Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:38 pm BST

PDB ID	:	6ZKK / pdb_00006zkk
EMDB ID	:	EMD-11252
Title	:	Complex I inhibited by rotenone, closed
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	3.70 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:

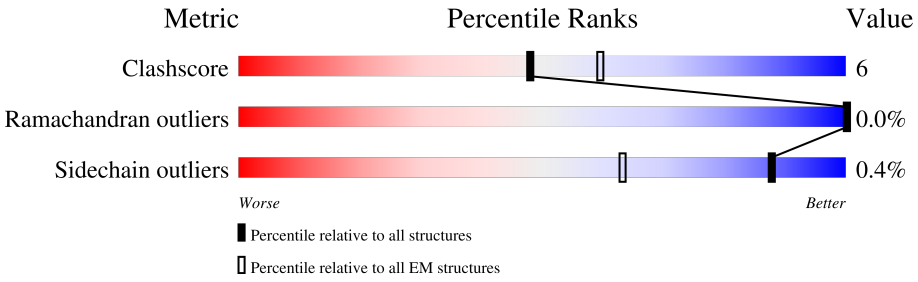
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.70 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	76% 17% 7%
2	2	246	77% 10% 13%
3	3	727	78% 16% 5%
4	4	463	76% 16% 7%
5	5	266	62% 17% 22%
6	6	223	57% 13% 30%
7	9	217	69% 12% 19%
8	A	115	84% 16%
9	H	318	81% 18%

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Mol	Chain	Length	Quality of chain
10	J	175	85% 15%
11	K	98	76% 24%
12	L	606	85% 15%
13	M	459	84% 16%
14	N	347	82% 18%
15	V	141	89% 9%
16	W	189	65% 9% 26%
17	X	157	49% 6% 45%
17	j	157	52% 48%
18	Y	172	93% 6%
19	Z	175	89% 9%
20	a	109	40% 60%
21	b	124	77% 23%
22	c	170	74% 26%
23	d	380	88% 11%
24	e	99	87% 13%
25	f	116	97%
26	g	140	81% 19%
27	h	114	83% 16%
28	i	145	100%
29	k	355	90% 10%
30	l	106	99%
31	m	84	94% 5%
32	n	98	81% 19%
33	o	122	98%

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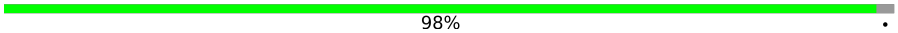
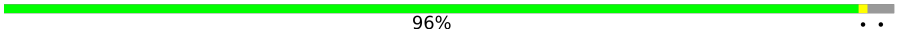
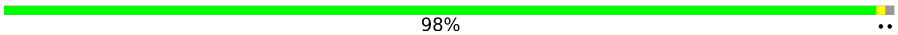
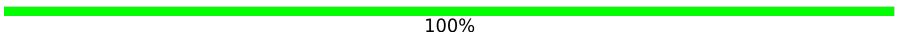
Mol	Chain	Length	Quality of chain
34	p	130	
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1	501	-	-	X	-
53	CDL	L	1004	X	-	-	-
53	CDL	L	1005	X	-	-	-
53	CDL	M	504	X	-	-	-
53	CDL	x	101	X	-	-	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 67950 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		

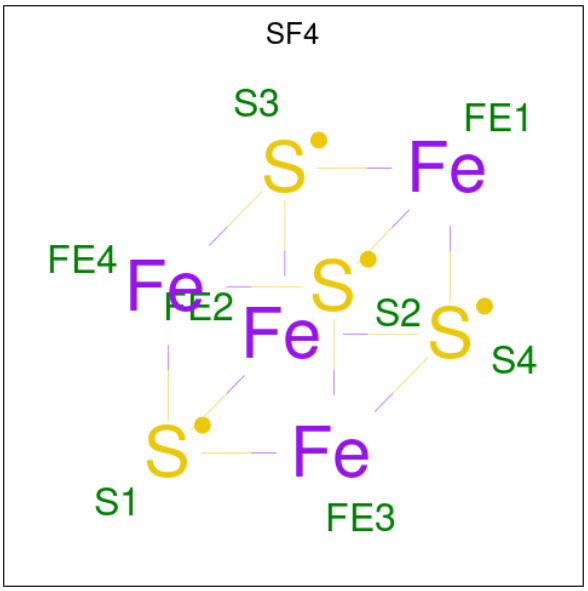
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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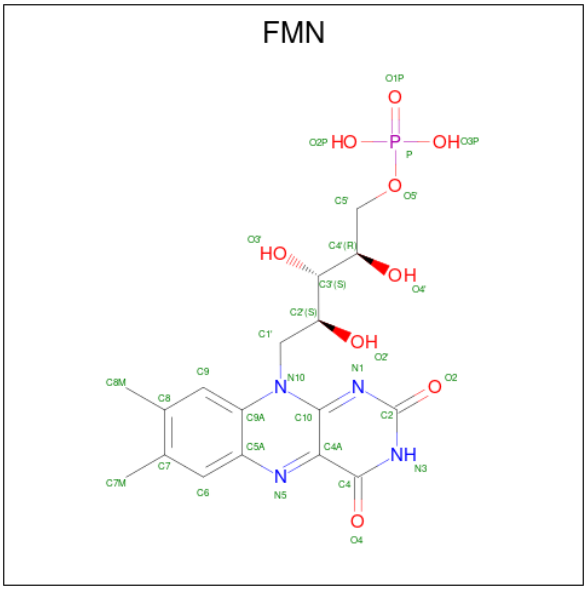
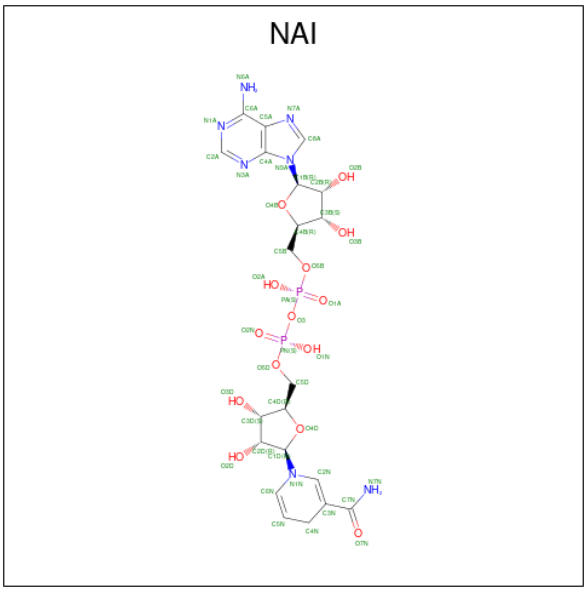
Mol	Chain	Residues	Atoms	AltConf
45	9	1	Total Fe S 8 4 4	0
45	9	1	Total Fe S 8 4 4	0

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



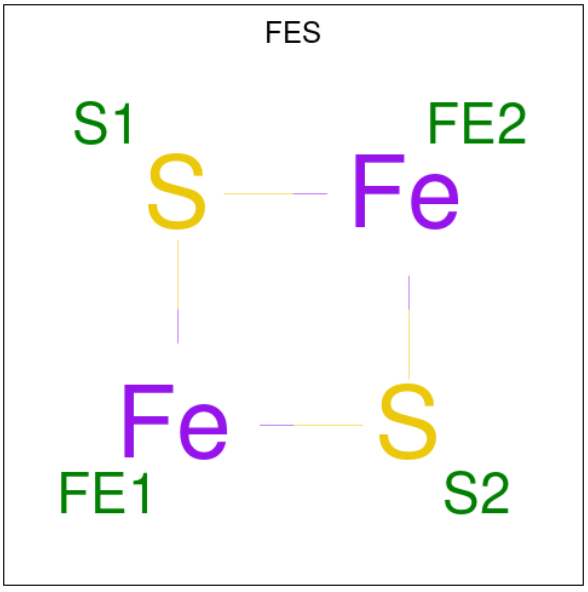
Mol	Chain	Residues	Atoms	AltConf
46	1	1	Total C N O P 31 17 4 9 1	0

- 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).

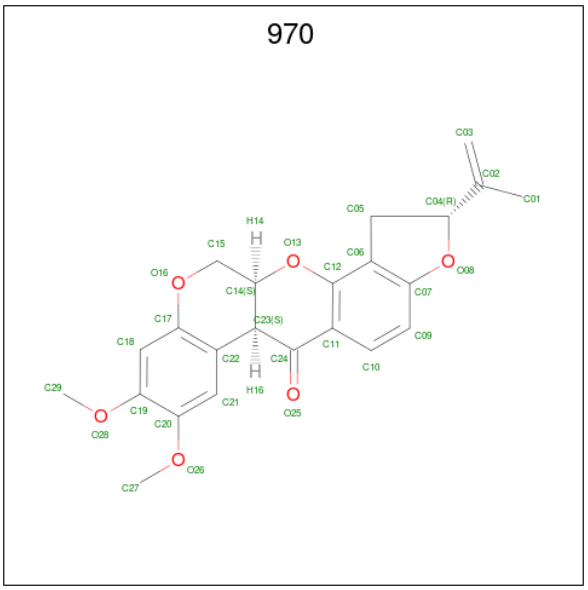


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

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

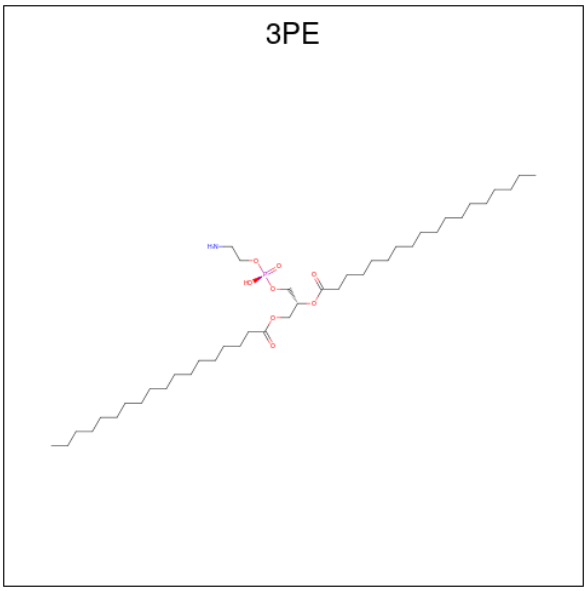
Mol	Chain	Residues	Atoms	AltConf
49	3	1	Total K 1 1	0

- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: $C_{23}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
50	4	1	Total C O 29 23 6	0

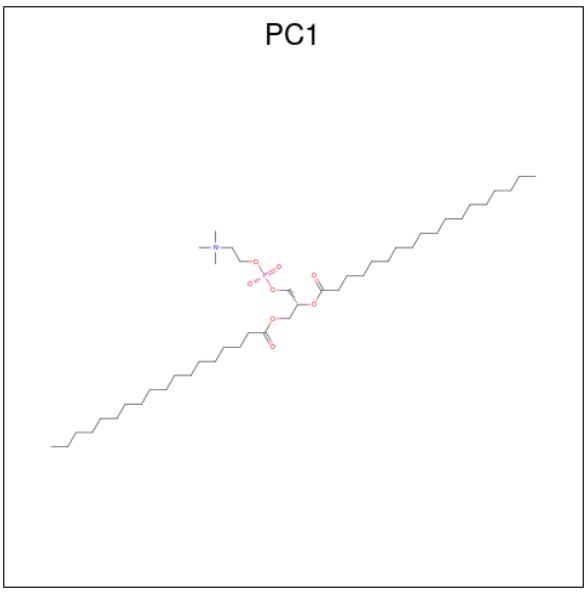
- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
51	4	1	Total C N O P 40 30 1 8 1	0
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 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

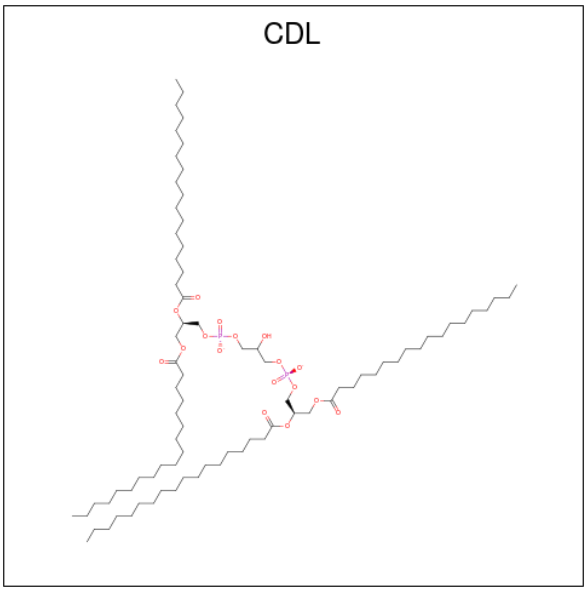
- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula: $C_{44}H_{88}NO_8P$).



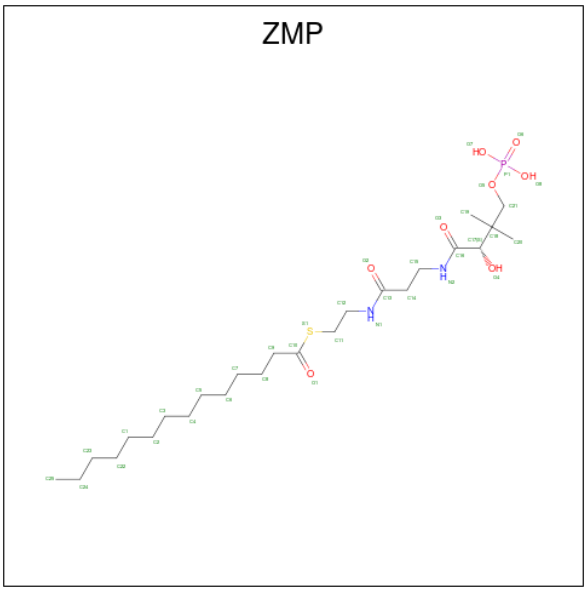
Mol	Chain	Residues	Atoms					AltConf
52	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

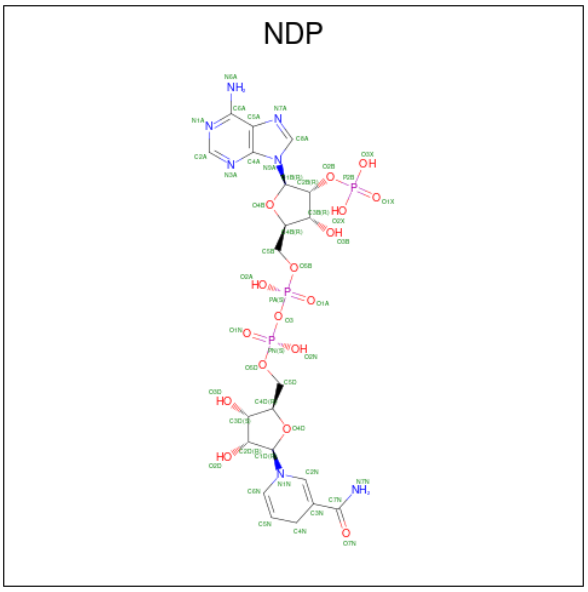


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
54	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

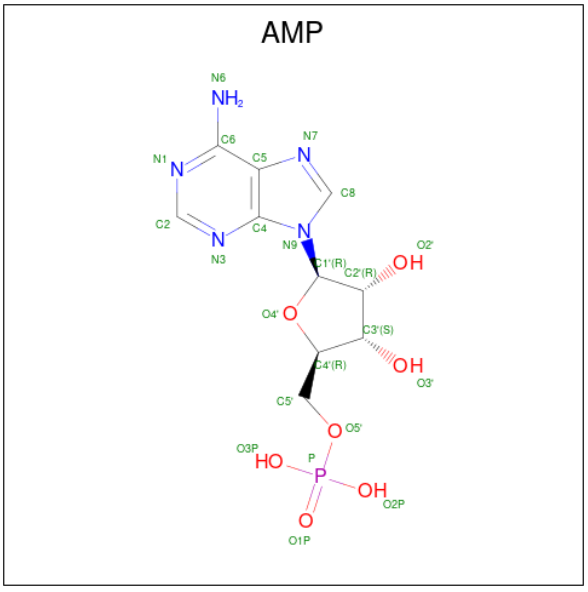
Mol	Chain	Residues	Atoms		AltConf
55	b	1	Total	Zn	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



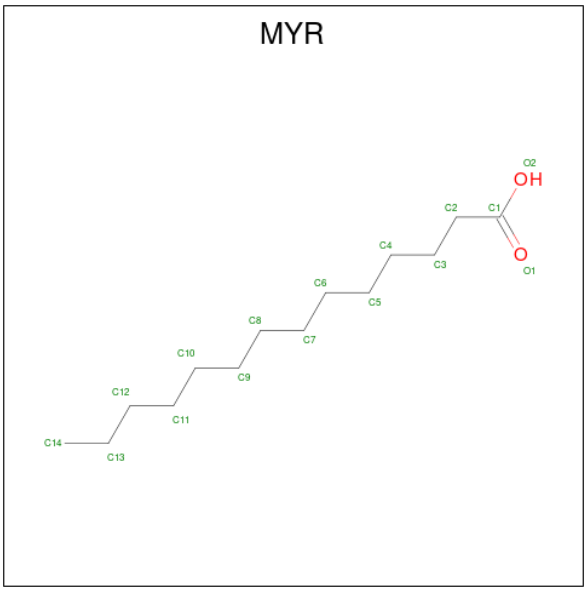
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



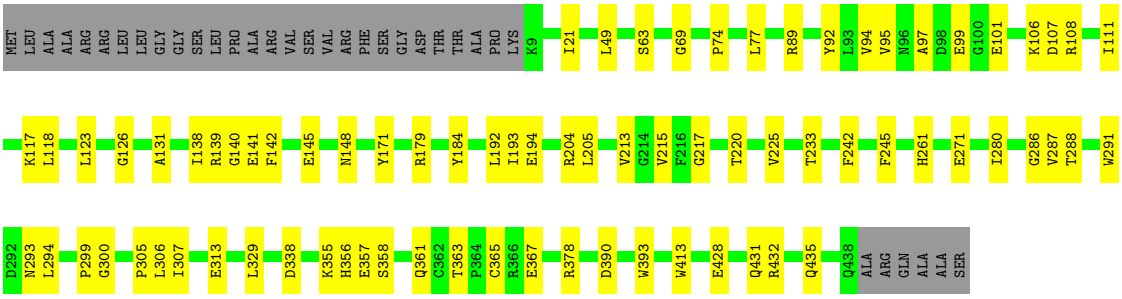
Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

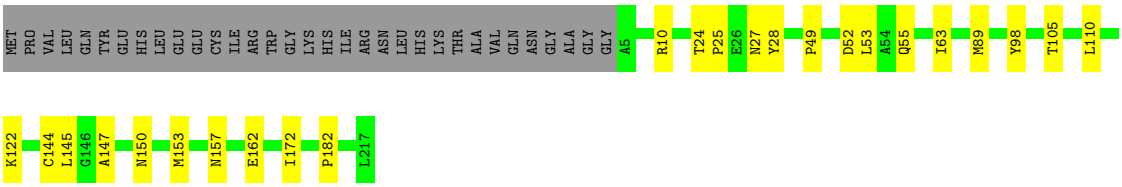
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



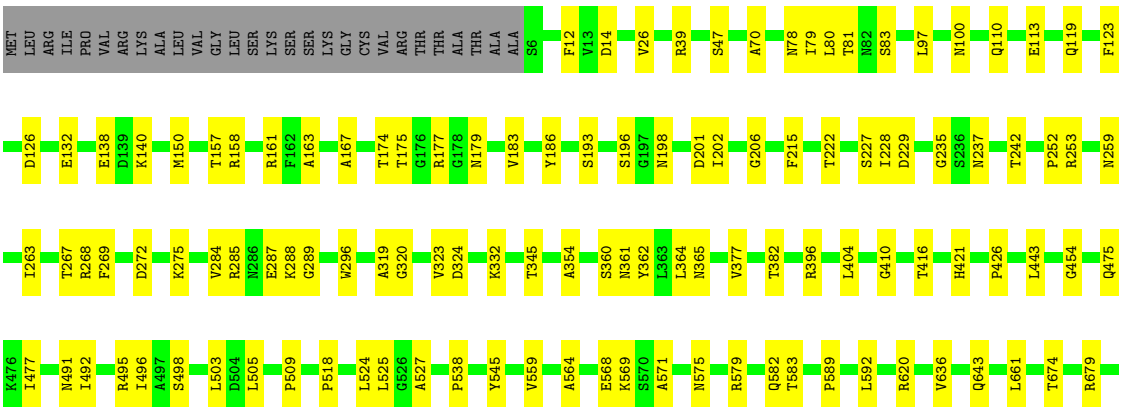
• Molecule 2: Mitochondrial complex I, 24 kDa subunit

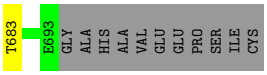
Chain 2:



• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

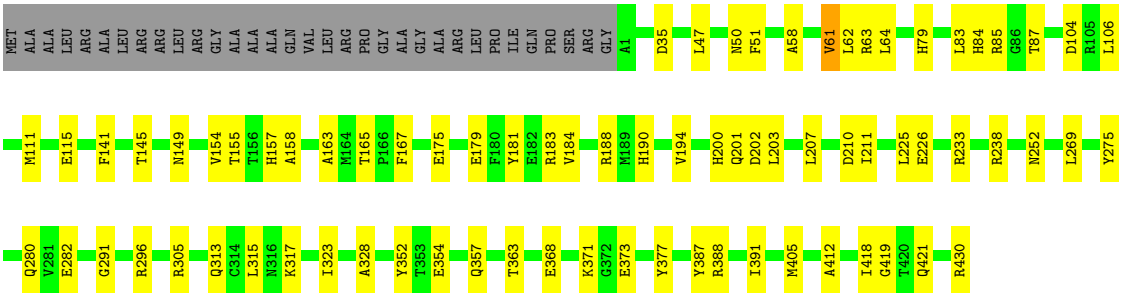
Chain 3:





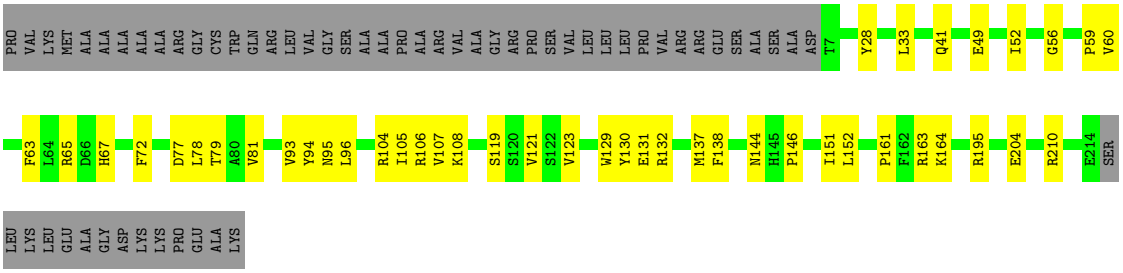
• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:



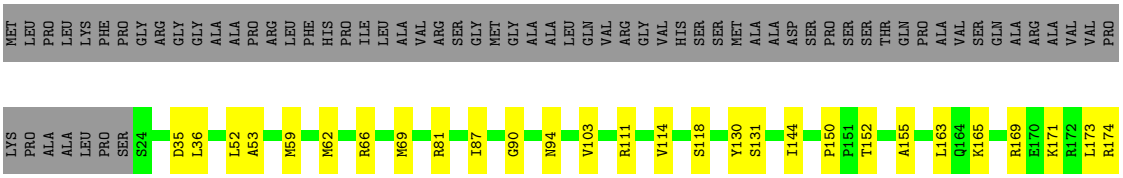
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:



• Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:

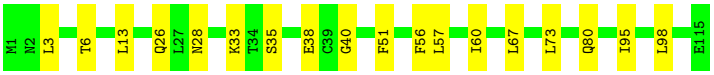


• Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:

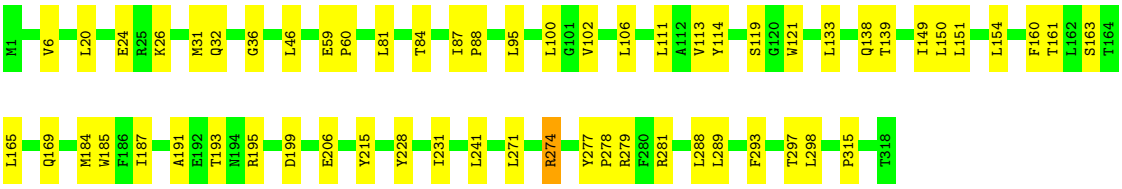
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A:



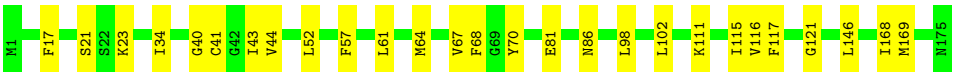
• Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

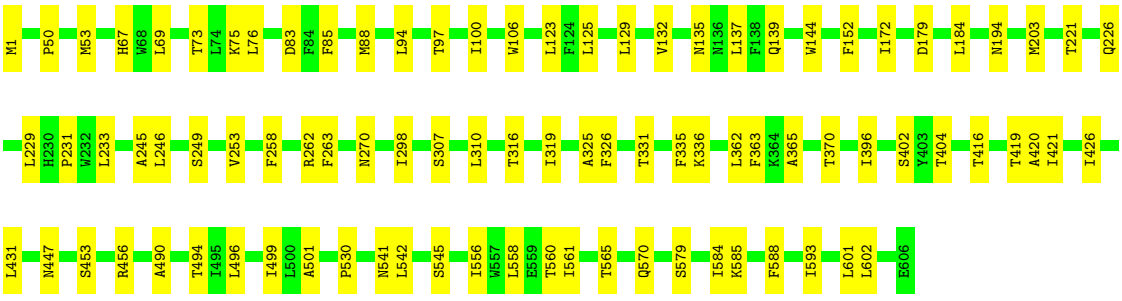


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

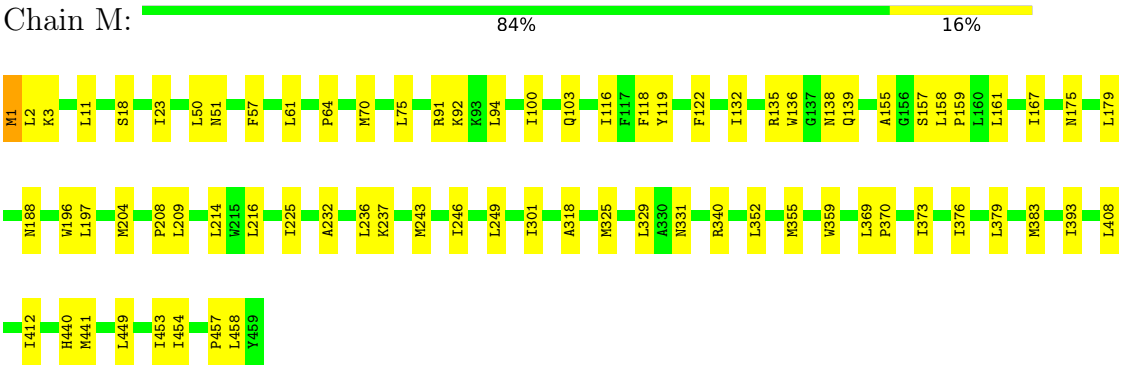
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



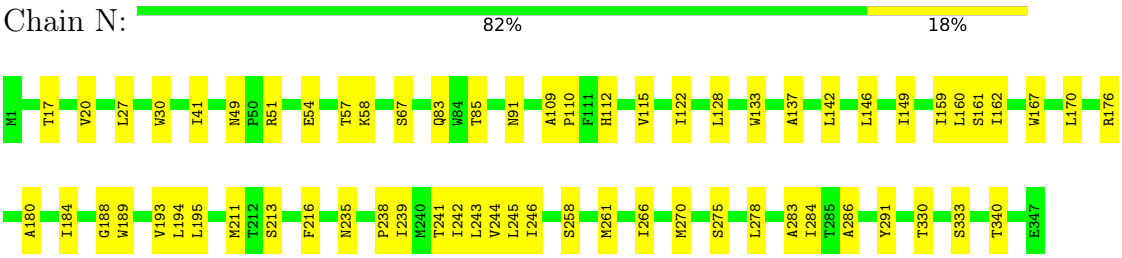
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



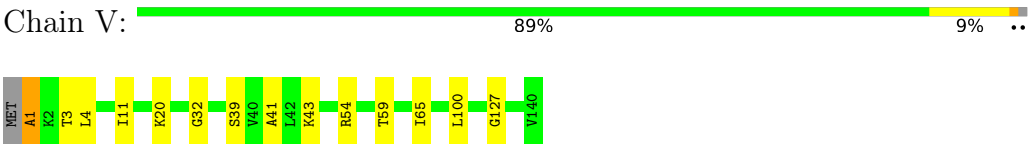
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



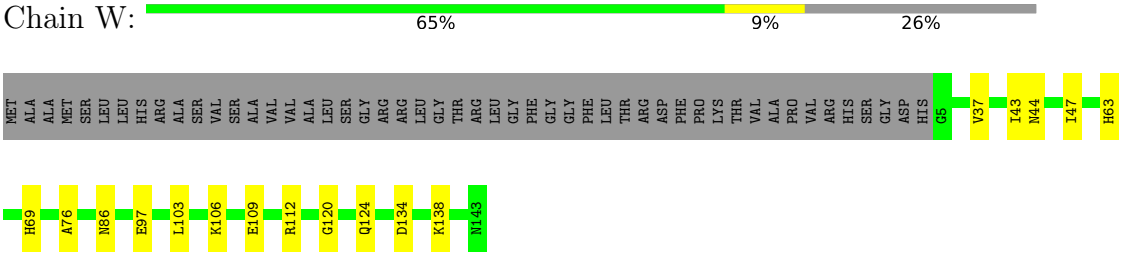
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V:



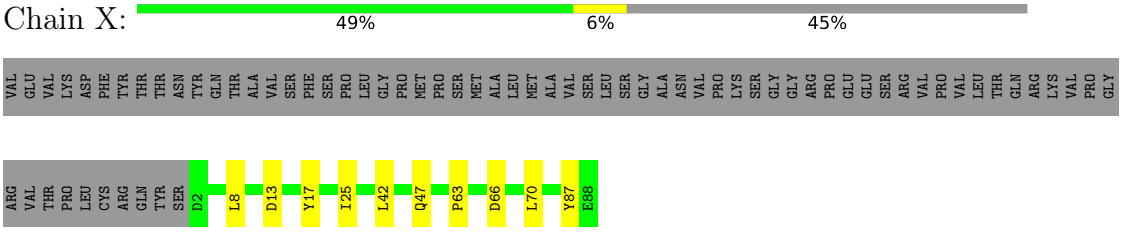
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W:



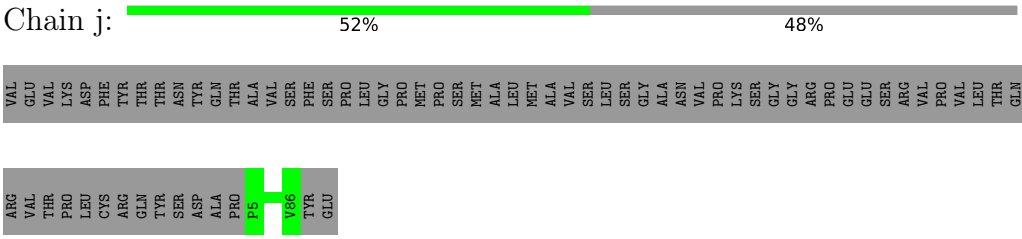
• Molecule 17: Acyl carrier protein

Chain X:



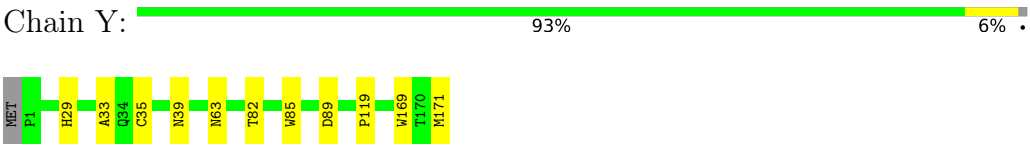
• Molecule 17: Acyl carrier protein

Chain j:



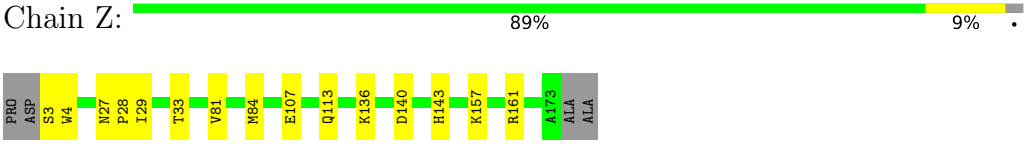
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:



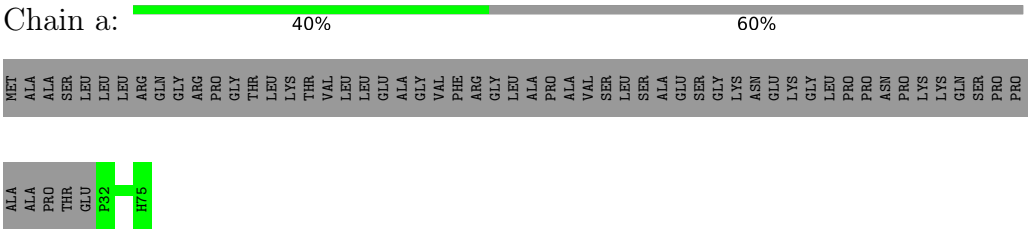
• Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:



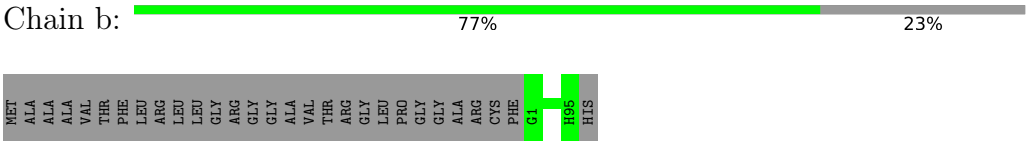
• Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:



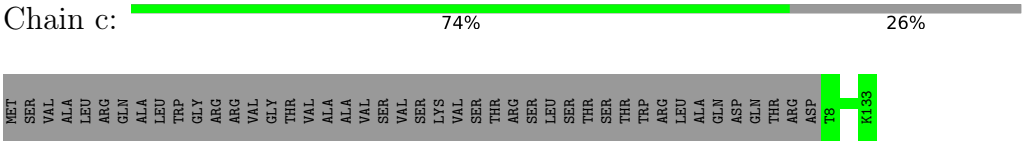
• Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:



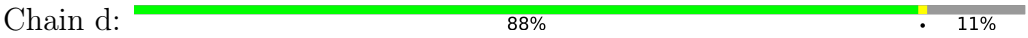
• Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

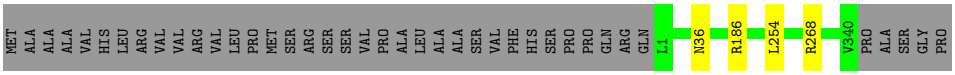
Chain c:



• Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

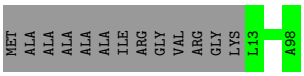
Chain d:





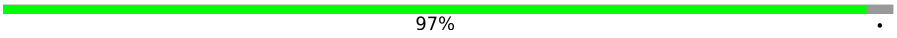
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

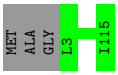
Chain e:



• Molecule 25: Mitochondrial complex I, B13 subunit

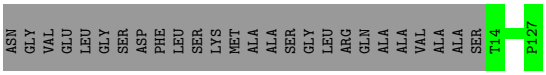
Chain f:





• Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:

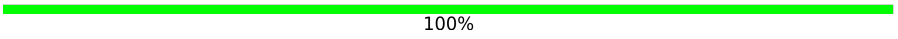


• Molecule 27: Mitochondrial complex I, B14.5a subunit

Chain h:

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

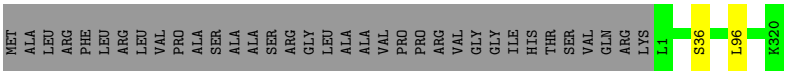
Chain i:



There are no outlier residues recorded for this chain.

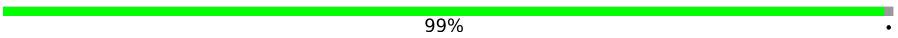
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:



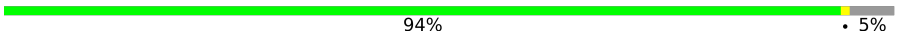
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

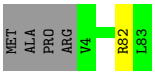
Chain l:



• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

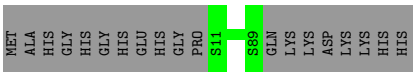
Chain m:





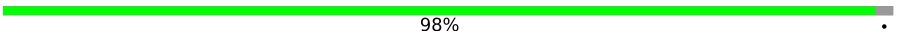
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n:



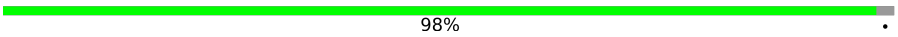
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:



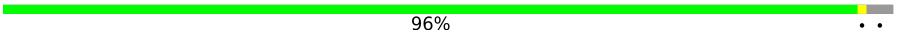
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

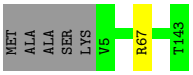
Chain p:



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

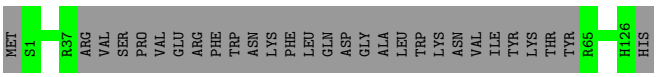
Chain q:





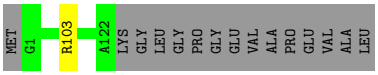
• Molecule 36: Mitochondrial complex I, B17 subunit

Chain r:



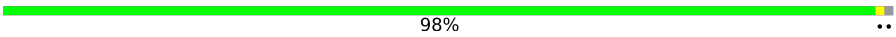
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain s:



• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain t:



• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u:

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

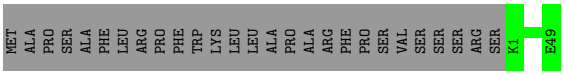
Chain v:

• Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w:

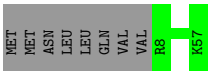
• Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x:



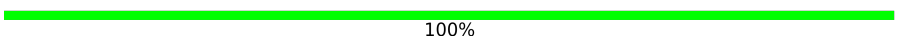
• Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y:



• Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7162	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: 3PE, NDP, K, FMN, PC1, 970, AYA, CDL, FES, SEP, 2MR, ZMP, AMP, NAI, ZN, MYR, SF4, FME

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	0.35	0/3386	0.56	0/4575
2	2	0.33	0/1695	0.54	0/2306
3	3	0.34	0/5362	0.55	0/7266
4	4	0.38	0/3535	0.56	0/4791
5	5	0.35	0/1776	0.55	2/2417 (0.1%)
6	6	0.41	0/1278	0.56	0/1728
7	9	0.39	0/1445	0.56	0/1956
8	A	0.33	0/947	0.63	2/1296 (0.2%)
9	H	0.35	0/2603	0.64	0/3561
10	J	0.36	0/1378	0.65	2/1868 (0.1%)
11	K	0.31	0/749	0.62	0/1014
12	L	0.32	0/4925	0.56	0/6700
13	M	0.33	0/3731	0.61	1/5085 (0.0%)
14	N	0.34	0/2787	0.59	1/3795 (0.0%)
15	V	0.27	0/1041	0.51	0/1412
16	W	0.30	0/1188	0.52	0/1607
17	X	0.27	0/713	0.51	0/963
17	j	0.29	0/670	0.51	0/902
18	Y	0.30	0/1440	0.53	0/1942
19	Z	0.30	0/1475	0.50	0/1989
20	a	0.28	0/383	0.48	0/518
21	b	0.32	0/749	0.47	0/1009
22	c	0.30	0/1047	0.51	0/1415
23	d	0.30	0/2824	0.55	1/3830 (0.0%)
24	e	0.28	0/702	0.51	0/945
25	f	0.29	0/937	0.51	0/1271
26	g	0.32	0/993	0.52	0/1336
27	h	0.31	0/779	0.55	0/1053
28	i	0.33	0/1250	0.51	0/1698
29	k	0.30	0/2646	0.50	1/3579 (0.0%)
30	l	0.30	0/896	0.52	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	m	0.28	0/647	0.49	0/890
32	n	0.30	0/653	0.45	0/882
33	o	0.32	0/1035	0.49	0/1398
34	p	0.28	0/1085	0.49	0/1467
35	q	0.30	0/1171	0.50	0/1579
36	r	0.29	0/874	0.52	0/1188
37	s	0.27	0/1072	0.48	0/1436
38	t	0.30	0/1573	0.51	1/2130 (0.0%)
39	u	0.30	0/590	0.47	0/810
40	v	0.29	0/1361	0.52	1/1861 (0.1%)
41	w	0.30	0/872	0.51	0/1185
42	x	0.27	0/425	0.41	0/576
43	y	0.27	0/449	0.50	0/605
44	z	0.36	0/591	0.52	0/795
All	All	0.33	0/67728	0.55	12/91829 (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	1
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	254	LEU	CA-CB-CG	6.64	130.56	115.30
10	J	146	LEU	CA-CB-CG	6.30	129.79	115.30
5	5	52	ILE	C-N-CA	6.28	137.40	121.70
10	J	52	LEU	CA-CB-CG	5.94	128.96	115.30
8	A	3	LEU	CA-CB-CG	5.83	128.72	115.30
40	v	93	PRO	C-N-CA	5.48	135.41	121.70
14	N	146	LEU	CA-CB-CG	5.44	127.81	115.30
5	5	144	ASN	C-N-CA	5.21	134.73	121.70
8	A	13	LEU	CA-CB-CG	5.16	127.16	115.30
29	k	96	LEU	CA-CB-CG	5.11	127.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	t	152	ALA	C-N-CA	5.08	134.39	121.70
13	M	458	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (4) 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

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	53	0
2	2	1655	0	1668	14	0
3	3	5275	0	5300	66	0
4	4	3457	0	3397	56	0
5	5	1726	0	1676	27	0
6	6	1247	0	1259	20	0
7	9	1414	0	1371	20	0
8	A	922	0	953	17	0
9	H	2528	0	2641	43	0
10	J	1344	0	1364	19	0
11	K	749	0	793	20	0
12	L	4807	0	4949	55	0
13	M	3647	0	3849	46	0
14	N	2723	0	2930	43	0
15	V	1028	0	1036	10	0
16	W	1155	0	1177	11	0
17	X	701	0	692	5	0
17	j	660	0	663	0	0
18	Y	1403	0	1392	7	0
19	Z	1441	0	1419	9	0
20	a	371	0	344	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	3	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	0	0
47	1	44	0	27	2	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	4	29	0	0	0	0
51	4	40	0	54	1	0
51	6	51	0	82	3	0
51	A	51	0	82	0	0
51	J	91	0	136	2	0
51	L	82	0	118	1	0
51	M	44	0	65	1	0
51	N	51	0	82	0	0
51	V	64	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	i	51	0	82	0	0
51	o	31	0	36	0	0
52	6	46	0	69	1	0
52	9	54	0	88	4	0
52	L	54	0	88	5	0
52	M	108	0	176	8	0
53	L	185	0	276	12	0
53	M	100	0	156	3	0
53	N	90	0	133	7	0
53	V	94	0	141	4	0
53	W	100	0	156	7	0
53	h	58	0	60	0	0
53	x	75	0	97	0	0
54	X	31	0	34	1	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	0	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67950	0	68834	489	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 6.

All (489) 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)
14:N:242:ILE:HG23	53:N:402:CDL:H791	1.73	0.71
5:5:129:TRP:O	5:5:132:ARG:HB3	1.92	0.70
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.74	0.69
11:K:70:GLU:O	11:K:73:LEU:HB3	1.92	0.68
4:4:405:MET:SD	4:4:421:GLN:NE2	2.68	0.66
4:4:58:ALA:HB1	4:4:62:LEU:HB3	1.78	0.64
13:M:139:GLN:HG3	13:M:340:ARG:HH22	1.62	0.64
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.80	0.64
11:K:77:LEU:HD21	14:N:57:THR:HA	1.80	0.64
1:1:213:VAL:HG13	1:1:217:GLY:HA2	1.81	0.62
3:3:193:SER:H	3:3:196:SER:HB3	1.64	0.62
12:L:363:PHE:HA	12:L:370:THR:HG21	1.81	0.61
6:6:81:ARG:NH2	8:A:35:SER:O	2.32	0.61
9:H:100:LEU:HD23	9:H:160:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:77:ASP:HB3	5:5:95:ASN:HD22	1.65	0.61
4:4:226:GLU:OE1	4:4:305:ARG:NH2	2.33	0.61
14:N:30:TRP:NE1	14:N:67:SER:OG	2.34	0.61
18:Y:29:HIS:HB3	18:Y:119:PRO:HD2	1.81	0.60
1:1:245:PHE:HB3	1:1:271:GLU:HG3	1.84	0.60
17:X:25:ILE:HD11	17:X:42:LEU:HD11	1.84	0.60
52:6:202:PC1:H121	8:A:26:GLN:HG2	1.82	0.60
4:4:63:ARG:HB3	4:4:79:HIS:HB2	1.84	0.60
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.84	0.59
7:9:94:ILE:HA	7:9:108:ARG:O	2.03	0.59
53:L:1005:CDL:H642	53:L:1005:CDL:H562	1.84	0.59
52:M:502:PC1:H272	53:W:201:CDL:H402	1.85	0.59
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.68	0.59
12:L:453:SER:HA	12:L:456:ARG:HH21	1.68	0.59
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.36	0.58
3:3:163:ALA:HA	3:3:167:ALA:HB3	1.85	0.58
13:M:94:LEU:HD13	53:N:402:CDL:H762	1.85	0.58
1:1:97:ALA:HB1	1:1:111:ILE:HD11	1.84	0.58
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.84	0.58
9:H:165:LEU:HD21	9:H:241:LEU:HA	1.84	0.58
16:W:44:ASN:OD1	16:W:69:HIS:NE2	2.37	0.58
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.35	0.58
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.37	0.58
8:A:56:PHE:O	10:J:70:TYR:OH	2.21	0.58
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.86	0.58
1:1:194:GLU:OE2	1:1:204:ARG:NE	2.36	0.57
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.35	0.57
6:6:118:SER:N	45:6:201:SF4:S4	2.78	0.57
13:M:159:PRO:HD3	14:N:284:ILE:HD11	1.86	0.57
8:A:57:LEU:HD21	10:J:169:MET:HG2	1.86	0.57
9:H:114:TYR:OH	10:J:61:LEU:O	2.23	0.57
4:4:163:ALA:HB2	9:H:278:PRO:HG3	1.86	0.57
1:1:89:ARG:NH1	1:1:217:GLY:O	2.37	0.57
1:1:361:GLN:N	45:1:501:SF4:S4	2.75	0.57
4:4:51:PHE:HB3	4:4:64:LEU:HB2	1.87	0.57
8:A:67:LEU:HD22	11:K:65:VAL:HA	1.85	0.57
9:H:87:ILE:HG22	9:H:95:LEU:HD23	1.86	0.57
5:5:65:ARG:NH1	5:5:123:VAL:O	2.38	0.57
4:4:233:ARG:NH2	7:9:23:GLN:O	2.37	0.57
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.87	0.57
12:L:231:PRO:HB3	12:L:530:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.86	0.56
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.87	0.56
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.38	0.56
3:3:360:SER:O	3:3:365:ASN:ND2	2.34	0.56
10:J:81:GLU:OE1	11:K:23:ARG:NH2	2.38	0.56
51:J:201:3PE:H2G1	51:J:201:3PE:H3A1	1.86	0.56
11:K:66:PHE:HA	11:K:69:CYS:HB3	1.88	0.56
12:L:421:ILE:HG12	12:L:501:ALA:HB2	1.86	0.56
52:L:1003:PC1:H271	52:M:502:PC1:H281	1.87	0.56
1:1:21:ILE:O	1:1:117:LYS:NZ	2.38	0.56
4:4:165:THR:HG23	9:H:32:GLN:HG2	1.86	0.56
7:9:23:GLN:HG3	7:9:28:THR:HB	1.87	0.56
16:W:63:HIS:NE2	16:W:76:ALA:O	2.39	0.56
3:3:524:LEU:HB2	3:3:545:TYR:HA	1.88	0.56
3:3:110:GLN:NE2	3:3:113:GLU:O	2.39	0.56
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.87	0.56
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.87	0.56
52:L:1003:PC1:H2A1	53:L:1005:CDL:H841	1.88	0.55
14:N:122:ILE:O	14:N:176:ARG:NH1	2.39	0.55
5:5:137:MET:HA	5:5:161:PRO:HD2	1.87	0.55
13:M:373:ILE:HG22	13:M:376:ILE:HD12	1.87	0.55
1:1:358:SER:OG	1:1:365:CYS:SG	2.63	0.55
3:3:323:VAL:HG11	3:3:525:LEU:HD13	1.89	0.55
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.39	0.55
1:1:69:GLY:O	47:1:503:NAI:N7N	2.37	0.55
1:1:299:PRO:HD3	1:1:306:LEU:HA	1.88	0.55
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.88	0.55
8:A:80:GLN:NE2	9:H:315:PRO:O	2.39	0.55
14:N:238:PRO:HB2	53:N:402:CDL:HB4	1.86	0.55
14:N:246:ILE:HD13	53:N:402:CDL:H591	1.89	0.55
17:X:47:GLN:NE2	17:X:70:LEU:O	2.39	0.55
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.38	0.55
4:4:184:VAL:O	7:9:60:ARG:NH1	2.37	0.55
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.40	0.55
1:1:287:VAL:HG21	1:1:294:LEU:HB2	1.88	0.54
4:4:64:LEU:HD11	4:4:418:ILE:HD11	1.89	0.54
9:H:20:LEU:HD21	9:H:231:ILE:HD11	1.89	0.54
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.87	0.54
53:M:504:CDL:OB4	18:Y:171:MET:SD	2.64	0.54
1:1:94:VAL:HG11	1:1:192:LEU:HD21	1.88	0.54
10:J:67:VAL:HG11	11:K:31:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:6:203:3PE:H242	9:H:46:LEU:HD21	1.90	0.54
10:J:41:CYS:HA	10:J:44:VAL:HG12	1.90	0.54
16:W:44:ASN:ND2	53:W:201:CDL:OB4	2.39	0.54
3:3:47:SER:O	3:3:161:ARG:NH1	2.40	0.54
9:H:102:VAL:HG11	9:H:154:LEU:HD11	1.89	0.54
9:H:169:GLN:NE2	9:H:241:LEU:O	2.41	0.54
11:K:64:LEU:O	11:K:67:ALA:HB3	2.07	0.54
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.88	0.54
3:3:396:ARG:NH1	3:3:416:THR:O	2.41	0.54
3:3:158:ARG:NH1	3:3:202:ILE:O	2.39	0.54
11:K:93:LEU:HB3	14:N:54:GLU:HG3	1.88	0.54
13:M:453:ILE:HG13	13:M:454:ILE:HG23	1.88	0.54
52:9:401:PC1:H32	9:H:288:LEU:HD11	1.89	0.54
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.39	0.54
15:V:39:SER:OG	15:V:54:ARG:NH2	2.41	0.54
3:3:174:THR:HG22	3:3:183:VAL:HG22	1.89	0.53
14:N:189:TRP:HZ2	14:N:286:ALA:HB2	1.73	0.53
3:3:674:THR:O	3:3:679:ARG:NH1	2.42	0.53
12:L:88:MET:HB2	12:L:326:PHE:HE2	1.74	0.53
52:L:1003:PC1:H3B2	53:W:201:CDL:H131	1.91	0.53
9:H:20:LEU:HD23	9:H:228:TYR:HB3	1.91	0.53
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.91	0.53
9:H:81:LEU:HA	9:H:84:THR:HG22	1.90	0.53
10:J:23:LYS:O	11:K:23:ARG:NH1	2.42	0.53
5:5:195:ARG:NH2	7:9:92:ILE:O	2.36	0.52
4:4:190:HIS:HD2	6:6:150:PRO:HD3	1.73	0.52
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.91	0.52
8:A:67:LEU:HD11	11:K:68:ALA:HB3	1.90	0.52
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.91	0.52
2:2:172:ILE:HG23	2:2:182:PRO:HG2	1.92	0.52
16:W:43:ILE:HG12	16:W:47:ILE:HD12	1.90	0.52
4:4:35:ASP:O	14:N:49:ASN:ND2	2.42	0.52
4:4:83:LEU:HD11	6:6:53:ALA:HB2	1.91	0.52
8:A:73:LEU:HD12	9:H:151:LEU:HD13	1.91	0.52
1:1:141:GLU:HG2	2:2:145:LEU:HD22	1.90	0.52
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.92	0.52
3:3:426:PRO:HG3	3:3:661:LEU:HG	1.92	0.52
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.92	0.52
13:M:352:LEU:HB3	13:M:355:MET:HB3	1.91	0.52
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.43	0.52
9:H:206:GLU:OE1	9:H:279:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:158:LEU:HD23	14:N:283:ALA:HB1	1.92	0.52
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.28	0.51
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.91	0.51
3:3:518:PRO:HB2	3:3:538:PRO:HD3	1.92	0.51
1:1:365:CYS:HB2	45:1:501:SF4:S3	2.50	0.51
2:2:10:ARG:NH2	3:3:138:GLU:OE2	2.44	0.51
3:3:228:ILE:HB	3:3:583:THR:HG22	1.92	0.51
3:3:365:ASN:N	3:3:491:ASN:OD1	2.44	0.51
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.74	0.51
7:9:132:VAL:HG21	7:9:165:ILE:HG21	1.91	0.51
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.92	0.51
1:1:299:PRO:HG3	1:1:307:ILE:HG12	1.92	0.51
3:3:206:GLY:N	45:3:801:SF4:S2	2.76	0.51
9:H:289:LEU:HA	9:H:293:PHE:HB2	1.92	0.51
11:K:60:PRO:O	11:K:63:LEU:HB3	2.10	0.51
12:L:139:GLN:HG3	53:L:1005:CDL:H873	1.92	0.51
53:L:1005:CDL:H741	13:M:369:LEU:HD21	1.92	0.51
14:N:211:MET:HG2	14:N:333:SER:HB2	1.92	0.51
8:A:98:LEU:HD22	9:H:298:LEU:HD11	1.92	0.51
2:2:55:GLN:NE2	2:2:89:MET:O	2.44	0.51
9:H:161:THR:HG22	9:H:163:SER:H	1.76	0.51
1:1:126:GLY:HA2	1:1:131:ALA:HB3	1.92	0.50
13:M:1:FME:O1	13:M:3:LYS:NZ	2.43	0.50
14:N:128:LEU:HD13	14:N:216:PHE:HB2	1.93	0.50
1:1:140:GLY:O	1:1:179:ARG:NH2	2.40	0.50
12:L:106:TRP:HD1	12:L:447:ASN:HD22	1.58	0.50
12:L:579:SER:O	15:V:43:LYS:NZ	2.43	0.50
3:3:285:ARG:NH1	3:3:289:GLY:O	2.44	0.50
1:1:118:LEU:HD13	1:1:225:VAL:HG13	1.93	0.50
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.39	0.50
3:3:524:LEU:HD22	3:3:527:ALA:HB3	1.94	0.50
1:1:95:VAL:HG11	1:1:118:LEU:HD11	1.94	0.50
13:M:179:LEU:HB3	13:M:249:LEU:HD21	1.94	0.50
4:4:47:LEU:HD13	8:A:51:PHE:HD1	1.75	0.50
4:4:280:GLN:O	4:4:317:LYS:NZ	2.40	0.50
11:K:95:LEU:O	14:N:51:ARG:NH1	2.45	0.50
13:M:70:MET:HG2	13:M:103:GLN:HE21	1.77	0.50
16:W:103:LEU:HD23	16:W:106:LYS:HD2	1.93	0.49
16:W:109:GLU:OE2	16:W:112:ARG:NH2	2.43	0.49
3:3:222:THR:HA	3:3:242:THR:O	2.12	0.49
3:3:319:ALA:HB3	3:3:345:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:158:ALA:HB1	4:4:163:ALA:HB3	1.93	0.49
13:M:61:LEU:HB2	13:M:457:PRO:HG3	1.94	0.49
13:M:2:LEU:HD11	53:M:504:CDL:H142	1.95	0.49
4:4:188:ARG:HH21	6:6:152:THR:HB	1.77	0.49
13:M:155:ALA:HB1	52:M:503:PC1:H2H2	1.95	0.49
17:X:63:PRO:HG2	17:X:66:ASP:HB2	1.94	0.49
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.95	0.49
12:L:249:SER:HB2	12:L:336:LYS:HG3	1.94	0.49
16:W:134:ASP:O	16:W:138:LYS:NZ	2.45	0.49
52:L:1003:PC1:H262	53:W:201:CDL:H621	1.95	0.49
14:N:112:HIS:HB2	14:N:184:ILE:HD13	1.93	0.49
3:3:12:PHE:HB2	3:3:78:ASN:HA	1.95	0.49
7:9:92:ILE:HA	7:9:110:ASP:O	2.13	0.49
12:L:69:LEU:HD23	12:L:76:LEU:HD12	1.95	0.49
52:L:1003:PC1:H2B1	13:M:449:LEU:HD23	1.94	0.49
53:L:1004:CDL:H362	53:L:1004:CDL:H542	1.93	0.49
13:M:232:ALA:O	13:M:237:LYS:NZ	2.39	0.49
16:W:120:GLY:O	16:W:124:GLN:NE2	2.45	0.49
6:6:35:ASP:HB3	51:6:203:3PE:H331	1.93	0.48
15:V:11:ILE:HB	15:V:20:LYS:HD3	1.94	0.48
15:V:32:GLY:HA3	15:V:59:THR:HA	1.94	0.48
1:1:432:ARG:HA	1:1:435:GLN:HG3	1.95	0.48
15:V:1:AYA:HA	15:V:4:LEU:HD23	1.95	0.48
1:1:139:ARG:NH2	2:2:144:CYS:O	2.39	0.48
6:6:36:LEU:HD22	51:6:203:3PE:H3A1	1.95	0.48
9:H:111:LEU:HD22	10:J:57:PHE:HZ	1.79	0.48
51:J:202:3PE:O14	12:L:585:LYS:NZ	2.44	0.48
12:L:362:LEU:HA	12:L:365:ALA:HB3	1.95	0.48
12:L:584:ILE:HG12	14:N:58:LYS:HG2	1.95	0.48
53:L:1005:CDL:H232	53:W:201:CDL:H752	1.95	0.48
6:6:165:LYS:O	6:6:169:ARG:NH1	2.46	0.48
7:9:69:ARG:NH1	7:9:73:GLY:O	2.44	0.48
12:L:245:ALA:O	12:L:249:SER:OG	2.31	0.48
4:4:211:ILE:HG22	4:4:315:LEU:HD11	1.96	0.48
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.78	0.48
10:J:17:PHE:O	10:J:21:SER:CB	2.62	0.48
53:L:1004:CDL:H162	53:V:203:CDL:H541	1.96	0.48
3:3:410:GLY:O	3:3:421:HIS:NE2	2.43	0.48
4:4:238:ARG:NH1	9:H:279:ARG:O	2.46	0.48
5:5:93:VAL:HG22	5:5:108:LYS:HG2	1.96	0.48
12:L:402:SER:OG	12:L:404:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.95	0.48
3:3:332:LYS:NZ	3:3:505:LEU:O	2.47	0.48
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.95	0.48
9:H:121:TRP:HB2	10:J:68:PHE:HZ	1.79	0.48
12:L:316:THR:HA	12:L:319:ILE:HG12	1.96	0.48
12:L:558:LEU:HB3	13:M:214:LEU:HD21	1.96	0.48
3:3:495:ARG:HG3	3:3:496:ILE:HG12	1.95	0.48
12:L:50:PRO:HA	12:L:53:MET:HG2	1.95	0.48
13:M:318:ALA:HB2	13:M:373:ILE:HG13	1.94	0.48
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.95	0.47
12:L:556:ILE:O	12:L:560:THR:N	2.47	0.47
4:4:106:LEU:HD13	4:4:391:ILE:HG21	1.96	0.47
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.49	0.47
3:3:382:THR:HB	3:3:454:GLY:HA3	1.95	0.47
5:5:79:THR:HB	5:5:93:VAL:HB	1.97	0.47
52:M:503:PC1:H2E1	14:N:284:ILE:HG13	1.97	0.47
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.96	0.47
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.95	0.47
12:L:152:PHE:HB2	12:L:172:ILE:HD11	1.96	0.47
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.96	0.47
4:4:84:HIS:NE2	6:6:130:TYR:OH	2.36	0.47
14:N:270:MET:O	14:N:275:SER:OG	2.27	0.47
3:3:26:VAL:HG13	3:3:79:ILE:HD13	1.95	0.47
19:Z:81:VAL:HA	19:Z:84:MET:HG2	1.97	0.47
4:4:61:VAL:HG21	4:4:83:LEU:HB2	1.95	0.47
4:4:154:VAL:HG11	4:4:225:LEU:HD21	1.95	0.47
8:A:28:ASN:O	8:A:33:LYS:NZ	2.43	0.47
53:L:1005:CDL:H832	52:M:502:PC1:H2E1	1.97	0.47
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.96	0.47
1:1:97:ALA:HB3	1:1:138:ILE:HA	1.96	0.47
13:M:50:LEU:HA	16:W:86:ASN:HD21	1.80	0.47
14:N:110:PRO:HD3	14:N:160:LEU:HD23	1.96	0.47
14:N:193:VAL:HB	14:N:266:ILE:HG23	1.97	0.47
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.33	0.47
5:5:94:TYR:HB2	5:5:107:VAL:HB	1.96	0.47
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.97	0.47
14:N:20:VAL:HG11	14:N:137:ALA:HB1	1.97	0.47
1:1:139:ARG:NE	1:1:141:GLU:OE1	2.48	0.46
1:1:390:ASP:O	1:1:393:TRP:HB3	2.16	0.46
5:5:121:VAL:HG21	5:5:146:PRO:HD3	1.97	0.46
7:9:158:GLY:O	7:9:162:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:9:401:PC1:H351	9:H:187:ILE:HD12	1.97	0.46
9:H:6:VAL:HG22	9:H:95:LEU:HD21	1.97	0.46
13:M:119:TYR:HE1	13:M:157:SER:HB2	1.80	0.46
14:N:245:LEU:HD23	53:N:402:CDL:H792	1.97	0.46
3:3:284:VAL:HG12	3:3:559:VAL:HG13	1.97	0.46
5:5:79:THR:O	5:5:93:VAL:N	2.39	0.46
1:1:205:LEU:HD22	3:3:70:ALA:HB3	1.98	0.46
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.97	0.46
1:1:49:LEU:HD11	1:1:123:LEU:HD21	1.98	0.46
2:2:105:THR:OG1	48:2:300:FES:S2	2.74	0.46
9:H:106:LEU:HD22	9:H:150:LEU:HD23	1.97	0.46
12:L:69:LEU:HB3	12:L:76:LEU:HB2	1.98	0.46
5:5:138:PHE:O	5:5:163:ARG:NE	2.49	0.46
15:V:1:AYA:HM2	15:V:3:THR:HG22	1.97	0.46
18:Y:85:TRP:O	18:Y:89:ASP:HB2	2.16	0.46
1:1:99:GLU:OE2	1:1:106:LYS:N	2.48	0.46
4:4:233:ARG:HH11	52:9:401:PC1:H2	1.81	0.46
5:5:78:LEU:HB3	5:5:130:TYR:HB3	1.98	0.46
12:L:561:ILE:O	12:L:565:THR:OG1	2.33	0.46
13:M:408:LEU:O	13:M:412:ILE:N	2.49	0.46
8:A:6:THR:HG21	9:H:87:ILE:HG21	1.98	0.46
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.96	0.46
3:3:14:ASP:OD2	3:3:81:THR:OG1	2.34	0.45
53:L:1004:CDL:H152	53:V:203:CDL:H712	1.97	0.45
3:3:475:GLN:NE2	3:3:643:GLN:OE1	2.38	0.45
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.51	0.45
14:N:239:ILE:HA	14:N:242:ILE:HD12	1.98	0.45
3:3:564:ALA:HB3	3:3:569:LYS:HD3	1.98	0.45
9:H:199:ASP:HB2	9:H:279:ARG:HD2	1.98	0.45
10:J:34:ILE:HG13	10:J:64:MET:HG3	1.98	0.45
19:Z:143:HIS:O	19:Z:157:LYS:NZ	2.39	0.45
3:3:503:LEU:HD21	3:3:509:PRO:HB3	1.99	0.45
4:4:145:THR:HG1	4:4:181:TYR:HH	1.62	0.45
6:6:62:MET:SD	6:6:69:MET:HB3	2.57	0.45
10:J:23:LYS:NZ	11:K:18:GLY:O	2.41	0.45
11:K:79:VAL:O	11:K:83:ASN:N	2.50	0.45
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.97	0.45
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.99	0.45
17:X:8:LEU:H	17:X:87:TYR:HE2	1.64	0.45
4:4:145:THR:OG1	4:4:181:TYR:OH	2.28	0.45
9:H:119:SER:HB2	9:H:215:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:496:LEU:HD23	12:L:499:ILE:HD12	1.98	0.45
3:3:287:GLU:HG2	3:3:288:LYS:HG3	1.98	0.45
3:3:296:TRP:HE1	3:3:592:LEU:HB3	1.81	0.45
6:6:155:ALA:HB2	7:9:137:PHE:HD2	1.82	0.45
12:L:331:THR:HG22	12:L:335:PHE:HE1	1.82	0.45
4:4:111:MET:SD	4:4:111:MET:N	2.88	0.45
12:L:73:THR:HB	12:L:194:ASN:HD21	1.82	0.45
13:M:243:MET:HA	13:M:246:ILE:HG22	1.99	0.45
5:5:204:GLU:OE2	5:5:210:ARG:NE	2.50	0.45
9:H:26:LYS:HG2	9:H:36:GLY:HA3	1.99	0.45
1:1:99:GLU:OE2	1:1:107:ASP:N	2.47	0.44
4:4:387:TYR:CZ	5:5:164:LYS:HE3	2.52	0.44
8:A:95:ILE:HG23	9:H:298:LEU:HD22	1.99	0.44
12:L:396:ILE:HG21	12:L:490:ALA:HB2	1.98	0.44
13:M:175:ASN:HD22	16:W:97:GLU:HG3	1.82	0.44
1:1:21:ILE:HG12	1:1:233:THR:HG21	1.99	0.44
1:1:261:HIS:ND1	1:1:338:ASP:OD1	2.51	0.44
4:4:141:PHE:O	4:4:145:THR:OG1	2.35	0.44
9:H:184:MET:SD	9:H:297:THR:OG1	2.75	0.44
13:M:116:ILE:HD11	13:M:161:LEU:HD12	1.99	0.44
1:1:363:THR:HG21	3:3:97:LEU:HG	1.98	0.44
9:H:87:ILE:HG13	9:H:88:PRO:HD3	2.00	0.44
14:N:109:ALA:HB3	14:N:161:SER:HA	2.00	0.44
14:N:128:LEU:HD11	14:N:213:SER:HA	1.98	0.44
3:3:269:PHE:HB3	3:3:683:THR:HG21	2.00	0.44
4:4:87:THR:HG21	4:4:106:LEU:HD21	2.00	0.44
5:5:72:PHE:HB3	5:5:96:LEU:HB3	1.99	0.44
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.99	0.44
19:Z:3:SER:OG	19:Z:4:TRP:N	2.50	0.44
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.82	0.44
4:4:412:ALA:HB3	9:H:281:ARG:HG3	1.99	0.44
9:H:59:GLU:HA	9:H:60:PRO:HD3	1.89	0.44
12:L:221:THR:HG22	12:L:229:LEU:HB2	1.99	0.44
15:V:127:GLY:HA3	51:V:202:3PE:H342	2.00	0.44
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.98	0.44
13:M:91:ARG:HD3	13:M:135:ARG:HH21	1.83	0.44
1:1:131:ALA:O	1:1:171:TYR:OH	2.34	0.44
1:1:356:HIS:O	3:3:177:ARG:NH2	2.50	0.44
5:5:60:VAL:O	5:5:63:PHE:HB3	2.18	0.44
14:N:258:SER:O	14:N:261:MET:HB3	2.18	0.44
3:3:237:ASN:OD1	3:3:253:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:56:GLY:HA2	5:5:59:PRO:HD2	2.00	0.43
6:6:144:ILE:HG13	6:6:163:LEU:HB2	2.00	0.43
9:H:195:ARG:HH12	9:H:274:ARG:HH11	1.65	0.43
13:M:23:ILE:HD11	13:M:92:LYS:HD2	2.00	0.43
13:M:196:TRP:HE3	13:M:197:LEU:HD12	1.83	0.43
9:H:293:PHE:O	9:H:297:THR:OG1	2.28	0.43
1:1:261:HIS:NE2	2:2:110:LEU:O	2.41	0.43
2:2:147:ALA:HB3	2:2:153:MET:HG2	1.99	0.43
3:3:324:ASP:OD1	3:3:324:ASP:N	2.44	0.43
5:5:41:GLN:NE2	5:5:49:GLU:OE1	2.48	0.43
12:L:420:ALA:HB2	12:L:494:THR:HG23	1.99	0.43
3:3:140:LYS:HD3	3:3:150:MET:HG3	2.00	0.43
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.83	0.43
4:4:373:GLU:OE2	5:5:104:ARG:NH1	2.52	0.43
12:L:67:HIS:NE2	12:L:75:LYS:HG3	2.34	0.43
12:L:601:LEU:O	15:V:1:AYA:N	2.46	0.43
53:L:1005:CDL:H251	53:L:1005:CDL:H201	1.99	0.43
4:4:363:THR:O	4:4:377:TYR:HA	2.18	0.43
3:3:80:LEU:HB3	3:3:83:SER:HB3	1.99	0.43
3:3:175:THR:HG21	3:3:186:TYR:HB2	2.00	0.43
3:3:354:ALA:HB3	3:3:361:ASN:HD21	1.84	0.43
5:5:49:GLU:HG2	5:5:106:ARG:HD2	2.01	0.43
3:3:568:GLU:HB3	3:3:589:PRO:HG3	1.99	0.43
10:J:17:PHE:O	10:J:21:SER:OG	2.32	0.43
8:A:51:PHE:HD2	9:H:133:LEU:HD12	1.84	0.43
9:H:24:GLU:HA	9:H:271:LEU:HD13	2.00	0.43
14:N:149:ILE:HB	14:N:195:LEU:HD21	1.99	0.43
3:3:272:ASP:HA	3:3:275:LYS:HG2	2.00	0.43
4:4:323:ILE:H	4:4:323:ILE:HG13	1.71	0.43
10:J:98:LEU:O	10:J:102:LEU:HB2	2.19	0.43
53:N:402:CDL:H851	53:N:402:CDL:H821	1.88	0.43
13:M:167:ILE:HD13	13:M:249:LEU:HD13	2.00	0.42
1:1:74:PRO:HB2	1:1:77:LEU:HB3	2.01	0.42
12:L:203:MET:HB2	19:Z:113:GLN:HG3	2.00	0.42
13:M:216:LEU:HD11	13:M:236:LEU:HD11	2.00	0.42
1:1:92:TYR:O	1:1:220:THR:HA	2.19	0.42
1:1:300:GLY:HA3	1:1:329:LEU:O	2.19	0.42
2:2:25:PRO:HA	2:2:28:TYR:HD2	1.84	0.42
3:3:215:PHE:HA	7:9:104:ARG:NH1	2.34	0.42
12:L:602:LEU:HD21	53:V:203:CDL:H422	2.01	0.42
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:184:LEU:HD13	13:M:393:ILE:HG21	2.02	0.42
1:1:49:LEU:HD21	1:1:123:LEU:HG	2.02	0.42
4:4:155:THR:HB	4:4:167:PHE:HA	2.01	0.42
12:L:416:THR:O	12:L:419:THR:OG1	2.33	0.42
52:M:502:PC1:H3D2	52:M:502:PC1:H3A1	1.87	0.42
3:3:235:GLY:HA3	3:3:575:ASN:HB3	2.01	0.42
8:A:60:ILE:HG21	10:J:168:ILE:HG21	2.02	0.42
9:H:138:GLN:NE2	9:H:191:ALA:O	2.39	0.42
13:M:132:ILE:HA	13:M:136:TRP:HE3	1.84	0.42
13:M:225:ILE:HD13	13:M:331:ASN:HB2	2.02	0.42
3:3:579:ARG:HE	3:3:636:VAL:HG23	1.85	0.42
1:1:99:GLU:OE1	1:1:108:ARG:N	2.53	0.42
3:3:320:GLY:O	3:3:498:SER:OG	2.34	0.42
51:L:1001:3PE:H262	51:L:1001:3PE:H231	1.82	0.42
7:9:41:LEU:HD13	9:H:31:MET:HG3	2.01	0.42
12:L:542:LEU:HA	12:L:545:SER:HB2	2.02	0.42
14:N:142:LEU:HB3	14:N:194:LEU:HD21	2.02	0.42
14:N:162:ILE:HG13	14:N:188:GLY:HA3	2.02	0.42
4:4:200:HIS:ND1	4:4:201:GLN:HB2	2.35	0.42
9:H:113:VAL:HG21	9:H:139:THR:HG21	2.01	0.42
52:M:502:PC1:H251	53:W:201:CDL:H381	2.01	0.42
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.85	0.41
3:3:227:SER:OG	3:3:228:ILE:N	2.53	0.41
3:3:377:VAL:HG23	3:3:404:LEU:HD11	2.02	0.41
4:4:203:LEU:HD22	4:4:207:LEU:HD23	2.01	0.41
7:9:69:ARG:HG2	7:9:75:GLU:HA	2.01	0.41
53:L:1004:CDL:H572	53:L:1004:CDL:H251	2.02	0.41
52:M:502:PC1:H153	52:M:502:PC1:H111	1.89	0.41
10:J:17:PHE:O	10:J:21:SER:HB2	2.20	0.41
11:K:20:LEU:HD12	12:L:588:PHE:HD1	1.86	0.41
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.53	0.41
1:1:280:ILE:HG22	1:1:286:GLY:HA2	2.03	0.41
1:1:355:LYS:HE2	1:1:355:LYS:HB2	1.92	0.41
12:L:144:TRP:NE1	12:L:179:ASP:OD1	2.53	0.41
13:M:11:LEU:HB3	13:M:100:ILE:HD13	2.03	0.41
18:Y:33:ALA:HB2	18:Y:119:PRO:HG3	2.02	0.41
1:1:193:ILE:HG23	1:1:215:VAL:HA	2.03	0.41
1:1:365:CYS:HB3	45:1:501:SF4:S3	2.57	0.41
12:L:85:PHE:HB3	12:L:258:PHE:HE1	1.86	0.41
53:V:203:CDL:H331	53:V:203:CDL:H181	2.02	0.41
2:2:49:PRO:O	2:2:52:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:362:TYR:HA	3:3:492:ILE:HD12	2.03	0.41
4:4:202:ASP:HA	4:4:323:ILE:HG21	2.02	0.41
6:6:52:LEU:HB2	6:6:90:GLY:HA3	2.02	0.41
13:M:51:ASN:HA	13:M:57:PHE:HB2	2.03	0.41
13:M:204:MET:O	13:M:209:LEU:N	2.54	0.41
1:1:288:THR:O	1:1:293:ASN:ND2	2.52	0.41
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.85	0.41
4:4:104:ASP:HB3	4:4:190:HIS:HD1	1.84	0.41
52:9:401:PC1:H362	9:H:277:TYR:CE2	2.56	0.41
12:L:129:LEU:HA	12:L:132:VAL:HG22	2.02	0.41
4:4:157:HIS:ND1	4:4:419:GLY:HA3	2.35	0.41
11:K:43:LEU:HD12	11:K:43:LEU:HA	1.90	0.41
12:L:75:LYS:HE2	19:Z:107:GLU:HG2	2.02	0.41
13:M:188:ASN:OD1	51:M:501:3PE:N	2.48	0.41
54:X:101:ZMP:H17	54:X:101:ZMP:H15	1.64	0.41
2:2:27:ASN:HB3	2:2:53:LEU:HD21	2.02	0.41
3:3:157:THR:O	3:3:161:ARG:NE	2.47	0.41
4:4:158:ALA:O	4:4:163:ALA:N	2.54	0.41
7:9:64:GLU:OE1	7:9:136:ASN:ND2	2.54	0.41
11:K:59:MET:HG2	14:N:27:LEU:HD22	2.01	0.41
14:N:17:THR:OG1	14:N:133:TRP:NE1	2.52	0.41
1:1:291:TRP:NE1	1:1:313:GLU:OE1	2.48	0.41
1:1:305:PRO:HG3	1:1:413:TRP:HB3	2.02	0.41
4:4:50:ASN:HB3	8:A:38:GLU:HG3	2.03	0.41
4:4:291:GLY:O	4:4:296:ARG:NH1	2.52	0.41
5:5:119:SER:OG	5:5:131:GLU:OE2	2.30	0.41
10:J:117:PHE:HE1	14:N:91:ASN:HD21	1.68	0.41
12:L:362:LEU:O	12:L:370:THR:OG1	2.30	0.41
13:M:329:LEU:HB3	13:M:359:TRP:CZ2	2.55	0.41
14:N:83:GLN:OE1	14:N:85:THR:N	2.49	0.41
14:N:193:VAL:HG11	14:N:266:ILE:HG12	2.03	0.41
14:N:241:THR:HA	14:N:244:VAL:HG22	2.03	0.41
19:Z:136:LYS:NZ	19:Z:140:ASP:OD2	2.53	0.41
4:4:175:GLU:OE2	4:4:188:ARG:NH1	2.54	0.41
51:4:502:3PE:O14	14:N:291:TYR:OH	2.37	0.41
6:6:103:VAL:HG23	8:A:40:GLY:HA2	2.03	0.41
6:6:173:LEU:HA	6:6:176:TRP:HB3	2.03	0.41
12:L:298:ILE:HG13	12:L:426:ILE:HD12	2.02	0.41
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.56	0.41
13:M:118:PHE:O	13:M:122:PHE:CB	2.69	0.41
13:M:208:PRO:HG3	13:M:216:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:78:ILE:H	7:9:78:ILE:HG13	1.62	0.40
12:L:253:VAL:HB	12:L:310:LEU:HD11	2.03	0.40
14:N:159:ILE:HG21	14:N:278:LEU:HD11	2.03	0.40
14:N:261:MET:HG3	14:N:340:THR:HG23	2.03	0.40
17:X:13:ASP:O	17:X:17:TYR:HB2	2.21	0.40
19:Z:27:ASN:HA	19:Z:28:PRO:HD3	1.91	0.40
6:6:87:ILE:HG12	6:6:114:VAL:HB	2.03	0.40
53:M:504:CDL:H741	18:Y:169:TRP:HE1	1.85	0.40
14:N:170:LEU:HD22	14:N:291:TYR:HD2	1.86	0.40
19:Z:29:ILE:O	19:Z:33:THR:OG1	2.33	0.40
1:1:63:SER:HB2	1:1:242:PHE:HD2	1.86	0.40
10:J:111:LYS:O	10:J:121:GLY:N	2.54	0.40
11:K:56:ALA:O	11:K:59:MET:HB3	2.21	0.40
13:M:379:LEU:O	13:M:383:MET:HG2	2.22	0.40
53:N:402:CDL:H341	53:N:402:CDL:H552	2.03	0.40
16:W:37:VAL:HG11	53:W:201:CDL:H862	2.04	0.40
4:4:115:GLU:HB3	4:4:194:VAL:HB	2.03	0.40
11:K:31:LEU:HD23	11:K:31:LEU:HA	1.91	0.40
13:M:325:MET:SD	13:M:441:MET:HB2	2.61	0.40
3:3:229:ASP:OD2	3:3:267:THR:OG1	2.30	0.40
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.47	0.40
5:5:28:TYR:OH	5:5:67:HIS:NE2	2.50	0.40
6:6:94:ASN:HD22	6:6:131:SER:HA	1.87	0.40
12:L:123:LEU:HD13	53:L:1005:CDL:H712	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	408 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	211/246 (86%)	195 (92%)	16 (8%)	0	100	100
3	3	686/727 (94%)	641 (93%)	45 (7%)	0	100	100
4	4	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
5	5	206/266 (77%)	190 (92%)	16 (8%)	0	100	100
6	6	154/223 (69%)	148 (96%)	6 (4%)	0	100	100
7	9	174/217 (80%)	159 (91%)	15 (9%)	0	100	100
8	A	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
9	H	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
10	J	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	22	54
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	564 (93%)	40 (7%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	V	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
16	W	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
17	X	85/157 (54%)	80 (94%)	5 (6%)	0	100	100
17	j	80/157 (51%)	73 (91%)	7 (9%)	0	100	100
18	Y	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
21	b	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
22	c	124/170 (73%)	122 (98%)	2 (2%)	0	100	100
23	d	338/380 (89%)	318 (94%)	20 (6%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
25	f	111/116 (96%)	107 (96%)	4 (4%)	0	100	100
26	g	112/140 (80%)	109 (97%)	3 (3%)	0	100	100
27	h	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
28	i	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
29	k	317/355 (89%)	299 (94%)	18 (6%)	0	100	100
30	l	103/106 (97%)	94 (91%)	9 (9%)	0	100	100
31	m	78/84 (93%)	72 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	n	77/98 (79%)	73 (95%)	4 (5%)	0	100	100
33	o	118/122 (97%)	115 (98%)	3 (2%)	0	100	100
34	p	126/130 (97%)	119 (94%)	7 (6%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
37	s	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
38	t	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
39	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
40	v	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
41	w	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
42	x	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
43	y	48/58 (83%)	48 (100%)	0	0	100	100
44	z	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	8131/9247 (88%)	7712 (95%)	418 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	116	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	343 (100%)	1 (0%)	91	94
2	2	183/210 (87%)	182 (100%)	1 (0%)	86	92
3	3	578/608 (95%)	576 (100%)	2 (0%)	91	94
4	4	370/391 (95%)	367 (99%)	3 (1%)	79	85
5	5	189/230 (82%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	6	132/181 (73%)	130 (98%)	2 (2%)	60 75
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 79
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 94
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%)	291 (99%)	3 (1%)	73 82
24	e	76/82 (93%)	76 (100%)	0	100 100
25	f	101/102 (99%)	101 (100%)	0	100 100
26	g	107/124 (86%)	107 (100%)	0	100 100
27	h	84/96 (88%)	84 (100%)	0	100 100
28	i	131/131 (100%)	131 (100%)	0	100 100
29	k	283/309 (92%)	283 (100%)	0	100 100
30	l	94/95 (99%)	94 (100%)	0	100 100
31	m	69/72 (96%)	68 (99%)	1 (1%)	62 76
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 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	r	95/122 (78%)	95 (100%)	0	100 100
37	s	110/120 (92%)	109 (99%)	1 (1%)	75 84
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%)	7163 (100%)	26 (0%)	88 93

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

Mol	Chain	Res	Type
1	1	148	ASN
2	2	122	LYS
3	3	39	ARG
3	3	179	ASN
4	4	61	VAL
4	4	252	ASN
4	4	430	ARG
6	6	59	MET
6	6	111	ARG
9	H	193	THR
9	H	274	ARG
10	J	86	ASN
11	K	50	ASN
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
23	d	186	ARG
23	d	268	ARG
31	m	82	ARG
35	q	67	ARG
37	s	103	ARG

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Mol	Chain	Res	Type
38	t	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
2	2	42	HIS
3	3	100	ASN
3	3	179	ASN
3	3	535	GLN
4	4	149	ASN
4	4	252	ASN
5	5	95	ASN
6	6	82	GLN
7	9	156	ASN
9	H	230	ASN
10	J	46	ASN
10	J	86	ASN
11	K	52	HIS
11	K	83	ASN
12	L	135	ASN
12	L	199	GLN
12	L	210	ASN
12	L	248	HIS
12	L	270	ASN
13	M	138	ASN
13	M	333	ASN
18	Y	63	ASN
19	Z	55	HIS
20	a	40	ASN
21	b	95	HIS
22	c	29	HIS
22	c	44	ASN
23	d	87	HIS
23	d	288	HIS
25	f	36	HIS
26	g	98	GLN
28	i	5	GLN
29	k	114	HIS
29	k	141	GLN
29	k	153	ASN
30	l	33	HIS

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Mol	Chain	Res	Type
33	o	46	ASN
33	o	117	HIS
34	p	78	ASN
38	t	138	GLN
44	z	40	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	$\#\|Z\| > 2$
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	1.12	1 (14%)
15	AYA	V	1	15	6,7,8	1.16	0	5,8,10	2.00	2 (40%)
29	SEP	k	36	29	8,9,10	1.52	1 (12%)	8,12,14	1.78	2 (25%)
13	FME	M	1	13	8,9,10	1.01	1 (12%)	7,9,11	0.86	0
4	2MR	4	85	4	10,12,13	2.34	3 (30%)	5,13,15	1.69	1 (20%)
11	FME	K	1	11	8,9,10	0.99	1 (12%)	7,9,11	0.81	0
27	AYA	h	1	27	6,7,8	1.14	1 (16%)	5,8,10	1.69	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L	1	12	-	3/7/9/11	-
15	AYA	V	1	15	-	2/4/6/8	-

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	4.80	1.44	1.34
4	4	85	2MR	CZ-NH2	4.73	1.43	1.33
29	k	36	SEP	P-O1P	3.34	1.61	1.50
13	M	1	FME	CA-N	-2.16	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.10	1.42	1.46
27	h	1	AYA	CA-N	-2.02	1.44	1.46
11	K	1	FME	CA-N	-2.01	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	h	1	AYA	CB-CA-N	3.55	113.56	109.61
29	k	36	SEP	P-OG-CB	-3.34	109.09	118.30
29	k	36	SEP	OG-CB-CA	3.31	111.36	108.14
15	V	1	AYA	CB-CA-N	3.30	113.28	109.61
4	4	85	2MR	NE-CZ-NH2	-2.93	116.80	119.48
12	L	1	FME	C-CA-N	2.34	113.95	109.73
15	V	1	AYA	CA-N-CT	2.24	124.78	121.52

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	1	AYA	3	0
13	M	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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	$\#\|Z\| > 2$
50	970	4	501	-	33,33,33	0.42	0	48,50,50	0.57	0
52	PC1	L	1003	-	53,53,53	0.32	0	59,61,61	0.62	2 (3%)
53	CDL	L	1004	-	84,84,99	0.28	0	90,96,111	0.22	0
52	PC1	M	503	-	53,53,53	0.30	0	59,61,61	0.36	0
45	SF4	6	201	6	0,12,12	-	-	-		
45	SF4	9	403	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	3PE	N	401	-	50,50,50	0.34	0	53,55,55	0.55	1 (1%)
51	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.33	0
51	3PE	J	201	-	50,50,50	0.32	0	53,55,55	0.37	0
51	3PE	V	201	-	26,26,50	0.48	0	30,31,55	0.48	1 (3%)
51	3PE	A	201	-	50,50,50	0.32	0	53,55,55	0.33	0
51	3PE	M	501	-	43,43,50	0.34	0	46,48,55	0.40	0
47	NAI	1	503	-	42,48,48	0.60	0	47,73,73	1.99	4 (8%)
53	CDL	L	1005	-	99,99,99	0.25	0	105,111,111	0.30	0
51	3PE	J	202	-	39,39,50	0.35	0	42,44,55	0.48	0
48	FES	3	803	3	0,4,4	-	-	-		
52	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.37	0
53	CDL	W	201	-	99,99,99	0.26	0	105,111,111	0.30	0
45	SF4	9	402	7	0,12,12	-	-	-		
52	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.51	1 (1%)
53	CDL	x	101	-	74,74,99	0.30	0	80,86,111	0.43	1 (1%)
53	CDL	h	201	-	57,57,99	0.30	0	63,69,111	0.34	0
45	SF4	3	802	3	0,12,12	-	-	-		
51	3PE	L	1002	-	30,30,50	0.41	0	33,35,55	0.78	2 (6%)
53	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.27	0
53	CDL	N	402	-	89,89,99	0.29	0	95,101,111	0.40	0
45	SF4	1	501	1	0,12,12	-	-	-		
51	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.31	0
51	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.32	0
48	FES	2	300	2	0,4,4	-	-	-		
54	ZMP	X	101	17	24,30,36	0.84	1 (4%)	29,37,45	0.94	1 (3%)
56	NDP	d	401	-	45,52,52	0.52	0	53,80,80	0.62	1 (1%)
57	AMP	k	501	-	22,25,25	0.88	1 (4%)	25,38,38	1.19	2 (8%)
51	3PE	4	502	-	39,39,50	0.33	0	42,44,55	0.35	0
51	3PE	o	501	-	30,30,50	0.37	0	33,35,55	0.37	0
52	PC1	M	502	-	53,53,53	0.28	0	59,61,61	0.37	0
46	FMN	1	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.29	8 (16%)
54	ZMP	g	201	-	27,33,36	0.66	1 (3%)	32,40,45	1.22	3 (9%)
45	SF4	3	801	3	0,12,12	-	-	-		
58	MYR	s	201	37	14,14,15	0.19	0	13,13,15	0.21	0
51	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.27	0
53	CDL	M	504	-	99,99,99	0.28	0	105,111,111	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	970	4	501	-	-	4/8/41/41	0/5/5/5
53	CDL	L	1004	-	1/1/9/9	28/95/95/110	-
52	PC1	L	1003	-	-	16/57/57/57	-
52	PC1	M	503	-	-	21/57/57/57	-
45	SF4	6	201	6	-	-	0/6/5/5
45	SF4	9	403	7	-	-	0/6/5/5
51	3PE	N	401	-	-	18/54/54/54	-
51	3PE	L	1001	-	-	9/54/54/54	-
51	3PE	J	201	-	-	13/54/54/54	-
51	3PE	V	201	-	-	3/27/27/54	-
51	3PE	A	201	-	-	13/54/54/54	-
51	3PE	M	501	-	-	11/47/47/54	-
47	NAI	1	503	-	-	8/25/72/72	0/5/5/5
53	CDL	L	1005	-	1/1/9/9	34/110/110/110	-
51	3PE	J	202	-	-	17/43/43/54	-
53	CDL	W	201	-	-	21/110/110/110	-
52	PC1	6	202	-	-	11/49/49/57	-
48	FES	3	803	3	-	-	0/1/1/1
52	PC1	9	401	-	-	17/57/57/57	-
45	SF4	9	402	7	-	-	0/6/5/5
53	CDL	x	101	-	2/2/9/9	15/85/85/110	-
53	CDL	h	201	-	-	20/68/68/110	-
45	SF4	3	802	3	-	-	0/6/5/5
51	3PE	L	1002	-	-	12/34/34/54	-
53	CDL	V	203	-	-	25/104/104/110	-
53	CDL	N	402	-	-	29/100/100/110	-
45	SF4	1	501	1	-	-	0/6/5/5
51	3PE	V	202	-	-	9/40/40/54	-
51	3PE	6	203	-	-	10/54/54/54	-
48	FES	2	300	2	-	-	0/1/1/1
54	ZMP	X	101	17	-	12/35/37/43	-
56	NDP	d	401	-	-	6/30/77/77	0/5/5/5
57	AMP	k	501	-	-	3/6/26/26	0/3/3/3
51	3PE	4	502	-	-	9/43/43/54	-
51	3PE	o	501	-	-	5/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PC1	M	502	-	-	10/57/57/57	-
46	FMN	1	502	-	-	5/18/18/18	0/3/3/3
54	ZMP	g	201	-	-	7/38/40/43	-
58	MYR	s	201	37	-	0/11/12/13	-
45	SF4	3	801	3	-	-	0/6/5/5
51	3PE	i	201	-	-	13/54/54/54	-
53	CDL	M	504	-	1/1/9/9	29/110/110/110	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	502	FMN	C4A-N5	3.52	1.37	1.30
54	X	101	ZMP	C9-C10	2.93	1.53	1.50
57	k	501	AMP	C5-C4	2.37	1.47	1.40
54	g	201	ZMP	C9-C10	2.30	1.53	1.50
46	1	502	FMN	C10-N1	2.12	1.37	1.33

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	-9.67	71.29	109.07
47	1	503	NAI	O2A-PA-O1A	-8.08	72.31	112.24
46	1	502	FMN	C4-N3-C2	-3.43	119.30	125.64
57	k	501	AMP	N3-C2-N1	-3.21	123.67	128.68
54	g	201	ZMP	O1-C10-C9	-3.03	120.41	123.99
46	1	502	FMN	C4A-C10-N10	2.86	120.66	116.48
54	g	201	ZMP	C14-C15-N2	-2.80	106.24	111.90
46	1	502	FMN	C4A-C4-N3	2.72	120.11	113.19
46	1	502	FMN	O4-C4-C4A	-2.68	119.50	126.60
47	1	503	NAI	O2A-PA-O5B	2.66	120.11	107.75
57	k	501	AMP	C4-C5-N7	-2.62	106.67	109.40
54	g	201	ZMP	C15-C14-C13	-2.56	108.10	112.36
51	N	401	3PE	C2-O21-C21	2.46	123.86	117.79
54	X	101	ZMP	O1-C10-C9	-2.45	121.09	123.99
51	L	1002	3PE	C2-O21-C21	2.44	123.79	117.79
52	L	1003	PC1	C2-O21-C21	2.43	123.78	117.79
46	1	502	FMN	C4A-C10-N1	-2.43	119.10	124.73
47	1	503	NAI	C5A-C6A-N6A	2.30	123.85	120.35
56	d	401	NDP	C5A-C6A-N6A	2.30	123.85	120.35
52	9	401	PC1	C2-O21-C21	2.17	123.14	117.79
51	L	1002	3PE	O21-C2-C1	2.16	116.21	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	1	502	FMN	C5A-C9A-N10	2.14	120.17	117.95
52	L	1003	PC1	O21-C2-C1	2.12	116.09	108.40
51	V	201	3PE	O12-P-O14	2.11	118.96	110.68
46	1	502	FMN	C4-C4A-C10	2.10	120.31	116.79
46	1	502	FMN	C10-C4A-N5	-2.08	120.45	124.86
53	x	101	CDL	CB4-OB6-CB5	2.06	122.87	117.79

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	1004	CDL	CB4
53	L	1005	CDL	CB4
53	M	504	CDL	CB4
53	x	101	CDL	CA4
53	x	101	CDL	CB4

All (463) 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-O1P
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
50	4	501	970	C01-C02-C04-C05
50	4	501	970	C01-C02-C04-O08
50	4	501	970	C03-C02-C04-C05
50	4	501	970	C03-C02-C04-O08
51	4	502	3PE	C1-O11-P-O12
51	4	502	3PE	C1-O11-P-O14
51	4	502	3PE	C11-O13-P-O11
51	4	502	3PE	C11-O13-P-O12
51	4	502	3PE	C11-O13-P-O14
51	6	203	3PE	C11-O13-P-O12
51	A	201	3PE	C1-O11-P-O12
51	A	201	3PE	C1-O11-P-O13
51	A	201	3PE	C1-O11-P-O14
51	J	201	3PE	C11-O13-P-O12
51	J	202	3PE	C11-O13-P-O14
51	J	202	3PE	O13-C11-C12-N
51	L	1001	3PE	O13-C11-C12-N
51	L	1002	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
51	L	1002	3PE	C2-C1-O11-P
51	L	1002	3PE	O13-C11-C12-N
51	M	501	3PE	C1-O11-P-O14
51	N	401	3PE	C11-O13-P-O12
51	N	401	3PE	C11-O13-P-O14
51	N	401	3PE	O13-C11-C12-N
51	V	201	3PE	C1-O11-P-O12
51	V	201	3PE	C1-O11-P-O13
51	V	202	3PE	C1-O11-P-O12
51	V	202	3PE	C1-O11-P-O13
51	V	202	3PE	C1-O11-P-O14
51	i	201	3PE	C1-O11-P-O12
51	i	201	3PE	C11-O13-P-O12
51	i	201	3PE	O13-C11-C12-N
51	o	501	3PE	C1-O11-P-O12
51	o	501	3PE	C1-O11-P-O14
52	9	401	PC1	C1-O11-P-O12
52	9	401	PC1	C1-O11-P-O14
52	9	401	PC1	C1-O11-P-O13
52	L	1003	PC1	C1-O11-P-O12
52	M	503	PC1	C11-O13-P-O11
52	M	503	PC1	C1-O11-P-O12
53	L	1004	CDL	CA3-OA5-PA1-OA3
53	L	1004	CDL	CB2-OB2-PB2-OB3
53	L	1004	CDL	CB2-OB2-PB2-OB4
53	L	1004	CDL	CB2-OB2-PB2-OB5
53	L	1004	CDL	CB3-OB5-PB2-OB3
53	L	1005	CDL	CA3-OA5-PA1-OA3
53	L	1005	CDL	CA3-OA5-PA1-OA4
53	L	1005	CDL	CB3-OB5-PB2-OB2
53	L	1005	CDL	CB3-OB5-PB2-OB3
53	L	1005	CDL	CB3-OB5-PB2-OB4
53	M	504	CDL	CA2-OA2-PA1-OA3
53	M	504	CDL	CB2-OB2-PB2-OB3
53	M	504	CDL	CB3-OB5-PB2-OB3
53	N	402	CDL	CB3-OB5-PB2-OB2
53	N	402	CDL	CB3-OB5-PB2-OB3
53	N	402	CDL	CB3-OB5-PB2-OB4
53	V	203	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CB3-OB5-PB2-OB3
53	V	203	CDL	CB3-OB5-PB2-OB4
53	W	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
53	W	201	CDL	CA2-OA2-PA1-OA4
53	W	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CA2-C1-CB2-OB2
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB2-OB2-PB2-OB4
53	h	201	CDL	CB3-OB5-PB2-OB2
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	CB3-OB5-PB2-OB4
53	x	101	CDL	CA2-OA2-PA1-OA3
53	x	101	CDL	CA3-OA5-PA1-OA2
53	x	101	CDL	CA3-OA5-PA1-OA3
53	x	101	CDL	CA3-OA5-PA1-OA4
53	x	101	CDL	CB2-OB2-PB2-OB3
53	x	101	CDL	CB2-OB2-PB2-OB5
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	O3-C16-C17-O4
54	X	101	ZMP	C17-C16-N2-C15
54	X	101	ZMP	C12-C11-S1-C10
54	g	201	ZMP	C17-C18-C21-O5
54	g	201	ZMP	S1-C11-C12-N1
54	g	201	ZMP	O1-C10-S1-C11
54	g	201	ZMP	C9-C10-S1-C11
57	k	501	AMP	C3'-C4'-C5'-O5'
54	X	101	ZMP	O3-C16-N2-C15
53	L	1005	CDL	C1-CA2-OA2-PA1
52	6	202	PC1	C11-C12-N-C14
52	6	202	PC1	C11-C12-N-C15
53	L	1004	CDL	C33-C34-C35-C36
53	h	201	CDL	O1-C1-CB2-OB2
53	x	101	CDL	O1-C1-CA2-OA2
51	M	501	3PE	C31-C32-C33-C34
47	1	503	NAI	C2D-C1D-N1N-C2N
51	J	201	3PE	C21-C22-C23-C24
53	N	402	CDL	CB5-C51-C52-C53
57	k	501	AMP	O4'-C4'-C5'-O5'
52	L	1003	PC1	C2-C1-O11-P
53	W	201	CDL	CB5-C51-C52-C53
51	4	502	3PE	C1-O11-P-O13
51	J	201	3PE	C1-O11-P-O13
51	J	202	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
51	L	1002	3PE	C1-O11-P-O13
51	M	501	3PE	C1-O11-P-O13
51	N	401	3PE	C1-O11-P-O13
51	N	401	3PE	C11-O13-P-O11
51	V	202	3PE	C11-O13-P-O11
51	i	201	3PE	C1-O11-P-O13
51	o	501	3PE	C1-O11-P-O13
52	9	401	PC1	C11-O13-P-O11
53	L	1004	CDL	CB3-OB5-PB2-OB2
53	L	1005	CDL	CA2-OA2-PA1-OA5
53	L	1005	CDL	CA3-OA5-PA1-OA2
53	M	504	CDL	CA2-OA2-PA1-OA5
53	M	504	CDL	CB3-OB5-PB2-OB2
53	V	203	CDL	CA3-OA5-PA1-OA2
53	V	203	CDL	CB2-OB2-PB2-OB5
53	V	203	CDL	CB3-OB5-PB2-OB2
53	W	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB2-OB2-PB2-OB5
53	x	101	CDL	CA2-OA2-PA1-OA5
52	9	401	PC1	C39-C3A-C3B-C3C
53	L	1004	CDL	C13-C14-C15-C16
53	V	203	CDL	C39-C40-C41-C42
51	A	201	3PE	C2C-C2D-C2E-C2F
53	L	1005	CDL	C56-C57-C58-C59
53	M	504	CDL	C52-C53-C54-C55
53	L	1005	CDL	C41-C42-C43-C44
53	V	203	CDL	C79-C80-C81-C82
52	9	401	PC1	C2B-C2C-C2D-C2E
54	X	101	ZMP	C6-C7-C8-C9
51	A	201	3PE	C2E-C2F-C2G-C2H
53	L	1005	CDL	C77-C78-C79-C80
53	L	1005	CDL	C22-C23-C24-C25
52	M	503	PC1	C3A-C3B-C3C-C3D
53	W	201	CDL	C35-C36-C37-C38
53	M	504	CDL	CB5-C51-C52-C53
47	1	503	NAI	C2D-C1D-N1N-C6N
53	M	504	CDL	C36-C37-C38-C39
51	L	1001	3PE	O11-C1-C2-C3
53	x	101	CDL	OB5-CB3-CB4-CB6
51	V	201	3PE	C22-C23-C24-C25
51	i	201	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
53	M	504	CDL	C63-C64-C65-C66
53	W	201	CDL	C82-C83-C84-C85
53	N	402	CDL	C78-C79-C80-C81
53	L	1005	CDL	C21-C22-C23-C24
51	N	401	3PE	C36-C37-C38-C39
52	L	1003	PC1	C38-C39-C3A-C3B
53	V	203	CDL	C71-C72-C73-C74
53	L	1004	CDL	C77-C78-C79-C80
51	6	203	3PE	C36-C37-C38-C39
53	N	402	CDL	C52-C53-C54-C55
52	6	202	PC1	C11-C12-N-C13
53	L	1005	CDL	CB5-C51-C52-C53
51	A	201	3PE	C38-C39-C3A-C3B
51	L	1001	3PE	C34-C35-C36-C37
51	N	401	3PE	C2B-C2C-C2D-C2E
51	J	202	3PE	C34-C35-C36-C37
53	M	504	CDL	C82-C83-C84-C85
53	M	504	CDL	CA5-C11-C12-C13
53	L	1004	CDL	OA6-CA4-CA6-OA8
53	L	1005	CDL	C35-C36-C37-C38
52	M	502	PC1	C35-C36-C37-C38
51	J	201	3PE	C11-O13-P-O11
51	L	1002	3PE	C11-O13-P-O11
53	N	402	CDL	CB2-OB2-PB2-OB5
52	L	1003	PC1	O11-C1-C2-C3
53	V	203	CDL	OA5-CA3-CA4-CA6
51	J	202	3PE	C32-C33-C34-C35
53	M	504	CDL	C57-C58-C59-C60
53	L	1004	CDL	CB3-CB4-CB6-OB8
53	h	201	CDL	CB3-CB4-CB6-OB8
53	M	504	CDL	C80-C81-C82-C83
52	L	1003	PC1	C2A-C2B-C2C-C2D
51	o	501	3PE	C31-C32-C33-C34
53	N	402	CDL	C84-C85-C86-C87
53	V	203	CDL	OA5-CA3-CA4-OA6
53	M	504	CDL	O1-C1-CB2-OB2
53	L	1005	CDL	OA6-CA4-CA6-OA8
53	W	201	CDL	C31-C32-C33-C34
52	L	1003	PC1	C23-C24-C25-C26
52	M	502	PC1	C3E-C3F-C3G-C3H
51	J	202	3PE	C26-C27-C28-C29
51	N	401	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
53	L	1004	CDL	C71-C72-C73-C74
53	M	504	CDL	C12-C13-C14-C15
51	J	201	3PE	O11-C1-C2-C3
52	M	503	PC1	O11-C1-C2-C3
53	W	201	CDL	OB5-CB3-CB4-CB6
51	o	501	3PE	O13-C11-C12-N
51	4	502	3PE	C1-C2-C3-O31
53	L	1004	CDL	CA3-CA4-CA6-OA8
53	L	1005	CDL	CA3-CA4-CA6-OA8
53	M	504	CDL	CA3-CA4-CA6-OA8
53	N	402	CDL	CA3-CA4-CA6-OA8
53	N	402	CDL	CB3-CB4-CB6-OB8
51	L	1001	3PE	C36-C37-C38-C39
53	N	402	CDL	CA2-OA2-PA1-OA5
53	V	203	CDL	CB7-C71-C72-C73
53	N	402	CDL	C62-C63-C64-C65
51	L	1001	3PE	O11-C1-C2-O21
51	L	1002	3PE	O11-C1-C2-O21
53	W	201	CDL	OB5-CB3-CB4-OB6
51	4	502	3PE	O21-C2-C3-O31
53	N	402	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OB6-CB4-CB6-OB8
52	M	503	PC1	C2C-C2D-C2E-C2F
53	N	402	CDL	C71-C72-C73-C74
52	M	503	PC1	C2-C1-O11-P
53	N	402	CDL	CB4-CB3-OB5-PB2
51	6	203	3PE	C39-C3A-C3B-C3C
51	J	201	3PE	C2D-C2E-C2F-C2G
53	L	1004	CDL	C79-C80-C81-C82
47	1	503	NAI	PN-O3-PA-O5B
53	M	504	CDL	OB5-CB3-CB4-CB6
53	N	402	CDL	OB5-CB3-CB4-CB6
47	1	503	NAI	O4D-C1D-N1N-C2N
53	W	201	CDL	C19-C20-C21-C22
51	J	202	3PE	C31-C32-C33-C34
52	6	202	PC1	C3B-C3C-C3D-C3E
53	N	402	CDL	C76-C77-C78-C79
52	6	202	PC1	C24-C25-C26-C27
53	L	1005	CDL	CA7-C31-C32-C33
51	M	501	3PE	C2-C1-O11-P
51	J	201	3PE	O11-C1-C2-O21
52	L	1003	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
52	M	503	PC1	O11-C1-C2-O21
53	L	1004	CDL	OA5-CA3-CA4-OA6
53	L	1004	CDL	C52-C53-C54-C55
53	V	203	CDL	C78-C79-C80-C81
54	X	101	ZMP	C16-C17-C18-C20
53	L	1004	CDL	OB6-CB4-CB6-OB8
53	V	203	CDL	C20-C21-C22-C23
53	L	1004	CDL	C73-C74-C75-C76
52	9	401	PC1	C34-C35-C36-C37
47	1	503	NAI	O4D-C1D-N1N-C6N
51	6	203	3PE	C11-O13-P-O11
51	i	201	3PE	C11-O13-P-O11
53	L	1004	CDL	CA3-OA5-PA1-OA2
53	N	402	CDL	CA3-OA5-PA1-OA2
53	W	201	CDL	CB3-OB5-PB2-OB2
47	1	503	NAI	C5B-O5B-PA-O2A
51	6	203	3PE	C11-O13-P-O14
51	J	201	3PE	C1-O11-P-O14
51	J	201	3PE	C11-O13-P-O14
51	J	202	3PE	C1-O11-P-O14
51	L	1002	3PE	C1-O11-P-O14
51	L	1002	3PE	C11-O13-P-O14
51	M	501	3PE	C1-O11-P-O12
51	N	401	3PE	C1-O11-P-O12
51	N	401	3PE	C1-O11-P-O14
51	V	202	3PE	C11-O13-P-O14
51	i	201	3PE	C1-O11-P-O14
51	i	201	3PE	C11-O13-P-O14
52	9	401	PC1	C11-O13-P-O14
52	L	1003	PC1	C1-O11-P-O14
52	M	503	PC1	C11-O13-P-O12
53	L	1004	CDL	CB3-OB5-PB2-OB4
53	L	1005	CDL	CA2-OA2-PA1-OA3
53	L	1005	CDL	CA2-OA2-PA1-OA4
53	M	504	CDL	CA2-OA2-PA1-OA4
53	N	402	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CA3-OA5-PA1-OA3
53	V	203	CDL	CA3-OA5-PA1-OA4
53	W	201	CDL	CA3-OA5-PA1-OA3
53	x	101	CDL	CA2-OA2-PA1-OA4
56	d	401	NDP	C2N-C3N-C7N-N7N
53	N	402	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
52	6	202	PC1	O11-C1-C2-C3
53	L	1004	CDL	OA5-CA3-CA4-CA6
52	6	202	PC1	O11-C1-C2-O21
53	M	504	CDL	OB5-CB3-CB4-OB6
53	V	203	CDL	OB5-CB3-CB4-OB6
54	X	101	ZMP	S1-C11-C12-N1
52	9	401	PC1	C3D-C3E-C3F-C3G
52	M	503	PC1	C25-C26-C27-C28
53	M	504	CDL	C83-C84-C85-C86
52	M	503	PC1	C11-C12-N-C14
53	h	201	CDL	CA7-C31-C32-C33
51	J	202	3PE	C1-C2-C3-O31
52	9	401	PC1	O13-C11-C12-N
52	M	502	PC1	O13-C11-C12-N
52	M	503	PC1	C39-C3A-C3B-C3C
54	X	101	ZMP	O4-C17-C18-C21
56	d	401	NDP	C2N-C3N-C7N-O7N
51	J	202	3PE	O21-C2-C3-O31
53	M	504	CDL	OA6-CA4-CA6-OA8
51	N	401	3PE	C24-C25-C26-C27
52	6	202	PC1	C23-C24-C25-C26
53	M	504	CDL	C1-CB2-OB2-PB2
51	V	202	3PE	C32-C33-C34-C35
52	L	1003	PC1	C1-C2-O21-C21
53	V	203	CDL	OB5-CB3-CB4-CB6
52	M	502	PC1	C31-C32-C33-C34
53	L	1005	CDL	CA4-CA3-OA5-PA1
53	N	402	CDL	C1-CA2-OA2-PA1
57	k	501	AMP	C5'-O5'-P-O1P
53	x	101	CDL	OB5-CB3-CB4-OB6
52	M	503	PC1	C11-C12-N-C13
51	i	201	3PE	C2B-C2C-C2D-C2E
51	J	202	3PE	C29-C2A-C2B-C2C
51	N	401	3PE	O21-C2-C3-O31
52	L	1003	PC1	C2B-C2C-C2D-C2E
51	A	201	3PE	C11-O13-P-O11
51	J	202	3PE	C11-O13-P-O11
51	L	1001	3PE	C11-O13-P-O11
51	M	501	3PE	C11-O13-P-O11
52	L	1003	PC1	C1-O11-P-O13
53	L	1005	CDL	CB2-OB2-PB2-OB5
52	L	1003	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
52	6	202	PC1	C36-C37-C38-C39
52	9	401	PC1	C23-C24-C25-C26
56	d	401	NDP	O4D-C1D-N1N-C6N
51	6	203	3PE	C21-C22-C23-C24
51	J	202	3PE	C25-C26-C27-C28
51	J	202	3PE	C27-C28-C29-C2A
53	W	201	CDL	CB7-C71-C72-C73
53	L	1004	CDL	C32-C33-C34-C35
51	J	201	3PE	C3A-C3B-C3C-C3D
52	M	502	PC1	C26-C27-C28-C29
52	9	401	PC1	C3A-C3B-C3C-C3D
51	L	1002	3PE	O11-C1-C2-C3
52	M	503	PC1	C3B-C3C-C3D-C3E
52	M	503	PC1	C27-C28-C29-C2A
53	L	1005	CDL	C58-C59-C60-C61
51	N	401	3PE	C3A-C3B-C3C-C3D
51	M	501	3PE	C37-C38-C39-C3A
51	J	201	3PE	O21-C2-C3-O31
53	V	203	CDL	OA6-CA4-CA6-OA8
53	L	1005	CDL	CB2-C1-CA2-OA2
53	V	203	CDL	C19-C20-C21-C22
54	g	201	ZMP	C19-C18-C21-O5
54	g	201	ZMP	C20-C18-C21-O5
52	9	401	PC1	C3-C2-O21-C21
52	M	503	PC1	C11-C12-N-C15
52	M	503	PC1	C2E-C2F-C2G-C2H
52	6	202	PC1	C38-C39-C3A-C3B
53	L	1005	CDL	C73-C74-C75-C76
52	M	502	PC1	O11-C1-C2-C3
51	N	401	3PE	C27-C28-C29-C2A
52	L	1003	PC1	C36-C37-C38-C39
51	J	201	3PE	C2B-C2C-C2D-C2E
53	W	201	CDL	C22-C23-C24-C25
51	J	201	3PE	C27-C28-C29-C2A
51	M	501	3PE	C39-C3A-C3B-C3C
53	V	203	CDL	CA2-C1-CB2-OB2
51	A	201	3PE	C39-C3A-C3B-C3C
51	6	203	3PE	C25-C26-C27-C28
52	9	401	PC1	C3E-C3F-C3G-C3H
53	N	402	CDL	C53-C54-C55-C56
52	M	502	PC1	O11-C1-C2-O21
53	L	1004	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
52	M	503	PC1	O31-C31-C32-C33
53	W	201	CDL	C53-C54-C55-C56
52	M	502	PC1	C11-C12-N-C15
52	L	1003	PC1	O31-C31-C32-C33
51	V	202	3PE	O13-C11-C12-N
53	L	1004	CDL	C1-CA2-OA2-PA1
53	N	402	CDL	C72-C73-C74-C75
51	A	201	3PE	O21-C2-C3-O31
52	9	401	PC1	O21-C2-C3-O31
51	i	201	3PE	C28-C29-C2A-C2B
51	M	501	3PE	C32-C31-O31-C3
53	V	203	CDL	C32-C31-CA7-OA8
53	L	1005	CDL	C34-C35-C36-C37
56	d	401	NDP	C2D-C1D-N1N-C6N
53	L	1004	CDL	C78-C79-C80-C81
51	A	201	3PE	O21-C21-C22-C23
51	L	1002	3PE	C1-C2-O21-C21
51	N	401	3PE	C3-C2-O21-C21
53	x	101	CDL	C18-C19-C20-C21
51	M	501	3PE	O21-C21-C22-C23
53	W	201	CDL	C73-C74-C75-C76
51	N	401	3PE	O21-C21-C22-C23
52	M	503	PC1	O21-C21-C22-C23
53	M	504	CDL	C72-C71-CB7-OB8
51	i	201	3PE	O21-C21-C22-C23
53	L	1005	CDL	C72-C71-CB7-OB8
51	i	201	3PE	C36-C37-C38-C39
52	9	401	PC1	C29-C2A-C2B-C2C
54	X	101	ZMP	C16-C17-C18-C19
53	N	402	CDL	C32-C31-CA7-OA8
51	V	202	3PE	O31-C31-C32-C33
53	L	1005	CDL	C12-C11-CA5-OA6
53	L	1005	CDL	C32-C31-CA7-OA8
53	M	504	CDL	C32-C31-CA7-OA8
53	h	201	CDL	C52-C51-CB5-OB6
54	X	101	ZMP	O4-C17-C18-C19
56	d	401	NDP	C2B-O2B-P2B-O2X
51	L	1001	3PE	C35-C36-C37-C38
52	6	202	PC1	C21-C22-C23-C24
51	6	203	3PE	C38-C39-C3A-C3B
53	h	201	CDL	C57-C58-C59-C60
53	h	201	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
52	M	503	PC1	C2B-C2C-C2D-C2E
54	g	201	ZMP	C2-C1-C22-C23
53	L	1005	CDL	C33-C34-C35-C36
56	d	401	NDP	O4B-C4B-C5B-O5B
53	L	1004	CDL	CB7-C71-C72-C73
47	1	503	NAI	PN-O3-PA-O1A
51	N	401	3PE	C28-C29-C2A-C2B
53	L	1005	CDL	C72-C71-CB7-OB9
53	L	1005	CDL	C84-C85-C86-C87
52	M	503	PC1	C26-C27-C28-C29
53	V	203	CDL	C32-C31-CA7-OA9
54	X	101	ZMP	C2-C3-C4-C5
51	A	201	3PE	C3D-C3E-C3F-C3G
53	N	402	CDL	C61-C62-C63-C64
53	M	504	CDL	C72-C71-CB7-OB9
53	x	101	CDL	C52-C51-CB5-OB6
53	V	203	CDL	O1-C1-CB2-OB2
51	M	501	3PE	O22-C21-C22-C23
51	A	201	3PE	O22-C21-C22-C23
53	h	201	CDL	C52-C51-CB5-OB7
47	1	503	NAI	C2N-C3N-C7N-N7N
51	A	201	3PE	C11-O13-P-O14
51	J	202	3PE	C11-O13-P-O12
52	L	1003	PC1	C11-C12-N-C15
52	M	503	PC1	C1-O11-P-O14
53	N	402	CDL	CA3-OA5-PA1-OA3
53	N	402	CDL	C32-C31-CA7-OA9
51	V	202	3PE	O32-C31-C32-C33
51	N	401	3PE	O22-C21-C22-C23
52	L	1003	PC1	C35-C36-C37-C38
51	J	202	3PE	C12-C11-O13-P
53	N	402	CDL	CB6-CB4-OB6-CB5
51	i	201	3PE	O22-C21-C22-C23
53	L	1005	CDL	C12-C11-CA5-OA7
51	L	1002	3PE	O21-C21-C22-C23
51	J	202	3PE	C21-C22-C23-C24
52	M	502	PC1	C11-C12-N-C14
53	h	201	CDL	C12-C11-CA5-OA6
53	x	101	CDL	C72-C71-CB7-OB8
53	L	1005	CDL	C32-C31-CA7-OA9
53	L	1004	CDL	C32-C31-CA7-OA8
53	M	504	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
53	W	201	CDL	C32-C31-CA7-OA8
53	x	101	CDL	CB2-C1-CA2-OA2
53	h	201	CDL	C56-C57-C58-C59
53	M	504	CDL	C32-C31-CA7-OA9
51	6	203	3PE	C2D-C2E-C2F-C2G
53	N	402	CDL	CA4-CA3-OA5-PA1
53	M	504	CDL	CA7-C31-C32-C33
51	L	1002	3PE	O22-C21-C22-C23
51	L	1001	3PE	C24-C25-C26-C27
52	9	401	PC1	C3F-C3G-C3H-C3I
51	4	502	3PE	O21-C21-C22-C23
53	W	201	CDL	C12-C11-CA5-OA6
53	L	1004	CDL	C32-C31-CA7-OA9
51	L	1001	3PE	C38-C39-C3A-C3B
52	M	502	PC1	C28-C29-C2A-C2B
53	W	201	CDL	C32-C31-CA7-OA9
53	V	203	CDL	C11-C12-C13-C14
53	W	201	CDL	C12-C11-CA5-OA7
53	M	504	CDL	C22-C23-C24-C25
51	6	203	3PE	O21-C21-C22-C23

There are no ring outliers.

24 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	L	1003	PC1	5	0
53	L	1004	CDL	4	0
52	M	503	PC1	2	0
45	6	201	SF4	1	0
51	L	1001	3PE	1	0
51	J	201	3PE	1	0
51	M	501	3PE	1	0
47	1	503	NAI	2	0
53	L	1005	CDL	8	0
51	J	202	3PE	1	0
52	6	202	PC1	1	0
53	W	201	CDL	7	0
52	9	401	PC1	4	0
53	V	203	CDL	4	0
53	N	402	CDL	7	0
45	1	501	SF4	3	0
51	V	202	3PE	1	0

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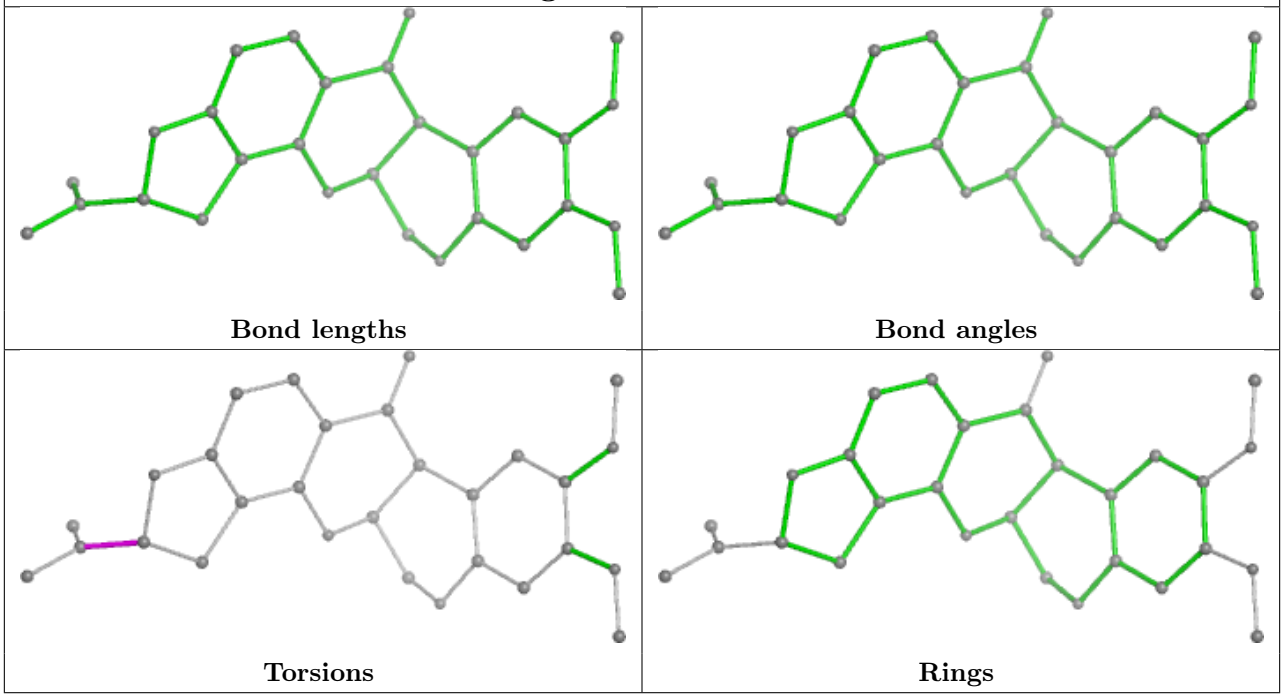
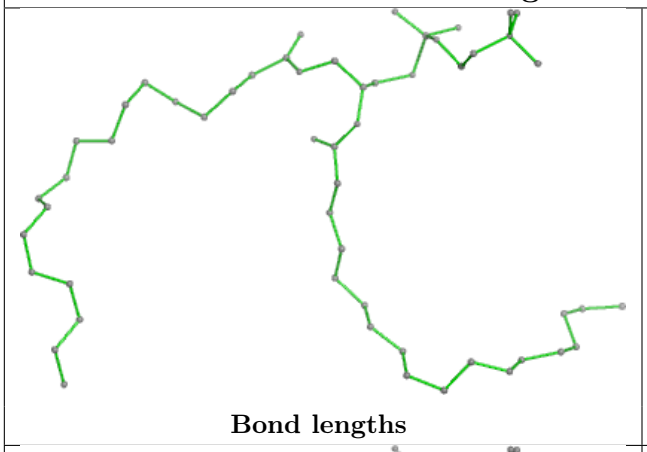
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	6	203	3PE	3	0
48	2	300	FES	1	0
54	X	101	ZMP	1	0
51	4	502	3PE	1	0
52	M	502	PC1	6	0
45	3	801	SF4	1	0
53	M	504	CDL	3	0

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.

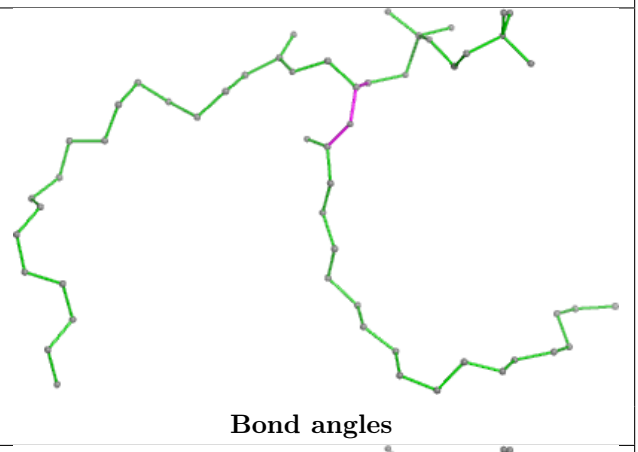
Ligand 970 4 501



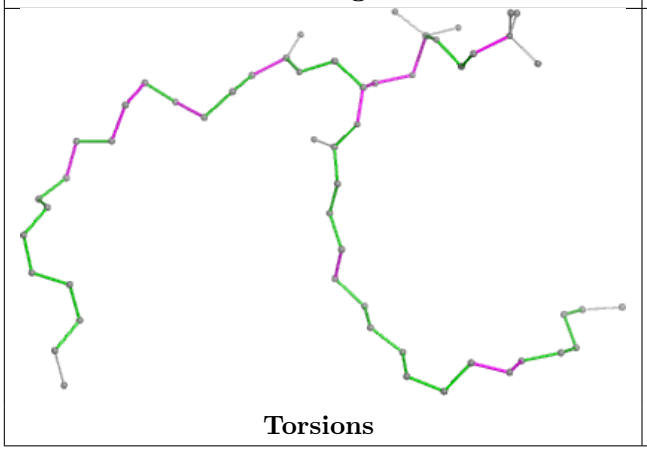
Ligand PC1 L 1003



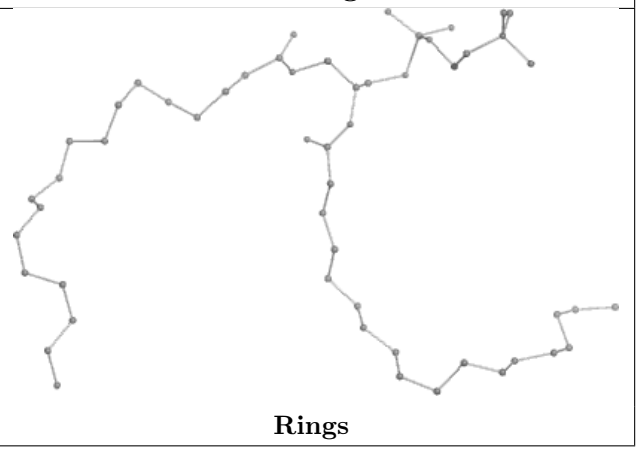
Bond lengths



Bond angles

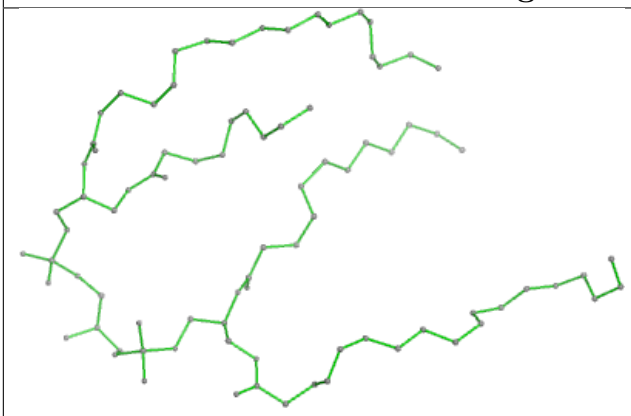


Torsions

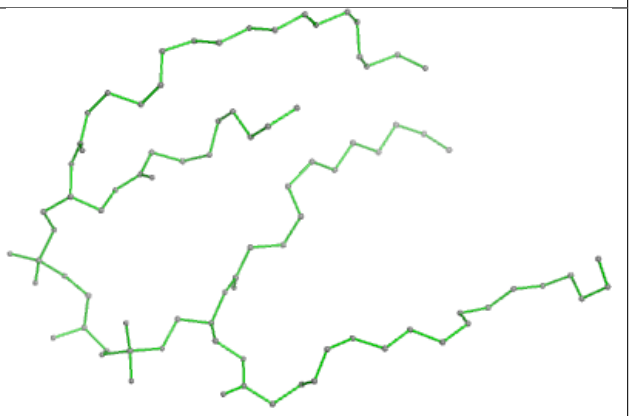


Rings

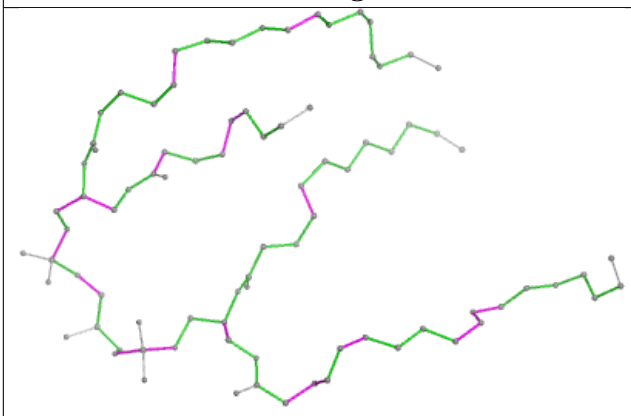
Ligand CDL L 1004



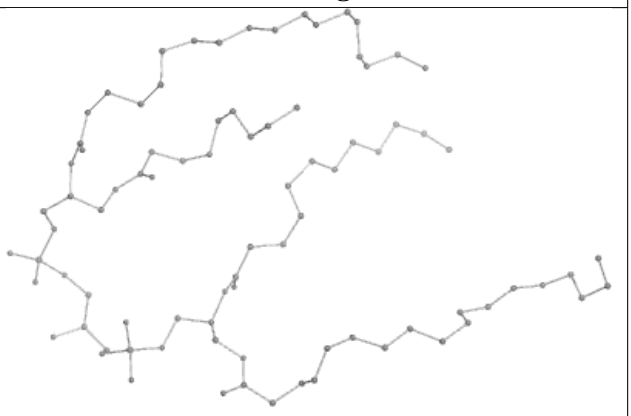
Bond lengths



Bond angles

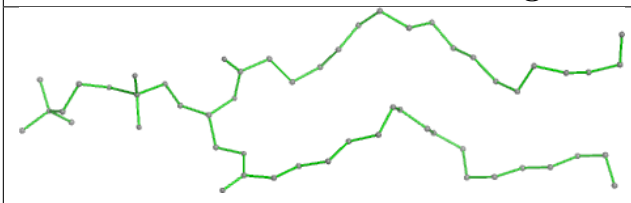


Torsions

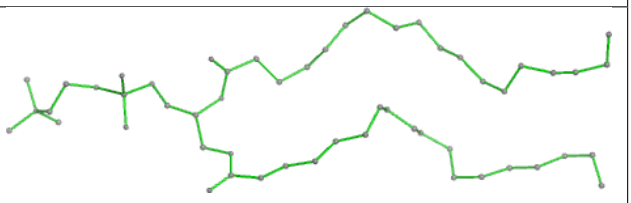


Rings

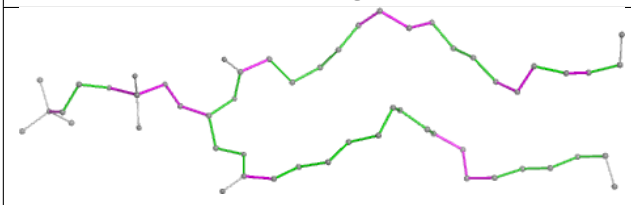
Ligand PC1 M 503



Bond lengths



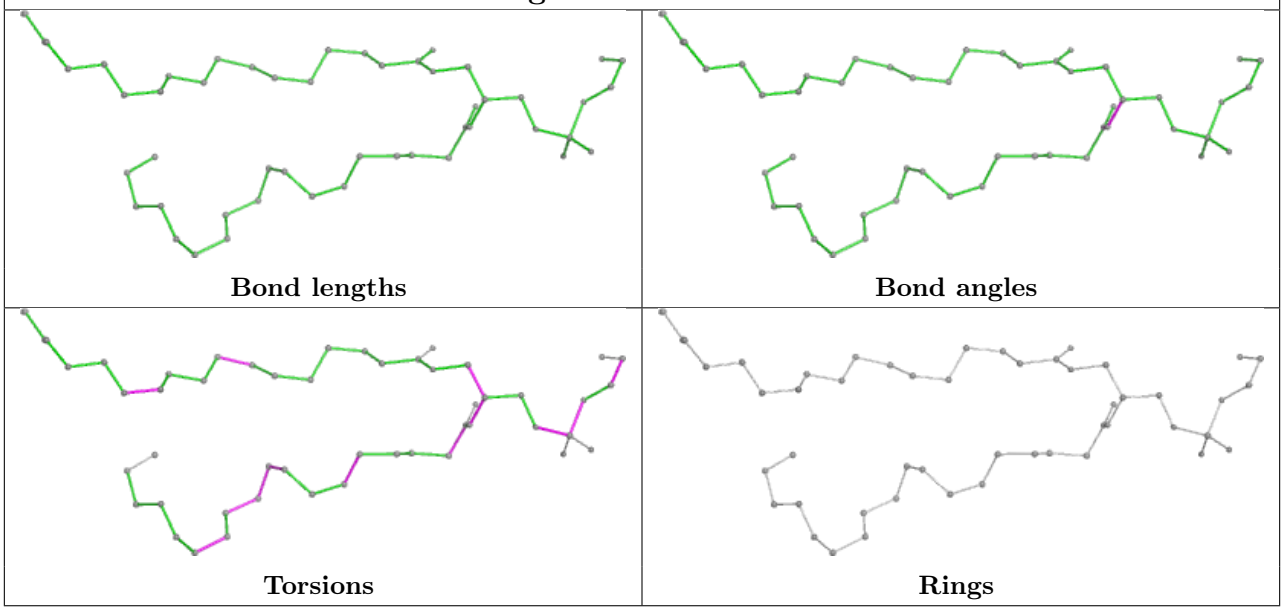
Bond angles



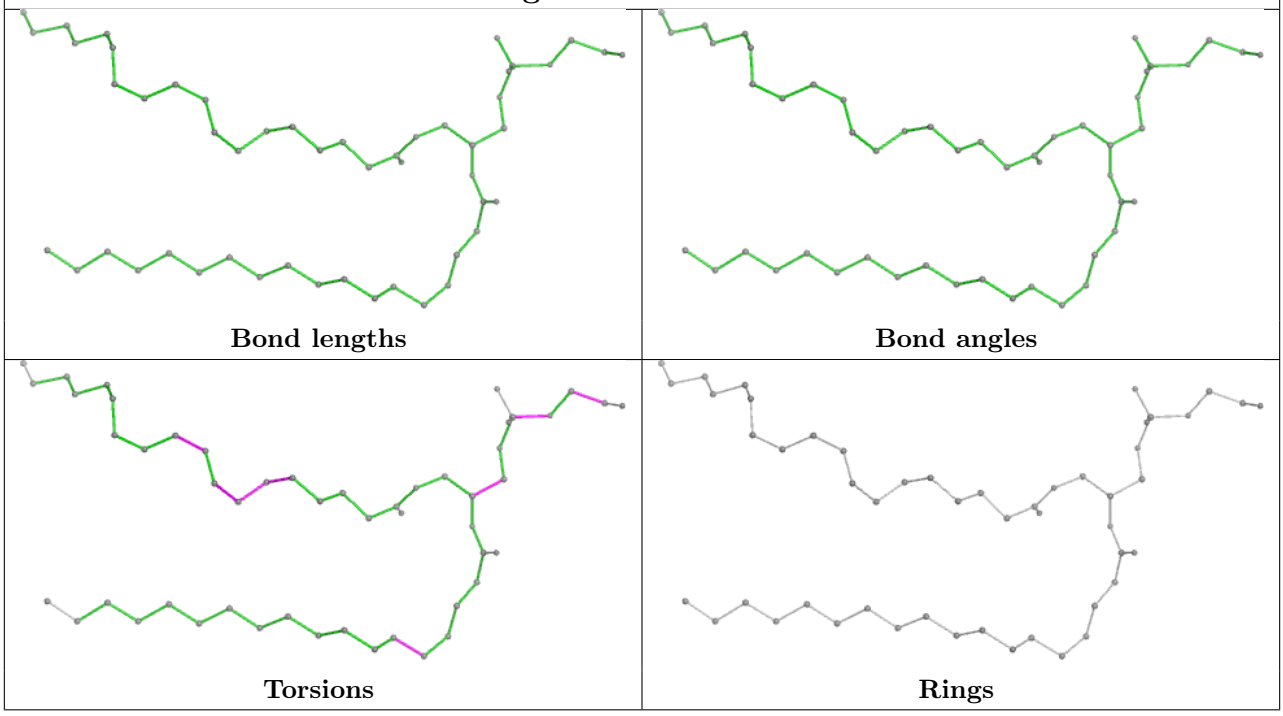
Torsions

Rings

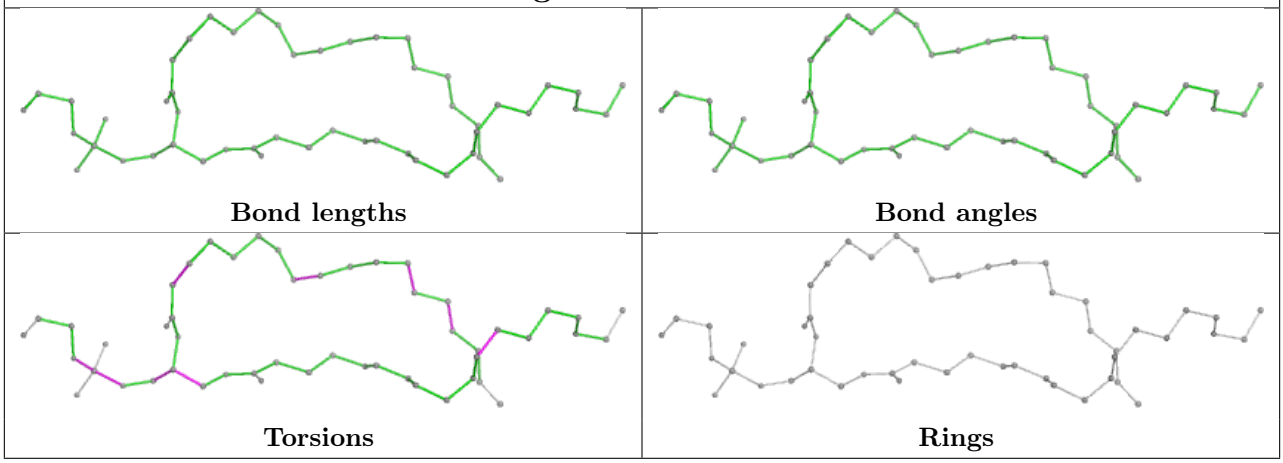
Ligand 3PE N 401



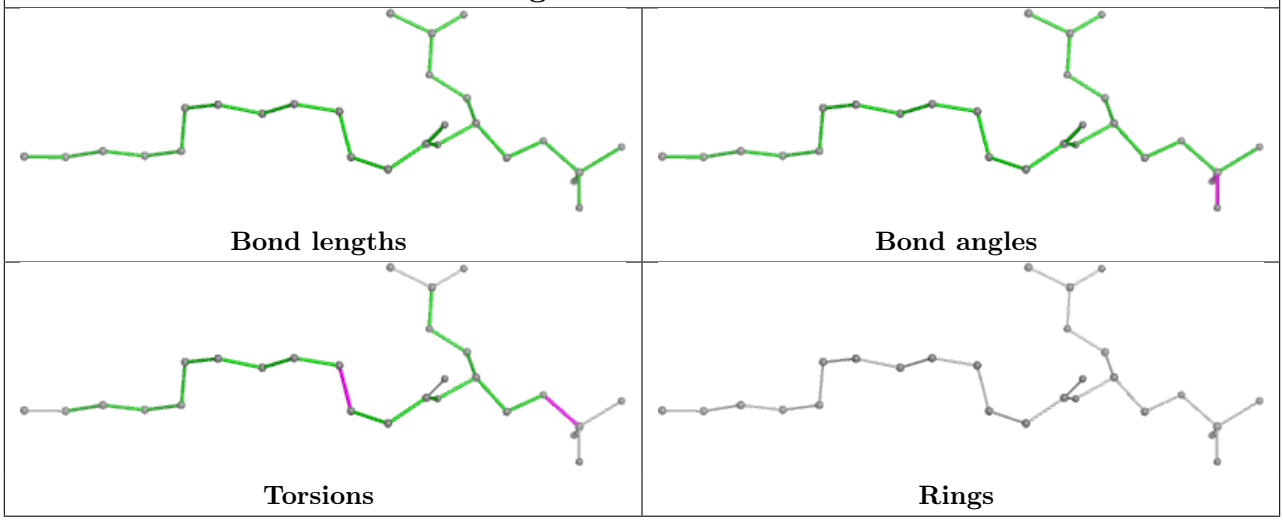
Ligand 3PE L 1001



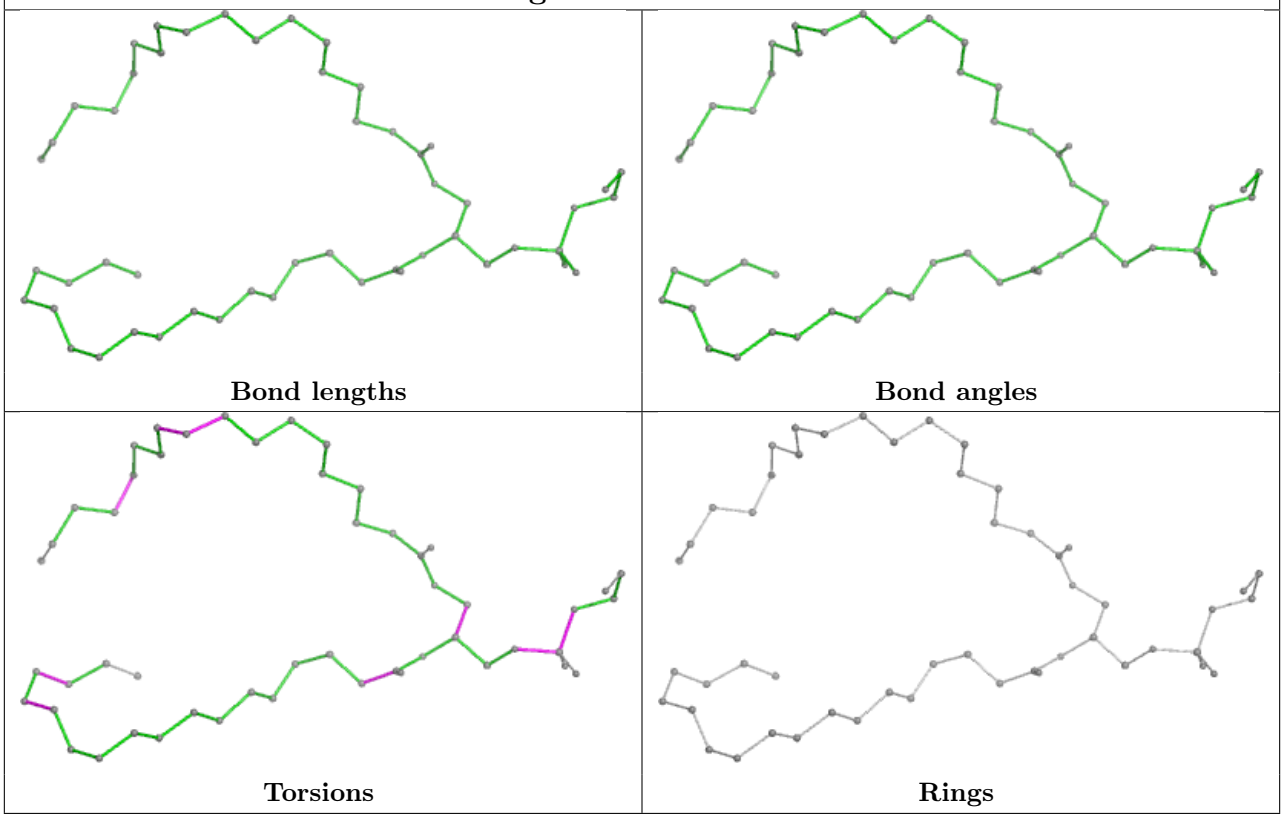
Ligand 3PE J 201



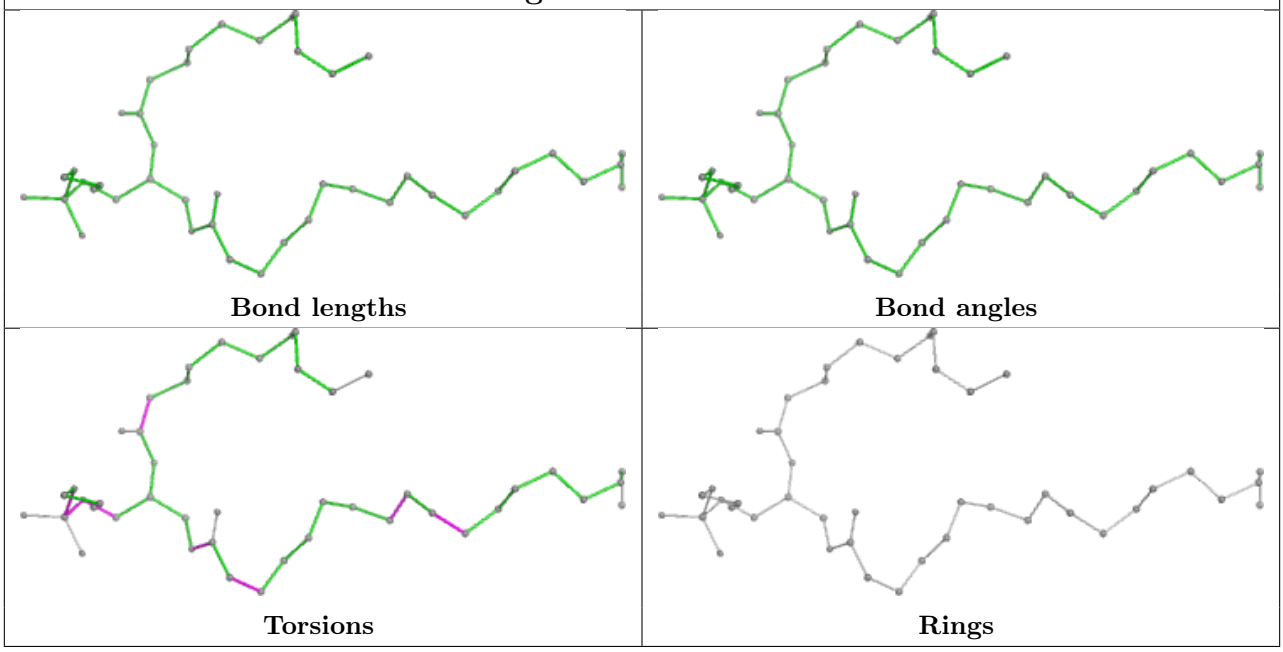
Ligand 3PE V 201



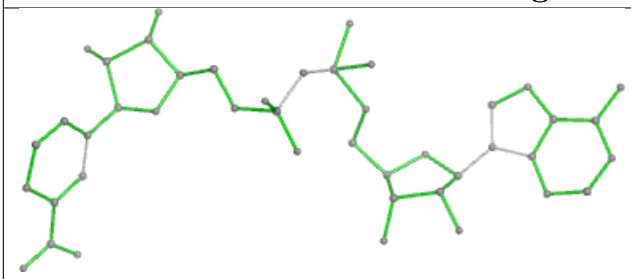
Ligand 3PE A 201



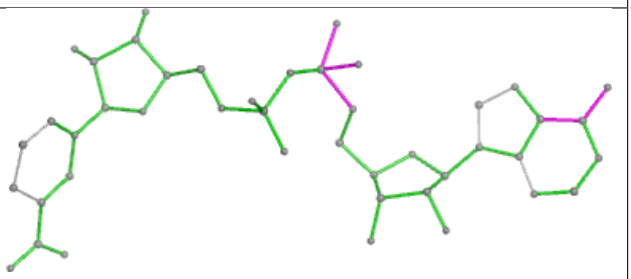
Ligand 3PE M 501



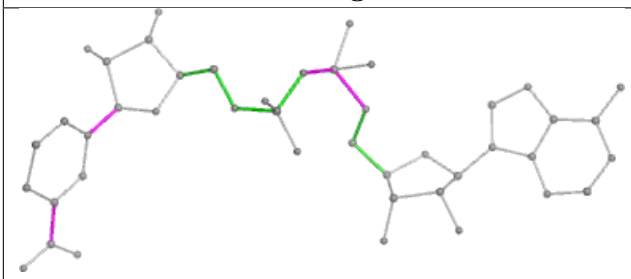
Ligand NAI 1 503



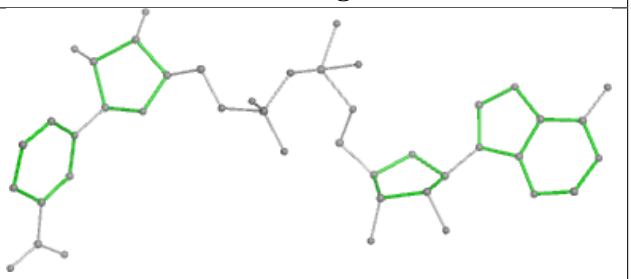
Bond lengths



Bond angles

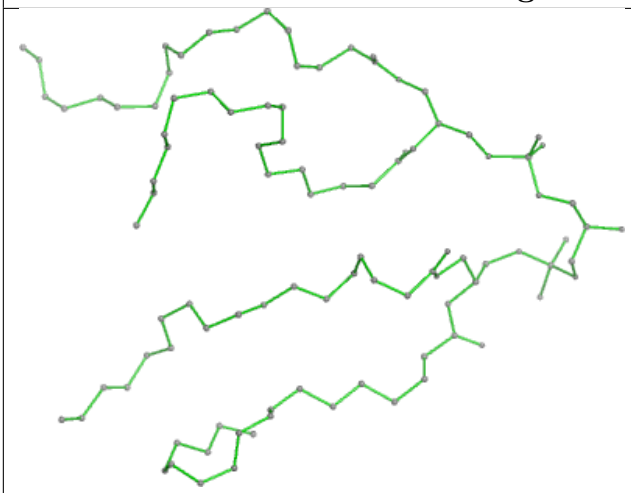


Torsions



Rings

Ligand CDL L 1005



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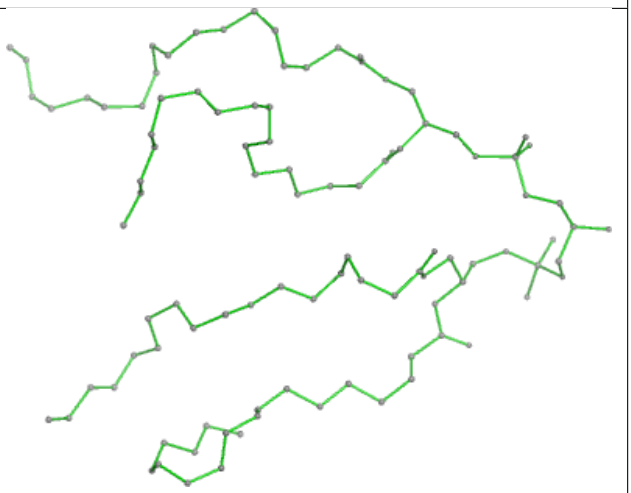
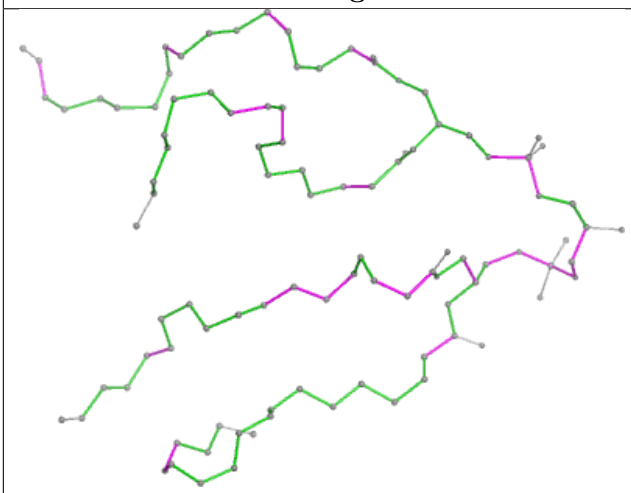
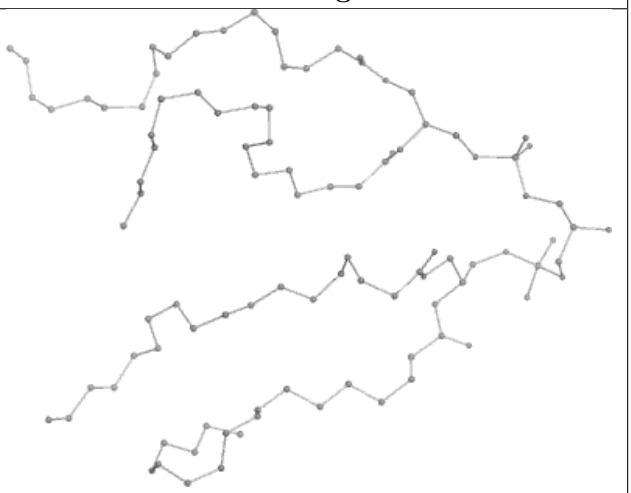


Bond angles

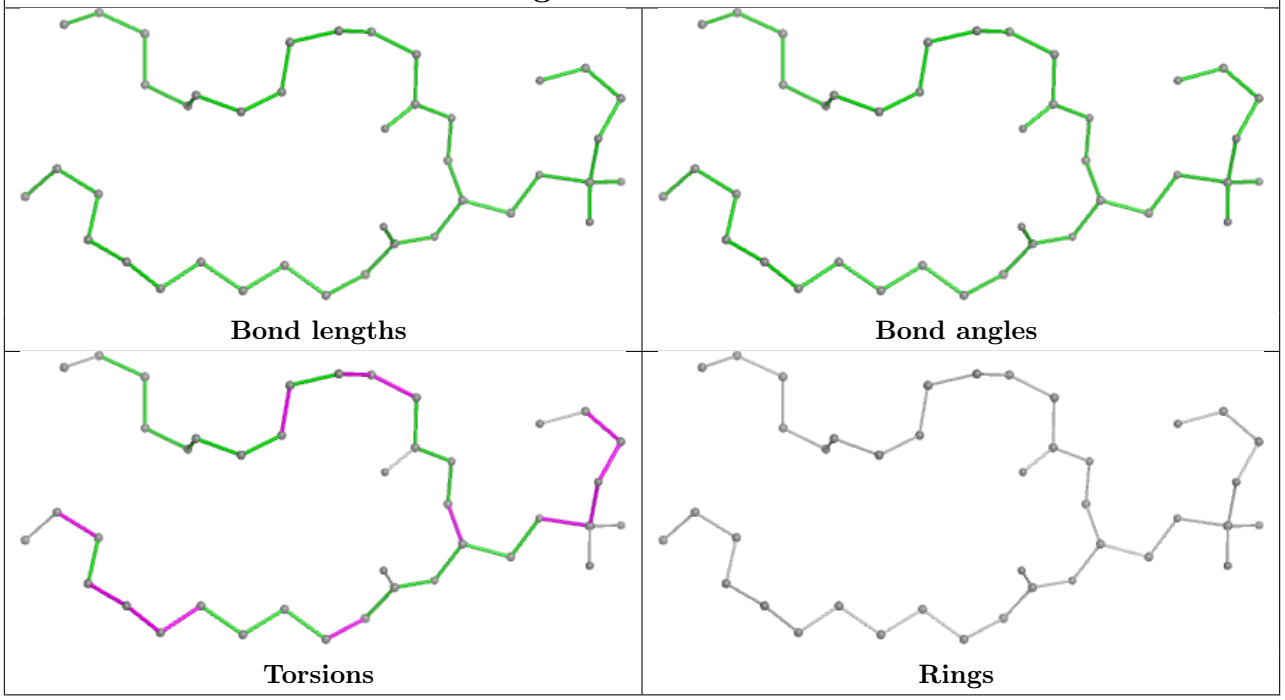


Torsions

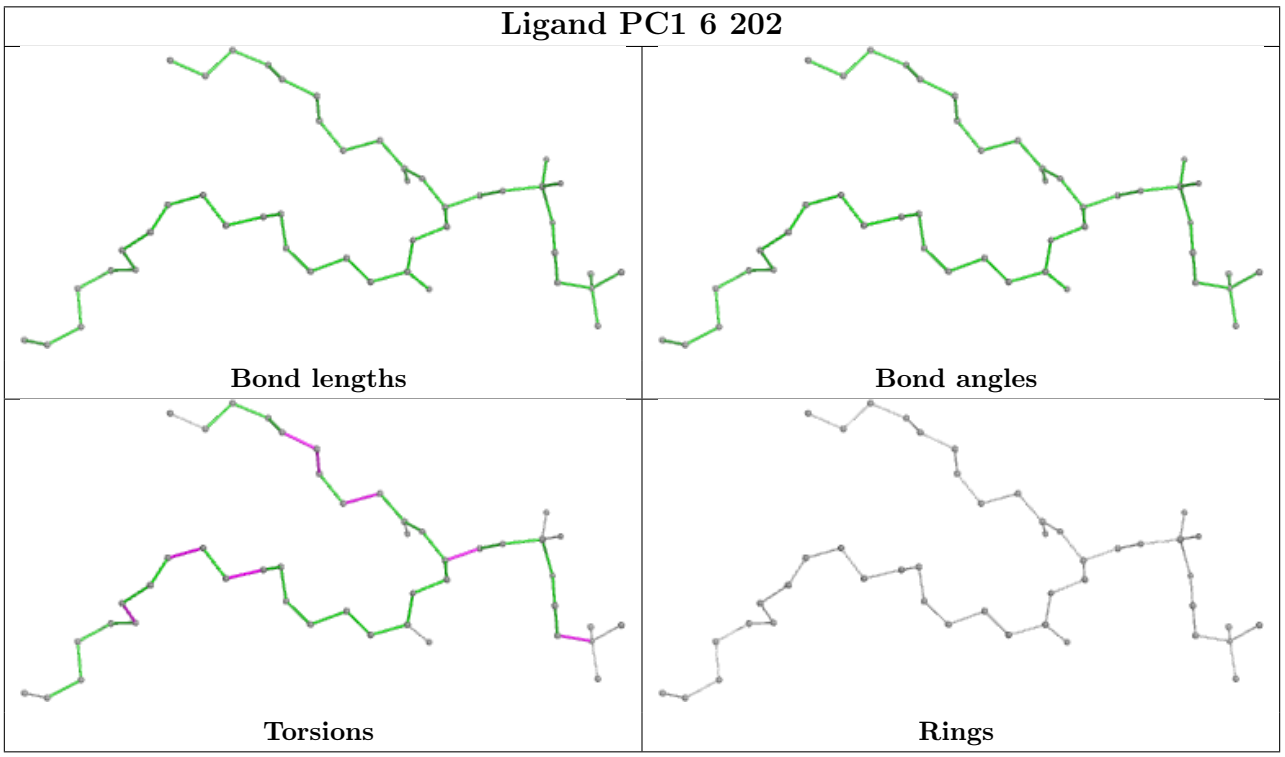


Rings

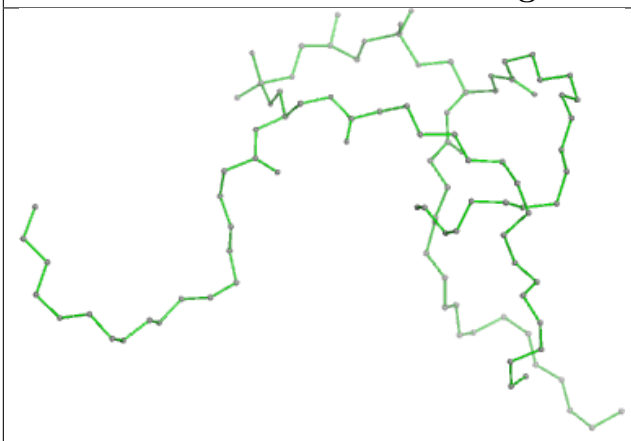
Ligand 3PE J 202



Ligand PC1 6 202



Ligand CDL W 201



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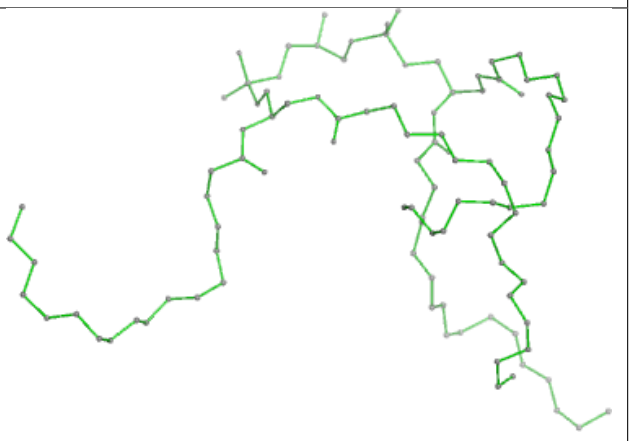
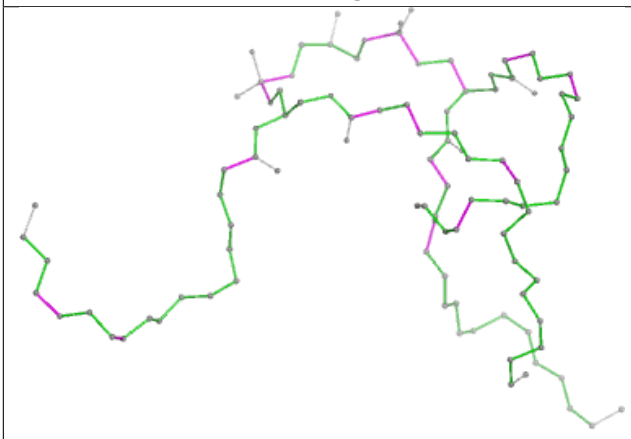
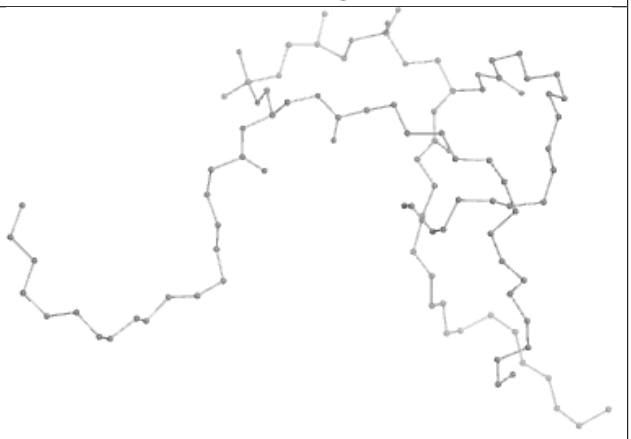


Bond angles

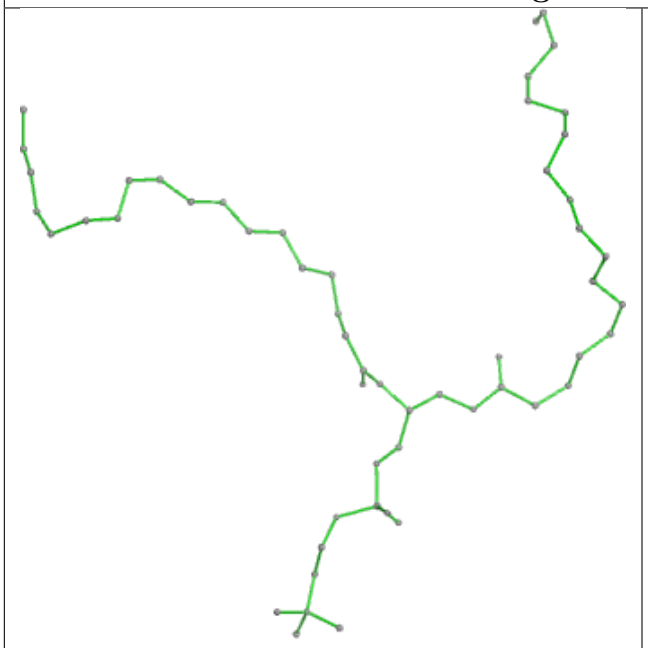


Torsions

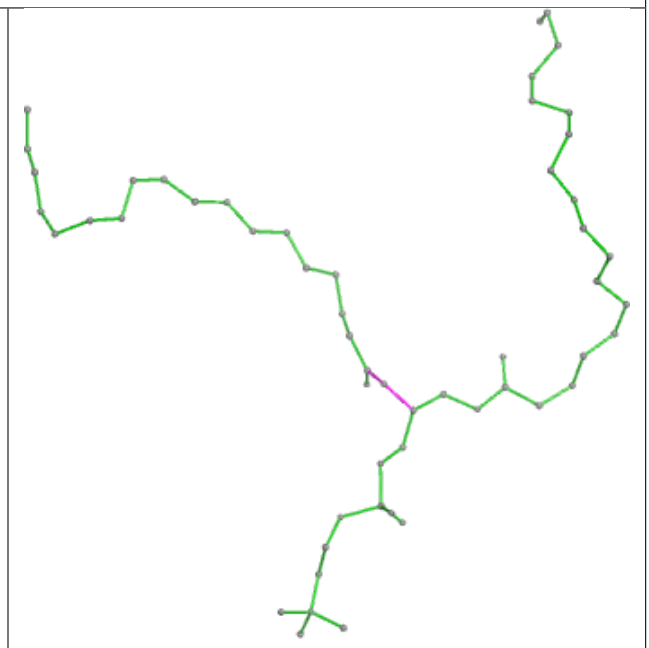


Rings

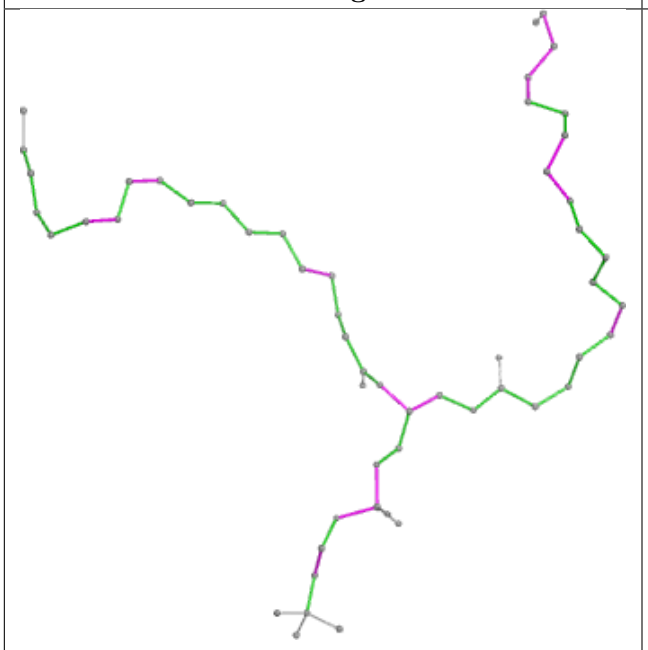
Ligand PC1 9 401



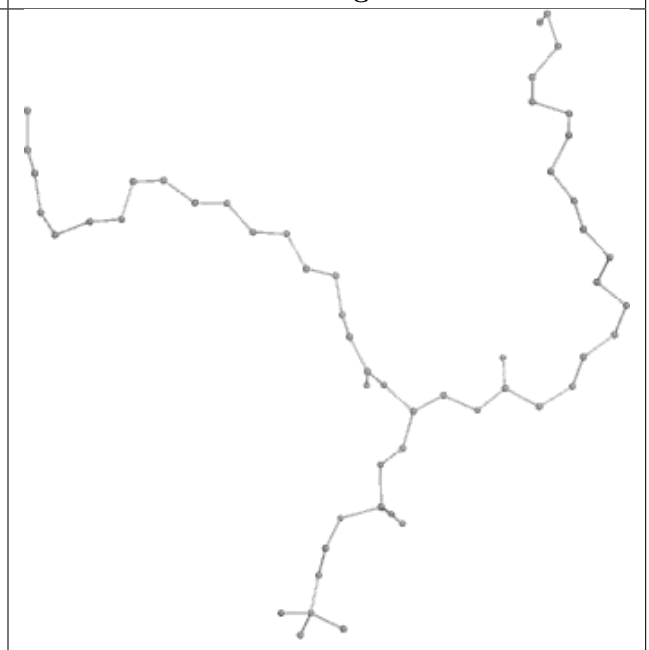
Bond lengths



Bond angles

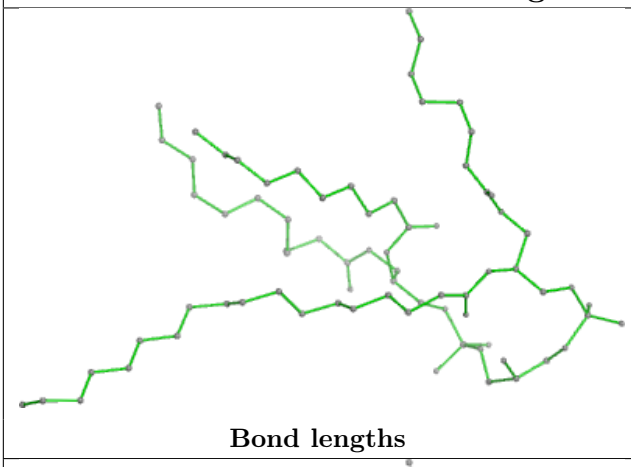


Torsions

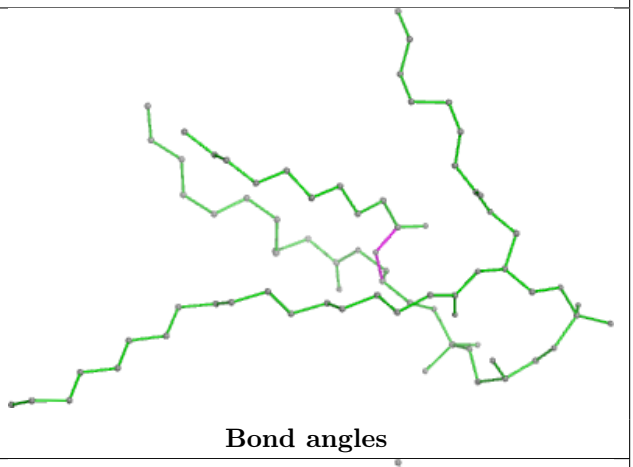


Rings

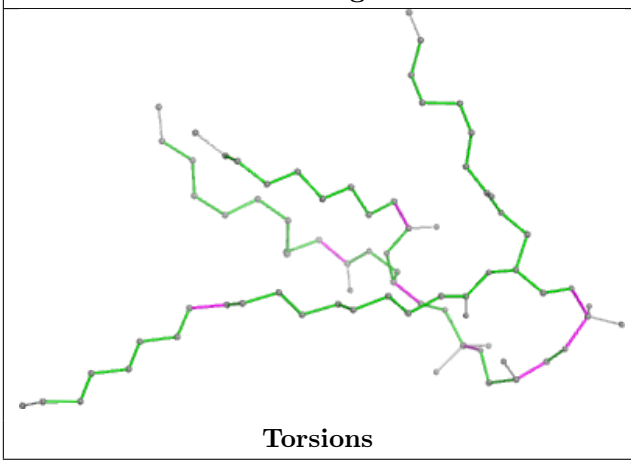
Ligand CDL x 101



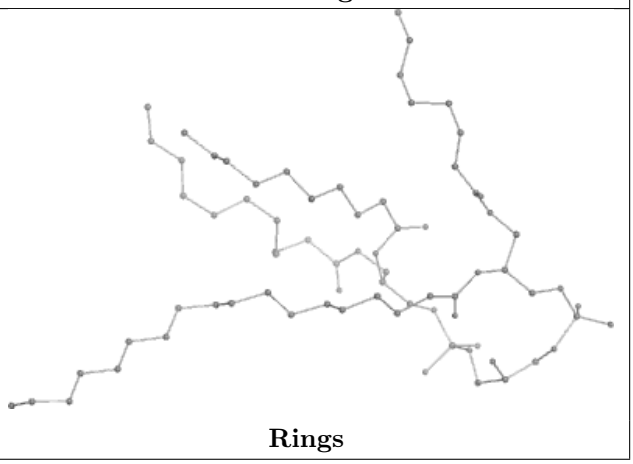
Bond lengths



Bond angles

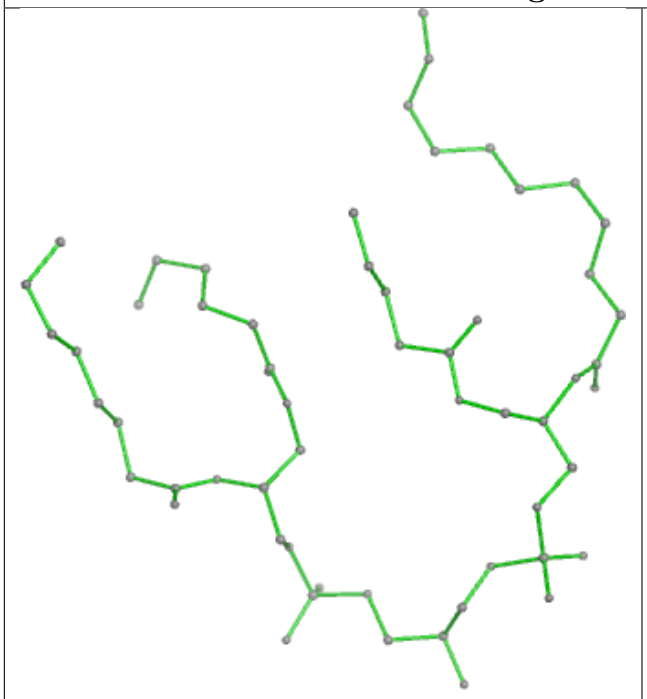


Torsions



Rings

Ligand CDL h 201



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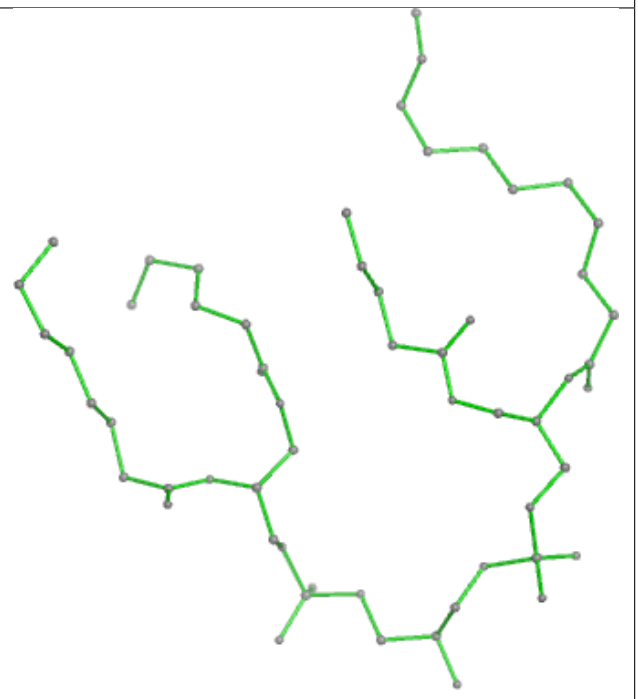
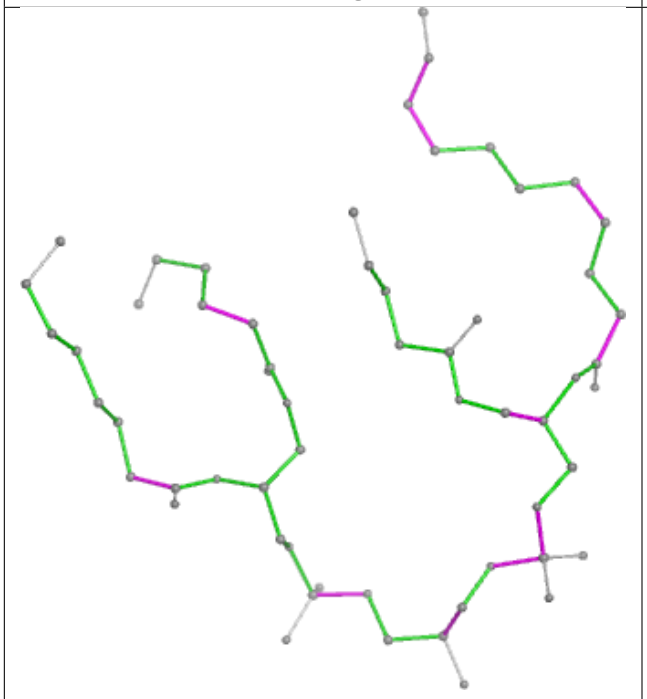
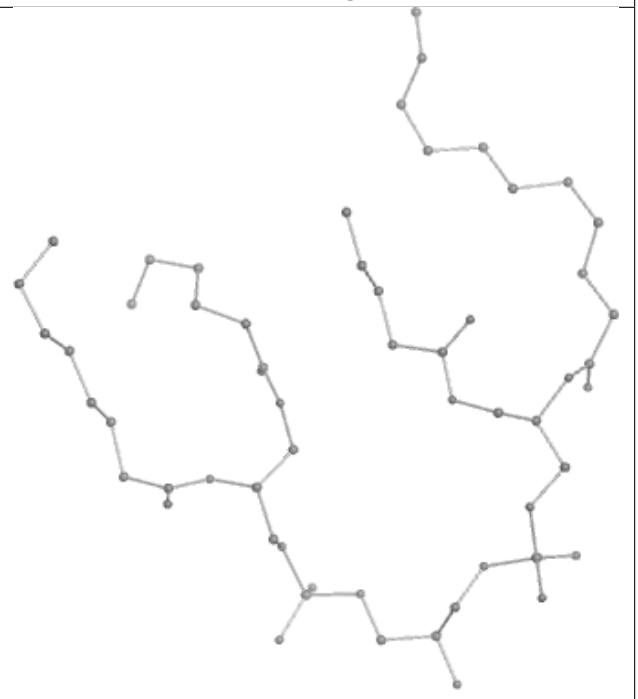


Bond angles

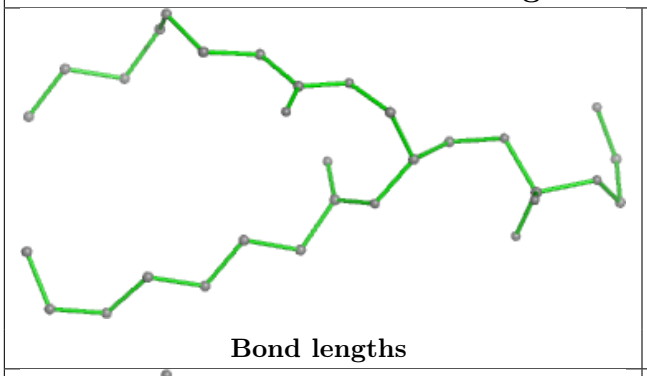


Torsions

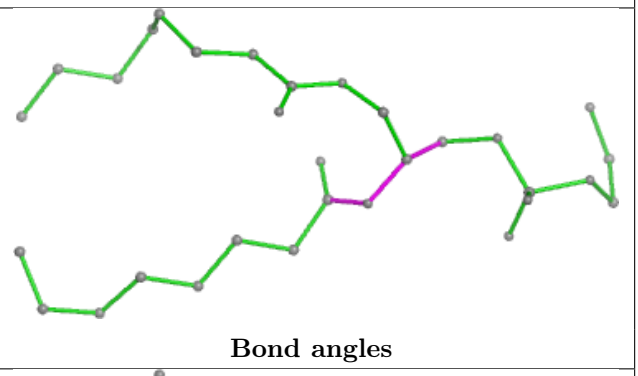


Rings

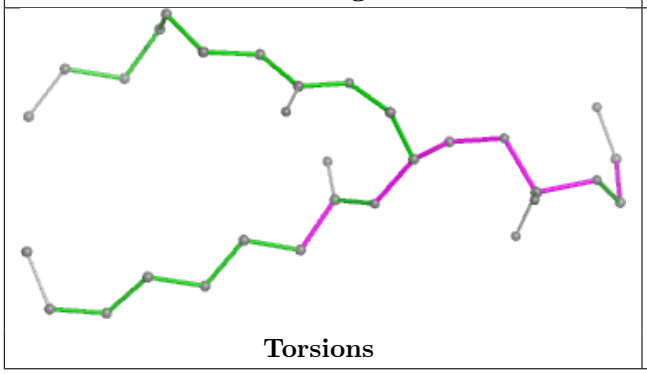
Ligand 3PE L 1002



Bond lengths



Bond angles



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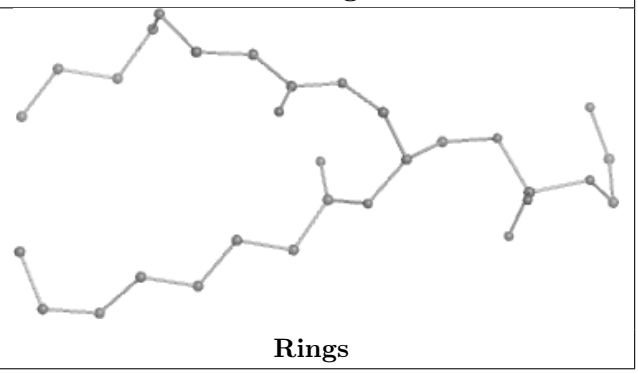
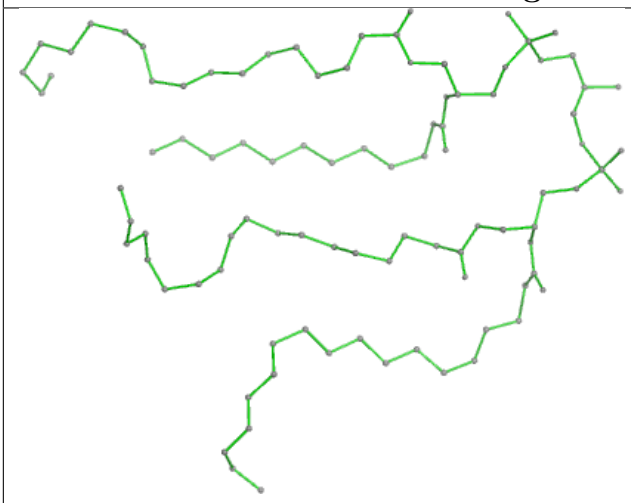
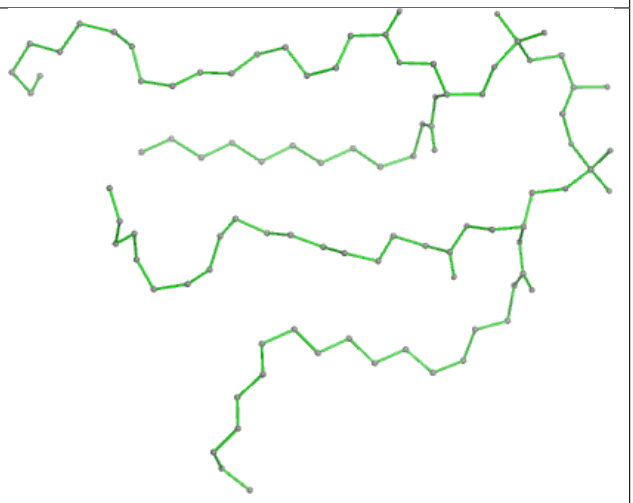


Rings

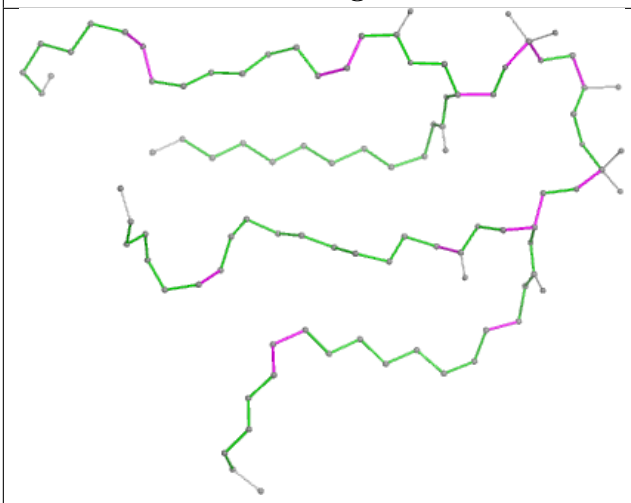
Ligand CDL V 203



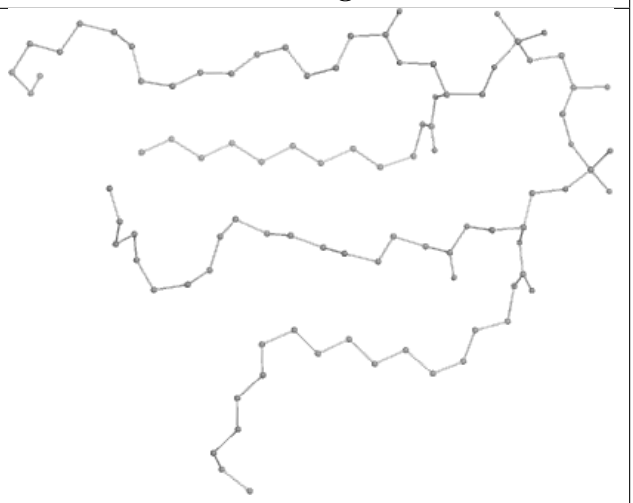
Bond lengths



Bond angles

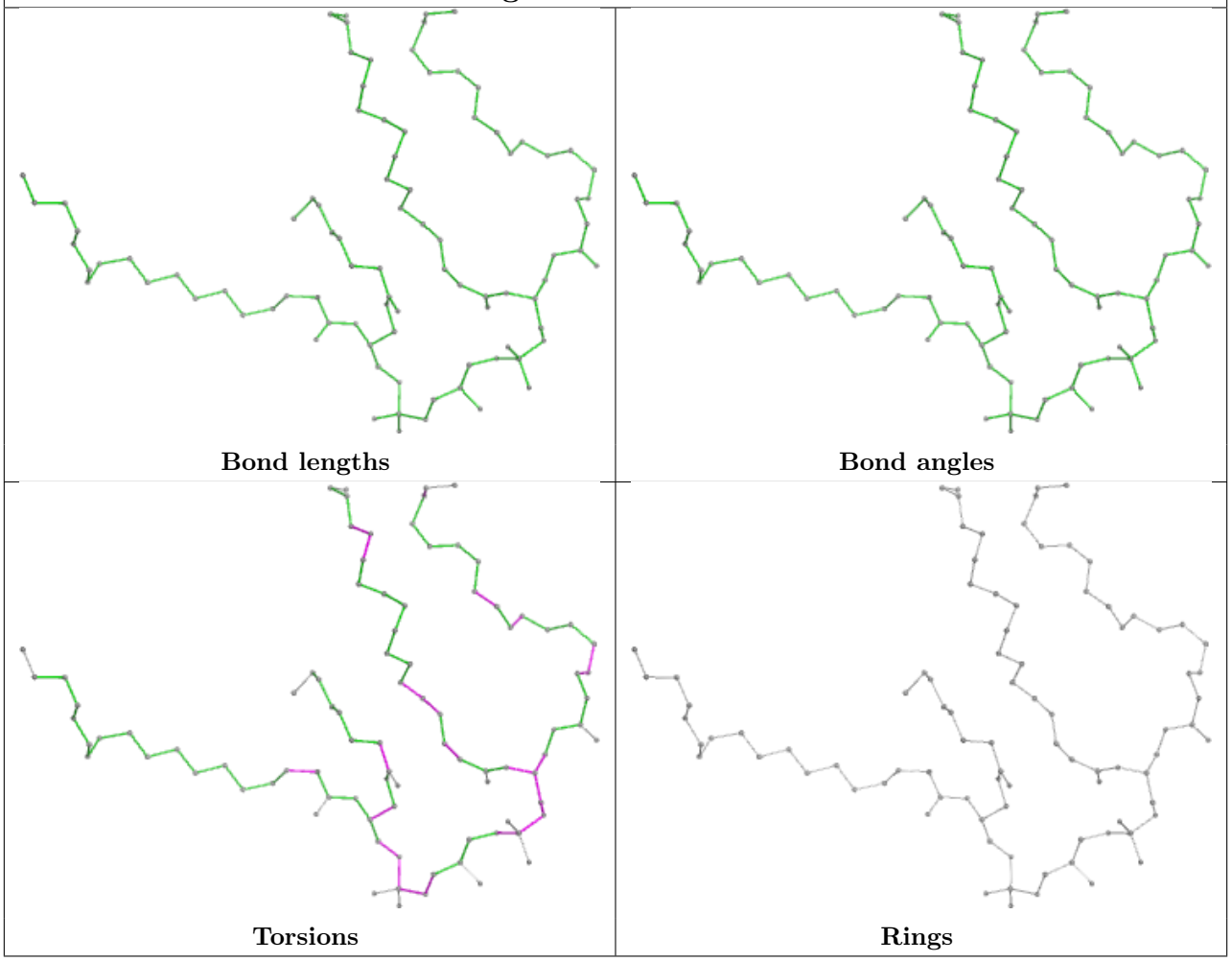


Torsions

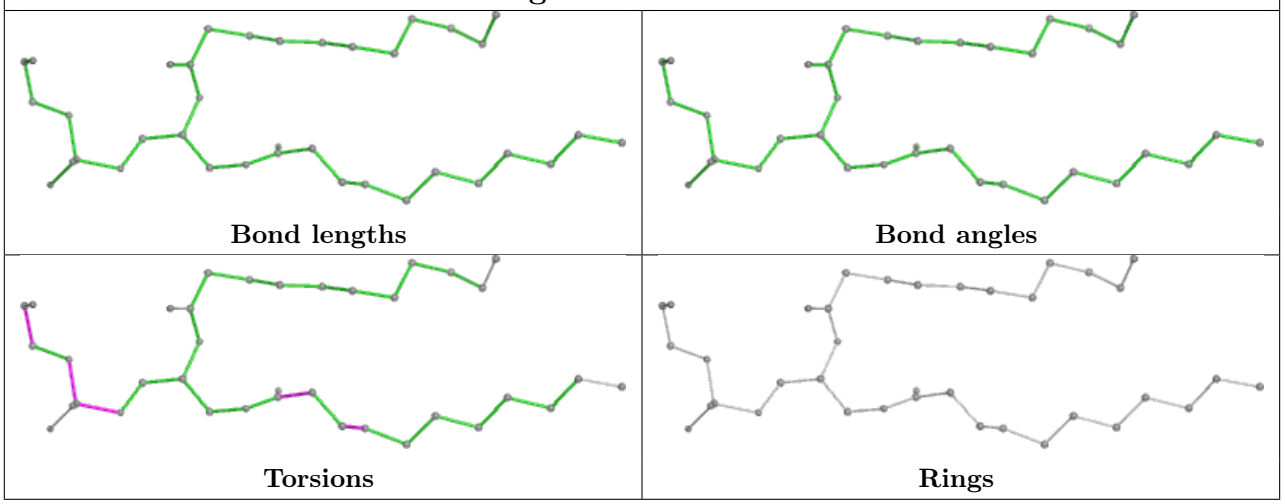


Rings

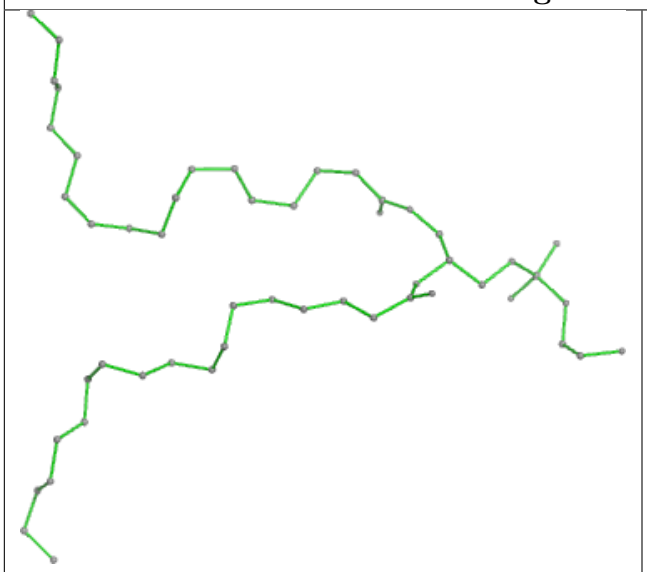
Ligand CDL N 402



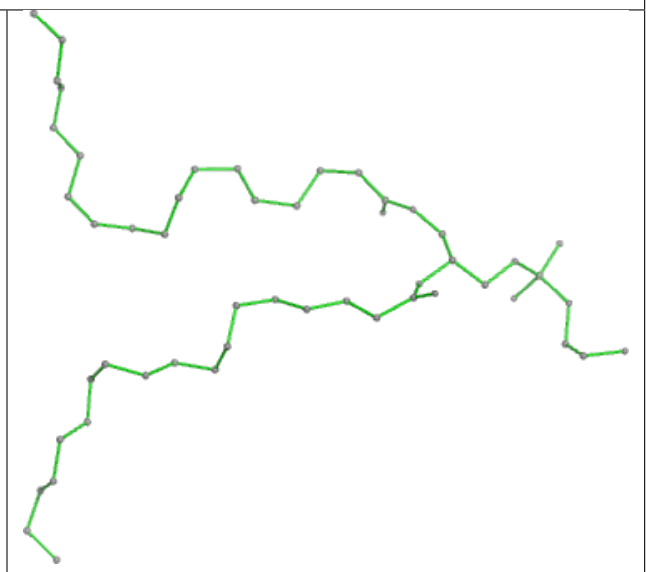
Ligand 3PE V 202



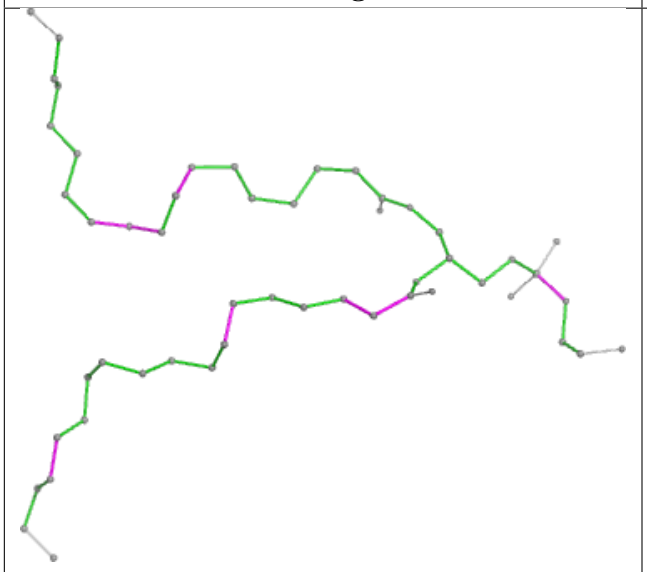
Ligand 3PE 6 203



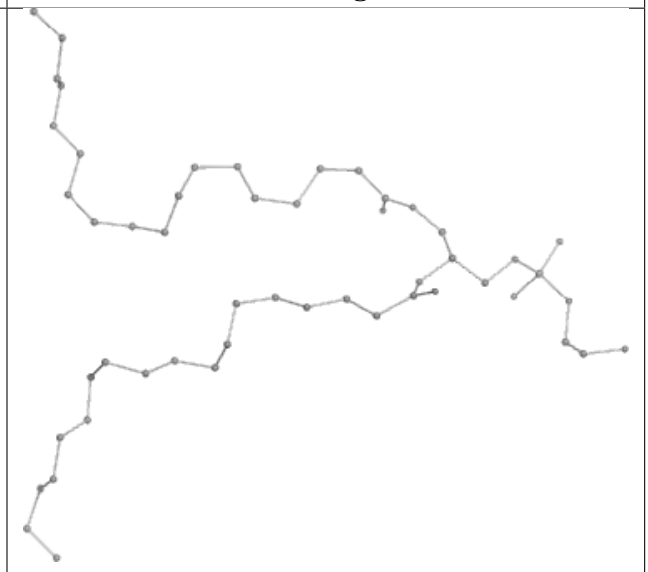
Bond lengths



Bond angles

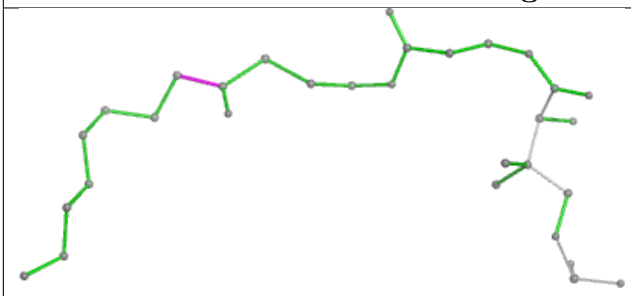


Torsions

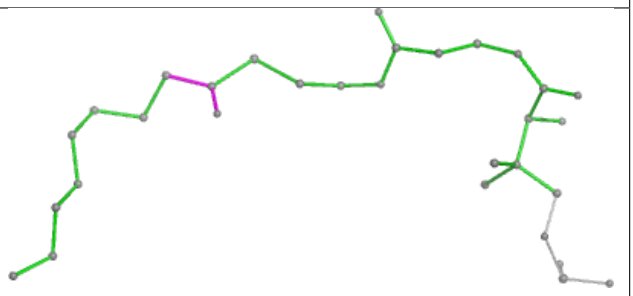


Rings

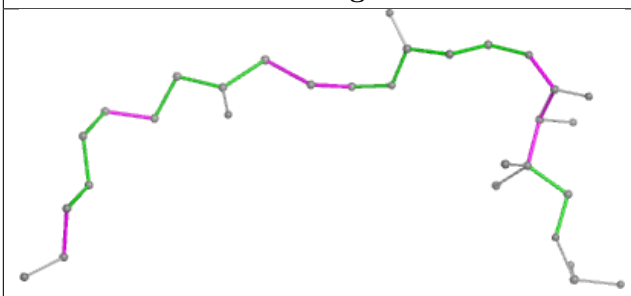
Ligand ZMP X 101



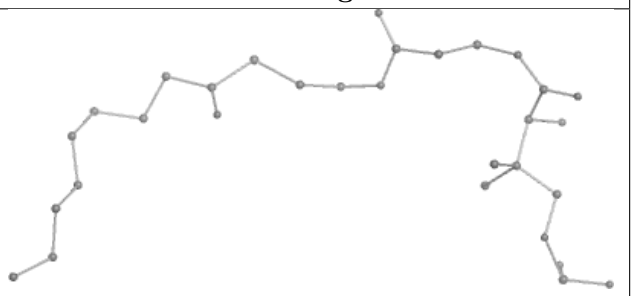
Bond lengths



Bond angles

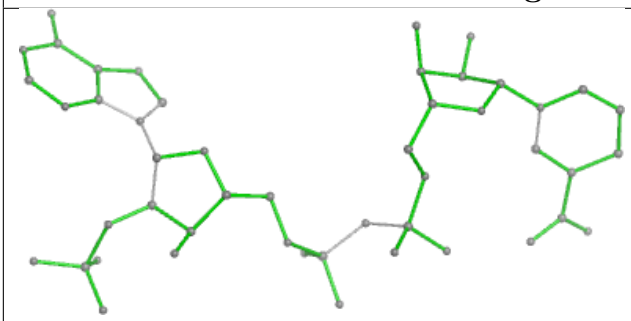


Torsions

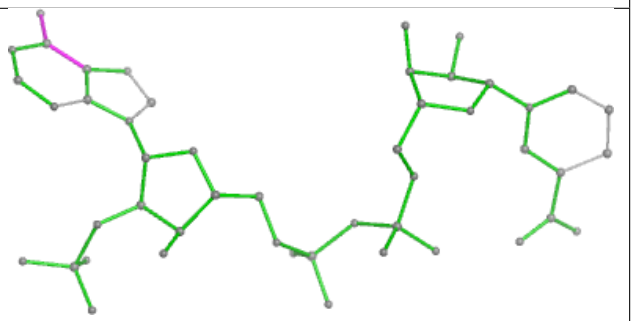


Rings

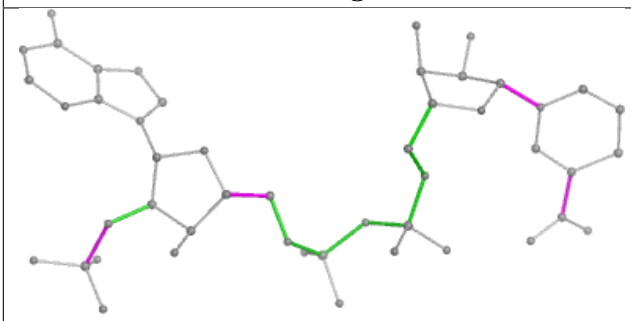
Ligand NDP d 401



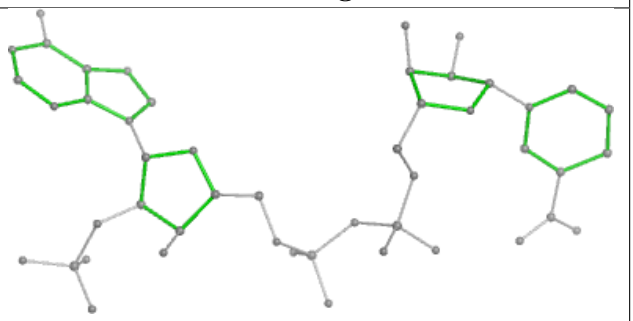
Bond lengths



Bond angles

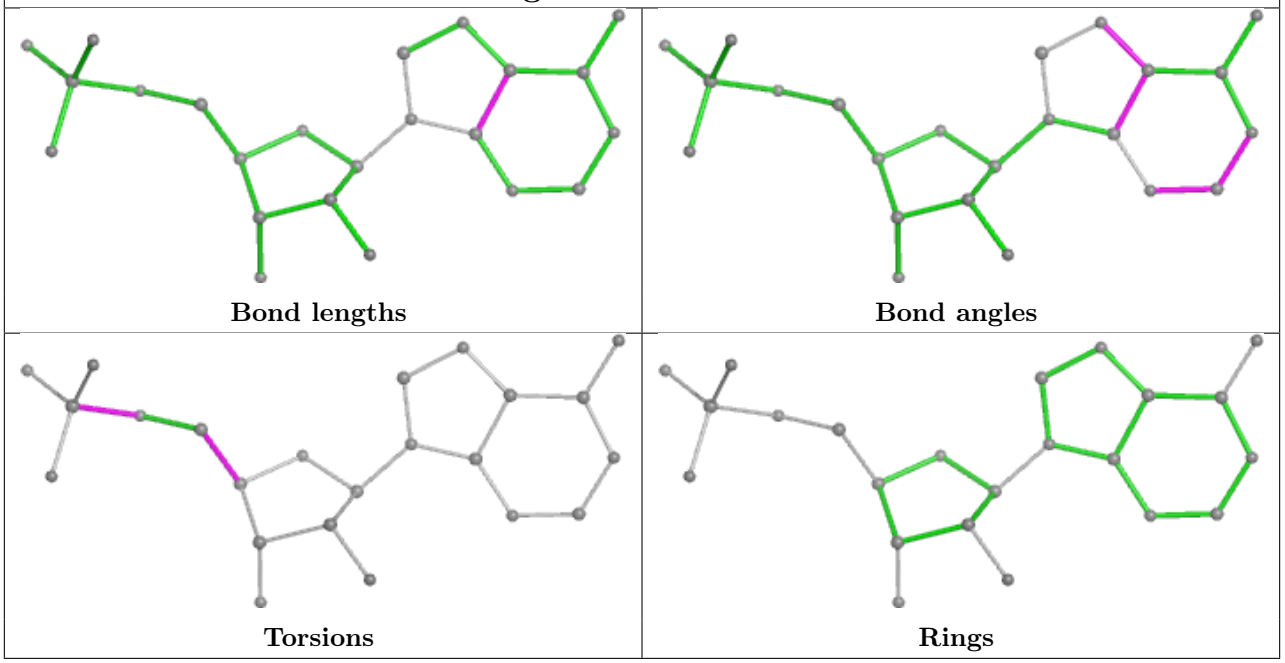


Torsions

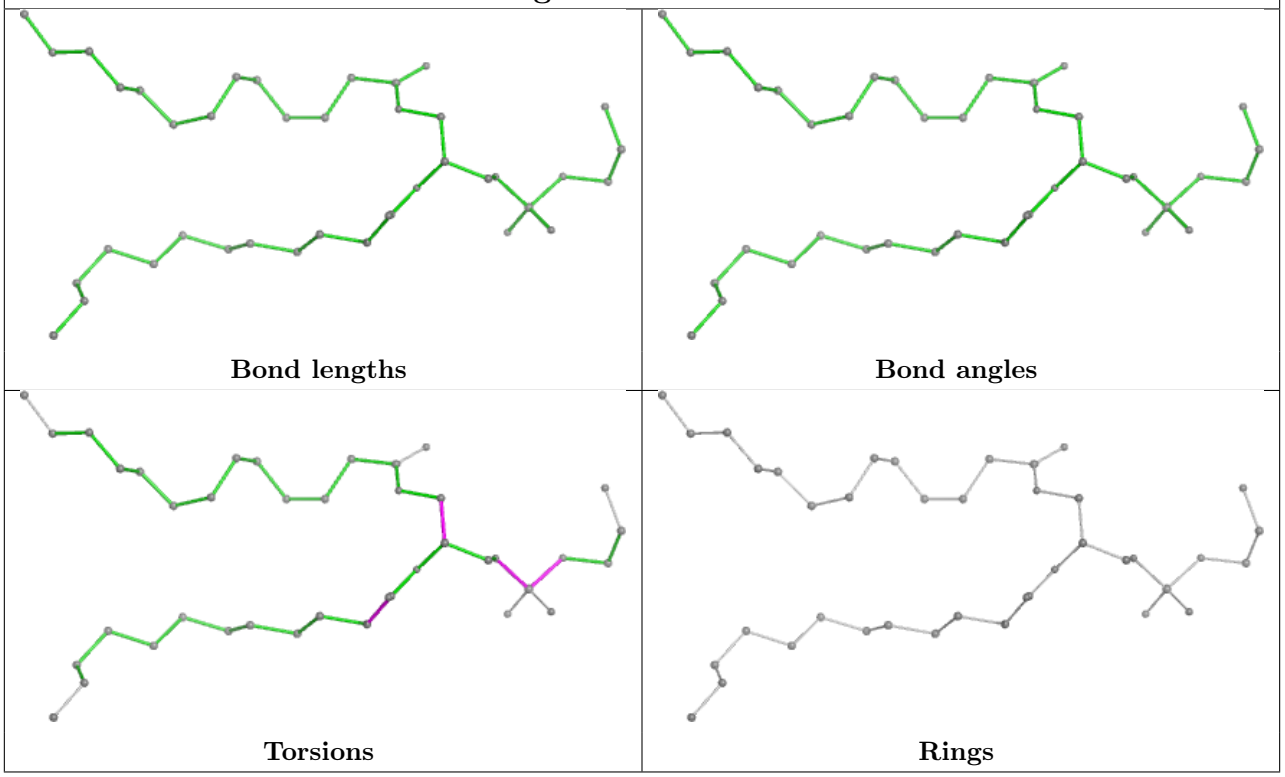


Rings

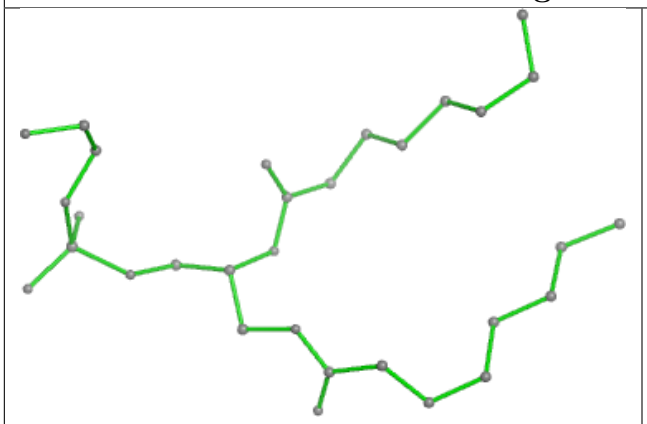
Ligand AMP k 501



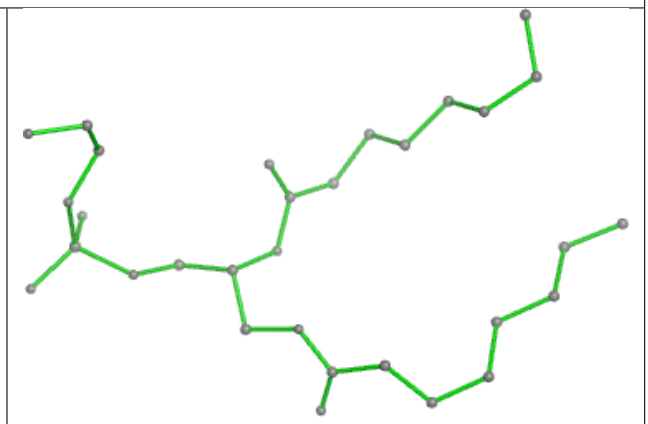
Ligand 3PE 4 502



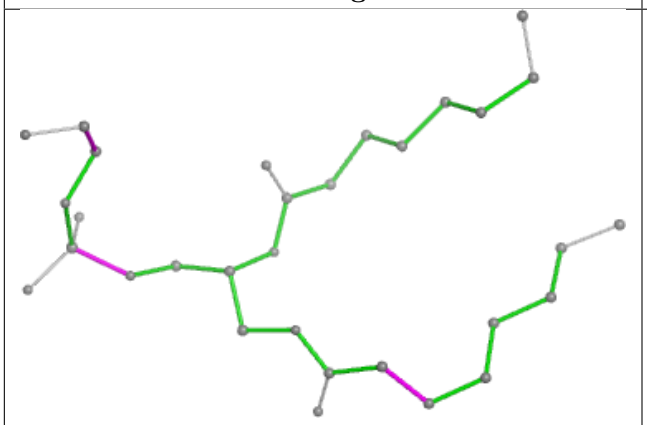
Ligand 3PE o 501



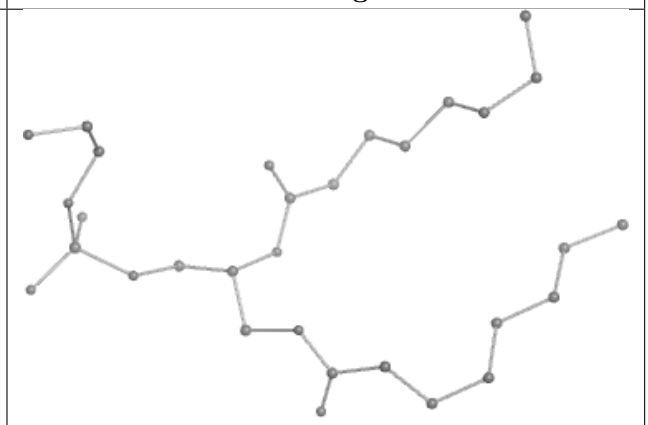
Bond lengths



Bond angles

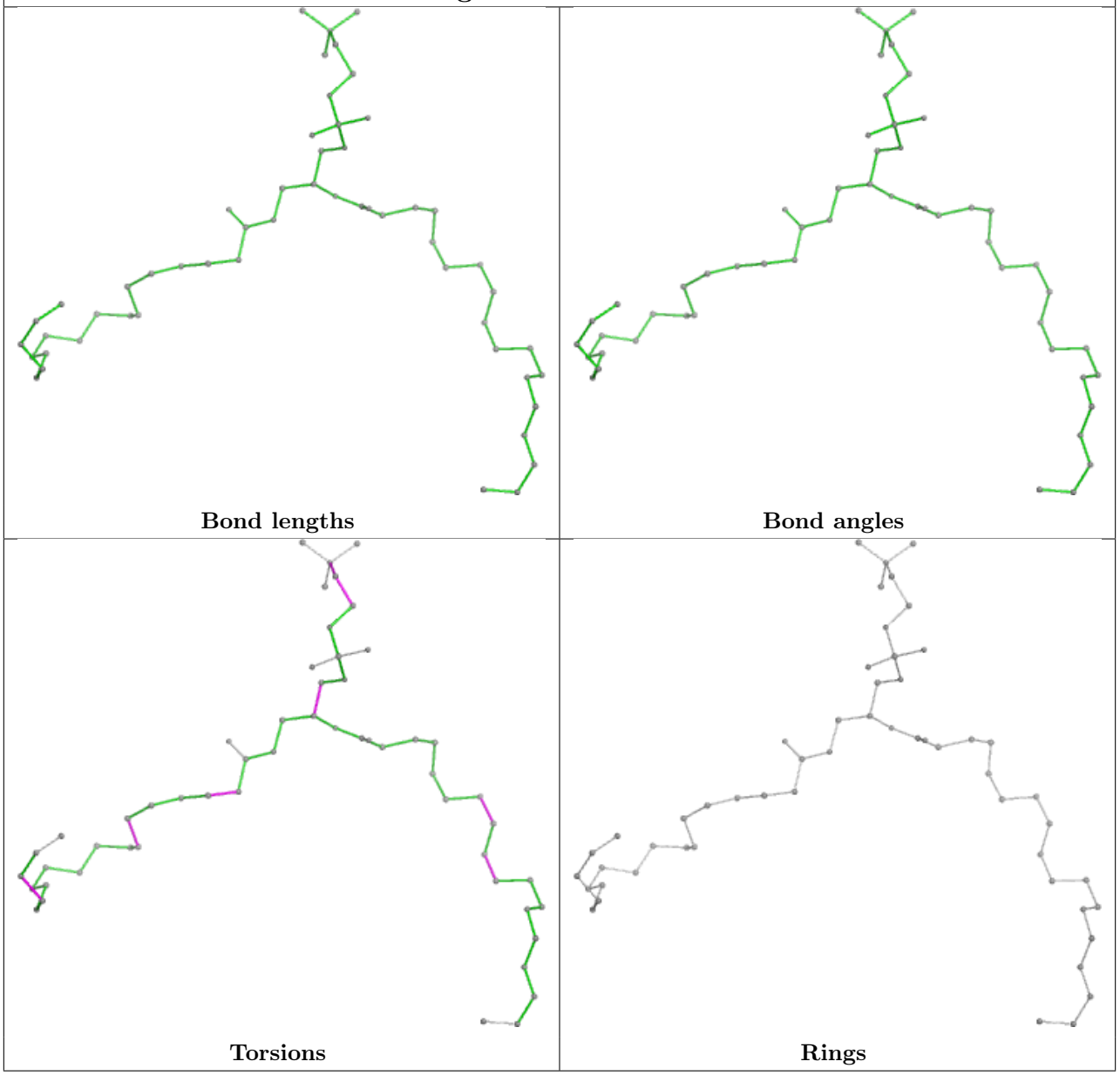


Torsions

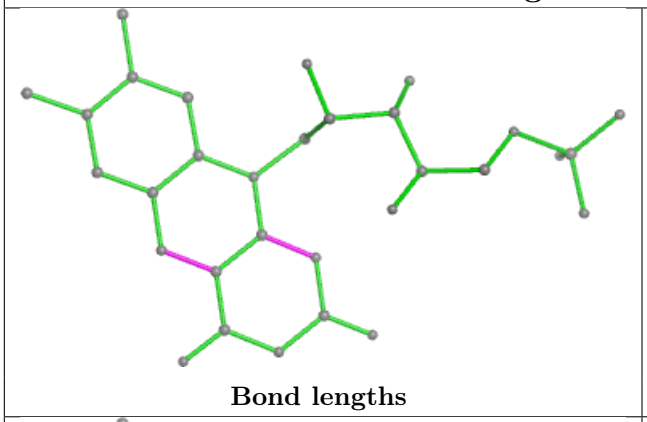


Rings

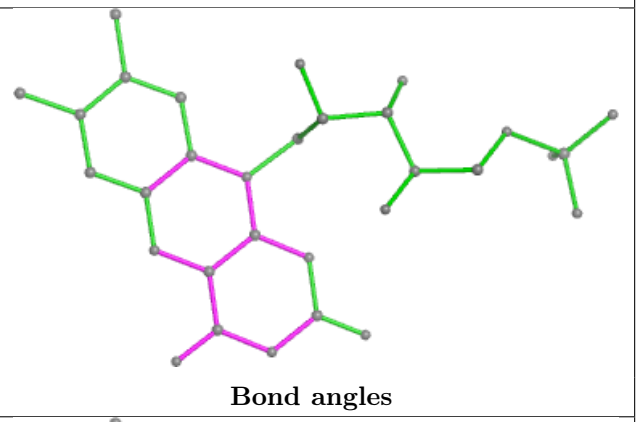
Ligand PC1 M 502



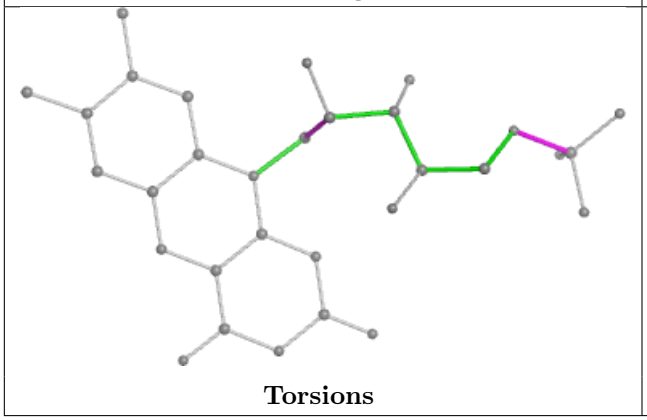
Ligand FMN 1 502



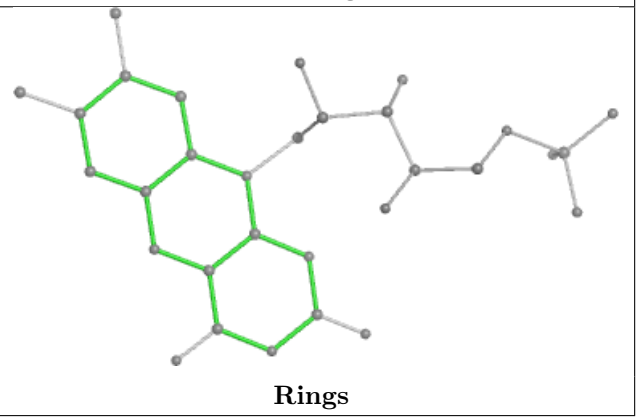
Bond lengths



Bond angles

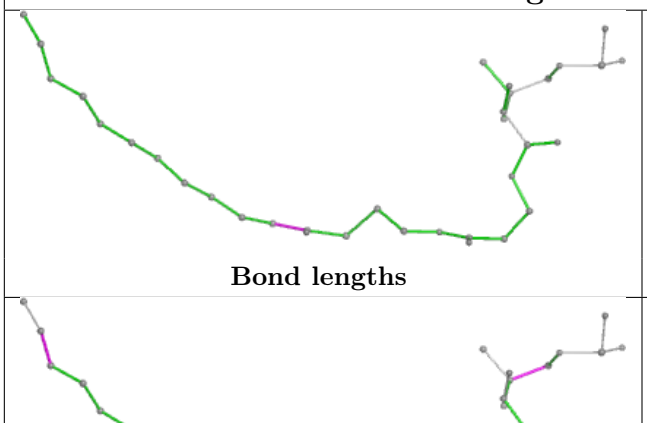


Torsions

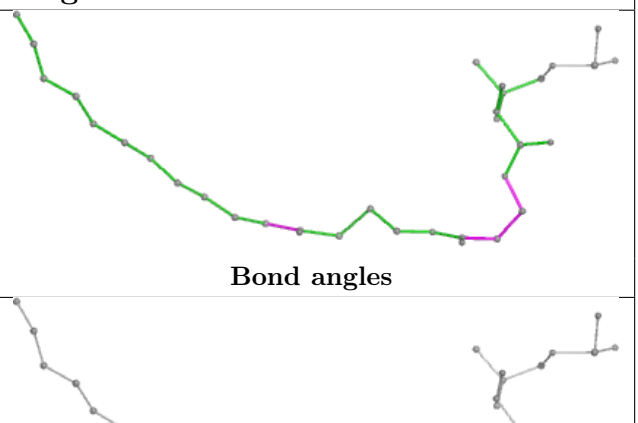


Rings

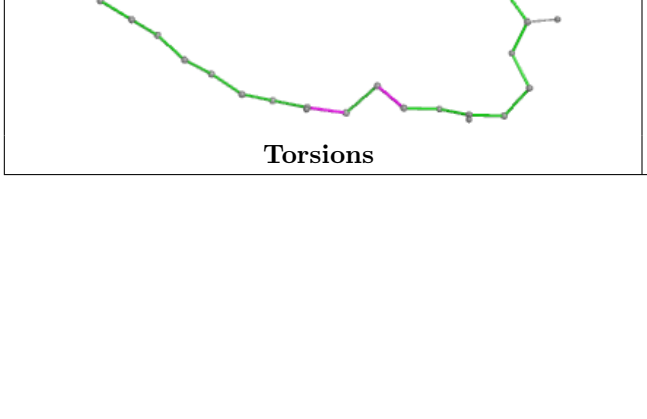
Ligand ZMP g 201



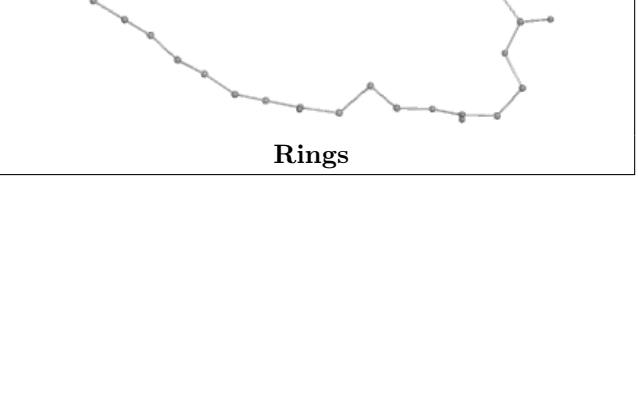
Bond lengths



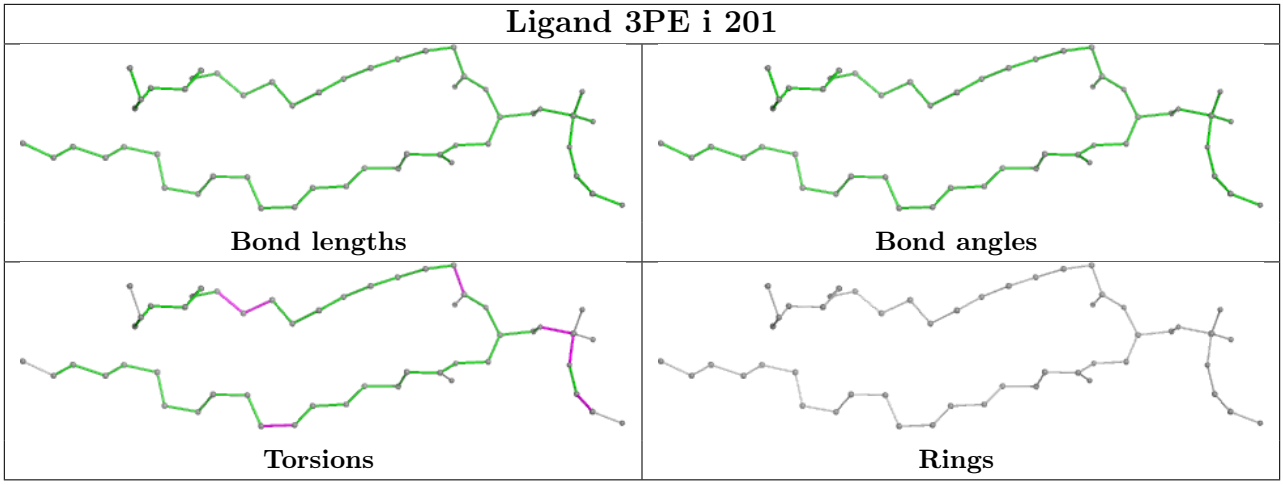
Bond angles

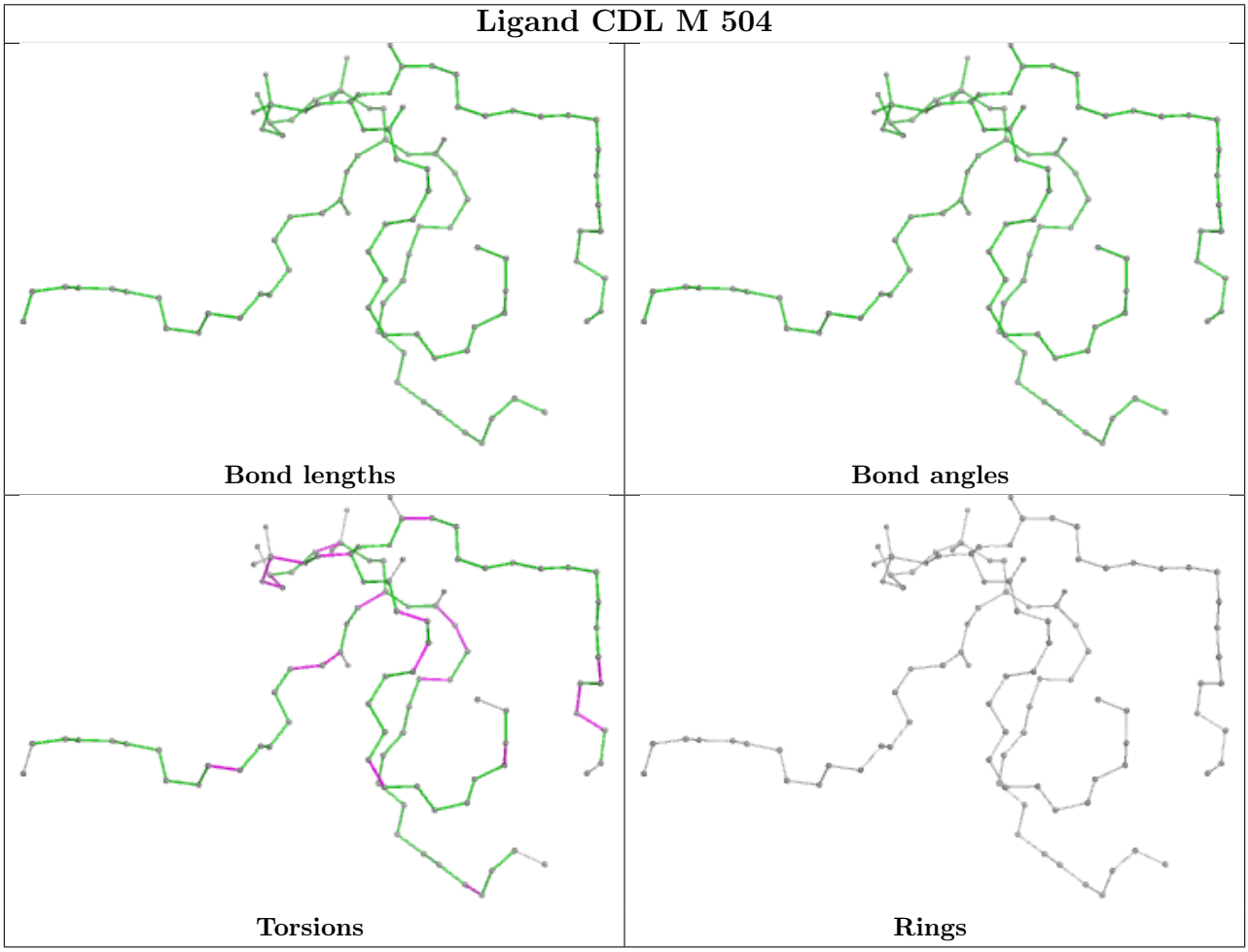


Torsions



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-11252. 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.