Full wwPDB EM Validation Report ⓘ

Jun 17, 2024 – 10:27 am BST

PDB ID	:	8Q1U
EMDB ID	:	EMD-18067
Title	:	Inward-facing, open1 proteoliposome complex I at 3.3 A, after deactivation treatment. Initially purified in LMNG.
Authors	:	Grba, D.N.; Hirst, J.
Deposited on	:	2023-08-01
Resolution	:	3.30 Å(reported)
Based on initial model	:	7QSN

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

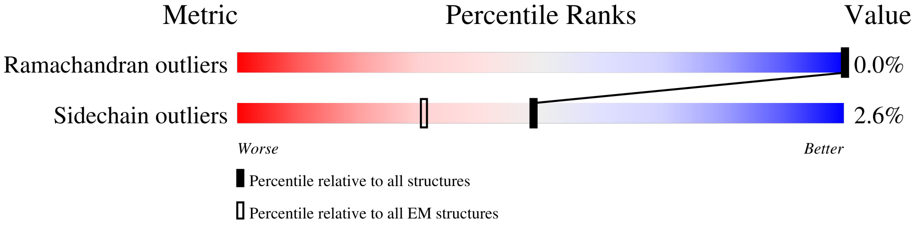
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

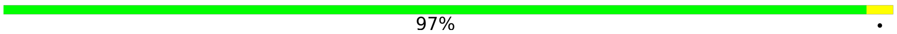
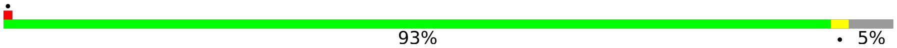
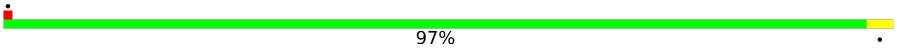
The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	 97% •
2	B	216	 69% • 28%
3	C	266	 77% • 22%
4	D	463	 89% • 9%
5	E	249	 84% • 14%
6	F	464	 • 91% • 7%
7	G	727	 • 93% • 5%
8	H	318	 • 97% •
9	I	212	 82% • 17%

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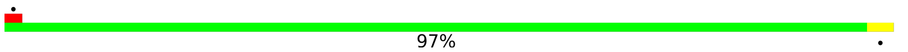
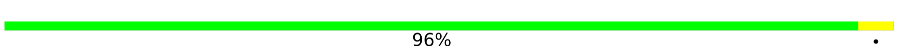
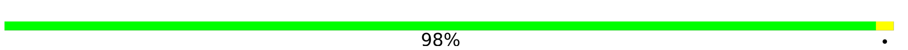
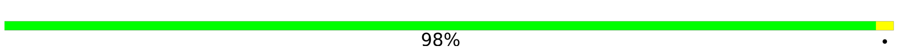
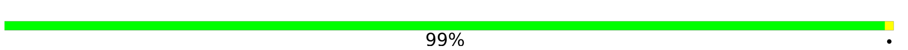
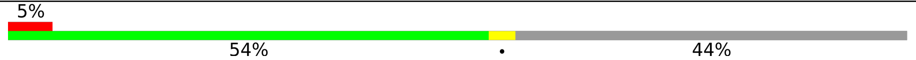
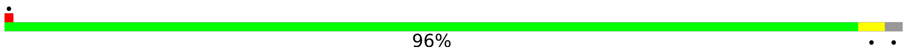
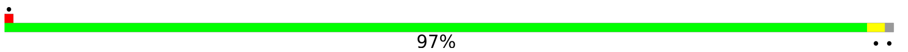
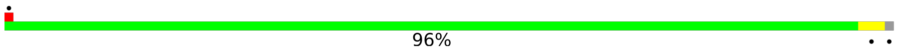
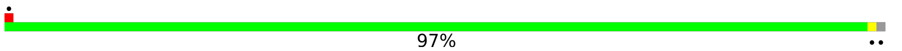
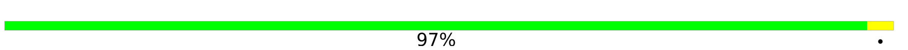
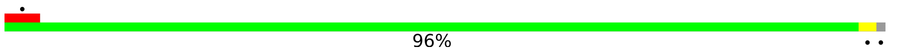
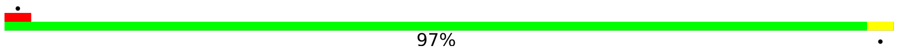
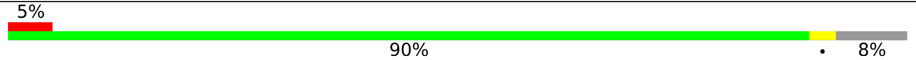
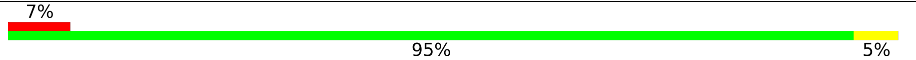
Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	

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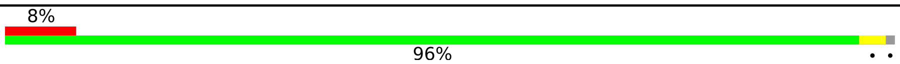
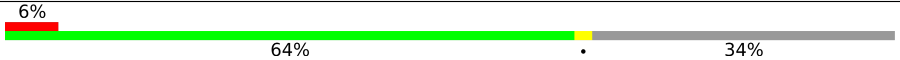
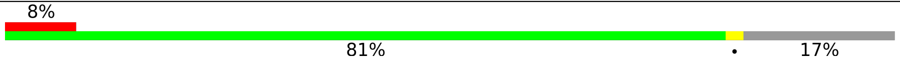
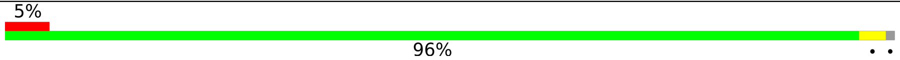
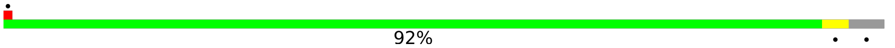
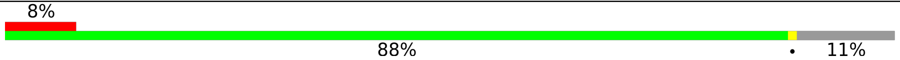
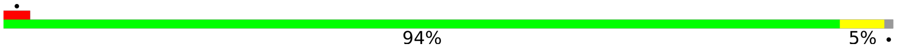
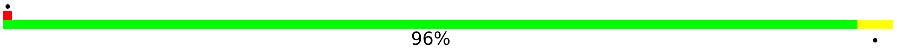
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 69145 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	115	921	622	133	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	421	3392	2168	584	615	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1659	1059	278	312	10	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	432	3326	2096	594	616	20	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	691	5298	3318	925	1016	39	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	318	2509	1681	385	420	23	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	175	1345	906	191	236	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	98	745	486	112	131	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4802	3195	737	827	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3654	2436	570	609	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	347	2733	1817	416	457	43	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	339	2728	1765	484	474	5	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	129	1049	659	188	199	3	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total 740	C 454	N 140	O 143	S 3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total 707	C 454	N 104	O 144	S 5	0	0
20	U	88	Total 707	C 454	N 104	O 144	S 5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total 923	C 597	N 156	O 167	S 3	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	116	Total 982	C 628	N 182	O 168	S 4	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total 1402	C 887	N 253	O 252	S 10	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			654	427	109	116	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	98	Total	C	N	O	S	0	0
			825	521	157	141	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	57	492	322	86	82	2	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	101	846	544	140	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1154	759	196	197	2	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	127	1097	722	191	183	1	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	71	597	390	99	107	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	81	653	427	110	114	2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total 1314	C 850	N 216	O 240	S 8	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	128	Total 1070	C 686	N 188	O 196	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total 1487	C 952	N 272	O 256	S 7	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total 1048	C 653	N 201	O 185	S 9	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	174	Total 1458	C 913	N 269	O 268	S 8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total 1212	C 780	N 216	O 211	S 5	0	0

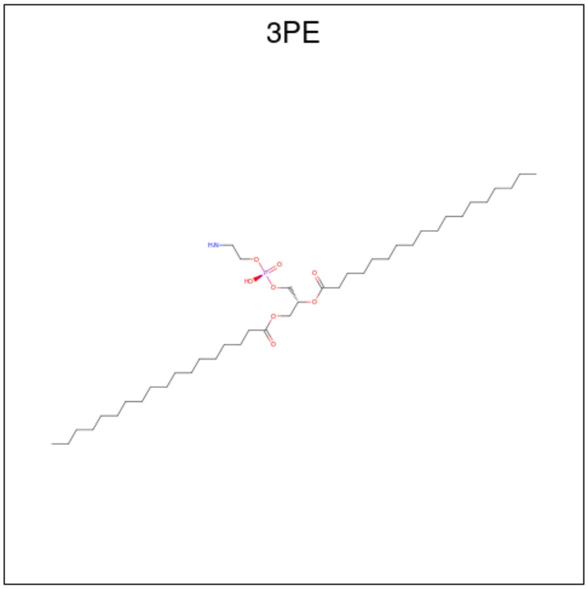
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	95	776	490	144	139	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	A	1	34	24	1	8	1	0
45	I	1	36	26	1	8	1	0
45	J	1	33	23	1	8	1	0
45	K	1	44	34	1	8	1	0
45	L	1	35	25	1	8	1	0
45	L	1	44	34	1	8	1	0
45	L	1	46	36	1	8	1	0

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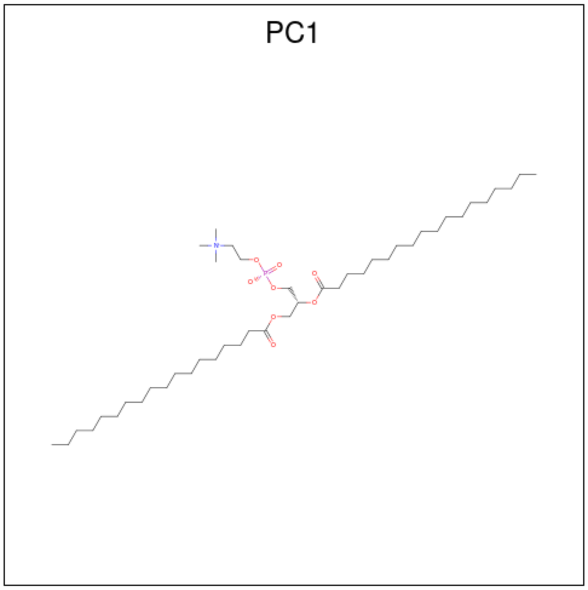
Mol	Chain	Residues	Atoms	AltConf
45	L	1	Total C N O P 37 27 1 8 1	0
45	M	1	Total C N O P 50 40 1 8 1	0
45	N	1	Total C N O P 49 39 1 8 1	0
45	N	1	Total C N O P 45 35 1 8 1	0
45	N	1	Total C N O P 45 35 1 8 1	0
45	Y	1	Total C N O P 27 17 1 8 1	0
45	Y	1	Total C N O P 51 41 1 8 1	0
45	Y	1	Total C N O P 51 41 1 8 1	0
45	Y	1	Total C N O P 36 26 1 8 1	0
45	Z	1	Total C N O P 45 35 1 8 1	0
45	b	1	Total C N O P 47 37 1 8 1	0
45	d	1	Total C N O P 49 39 1 8 1	0
45	g	1	Total C N O P 29 19 1 8 1	0
45	i	1	Total C N O P 45 35 1 8 1	0
45	m	1	Total C N O P 41 31 1 8 1	0
45	m	1	Total C N O P 33 23 1 8 1	0
45	o	1	Total C N O P 35 25 1 8 1	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 35 25 1 8 1	0
46	A	1	Total C N O P 35 25 1 8 1	0
46	H	1	Total C N O P 48 38 1 8 1	0
46	H	1	Total C N O P 39 29 1 8 1	0
46	I	1	Total C N O P 54 44 1 8 1	0
46	I	1	Total C N O P 37 27 1 8 1	0
46	L	1	Total C N O P 47 37 1 8 1	0
46	M	1	Total C N O P 44 34 1 8 1	0
46	M	1	Total C N O P 26 16 1 8 1	0
46	P	1	Total C N O P 46 36 1 8 1	0
46	Y	1	Total C N O P 40 30 1 8 1	0
46	d	1	Total C N O P 39 29 1 8 1	0
46	h	1	Total C N O P 31 21 1 8 1	0
46	q	1	Total C N O P 48 38 1 8 1	0

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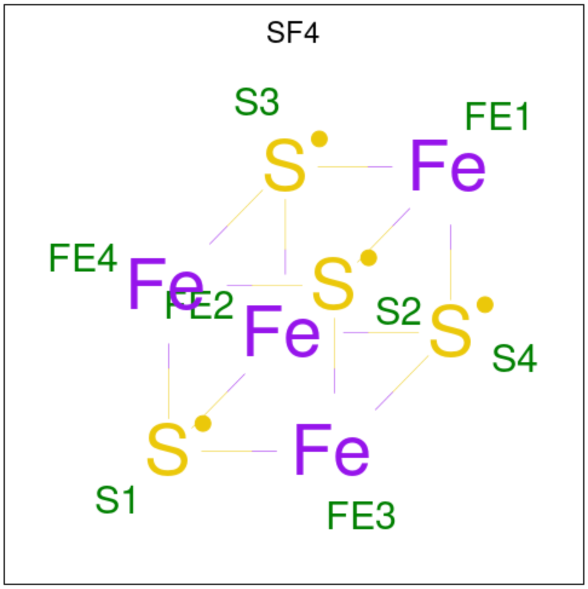
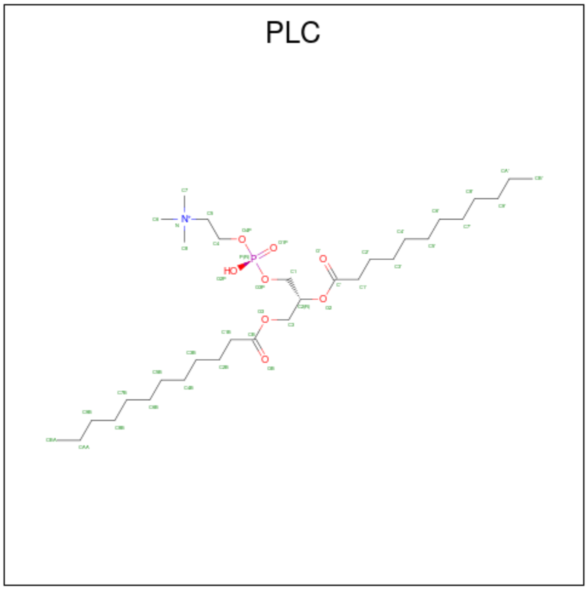
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	q	1	30	20	1	8	1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



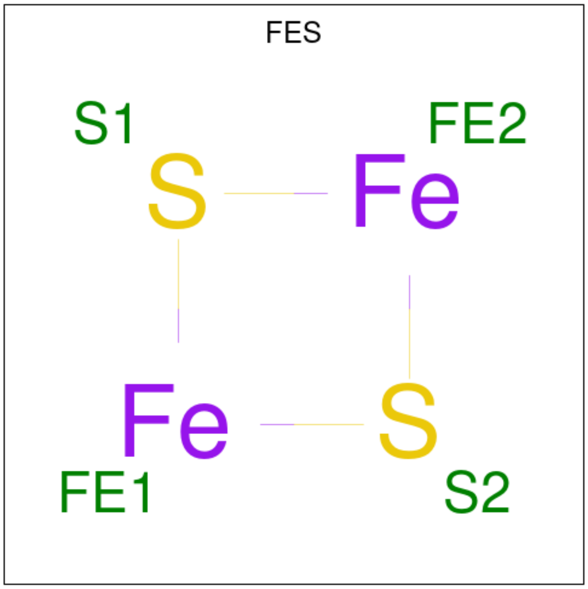
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	8	4	4	0
47	F	1	8	4	4	0
47	G	1	8	4	4	0
47	G	1	8	4	4	0
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



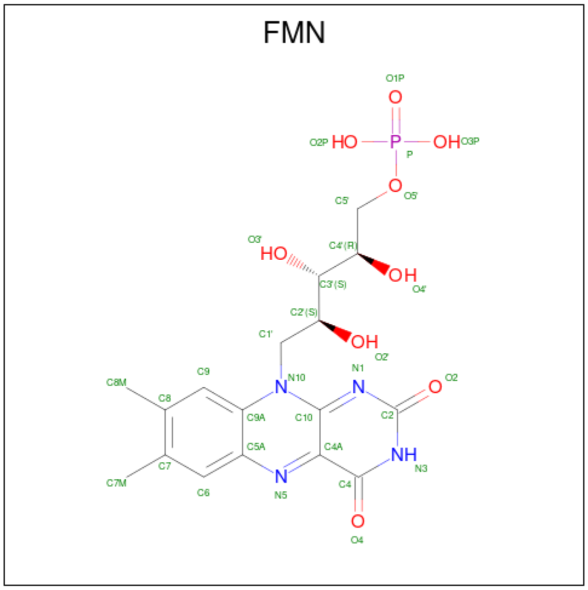
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total 38	C 28	N 1	O 8	P 1	0
48	L	1	Total 27	C 17	N 1	O 8	P 1	0
48	N	1	Total 26	C 16	N 1	O 8	P 1	0
48	b	1	Total 32	C 22	N 1	O 8	P 1	0
48	g	1	Total 32	C 22	N 1	O 8	P 1	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	E	1	4	2	2	0
49	G	1	4	2	2	0

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

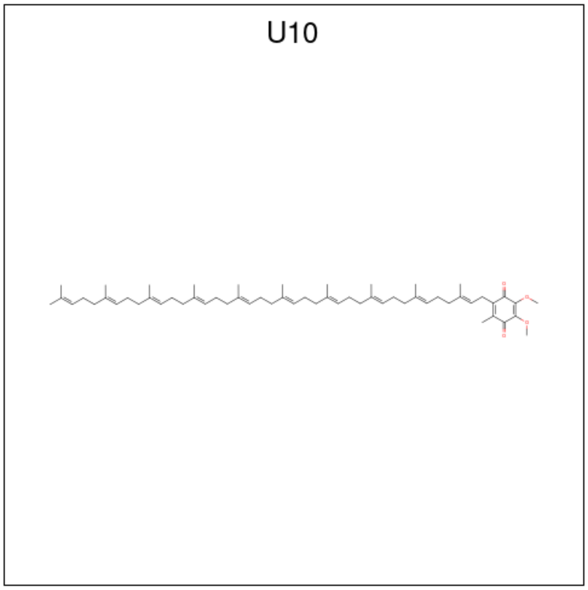


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	F	1	31	17	4	9	1	0

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

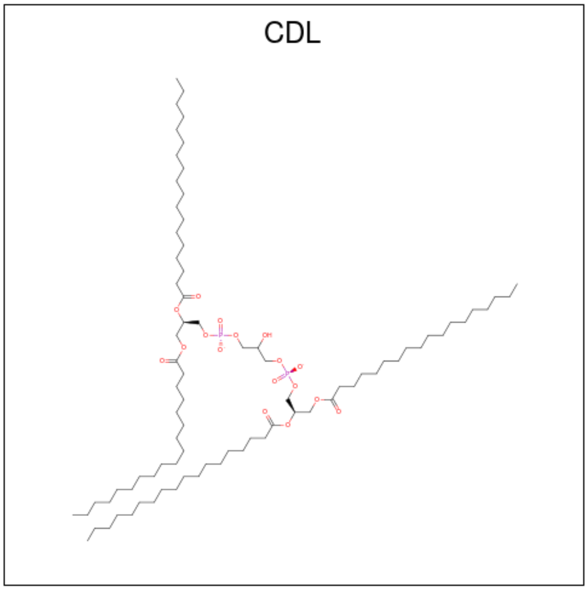
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
51	G	1	1	1	0

- Molecule 52 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	H	1	28	24	4	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	J	1	36	17	17	2	0
53	L	1	87	68	17	2	0
53	M	1	91	72	17	2	0

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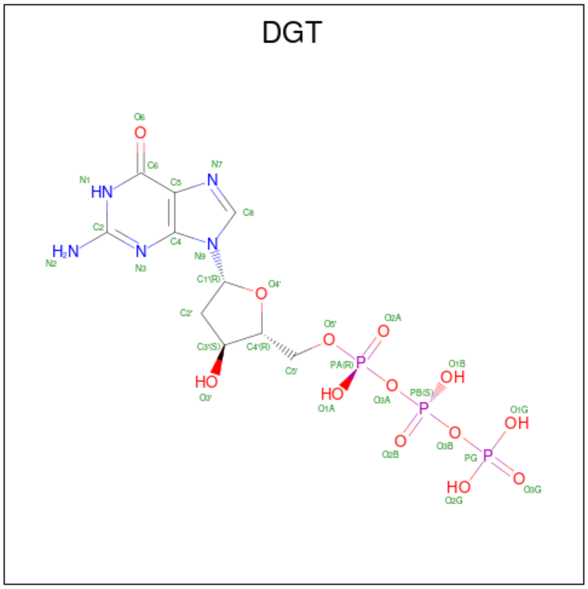
Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total 74	C 55	O 17	P 2	0
53	X	1	Total 87	C 68	O 17	P 2	0
53	d	1	Total 65	C 46	O 17	P 2	0
53	h	1	Total 80	C 61	O 17	P 2	0
53	q	1	Total 61	C 42	O 17	P 2	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total 1	Zn 1	0
54	R	1	Total 1	Zn 1	0

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

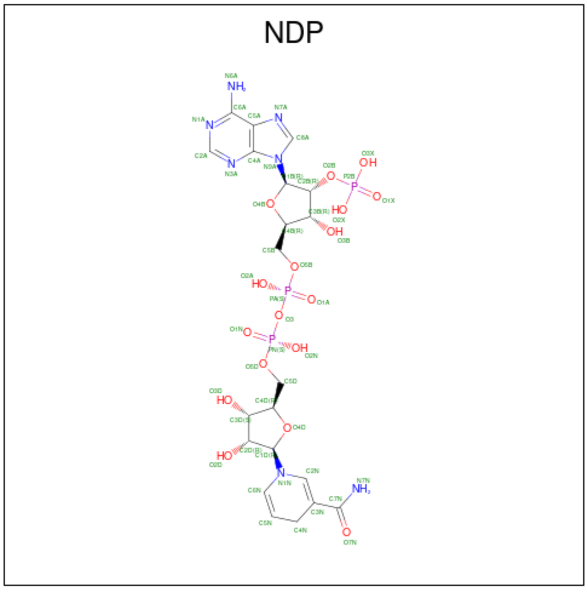


Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

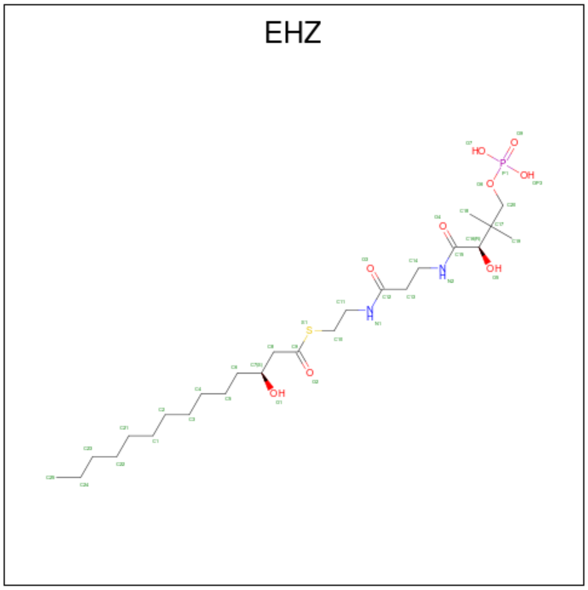
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	O	1	1	1	0

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



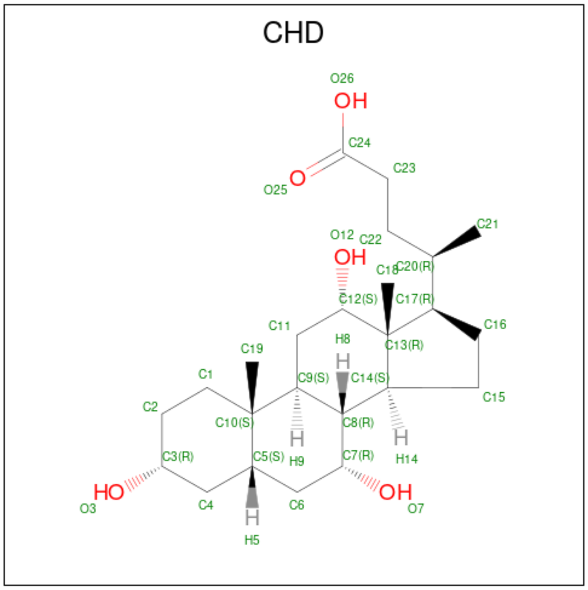
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	P	1	48	21	7	17	3	0

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



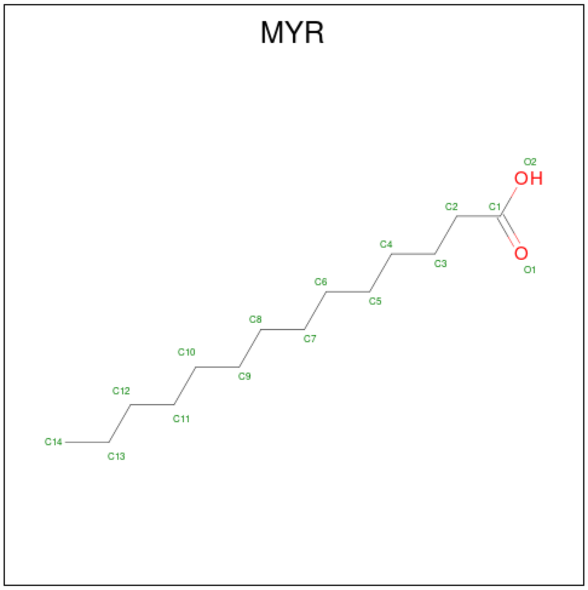
Mol	Chain	Residues	Atoms	AltConf
58	T	1	Total C N O P S 37 25 2 8 1 1	0
58	U	1	Total C N O P S 37 25 2 8 1 1	0

- Molecule 59 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	AltConf
59	i	1	Total C O 29 24 5	0

- Molecule 60 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).

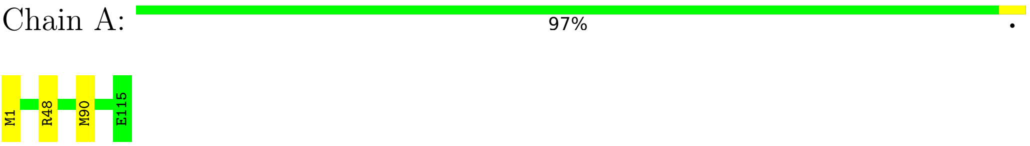


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
60	o	1	15	14	1	0

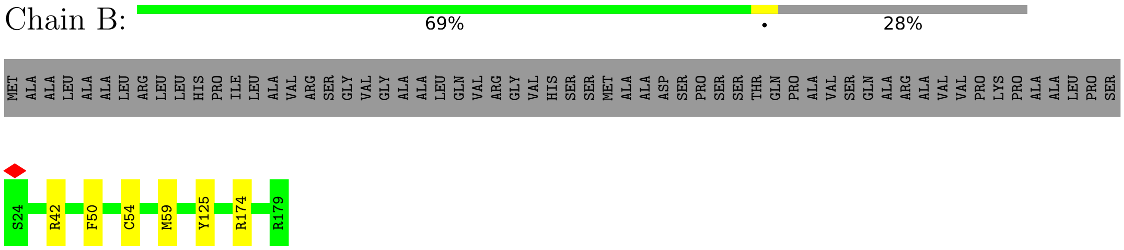
3 Residue-property plots ⓘ

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

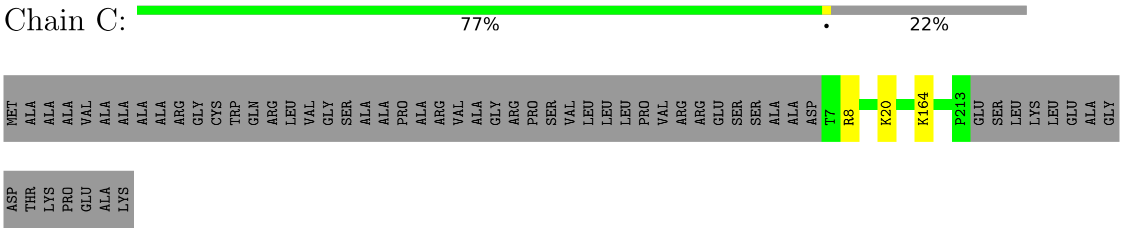
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



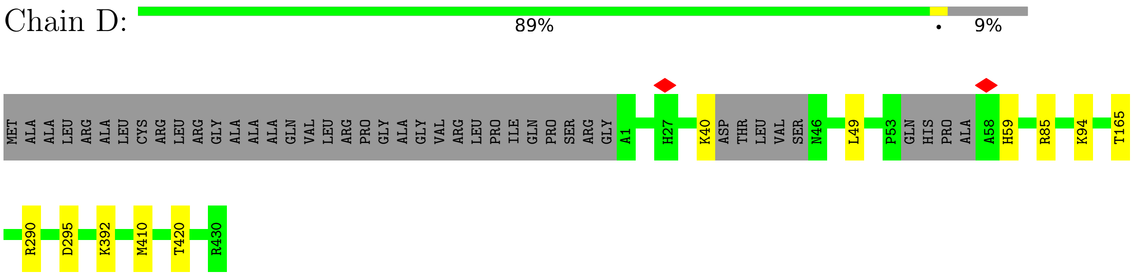
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

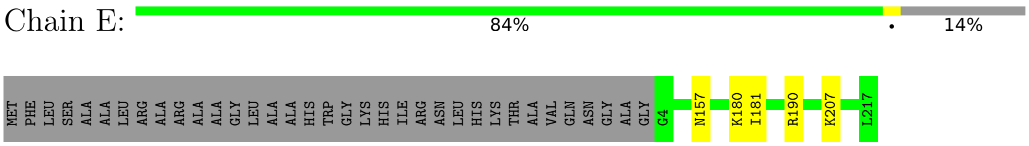


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



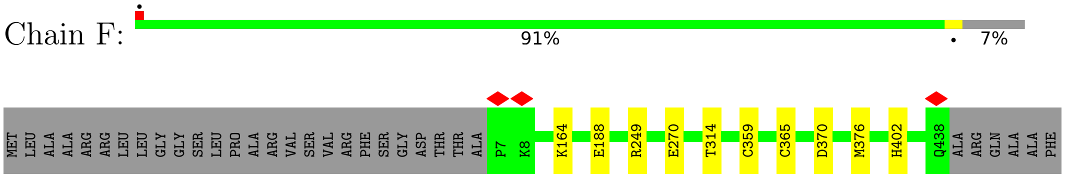
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



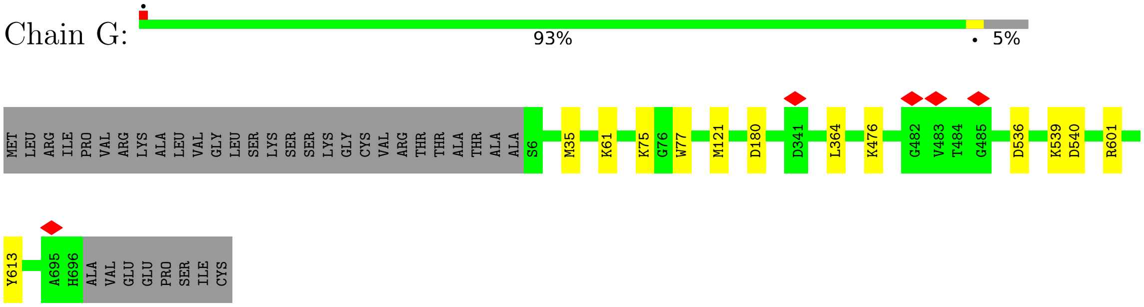
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



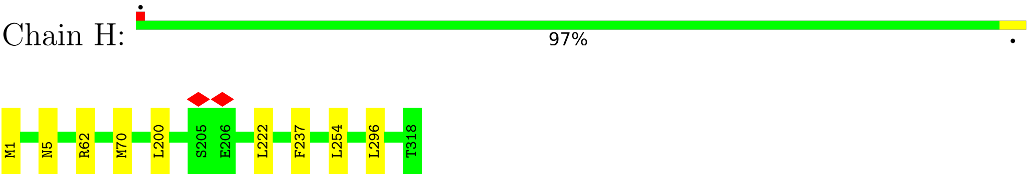
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



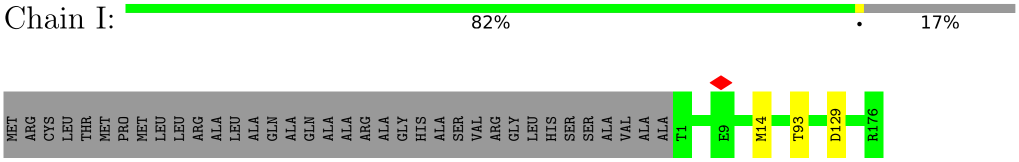
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



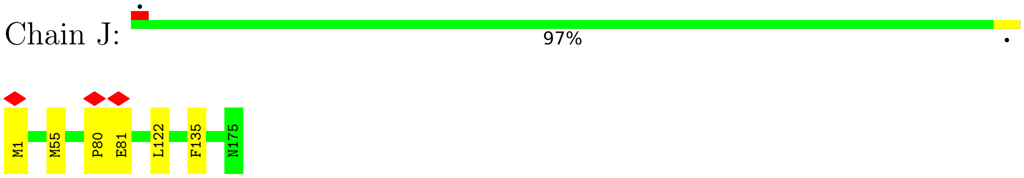
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



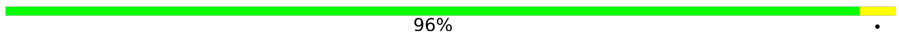
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

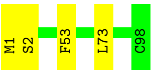
Chain J:



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

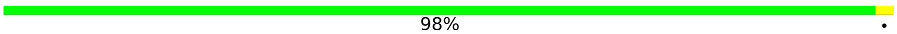
Chain K:

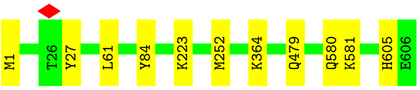




- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

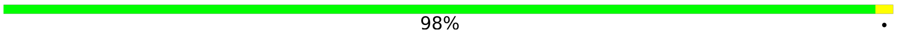
Chain L:

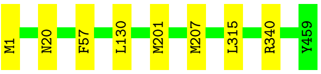




- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

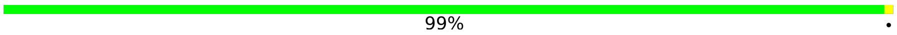
Chain M:

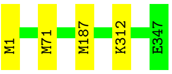




- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

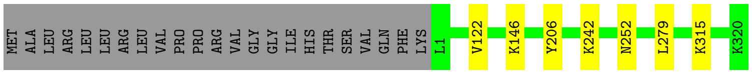
Chain N:





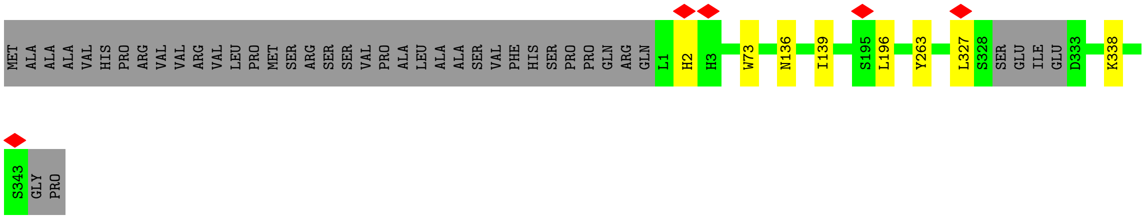
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



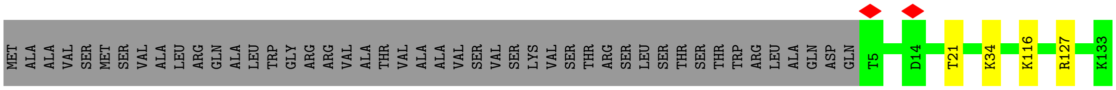
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



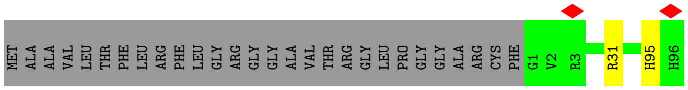
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



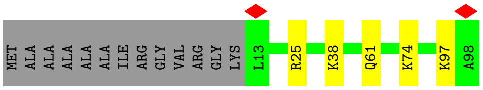
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



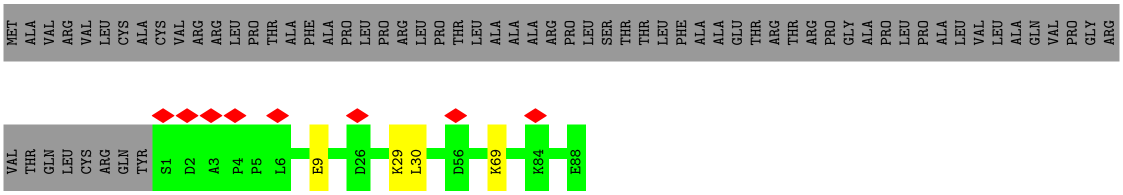
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



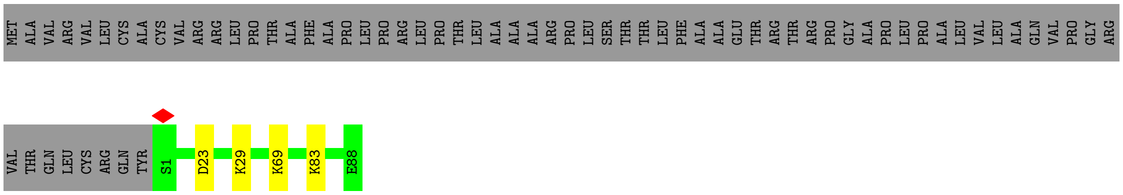
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



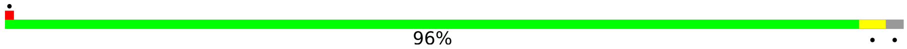
- Molecule 20: Acyl carrier protein, mitochondrial

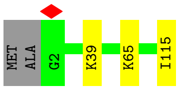
Chain U:



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

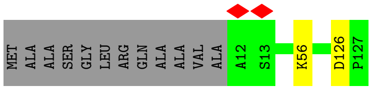
Chain V:





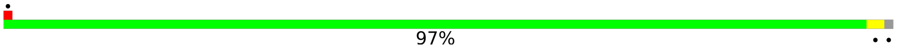
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

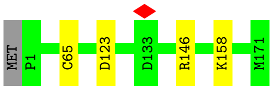
Chain W:



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

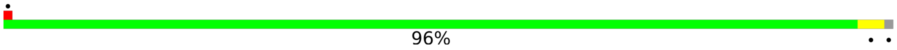
Chain X:

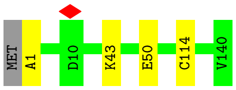




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

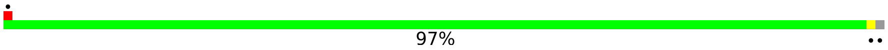
Chain Y:

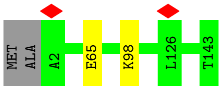




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

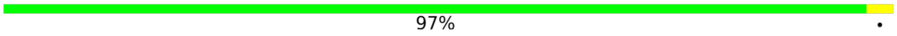
Chain Z:

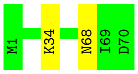




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

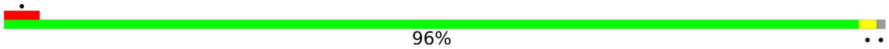
Chain a:

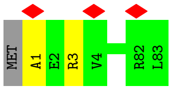




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

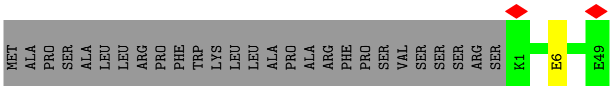
Chain b:





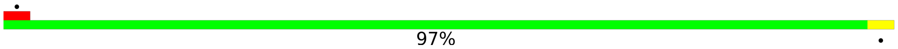
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

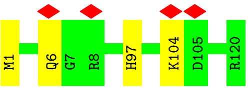
Chain c:



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

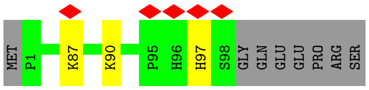
Chain d:





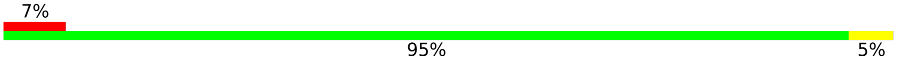
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

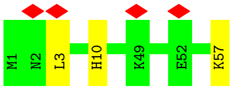
Chain e:



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:





- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

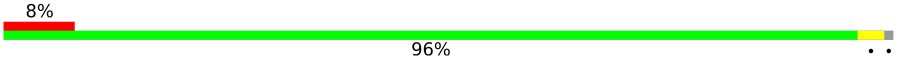
Chain g:

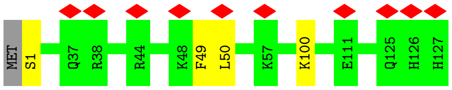
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

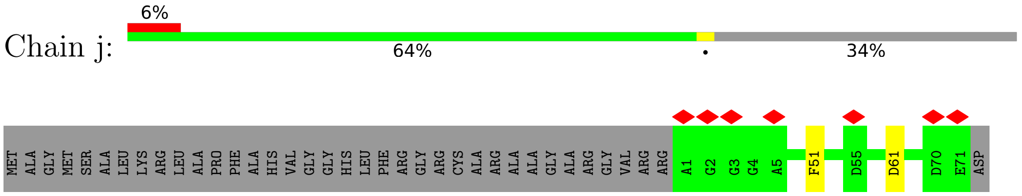
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:

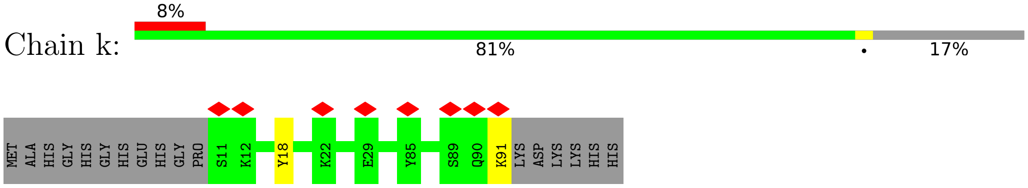




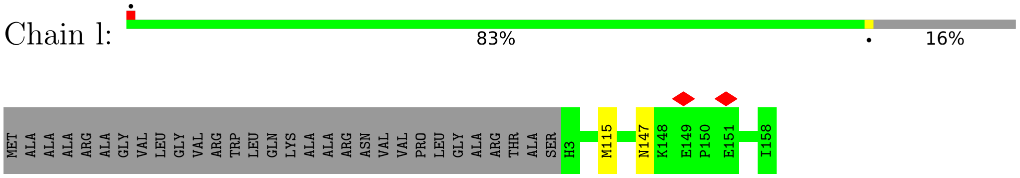
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



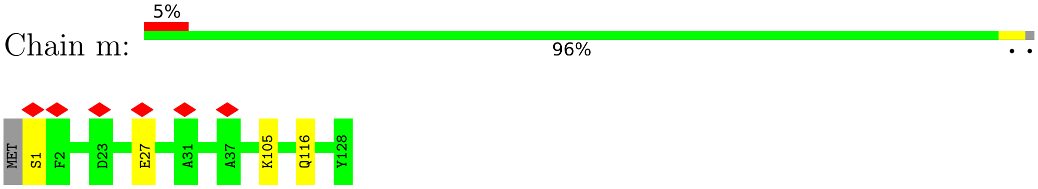
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



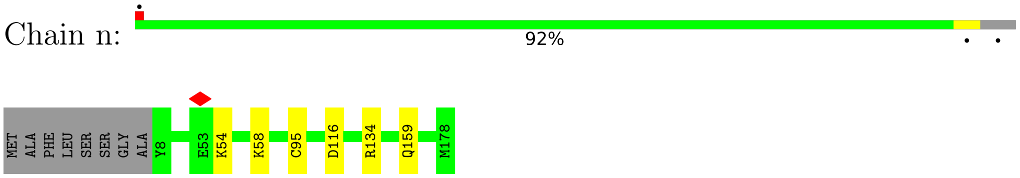
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



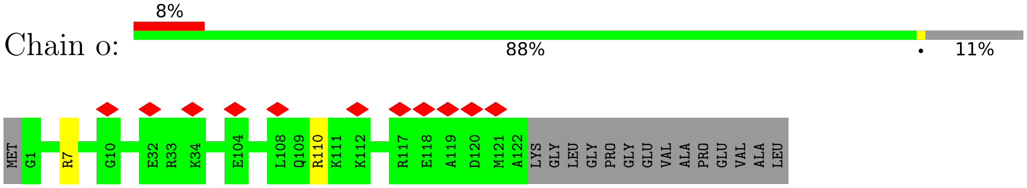
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



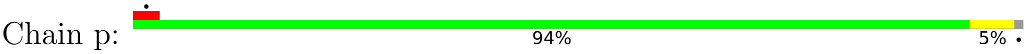
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

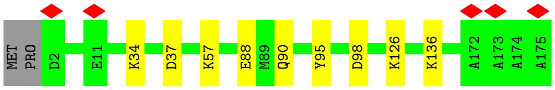


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



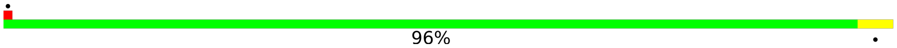
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

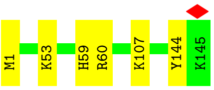




- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

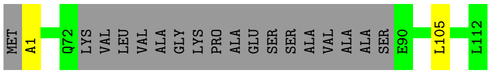
Chain q:





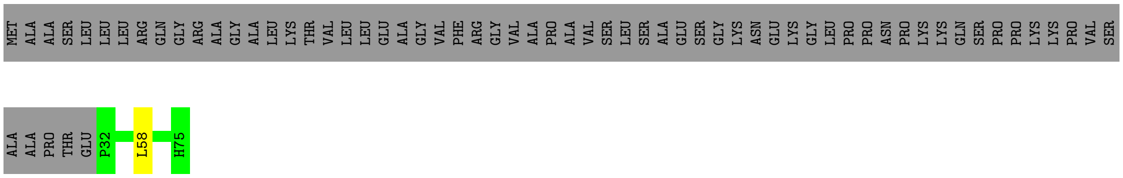
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14905	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 ($e^-/\text{Å}^2$)	40, 40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, U10, CDL, AYA, K, PLC, AME, FES, CHD, DGT, PC1, SAC, MG, ZN, FME, NDP, FMN, EHZ, 3PE, MYR, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/936	0.42	0/1281
2	B	0.35	0/1278	0.53	0/1728
3	C	0.34	0/1772	0.51	0/2413
4	D	0.33	0/3466	0.48	0/4692
5	E	0.30	0/1699	0.46	0/2312
6	F	0.29	0/3401	0.50	0/4595
7	G	0.29	0/5387	0.50	0/7301
8	H	0.30	0/2571	0.44	0/3513
9	I	0.36	0/1445	0.53	0/1956
10	J	0.31	0/1370	0.42	0/1859
11	K	0.29	0/745	0.42	0/1008
12	L	0.28	0/4920	0.42	0/6694
13	M	0.29	0/3738	0.43	0/5097
14	N	0.29	0/2792	0.43	0/3800
15	O	0.29	0/2651	0.43	0/3587
16	P	0.28	0/2804	0.49	0/3803
17	Q	0.29	0/1072	0.51	0/1449
18	R	0.32	0/753	0.51	0/1014
19	S	0.25	0/702	0.52	0/945
20	T	0.25	0/719	0.41	0/971
20	U	0.26	0/719	0.39	0/971
21	V	0.27	0/943	0.42	0/1277
22	W	0.28	0/1006	0.49	0/1352
23	X	0.28	0/1439	0.48	0/1942
24	Y	0.26	0/1042	0.46	0/1414
25	Z	0.30	0/1186	0.51	0/1599
26	a	0.32	0/584	0.52	0/786
27	b	0.28	0/667	0.45	0/916
28	c	0.28	0/427	0.42	0/579
29	d	0.32	0/1018	0.48	0/1375
30	e	0.27	0/846	0.50	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
31	f	0.27	0/505	0.48	0/681
32	g	0.29	0/873	0.45	0/1186
33	h	0.29	0/1188	0.47	0/1607
34	i	0.27	0/1127	0.46	0/1534
35	j	0.26	0/624	0.45	0/855
36	k	0.25	0/672	0.43	0/906
37	l	0.28	0/1369	0.45	0/1873
38	m	0.29	0/1088	0.51	0/1472
39	n	0.26	0/1540	0.48	0/2085
40	o	0.26	0/1073	0.51	0/1437
41	p	0.28	0/1491	0.49	0/2011
42	q	0.32	0/1242	0.50	0/1688
43	r	0.30	0/789	0.49	0/1068
44	s	0.28	0/383	0.48	0/518
All	All	0.29	0/68062	0.47	0/92281

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	154/216 (71%)	145 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	205/266 (77%)	196 (96%)	9 (4%)	0	100	100
4	D	414/463 (89%)	396 (96%)	18 (4%)	0	100	100
5	E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	29	61
6	F	430/464 (93%)	407 (95%)	23 (5%)	0	100	100
7	G	689/727 (95%)	646 (94%)	43 (6%)	0	100	100
8	H	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	163 (94%)	9 (5%)	1 (1%)	25	57
11	K	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	15	46
12	L	604/606 (100%)	572 (95%)	32 (5%)	0	100	100
13	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
14	N	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
15	O	318/343 (93%)	306 (96%)	12 (4%)	0	100	100
16	P	335/380 (88%)	319 (95%)	16 (5%)	0	100	100
17	Q	127/175 (73%)	122 (96%)	5 (4%)	0	100	100
18	R	94/124 (76%)	88 (94%)	6 (6%)	0	100	100
19	S	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	81 (94%)	5 (6%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
22	W	114/128 (89%)	109 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	138 (100%)	0	0	100	100
25	Z	140/144 (97%)	136 (97%)	4 (3%)	0	100	100
26	a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
30	e	96/106 (91%)	90 (94%)	6 (6%)	0	100	100
31	f	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	8	35
32	g	99/154 (64%)	91 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	i	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
35	j	69/108 (64%)	64 (93%)	5 (7%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	p	172/176 (98%)	168 (98%)	4 (2%)	0	100	100
42	q	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
43	r	91/113 (80%)	85 (93%)	6 (7%)	0	100	100
44	s	42/109 (38%)	39 (93%)	3 (7%)	0	100	100
All	All	8175/9213 (89%)	7805 (96%)	366 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	157	ASN
10	J	80	PRO
11	K	2	SER
31	f	3	LEU

5.3.2 Protein sidechains ⓘ

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	A	100/100 (100%)	98 (98%)	2 (2%)	55	76
2	B	132/175 (75%)	126 (96%)	6 (4%)	27	58
3	C	188/228 (82%)	185 (98%)	3 (2%)	62	79
4	D	362/392 (92%)	352 (97%)	10 (3%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	183/205 (89%)	179 (98%)	4 (2%)	52	74
6	F	346/368 (94%)	336 (97%)	10 (3%)	42	69
7	G	579/608 (95%)	566 (98%)	13 (2%)	52	74
8	H	274/274 (100%)	266 (97%)	8 (3%)	42	69
9	I	151/175 (86%)	148 (98%)	3 (2%)	55	76
10	J	141/141 (100%)	137 (97%)	4 (3%)	43	70
11	K	85/85 (100%)	83 (98%)	2 (2%)	49	73
12	L	533/533 (100%)	523 (98%)	10 (2%)	57	77
13	M	412/412 (100%)	405 (98%)	7 (2%)	60	78
14	N	315/315 (100%)	312 (99%)	3 (1%)	76	86
15	O	283/303 (93%)	276 (98%)	7 (2%)	47	72
16	P	293/327 (90%)	285 (97%)	8 (3%)	44	71
17	Q	116/153 (76%)	112 (97%)	4 (3%)	37	65
18	R	79/97 (81%)	77 (98%)	2 (2%)	47	72
19	S	76/82 (93%)	71 (93%)	5 (7%)	16	46
20	T	81/135 (60%)	77 (95%)	4 (5%)	25	56
20	U	81/135 (60%)	77 (95%)	4 (5%)	25	56
21	V	101/102 (99%)	98 (97%)	3 (3%)	41	68
22	W	108/114 (95%)	106 (98%)	2 (2%)	57	77
23	X	154/155 (99%)	150 (97%)	4 (3%)	46	71
24	Y	101/102 (99%)	98 (97%)	3 (3%)	41	68
25	Z	120/121 (99%)	118 (98%)	2 (2%)	60	78
26	a	59/59 (100%)	57 (97%)	2 (3%)	37	65
27	b	71/72 (99%)	70 (99%)	1 (1%)	67	82
28	c	45/68 (66%)	44 (98%)	1 (2%)	52	74
29	d	105/105 (100%)	102 (97%)	3 (3%)	42	69
30	e	89/96 (93%)	86 (97%)	3 (3%)	37	65
31	f	54/54 (100%)	52 (96%)	2 (4%)	34	63
32	g	92/131 (70%)	89 (97%)	3 (3%)	38	66
33	h	121/158 (77%)	119 (98%)	2 (2%)	60	78
34	i	120/121 (99%)	117 (98%)	3 (2%)	47	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	j	61/84 (73%)	59 (97%)	2 (3%)	38	66
36	k	63/76 (83%)	61 (97%)	2 (3%)	39	67
37	l	140/159 (88%)	138 (99%)	2 (1%)	67	82
38	m	113/114 (99%)	110 (97%)	3 (3%)	44	71
39	n	156/161 (97%)	150 (96%)	6 (4%)	33	62
40	o	110/120 (92%)	108 (98%)	2 (2%)	59	78
41	p	155/157 (99%)	146 (94%)	9 (6%)	20	50
42	q	130/130 (100%)	125 (96%)	5 (4%)	33	62
43	r	85/97 (88%)	84 (99%)	1 (1%)	71	83
44	s	43/92 (47%)	42 (98%)	1 (2%)	50	73
All	All	7206/7891 (91%)	7020 (97%)	186 (3%)	49	71

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	90	MET
2	B	42	ARG
2	B	50	PHE
2	B	54	CYS
2	B	59	MET
2	B	125	TYR
2	B	174	ARG
3	C	8	ARG
3	C	20	LYS
3	C	164	LYS
4	D	40	LYS
4	D	49	LEU
4	D	59	HIS
4	D	94	LYS
4	D	165	THR
4	D	290	ARG
4	D	295	ASP
4	D	392	LYS
4	D	410	MET
4	D	420	THR
5	E	180	LYS
5	E	181	ILE

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Mol	Chain	Res	Type
5	E	190	ARG
5	E	207	LYS
6	F	164	LYS
6	F	188	GLU
6	F	249	ARG
6	F	270	GLU
6	F	314	THR
6	F	359	CYS
6	F	365	CYS
6	F	370	ASP
6	F	376	MET
6	F	402	HIS
7	G	35	MET
7	G	61	LYS
7	G	75	LYS
7	G	77	TRP
7	G	121	MET
7	G	180	ASP
7	G	364	LEU
7	G	476	LYS
7	G	536	ASP
7	G	539	LYS
7	G	540	ASP
7	G	601	ARG
7	G	613	TYR
8	H	5	ASN
8	H	62	ARG
8	H	70	MET
8	H	200	LEU
8	H	222	LEU
8	H	237	PHE
8	H	254	LEU
8	H	296	LEU
9	I	14	MET
9	I	93	THR
9	I	129	ASP
10	J	55	MET
10	J	81	GLU
10	J	122	LEU
10	J	135	PHE
11	K	53	PHE
11	K	73	LEU

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Mol	Chain	Res	Type
12	L	27	TYR
12	L	61	LEU
12	L	84	TYR
12	L	223	LYS
12	L	252	MET
12	L	364	LYS
12	L	479	GLN
12	L	580	GLN
12	L	581	LYS
12	L	605	HIS
13	M	20	ASN
13	M	57	PHE
13	M	130	LEU
13	M	201	MET
13	M	207	MET
13	M	315	LEU
13	M	340	ARG
14	N	71	MET
14	N	187	MET
14	N	312	LYS
15	O	122	VAL
15	O	146	LYS
15	O	206	TYR
15	O	242	LYS
15	O	252	ASN
15	O	279	LEU
15	O	315	LYS
16	P	2	HIS
16	P	73	TRP
16	P	136	ASN
16	P	139	ILE
16	P	196	LEU
16	P	263	TYR
16	P	327	LEU
16	P	338	LYS
17	Q	21	THR
17	Q	34	LYS
17	Q	116	LYS
17	Q	127	ARG
18	R	31	ARG
18	R	95	HIS
19	S	25	ARG

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Mol	Chain	Res	Type
19	S	38	LYS
19	S	61	GLN
19	S	74	LYS
19	S	97	LYS
20	T	9	GLU
20	T	29	LYS
20	T	30	LEU
20	T	69	LYS
20	U	23	ASP
20	U	29	LYS
20	U	69	LYS
20	U	83	LYS
21	V	39	LYS
21	V	65	LYS
21	V	115	ILE
22	W	56	LYS
22	W	126	ASP
23	X	65	CYS
23	X	123	ASP
23	X	146	ARG
23	X	158	LYS
24	Y	43	LYS
24	Y	50	GLU
24	Y	114	CYS
25	Z	65	GLU
25	Z	98	LYS
26	a	34	LYS
26	a	68	ASN
27	b	3	ARG
28	c	6	GLU
29	d	6	GLN
29	d	97	HIS
29	d	104	LYS
30	e	87	LYS
30	e	90	LYS
30	e	97	HIS
31	f	10	HIS
31	f	57	LYS
32	g	26	TRP
32	g	43	ASP
32	g	84	ARG
33	h	106	LYS

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Mol	Chain	Res	Type
33	h	130	LYS
34	i	49	PHE
34	i	50	LEU
34	i	100	LYS
35	j	51	PHE
35	j	61	ASP
36	k	18	TYR
36	k	91	LYS
37	l	115	MET
37	l	147	ASN
38	m	27	GLU
38	m	105	LYS
38	m	116	GLN
39	n	54	LYS
39	n	58	LYS
39	n	95	CYS
39	n	116	ASP
39	n	134	ARG
39	n	159	GLN
40	o	7	ARG
40	o	110	ARG
41	p	34	LYS
41	p	37	ASP
41	p	57	LYS
41	p	88	GLU
41	p	90	GLN
41	p	95	TYR
41	p	98	ASP
41	p	126	LYS
41	p	136	LYS
42	q	53	LYS
42	q	59	HIS
42	q	60	ARG
42	q	107	LYS
42	q	144	TYR
43	r	105	LEU
44	s	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
7	G	255	HIS

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Mol	Chain	Res	Type
7	G	475	GLN
12	L	446	ASN
13	M	293	HIS
13	M	399	ASN
34	i	66	HIS
42	q	113	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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	$\#\|Z\| > 2$
38	SAC	m	1	38	7,8,9	1.65	1 (14%)	8,9,11	1.32	1 (12%)
27	AYA	b	1	27	6,7,8	1.81	1 (16%)	5,8,10	1.45	1 (20%)
8	FME	H	1	8	8,9,10	1.49	1 (12%)	7,9,11	1.73	3 (42%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.74	3 (42%)
4	2MR	D	85	4	10,12,13	2.38	2 (20%)	5,13,15	1.26	1 (20%)
29	AME	d	1	29	9,10,11	1.45	1 (11%)	9,11,13	1.64	2 (22%)
42	AME	q	1	42	9,10,11	1.46	1 (11%)	9,11,13	1.73	3 (33%)
14	FME	N	1	14	8,9,10	1.48	1 (12%)	7,9,11	1.66	2 (28%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	7,9,11	1.51	1 (14%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	7,9,11	1.64	2 (28%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	7,9,11	1.66	2 (28%)
12	FME	L	1	12	8,9,10	1.50	1 (12%)	7,9,11	1.67	2 (28%)
24	AYA	Y	1	24	6,7,8	1.80	2 (33%)	5,8,10	1.32	1 (20%)
34	SAC	i	1	34	7,8,9	1.68	1 (14%)	8,9,11	1.57	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
43	AYA	r	1	43	6,7,8	1.82	1 (16%)	5,8,10	1.33	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
38	SAC	m	1	38	-	3/7/8/10	-
27	AYA	b	1	27	-	0/4/6/8	-
8	FME	H	1	8	-	3/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
29	AME	d	1	29	-	1/9/10/12	-
42	AME	q	1	42	-	2/9/10/12	-
14	FME	N	1	14	-	3/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
13	FME	M	1	13	-	3/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
34	SAC	i	1	34	-	5/7/8/10	-
43	AYA	r	1	43	-	0/4/6/8	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.13	1.44	1.33
4	D	85	2MR	CZ-NE	5.13	1.45	1.34
11	K	1	FME	CN-N	3.68	1.45	1.33
13	M	1	FME	CN-N	3.67	1.45	1.33
10	J	1	FME	CN-N	3.67	1.45	1.33
12	L	1	FME	CN-N	3.63	1.45	1.33
14	N	1	FME	CN-N	3.62	1.45	1.33
1	A	1	FME	CN-N	3.61	1.45	1.33
8	H	1	FME	CN-N	3.57	1.45	1.33
34	i	1	SAC	C1A-N	3.39	1.46	1.34
38	m	1	SAC	C1A-N	3.29	1.45	1.34
27	b	1	AYA	CT-N	3.28	1.45	1.34
43	r	1	AYA	CT-N	3.27	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	q	1	AME	CT1-N	3.24	1.45	1.34
29	d	1	AME	CT1-N	3.24	1.45	1.34
24	Y	1	AYA	CT-N	3.23	1.45	1.34
24	Y	1	AYA	OT-CT	-2.02	1.18	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	C2A-C1A-N	3.28	121.66	116.10
42	q	1	AME	CE-SD-CG	2.90	110.38	100.40
29	d	1	AME	CE-SD-CG	2.84	110.15	100.40
1	A	1	FME	CE-SD-CG	2.74	109.81	100.40
10	J	1	FME	CE-SD-CG	2.73	109.77	100.40
11	K	1	FME	CE-SD-CG	2.73	109.77	100.40
12	L	1	FME	CE-SD-CG	2.67	109.58	100.40
13	M	1	FME	CE-SD-CG	2.59	109.30	100.40
42	q	1	AME	CT2-CT1-N	2.49	120.31	116.10
14	N	1	FME	CE-SD-CG	2.49	108.94	100.40
29	d	1	AME	CT2-CT1-N	2.44	120.23	116.10
42	q	1	AME	CA-N-CT1	-2.40	118.72	123.15
38	m	1	SAC	C2A-C1A-N	2.38	120.12	116.10
8	H	1	FME	CE-SD-CG	2.37	108.56	100.40
43	r	1	AYA	CM-CT-N	2.37	120.11	116.10
27	b	1	AYA	CM-CT-N	2.34	120.06	116.10
8	H	1	FME	CA-N-CN	-2.34	119.23	122.82
14	N	1	FME	CA-N-CN	-2.26	119.35	122.82
24	Y	1	AYA	CM-CT-N	2.17	119.77	116.10
8	H	1	FME	O1-CN-N	-2.16	119.57	125.27
1	A	1	FME	CA-N-CN	-2.16	119.50	122.82
4	D	85	2MR	CD-NE-CZ	-2.16	119.36	123.41
1	A	1	FME	O1-CN-N	-2.11	119.71	125.27
12	L	1	FME	O1-CN-N	-2.08	119.80	125.27
10	J	1	FME	O1-CN-N	-2.03	119.93	125.27
13	M	1	FME	O1-CN-N	-2.01	119.98	125.27

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CA-N-CN
10	J	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
34	i	1	SAC	O-C-CA-CB
34	i	1	SAC	C-CA-CB-OG
38	m	1	SAC	O-C-CA-CB
38	m	1	SAC	N-CA-CB-OG
38	m	1	SAC	C-CA-CB-OG
42	q	1	AME	O-C-CA-CB
10	J	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
8	H	1	FME	N-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
34	i	1	SAC	N-CA-CB-OG
1	A	1	FME	C-CA-CB-CG
42	q	1	AME	N-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
8	H	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CG-SD-CE
14	N	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
11	K	1	FME	C-CA-CB-CG
14	N	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 72 ligands modelled in this entry, 4 are monoatomic - leaving 68 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	$\#\|Z\| > 2$
53	CDL	L	701	-	86,86,99	0.94	7 (8%)	92,98,111	1.13	4 (4%)
46	PC1	I	204	-	53,53,53	0.94	4 (7%)	59,61,61	0.97	2 (3%)
46	PC1	A	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.02	2 (5%)
46	PC1	h	202	-	30,30,53	1.22	4 (13%)	36,38,61	1.06	2 (5%)
47	SF4	B	201	2	0,12,12	-	-	-		
45	3PE	N	404	-	44,44,50	0.91	4 (9%)	47,49,55	1.03	2 (4%)
45	3PE	Y	204	-	35,35,50	1.01	4 (11%)	38,40,55	1.21	2 (5%)
45	3PE	m	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.13	2 (4%)
45	3PE	K	101	-	43,43,50	0.92	3 (6%)	46,48,55	1.11	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		
47	SF4	G	801	7	0,12,12	-	-	-		
45	3PE	L	703	-	43,43,50	0.92	4 (9%)	46,48,55	1.09	2 (4%)
45	3PE	Z	201	-	44,44,50	0.91	4 (9%)	47,49,55	1.05	2 (4%)
46	PC1	d	203	-	38,38,53	1.10	4 (10%)	44,46,61	1.01	2 (4%)
46	PC1	Y	205	-	39,39,53	1.08	4 (10%)	45,47,61	1.05	2 (4%)
53	CDL	J	201	-	35,35,99	1.32	6 (17%)	41,47,111	1.44	3 (7%)
46	PC1	A	203	-	34,34,53	1.15	4 (11%)	40,42,61	1.05	2 (5%)
57	NDP	P	501	-	45,52,52	4.24	23 (51%)	53,80,80	2.09	5 (9%)
48	PLC	L	707	-	26,26,41	0.61	0	32,34,49	0.61	0
45	3PE	Y	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
45	3PE	I	203	-	35,35,50	1.01	4 (11%)	38,40,55	1.15	2 (5%)
58	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.59	5 (14%)
60	MYR	o	201	40	14,14,15	0.46	0	13,13,15	0.86	0
49	FES	G	803	7	0,4,4	-	-	-		
45	3PE	N	403	-	44,44,50	0.91	4 (9%)	47,49,55	1.05	2 (4%)
45	3PE	J	202	-	32,32,50	1.06	4 (12%)	35,37,55	1.10	2 (5%)
46	PC1	q	202	46	47,47,53	1.00	4 (8%)	53,55,61	0.97	2 (3%)
46	PC1	L	706	-	46,46,53	0.99	4 (8%)	52,54,61	1.06	2 (3%)
55	DGT	O	401	56	26,33,33	2.66	8 (30%)	32,52,52	1.68	10 (31%)
45	3PE	g	201	-	28,28,50	1.13	4 (14%)	31,33,55	1.32	3 (9%)
45	3PE	i	202	-	44,44,50	0.90	4 (9%)	47,49,55	1.09	2 (4%)
53	CDL	M	602	-	90,90,99	0.91	7 (7%)	96,102,111	1.13	4 (4%)
47	SF4	G	802	7	0,12,12	-	-	-		
45	3PE	A	201	-	33,33,50	1.03	4 (12%)	36,38,55	1.18	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	FES	E	301	5	0,4,4	-	-	-		
46	PC1	M	604	-	43,43,53	1.02	4 (9%)	49,51,61	1.04	2 (4%)
46	PC1	M	605	-	25,25,53	1.33	4 (16%)	31,33,61	1.05	2 (6%)
47	SF4	I	202	9	0,12,12	-	-	-		
45	3PE	L	704	-	45,45,50	0.92	4 (8%)	48,50,55	1.10	2 (4%)
45	3PE	Y	201	-	26,26,50	1.15	4 (15%)	29,31,55	1.11	2 (6%)
45	3PE	Y	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
47	SF4	I	201	9	0,12,12	-	-	-		
50	FMN	F	501	-	33,33,33	2.73	10 (30%)	48,50,50	1.72	11 (22%)
52	U10	H	401	-	28,28,63	2.00	14 (50%)	34,37,79	1.99	7 (20%)
48	PLC	b	102	-	31,31,41	0.56	0	37,39,49	0.61	0
45	3PE	N	402	-	48,48,50	0.88	4 (8%)	51,53,55	1.07	2 (3%)
59	CHD	i	201	-	32,32,32	3.20	10 (31%)	51,51,51	2.38	17 (33%)
46	PC1	H	403	-	38,38,53	1.09	4 (10%)	44,46,61	1.01	2 (4%)
48	PLC	g	202	-	31,31,41	0.58	0	37,39,49	0.57	0
53	CDL	h	201	-	79,79,99	0.97	8 (10%)	85,91,111	1.11	4 (4%)
46	PC1	H	402	-	47,47,53	1.00	4 (8%)	53,55,61	1.04	2 (3%)
46	PC1	P	502	46	45,45,53	1.02	3 (6%)	51,53,61	1.02	3 (5%)
53	CDL	d	201	-	64,64,99	1.07	8 (12%)	70,76,111	1.13	4 (5%)
53	CDL	q	201	-	60,60,99	1.11	7 (11%)	66,72,111	1.15	4 (6%)
45	3PE	m	202	-	32,32,50	1.05	4 (12%)	35,37,55	1.14	2 (5%)
45	3PE	o	202	-	34,34,50	0.96	3 (8%)	37,39,55	1.08	1 (2%)
53	CDL	N	401	-	73,73,99	1.00	8 (10%)	79,85,111	1.12	4 (5%)
58	EHZ	T	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.73	9 (25%)
48	PLC	B	202	-	37,37,41	0.52	0	43,45,49	0.55	0
46	PC1	I	205	-	36,36,53	1.12	4 (11%)	42,44,61	1.02	2 (4%)
46	PC1	q	203	-	29,29,53	1.24	4 (13%)	35,37,61	1.13	2 (5%)
45	3PE	d	202	-	48,48,50	0.88	4 (8%)	51,53,55	1.08	2 (3%)
45	3PE	L	705	-	36,36,50	0.99	4 (11%)	39,41,55	1.15	2 (5%)
48	PLC	N	405	-	25,25,41	0.62	0	31,33,49	0.63	0
45	3PE	L	702	-	34,34,50	0.96	3 (8%)	37,39,55	1.12	1 (2%)
45	3PE	M	603	-	49,49,50	0.88	3 (6%)	52,54,55	1.01	2 (3%)
53	CDL	X	201	-	86,86,99	0.93	8 (9%)	92,98,111	1.10	4 (4%)
45	3PE	b	101	-	46,46,50	0.89	4 (8%)	49,51,55	1.06	2 (4%)

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
53	CDL	L	701	-	-	31/97/97/110	-
46	PC1	I	204	-	-	20/57/57/57	-
46	PC1	A	202	-	-	20/38/38/57	-
46	PC1	h	202	-	-	14/34/34/57	-
47	SF4	B	201	2	-	-	0/6/5/5
45	3PE	N	404	-	-	21/48/48/54	-
45	3PE	Y	204	-	-	20/39/39/54	-
45	3PE	m	201	-	-	15/44/44/54	-
45	3PE	K	101	-	-	18/47/47/54	-
47	SF4	F	502	6	-	-	0/6/5/5
47	SF4	G	801	7	-	-	0/6/5/5
45	3PE	L	703	-	-	20/47/47/54	-
45	3PE	Z	201	-	-	24/48/48/54	-
46	PC1	d	203	-	-	15/42/42/57	-
46	PC1	Y	205	-	-	12/43/43/57	-
53	CDL	J	201	-	-	19/42/42/110	-
46	PC1	A	203	-	-	11/38/38/57	-
57	NDP	P	501	-	-	14/30/77/77	0/5/5/5
48	PLC	L	707	-	-	11/30/30/45	-
45	3PE	Y	202	-	-	30/54/54/54	-
45	3PE	I	203	-	-	19/39/39/54	-
58	EHZ	U	101	20	-	10/42/44/45	-
60	MYR	o	201	40	-	3/11/12/13	-
49	FES	G	803	7	-	-	0/1/1/1
45	3PE	N	403	-	-	31/48/48/54	-
45	3PE	J	202	-	-	22/36/36/54	-
46	PC1	q	202	46	-	14/51/51/57	-
46	PC1	L	706	-	-	23/50/50/57	-
55	DGT	O	401	56	-	8/18/34/34	0/3/3/3
45	3PE	g	201	-	-	10/31/31/54	-
45	3PE	i	202	-	-	22/48/48/54	-
53	CDL	M	602	-	-	43/101/101/110	-
47	SF4	G	802	7	-	-	0/6/5/5
45	3PE	A	201	-	-	10/37/37/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FES	E	301	5	-	-	0/1/1/1
46	PC1	M	604	-	-	23/47/47/57	-
46	PC1	M	605	-	-	18/29/29/57	-
47	SF4	I	202	9	-	-	0/6/5/5
45	3PE	L	704	-	-	25/49/49/54	-
45	3PE	Y	201	-	-	13/30/30/54	-
45	3PE	Y	203	-	-	21/54/54/54	-
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
47	SF4	I	201	9	-	-	0/6/5/5
52	U10	H	401	-	-	2/21/45/87	0/1/1/1
48	PLC	b	102	-	-	14/35/35/45	-
45	3PE	N	402	-	-	26/52/52/54	-
59	CHD	i	201	-	-	2/9/74/74	0/4/4/4
46	PC1	H	403	-	-	17/42/42/57	-
48	PLC	g	202	-	-	8/34/34/45	-
53	CDL	h	201	-	-	33/90/90/110	-
46	PC1	H	402	-	-	19/51/51/57	-
46	PC1	P	502	46	-	15/49/49/57	-
53	CDL	d	201	-	-	33/75/75/110	-
53	CDL	q	201	-	-	26/71/71/110	-
45	3PE	m	202	-	-	14/36/36/54	-
45	3PE	o	202	-	-	14/37/37/54	-
53	CDL	N	401	-	-	31/84/84/110	-
58	EHZ	T	101	20	-	12/42/44/45	-
48	PLC	B	202	-	-	15/41/41/45	-
46	PC1	I	205	-	-	14/40/40/57	-
46	PC1	q	203	-	-	15/33/33/57	-
45	3PE	d	202	-	-	18/52/52/54	-
45	3PE	L	705	-	-	16/40/40/54	-
48	PLC	N	405	-	-	10/28/28/45	-
45	3PE	L	702	-	-	15/37/37/54	-
45	3PE	M	603	-	-	23/53/53/54	-
53	CDL	X	201	-	-	46/97/97/110	-
45	3PE	b	101	-	-	15/50/50/54	-

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	O4B-C1B	14.70	1.61	1.41
57	P	501	NDP	C6N-C5N	11.88	1.54	1.33
59	i	201	CHD	C11-C12	8.63	1.67	1.53
57	P	501	NDP	C7N-N7N	8.34	1.55	1.33
55	O	401	DGT	O6-C6	8.33	1.40	1.23
57	P	501	NDP	O4D-C1D	8.22	1.61	1.42
57	P	501	NDP	C2D-C1D	-7.25	1.30	1.53
59	i	201	CHD	C16-C15	7.22	1.73	1.54
50	F	501	FMN	C4A-N5	7.14	1.44	1.30
50	F	501	FMN	C10-N1	6.44	1.46	1.33
57	P	501	NDP	O4D-C4D	-6.41	1.30	1.45
59	i	201	CHD	C20-C17	-6.17	1.43	1.54
58	U	101	EHZ	C15-N2	5.41	1.45	1.33
58	T	101	EHZ	C12-N1	5.35	1.45	1.33
58	U	101	EHZ	C12-N1	5.30	1.45	1.33
57	P	501	NDP	O4B-C4B	-5.24	1.33	1.45
58	T	101	EHZ	C15-N2	5.23	1.45	1.33
50	F	501	FMN	C5A-N5	5.22	1.49	1.39
59	i	201	CHD	O12-C12	-5.18	1.35	1.43
59	i	201	CHD	C8-C9	5.10	1.63	1.53
57	P	501	NDP	P2B-O2B	5.09	1.68	1.59
59	i	201	CHD	C13-C17	4.98	1.64	1.55
50	F	501	FMN	C9A-N10	4.93	1.49	1.41
55	O	401	DGT	C2-N2	4.75	1.45	1.34
50	F	501	FMN	C2-N1	4.67	1.47	1.36
55	O	401	DGT	C2-N1	4.63	1.49	1.37
57	P	501	NDP	C2N-C3N	4.62	1.47	1.34
59	i	201	CHD	C6-C5	4.51	1.61	1.53
55	O	401	DGT	C2-N3	4.36	1.43	1.33
50	F	501	FMN	C2-N3	4.17	1.48	1.39
59	i	201	CHD	C15-C14	4.10	1.62	1.54
57	P	501	NDP	O7N-C7N	-4.07	1.14	1.24
57	P	501	NDP	O2D-C2D	3.99	1.52	1.43
59	i	201	CHD	C6-C7	3.81	1.59	1.52
57	P	501	NDP	C6A-N6A	3.79	1.47	1.34
50	F	501	FMN	C4-N3	3.66	1.45	1.38
50	F	501	FMN	C10-N10	3.65	1.45	1.37
57	P	501	NDP	C5A-C4A	-3.63	1.31	1.40
57	P	501	NDP	C4N-C3N	3.22	1.56	1.49
52	H	401	U10	C4-C5	-3.17	1.39	1.48
52	H	401	U10	C3-C2	-3.08	1.40	1.48
50	F	501	FMN	O2-C2	-3.00	1.18	1.24
52	H	401	U10	C7-C8	2.93	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	O	401	DGT	C5-C6	-2.91	1.41	1.47
50	F	501	FMN	O4-C4	-2.80	1.18	1.23
46	P	502	PC1	O21-C2	-2.78	1.39	1.46
55	O	401	DGT	C1'-N9	-2.76	1.41	1.49
53	M	602	CDL	OB6-CB4	-2.75	1.39	1.46
52	H	401	U10	C21-C19	2.74	1.57	1.50
57	P	501	NDP	C2A-N3A	2.73	1.36	1.32
53	L	701	CDL	OA6-CA4	-2.72	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.71	1.39	1.46
57	P	501	NDP	C4N-C5N	2.69	1.55	1.48
53	h	201	CDL	OA6-CA4	-2.68	1.39	1.46
46	I	204	PC1	O21-C2	-2.65	1.40	1.46
45	M	603	3PE	O21-C2	-2.64	1.40	1.46
45	K	101	3PE	O21-C2	-2.64	1.40	1.46
57	P	501	NDP	O3B-C3B	-2.61	1.36	1.43
53	X	201	CDL	OB6-CB4	-2.61	1.40	1.46
53	N	401	CDL	OB6-CB4	-2.58	1.40	1.46
53	h	201	CDL	OB6-CB4	-2.57	1.40	1.46
53	J	201	CDL	OA6-CA4	-2.56	1.40	1.46
46	h	202	PC1	O21-C2	-2.56	1.40	1.46
46	L	706	PC1	O21-C2	-2.56	1.40	1.46
53	L	701	CDL	OB6-CB4	-2.56	1.40	1.46
46	d	203	PC1	O21-C2	-2.55	1.40	1.46
46	q	203	PC1	O21-C2	-2.54	1.40	1.46
57	P	501	NDP	O3D-C3D	-2.54	1.37	1.43
53	q	201	CDL	OB6-CB4	-2.54	1.40	1.46
45	L	702	3PE	O21-C2	-2.53	1.40	1.46
45	A	201	3PE	O21-C2	-2.53	1.40	1.46
46	M	604	PC1	O21-C2	-2.53	1.40	1.46
53	d	201	CDL	OB8-CB7	2.52	1.40	1.33
45	I	203	3PE	O21-C2	-2.52	1.40	1.46
59	i	201	CHD	C13-C12	-2.52	1.50	1.54
45	J	202	3PE	O21-C2	-2.52	1.40	1.46
53	M	602	CDL	OA6-CA4	-2.51	1.40	1.46
45	m	202	3PE	O21-C2	-2.51	1.40	1.46
46	q	202	PC1	O21-C2	-2.51	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.51	1.40	1.46
45	N	402	3PE	O21-C2	-2.51	1.40	1.46
53	J	201	CDL	OB6-CB4	-2.51	1.40	1.46
45	L	703	3PE	O21-C2	-2.50	1.40	1.46
45	Y	202	3PE	O21-C2	-2.50	1.40	1.46
45	g	201	3PE	O21-C2	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	q	203	PC1	O31-C31	2.49	1.40	1.33
53	q	201	CDL	OB8-CB7	2.49	1.40	1.33
53	d	201	CDL	OB6-CB4	-2.49	1.40	1.46
45	N	404	3PE	O21-C2	-2.49	1.40	1.46
53	X	201	CDL	OB8-CB6	-2.48	1.39	1.45
53	h	201	CDL	OB8-CB7	2.48	1.40	1.33
45	d	202	3PE	O21-C2	-2.47	1.40	1.46
45	L	704	3PE	O31-C31	2.47	1.40	1.33
53	X	201	CDL	OA6-CA4	-2.47	1.40	1.46
46	M	605	PC1	O21-C2	-2.46	1.40	1.46
45	Y	203	3PE	O31-C31	2.46	1.40	1.33
45	Z	201	3PE	O21-C2	-2.45	1.40	1.46
46	I	205	PC1	O21-C2	-2.45	1.40	1.46
45	L	704	3PE	O21-C2	-2.45	1.40	1.46
46	A	202	PC1	O31-C31	2.45	1.40	1.33
45	b	101	3PE	O21-C2	-2.45	1.40	1.46
52	H	401	U10	C15-C14	2.44	1.57	1.50
46	I	205	PC1	O31-C31	2.43	1.40	1.33
46	Y	205	PC1	O31-C31	2.43	1.40	1.33
45	m	201	3PE	O21-C2	-2.43	1.40	1.46
46	M	605	PC1	O31-C31	2.43	1.40	1.33
46	Y	205	PC1	O21-C2	-2.43	1.40	1.46
46	A	203	PC1	O21-C2	-2.43	1.40	1.46
52	H	401	U10	C11-C9	2.43	1.56	1.51
53	M	602	CDL	OA8-CA7	2.42	1.40	1.33
45	M	603	3PE	O31-C31	2.42	1.40	1.33
45	N	403	3PE	O21-C21	2.41	1.41	1.34
46	H	402	PC1	O21-C2	-2.41	1.40	1.46
45	N	404	3PE	O31-C31	2.41	1.40	1.33
46	q	202	PC1	O31-C31	2.41	1.40	1.33
53	X	201	CDL	OA8-CA7	2.41	1.40	1.33
53	N	401	CDL	OA8-CA7	2.40	1.40	1.33
58	T	101	EHZ	C9-S1	2.40	1.81	1.76
45	Z	201	3PE	O31-C31	2.40	1.40	1.33
46	H	403	PC1	O21-C2	-2.40	1.40	1.46
45	L	703	3PE	O31-C31	2.39	1.40	1.33
45	I	203	3PE	O31-C31	2.39	1.40	1.33
53	L	701	CDL	OB8-CB7	2.39	1.40	1.33
52	H	401	U10	C6-C1	2.39	1.39	1.35
45	Y	204	3PE	O31-C31	2.38	1.40	1.33
46	A	203	PC1	O31-C31	2.38	1.40	1.33
46	d	203	PC1	O31-C31	2.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	T	101	EHZ	O4-C15	-2.38	1.18	1.23
45	Y	204	3PE	O21-C2	-2.38	1.40	1.46
53	N	401	CDL	OB8-CB7	2.38	1.40	1.33
45	A	201	3PE	O31-C31	2.37	1.40	1.33
45	i	202	3PE	O31-C31	2.37	1.40	1.33
53	d	201	CDL	OA8-CA7	2.37	1.40	1.33
45	m	201	3PE	O31-C31	2.37	1.40	1.33
45	J	202	3PE	O31-C31	2.37	1.40	1.33
45	d	202	3PE	O31-C31	2.37	1.40	1.33
46	I	204	PC1	O31-C31	2.36	1.40	1.33
53	N	401	CDL	OA6-CA4	-2.36	1.40	1.46
53	h	201	CDL	OA8-CA7	2.36	1.40	1.33
53	L	701	CDL	OA8-CA7	2.36	1.40	1.33
58	U	101	EHZ	C9-S1	2.36	1.81	1.76
46	M	604	PC1	O31-C31	2.36	1.40	1.33
45	o	202	3PE	O21-C2	-2.35	1.40	1.46
45	Y	201	3PE	O21-C2	-2.35	1.40	1.46
46	H	402	PC1	O31-C31	2.34	1.40	1.33
46	h	202	PC1	O31-C31	2.34	1.40	1.33
45	L	705	3PE	O21-C2	-2.34	1.40	1.46
52	H	401	U10	C7-C6	2.34	1.55	1.51
53	q	201	CDL	OA8-CA7	2.34	1.40	1.33
45	Y	201	3PE	O31-C31	2.33	1.40	1.33
45	m	202	3PE	O31-C31	2.33	1.40	1.33
45	b	101	3PE	O31-C31	2.32	1.40	1.33
45	N	402	3PE	O31-C31	2.32	1.40	1.33
46	H	403	PC1	O31-C3	-2.32	1.39	1.45
58	T	101	EHZ	O3-C12	-2.31	1.18	1.23
57	P	501	NDP	PA-O5B	2.29	1.68	1.59
45	i	202	3PE	O21-C2	-2.29	1.40	1.46
58	U	101	EHZ	O3-C12	-2.29	1.18	1.23
46	A	202	PC1	O21-C2	-2.28	1.40	1.46
46	P	502	PC1	O31-C31	2.28	1.40	1.33
45	g	201	3PE	O21-C21	2.28	1.40	1.35
45	Y	202	3PE	O31-C31	2.28	1.40	1.33
45	g	201	3PE	O31-C31	2.28	1.40	1.33
52	H	401	U10	C6-C5	-2.27	1.40	1.46
53	J	201	CDL	OA6-CA5	2.26	1.40	1.35
46	L	706	PC1	O31-C3	-2.26	1.40	1.45
45	K	101	3PE	O31-C31	2.25	1.39	1.33
53	d	201	CDL	OA8-CA6	-2.25	1.40	1.45
46	H	403	PC1	O31-C31	2.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	L	706	PC1	O31-C31	2.24	1.39	1.33
45	Y	202	3PE	O31-C3	-2.24	1.40	1.45
57	P	501	NDP	C5B-C4B	2.24	1.58	1.51
58	U	101	EHZ	O4-C15	-2.24	1.18	1.23
53	J	201	CDL	OB6-CB5	2.24	1.40	1.35
53	M	602	CDL	OB8-CB6	-2.23	1.40	1.45
45	N	403	3PE	O31-C3	-2.23	1.40	1.45
45	L	705	3PE	O31-C31	2.23	1.39	1.33
45	N	403	3PE	O31-C31	2.23	1.39	1.33
46	I	205	PC1	O21-C21	2.23	1.40	1.34
53	M	602	CDL	OB8-CB7	2.23	1.39	1.33
45	K	101	3PE	O31-C3	-2.23	1.40	1.45
45	L	705	3PE	O21-C21	2.22	1.40	1.34
45	o	202	3PE	O21-C21	2.22	1.40	1.34
45	N	402	3PE	O31-C3	-2.21	1.40	1.45
53	d	201	CDL	OB6-CB5	2.21	1.40	1.34
46	H	403	PC1	O21-C21	2.21	1.40	1.34
45	b	101	3PE	O31-C3	-2.21	1.40	1.45
53	N	401	CDL	OA6-CA5	2.21	1.40	1.34
57	P	501	NDP	C7N-C3N	2.21	1.53	1.48
45	L	705	3PE	O31-C3	-2.21	1.40	1.45
45	m	201	3PE	O21-C21	2.21	1.40	1.34
46	Y	205	PC1	O21-C21	2.21	1.40	1.34
46	P	502	PC1	O31-C3	-2.20	1.40	1.45
45	d	202	3PE	O31-C3	-2.20	1.40	1.45
53	N	401	CDL	OB8-CB6	-2.20	1.40	1.45
46	A	202	PC1	O21-C21	2.20	1.40	1.34
57	P	501	NDP	C6N-N1N	2.19	1.42	1.37
45	m	202	3PE	O31-C3	-2.19	1.40	1.45
53	L	701	CDL	OA8-CA6	-2.19	1.40	1.45
45	g	201	3PE	O31-C3	-2.19	1.40	1.45
53	q	201	CDL	OB8-CB6	-2.19	1.40	1.45
45	L	702	3PE	O31-C3	-2.19	1.40	1.45
53	L	701	CDL	OB8-CB6	-2.19	1.40	1.45
46	H	402	PC1	O21-C21	2.19	1.40	1.34
46	h	202	PC1	O21-C21	2.19	1.40	1.34
53	q	201	CDL	OA8-CA6	-2.19	1.40	1.45
46	A	202	PC1	O31-C3	-2.18	1.40	1.45
46	M	604	PC1	O31-C3	-2.18	1.40	1.45
57	P	501	NDP	P2B-O1X	2.18	1.57	1.50
45	o	202	3PE	O31-C3	-2.18	1.40	1.45
45	i	202	3PE	O21-C21	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	203	PC1	O21-C21	2.17	1.40	1.34
45	N	404	3PE	O21-C21	2.17	1.40	1.34
45	I	203	3PE	O31-C3	-2.17	1.40	1.45
53	h	201	CDL	OA8-CA6	-2.16	1.40	1.45
46	d	203	PC1	O31-C3	-2.16	1.40	1.45
45	b	101	3PE	O21-C21	2.16	1.40	1.34
45	N	403	3PE	O21-C2	-2.16	1.41	1.46
46	M	605	PC1	O21-C21	2.16	1.40	1.34
45	Y	203	3PE	O21-C2	-2.16	1.41	1.46
55	O	401	DGT	PG-O2G	-2.16	1.46	1.54
46	q	202	PC1	O21-C21	2.16	1.40	1.34
53	N	401	CDL	OB6-CB5	2.15	1.40	1.34
52	H	401	U10	O4-C4	2.15	1.42	1.36
53	X	201	CDL	OA8-CA6	-2.15	1.40	1.45
53	d	201	CDL	OA6-CA5	2.15	1.40	1.34
53	M	602	CDL	OA8-CA6	-2.14	1.40	1.45
45	Y	204	3PE	O21-C21	2.14	1.40	1.34
46	H	402	PC1	O31-C3	-2.14	1.40	1.45
55	O	401	DGT	PG-O1G	-2.14	1.46	1.54
53	M	602	CDL	OA6-CA5	2.14	1.40	1.34
45	J	202	3PE	O21-C21	2.14	1.40	1.34
46	h	202	PC1	O31-C3	-2.13	1.40	1.45
53	L	701	CDL	OB6-CB5	2.13	1.40	1.34
45	d	202	3PE	O21-C21	2.13	1.40	1.34
45	L	703	3PE	O31-C3	-2.13	1.40	1.45
53	h	201	CDL	OB6-CB5	2.13	1.40	1.34
45	J	202	3PE	O31-C3	-2.13	1.40	1.45
45	N	402	3PE	O21-C21	2.12	1.40	1.34
45	Y	203	3PE	O21-C21	2.12	1.40	1.34
45	I	203	3PE	O21-C21	2.12	1.40	1.34
52	H	401	U10	C1-C2	-2.12	1.39	1.47
45	Y	203	3PE	O31-C3	-2.12	1.40	1.45
46	q	202	PC1	O31-C3	-2.11	1.40	1.45
52	H	401	U10	C16-C14	2.11	1.55	1.51
46	L	706	PC1	O21-C21	2.11	1.40	1.34
45	L	704	3PE	O31-C3	-2.11	1.40	1.45
46	I	204	PC1	O31-C3	-2.11	1.40	1.45
45	m	201	3PE	O31-C3	-2.11	1.40	1.45
53	X	201	CDL	OA6-CA5	2.10	1.40	1.34
53	X	201	CDL	OB8-CB7	2.10	1.39	1.33
45	i	202	3PE	O31-C3	-2.10	1.40	1.45
45	L	704	3PE	O21-C21	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	I	205	PC1	O31-C3	-2.10	1.40	1.45
46	M	605	PC1	O31-C3	-2.10	1.40	1.45
53	h	201	CDL	OB8-CB6	-2.10	1.40	1.45
45	Z	201	3PE	O31-C3	-2.10	1.40	1.45
53	J	201	CDL	OB8-CB6	-2.10	1.40	1.45
52	H	401	U10	O3-C3	2.10	1.42	1.36
53	N	401	CDL	OA8-CA6	-2.09	1.40	1.45
46	I	204	PC1	O21-C21	2.09	1.40	1.34
45	L	703	3PE	O21-C21	2.09	1.40	1.34
46	q	203	PC1	O21-C21	2.09	1.40	1.34
45	m	202	3PE	O21-C21	2.08	1.40	1.34
45	N	404	3PE	O31-C3	-2.08	1.40	1.45
45	Z	201	3PE	O21-C21	2.08	1.40	1.34
46	A	203	PC1	O31-C3	-2.08	1.40	1.45
45	Y	204	3PE	O31-C3	-2.08	1.40	1.45
45	Y	201	3PE	O31-C3	-2.08	1.40	1.45
45	Y	201	3PE	O21-C21	2.08	1.40	1.34
53	d	201	CDL	OB8-CB6	-2.07	1.40	1.45
53	J	201	CDL	OA8-CA6	-2.07	1.40	1.45
45	M	603	3PE	O31-C3	-2.07	1.40	1.45
45	A	201	3PE	O31-C3	-2.07	1.40	1.45
46	d	203	PC1	O21-C21	2.06	1.40	1.34
45	L	702	3PE	O21-C21	2.06	1.40	1.34
53	q	201	CDL	OB6-CB5	2.06	1.40	1.34
46	M	604	PC1	O21-C21	2.06	1.40	1.34
46	Y	205	PC1	O31-C3	-2.06	1.40	1.45
45	A	201	3PE	O21-C21	2.05	1.40	1.34
53	X	201	CDL	OB6-CB5	2.05	1.40	1.34
45	Y	202	3PE	O21-C21	2.05	1.40	1.34
52	H	401	U10	C1M-C1	2.04	1.55	1.50
46	q	203	PC1	O31-C3	-2.04	1.40	1.45
53	h	201	CDL	OA6-CA5	2.02	1.40	1.34

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	P	501	NDP	C5A-C6A-N6A	8.63	133.47	120.35
59	i	201	CHD	C14-C13-C12	7.25	114.16	107.40
57	P	501	NDP	C1B-N9A-C4A	-7.17	114.04	126.64
59	i	201	CHD	C13-C17-C20	-7.00	111.14	119.50
52	H	401	U10	C7-C8-C9	-6.49	115.98	126.79
57	P	501	NDP	N6A-C6A-N1A	-6.12	105.86	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	T	101	EHZ	C8-C9-S1	5.64	120.61	113.63
58	U	101	EHZ	C8-C9-S1	5.63	120.59	113.63
57	P	501	NDP	N3A-C2A-N1A	-5.30	120.40	128.68
45	g	201	3PE	O21-C21-C22	4.98	120.25	111.09
53	J	201	CDL	OA6-CA5-C11	4.95	120.20	111.09
53	J	201	CDL	OB6-CB5-C51	4.94	120.18	111.09
52	H	401	U10	C12-C13-C14	-4.85	115.99	127.66
50	F	501	FMN	C9-C8-C7	4.73	126.44	119.67
59	i	201	CHD	C17-C13-C12	4.65	121.91	117.67
52	H	401	U10	C17-C18-C19	-4.49	112.41	127.75
45	L	705	3PE	O21-C21-C22	4.43	121.06	111.50
45	Y	204	3PE	O21-C21-C22	4.41	121.01	111.50
46	H	402	PC1	O21-C21-C22	4.38	120.94	111.50
45	i	202	3PE	O21-C21-C22	4.36	120.91	111.50
50	F	501	FMN	C7M-C7-C6	4.28	127.41	119.49
45	L	704	3PE	O21-C21-C22	4.27	120.71	111.50
53	h	201	CDL	OB6-CB5-C51	4.21	120.58	111.50
53	M	602	CDL	OA6-CA5-C11	4.20	120.55	111.50
45	A	201	3PE	O21-C21-C22	4.18	120.52	111.50
45	m	201	3PE	O21-C21-C22	4.18	120.51	111.50
46	L	706	PC1	O21-C21-C22	4.16	120.46	111.50
45	Y	202	3PE	O21-C21-C22	4.15	120.44	111.50
45	Y	203	3PE	O21-C21-C22	4.15	120.44	111.50
53	N	401	CDL	OB6-CB5-C51	4.14	120.43	111.50
46	q	203	PC1	O21-C21-C22	4.14	120.42	111.50
45	d	202	3PE	O21-C21-C22	4.13	120.41	111.50
45	N	402	3PE	O21-C21-C22	4.13	120.39	111.50
45	o	202	3PE	O21-C21-C22	4.09	120.31	111.50
53	d	201	CDL	OA6-CA5-C11	4.08	120.30	111.50
59	i	201	CHD	C18-C13-C17	-4.08	104.83	111.21
53	L	701	CDL	OB6-CB5-C51	4.08	120.29	111.50
45	L	702	3PE	O21-C21-C22	4.04	120.21	111.50
53	X	201	CDL	OB6-CB5-C51	4.02	120.17	111.50
45	b	101	3PE	O21-C21-C22	4.02	120.17	111.50
45	m	202	3PE	O21-C21-C22	4.01	120.13	111.50
45	K	101	3PE	O21-C21-C22	3.97	120.05	111.50
53	q	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
46	A	203	PC1	O21-C21-C22	3.95	120.02	111.50
46	h	202	PC1	O21-C21-C22	3.94	119.98	111.50
53	M	602	CDL	OB6-CB5-C51	3.93	119.98	111.50
46	P	502	PC1	O21-C21-C22	3.92	119.96	111.50
53	q	201	CDL	OA6-CA5-C11	3.92	119.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	N	403	3PE	O21-C21-C22	3.91	119.92	111.50
45	J	202	3PE	O21-C21-C22	3.91	119.92	111.50
45	Z	201	3PE	O21-C21-C22	3.90	119.91	111.50
46	I	204	PC1	O21-C21-C22	3.88	119.87	111.50
53	X	201	CDL	OA6-CA5-C11	3.88	119.86	111.50
53	h	201	CDL	OA6-CA5-C11	3.88	119.86	111.50
45	N	404	3PE	O21-C21-C22	3.86	119.83	111.50
46	I	205	PC1	O21-C21-C22	3.86	119.83	111.50
45	M	603	3PE	O21-C21-C22	3.83	119.75	111.50
59	i	201	CHD	C18-C13-C12	-3.82	105.18	109.07
46	M	604	PC1	O21-C21-C22	3.81	119.71	111.50
46	q	202	PC1	O21-C21-C22	3.81	119.71	111.50
46	d	203	PC1	O21-C21-C22	3.78	119.65	111.50
45	I	203	3PE	O21-C21-C22	3.78	119.65	111.50
45	L	703	3PE	O21-C21-C22	3.75	119.59	111.50
53	L	701	CDL	OA6-CA5-C11	3.71	119.50	111.50
46	Y	205	PC1	O21-C21-C22	3.64	119.36	111.50
53	N	401	CDL	OA6-CA5-C11	3.62	119.30	111.50
46	A	202	PC1	O21-C21-C22	3.61	119.29	111.50
53	d	201	CDL	OB6-CB5-C51	3.61	120.88	110.80
59	i	201	CHD	C1-C10-C5	3.46	112.89	107.77
59	i	201	CHD	C17-C13-C14	3.45	103.58	100.09
45	Y	201	3PE	O21-C21-C22	3.42	118.87	111.50
59	i	201	CHD	C18-C13-C14	-3.41	105.88	111.21
45	I	203	3PE	O31-C31-C32	3.37	120.22	111.38
45	Y	204	3PE	O31-C31-C32	3.35	120.17	111.38
50	F	501	FMN	C4-N3-C2	-3.33	119.49	125.64
46	M	605	PC1	O21-C21-C22	3.32	120.05	110.80
50	F	501	FMN	C8M-C8-C7	-3.31	113.96	120.74
58	T	101	EHZ	C13-C12-N1	3.16	121.75	116.42
46	H	403	PC1	O21-C21-C22	3.15	119.58	110.80
55	O	401	DGT	C5-C6-N1	3.09	119.41	113.95
52	H	401	U10	C10-C9-C11	3.06	120.43	115.27
57	P	501	NDP	PN-O3-PA	-3.04	122.40	132.83
55	O	401	DGT	C2-N1-C6	-3.03	119.52	125.10
55	O	401	DGT	PB-O3B-PG	-2.98	122.60	132.83
50	F	501	FMN	C4A-C10-N10	2.98	120.83	116.48
53	d	201	CDL	OB8-CB7-C71	2.97	121.24	111.91
59	i	201	CHD	C23-C22-C20	-2.97	109.09	114.52
59	i	201	CHD	C19-C10-C9	-2.93	107.15	111.18
45	Y	203	3PE	O31-C31-C32	2.93	121.09	111.91
55	O	401	DGT	O2G-PG-O3B	2.92	114.42	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	i	201	CHD	C6-C5-C4	-2.89	107.86	111.19
46	q	203	PC1	O31-C31-C32	2.88	120.94	111.91
53	L	701	CDL	OA8-CA7-C31	2.86	120.90	111.91
53	M	602	CDL	OA8-CA7-C31	2.86	120.88	111.91
45	Y	202	3PE	O31-C31-C32	2.83	120.78	111.91
55	O	401	DGT	C2'-C3'-C4'	2.80	108.59	102.76
45	L	704	3PE	O31-C31-C32	2.78	120.65	111.91
53	N	401	CDL	OA8-CA7-C31	2.76	120.58	111.91
46	A	202	PC1	O31-C31-C32	2.76	120.56	111.91
46	M	604	PC1	O31-C31-C32	2.74	120.50	111.91
45	L	703	3PE	O31-C31-C32	2.74	120.49	111.91
53	h	201	CDL	OB8-CB7-C71	2.73	120.47	111.91
45	N	403	3PE	O31-C31-C32	2.71	120.40	111.91
46	Y	205	PC1	O31-C31-C32	2.70	120.39	111.91
46	M	605	PC1	O31-C31-C32	2.69	120.34	111.91
55	O	401	DGT	O1G-PG-O3B	2.68	113.63	104.64
55	O	401	DGT	PA-O3A-PB	-2.68	123.63	132.83
53	L	701	CDL	OB8-CB7-C71	2.67	120.30	111.91
53	q	201	CDL	OA8-CA7-C31	2.67	120.28	111.91
45	A	201	3PE	O31-C31-C32	2.67	120.28	111.91
58	T	101	EHZ	C11-N1-C12	-2.67	117.89	122.84
46	I	204	PC1	O31-C31-C32	2.66	120.25	111.91
45	Y	201	3PE	O31-C31-C32	2.66	120.25	111.91
46	H	403	PC1	O31-C31-C32	2.65	120.24	111.91
50	F	501	FMN	C4A-C4-N3	2.65	119.92	113.19
53	X	201	CDL	OA8-CA7-C31	2.64	120.19	111.91
45	K	101	3PE	O31-C31-C32	2.62	120.14	111.91
45	m	201	3PE	O31-C31-C32	2.62	120.14	111.91
50	F	501	FMN	C6-C7-C8	-2.61	115.92	119.67
46	P	502	PC1	O31-C31-C32	2.60	120.06	111.91
46	A	203	PC1	O31-C31-C32	2.58	120.01	111.91
46	H	402	PC1	O31-C31-C32	2.58	120.01	111.91
45	i	202	3PE	O31-C31-C32	2.57	119.98	111.91
53	N	401	CDL	OB8-CB7-C71	2.56	119.94	111.91
46	d	203	PC1	O31-C31-C32	2.56	119.94	111.91
45	m	202	3PE	O31-C31-C32	2.56	119.93	111.91
50	F	501	FMN	O4-C4-C4A	-2.55	119.82	126.60
46	L	706	PC1	O31-C31-C32	2.55	119.92	111.91
45	L	705	3PE	O31-C31-C32	2.54	119.89	111.91
53	M	602	CDL	OB8-CB7-C71	2.54	119.87	111.91
59	i	201	CHD	C1-C2-C3	2.52	113.71	110.47
59	i	201	CHD	C4-C3-C2	2.52	113.56	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	I	205	PC1	O31-C31-C32	2.50	119.76	111.91
46	h	202	PC1	O31-C31-C32	2.50	119.75	111.91
59	i	201	CHD	C9-C11-C12	-2.50	111.01	114.30
45	Z	201	3PE	O31-C31-C32	2.49	119.72	111.91
45	J	202	3PE	O31-C31-C32	2.48	119.69	111.91
53	h	201	CDL	OA8-CA7-C31	2.48	119.68	111.91
59	i	201	CHD	C11-C9-C10	-2.48	111.17	113.73
45	g	201	3PE	O31-C31-C32	2.47	119.66	111.91
52	H	401	U10	C1M-C1-C6	-2.47	120.38	124.40
52	H	401	U10	C10-C9-C8	-2.47	117.35	123.68
45	N	404	3PE	O31-C31-C32	2.46	119.62	111.91
53	q	201	CDL	OB8-CB7-C71	2.45	119.59	111.91
45	N	402	3PE	O31-C31-C32	2.43	119.54	111.91
58	T	101	EHZ	C7-C8-C9	-2.42	108.37	113.89
52	H	401	U10	C15-C14-C16	2.42	119.34	115.27
59	i	201	CHD	C15-C14-C8	2.42	121.71	118.33
45	g	201	3PE	C2-O21-C21	-2.41	113.40	117.90
53	d	201	CDL	OA8-CA7-C31	2.41	119.46	111.91
45	M	603	3PE	O31-C31-C32	2.40	119.43	111.91
58	U	101	EHZ	C13-C12-N1	2.38	120.43	116.42
53	J	201	CDL	CA4-OA6-CA5	-2.36	113.49	117.90
45	b	101	3PE	O31-C31-C32	2.34	119.26	111.91
45	d	202	3PE	O31-C31-C32	2.32	119.19	111.91
53	X	201	CDL	OB8-CB7-C71	2.31	119.15	111.91
50	F	501	FMN	C10-C4A-N5	-2.29	120.00	124.86
58	T	101	EHZ	C10-S1-C9	2.27	108.94	101.87
58	T	101	EHZ	O2-C9-S1	-2.26	119.68	122.61
46	q	202	PC1	O31-C31-C32	2.26	118.99	111.91
58	T	101	EHZ	C19-C17-C16	2.23	112.68	108.82
55	O	401	DGT	O1A-PA-O2A	-2.22	101.26	112.24
50	F	501	FMN	C6-C5A-C9A	2.20	122.05	118.94
55	O	401	DGT	O1B-PB-O2B	-2.17	101.50	112.24
58	U	101	EHZ	O2-C9-S1	-2.17	119.80	122.61
58	T	101	EHZ	C14-C13-C12	-2.16	108.77	112.36
58	U	101	EHZ	C14-C13-C12	-2.13	108.80	112.36
58	U	101	EHZ	C7-C8-C9	-2.11	109.07	113.89
59	i	201	CHD	C5-C6-C7	-2.10	112.15	114.46
58	T	101	EHZ	O3-C12-N1	-2.09	119.06	123.01
55	O	401	DGT	O6-C6-C5	-2.09	120.29	124.37
46	P	502	PC1	C2-O21-C21	-2.04	112.78	117.79
50	F	501	FMN	C4A-C10-N1	-2.04	120.01	124.73

There are no chirality outliers.

All (1085) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	O22-C21-O21-C2
45	I	203	3PE	C1-O11-P-O12
45	I	203	3PE	C1-O11-P-O13
45	I	203	3PE	C1-O11-P-O14
45	I	203	3PE	O11-C1-C2-O21
45	J	202	3PE	C11-O13-P-O12
45	J	202	3PE	O13-C11-C12-N
45	K	101	3PE	C22-C21-O21-C2
45	L	702	3PE	C1-O11-P-O14
45	L	702	3PE	C11-O13-P-O14
45	L	702	3PE	O13-C11-C12-N
45	L	702	3PE	C22-C21-O21-C2
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	704	3PE	C1-O11-P-O14
45	L	704	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O14
45	L	704	3PE	O13-C11-C12-N
45	L	704	3PE	O22-C21-O21-C2
45	L	705	3PE	C22-C21-O21-C2
45	M	603	3PE	C1-O11-P-O13
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	O13-C11-C12-N
45	M	603	3PE	O11-C1-C2-O21
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13
45	N	402	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	N	403	3PE	C1-O11-P-O13
45	N	403	3PE	C1-O11-P-O14
45	N	403	3PE	C12-C11-O13-P
45	N	403	3PE	O21-C2-C3-O31
45	N	404	3PE	C11-O13-P-O11
45	N	404	3PE	C11-O13-P-O14
45	N	404	3PE	C12-C11-O13-P
45	Y	201	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O14
45	Y	202	3PE	C11-O13-P-O12
45	Y	202	3PE	C11-O13-P-O14
45	Y	202	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	Y	203	3PE	C1-O11-P-O12
45	Y	203	3PE	C1-O11-P-O14
45	Y	203	3PE	C11-O13-P-O12
45	Y	203	3PE	C11-O13-P-O14
45	Y	203	3PE	C3-C2-O21-C21
45	Y	203	3PE	C22-C21-O21-C2
45	Y	204	3PE	C1-O11-P-O12
45	Y	204	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O11
45	Y	204	3PE	C11-O13-P-O12
45	Y	204	3PE	C11-O13-P-O14
45	Y	204	3PE	O13-C11-C12-N
45	Y	204	3PE	C22-C21-O21-C2
45	Z	201	3PE	C1-O11-P-O12
45	Z	201	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O14
45	Z	201	3PE	C11-O13-P-O12
45	Z	201	3PE	O13-C11-C12-N
45	Z	201	3PE	O21-C2-C3-O31
45	d	202	3PE	C1-O11-P-O12
45	d	202	3PE	C1-O11-P-O14
45	i	202	3PE	C1-O11-P-O13
45	i	202	3PE	C22-C21-O21-C2
45	m	201	3PE	O22-C21-O21-C2
45	m	202	3PE	O22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
45	o	202	3PE	O22-C21-O21-C2
46	A	202	PC1	C11-O13-P-O14
46	A	202	PC1	C1-O11-P-O12
46	A	202	PC1	C1-O11-P-O14
46	A	202	PC1	C1-O11-P-O13
46	A	202	PC1	O13-C11-C12-N
46	A	202	PC1	C22-C21-O21-C2
46	A	203	PC1	C11-O13-P-O11
46	H	402	PC1	C11-O13-P-O12
46	H	402	PC1	C11-O13-P-O14
46	H	402	PC1	C11-O13-P-O11
46	H	403	PC1	O13-C11-C12-N
46	I	205	PC1	C11-O13-P-O14
46	I	205	PC1	C11-O13-P-O11
46	I	205	PC1	C1-O11-P-O12
46	I	205	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	I	205	PC1	C1-O11-P-O13
46	L	706	PC1	C11-O13-P-O14
46	L	706	PC1	C1-O11-P-O12
46	L	706	PC1	C1-O11-P-O14
46	L	706	PC1	C1-O11-P-O13
46	L	706	PC1	O13-C11-C12-N
46	M	604	PC1	C1-O11-P-O12
46	M	604	PC1	C1-O11-P-O13
46	M	604	PC1	O13-C11-C12-N
46	M	605	PC1	C11-O13-P-O12
46	M	605	PC1	C1-O11-P-O14
46	M	605	PC1	C1-O11-P-O13
46	M	605	PC1	C12-C11-O13-P
46	M	605	PC1	O11-C1-C2-O21
46	M	605	PC1	O22-C21-O21-C2
46	P	502	PC1	C11-O13-P-O11
46	P	502	PC1	C1-O11-P-O12
46	P	502	PC1	C1-O11-P-O14
46	P	502	PC1	C1-O11-P-O13
46	P	502	PC1	C22-C21-O21-C2
46	Y	205	PC1	C11-O13-P-O12
46	Y	205	PC1	C22-C21-O21-C2
46	h	202	PC1	C11-O13-P-O14
46	q	202	PC1	C11-O13-P-O12
46	q	202	PC1	C11-O13-P-O14
46	q	203	PC1	C11-O13-P-O14
46	q	203	PC1	C11-O13-P-O11
46	q	203	PC1	C1-O11-P-O12
46	q	203	PC1	C1-O11-P-O14
46	q	203	PC1	O22-C21-O21-C2
48	B	202	PLC	C1-O3P-P-O4P
48	L	707	PLC	C1-O3P-P-O2P
48	N	405	PLC	C4-O4P-P-O1P
48	N	405	PLC	C4-O4P-P-O2P
48	N	405	PLC	C4-O4P-P-O3P
48	b	102	PLC	C4-O4P-P-O1P
48	g	202	PLC	O2-C2-C3-O3
48	g	202	PLC	C1-O3P-P-O2P
53	J	201	CDL	C1-CA2-OA2-PA1
53	J	201	CDL	CA2-OA2-PA1-OA3
53	J	201	CDL	CA2-OA2-PA1-OA4
53	J	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	J	201	CDL	C51-CB5-OB6-CB4
53	L	701	CDL	C11-CA5-OA6-CA4
53	L	701	CDL	OB7-CB5-OB6-CB4
53	L	701	CDL	C51-CB5-OB6-CB4
53	M	602	CDL	C1-CA2-OA2-PA1
53	M	602	CDL	CA3-OA5-PA1-OA3
53	M	602	CDL	CA3-OA5-PA1-OA4
53	M	602	CDL	C51-CB5-OB6-CB4
53	N	401	CDL	CB3-OB5-PB2-OB2
53	N	401	CDL	CB3-OB5-PB2-OB3
53	N	401	CDL	CB3-OB5-PB2-OB4
53	N	401	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	C11-CA5-OA6-CA4
53	X	201	CDL	OA9-CA7-OA8-CA6
53	X	201	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CB2-OB2-PB2-OB4
53	X	201	CDL	CB3-OB5-PB2-OB4
53	X	201	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	CB3-OB5-PB2-OB2
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	d	201	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CB2-C1-CA2-OA2
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CA3-OA5-PA1-OA4
53	q	201	CDL	C11-CA5-OA6-CA4
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	CB3-OB5-PB2-OB2
53	q	201	CDL	CB3-OB5-PB2-OB3
53	q	201	CDL	CB3-OB5-PB2-OB4
53	q	201	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	C51-CB5-OB6-CB4
55	O	401	DGT	PB-O3B-PG-O1G
55	O	401	DGT	PB-O3B-PG-O2G
57	P	501	NDP	C5B-O5B-PA-O1A
57	P	501	NDP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
57	P	501	NDP	C5B-O5B-PA-O3
57	P	501	NDP	C2B-O2B-P2B-O1X
57	P	501	NDP	C5D-O5D-PN-O3
57	P	501	NDP	C5D-O5D-PN-O1N
57	P	501	NDP	C5D-O5D-PN-O2N
57	P	501	NDP	C3D-C4D-C5D-O5D
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	S1-C10-C11-N1
58	U	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
60	o	201	MYR	C1-C2-C3-C4
53	J	201	CDL	C11-CA5-OA6-CA4
45	L	703	3PE	O32-C31-O31-C3
46	d	203	PC1	O32-C31-O31-C3
53	d	201	CDL	OB9-CB7-OB8-CB6
45	N	402	3PE	C32-C31-O31-C3
46	d	203	PC1	C32-C31-O31-C3
53	d	201	CDL	C71-CB7-OB8-CB6
45	I	203	3PE	O32-C31-O31-C3
45	L	704	3PE	O32-C31-O31-C3
45	N	402	3PE	O32-C31-O31-C3
45	Y	202	3PE	O32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
46	A	202	PC1	O32-C31-O31-C3
46	M	604	PC1	O32-C31-O31-C3
46	M	605	PC1	O32-C31-O31-C3
46	q	203	PC1	O32-C31-O31-C3
53	L	701	CDL	OA9-CA7-OA8-CA6
53	M	602	CDL	OA9-CA7-OA8-CA6
53	d	201	CDL	OA9-CA7-OA8-CA6
53	J	201	CDL	OA7-CA5-OA6-CA4
53	J	201	CDL	OB7-CB5-OB6-CB4
45	K	101	3PE	O22-C21-O21-C2
45	L	702	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
45	Y	204	3PE	O22-C21-O21-C2
45	i	202	3PE	O22-C21-O21-C2
46	A	202	PC1	O22-C21-O21-C2
46	P	502	PC1	O22-C21-O21-C2
46	Y	205	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	h	202	PC1	O22-C21-O21-C2
53	L	701	CDL	OA7-CA5-OA6-CA4
53	M	602	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	OA7-CA5-OA6-CA4
53	q	201	CDL	OA7-CA5-OA6-CA4
45	g	201	3PE	C22-C21-O21-C2
48	B	202	PLC	C2-C3-O3-CB
45	I	203	3PE	C32-C31-O31-C3
45	L	703	3PE	C32-C31-O31-C3
45	L	704	3PE	C32-C31-O31-C3
45	Y	202	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
46	A	202	PC1	C32-C31-O31-C3
46	M	604	PC1	C32-C31-O31-C3
46	q	203	PC1	C32-C31-O31-C3
53	M	602	CDL	C31-CA7-OA8-CA6
53	X	201	CDL	C31-CA7-OA8-CA6
45	A	201	3PE	C22-C21-O21-C2
45	L	704	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
45	o	202	3PE	C22-C21-O21-C2
46	M	605	PC1	C22-C21-O21-C2
46	h	202	PC1	C22-C21-O21-C2
46	q	203	PC1	C22-C21-O21-C2
53	N	401	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	C51-CB5-OB6-CB4
45	L	702	3PE	O32-C31-O31-C3
45	d	202	3PE	C32-C31-O31-C3
46	H	403	PC1	C32-C31-O31-C3
46	M	605	PC1	C32-C31-O31-C3
46	h	202	PC1	C32-C31-O31-C3
53	L	701	CDL	C31-CA7-OA8-CA6
53	d	201	CDL	C31-CA7-OA8-CA6
45	o	202	3PE	O32-C31-O31-C3
45	L	705	3PE	O22-C21-O21-C2
46	H	403	PC1	O32-C31-O31-C3
46	h	202	PC1	O32-C31-O31-C3
53	N	401	CDL	OB9-CB7-OB8-CB6
45	L	702	3PE	C32-C31-O31-C3
45	o	202	3PE	C32-C31-O31-C3
53	J	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
45	N	403	3PE	C32-C31-O31-C3
48	B	202	PLC	C1B-CB-O3-C3
53	N	401	CDL	C71-CB7-OB8-CB6
45	d	202	3PE	O32-C31-O31-C3
45	Z	201	3PE	C22-C21-O21-C2
53	h	201	CDL	C11-CA5-OA6-CA4
57	P	501	NDP	O4B-C4B-C5B-O5B
57	P	501	NDP	O4D-C4D-C5D-O5D
53	J	201	CDL	OA9-CA7-OA8-CA6
45	Z	201	3PE	O22-C21-O21-C2
45	N	403	3PE	O32-C31-O31-C3
48	B	202	PLC	OB-CB-O3-C3
53	h	201	CDL	C71-CB7-OB8-CB6
59	i	201	CHD	C17-C20-C22-C23
53	M	602	CDL	C11-CA5-OA6-CA4
53	X	201	CDL	CB2-C1-CA2-OA2
53	h	201	CDL	OA7-CA5-OA6-CA4
59	i	201	CHD	C21-C20-C22-C23
53	h	201	CDL	OB9-CB7-OB8-CB6
45	A	201	3PE	C32-C31-O31-C3
46	Y	205	PC1	C32-C31-O31-C3
48	b	102	PLC	C1B-CB-O3-C3
53	M	602	CDL	C71-CB7-OB8-CB6
53	N	401	CDL	C31-CA7-OA8-CA6
53	J	201	CDL	C31-CA7-OA8-CA6
46	d	203	PC1	C21-C22-C23-C24
53	N	401	CDL	OB6-CB4-CB6-OB8
46	L	706	PC1	C32-C31-O31-C3
45	L	704	3PE	C31-C32-C33-C34
45	N	404	3PE	C32-C31-O31-C3
45	A	201	3PE	O32-C31-O31-C3
45	K	101	3PE	C31-C32-C33-C34
45	M	603	3PE	C21-C22-C23-C24
45	N	403	3PE	C21-C22-C23-C24
45	Y	203	3PE	C21-C22-C23-C24
46	I	205	PC1	C21-C22-C23-C24
46	M	604	PC1	C31-C32-C33-C34
46	q	203	PC1	C21-C22-C23-C24
48	B	202	PLC	C'-C1'-C2'-C3'
53	M	602	CDL	CA5-C11-C12-C13
53	J	201	CDL	OB9-CB7-OB8-CB6
53	M	602	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C31-C32-C33-C34
45	Y	203	3PE	C31-C32-C33-C34
45	i	202	3PE	C21-C22-C23-C24
53	L	701	CDL	CA5-C11-C12-C13
53	X	201	CDL	CA5-C11-C12-C13
53	d	201	CDL	CA5-C11-C12-C13
48	b	102	PLC	OB-CB-O3-C3
57	P	501	NDP	O4D-C1D-N1N-C6N
45	g	201	3PE	O22-C21-O21-C2
53	M	602	CDL	OB9-CB7-OB8-CB6
53	N	401	CDL	OA9-CA7-OA8-CA6
53	q	201	CDL	O1-C1-CA2-OA2
45	N	404	3PE	O32-C31-O31-C3
46	L	706	PC1	O32-C31-O31-C3
46	Y	205	PC1	O32-C31-O31-C3
46	H	403	PC1	C31-C32-C33-C34
46	I	204	PC1	C22-C21-O21-C2
45	I	203	3PE	C11-O13-P-O11
45	J	202	3PE	C11-O13-P-O11
45	K	101	3PE	C1-O11-P-O13
45	L	702	3PE	C11-O13-P-O11
45	L	704	3PE	C1-O11-P-O13
45	N	402	3PE	C11-O13-P-O11
45	N	403	3PE	C11-O13-P-O11
45	Y	202	3PE	C11-O13-P-O11
45	Y	203	3PE	C1-O11-P-O13
45	Y	203	3PE	C11-O13-P-O11
45	Y	204	3PE	C1-O11-P-O13
45	Z	201	3PE	C11-O13-P-O11
45	d	202	3PE	C1-O11-P-O13
45	m	202	3PE	C1-O11-P-O13
45	m	202	3PE	C11-O13-P-O11
46	A	202	PC1	C11-O13-P-O11
46	I	204	PC1	C1-O11-P-O13
46	L	706	PC1	C11-O13-P-O11
46	M	605	PC1	C11-O13-P-O11
46	Y	205	PC1	C11-O13-P-O11
46	q	202	PC1	C11-O13-P-O11
46	q	203	PC1	C1-O11-P-O13
48	L	707	PLC	C1-O3P-P-O4P
48	g	202	PLC	C1-O3P-P-O4P
53	L	701	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
53	M	602	CDL	CA3-OA5-PA1-OA2
53	M	602	CDL	CB2-OB2-PB2-OB5
53	X	201	CDL	CB2-OB2-PB2-OB5
53	X	201	CDL	CB3-OB5-PB2-OB2
53	h	201	CDL	CA2-OA2-PA1-OA5
48	N	405	PLC	C'-C1'-C2'-C3'
45	Y	204	3PE	C32-C31-O31-C3
53	N	401	CDL	CB7-C71-C72-C73
46	I	204	PC1	O22-C21-O21-C2
45	i	202	3PE	C32-C31-O31-C3
46	h	202	PC1	C22-C23-C24-C25
53	L	701	CDL	C37-C38-C39-C40
53	M	602	CDL	C32-C33-C34-C35
53	h	201	CDL	C74-C75-C76-C77
45	I	203	3PE	C22-C21-O21-C2
45	M	603	3PE	C22-C21-O21-C2
46	L	706	PC1	C22-C21-O21-C2
57	P	501	NDP	C3B-C4B-C5B-O5B
45	N	404	3PE	C2C-C2D-C2E-C2F
53	X	201	CDL	C78-C79-C80-C81
53	q	201	CDL	C51-C52-C53-C54
53	q	201	CDL	C71-C72-C73-C74
45	L	704	3PE	C23-C24-C25-C26
45	N	402	3PE	C24-C25-C26-C27
45	Y	204	3PE	C2C-C2D-C2E-C2F
46	h	202	PC1	C24-C25-C26-C27
53	M	602	CDL	C78-C79-C80-C81
45	I	203	3PE	O22-C21-O21-C2
53	h	201	CDL	C71-C72-C73-C74
60	o	201	MYR	C4-C5-C6-C7
45	d	202	3PE	C39-C3A-C3B-C3C
46	q	202	PC1	C38-C39-C3A-C3B
53	M	602	CDL	C56-C57-C58-C59
53	M	602	CDL	C83-C84-C85-C86
53	X	201	CDL	C37-C38-C39-C40
53	h	201	CDL	C31-C32-C33-C34
53	N	401	CDL	O1-C1-CB2-OB2
53	X	201	CDL	O1-C1-CA2-OA2
45	K	101	3PE	C33-C34-C35-C36
45	Z	201	3PE	C27-C28-C29-C2A
46	L	706	PC1	C37-C38-C39-C3A
53	L	701	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
45	d	202	3PE	C31-C32-C33-C34
53	M	602	CDL	CB5-C51-C52-C53
45	L	703	3PE	C2E-C2F-C2G-C2H
46	I	204	PC1	C36-C37-C38-C39
46	M	604	PC1	C24-C25-C26-C27
48	B	202	PLC	C3B-C4B-C5B-C6B
53	X	201	CDL	C57-C58-C59-C60
45	L	704	3PE	C36-C37-C38-C39
45	Z	201	3PE	C34-C35-C36-C37
46	H	402	PC1	C28-C29-C2A-C2B
46	I	205	PC1	C24-C25-C26-C27
45	N	404	3PE	C34-C35-C36-C37
46	H	403	PC1	C36-C37-C38-C39
46	d	203	PC1	C36-C37-C38-C39
45	o	202	3PE	C2E-C2F-C2G-C2H
46	A	203	PC1	C33-C34-C35-C36
48	g	202	PLC	C2'-C3'-C4'-C5'
53	X	201	CDL	C60-C61-C62-C63
45	M	603	3PE	O22-C21-O21-C2
46	L	706	PC1	O22-C21-O21-C2
53	d	201	CDL	OA7-CA5-OA6-CA4
53	d	201	CDL	C11-CA5-OA6-CA4
45	L	702	3PE	C27-C28-C29-C2A
45	N	402	3PE	C27-C28-C29-C2A
45	N	404	3PE	C23-C24-C25-C26
46	P	502	PC1	C25-C26-C27-C28
46	A	202	PC1	C21-C22-C23-C24
46	H	402	PC1	C21-C22-C23-C24
45	I	203	3PE	C28-C29-C2A-C2B
45	L	703	3PE	C33-C34-C35-C36
45	N	403	3PE	C39-C3A-C3B-C3C
45	N	403	3PE	C22-C23-C24-C25
45	N	403	3PE	C2C-C2D-C2E-C2F
45	Y	202	3PE	C35-C36-C37-C38
45	Y	203	3PE	C37-C38-C39-C3A
45	g	201	3PE	C35-C36-C37-C38
45	m	201	3PE	C25-C26-C27-C28
46	L	706	PC1	C3E-C3F-C3G-C3H
53	M	602	CDL	C12-C13-C14-C15
53	M	602	CDL	C71-C72-C73-C74
53	N	401	CDL	C16-C17-C18-C19
53	N	401	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
45	K	101	3PE	C35-C36-C37-C38
45	L	702	3PE	C2C-C2D-C2E-C2F
45	L	704	3PE	C24-C25-C26-C27
45	M	603	3PE	C32-C33-C34-C35
46	M	604	PC1	C28-C29-C2A-C2B
45	L	705	3PE	O13-C11-C12-N
45	N	404	3PE	O13-C11-C12-N
45	m	202	3PE	O13-C11-C12-N
45	J	202	3PE	C33-C34-C35-C36
45	N	403	3PE	C36-C37-C38-C39
45	Y	203	3PE	C3A-C3B-C3C-C3D
45	Y	204	3PE	C28-C29-C2A-C2B
53	X	201	CDL	C71-C72-C73-C74
46	L	706	PC1	C21-C22-C23-C24
45	i	202	3PE	O32-C31-O31-C3
46	H	403	PC1	C3C-C3D-C3E-C3F
46	L	706	PC1	C33-C34-C35-C36
53	L	701	CDL	C35-C36-C37-C38
53	h	201	CDL	C33-C34-C35-C36
45	M	603	3PE	C32-C31-O31-C3
46	I	205	PC1	C26-C27-C28-C29
58	U	101	EHZ	S1-C10-C11-N1
45	N	404	3PE	C26-C27-C28-C29
45	N	402	3PE	C28-C29-C2A-C2B
45	Y	202	3PE	C32-C33-C34-C35
45	Y	202	3PE	C3B-C3C-C3D-C3E
46	I	204	PC1	C22-C23-C24-C25
48	B	202	PLC	C1B-C2B-C3B-C4B
53	d	201	CDL	C72-C73-C74-C75
46	H	402	PC1	C31-C32-C33-C34
46	H	402	PC1	C22-C23-C24-C25
45	L	703	3PE	C35-C36-C37-C38
45	Y	202	3PE	C22-C23-C24-C25
45	d	202	3PE	C29-C2A-C2B-C2C
46	H	402	PC1	C32-C33-C34-C35
46	P	502	PC1	C3B-C3C-C3D-C3E
45	Y	204	3PE	O32-C31-O31-C3
45	m	201	3PE	C33-C34-C35-C36
53	M	602	CDL	O1-C1-CA2-OA2
46	I	204	PC1	C32-C33-C34-C35
45	b	101	3PE	C36-C37-C38-C39
46	h	202	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
48	g	202	PLC	C'-C1'-C2'-C3'
53	d	201	CDL	CA7-C31-C32-C33
53	N	401	CDL	CA2-C1-CB2-OB2
46	L	706	PC1	C3B-C3C-C3D-C3E
45	K	101	3PE	C27-C28-C29-C2A
45	Y	203	3PE	C32-C33-C34-C35
46	Y	205	PC1	C24-C25-C26-C27
45	M	603	3PE	O32-C31-O31-C3
45	N	404	3PE	C2A-C2B-C2C-C2D
45	d	202	3PE	C25-C26-C27-C28
46	I	204	PC1	C3A-C3B-C3C-C3D
46	L	706	PC1	C39-C3A-C3B-C3C
53	M	602	CDL	C75-C76-C77-C78
46	P	502	PC1	C31-C32-C33-C34
45	o	202	3PE	C2B-C2C-C2D-C2E
45	L	702	3PE	C29-C2A-C2B-C2C
53	N	401	CDL	C72-C73-C74-C75
53	d	201	CDL	C36-C37-C38-C39
45	N	403	3PE	C31-C32-C33-C34
46	I	204	PC1	C31-C32-C33-C34
45	i	202	3PE	C3E-C3F-C3G-C3H
58	U	101	EHZ	C1-C2-C3-C4
53	h	201	CDL	C58-C59-C60-C61
45	J	202	3PE	C32-C31-O31-C3
46	q	202	PC1	C32-C31-O31-C3
45	N	403	3PE	C34-C35-C36-C37
45	Y	202	3PE	C2C-C2D-C2E-C2F
45	m	201	3PE	C29-C2A-C2B-C2C
45	o	202	3PE	C2C-C2D-C2E-C2F
53	q	201	CDL	C13-C14-C15-C16
45	o	202	3PE	C27-C28-C29-C2A
45	N	402	3PE	C38-C39-C3A-C3B
45	N	402	3PE	C21-C22-C23-C24
53	N	401	CDL	CA5-C11-C12-C13
45	J	202	3PE	C22-C21-O21-C2
48	B	202	PLC	C1'-C'-O2-C2
53	N	401	CDL	C11-CA5-OA6-CA4
46	I	204	PC1	O11-C1-C2-O21
53	M	602	CDL	OB5-CB3-CB4-OB6
45	I	203	3PE	C2B-C2C-C2D-C2E
45	J	202	3PE	O22-C21-O21-C2
48	B	202	PLC	O'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C32-C33-C34-C35
45	m	202	3PE	C33-C34-C35-C36
46	L	706	PC1	C22-C23-C24-C25
45	Y	201	3PE	C21-C22-C23-C24
45	N	402	3PE	C36-C37-C38-C39
45	M	603	3PE	C39-C3A-C3B-C3C
53	N	401	CDL	OA7-CA5-OA6-CA4
45	I	203	3PE	C2C-C2D-C2E-C2F
45	m	201	3PE	C2E-C2F-C2G-C2H
48	b	102	PLC	C2-C3-O3-CB
45	i	202	3PE	C11-O13-P-O11
53	X	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB3-OB5-PB2-OB2
45	M	603	3PE	C2B-C2C-C2D-C2E
45	b	101	3PE	C2D-C2E-C2F-C2G
53	q	201	CDL	C71-CB7-OB8-CB6
45	L	704	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
53	N	401	CDL	OA5-CA3-CA4-CA6
45	b	101	3PE	C23-C24-C25-C26
45	b	101	3PE	C2A-C2B-C2C-C2D
53	L	701	CDL	C59-C60-C61-C62
45	N	402	3PE	C32-C33-C34-C35
45	L	705	3PE	C32-C33-C34-C35
58	T	101	EHZ	C22-C23-C24-C25
45	J	202	3PE	C1-C2-C3-O31
45	K	101	3PE	C32-C33-C34-C35
45	N	403	3PE	C1-C2-C3-O31
45	Y	201	3PE	C1-C2-C3-O31
45	g	201	3PE	C1-C2-C3-O31
45	m	201	3PE	C1-C2-C3-O31
46	h	202	PC1	C1-C2-C3-O31
48	b	102	PLC	C1-C2-C3-O3
48	g	202	PLC	C1-C2-C3-O3
53	N	401	CDL	CB3-CB4-CB6-OB8
58	U	101	EHZ	C22-C23-C24-C25
45	N	402	3PE	C22-C23-C24-C25
46	q	202	PC1	O32-C31-O31-C3
46	I	205	PC1	C33-C34-C35-C36
53	d	201	CDL	C40-C41-C42-C43
45	J	202	3PE	O32-C31-O31-C3
45	N	402	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
46	I	204	PC1	C26-C27-C28-C29
46	L	706	PC1	C24-C25-C26-C27
53	M	602	CDL	C34-C35-C36-C37
45	Y	201	3PE	C25-C26-C27-C28
53	L	701	CDL	C84-C85-C86-C87
53	X	201	CDL	C64-C65-C66-C67
45	Z	201	3PE	C37-C38-C39-C3A
48	N	405	PLC	C2'-C3'-C4'-C5'
53	N	401	CDL	C36-C37-C38-C39
46	I	204	PC1	C23-C24-C25-C26
53	q	201	CDL	OB9-CB7-OB8-CB6
45	N	404	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
45	L	705	3PE	C25-C26-C27-C28
46	M	605	PC1	O21-C2-C3-O31
53	M	602	CDL	OB6-CB4-CB6-OB8
45	N	404	3PE	C36-C37-C38-C39
45	o	202	3PE	C26-C27-C28-C29
45	N	403	3PE	C29-C2A-C2B-C2C
53	q	201	CDL	C31-CA7-OA8-CA6
45	M	603	3PE	C35-C36-C37-C38
45	i	202	3PE	C35-C36-C37-C38
45	L	704	3PE	C2A-C2B-C2C-C2D
45	L	703	3PE	O11-C1-C2-C3
45	M	603	3PE	O11-C1-C2-C3
45	N	403	3PE	O11-C1-C2-C3
45	g	201	3PE	O11-C1-C2-C3
46	I	204	PC1	O11-C1-C2-C3
46	M	605	PC1	O11-C1-C2-C3
48	L	707	PLC	O3P-C1-C2-C3
53	M	602	CDL	OB5-CB3-CB4-CB6
46	M	604	PC1	C2A-C2B-C2C-C2D
58	U	101	EHZ	C3-C4-C5-C6
45	L	705	3PE	C32-C31-O31-C3
45	d	202	3PE	C24-C25-C26-C27
45	d	202	3PE	C21-C22-C23-C24
46	q	202	PC1	C31-C32-C33-C34
45	A	201	3PE	C26-C27-C28-C29
53	d	201	CDL	C76-C77-C78-C79
45	b	101	3PE	C2C-C2D-C2E-C2F
45	Y	204	3PE	C1-C2-C3-O31
45	Z	201	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	A	202	PC1	C1-C2-C3-O31
46	H	403	PC1	C1-C2-C3-O31
46	q	203	PC1	C1-C2-C3-O31
48	B	202	PLC	C1-C2-C3-O3
53	X	201	CDL	CA3-CA4-CA6-OA8
53	M	602	CDL	C20-C21-C22-C23
45	M	603	3PE	C2E-C2F-C2G-C2H
53	X	201	CDL	C44-C45-C46-C47
45	L	703	3PE	C37-C38-C39-C3A
58	T	101	EHZ	N2-C15-C16-C17
45	g	201	3PE	C31-C32-C33-C34
45	Z	201	3PE	C28-C29-C2A-C2B
53	h	201	CDL	C37-C38-C39-C40
46	d	203	PC1	C34-C35-C36-C37
53	N	401	CDL	C74-C75-C76-C77
45	Y	204	3PE	O11-C1-C2-O21
46	H	402	PC1	O11-C1-C2-O21
48	b	102	PLC	O3P-C1-C2-O2
53	N	401	CDL	OA5-CA3-CA4-OA6
53	X	201	CDL	C31-C32-C33-C34
45	J	202	3PE	C23-C24-C25-C26
45	J	202	3PE	C24-C25-C26-C27
53	q	201	CDL	OA9-CA7-OA8-CA6
45	L	704	3PE	C27-C28-C29-C2A
45	J	202	3PE	O21-C2-C3-O31
45	d	202	3PE	O21-C2-C3-O31
45	o	202	3PE	O21-C2-C3-O31
46	A	202	PC1	O21-C2-C3-O31
46	q	203	PC1	O21-C2-C3-O31
48	L	707	PLC	O2-C2-C3-O3
48	N	405	PLC	O2-C2-C3-O3
53	X	201	CDL	OA6-CA4-CA6-OA8
53	d	201	CDL	OB6-CB4-CB6-OB8
45	N	404	3PE	C25-C26-C27-C28
53	N	401	CDL	C56-C57-C58-C59
53	h	201	CDL	C1-CA2-OA2-PA1
45	M	603	3PE	C2D-C2E-C2F-C2G
45	Y	203	3PE	C36-C37-C38-C39
58	T	101	EHZ	O2-C9-S1-C10
46	A	202	PC1	C31-C32-C33-C34
46	A	203	PC1	C32-C33-C34-C35
53	M	602	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
45	d	202	3PE	C22-C23-C24-C25
46	A	203	PC1	C23-C24-C25-C26
53	M	602	CDL	C58-C59-C60-C61
45	I	203	3PE	O11-C1-C2-C3
45	N	404	3PE	O11-C1-C2-C3
46	H	402	PC1	O11-C1-C2-C3
46	H	403	PC1	O11-C1-C2-C3
53	L	701	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	OA5-CA3-CA4-CA6
53	q	201	CDL	O1-C1-CB2-OB2
48	B	202	PLC	C7B-C8B-C9B-CAA
45	N	402	3PE	C2E-C2F-C2G-C2H
45	Y	202	3PE	C23-C24-C25-C26
53	L	701	CDL	C11-C12-C13-C14
53	h	201	CDL	C31-CA7-OA8-CA6
45	N	403	3PE	C26-C27-C28-C29
45	d	202	3PE	C37-C38-C39-C3A
45	N	404	3PE	C33-C34-C35-C36
45	N	402	3PE	C2C-C2D-C2E-C2F
45	M	603	3PE	C34-C35-C36-C37
53	q	201	CDL	CB3-CB4-OB6-CB5
58	T	101	EHZ	C8-C9-S1-C10
45	I	203	3PE	C2E-C2F-C2G-C2H
53	M	602	CDL	C72-C73-C74-C75
45	Z	201	3PE	C26-C27-C28-C29
53	q	201	CDL	CA5-C11-C12-C13
45	N	403	3PE	C2-C1-O11-P
45	Y	202	3PE	C1-C2-C3-O31
45	i	202	3PE	C1-C2-C3-O31
46	H	403	PC1	C2-C1-O11-P
46	d	203	PC1	C1-C2-C3-O31
53	M	602	CDL	CA3-CA4-CA6-OA8
45	A	201	3PE	O11-C1-C2-O21
45	N	403	3PE	O11-C1-C2-O21
45	g	201	3PE	O11-C1-C2-O21
53	L	701	CDL	OB5-CB3-CB4-OB6
53	X	201	CDL	OA5-CA3-CA4-OA6
45	o	202	3PE	C24-C25-C26-C27
53	X	201	CDL	CA7-C31-C32-C33
46	M	604	PC1	C2B-C2C-C2D-C2E
58	T	101	EHZ	O1-C7-C8-C9
58	U	101	EHZ	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
45	L	705	3PE	O32-C31-O31-C3
53	h	201	CDL	OA9-CA7-OA8-CA6
45	d	202	3PE	C28-C29-C2A-C2B
45	Y	201	3PE	O21-C2-C3-O31
45	Y	202	3PE	O21-C2-C3-O31
45	g	201	3PE	O21-C2-C3-O31
45	m	201	3PE	O21-C2-C3-O31
46	H	403	PC1	O21-C2-C3-O31
46	M	604	PC1	O21-C2-C3-O31
46	h	202	PC1	O21-C2-C3-O31
48	b	102	PLC	O2-C2-C3-O3
53	M	602	CDL	OA6-CA4-CA6-OA8
45	L	704	3PE	C37-C38-C39-C3A
46	I	204	PC1	C35-C36-C37-C38
45	L	704	3PE	C33-C34-C35-C36
48	g	202	PLC	C7'-C8'-C9'-CA'
53	M	602	CDL	C62-C63-C64-C65
45	L	703	3PE	C29-C2A-C2B-C2C
53	L	701	CDL	C62-C63-C64-C65
53	L	701	CDL	C78-C79-C80-C81
57	P	501	NDP	PN-O3-PA-O2A
45	b	101	3PE	C37-C38-C39-C3A
45	N	403	3PE	C2E-C2F-C2G-C2H
45	m	201	3PE	C23-C24-C25-C26
45	L	703	3PE	C1-O11-P-O13
45	Y	201	3PE	C1-O11-P-O13
45	Y	202	3PE	C1-O11-P-O13
45	o	202	3PE	C11-O13-P-O11
46	h	202	PC1	C11-O13-P-O11
48	B	202	PLC	C4-O4P-P-O3P
48	b	102	PLC	C4-O4P-P-O3P
53	J	201	CDL	CB2-OB2-PB2-OB5
53	M	602	CDL	CB3-OB5-PB2-OB2
53	X	201	CDL	CA3-OA5-PA1-OA2
53	N	401	CDL	C31-C32-C33-C34
45	L	705	3PE	C2-C1-O11-P
46	M	604	PC1	C2-C1-O11-P
46	M	605	PC1	C2-C1-O11-P
53	X	201	CDL	C1-CB2-OB2-PB2
45	Y	203	3PE	C2C-C2D-C2E-C2F
45	I	203	3PE	C11-O13-P-O12
45	I	203	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	J	202	3PE	C11-O13-P-O14
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	C1-O11-P-O14
45	L	702	3PE	C11-O13-P-O12
45	N	403	3PE	C11-O13-P-O14
45	Y	202	3PE	C1-O11-P-O12
45	Z	201	3PE	C11-O13-P-O14
45	b	101	3PE	C1-O11-P-O12
45	g	201	3PE	C11-O13-P-O12
45	i	202	3PE	C11-O13-P-O12
45	m	201	3PE	C1-O11-P-O12
45	m	202	3PE	C1-O11-P-O14
45	m	202	3PE	C11-O13-P-O12
46	I	204	PC1	C1-O11-P-O12
46	I	204	PC1	C1-O11-P-O14
46	I	205	PC1	C11-O13-P-O12
46	L	706	PC1	C11-O13-P-O12
46	M	604	PC1	C1-O11-P-O14
46	M	605	PC1	C11-O13-P-O14
46	M	605	PC1	C1-O11-P-O12
46	Y	205	PC1	C11-O13-P-O14
48	B	202	PLC	C1-O3P-P-O2P
53	L	701	CDL	CB3-OB5-PB2-OB3
53	L	701	CDL	CB3-OB5-PB2-OB4
53	M	602	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	C51-C52-C53-C54
45	d	202	3PE	C2F-C2G-C2H-C2I
46	A	202	PC1	C23-C24-C25-C26
53	L	701	CDL	C72-C73-C74-C75
48	N	405	PLC	C1B-CB-O3-C3
45	N	403	3PE	O13-C11-C12-N
45	b	101	3PE	O21-C21-C22-C23
45	M	603	3PE	C37-C38-C39-C3A
46	q	203	PC1	C32-C33-C34-C35
46	H	402	PC1	C33-C34-C35-C36
45	L	704	3PE	C32-C33-C34-C35
45	I	203	3PE	C12-C11-O13-P
45	L	702	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
45	L	704	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P
45	o	202	3PE	C12-C11-O13-P
46	A	202	PC1	C12-C11-O13-P
46	H	403	PC1	C12-C11-O13-P
46	L	706	PC1	C12-C11-O13-P
48	b	102	PLC	CB-C1B-C2B-C3B
46	I	205	PC1	C29-C2A-C2B-C2C
53	X	201	CDL	C81-C82-C83-C84
45	L	705	3PE	C36-C37-C38-C39
53	L	701	CDL	C64-C65-C66-C67
45	Z	201	3PE	C31-C32-C33-C34
53	X	201	CDL	CB7-C71-C72-C73
45	Y	202	3PE	O21-C21-C22-C23
53	d	201	CDL	C37-C38-C39-C40
53	h	201	CDL	C36-C37-C38-C39
45	L	703	3PE	O11-C1-C2-O21
45	L	704	3PE	O11-C1-C2-O21
45	b	101	3PE	O11-C1-C2-O21
48	L	707	PLC	O3P-C1-C2-O2
53	J	201	CDL	OB5-CB3-CB4-OB6
53	d	201	CDL	OA5-CA3-CA4-OA6
45	Y	202	3PE	C29-C2A-C2B-C2C
45	b	101	3PE	C29-C2A-C2B-C2C
46	H	403	PC1	C3A-C3B-C3C-C3D
53	X	201	CDL	C75-C76-C77-C78
45	Y	201	3PE	C22-C21-O21-C2
45	J	202	3PE	C35-C36-C37-C38
58	T	101	EHZ	C10-C11-N1-C12
45	Z	201	3PE	C29-C2A-C2B-C2C
46	A	203	PC1	O13-C11-C12-N
46	M	604	PC1	C1-C2-C3-O31
46	M	605	PC1	O13-C11-C12-N
48	N	405	PLC	C1-C2-C3-O3
48	b	102	PLC	O4P-C4-C5-N
53	M	602	CDL	CB3-CB4-CB6-OB8
58	T	101	EHZ	C16-C17-C20-O6
45	Y	201	3PE	O22-C21-O21-C2
45	i	202	3PE	O21-C2-C3-O31
46	d	203	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
48	B	202	PLC	O2-C2-C3-O3
46	I	205	PC1	C22-C23-C24-C25
53	d	201	CDL	C1-CA2-OA2-PA1
45	Y	202	3PE	C2D-C2E-C2F-C2G
46	P	502	PC1	C37-C38-C39-C3A
45	Y	203	3PE	C26-C27-C28-C29
45	Z	201	3PE	C2E-C2F-C2G-C2H
53	M	602	CDL	C79-C80-C81-C82
46	d	203	PC1	C39-C3A-C3B-C3C
53	h	201	CDL	C17-C18-C19-C20
45	N	402	3PE	O21-C21-C22-C23
45	Z	201	3PE	C2F-C2G-C2H-C2I
46	A	202	PC1	C24-C25-C26-C27
45	Y	202	3PE	C3F-C3G-C3H-C3I
53	X	201	CDL	C54-C55-C56-C57
53	d	201	CDL	C38-C39-C40-C41
45	J	202	3PE	C22-C23-C24-C25
45	N	404	3PE	C39-C3A-C3B-C3C
53	L	701	CDL	C39-C40-C41-C42
45	Y	201	3PE	C3-C2-O21-C21
45	Y	204	3PE	C3-C2-O21-C21
45	i	202	3PE	C1-C2-O21-C21
46	A	202	PC1	C3-C2-O21-C21
53	N	401	CDL	CA6-CA4-OA6-CA5
45	Y	202	3PE	O11-C1-C2-C3
48	b	102	PLC	O3P-C1-C2-C3
53	X	201	CDL	OA5-CA3-CA4-CA6
53	J	201	CDL	CB2-C1-CA2-OA2
46	d	203	PC1	C31-C32-C33-C34
53	h	201	CDL	C76-C77-C78-C79
46	H	403	PC1	C3F-C3G-C3H-C3I
53	L	701	CDL	C73-C74-C75-C76
50	F	501	FMN	C4'-C5'-O5'-P
53	N	401	CDL	C1-CA2-OA2-PA1
53	h	201	CDL	C55-C56-C57-C58
46	H	403	PC1	O11-C1-C2-O21
53	L	701	CDL	C72-C71-CB7-OB8
46	q	202	PC1	C27-C28-C29-C2A
46	L	706	PC1	C23-C24-C25-C26
46	Y	205	PC1	C37-C38-C39-C3A
45	i	202	3PE	C39-C3A-C3B-C3C
45	Y	204	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	A	203	PC1	O21-C2-C3-O31
53	N	401	CDL	OA6-CA4-CA6-OA8
45	J	202	3PE	C1-O11-P-O13
45	L	702	3PE	C1-O11-P-O13
45	N	404	3PE	C1-O11-P-O13
45	d	202	3PE	C11-O13-P-O11
46	H	402	PC1	C1-O11-P-O13
46	d	203	PC1	C11-O13-P-O11
48	b	102	PLC	C1-O3P-P-O4P
53	J	201	CDL	CA3-OA5-PA1-OA2
53	d	201	CDL	CB2-OB2-PB2-OB5
45	b	101	3PE	C24-C25-C26-C27
55	O	401	DGT	O4'-C4'-C5'-O5'
45	N	403	3PE	C2A-C2B-C2C-C2D
53	X	201	CDL	C34-C35-C36-C37
45	o	202	3PE	C1-C2-C3-O31
46	M	605	PC1	C1-C2-C3-O31
45	K	101	3PE	C29-C2A-C2B-C2C
46	H	403	PC1	C39-C3A-C3B-C3C
48	b	102	PLC	C3B-C4B-C5B-C6B
45	I	203	3PE	O31-C31-C32-C33
48	L	707	PLC	C2B-C1B-CB-O3
46	H	402	PC1	C22-C21-O21-C2
46	M	604	PC1	C11-C12-N-C13
55	O	401	DGT	PA-O3A-PB-O1B
45	m	201	3PE	C34-C35-C36-C37
45	M	603	3PE	C2-C1-O11-P
46	h	202	PC1	C2-C1-O11-P
53	J	201	CDL	CA4-CA3-OA5-PA1
46	H	402	PC1	O22-C21-O21-C2
46	d	203	PC1	C32-C33-C34-C35
45	M	603	3PE	C3D-C3E-C3F-C3G
45	g	201	3PE	O13-C11-C12-N
45	N	404	3PE	C35-C36-C37-C38
45	L	705	3PE	C22-C23-C24-C25
58	T	101	EHZ	O4-C15-C16-C17
45	L	704	3PE	C26-C27-C28-C29
46	d	203	PC1	C3B-C3C-C3D-C3E
45	I	203	3PE	O32-C31-C32-C33
46	P	502	PC1	C32-C33-C34-C35
45	A	201	3PE	C35-C36-C37-C38
45	L	703	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
46	H	403	PC1	C3E-C3F-C3G-C3H
46	Y	205	PC1	C38-C39-C3A-C3B
48	L	707	PLC	C'-C1'-C2'-C3'
46	M	604	PC1	C26-C27-C28-C29
45	b	101	3PE	C1-C2-C3-O31
45	d	202	3PE	C1-C2-C3-O31
46	I	204	PC1	C25-C26-C27-C28
45	K	101	3PE	O21-C21-C22-C23
53	h	201	CDL	C32-C33-C34-C35
45	L	705	3PE	C34-C35-C36-C37
45	L	705	3PE	C3-C2-O21-C21
46	Y	205	PC1	C1-C2-O21-C21
46	Y	205	PC1	C3-C2-O21-C21
48	L	707	PLC	C1-C2-O2-C'
48	b	102	PLC	C1-C2-O2-C'
53	X	201	CDL	CA3-CA4-OA6-CA5
53	h	201	CDL	C73-C74-C75-C76
46	M	604	PC1	C11-C12-N-C14
46	A	203	PC1	C21-C22-C23-C24
53	h	201	CDL	C54-C55-C56-C57
45	b	101	3PE	C1-O11-P-O13
46	A	202	PC1	C22-C23-C24-C25
58	U	101	EHZ	C2-C3-C4-C5
45	N	402	3PE	C3C-C3D-C3E-C3F
45	Y	202	3PE	C31-C32-C33-C34
45	N	402	3PE	O11-C1-C2-O21
46	q	202	PC1	C3A-C3B-C3C-C3D
48	L	707	PLC	C2B-C1B-CB-OB
45	m	202	3PE	C36-C37-C38-C39
53	L	701	CDL	C74-C75-C76-C77
53	J	201	CDL	OB5-CB3-CB4-CB6
45	L	704	3PE	C34-C35-C36-C37
53	M	602	CDL	C76-C77-C78-C79
45	L	705	3PE	C33-C34-C35-C36
53	h	201	CDL	C52-C53-C54-C55
45	M	603	3PE	C27-C28-C29-C2A
58	T	101	EHZ	C11-C10-S1-C9
46	L	706	PC1	O21-C2-C3-O31
53	N	401	CDL	C57-C58-C59-C60
45	N	402	3PE	C26-C27-C28-C29
46	d	203	PC1	C33-C34-C35-C36
60	o	201	MYR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	m	202	3PE	C22-C23-C24-C25
45	i	202	3PE	O21-C21-C22-C23
45	m	201	3PE	C31-C32-C33-C34
45	J	202	3PE	C32-C33-C34-C35
45	N	403	3PE	C32-C33-C34-C35
46	q	202	PC1	C37-C38-C39-C3A
45	i	202	3PE	C33-C34-C35-C36
46	h	202	PC1	O31-C31-C32-C33
46	A	203	PC1	C1-C2-C3-O31
53	d	201	CDL	CB3-CB4-CB6-OB8
46	q	203	PC1	C23-C24-C25-C26
53	M	602	CDL	OA5-CA3-CA4-OA6
45	L	705	3PE	C23-C24-C25-C26
46	I	205	PC1	C27-C28-C29-C2A
45	Y	204	3PE	O11-C1-C2-C3
52	H	401	U10	C12-C11-C9-C10
45	Y	202	3PE	C37-C38-C39-C3A
45	Y	203	3PE	C3F-C3G-C3H-C3I
53	M	602	CDL	C81-C82-C83-C84
45	N	403	3PE	C24-C25-C26-C27
53	N	401	CDL	C76-C77-C78-C79
45	Y	204	3PE	O31-C31-C32-C33
45	i	202	3PE	C25-C26-C27-C28
45	i	202	3PE	C28-C29-C2A-C2B
45	m	202	3PE	C34-C35-C36-C37
45	L	703	3PE	C28-C29-C2A-C2B
45	N	403	3PE	C33-C34-C35-C36
46	I	204	PC1	C3B-C3C-C3D-C3E
45	Z	201	3PE	C33-C34-C35-C36
46	M	604	PC1	O22-C21-O21-C2
55	O	401	DGT	PB-O3B-PG-O3G
58	T	101	EHZ	C18-C17-C20-O6
46	M	604	PC1	C11-C12-N-C15
46	A	202	PC1	C34-C35-C36-C37
46	q	202	PC1	C29-C2A-C2B-C2C
46	q	202	PC1	C33-C34-C35-C36
45	N	402	3PE	C23-C24-C25-C26
45	Y	202	3PE	C27-C28-C29-C2A
53	d	201	CDL	C42-C43-C44-C45
45	N	404	3PE	C32-C33-C34-C35
45	L	703	3PE	O31-C31-C32-C33
45	L	705	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	m	201	3PE	O31-C31-C32-C33
53	L	701	CDL	C57-C58-C59-C60
53	X	201	CDL	C72-C71-CB7-OB8
45	J	202	3PE	C26-C27-C28-C29
45	N	403	3PE	C23-C24-C25-C26
46	M	605	PC1	C32-C33-C34-C35
46	I	204	PC1	C2D-C2E-C2F-C2G
53	X	201	CDL	C51-C52-C53-C54
46	d	203	PC1	O11-C1-C2-O21
45	J	202	3PE	O21-C21-C22-C23
48	N	405	PLC	OB-CB-O3-C3
45	Y	203	3PE	C35-C36-C37-C38
46	A	203	PC1	O21-C21-C22-C23
46	P	502	PC1	C3A-C3B-C3C-C3D
45	Y	202	3PE	O31-C31-C32-C33
45	A	201	3PE	O11-C1-C2-C3
46	P	502	PC1	C26-C27-C28-C29
45	J	202	3PE	O31-C31-C32-C33
45	i	202	3PE	O31-C31-C32-C33
48	L	707	PLC	O2-C'-C1'-C2'
53	X	201	CDL	C32-C31-CA7-OA8
46	P	502	PC1	C33-C34-C35-C36
46	I	205	PC1	O21-C2-C3-O31
45	i	202	3PE	C3B-C3C-C3D-C3E
45	K	101	3PE	C3D-C3E-C3F-C3G
45	K	101	3PE	O31-C31-C32-C33
45	Y	201	3PE	O31-C31-C32-C33
46	H	402	PC1	O31-C31-C32-C33
46	M	604	PC1	C22-C21-O21-C2
53	X	201	CDL	C36-C37-C38-C39
53	h	201	CDL	CB4-CB3-OB5-PB2
45	M	603	3PE	C25-C26-C27-C28
53	L	701	CDL	C54-C55-C56-C57
45	N	402	3PE	C31-C32-C33-C34
53	d	201	CDL	CB7-C71-C72-C73
53	L	701	CDL	C61-C62-C63-C64
55	O	401	DGT	PB-O3A-PA-O1A
55	O	401	DGT	PB-O3A-PA-O2A
53	L	701	CDL	C32-C33-C34-C35
45	Y	202	3PE	C26-C27-C28-C29
45	L	703	3PE	O32-C31-C32-C33
45	L	705	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	Y	204	3PE	C2D-C2E-C2F-C2G
53	h	201	CDL	C75-C76-C77-C78
45	J	202	3PE	O22-C21-C22-C23
46	H	403	PC1	C35-C36-C37-C38
45	N	404	3PE	C38-C39-C3A-C3B
53	d	201	CDL	C74-C75-C76-C77
45	Y	202	3PE	O32-C31-C32-C33
53	M	602	CDL	C21-C22-C23-C24
45	A	201	3PE	C1-C2-C3-O31
53	J	201	CDL	CB3-CB4-CB6-OB8
53	d	201	CDL	C72-C71-CB7-OB8
53	X	201	CDL	C32-C31-CA7-OA9
45	L	702	3PE	C2-C1-O11-P
45	L	703	3PE	C2-C1-O11-P
45	L	704	3PE	C2-C1-O11-P
45	K	101	3PE	O32-C31-C32-C33
48	L	707	PLC	O'-C'-C1'-C2'
45	i	202	3PE	C11-O13-P-O14
45	m	202	3PE	C1-O11-P-O12
45	m	202	3PE	C11-O13-P-O14
46	P	502	PC1	C11-O13-P-O12
46	d	203	PC1	C11-O13-P-O14
48	B	202	PLC	C4-O4P-P-O2P
53	X	201	CDL	CA3-OA5-PA1-OA4
53	d	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CA3-OA5-PA1-OA3
55	O	401	DGT	C5'-O5'-PA-O2A
57	P	501	NDP	C2N-C3N-C7N-N7N
58	U	101	EHZ	C6-C7-C8-C9
46	A	203	PC1	O22-C21-C22-C23
45	Z	201	3PE	O21-C21-C22-C23
45	m	201	3PE	O32-C31-C32-C33
53	d	201	CDL	C33-C34-C35-C36
46	L	706	PC1	O31-C31-C32-C33
46	q	203	PC1	O31-C31-C32-C33
45	K	101	3PE	C37-C38-C39-C3A
45	b	101	3PE	C2E-C2F-C2G-C2H
53	h	201	CDL	C56-C57-C58-C59
45	K	101	3PE	C12-C11-O13-P
45	N	402	3PE	C12-C11-O13-P
45	m	202	3PE	C12-C11-O13-P
46	A	203	PC1	C12-C11-O13-P

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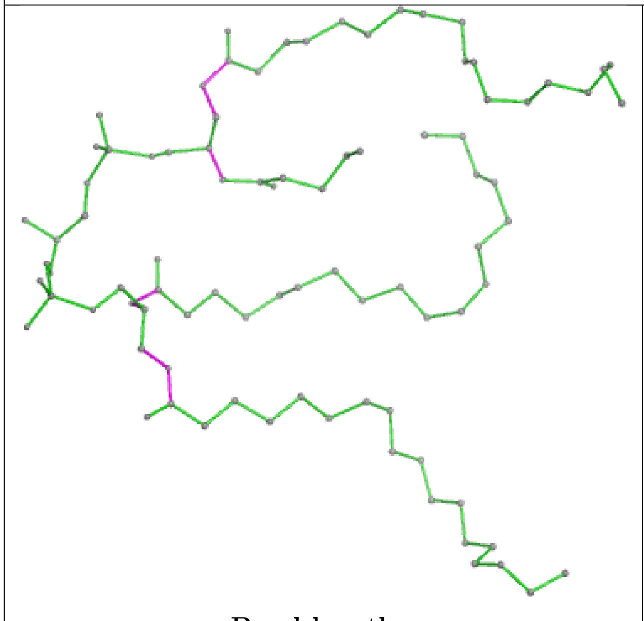
Mol	Chain	Res	Type	Atoms
48	N	405	PLC	C5-C4-O4P-P
48	g	202	PLC	C5-C4-O4P-P
53	X	201	CDL	CA6-CA4-OA6-CA5
53	X	201	CDL	C80-C81-C82-C83
53	M	602	CDL	C80-C81-C82-C83
46	q	202	PC1	C2B-C2C-C2D-C2E
46	M	604	PC1	O31-C31-C32-C33
46	q	202	PC1	O31-C31-C32-C33
53	d	201	CDL	C39-C40-C41-C42
46	M	604	PC1	C33-C34-C35-C36
53	q	201	CDL	C32-C31-CA7-OA8
45	K	101	3PE	C24-C25-C26-C27
50	F	501	FMN	N10-C1'-C2'-O2'
52	H	401	U10	C12-C11-C9-C8
45	i	202	3PE	O32-C31-C32-C33
45	N	403	3PE	O31-C31-C32-C33
46	h	202	PC1	O21-C21-C22-C23
45	J	202	3PE	O32-C31-C32-C33
45	Z	201	3PE	C25-C26-C27-C28
46	I	204	PC1	O31-C31-C32-C33
45	m	201	3PE	C22-C23-C24-C25
53	L	701	CDL	C58-C59-C60-C61
45	N	403	3PE	O32-C31-C32-C33
46	H	402	PC1	O32-C31-O31-C3
45	N	403	3PE	O21-C21-C22-C23
46	H	402	PC1	O21-C21-C22-C23
45	Y	201	3PE	C24-C25-C26-C27
45	Y	201	3PE	O32-C31-C32-C33
46	H	402	PC1	O32-C31-C32-C33
53	d	201	CDL	C72-C71-CB7-OB9
53	h	201	CDL	C11-C12-C13-C14
46	H	402	PC1	C32-C31-O31-C3
46	I	204	PC1	O32-C31-C32-C33
46	M	604	PC1	C29-C2A-C2B-C2C
45	L	704	3PE	O31-C31-C32-C33

There are no ring outliers.

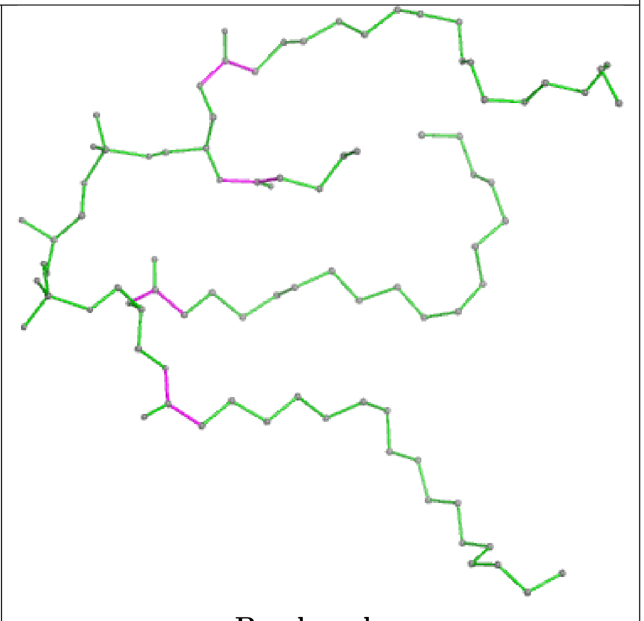
No monomer is involved in short contacts.

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

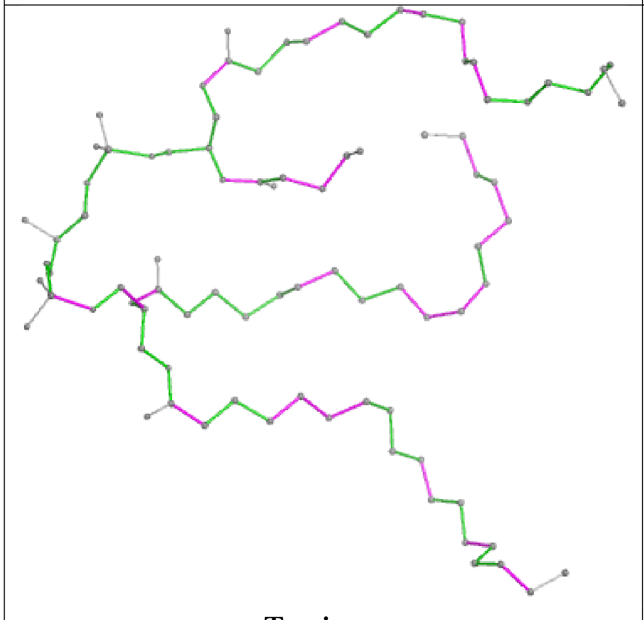
Ligand CDL L 701



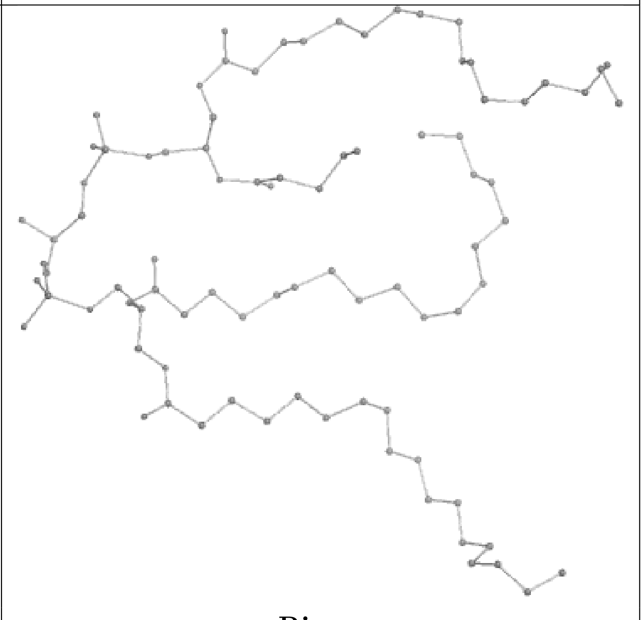
Bond lengths



Bond angles

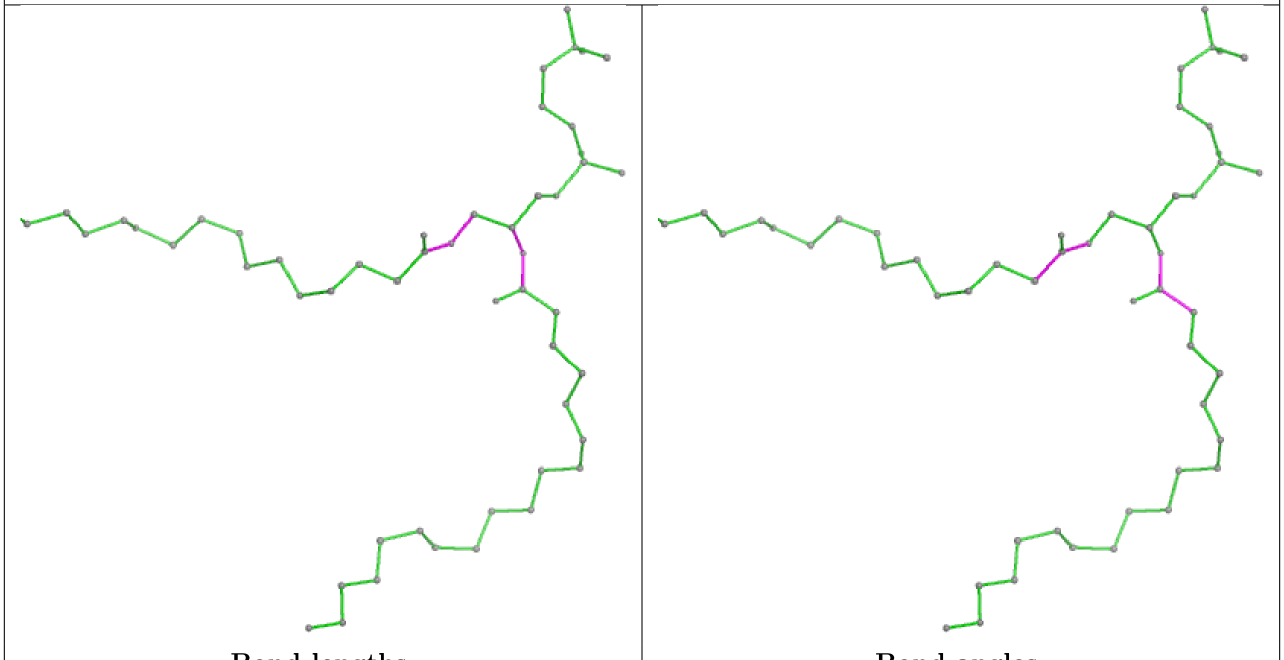


Torsions



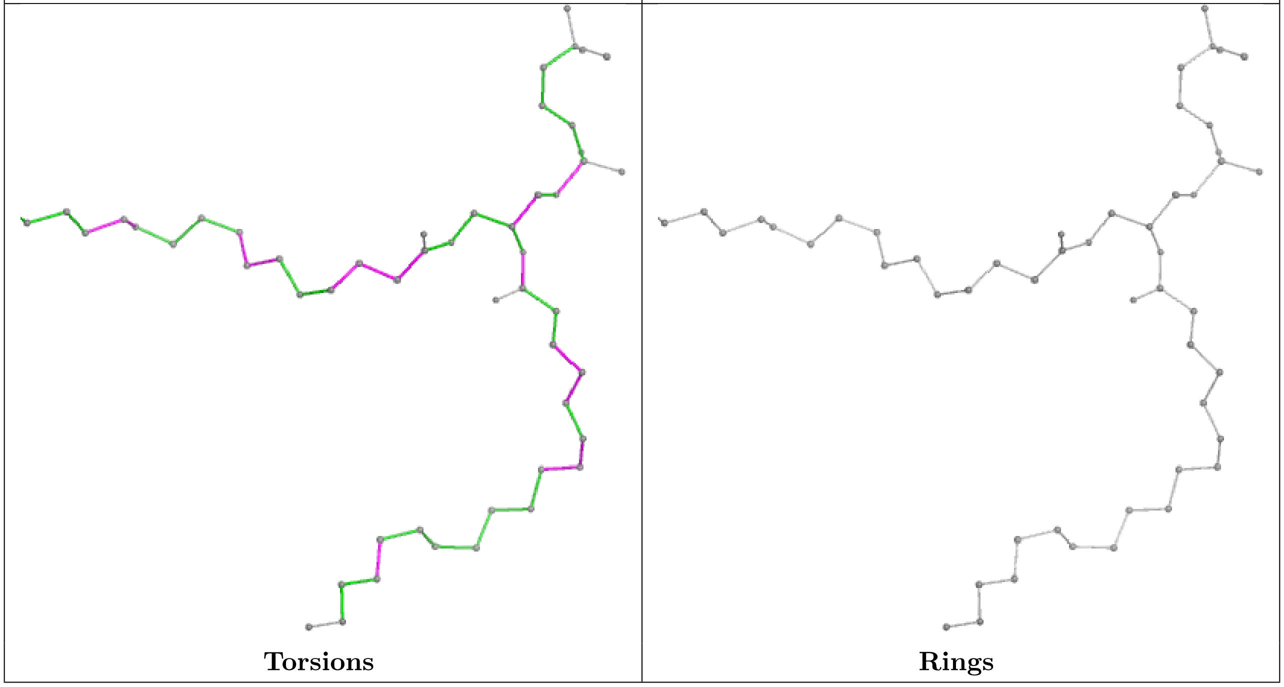
Rings

Ligand PC1 I 204



Bond lengths

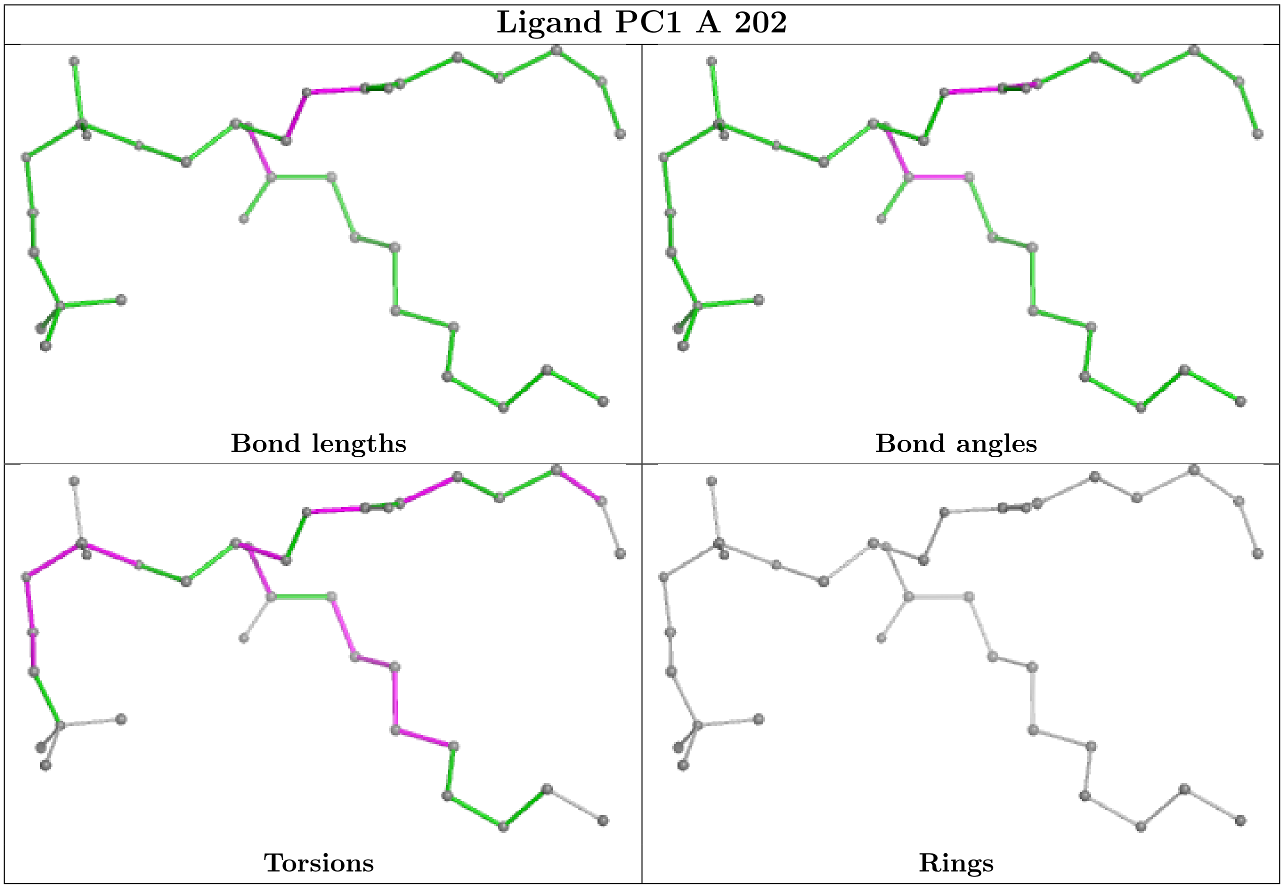
Bond angles



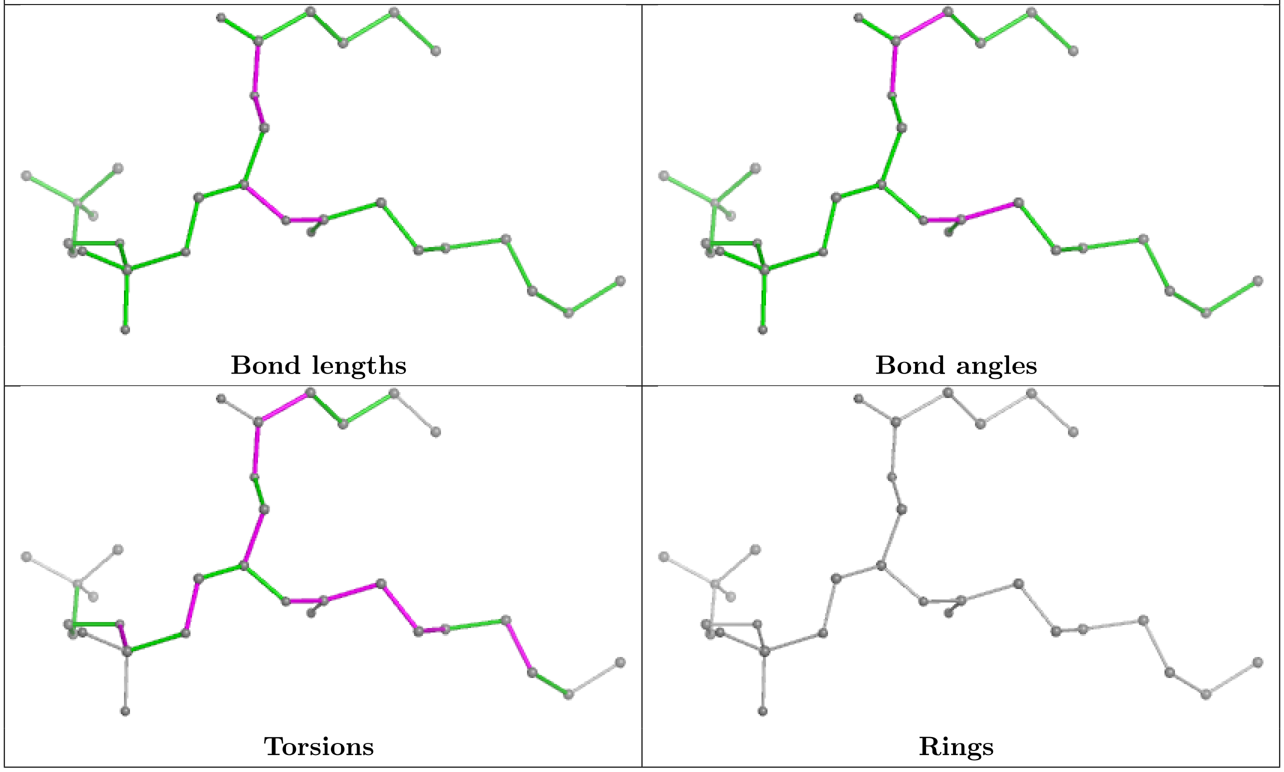
Torsions

Rings

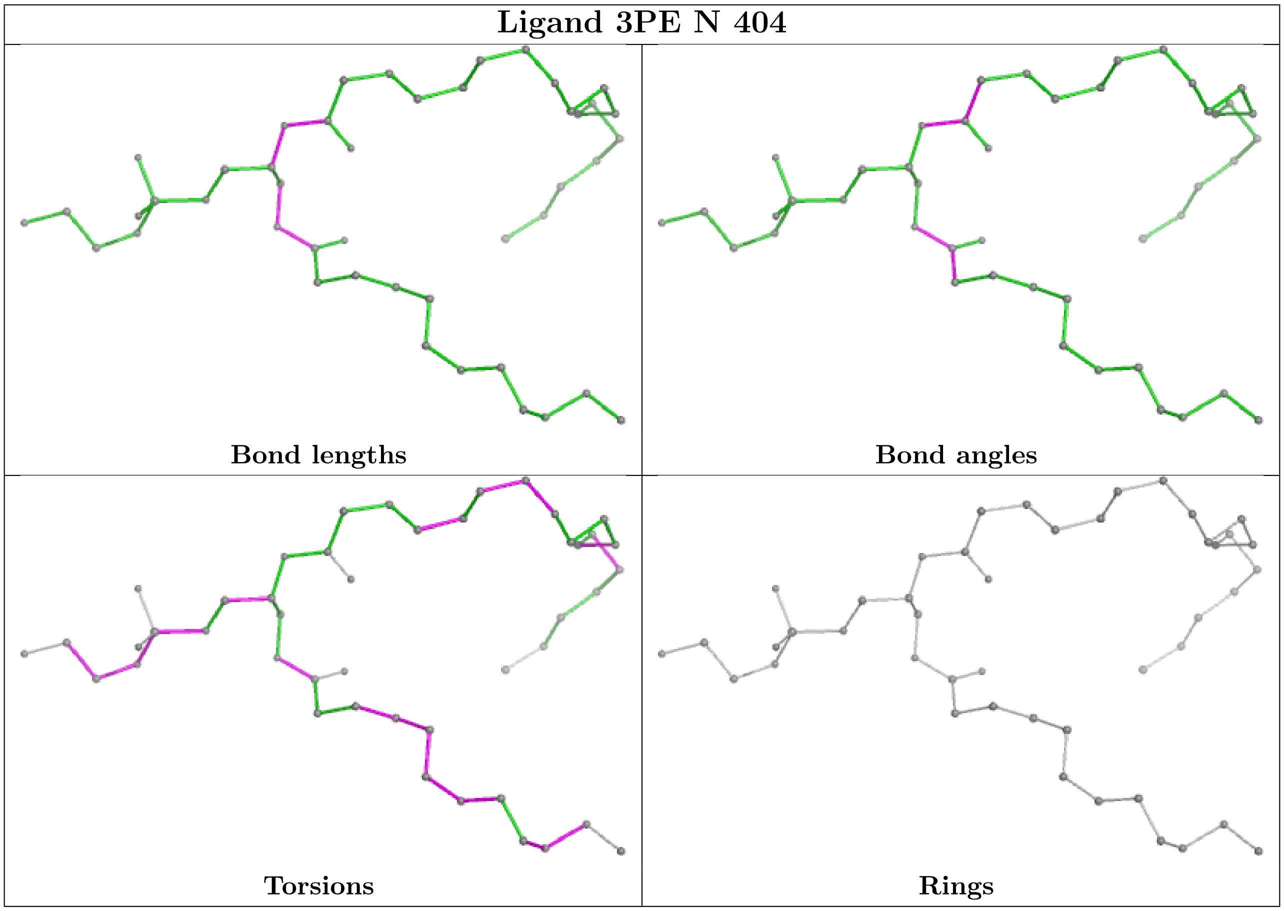
Ligand PC1 A 202



Ligand PC1 h 202



Ligand 3PE N 404



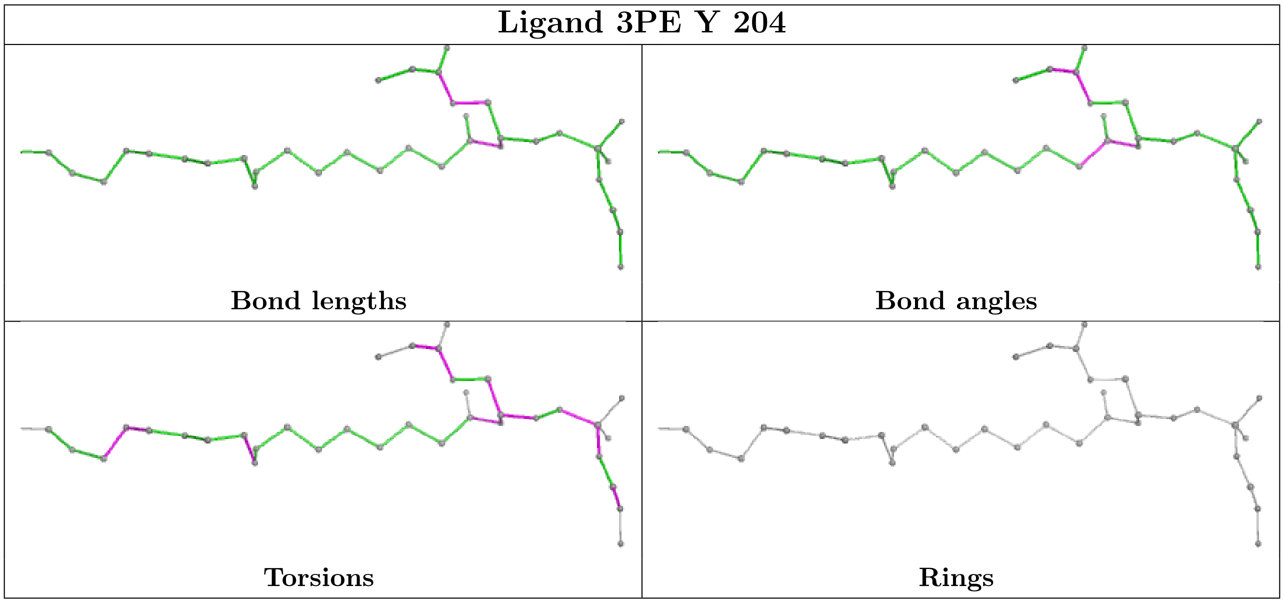
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Y 204



Bond lengths

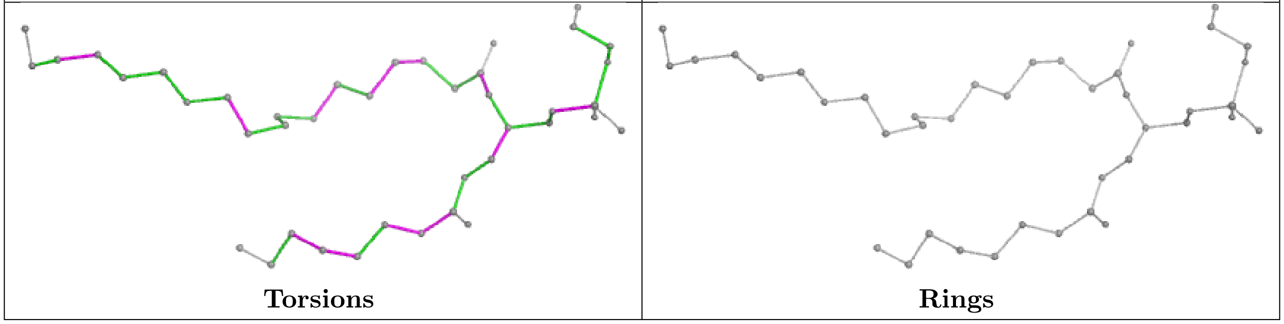
Bond angles

Torsions

Rings

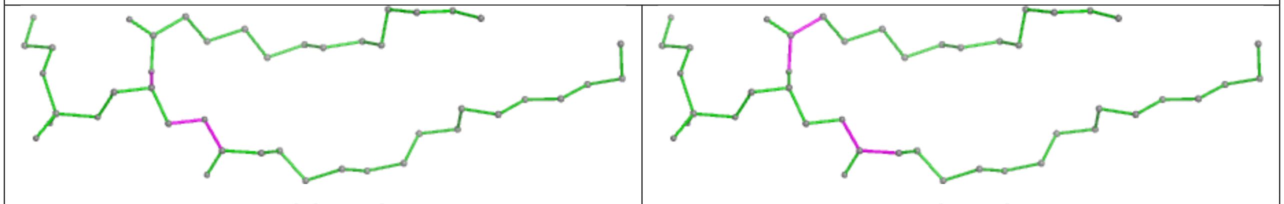
Ligand 3PE m 201

Bond lengths **Bond angles**

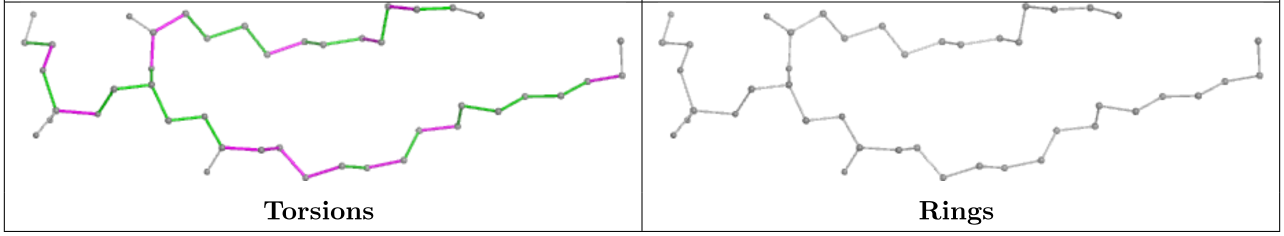


Torsions **Rings**

Ligand 3PE K 101

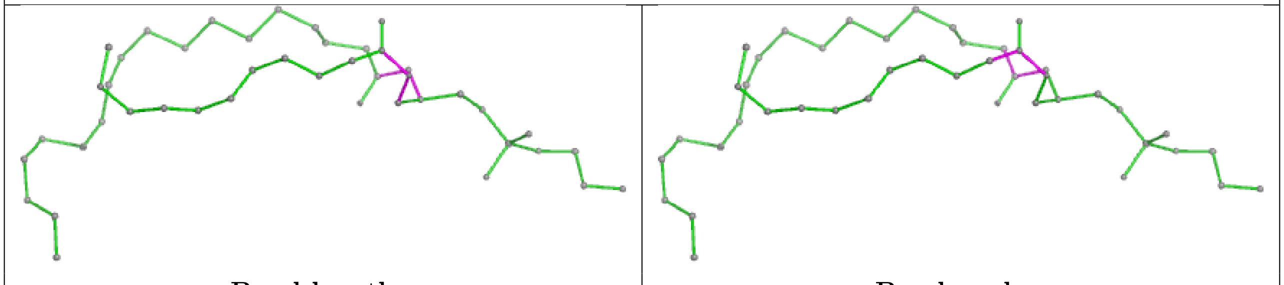


Bond lengths **Bond angles**

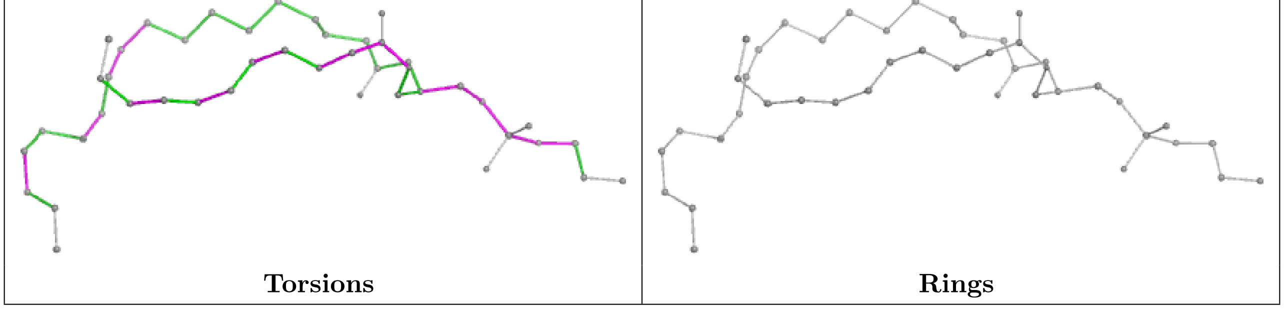


Torsions **Rings**

Ligand 3PE L 703

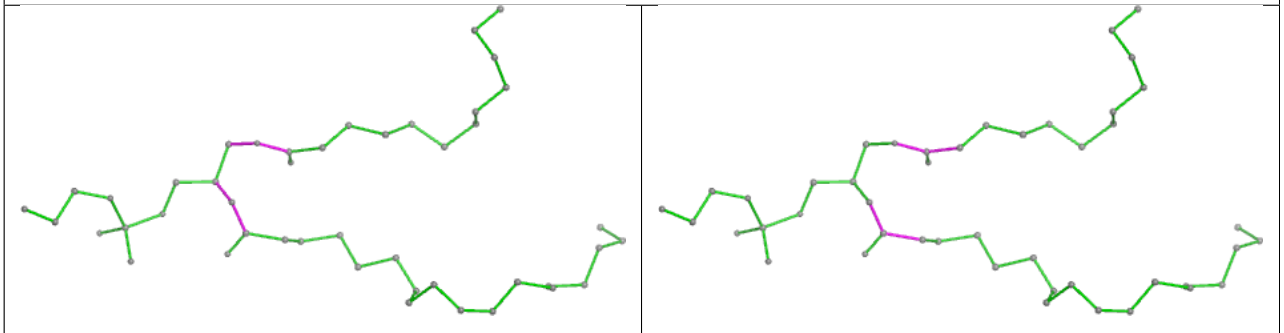


Bond lengths **Bond angles**

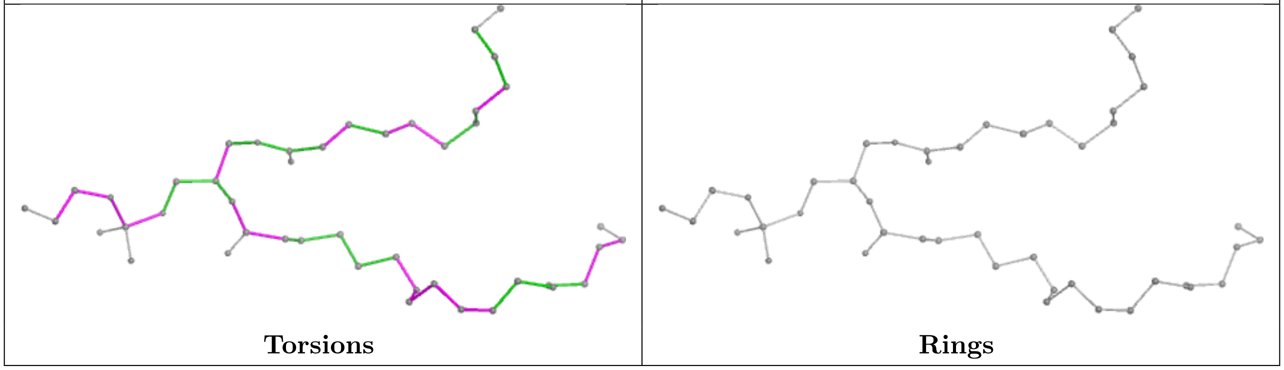


Torsions **Rings**

Ligand 3PE Z 201

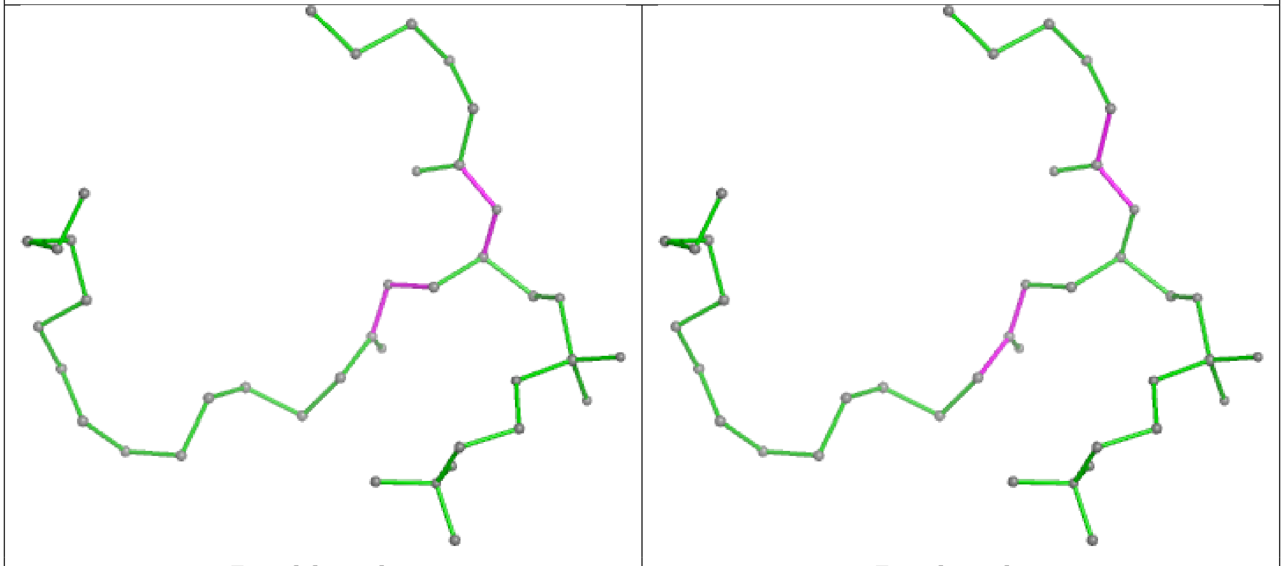


Bond lengths **Bond angles**



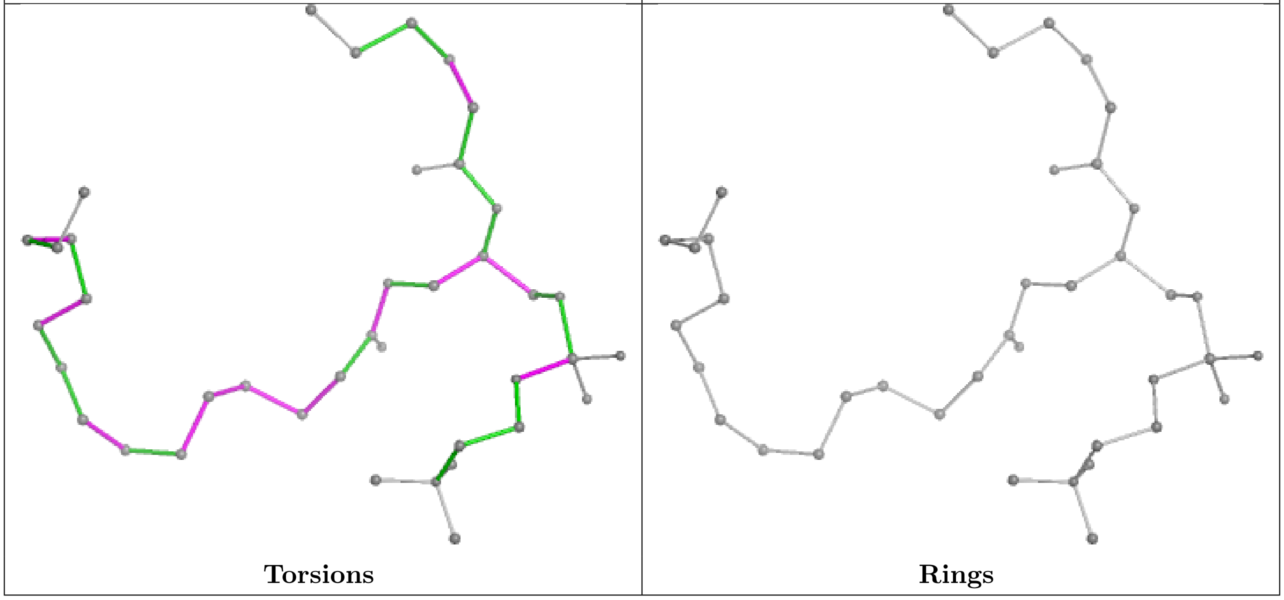
Torsions **Rings**

Ligand PC1 d 203



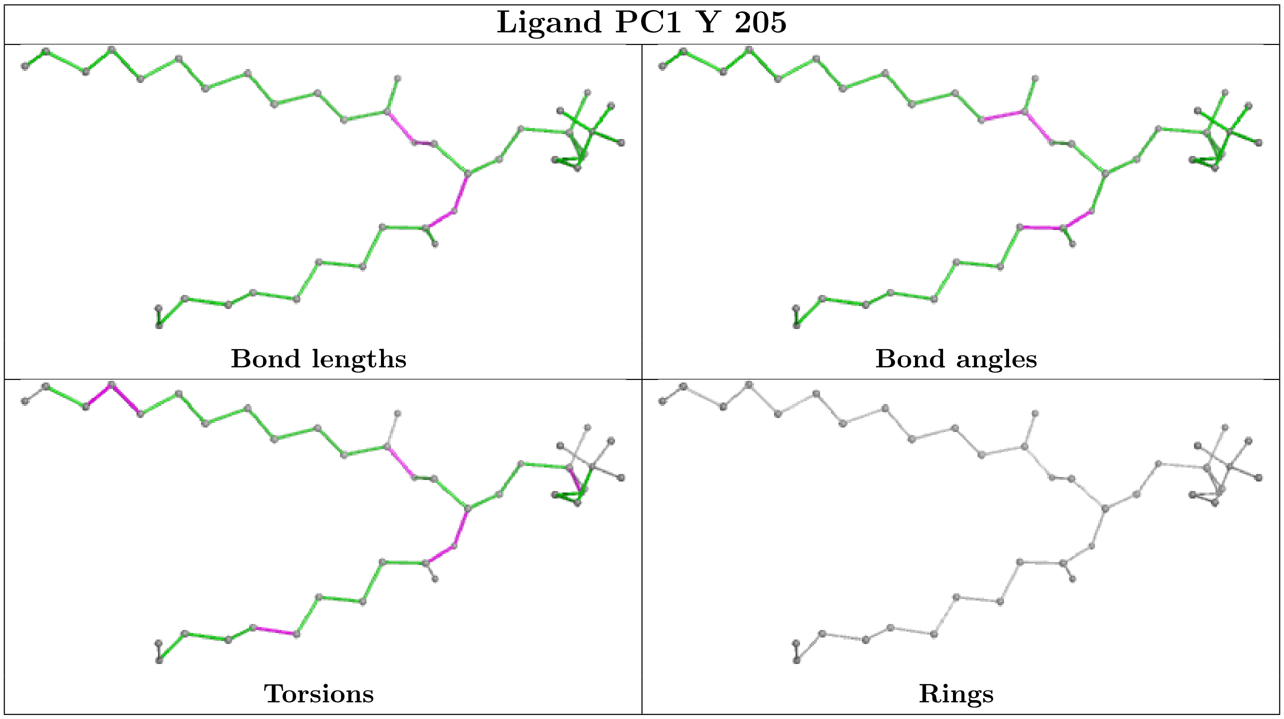
Bond lengths

Bond angles



Torsions

Rings



Ligand PC1 Y 205

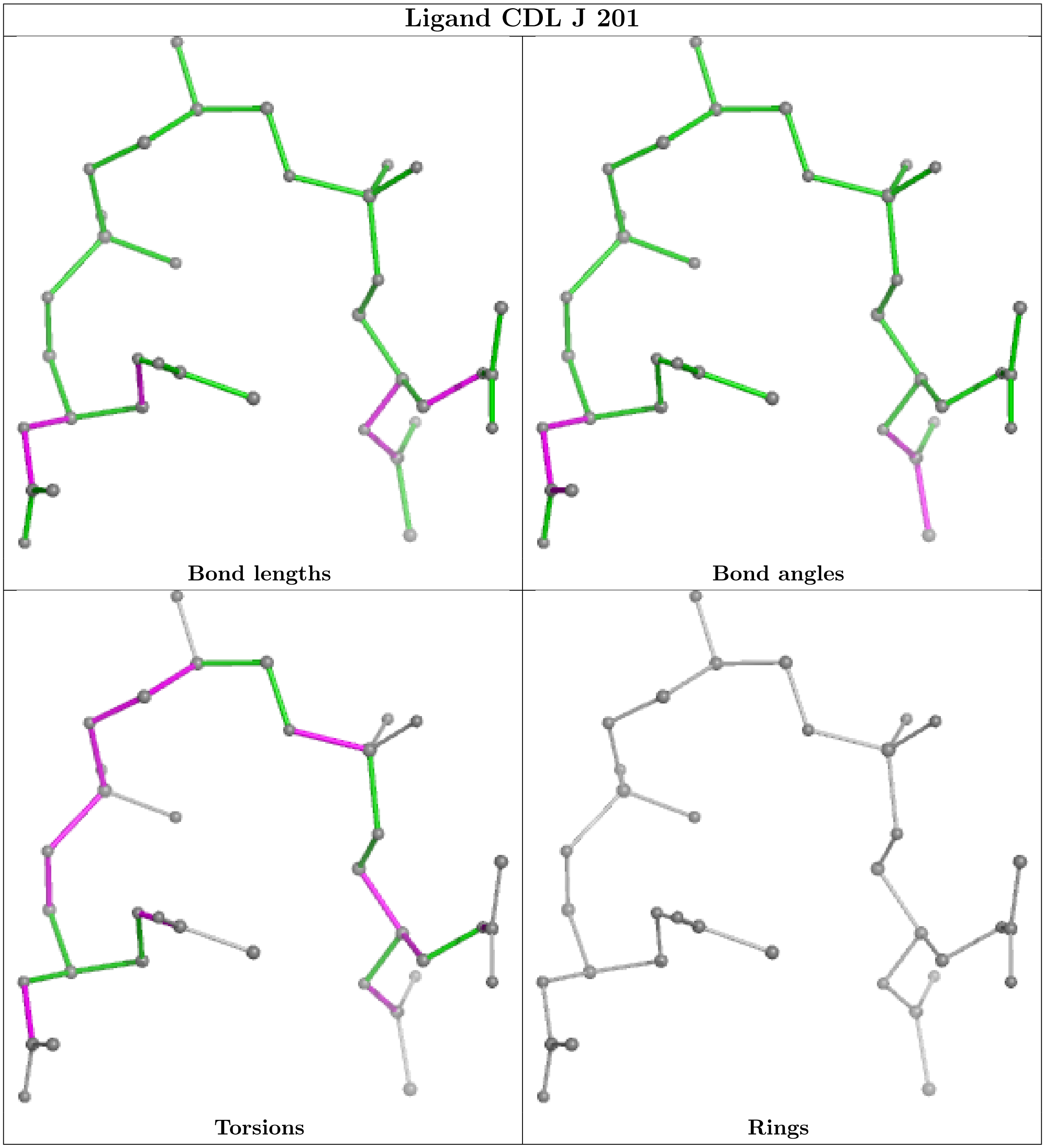
Bond lengths

Bond angles

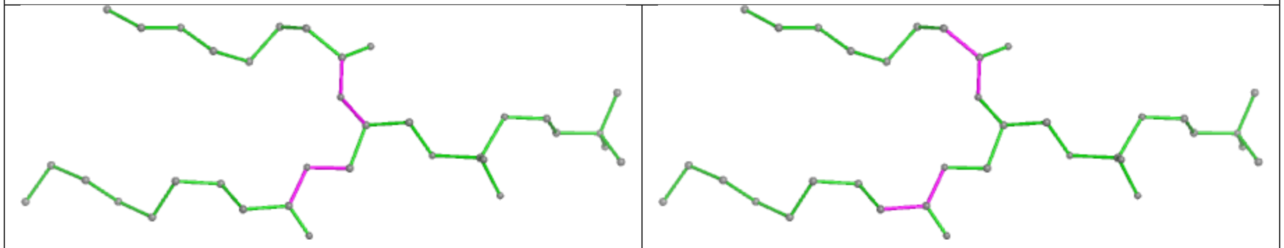
Torsions

Rings

Ligand CDL J 201

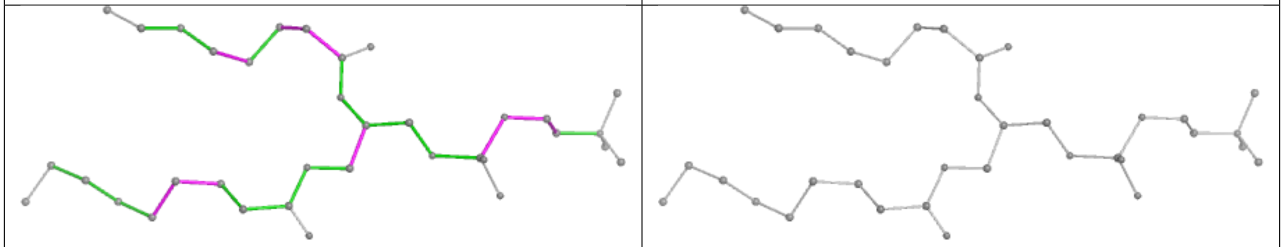


Ligand PC1 A 203



Bond lengths

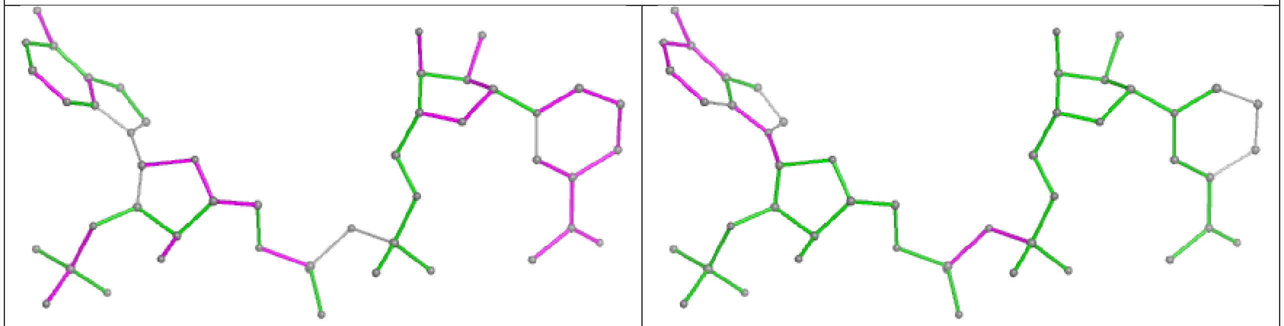
Bond angles



Torsions

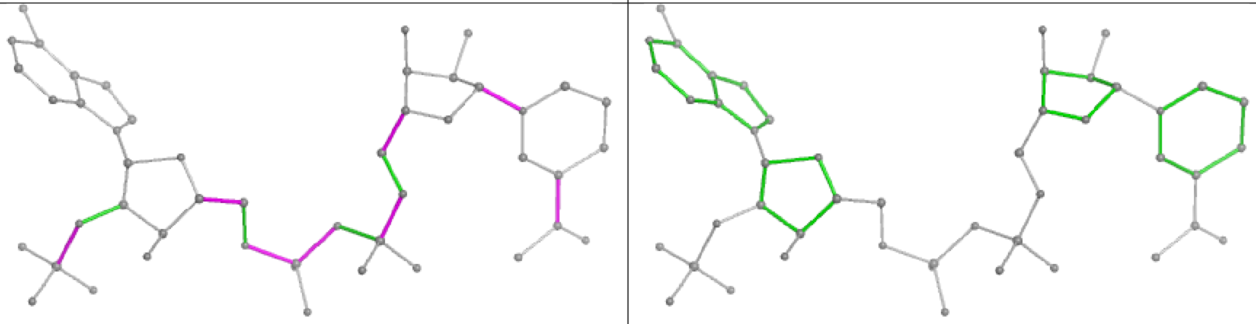
Rings

Ligand NDP P 501



Bond lengths

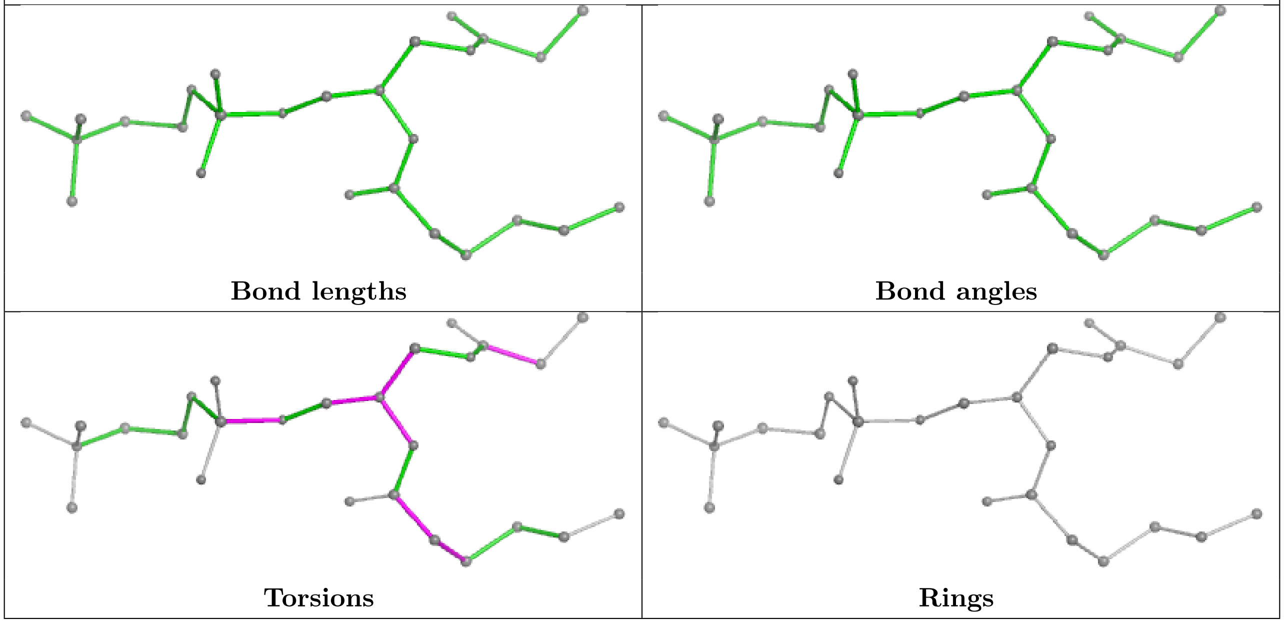
Bond angles



Torsions

Rings

Ligand PLC L 707



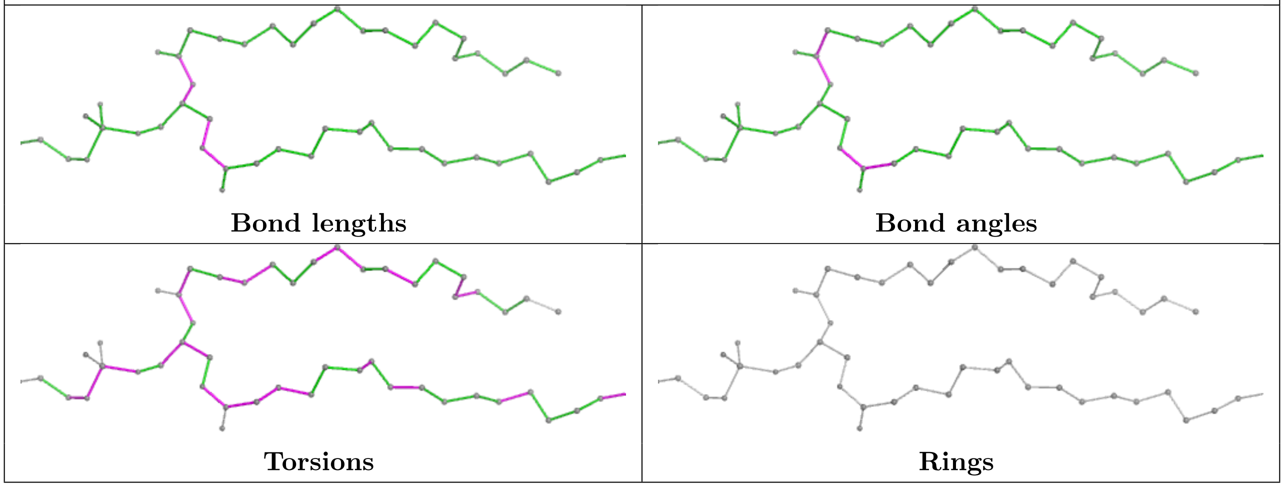
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Y 202



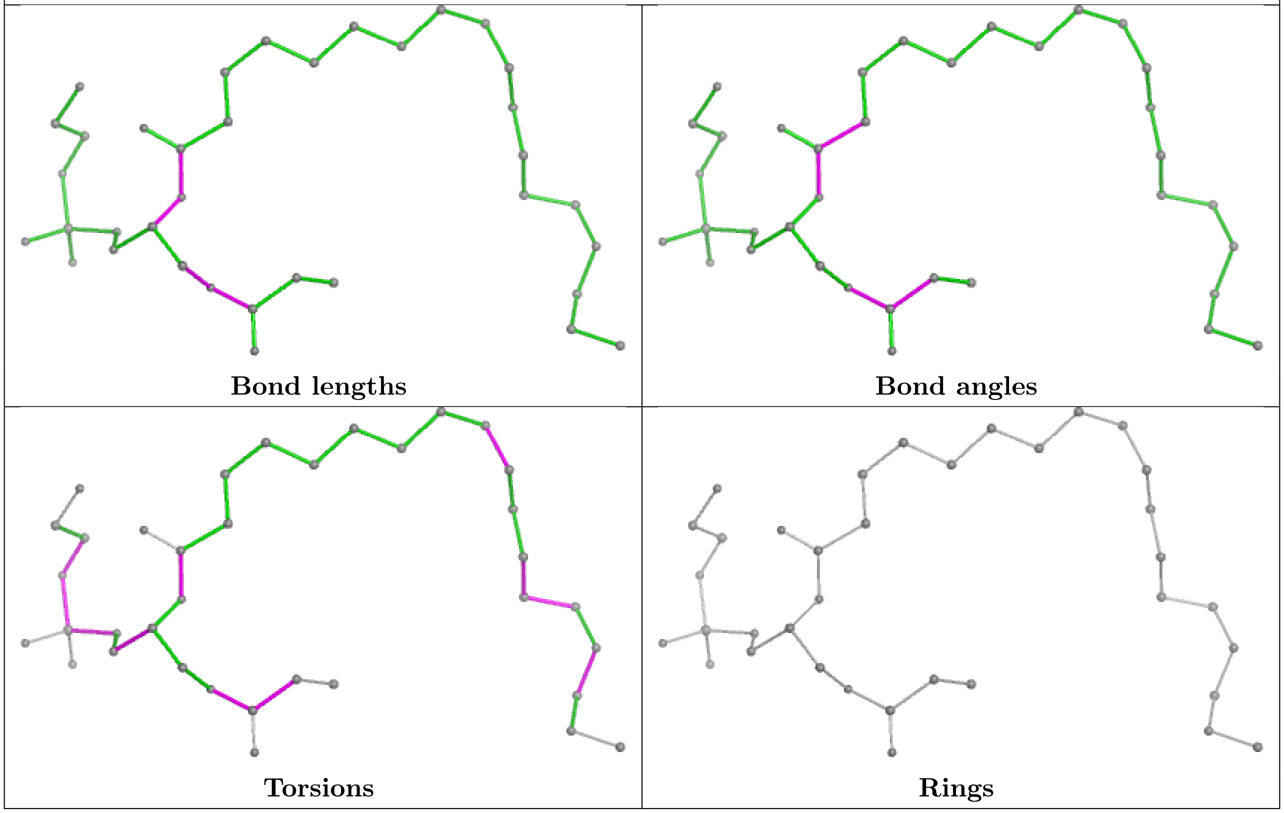
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE I 203



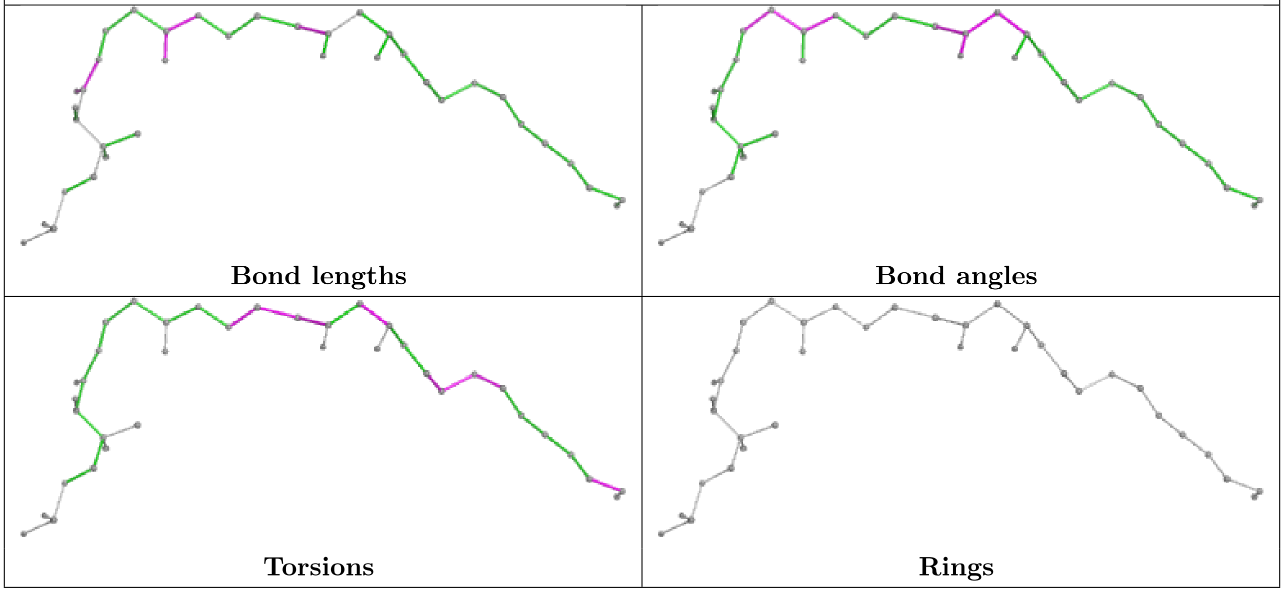
Bond lengths

Bond angles

Torsions

Rings

Ligand EHZ U 101



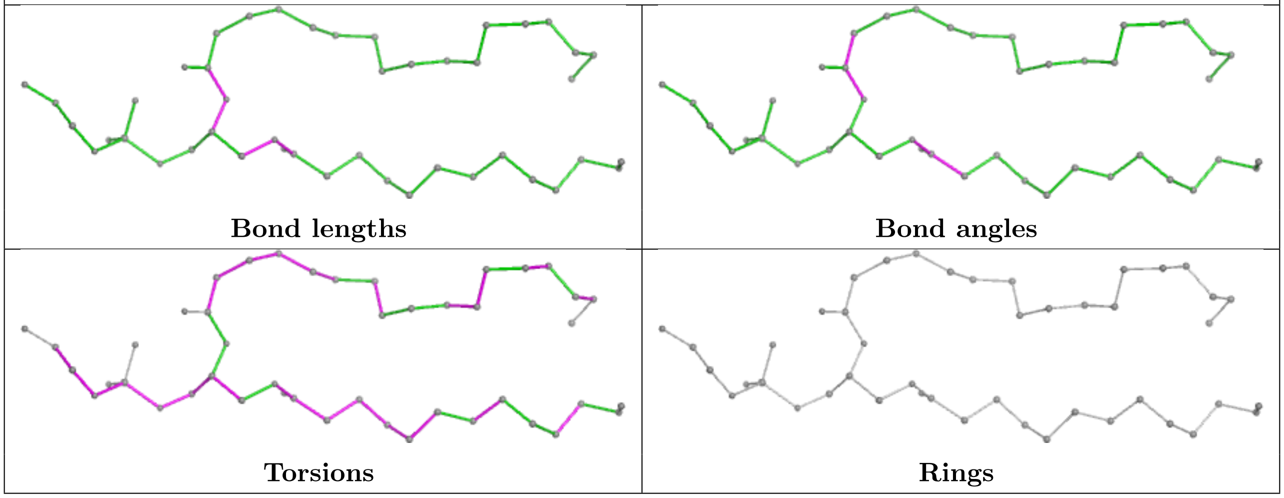
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE N 403


Bond lengths
Bond angles
Torsions
Rings

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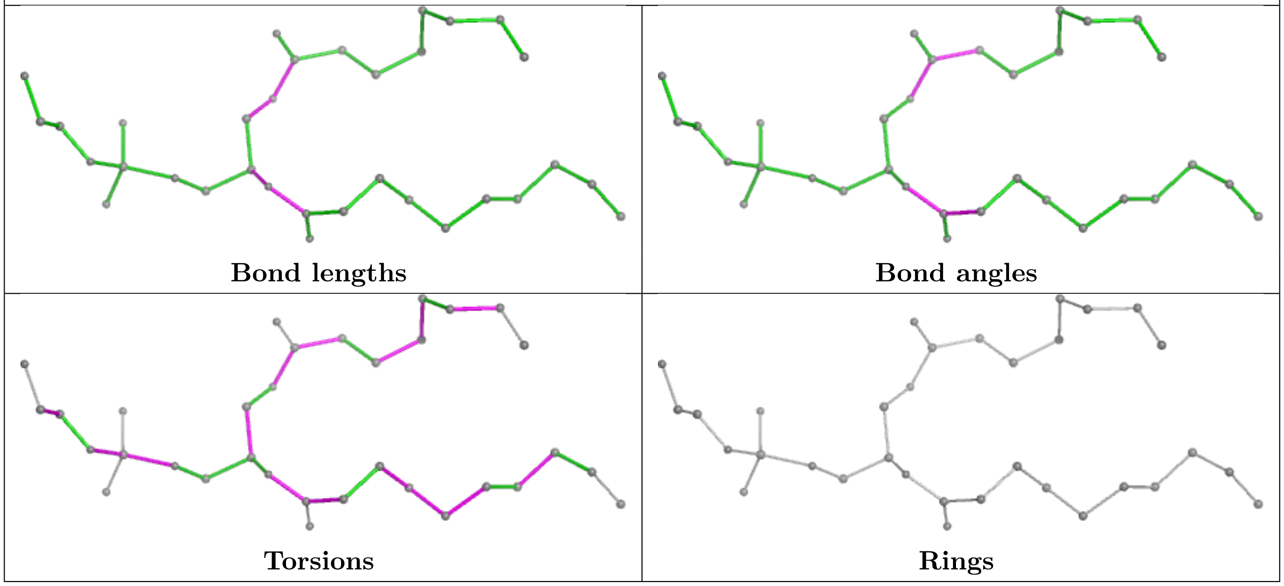
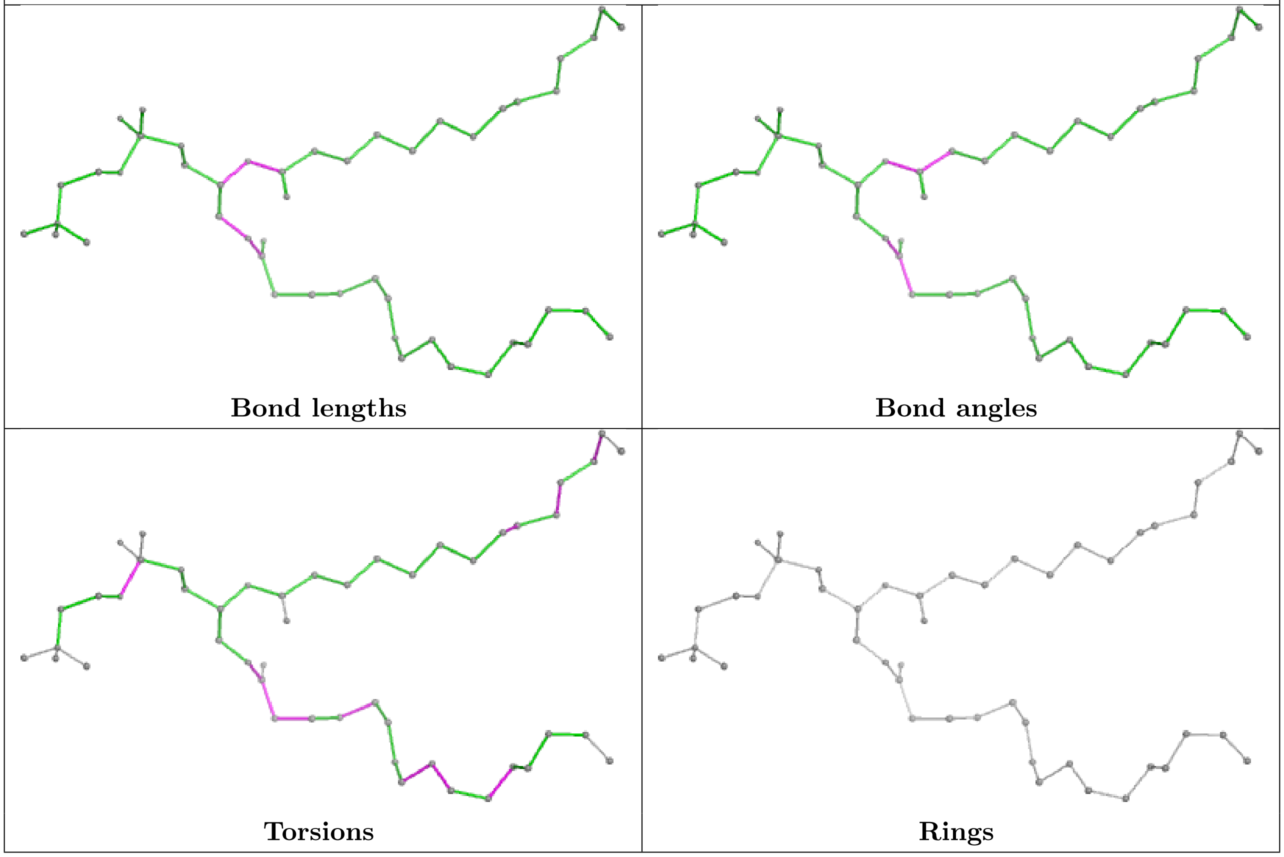

Bond lengths
Bond angles
Torsions
Rings

Ligand PC1 q 202



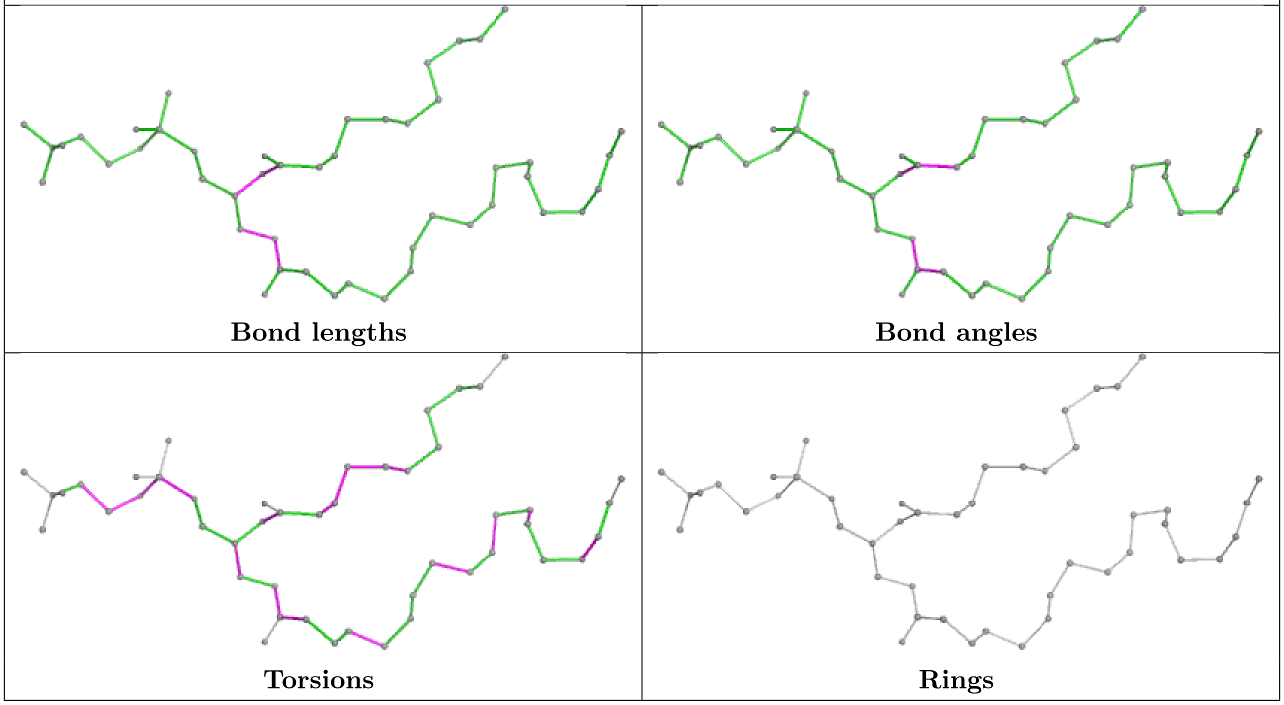
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 L 706



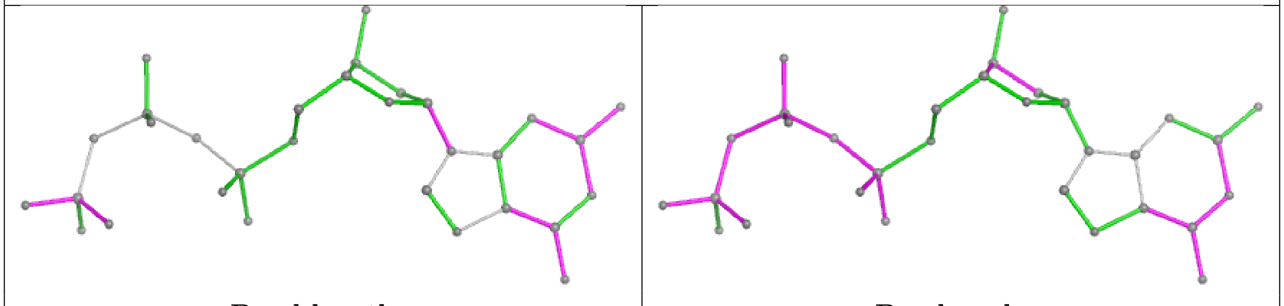
Bond lengths

Bond angles

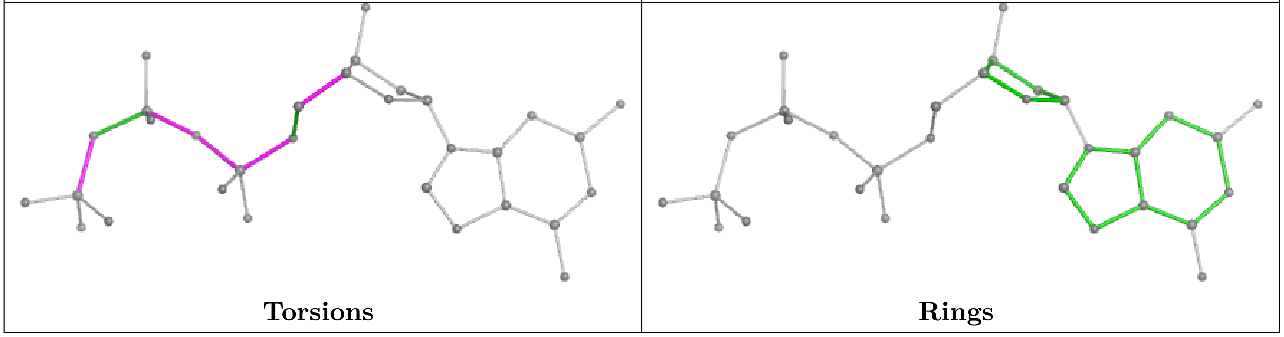
Torsions

Rings

Ligand DGT O 401

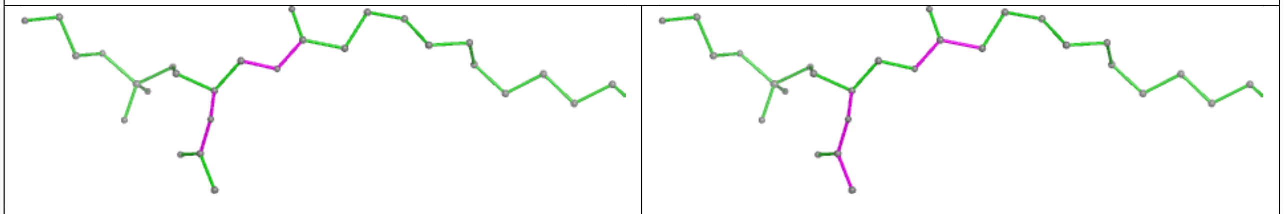


Bond lengths Bond angles

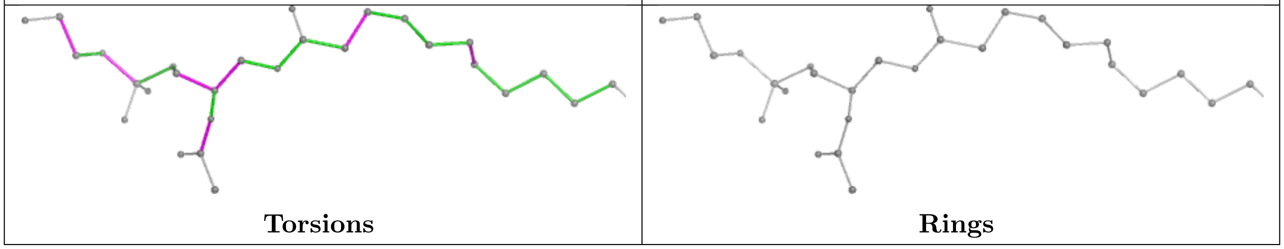


Torsions Rings

Ligand 3PE g 201

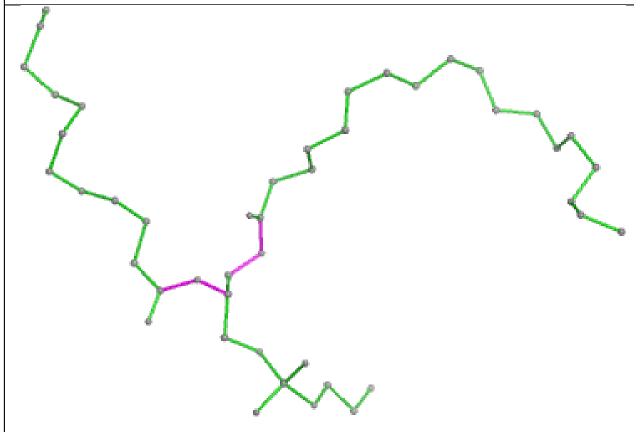


Bond lengths Bond angles

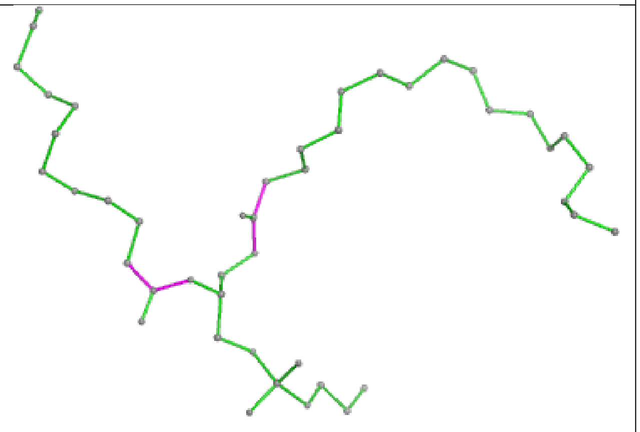


Torsions Rings

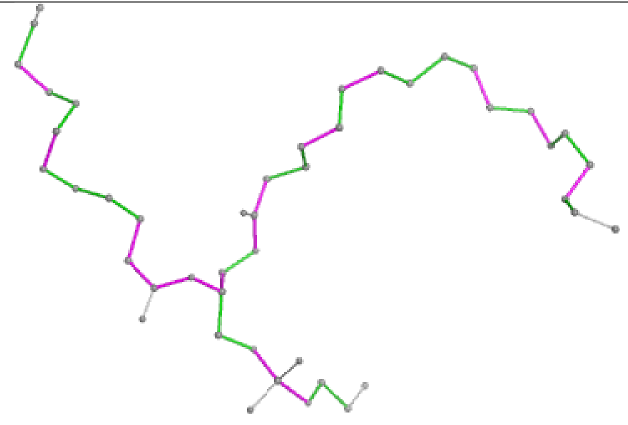
Ligand 3PE i 202



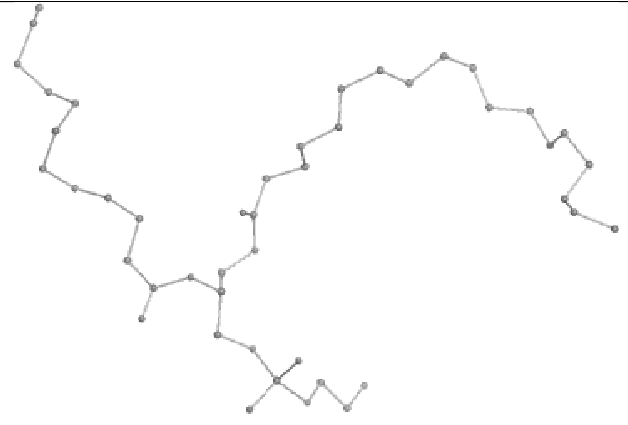
Bond lengths



Bond angles

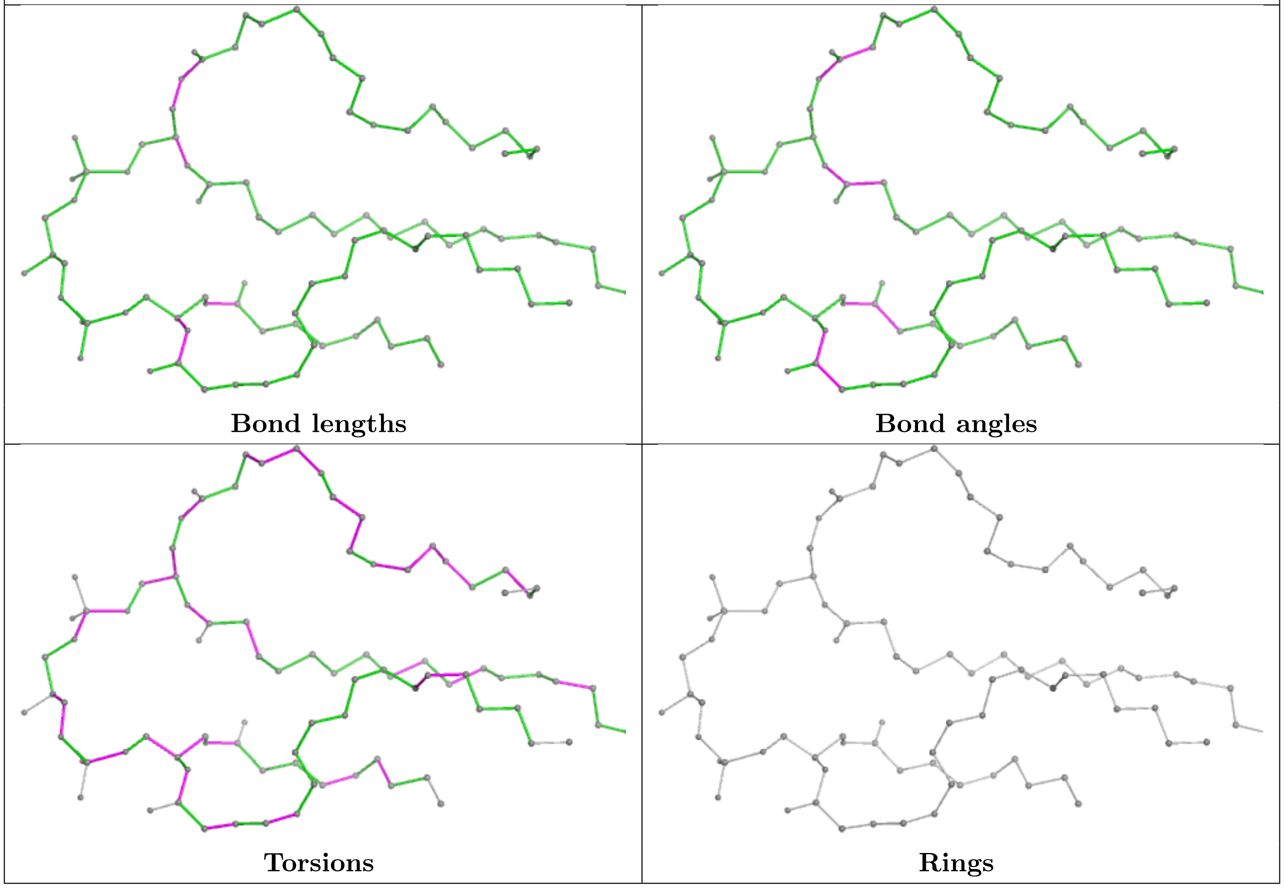


Torsions



Rings

Ligand CDL M 602



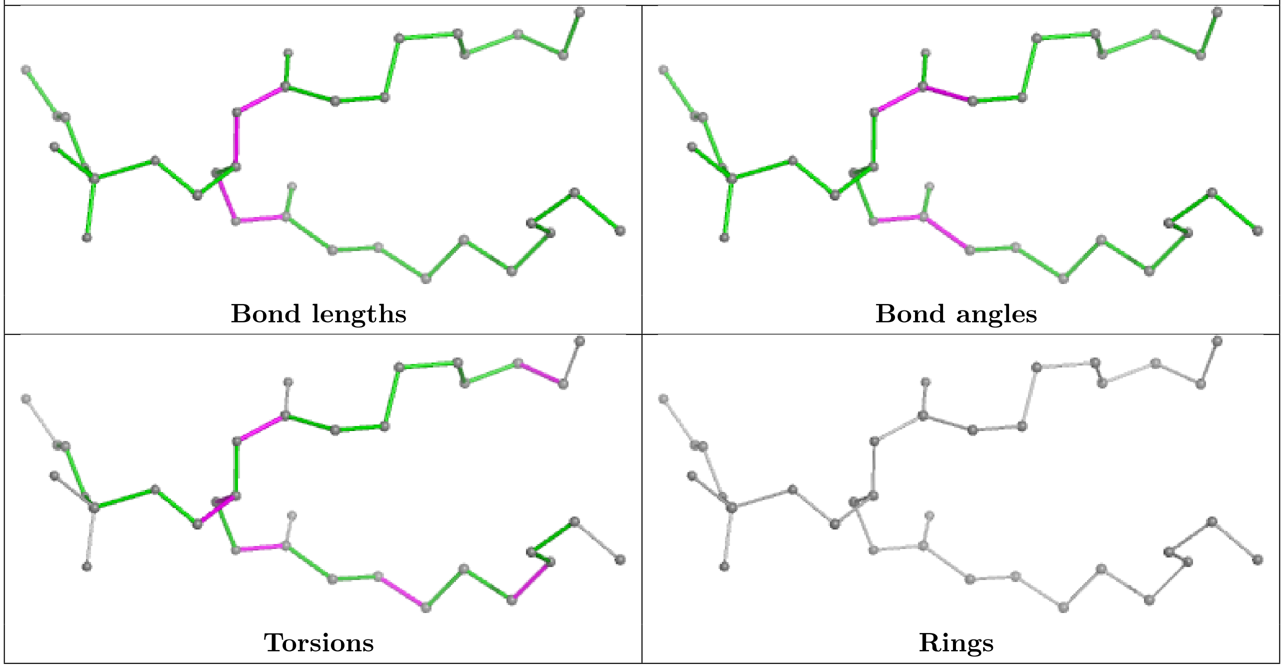
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE A 201



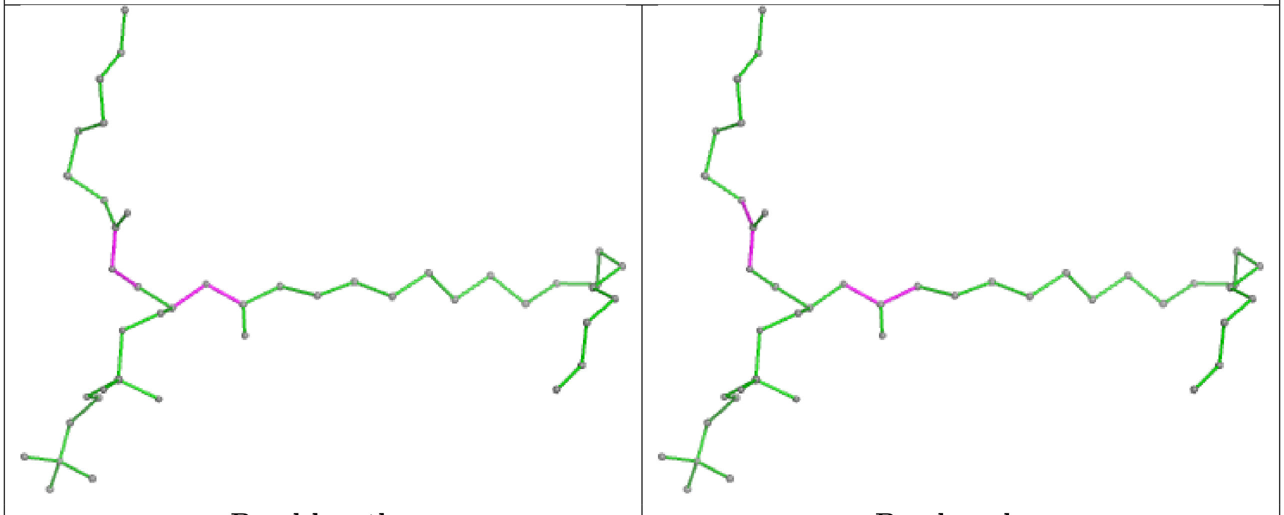
Bond lengths

Bond angles

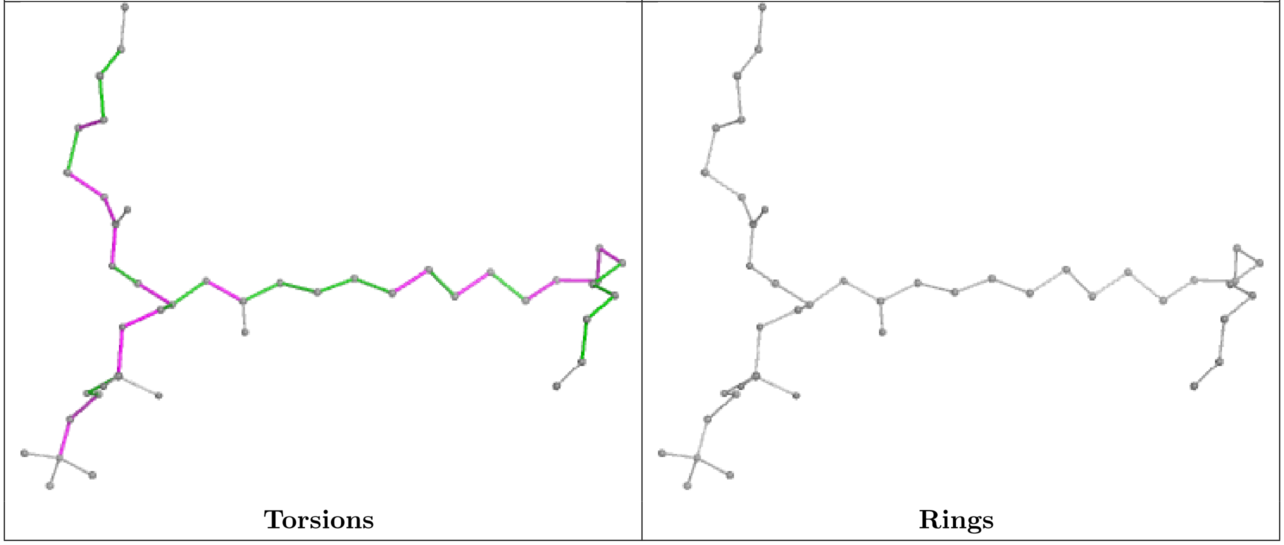
Torsions

Rings

Ligand PC1 M 604

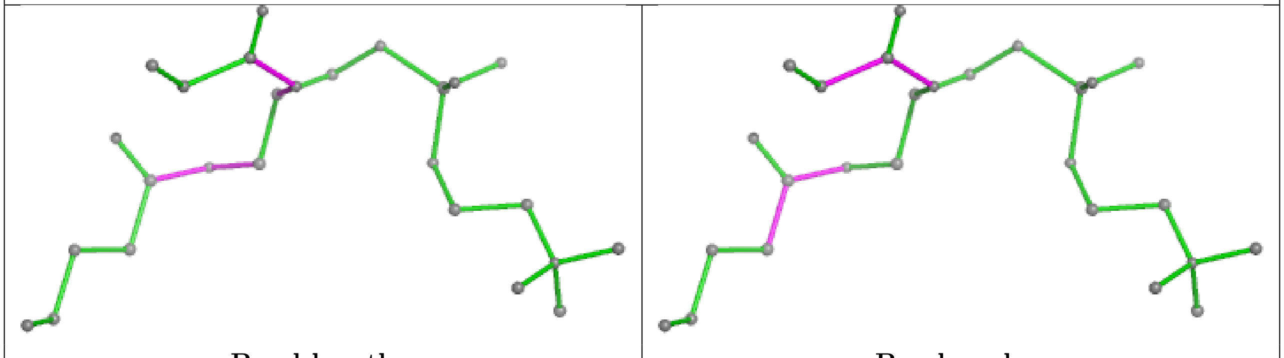


Bond lengths **Bond angles**



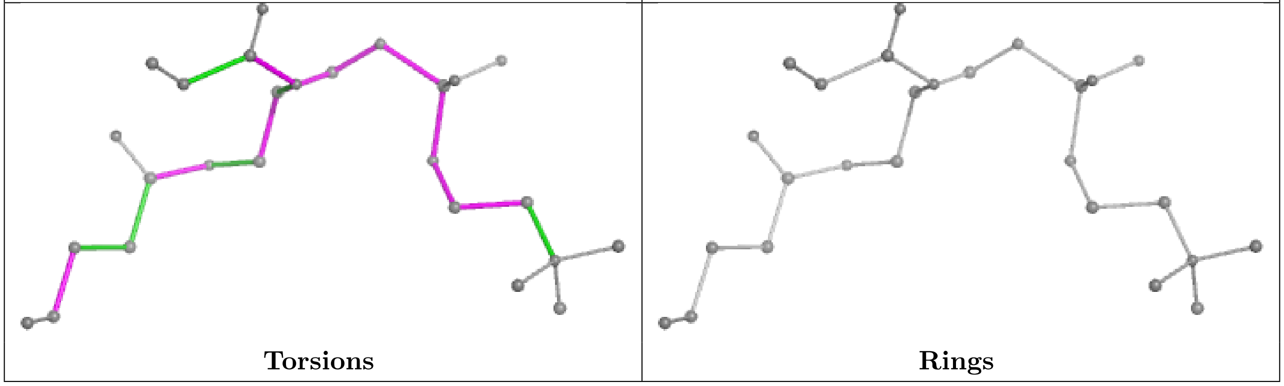
Torsions **Rings**

Ligand PC1 M 605



Bond lengths

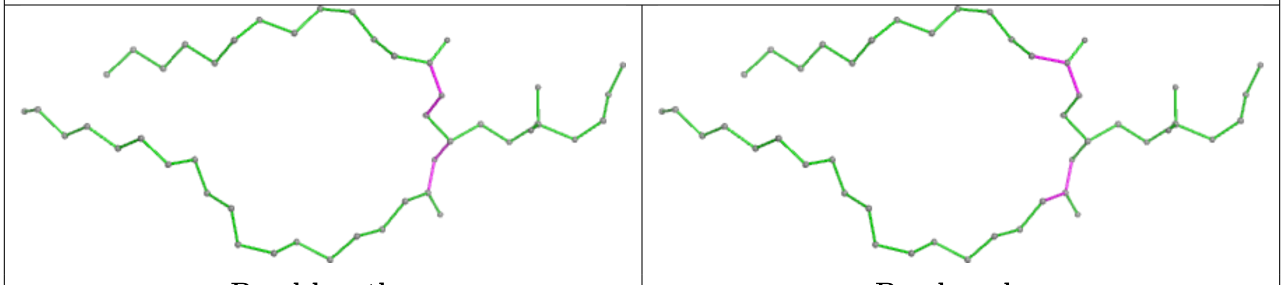
Bond angles



Torsions

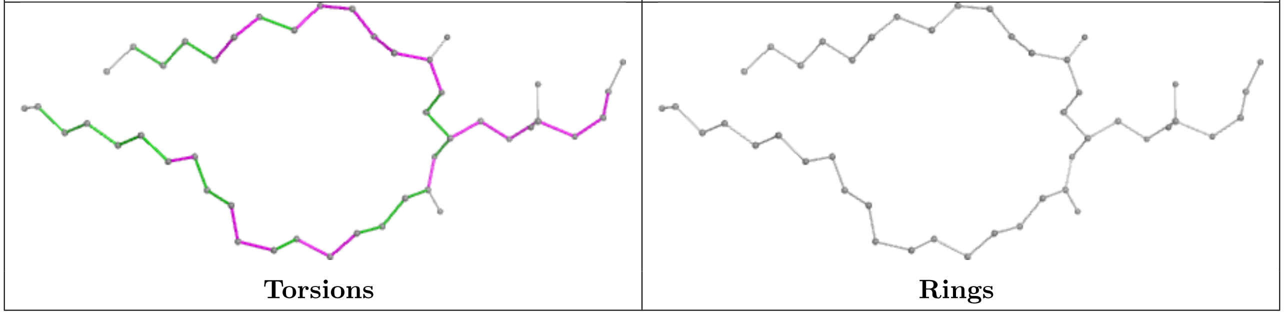
Rings

Ligand 3PE L 704



Bond lengths

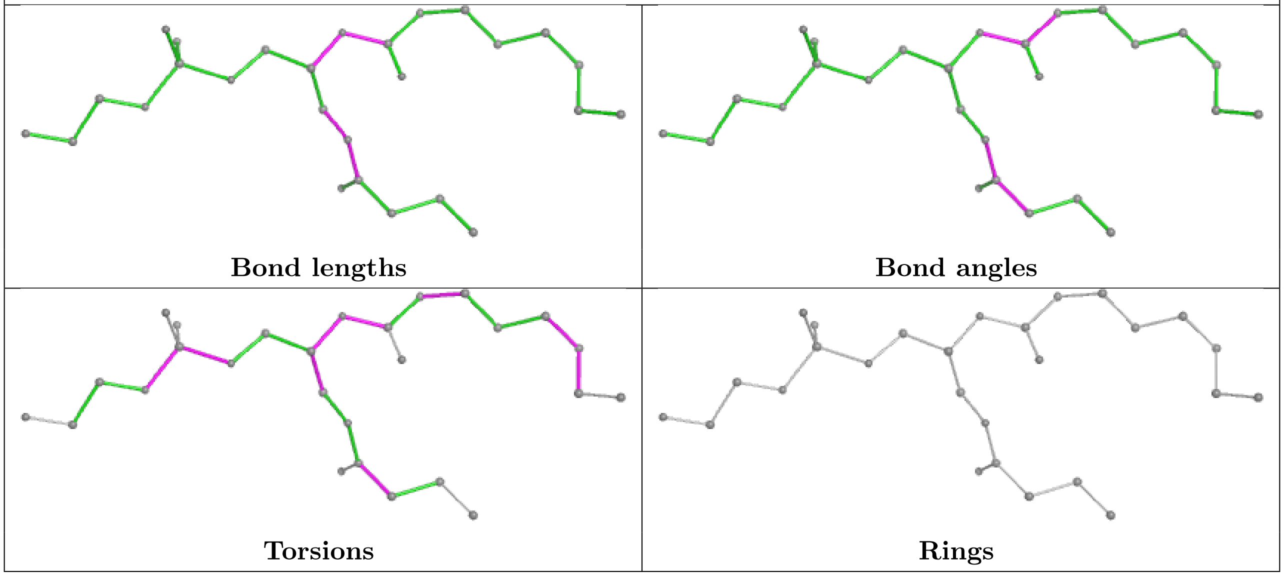
Bond angles



Torsions

Rings

Ligand 3PE Y 201



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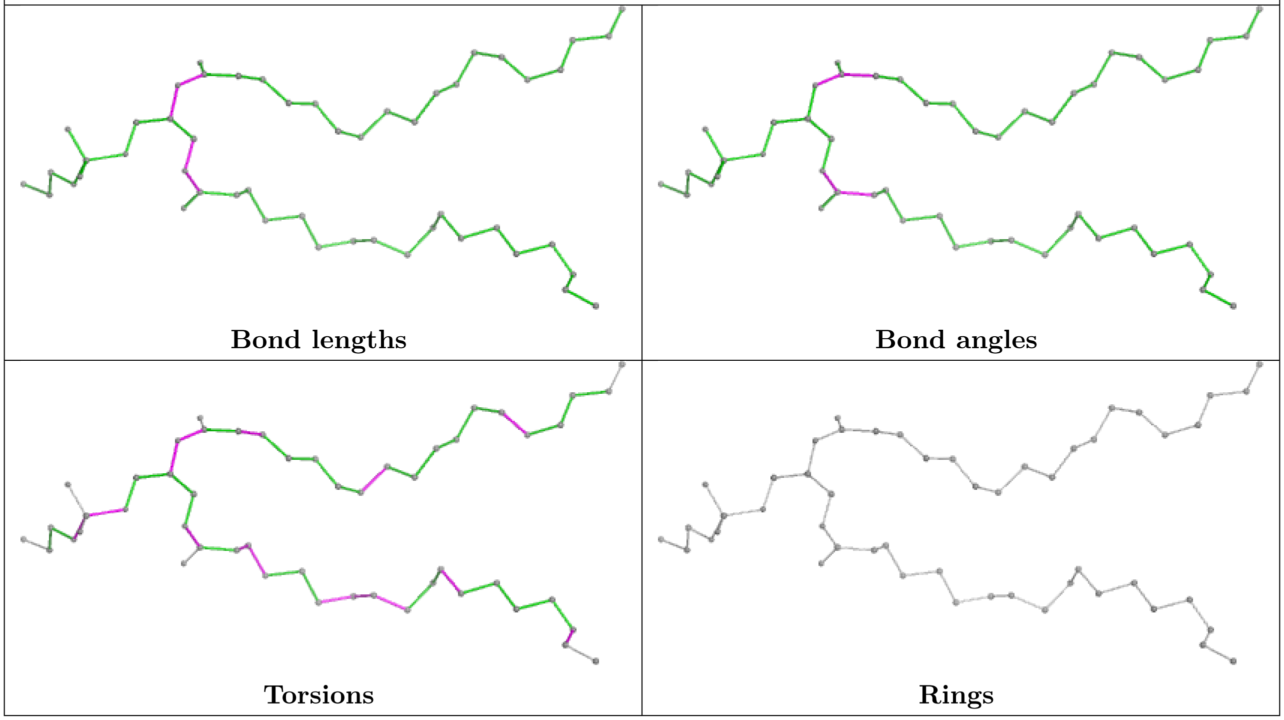
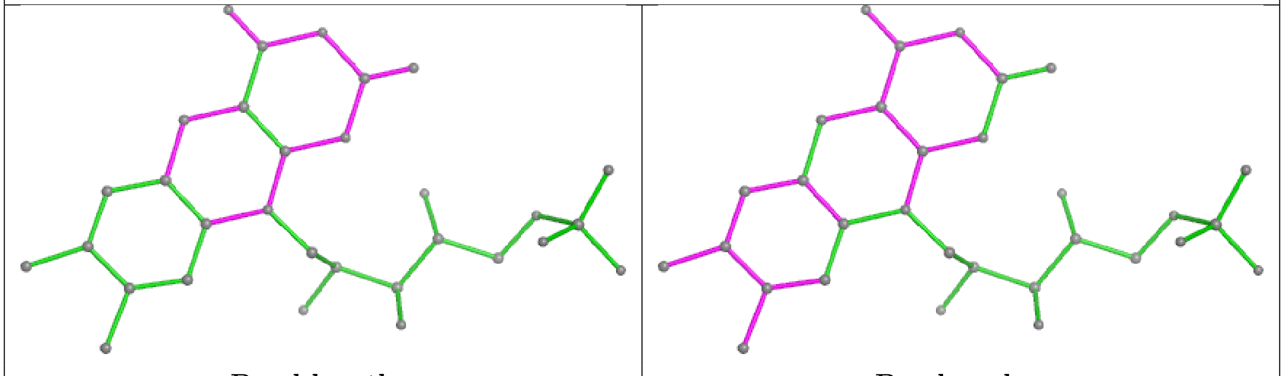
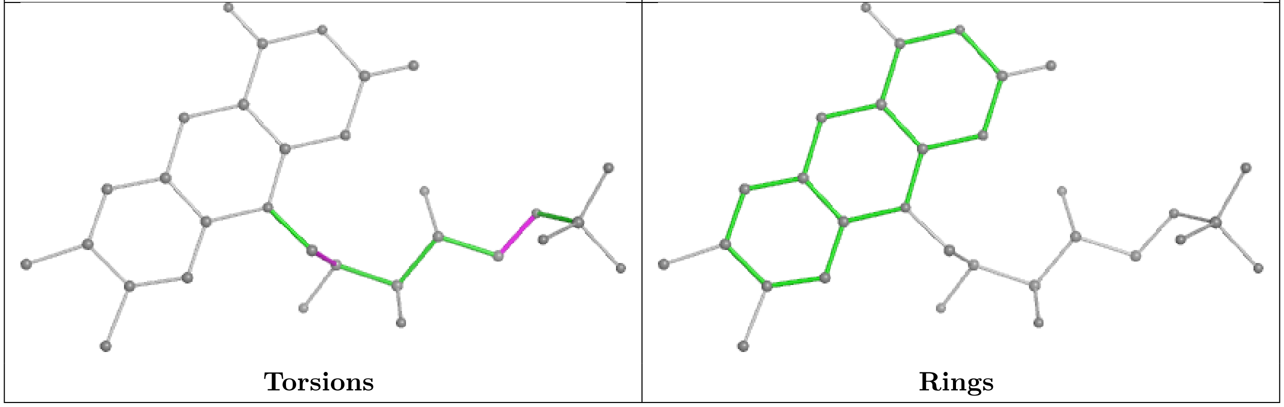


Ligand FMN F 501



Bond lengths

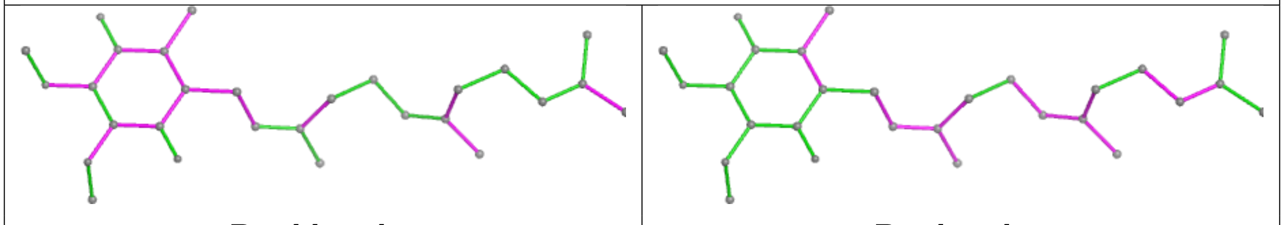
Bond angles



Torsions

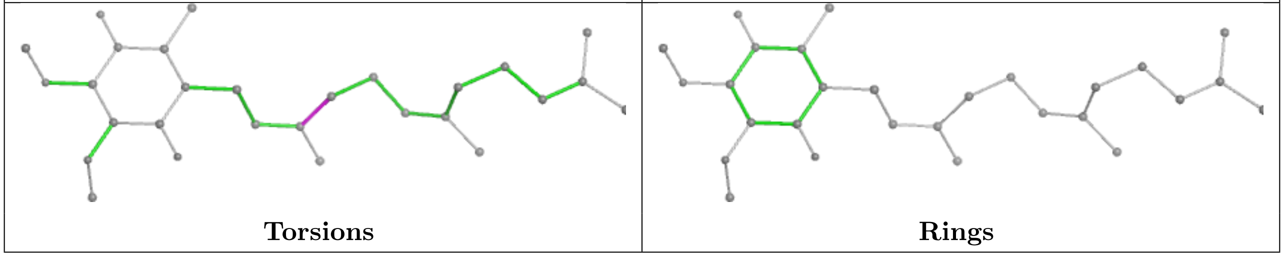
Rings

Ligand U10 H 401



Bond lengths

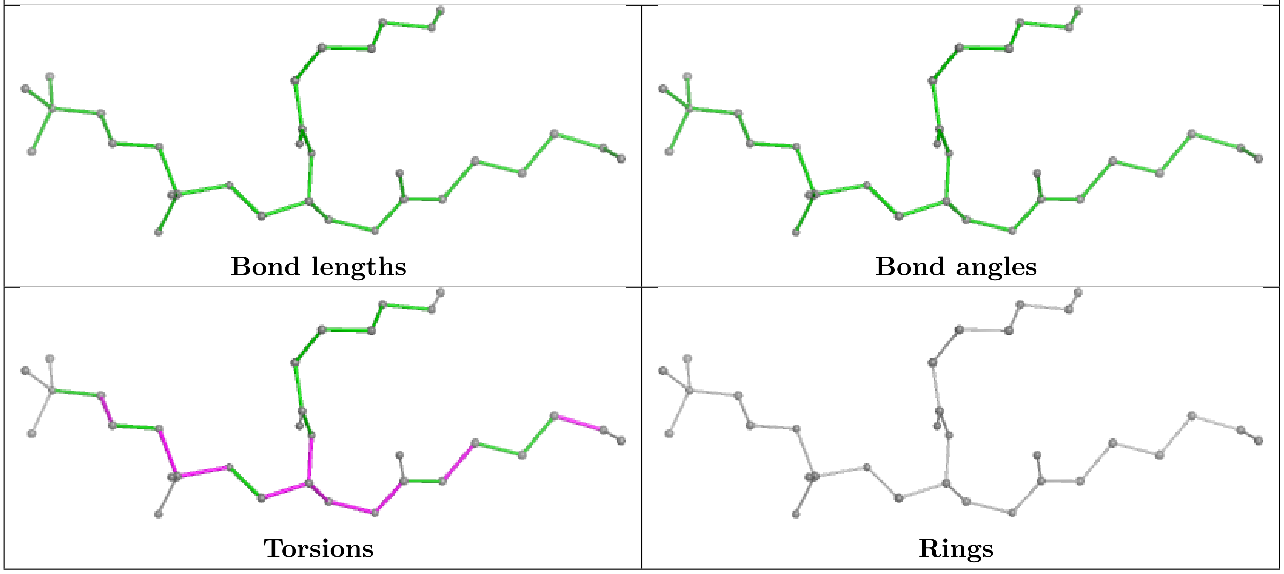
Bond angles



Torsions

Rings

Ligand PLC b 102



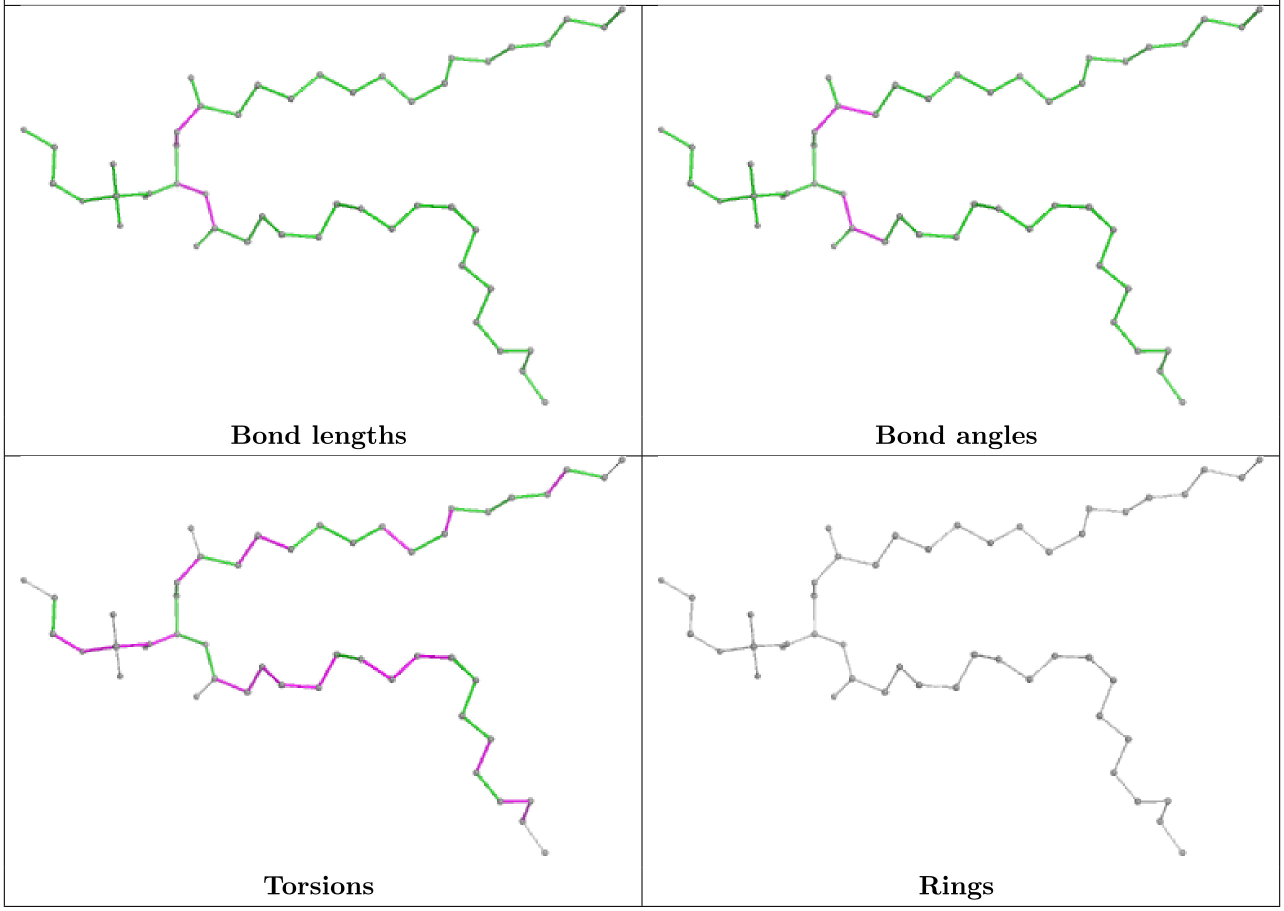
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE N 402



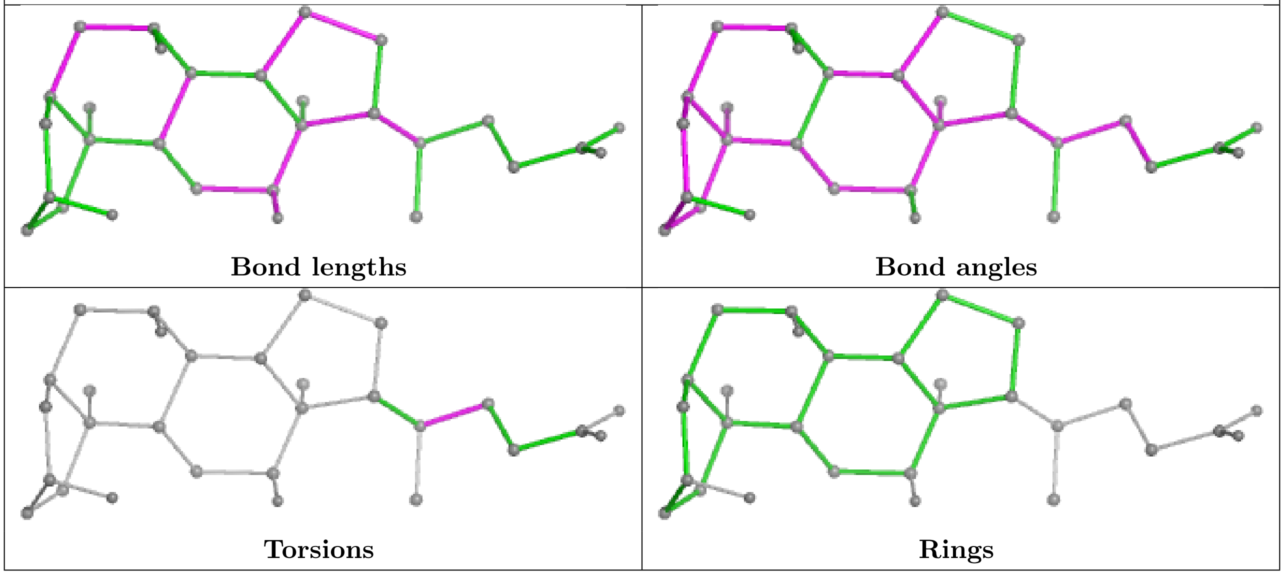
Bond lengths

Bond angles

Torsions

Rings

Ligand CHD i 201



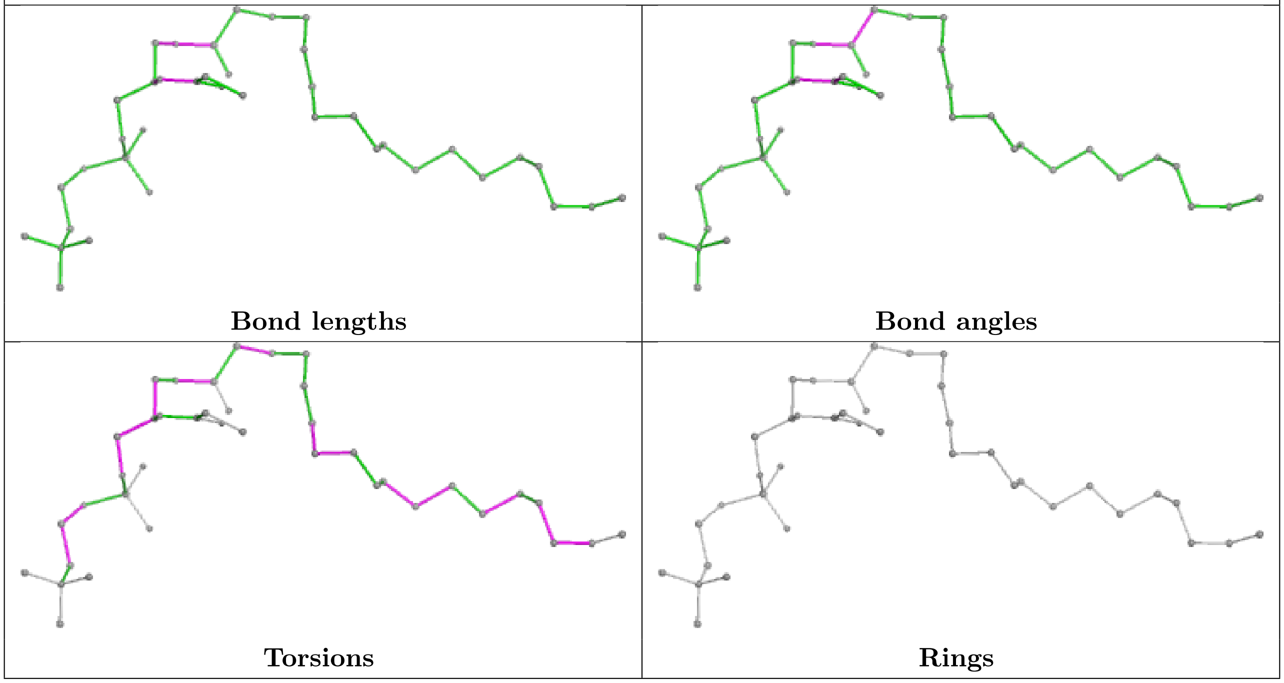
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 H 403



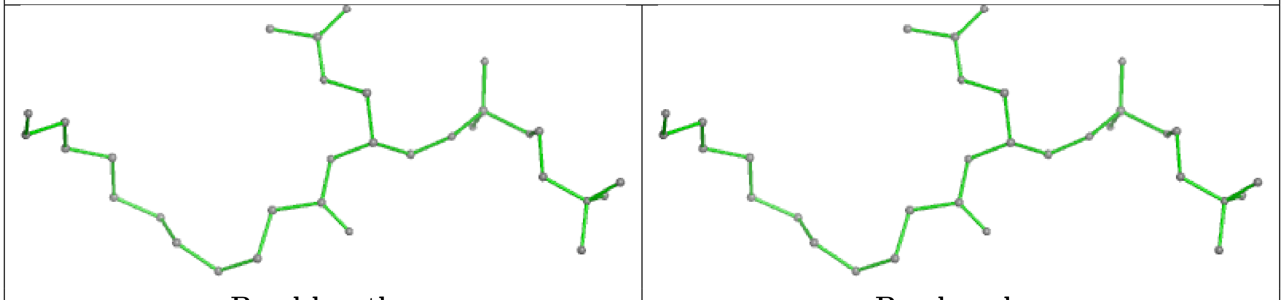
Bond lengths

Bond angles

Torsions

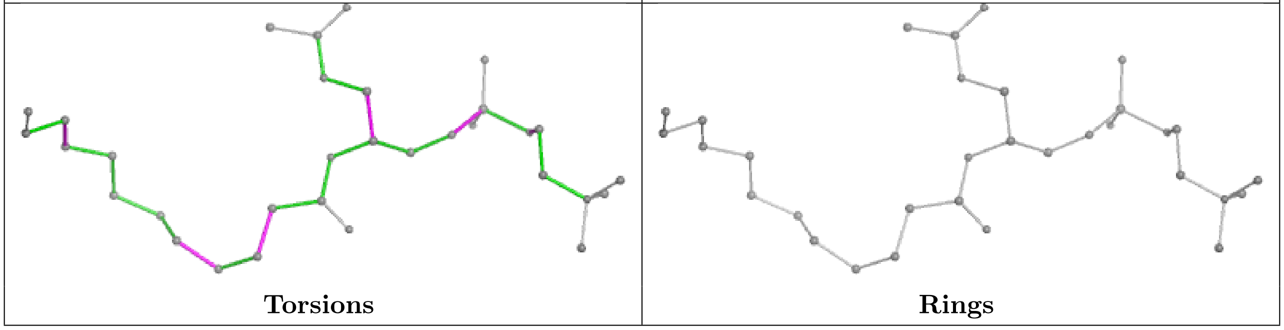
Rings

Ligand PLC g 202



Bond lengths

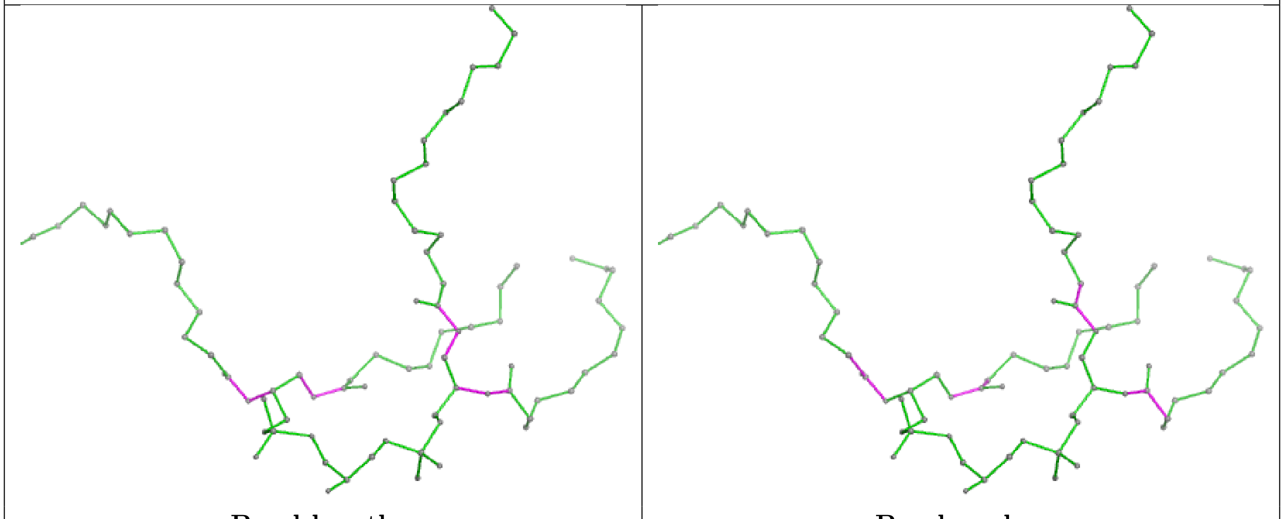
Bond angles



Torsions

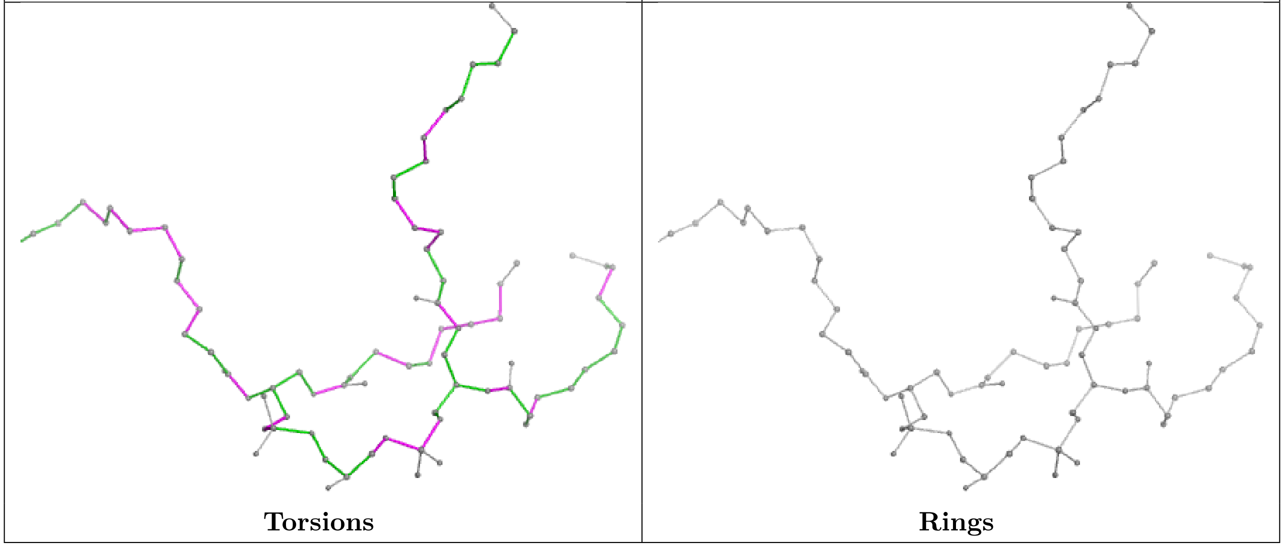
Rings

Ligand CDL h 201



Bond lengths

Bond angles



Torsions

Rings

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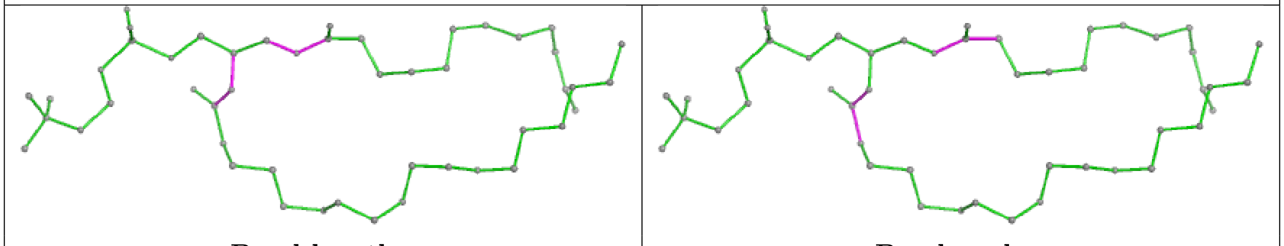
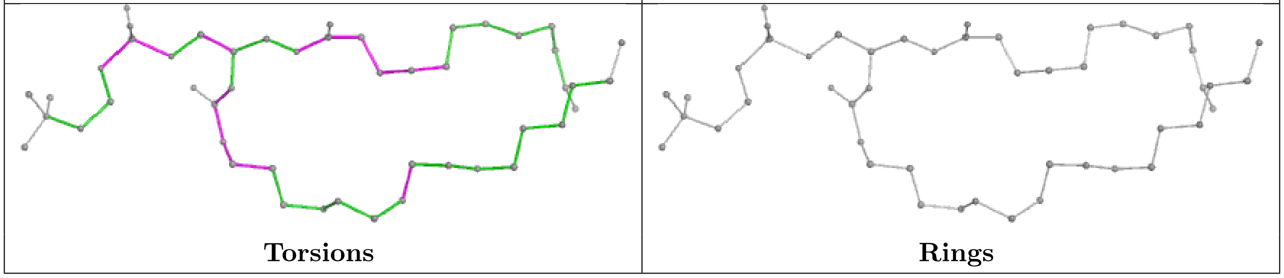


Bond lengths

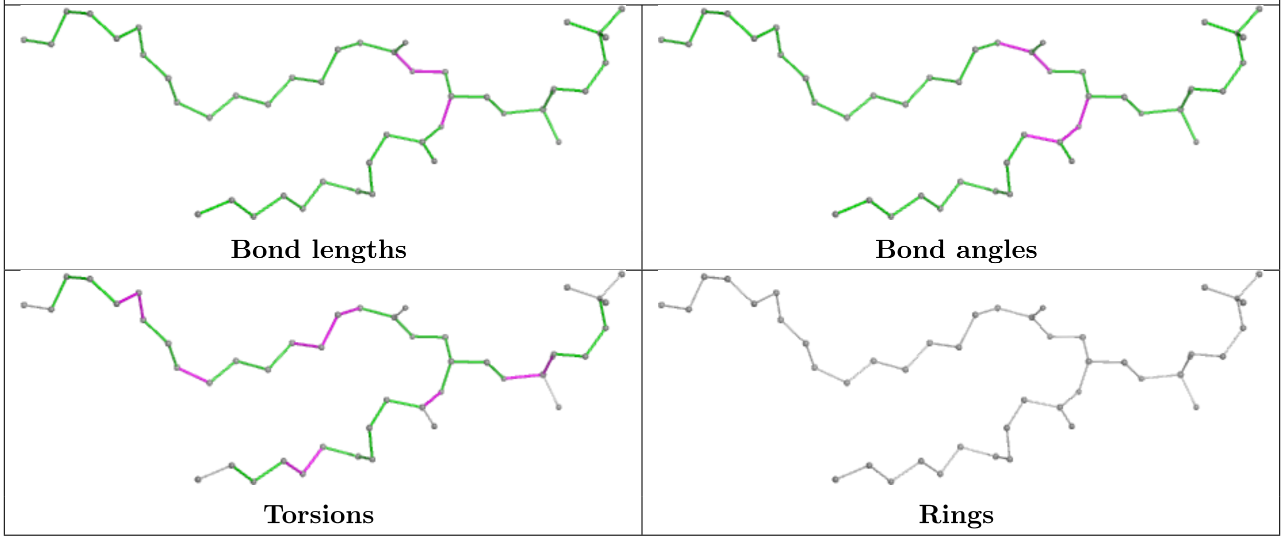
Bond angles



Torsions

Rings

Ligand PC1 P 502



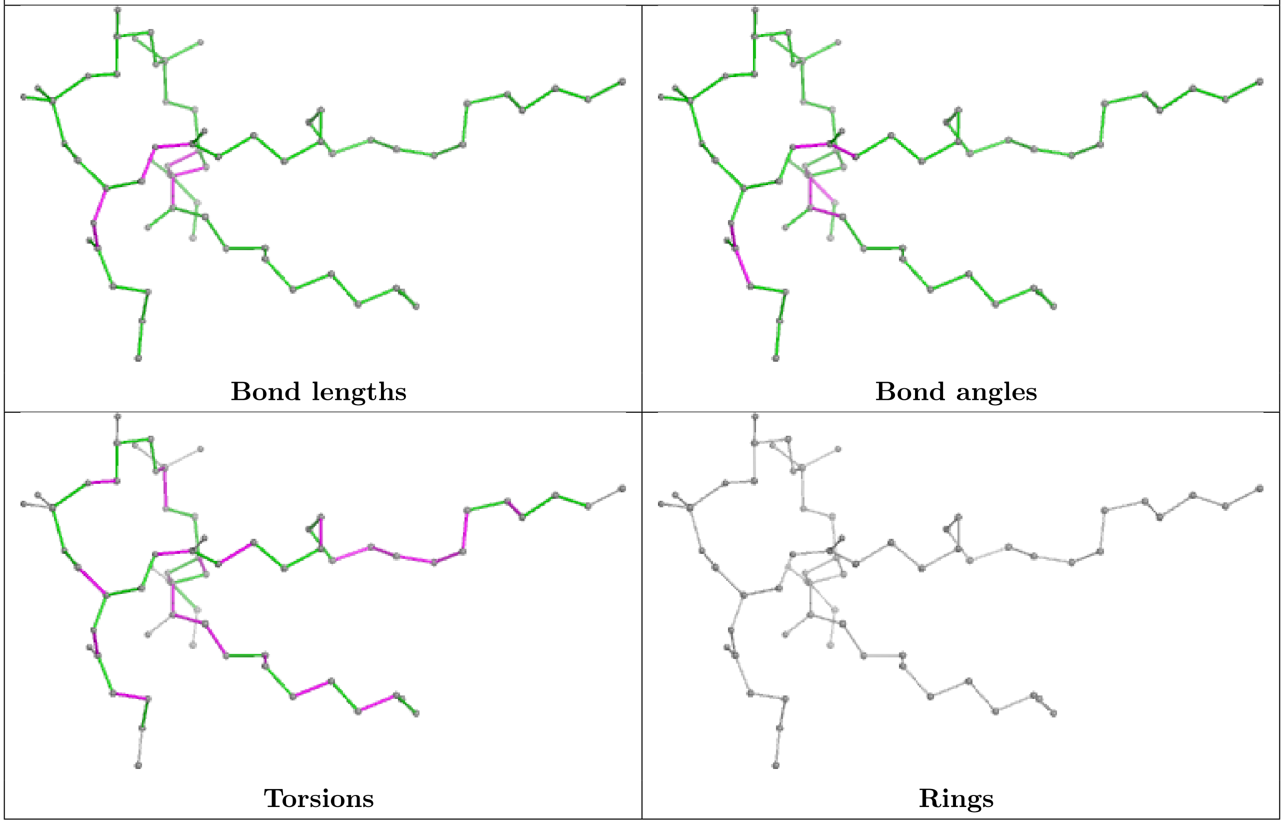
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL d 201



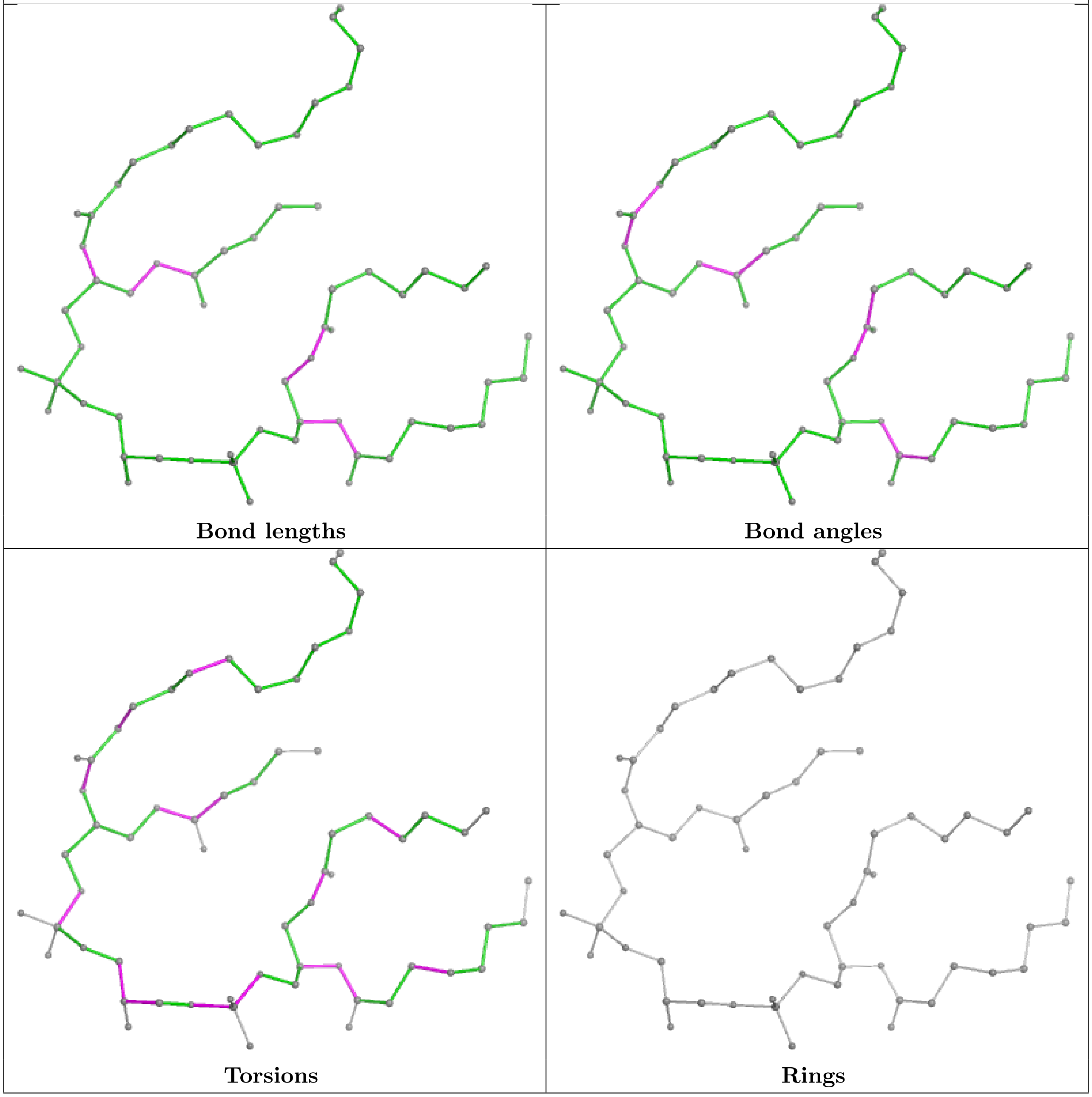
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL q 201



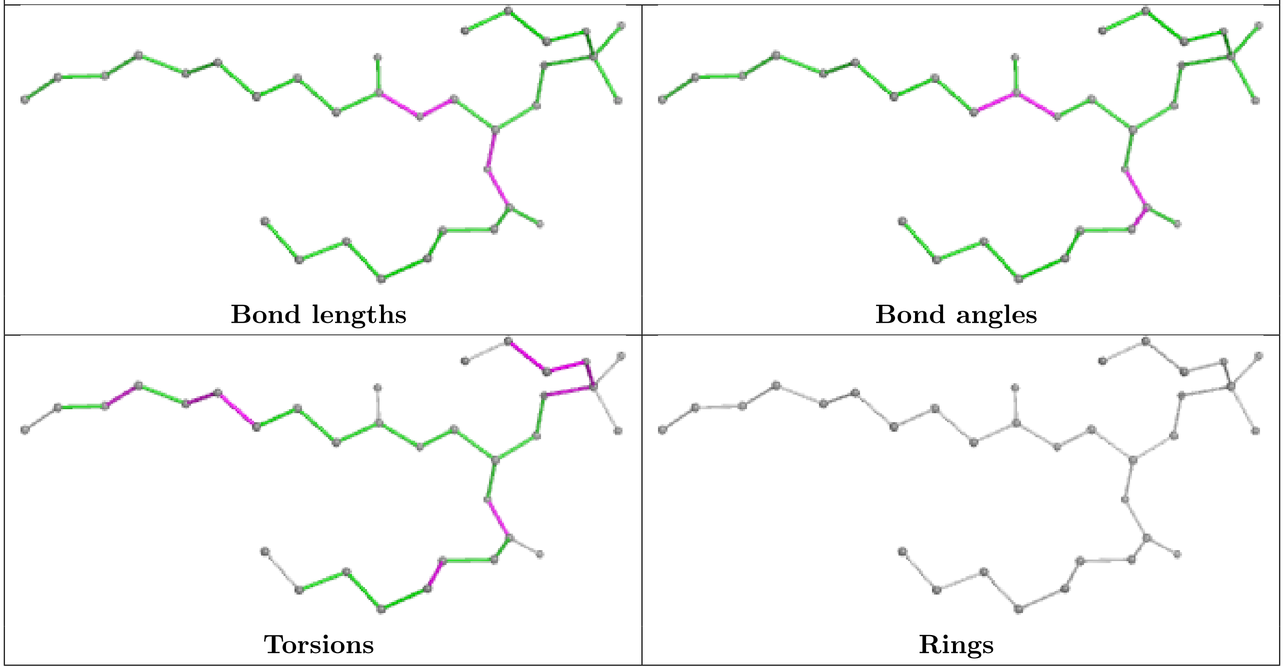
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE m 202



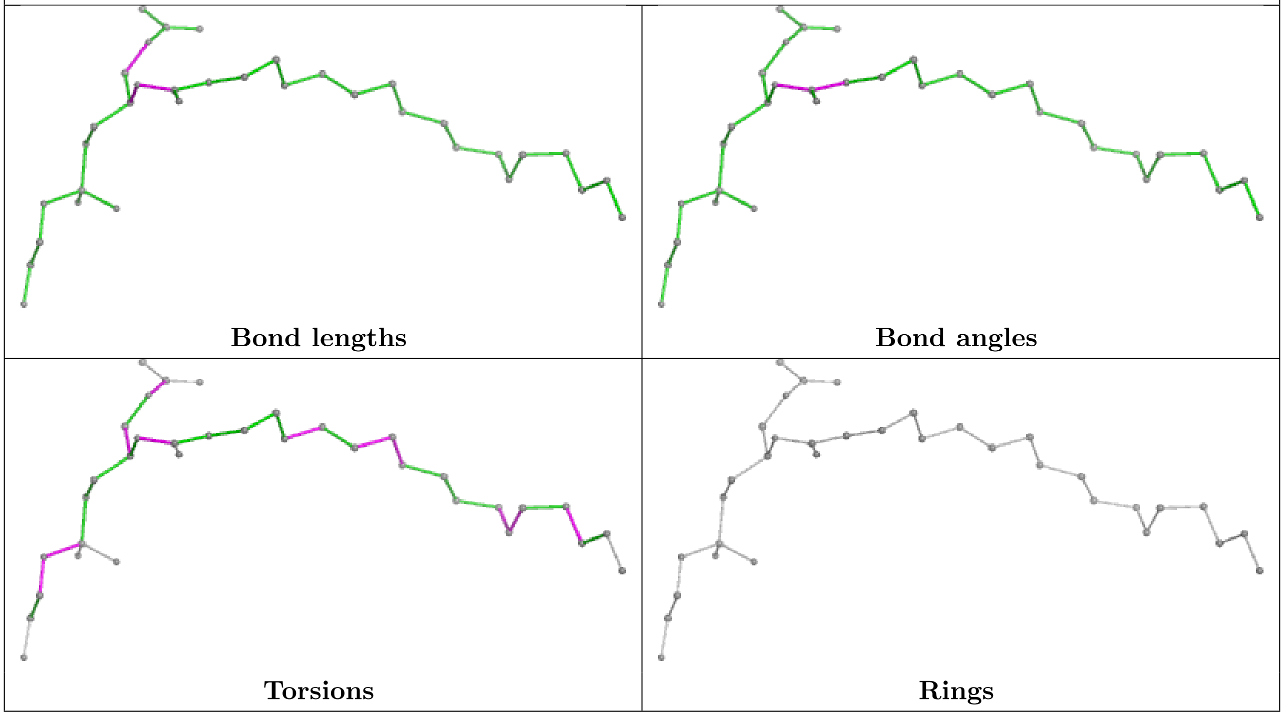
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE o 202



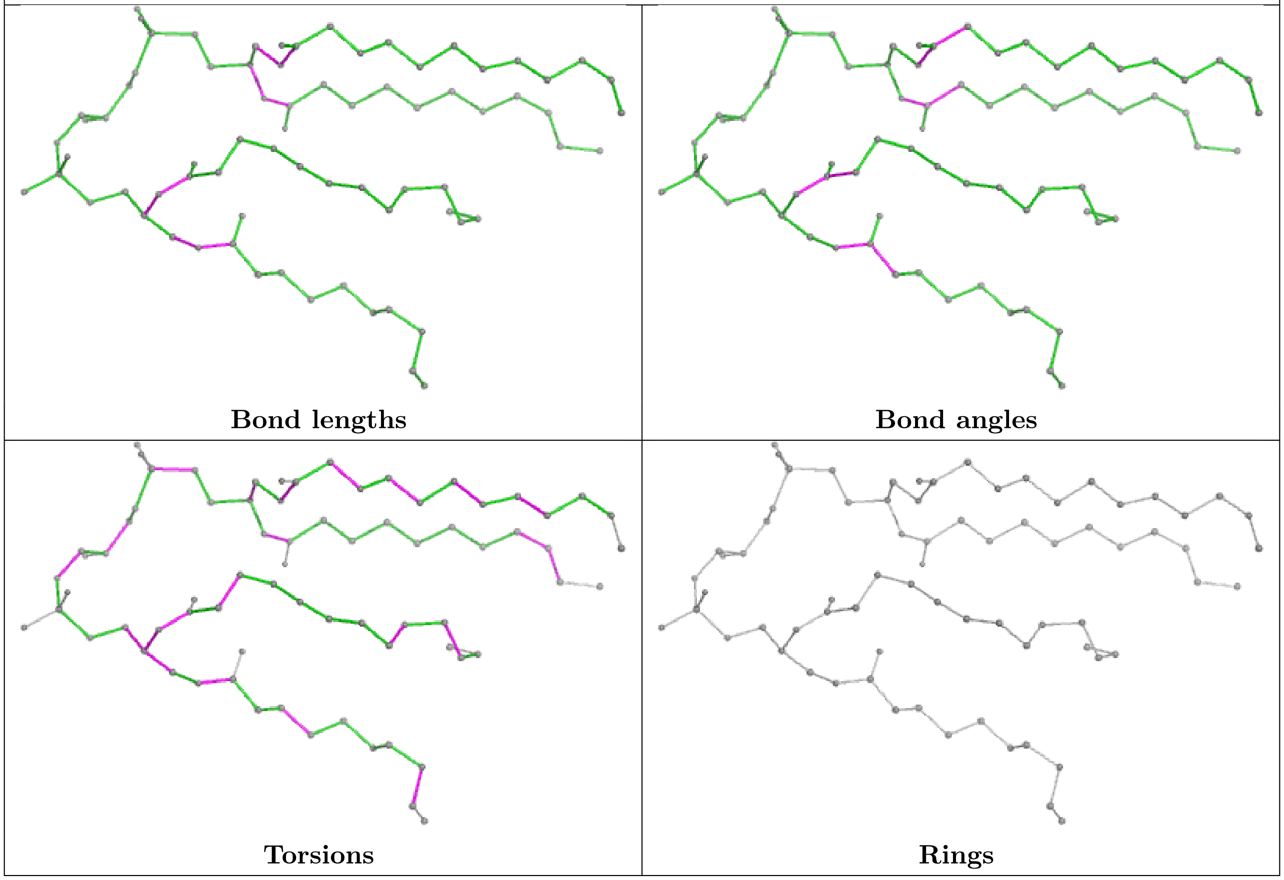
Bond lengths

Bond angles

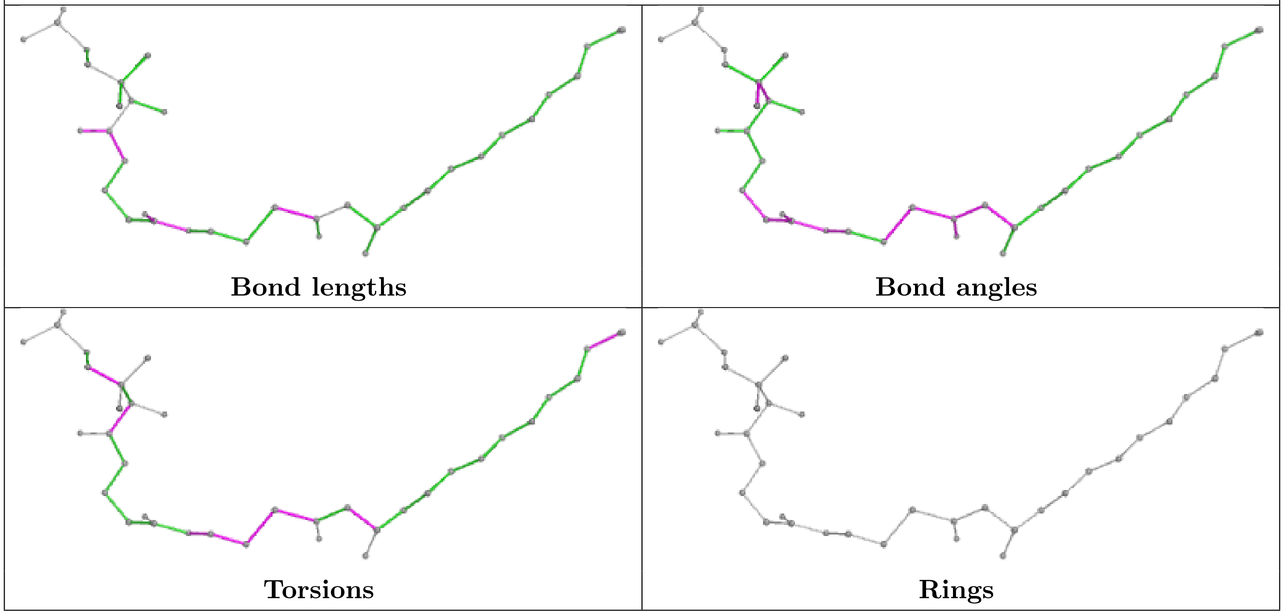
Torsions

Rings

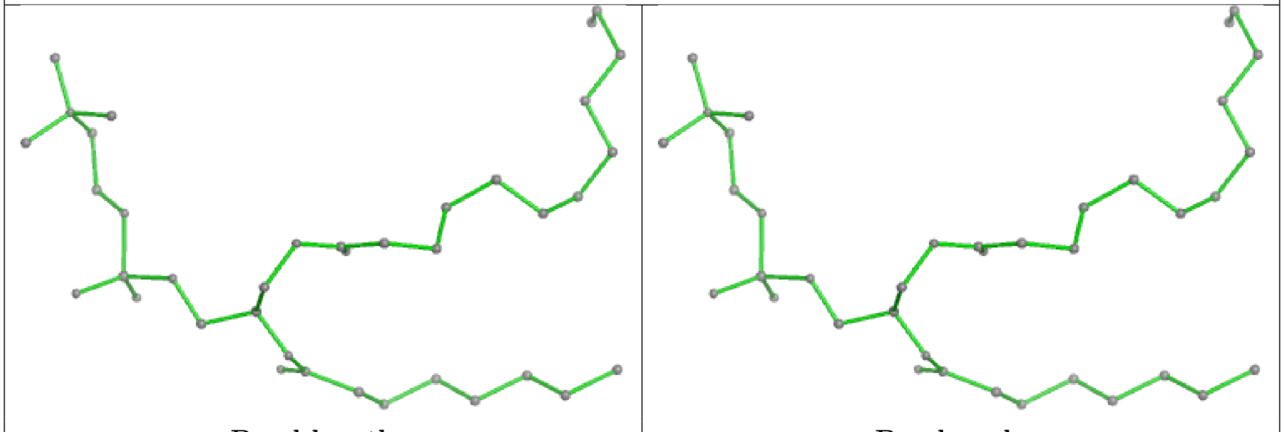
Ligand CDL N 401



Ligand EHZ T 101



Ligand PLC B 202



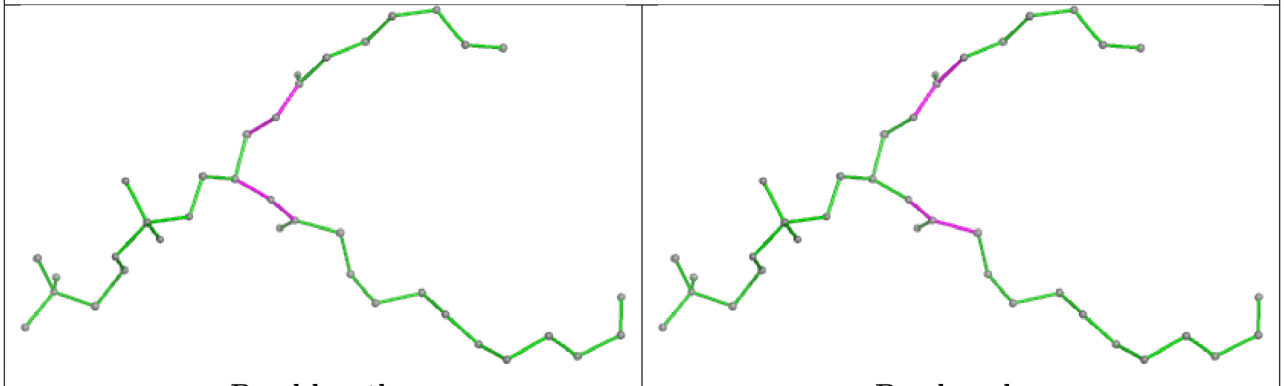
Bond lengths

Bond angles

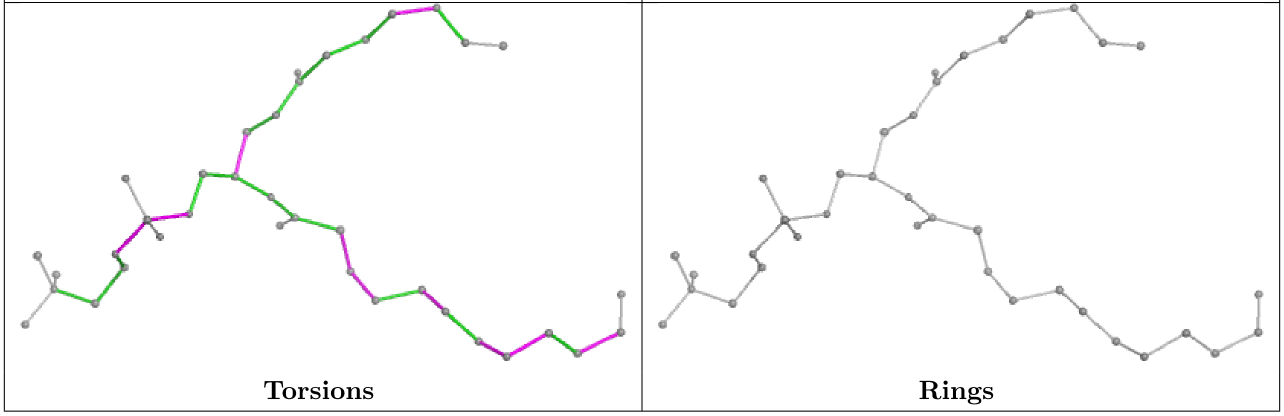
Torsions

Rings

Ligand PC1 I 205

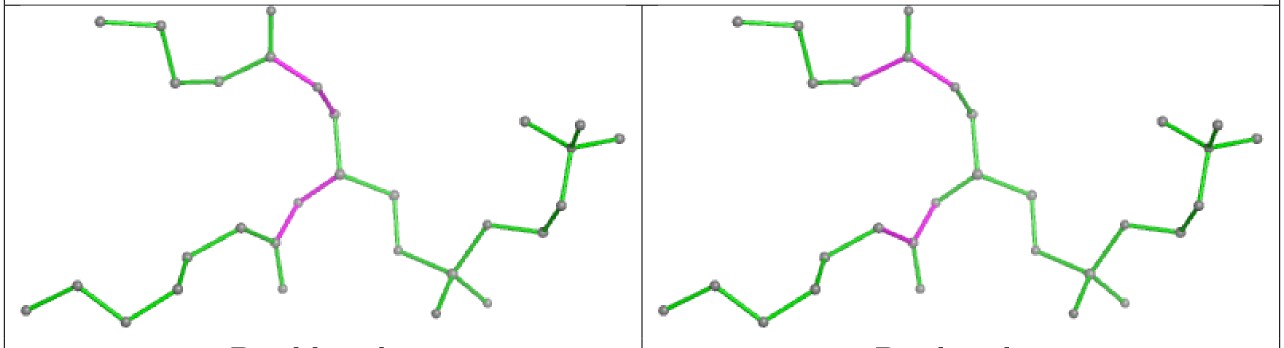


Bond lengths Bond angles



Torsions Rings

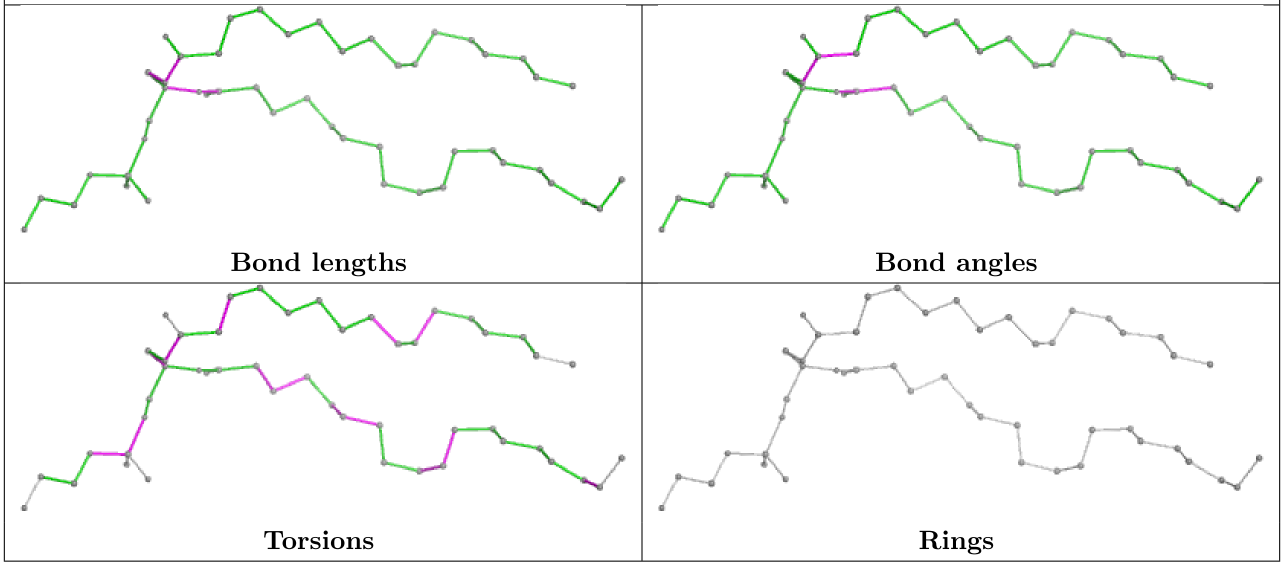
Ligand PC1 q 203



Bond lengths Bond angles

Torsions Rings

Ligand 3PE d 202



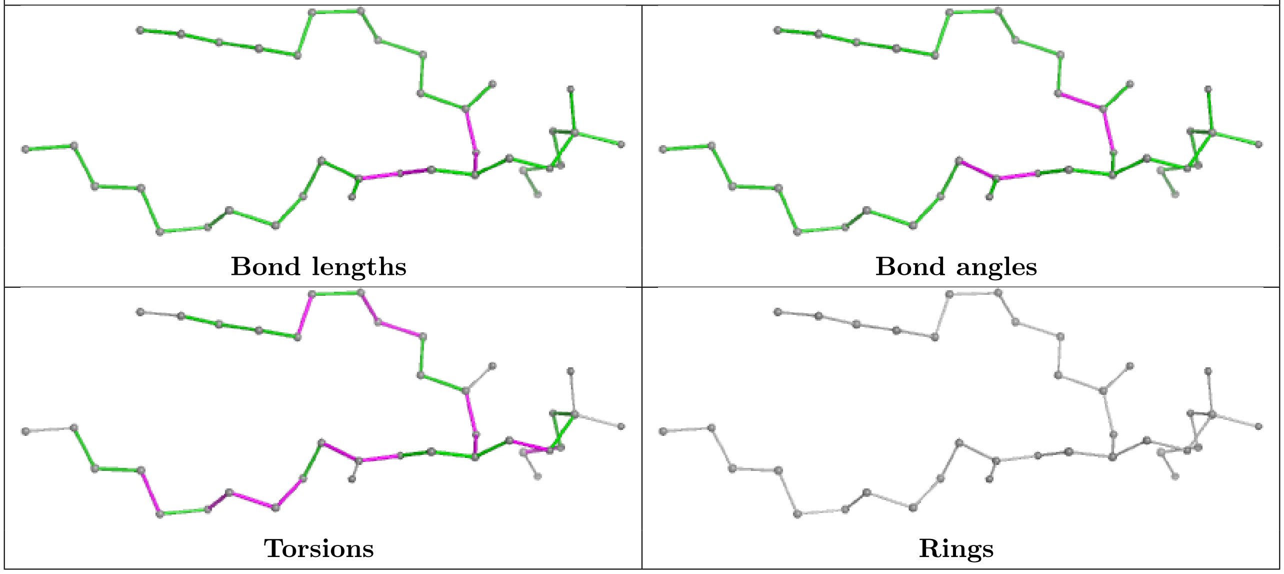
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE L 705



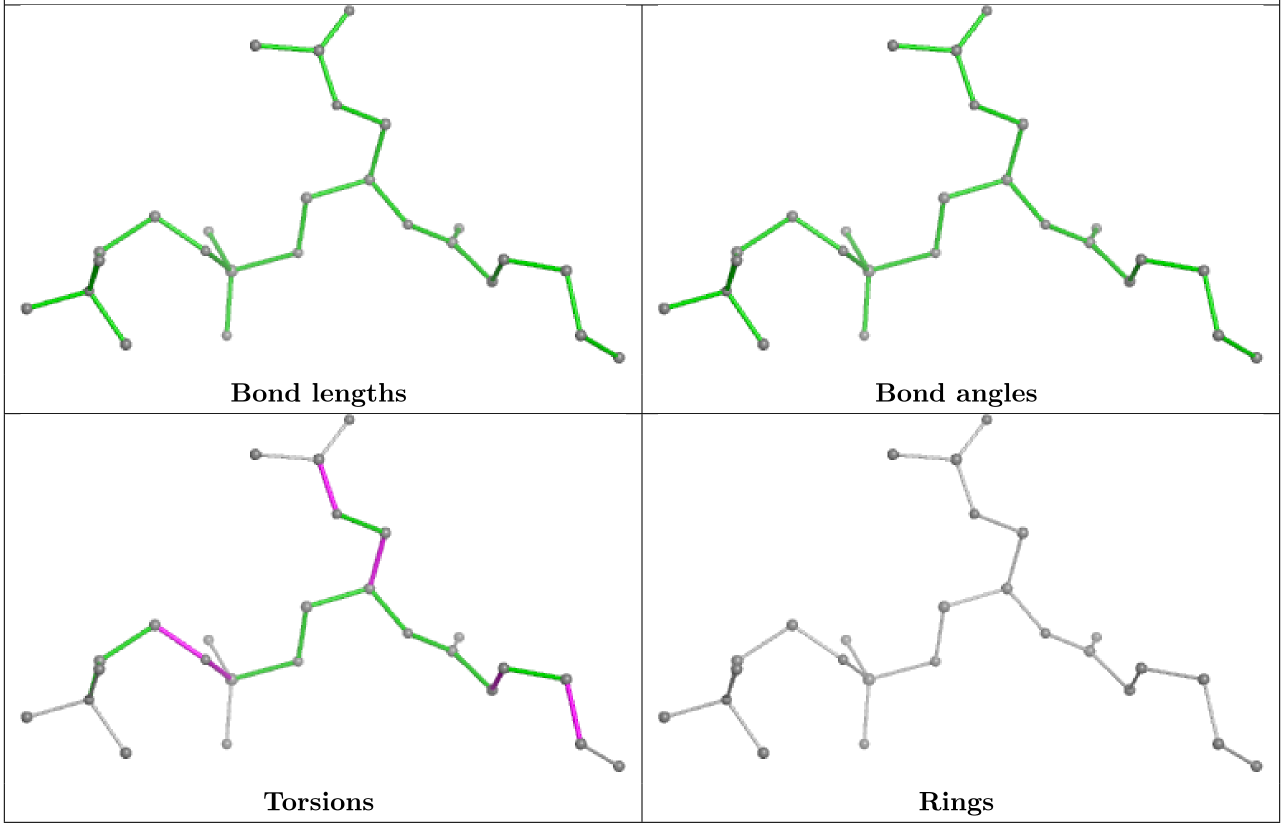
Bond lengths

Bond angles

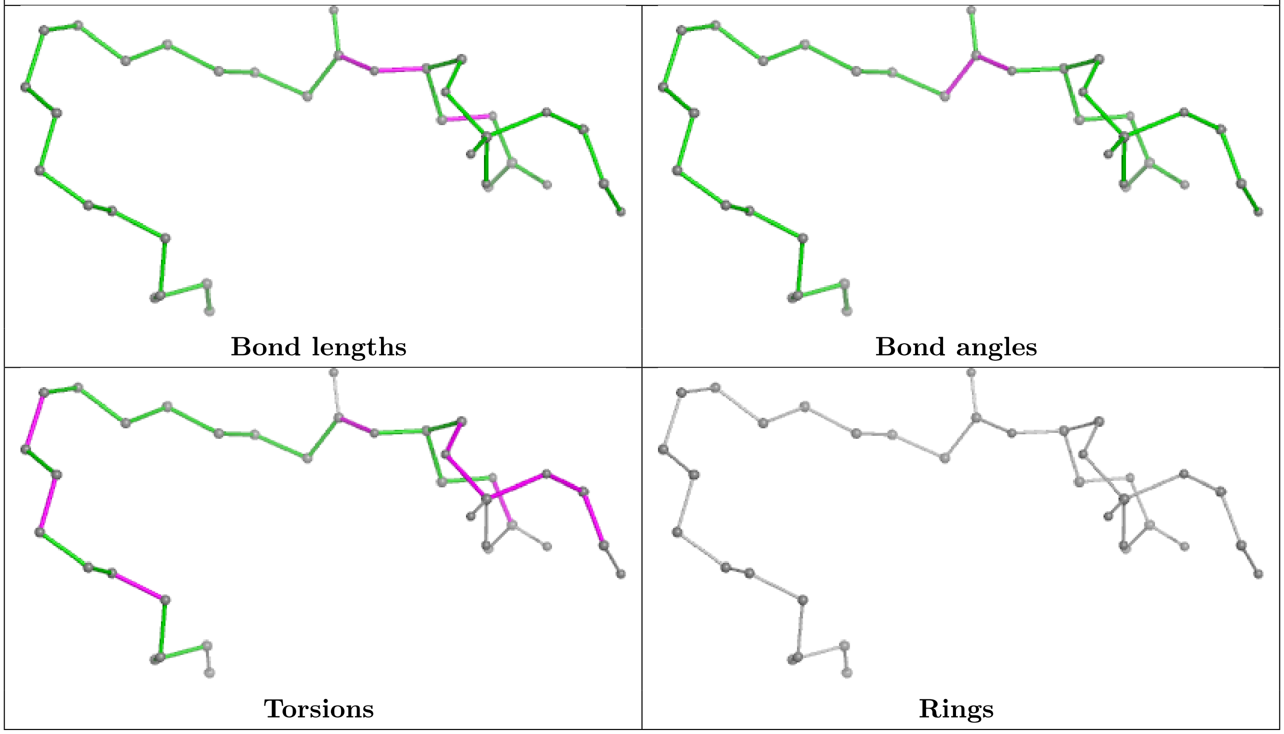
Torsions

Rings

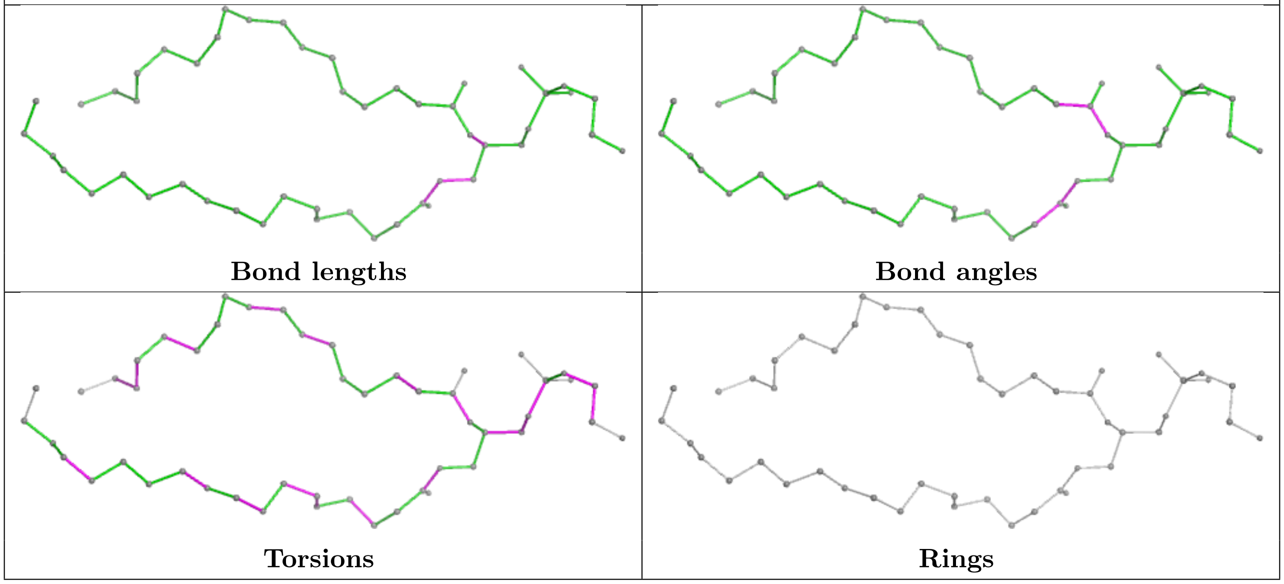
Ligand PLC N 405


Bond lengths
Bond angles
Torsions
Rings

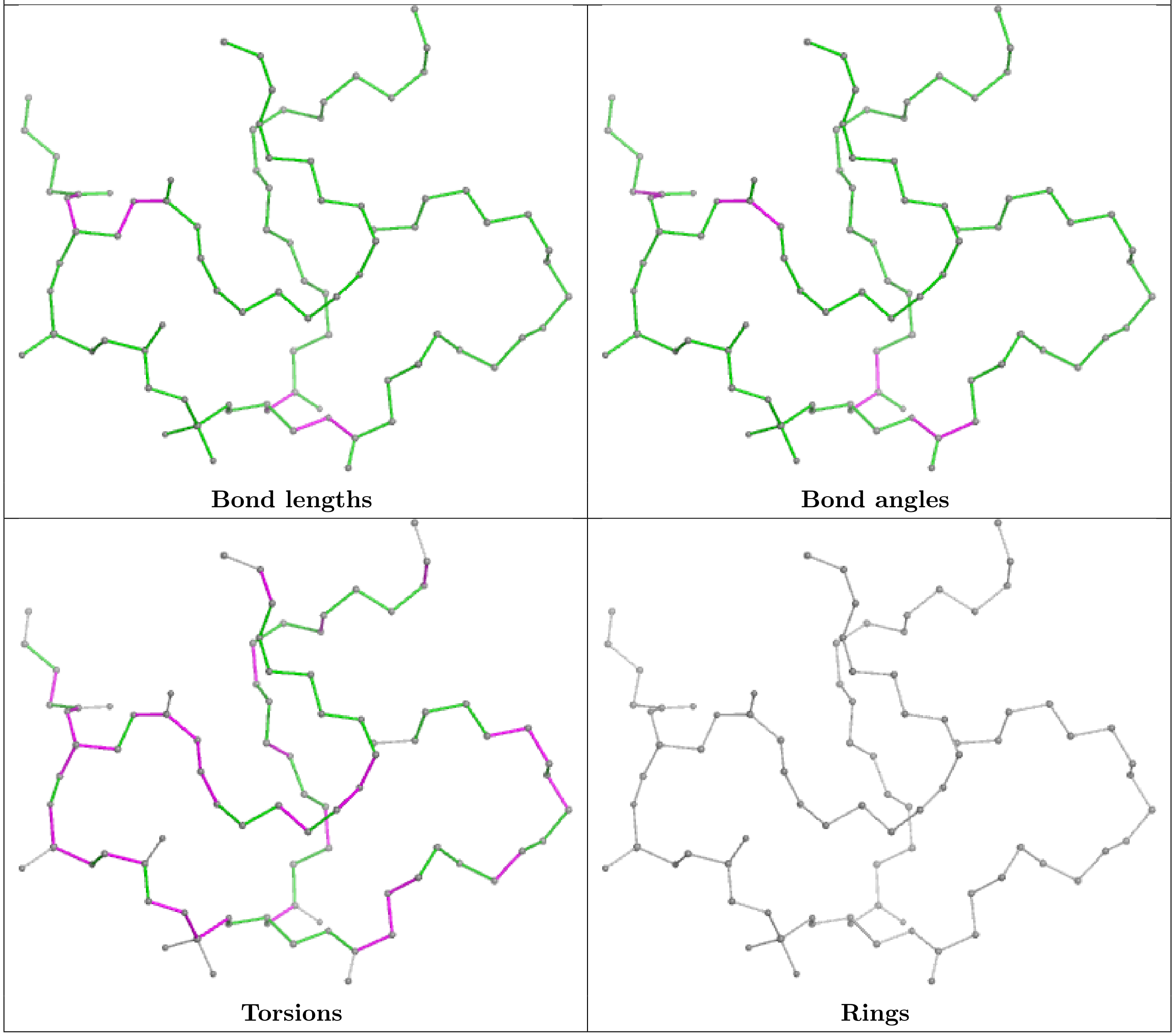
Ligand 3PE L 702


Bond lengths
Bond angles
Torsions
Rings

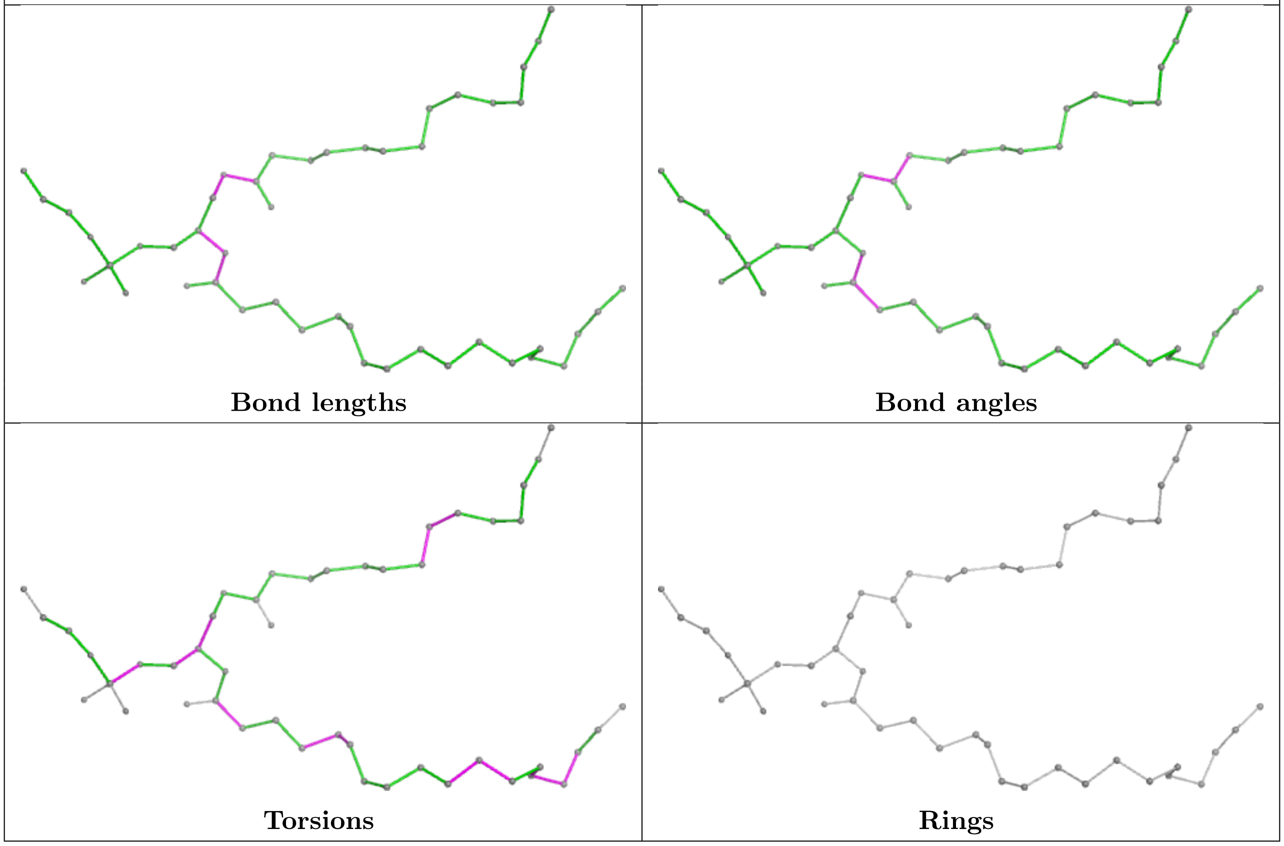
Ligand 3PE M 603



Ligand CDL X 201



Ligand 3PE b 101



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

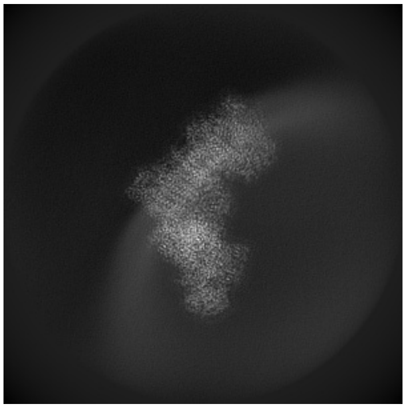
6 Map visualisation ⓘ

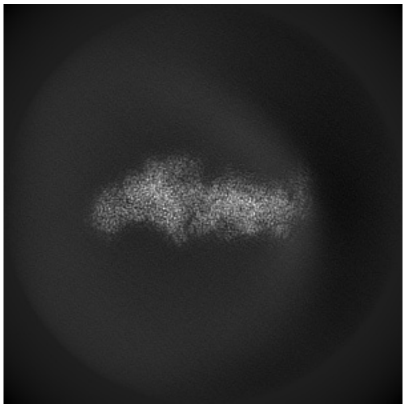
This section contains visualisations of the EMDB entry EMD-18067. These allow visual inspection of the internal detail of the map and identification of artifacts.

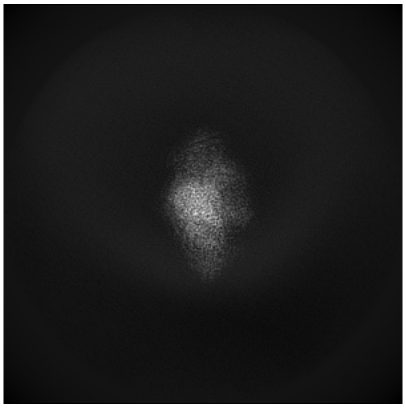
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

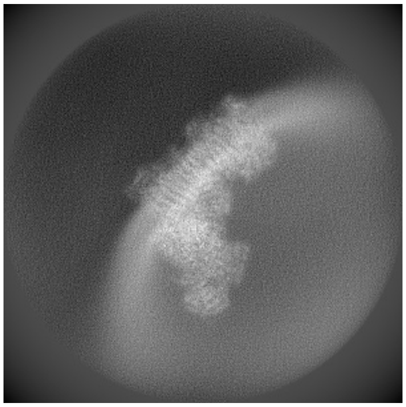
6.1.1 Primary map

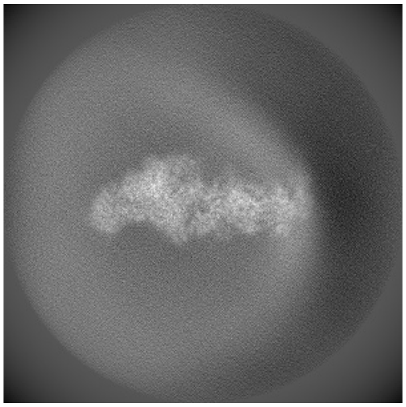

X

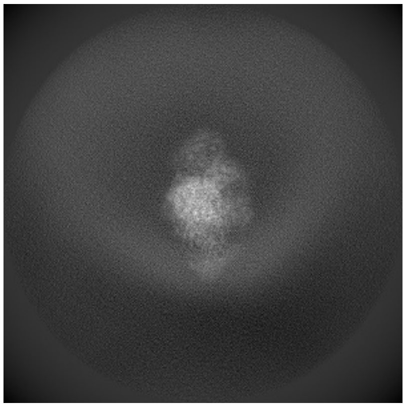

Y


Z

6.1.2 Raw map


X


Y

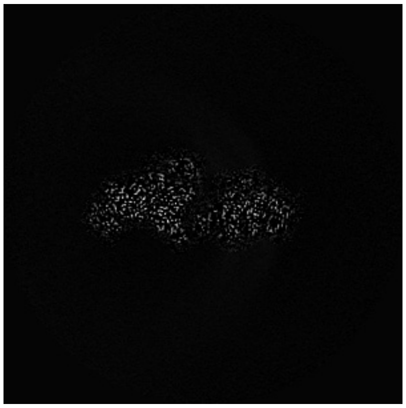

Z

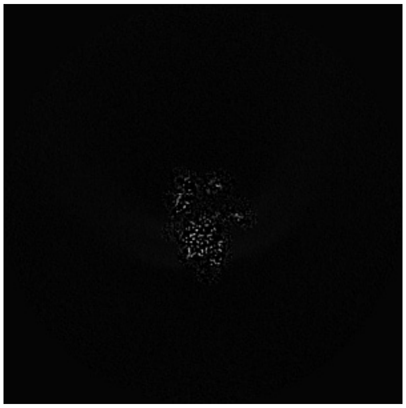
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

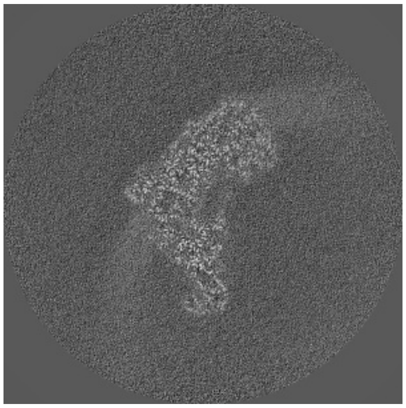
6.2.1 Primary map

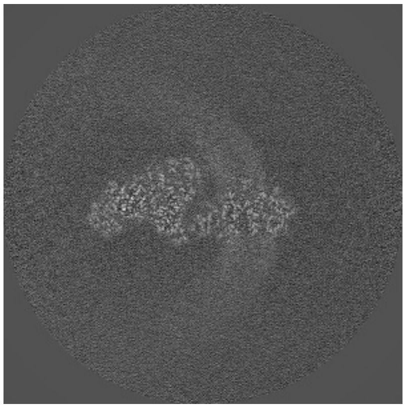

X Index: 240

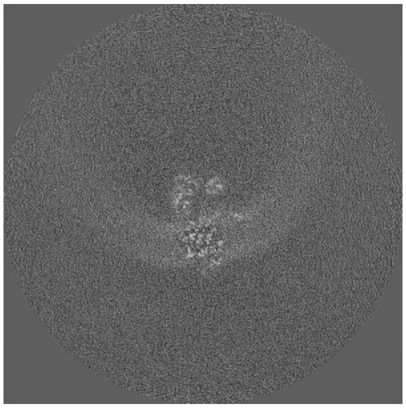

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240


Y Index: 240


Z Index: 240

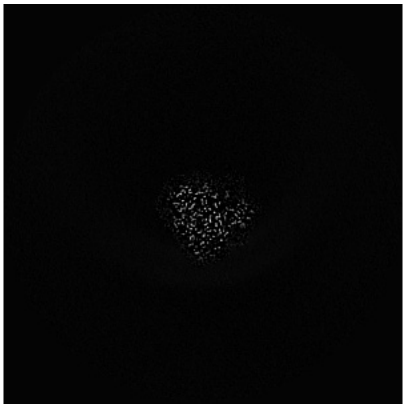
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map

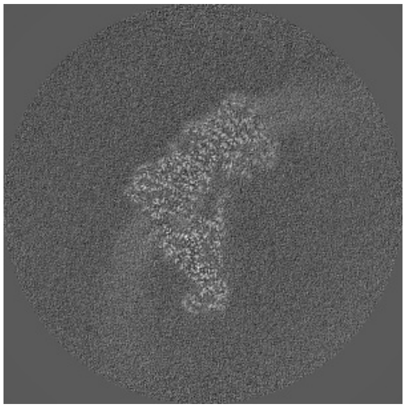
X Index: 243

Y Index: 230

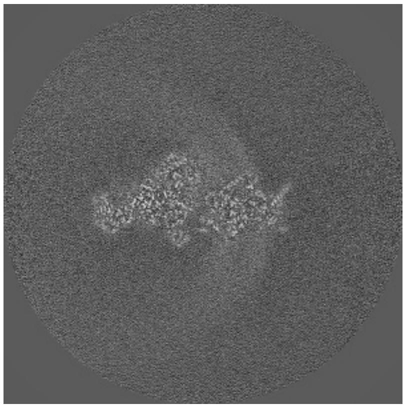


Z Index: 202

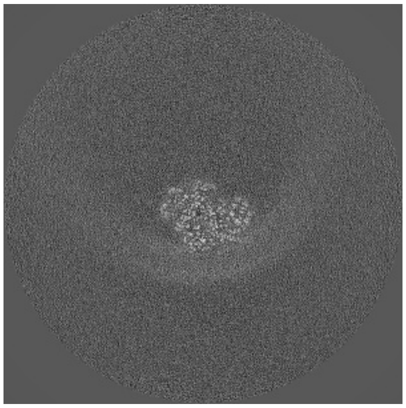
6.3.2 Raw map



X Index: 243



Y Index: 230

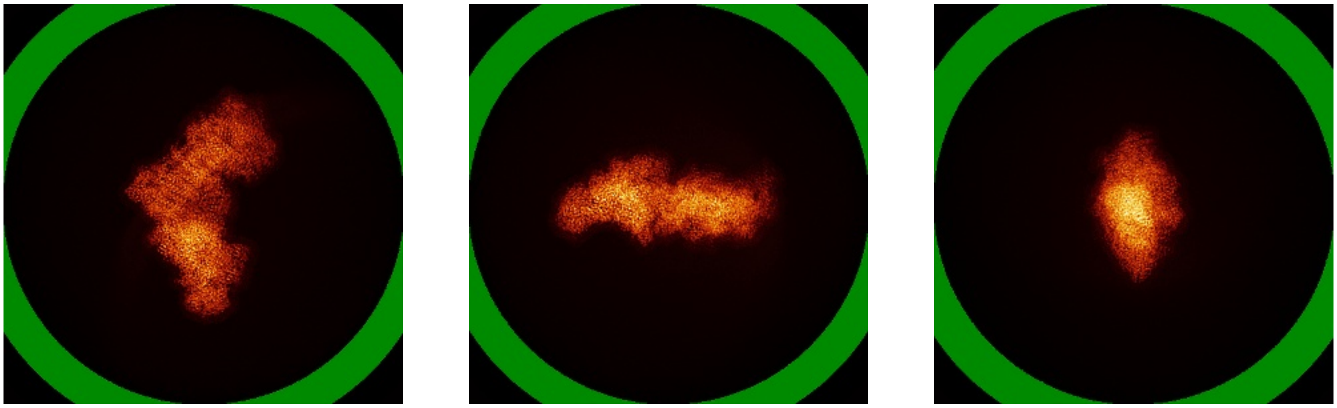


Z Index: 209

The images above show the largest variance slices of the map in three orthogonal directions.

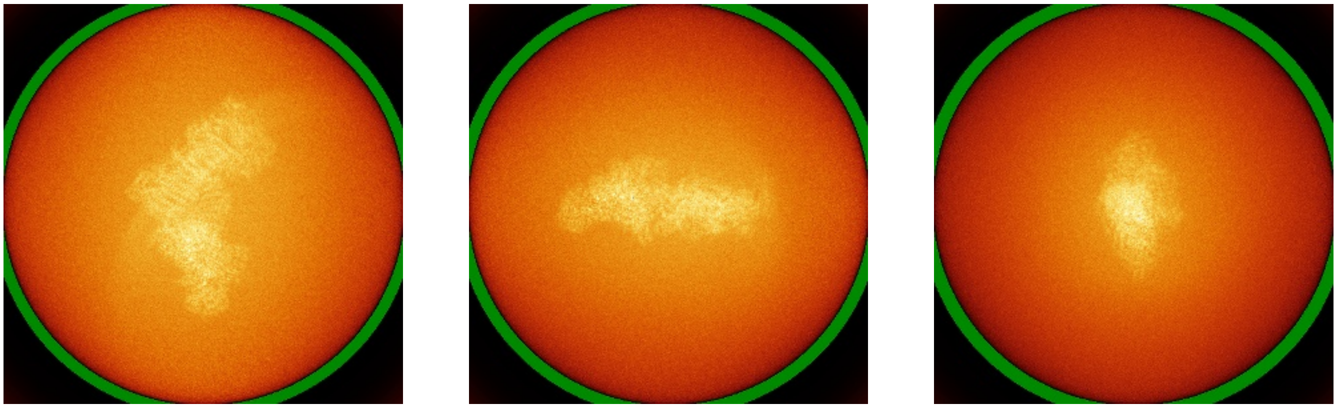
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



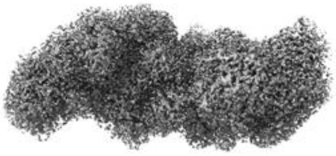
X Y Z

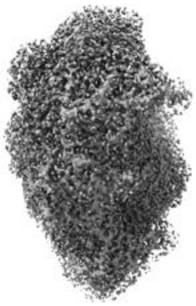
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

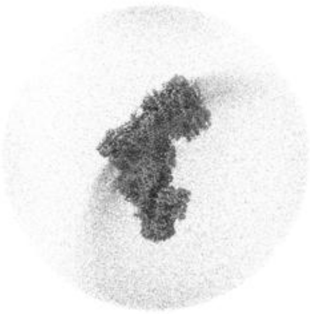

X

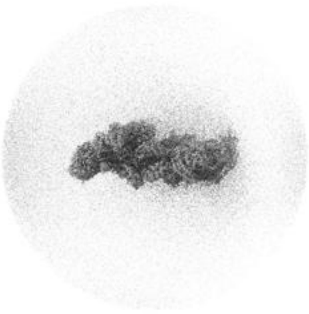

Y

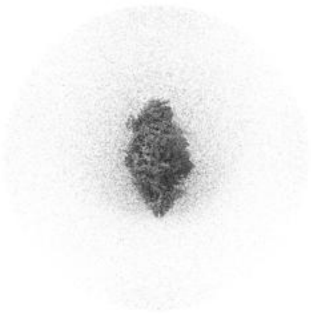

Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map


X


Y


Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

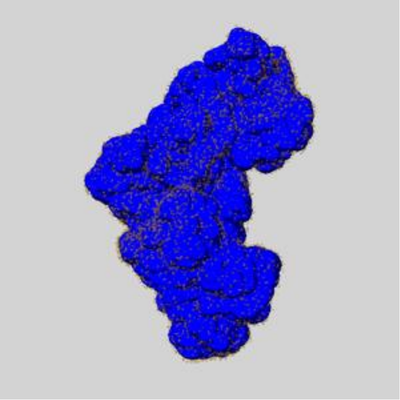
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

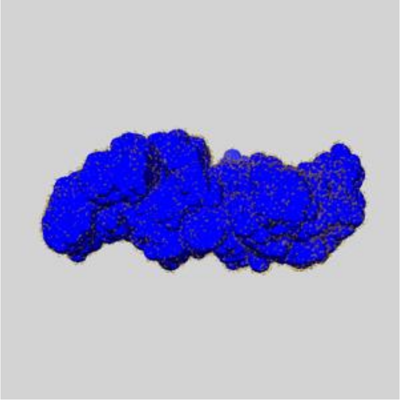
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

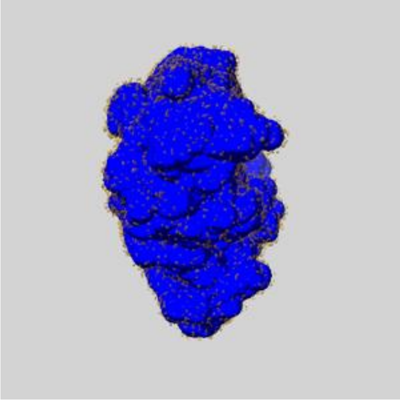
6.6.1 emd_18067_msk_1.map



X



Y

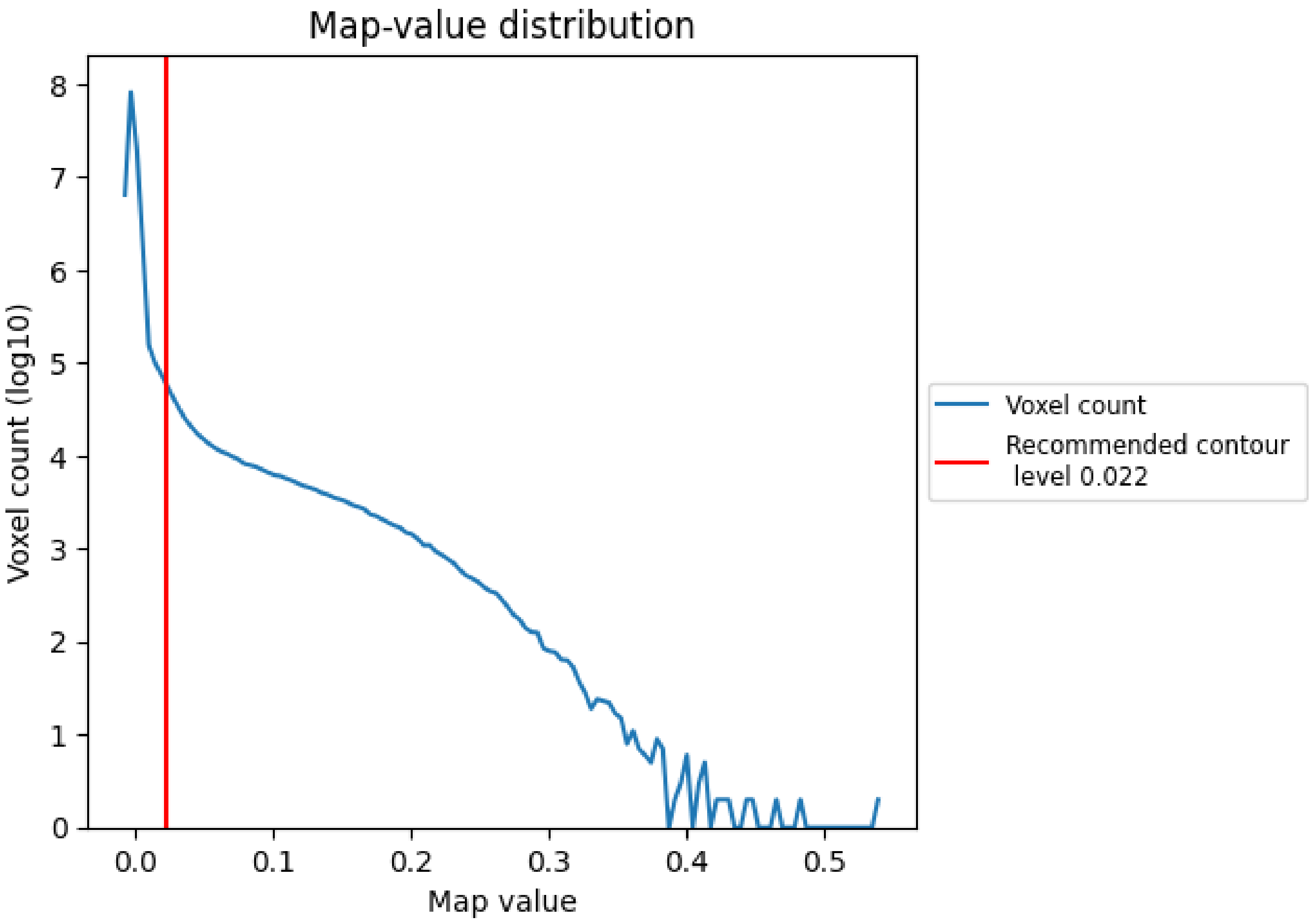


Z

7 Map analysis ⓘ

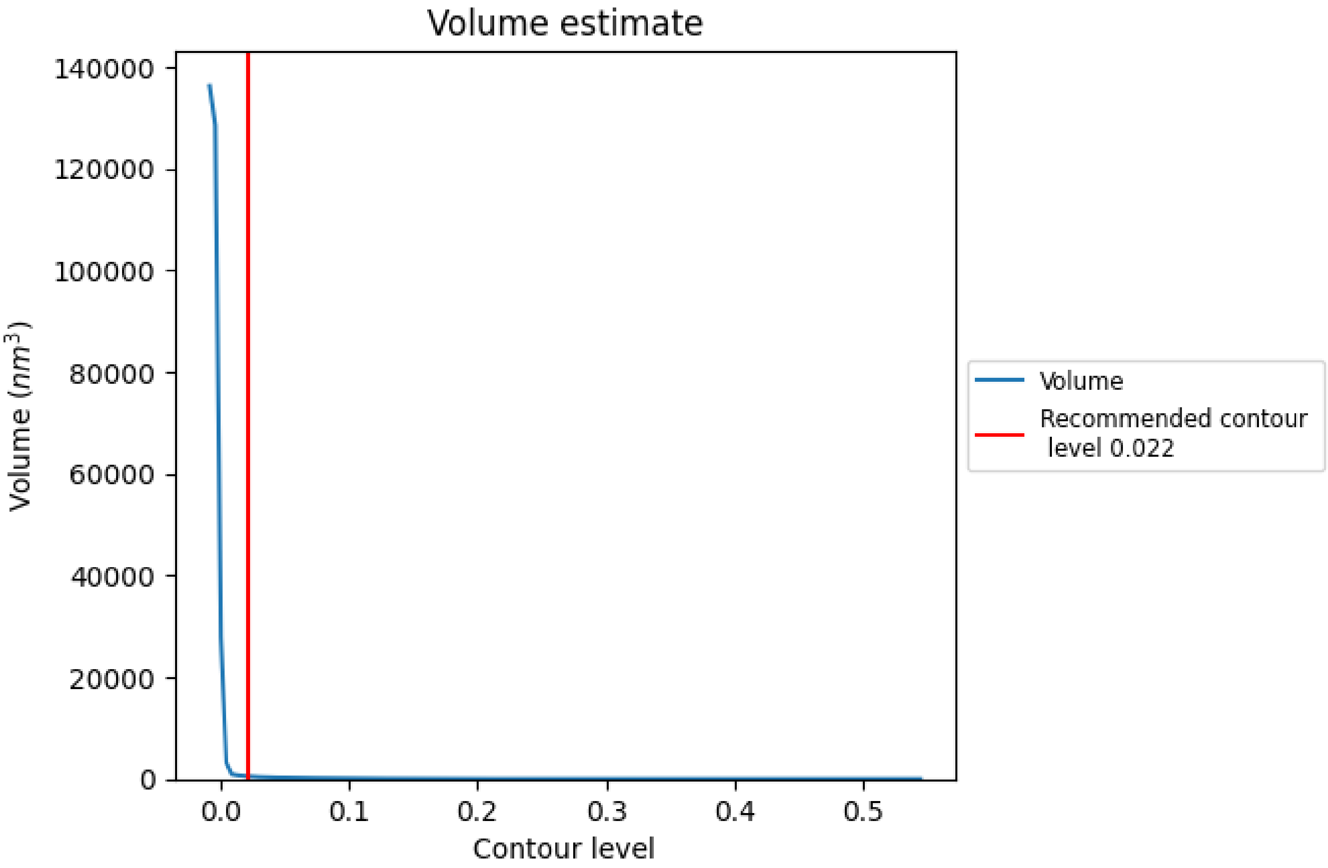
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

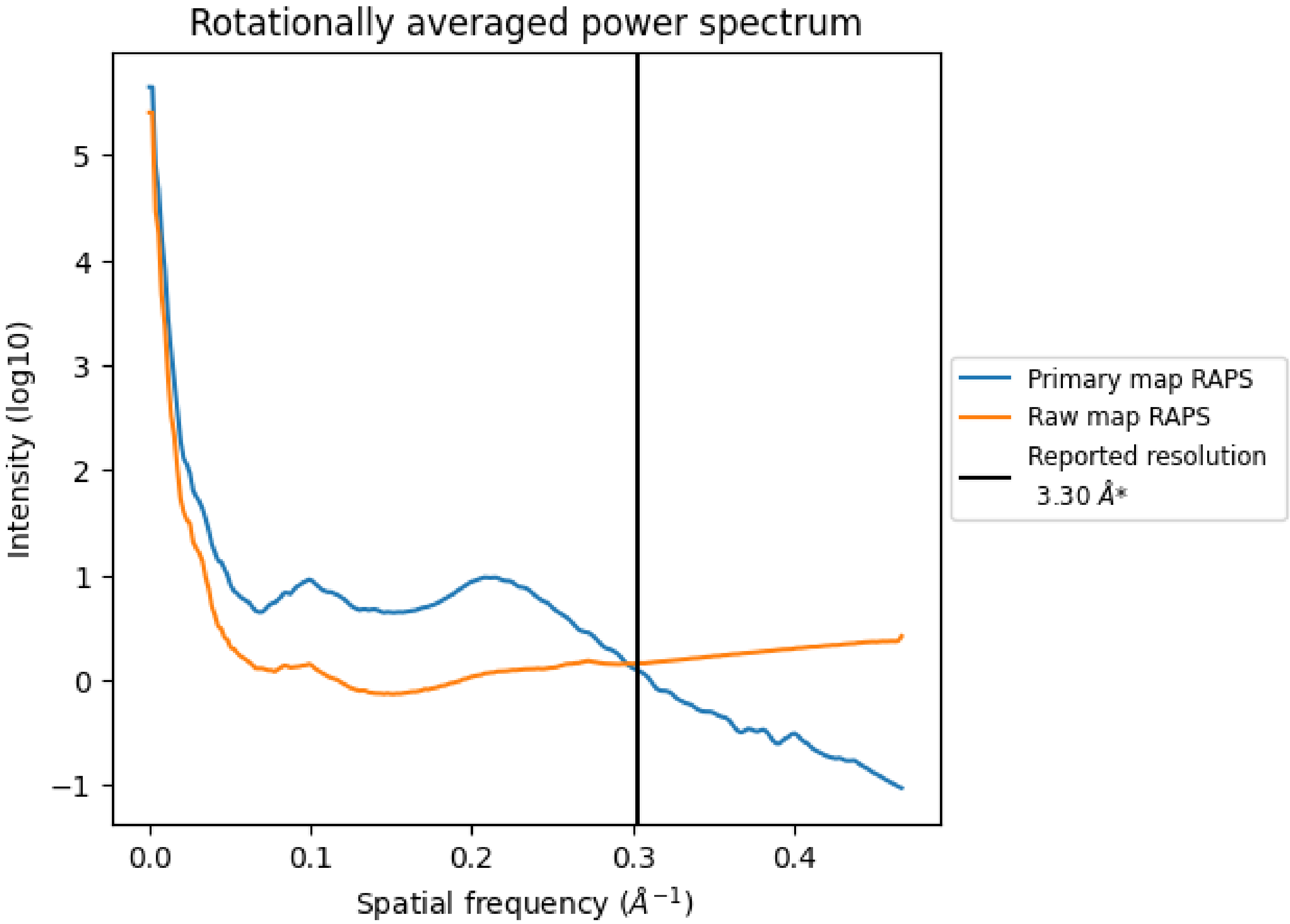
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 518 nm^3; this corresponds to an approximate mass of 468 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

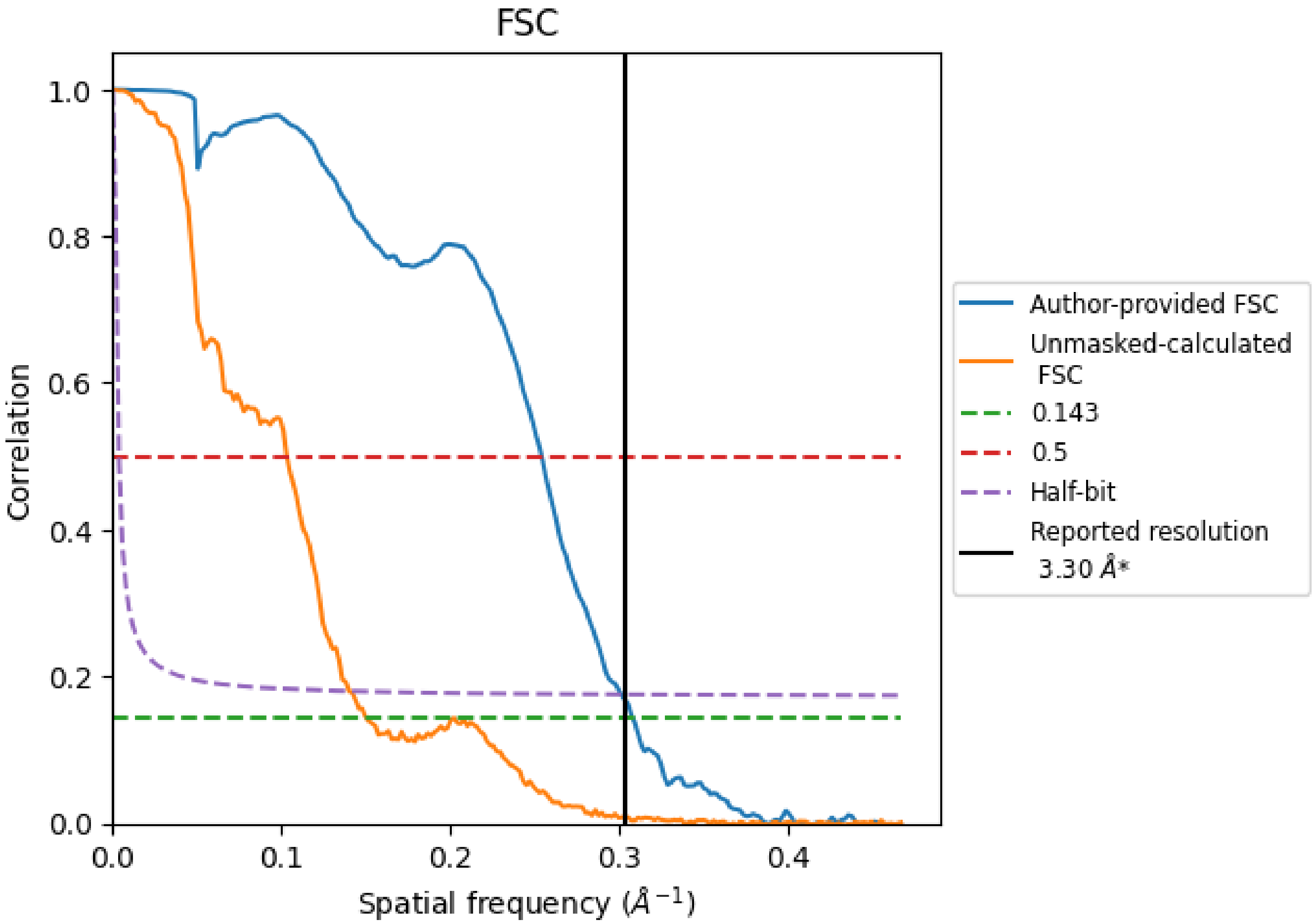


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates ⓘ

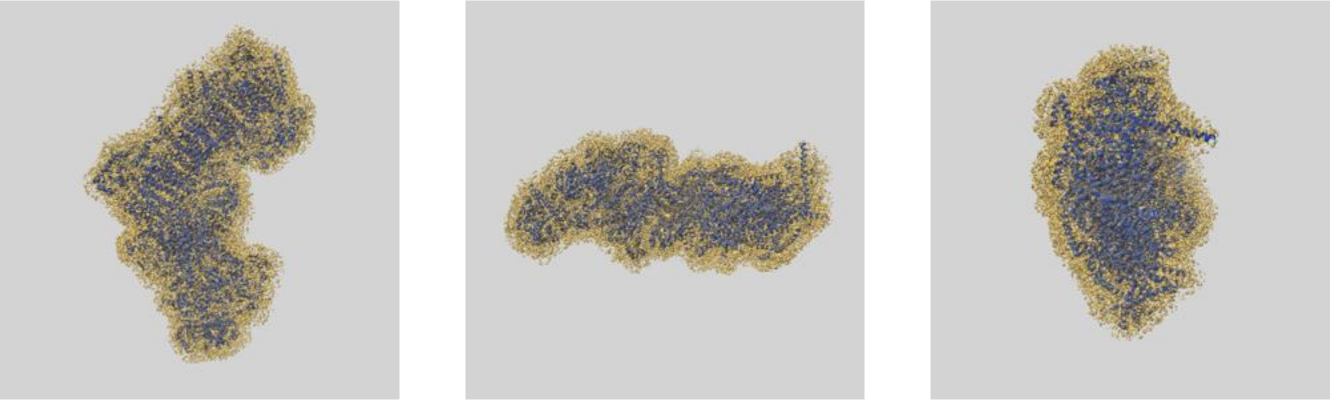
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.94	3.32
Unmasked-calculated*	6.65	9.69	7.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.65 differs from the reported value 3.3 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-18067 and PDB model 8Q1U. Per-residue inclusion information can be found in section 3 on page 23.

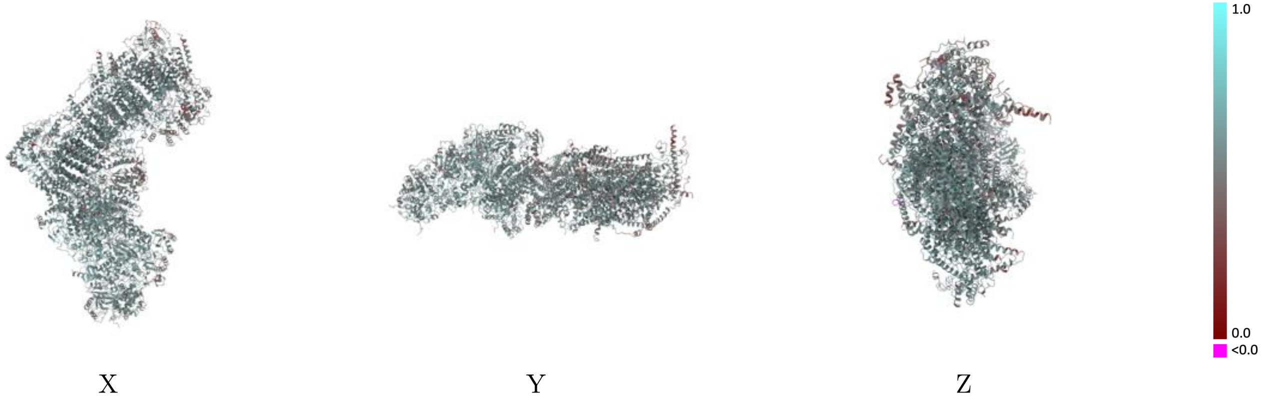
9.1 Map-model overlay (i)



X Y Z

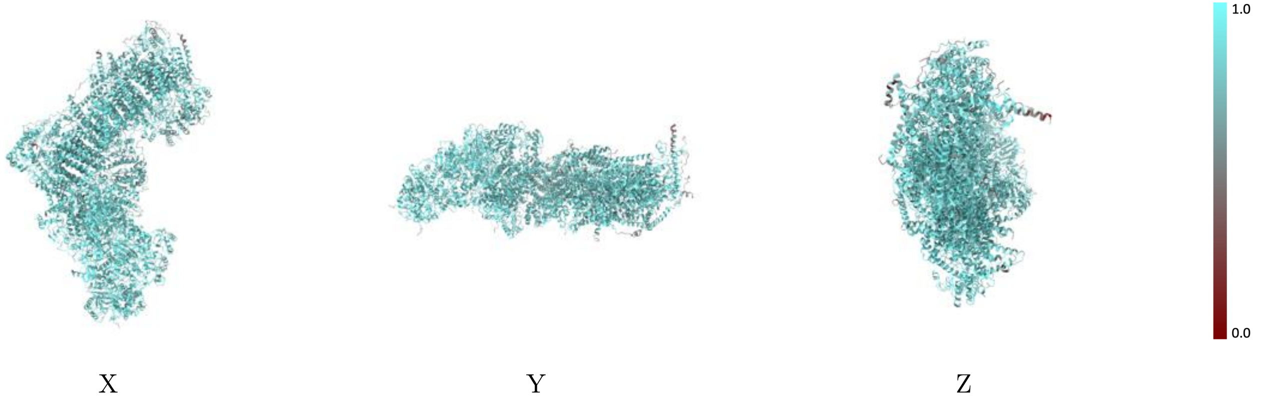
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



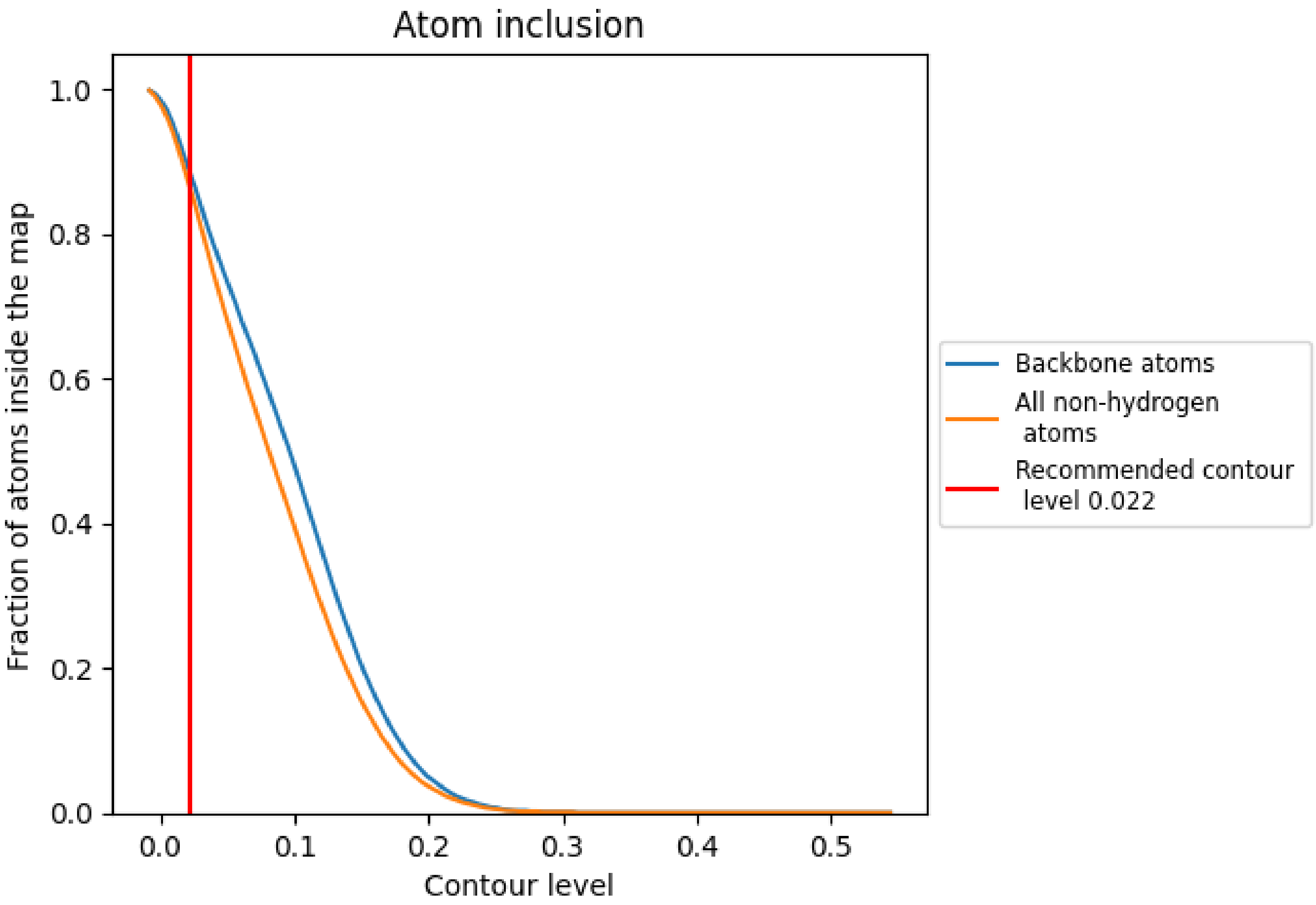
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.5500
A	0.8740	0.5630
B	0.9090	0.5860
C	0.9350	0.6060
D	0.9190	0.5940
E	0.8600	0.5330
F	0.8740	0.5550
G	0.8880	0.5680
H	0.8970	0.5740
I	0.9340	0.6080
J	0.8480	0.5390
K	0.9160	0.5740
L	0.8620	0.5480
M	0.9120	0.5880
N	0.9230	0.5910
O	0.8440	0.5240
P	0.8500	0.5360
Q	0.8950	0.5770
R	0.8850	0.5660
S	0.8120	0.5220
T	0.6980	0.4290
U	0.7670	0.4670
V	0.8570	0.5510
W	0.8730	0.5510
X	0.8610	0.5490
Y	0.8380	0.5220
Z	0.8520	0.5440
a	0.9020	0.5790
b	0.8440	0.5400
c	0.8300	0.5350
d	0.8630	0.5530
e	0.8140	0.5330
f	0.7540	0.4710
g	0.8280	0.5210
h	0.8720	0.5570

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.7400	0.4540
j	0.7700	0.4540
k	0.7170	0.4460
l	0.8370	0.5200
m	0.8200	0.5180
n	0.8200	0.5040
o	0.7420	0.4610
p	0.8170	0.5160
q	0.8880	0.5710
r	0.8920	0.5770
s	0.8540	0.5330