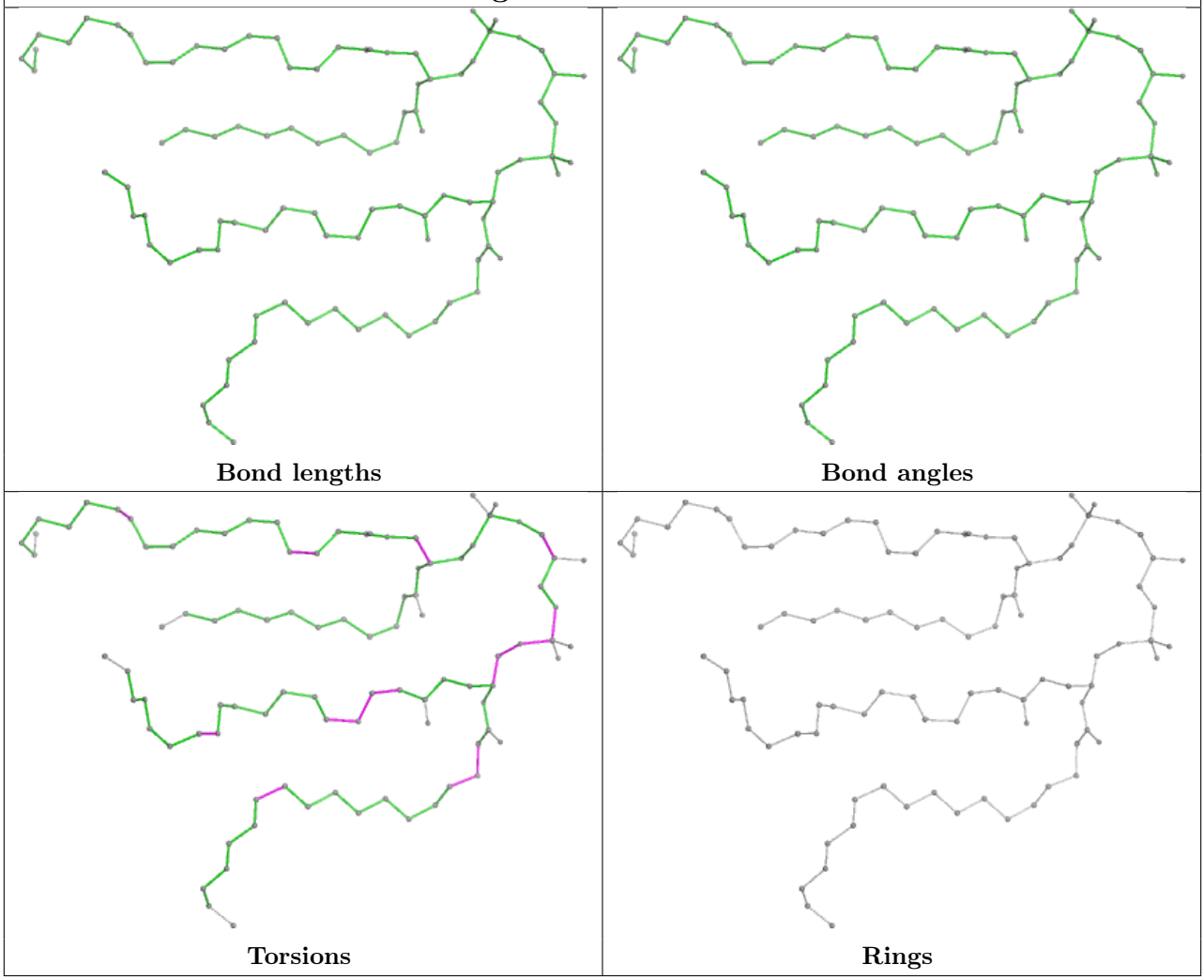

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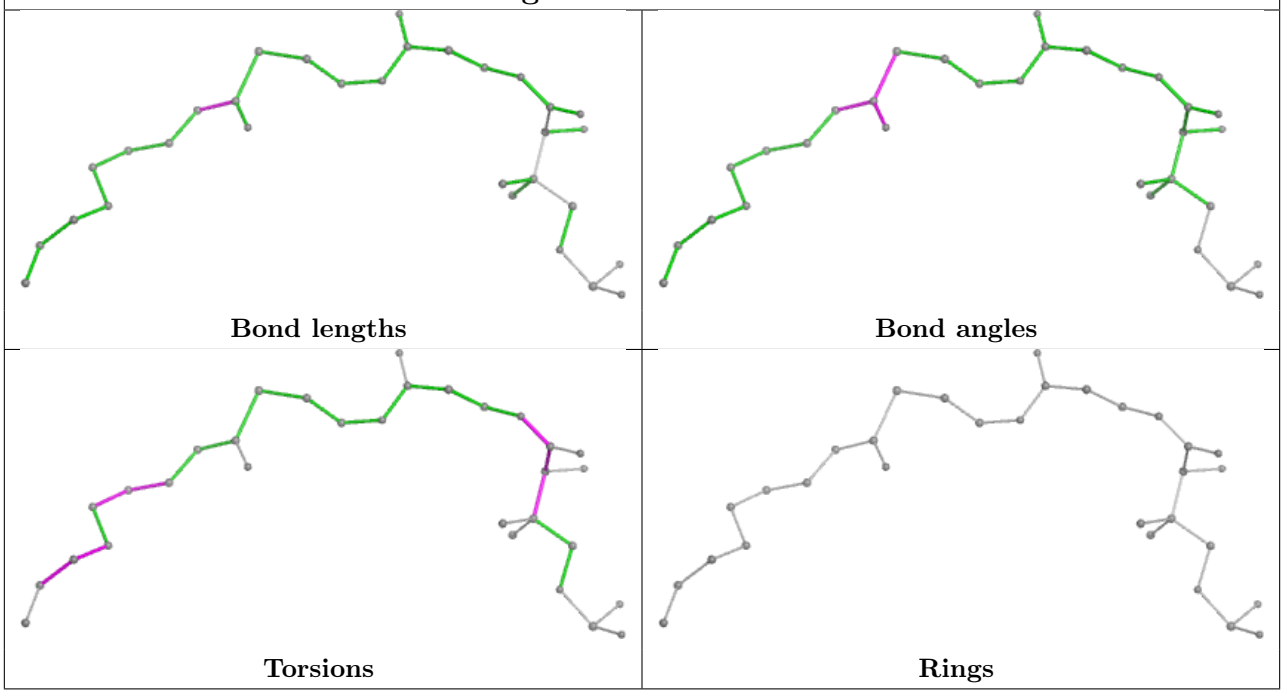
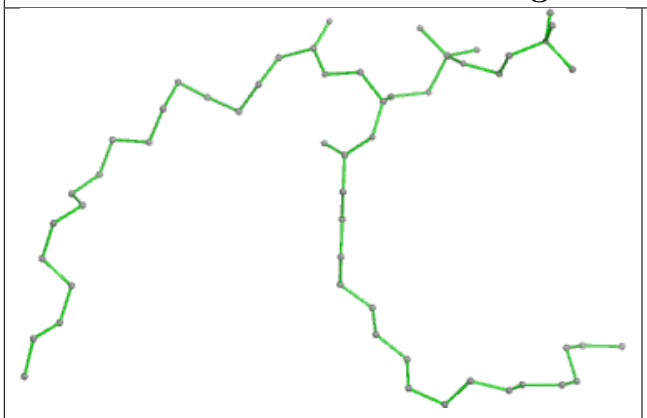
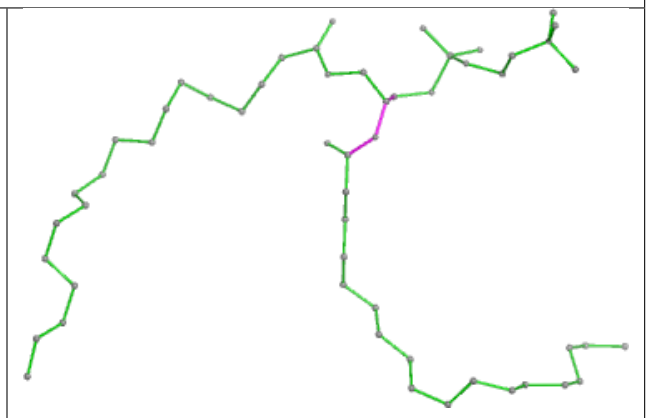


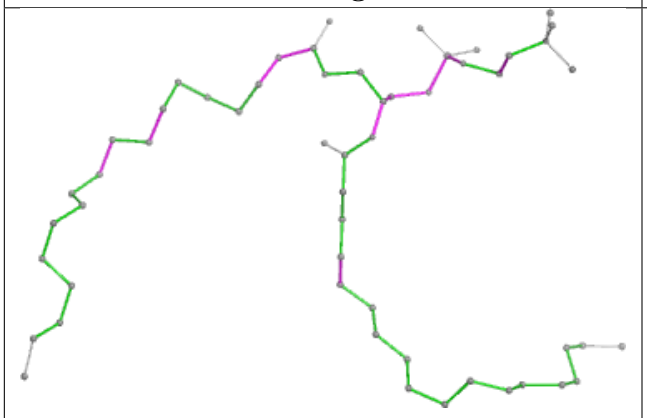
Ligand PC1 L 704



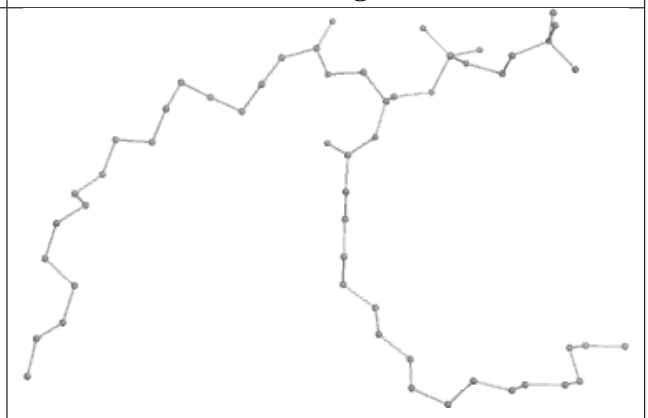
Bond lengths



Bond angles

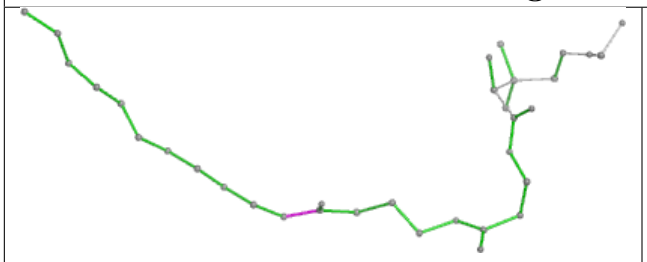


Torsions



Rings

Ligand ZMP g 201



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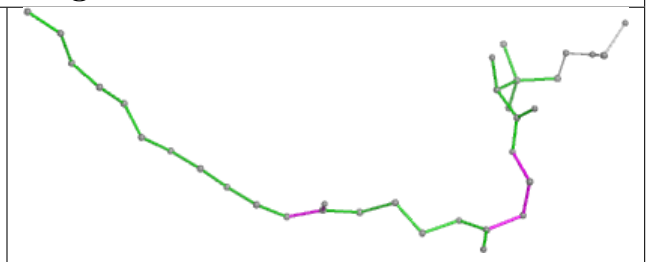
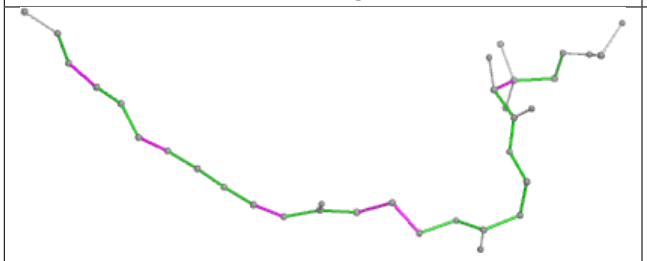
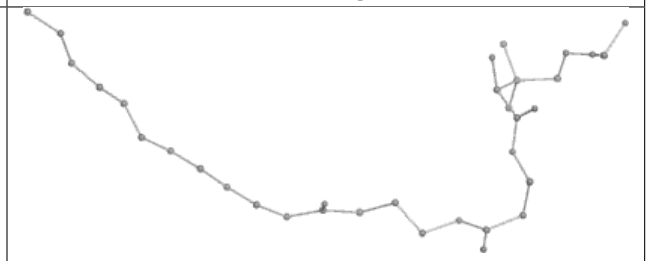


Bond angles

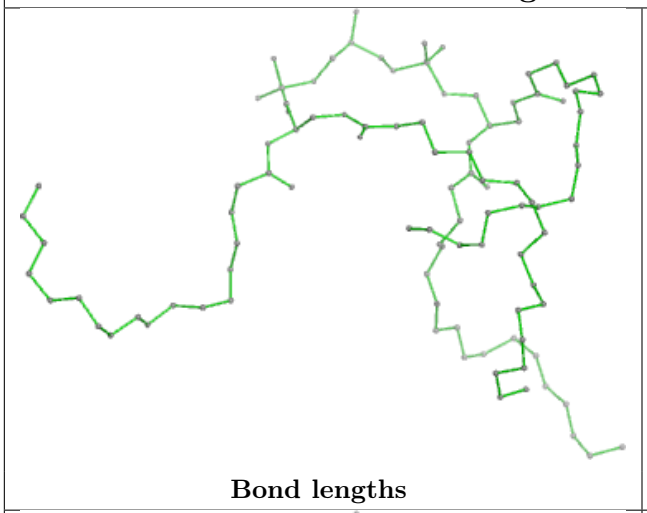


Torsions



Rings

Ligand CDL W 201



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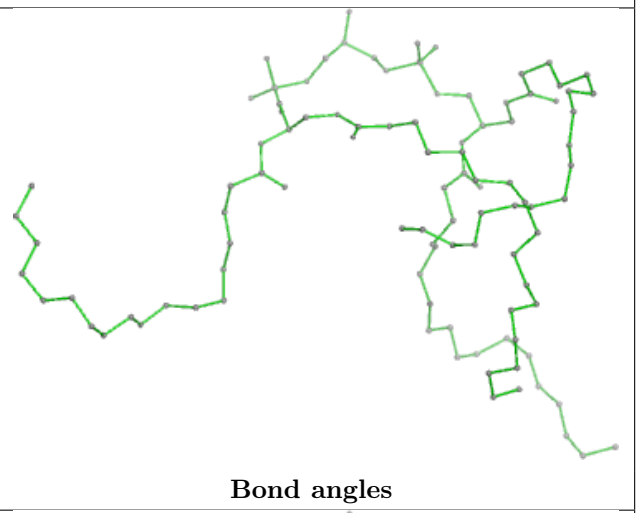
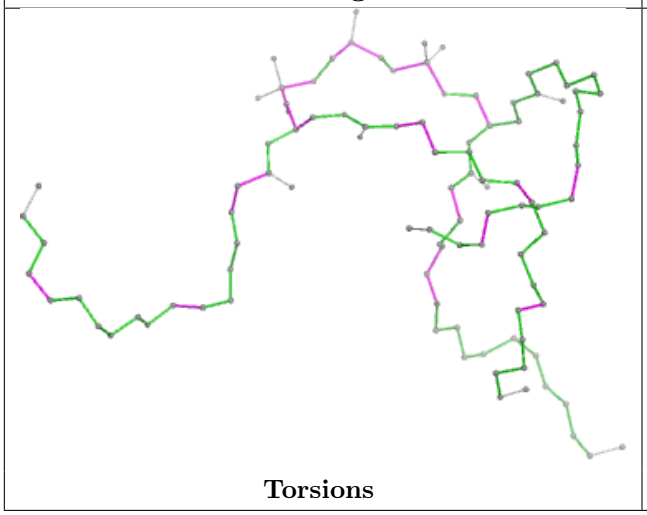
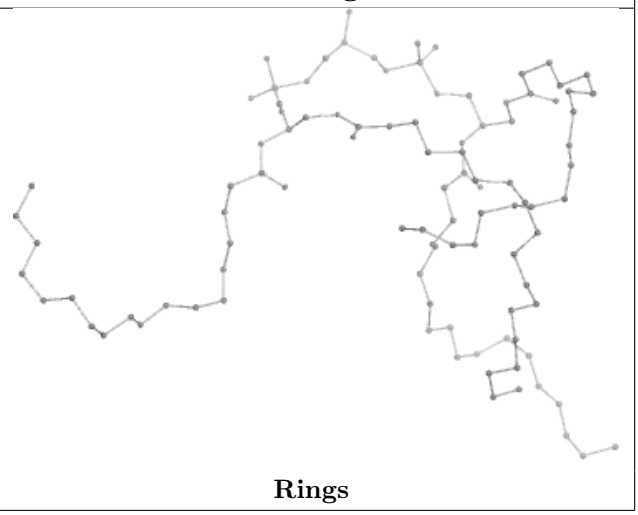


Bond angles

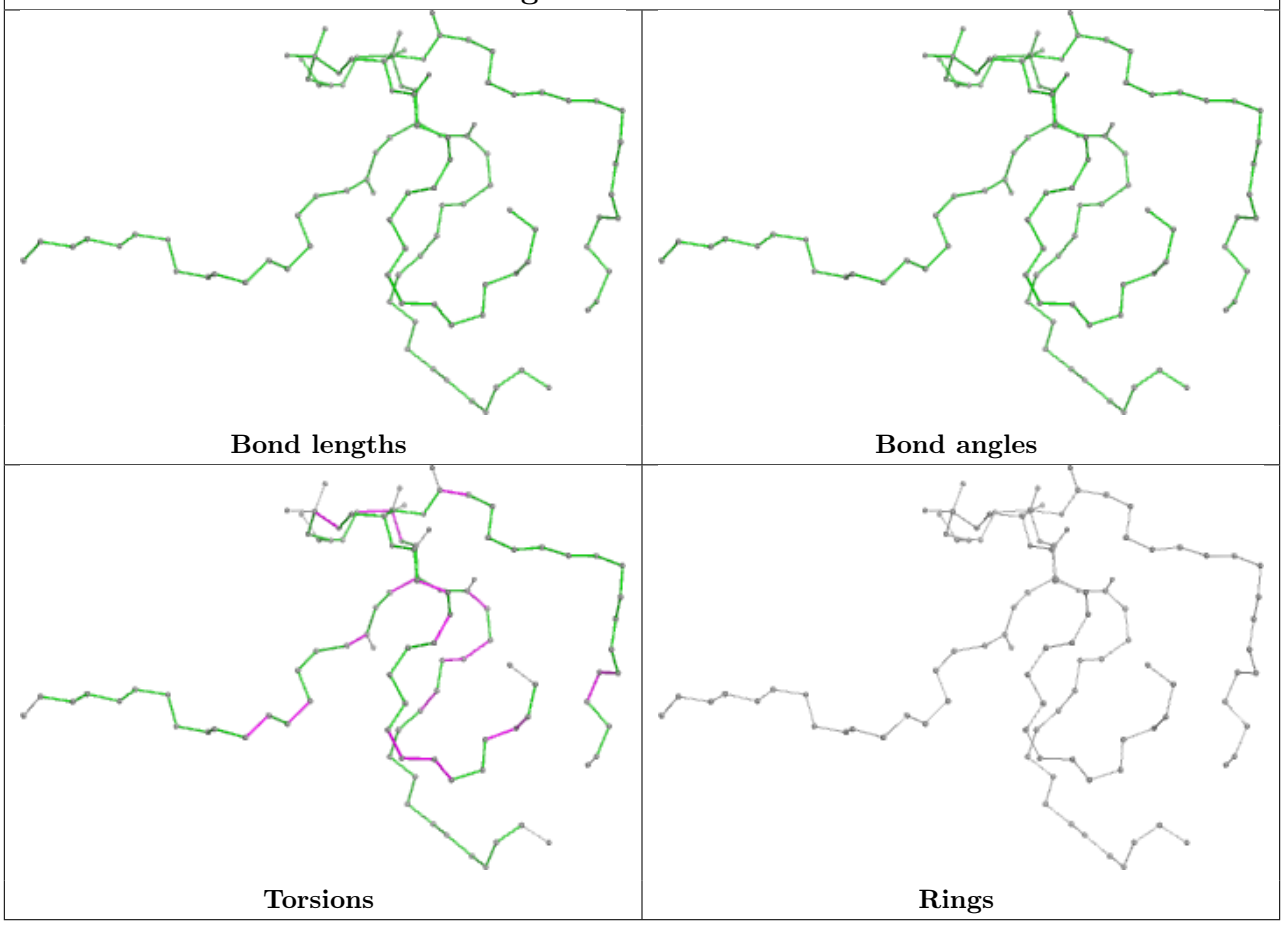


Torsions

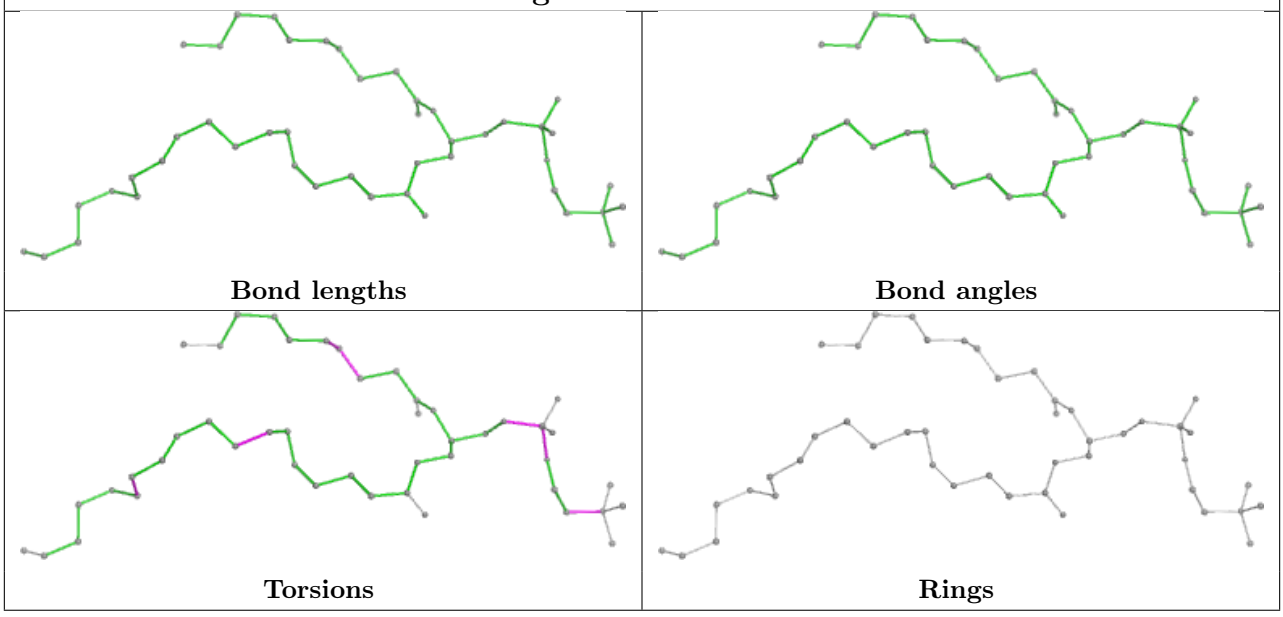


Rings

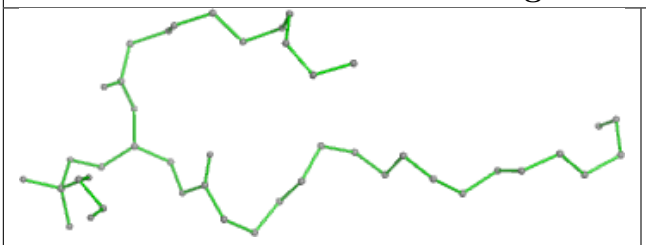
Ligand CDL M 503



Ligand PC1 6 202



Ligand 3PE M 501



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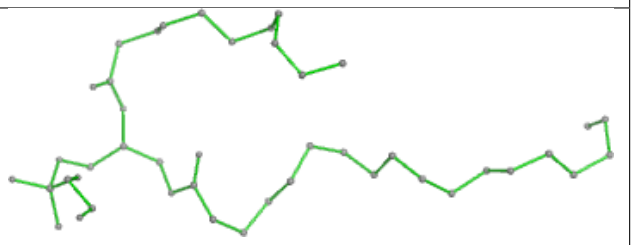
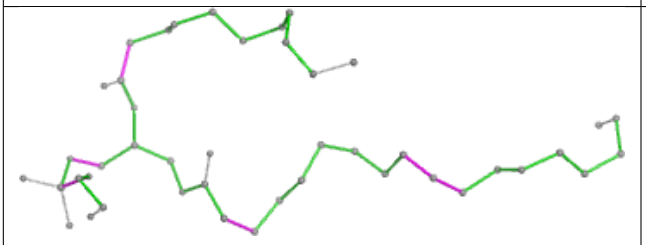


Bond angles



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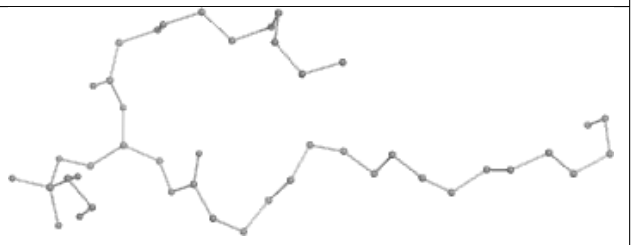
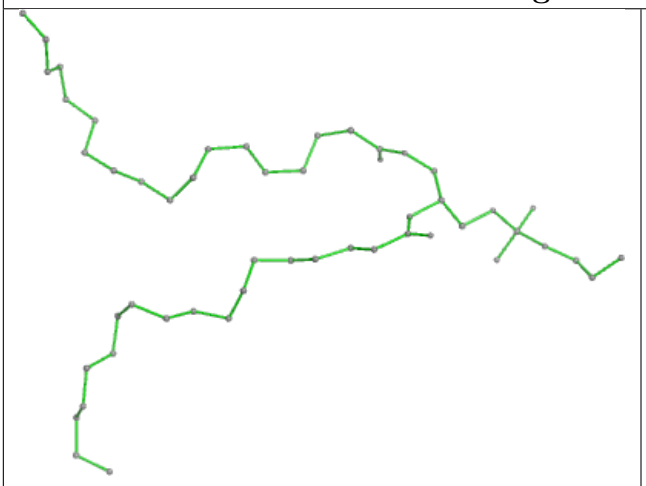
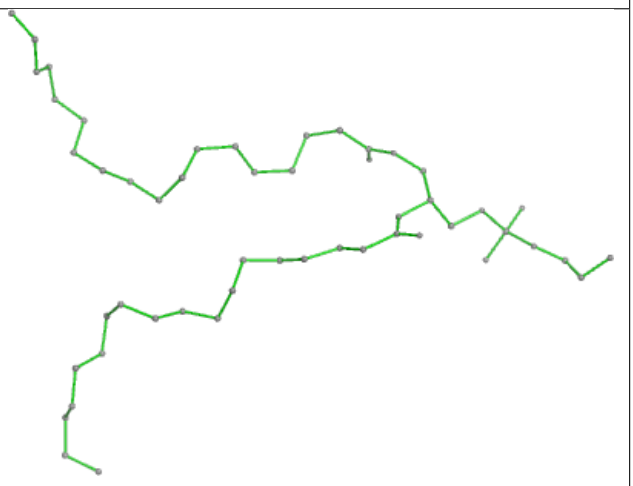


Rings

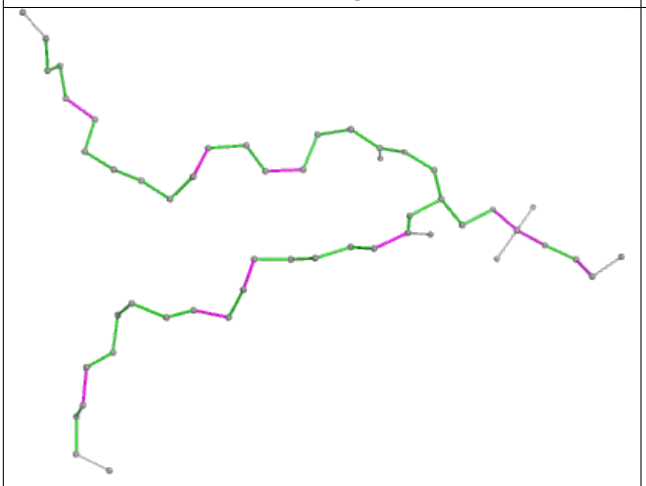
Ligand 3PE 6 203



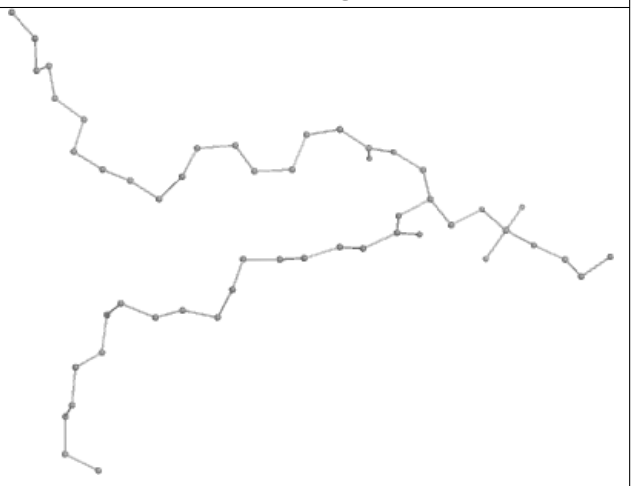
Bond lengths



Bond angles

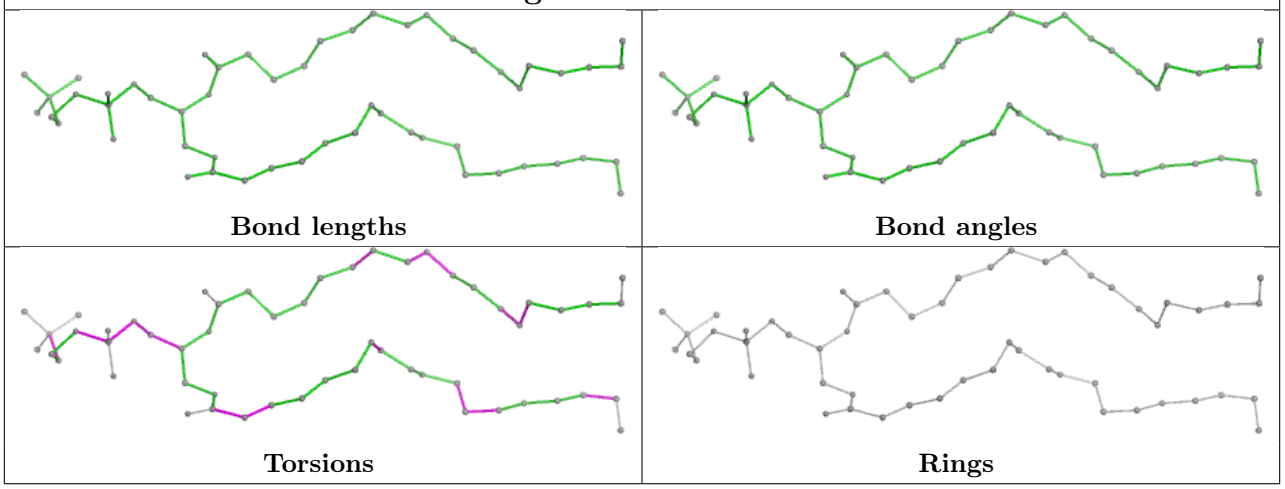


Torsions

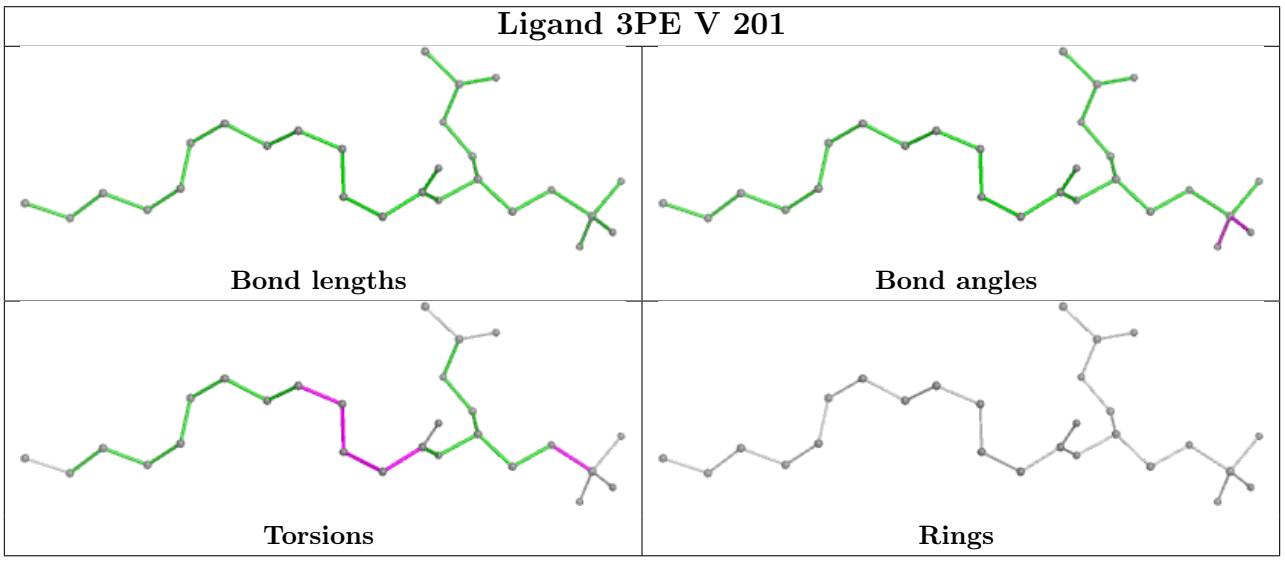


Rings

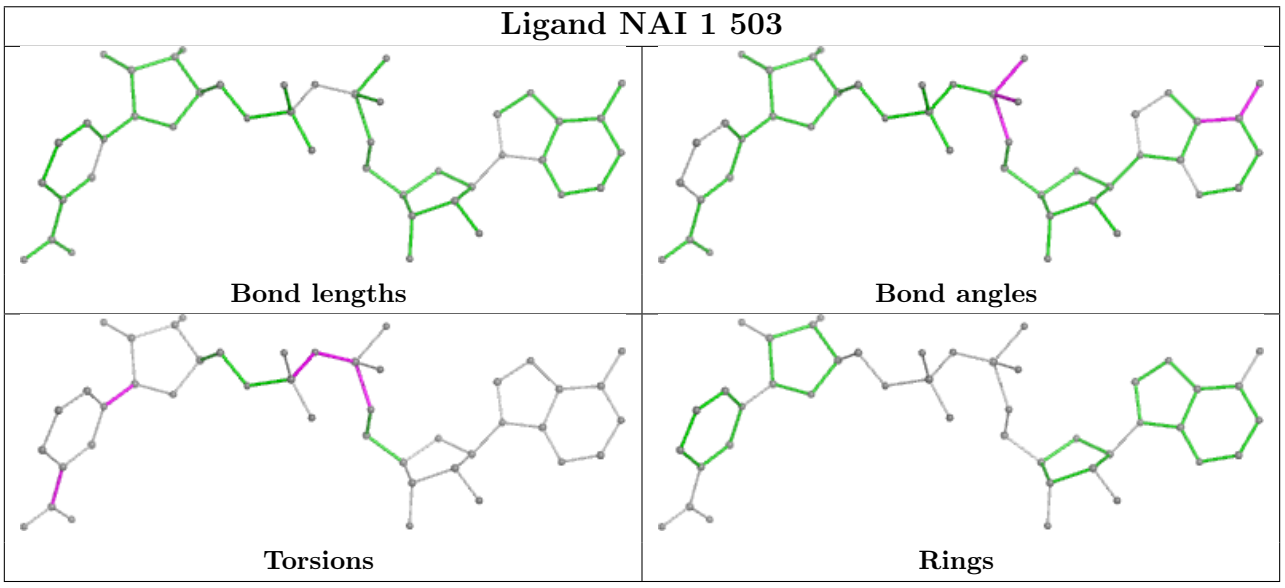
Ligand PC1 M 502



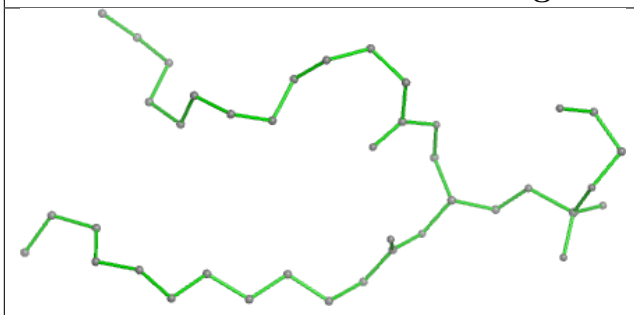
Ligand 3PE V 201



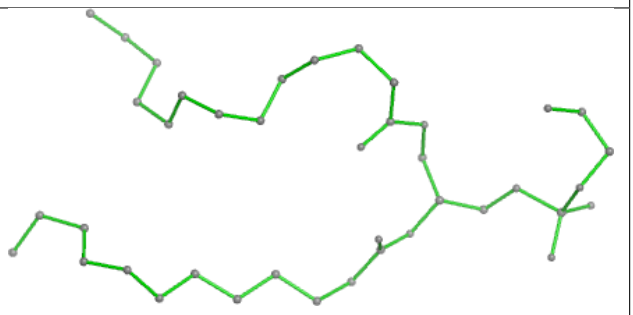
Ligand NAI 1 503



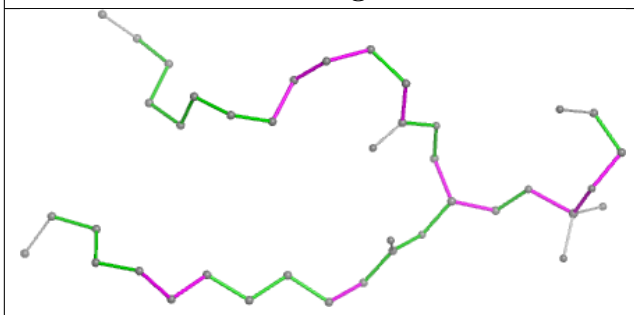
Ligand 3PE J 202



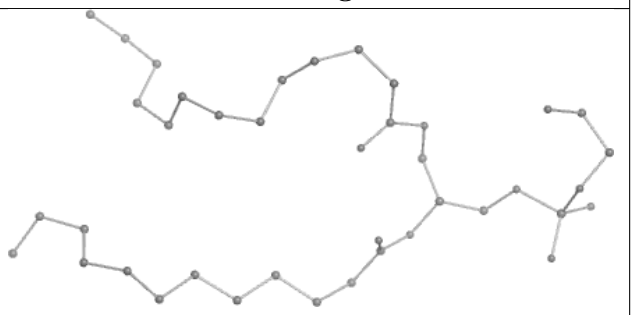
Bond lengths



Bond angles

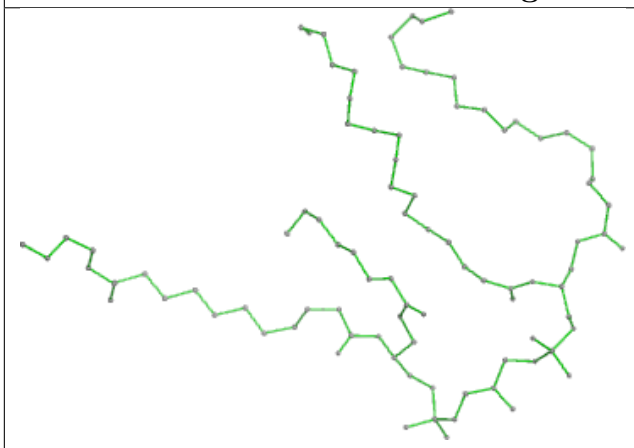


Torsions

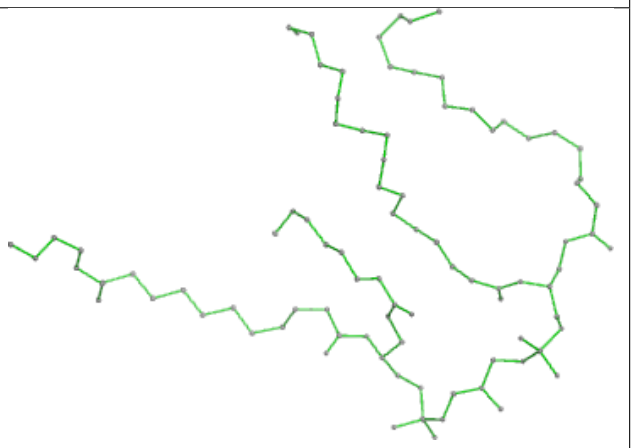


Rings

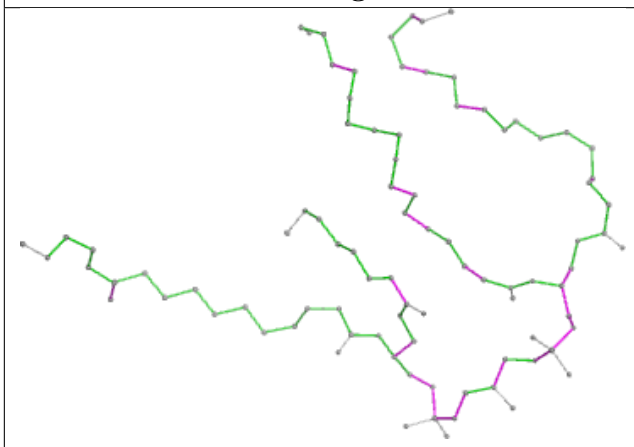
Ligand CDL M 504



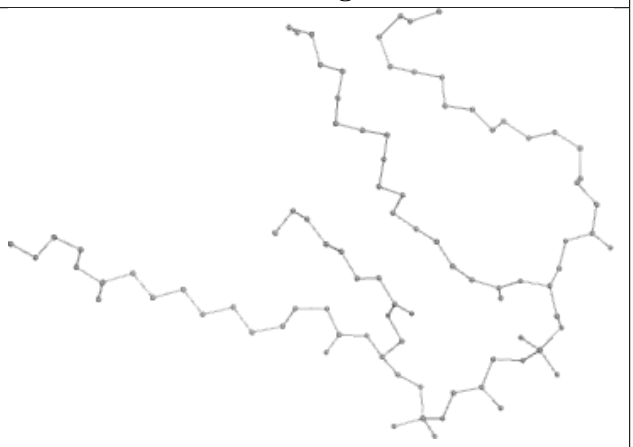
Bond lengths



Bond angles

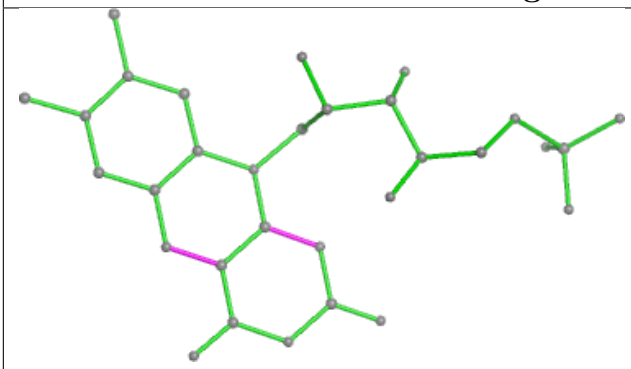


Torsions

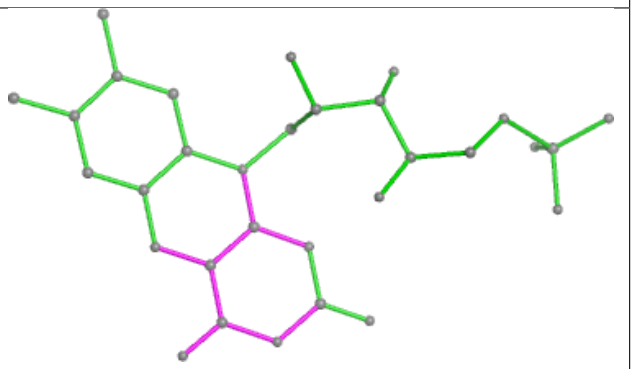


Rings

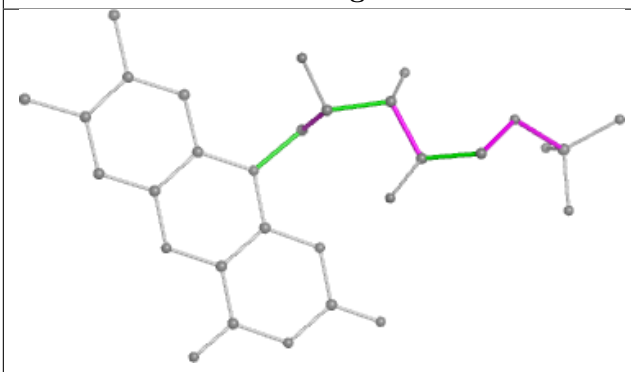
Ligand FMN 1 502



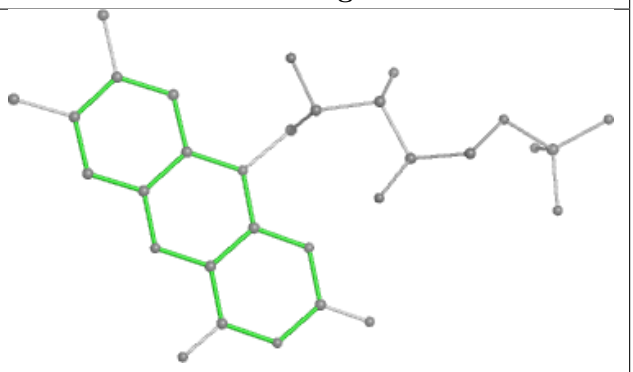
Bond lengths



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-11248. 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.