Full wwPDB EM Validation Report ⓘ

Feb 1, 2023 – 08:51 pm GMT

PDB ID	:	7R46
EMDB ID	:	EMD-14277
Title	:	Bovine complex I in the presence of IM1761092, deactive class ii (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.40 Å(reported)

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

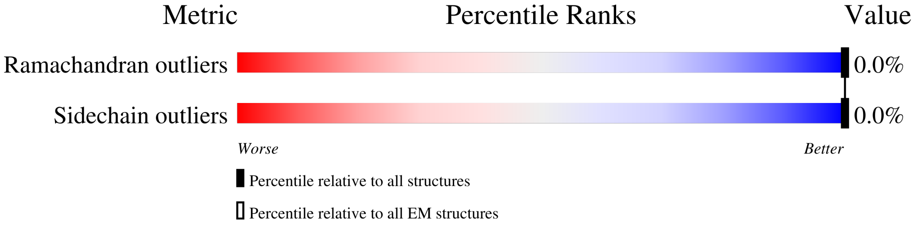
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance ⓘ

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

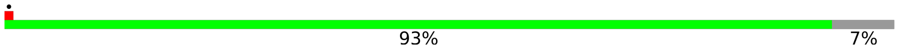
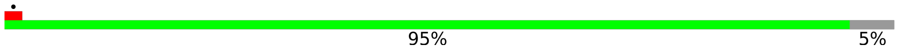
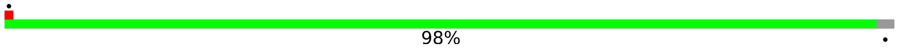
The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	
2	B	216	
3	C	266	
4	D	463	
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	

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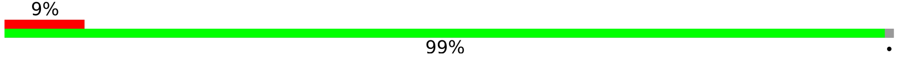
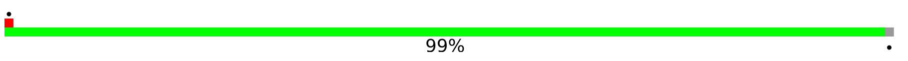
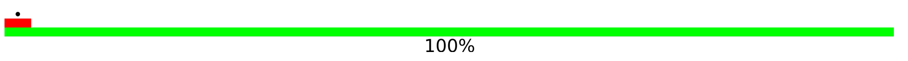
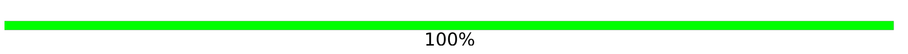
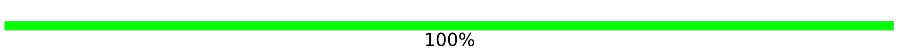
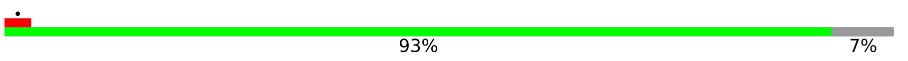
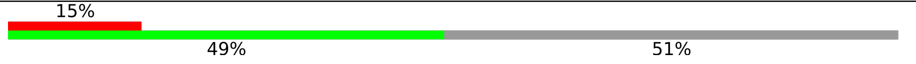
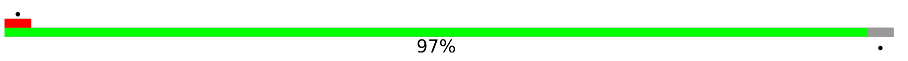
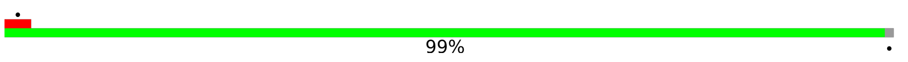
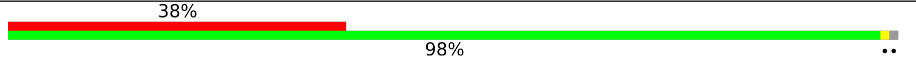
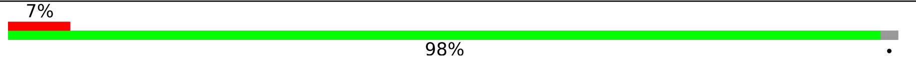
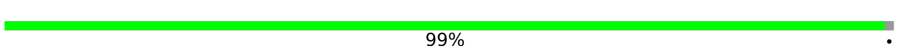
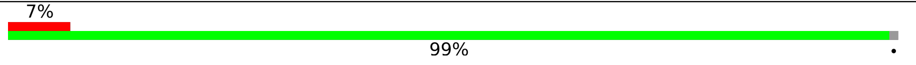
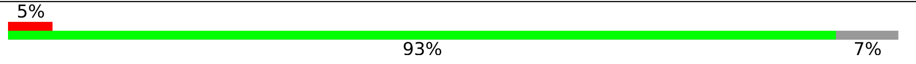
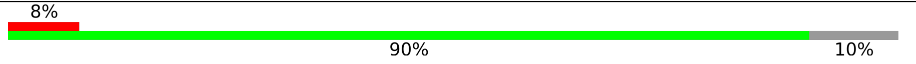
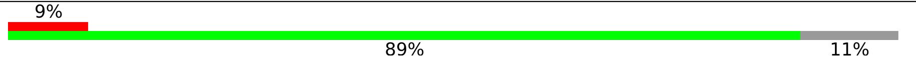
Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	

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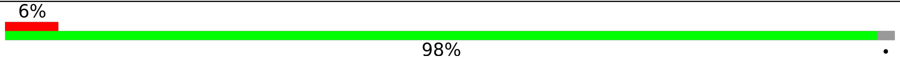
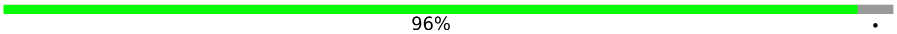
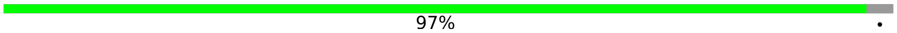
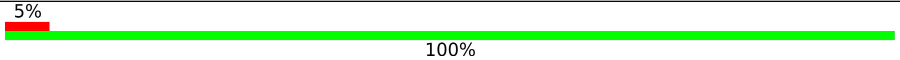
Mol	Chain	Length	Quality of chain
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 67614 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	101	814	555	118	136	5	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	155	1241	792	224	211	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	206	1714	1107	295	309	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	3395	2168	586	616	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	213	1655	1057	277	311	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	430	3310	2085	591	614	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	688	5279	3307	920	1013	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	312	2462	1651	378	410	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	174	1337	902	189	234	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	97	739	483	111	130	15	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	4784	3181	736	824	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	289	2298	1469	415	409	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	125	1016	641	181	191	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	94	Total 720	C 442	N 134	O 141	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	82	Total 663	C 416	N 124	O 121	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total 612	C 393	N 90	O 124	S 5	0	0
20	U	84	Total 681	C 439	N 100	O 137	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	112	Total 911	C 589	N 154	O 165	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	114	Total 971	C 622	N 180	O 165	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
			Total	C	N	O	S		
24	Y	140	1030	657	176	191	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	141	1152	740	201	202	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	69	561	361	103	92	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	83	651	425	109	115	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	48	405	268	69	68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	112	934	613	157	161	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	95	799	506	150	137	6	0	0

- 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	51	444	291	78	74	1	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	97	813	523	133	153	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	103	884	584	149	150	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	67	580	381	95	103	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	79	638	418	107	111	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	155	Total 1304	C 844	N 213	O 239	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	126	Total 1050	C 672	N 186	O 192	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	121	Total 1043	C 650	N 200	O 184	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	170	Total 1435	C 900	N 265	O 262	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 1209	C 778	N 216	O 210	S 5	0	0

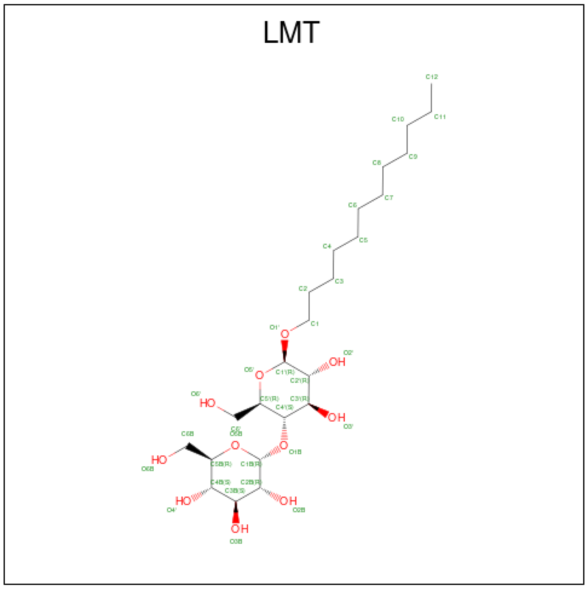
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	94	767	485	143	136	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	43	364	228	65	70	1	0	0

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	A	1	35	24	11	0
45	L	1	35	24	11	0
45	M	1	35	24	11	0
45	M	1	35	24	11	0
45	N	1	35	24	11	0
45	N	1	35	24	11	0
45	Y	1	35	24	11	0

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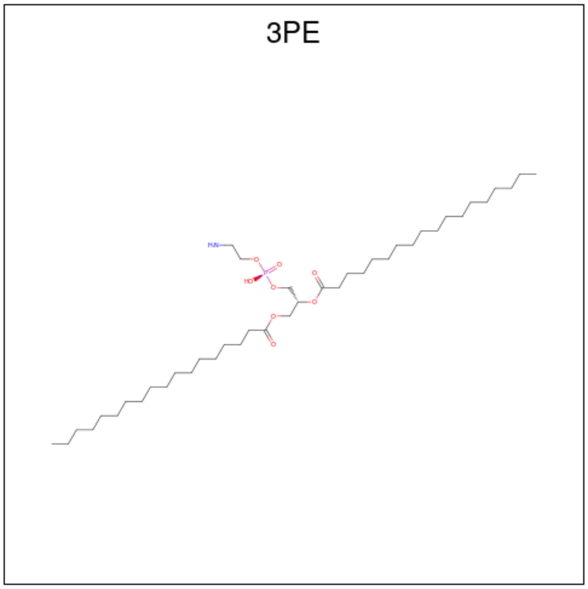
Mol	Chain	Residues	Atoms	AltConf
45	h	1	Total C O 35 24 11	0
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0
45	l	1	Total C O 35 24 11	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 40 30 1 8 1	0
46	B	1	Total C N O P 36 26 1 8 1	0
46	H	1	Total C N O P 24 14 1 8 1	0
46	I	1	Total C N O P 51 41 1 8 1	0
46	I	1	Total C N O P 31 21 1 8 1	0
46	L	1	Total C N O P 49 39 1 8 1	0
46	L	1	Total C N O P 45 35 1 8 1	0

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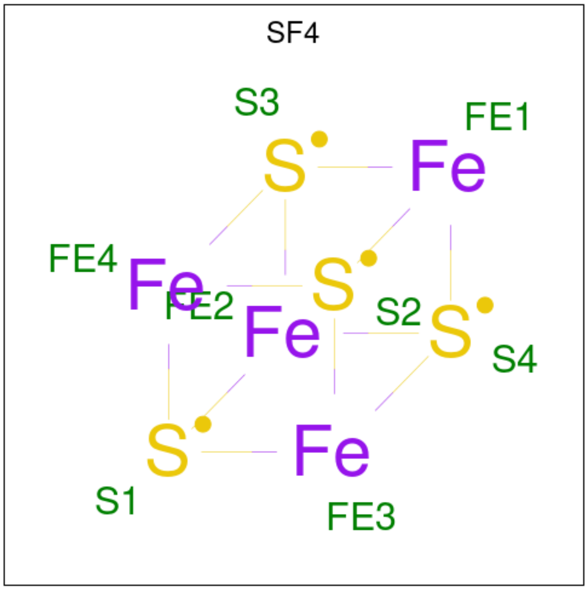
Mol	Chain	Residues	Atoms	AltConf
46	L	1	Total C N O P 29 19 1 8 1	0
46	N	1	Total C N O P 43 33 1 8 1	0
46	N	1	Total C N O P 41 31 1 8 1	0
46	Y	1	Total C N O P 46 36 1 8 1	0
46	Y	1	Total C N O P 35 25 1 8 1	0
46	Z	1	Total C N O P 25 15 1 8 1	0
46	d	1	Total C N O P 38 28 1 8 1	0

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



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

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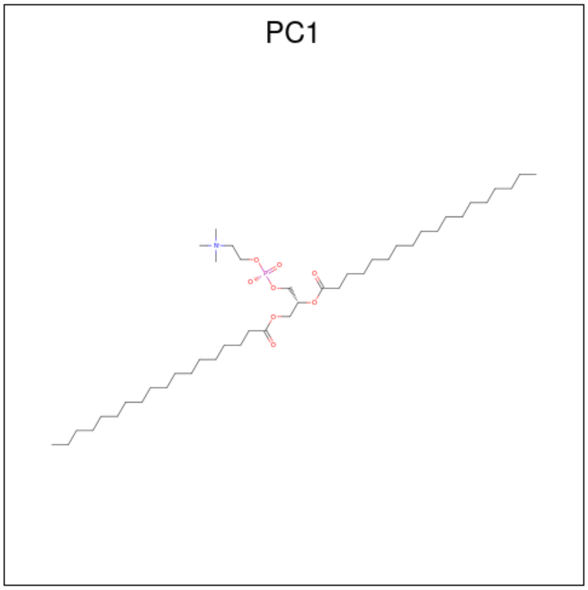
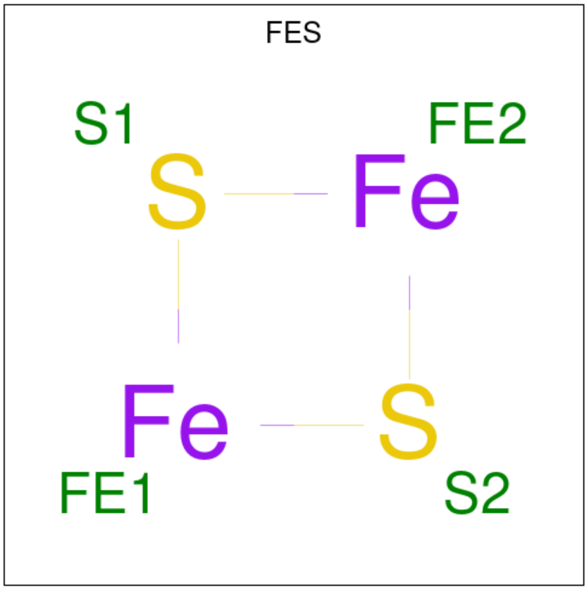
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total 8	Fe 4	S 4	0
47	I	1	Total 8	Fe 4	S 4	0

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



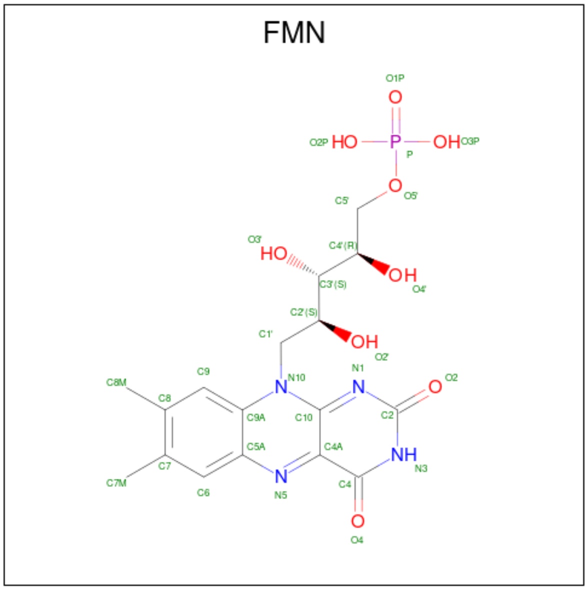
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total 35	C 25	N 1	O 8	P 1	0
48	g	1	Total 49	C 39	N 1	O 8	P 1	0

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



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

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

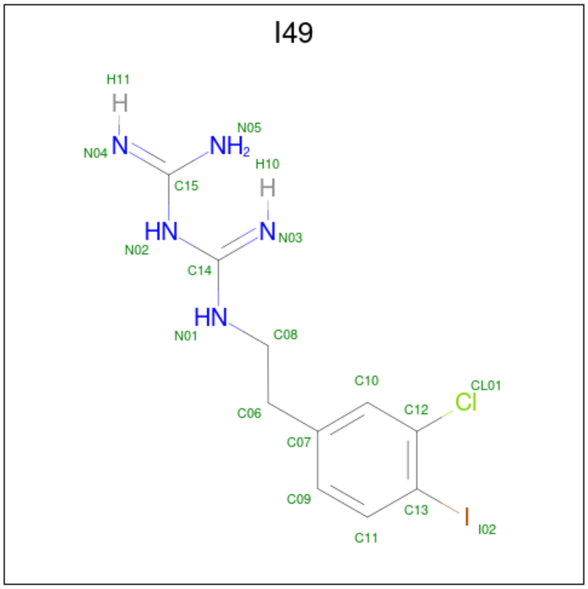


Mol	Chain	Residues	Atoms	AltConf
50	F	1	Total C N O P 31 17 4 9 1	0

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

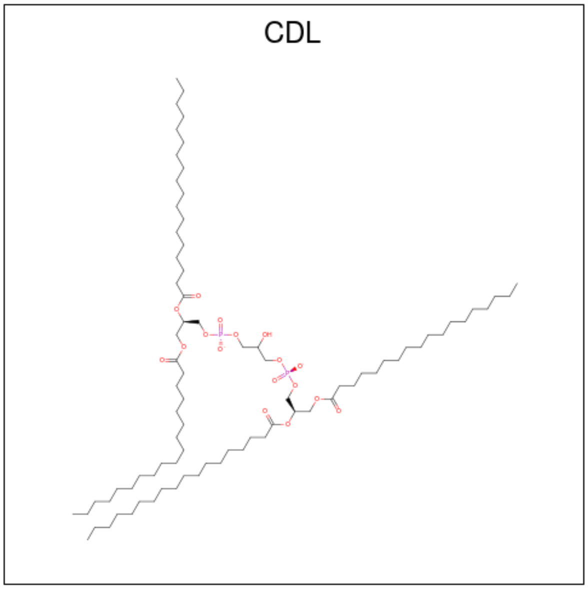
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
51	G	1	1	1	0

- Molecule 52 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



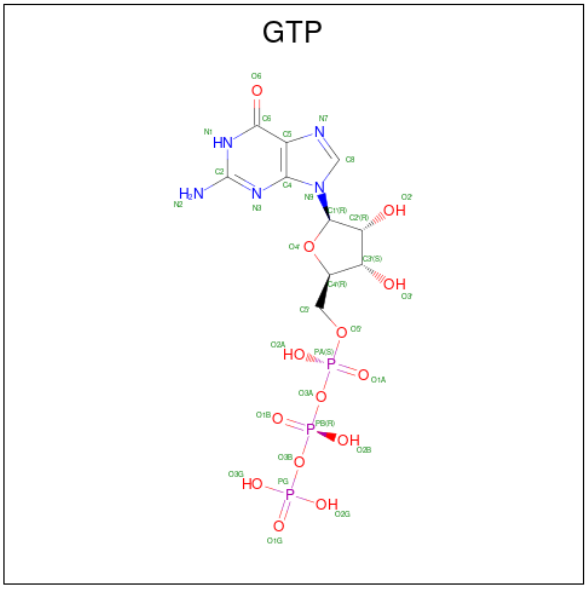
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	I	N	
52	H	1	17	10	1	1	5	0

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



Mol	Chain	Residues	Atoms				AltConf
53	K	1	Total 50	C 35	O 13	P 2	0
53	L	1	Total 64	C 45	O 17	P 2	0
53	X	1	Total 72	C 53	O 17	P 2	0
53	d	1	Total 65	C 46	O 17	P 2	0
53	h	1	Total 67	C 48	O 17	P 2	0
53	q	1	Total 61	C 42	O 17	P 2	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



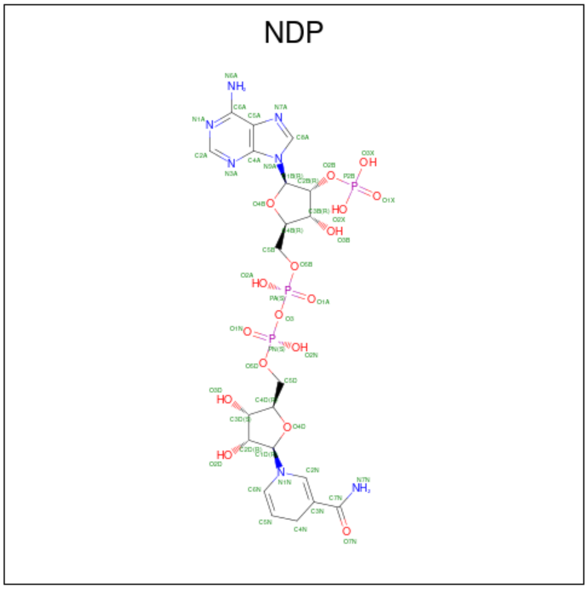
Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

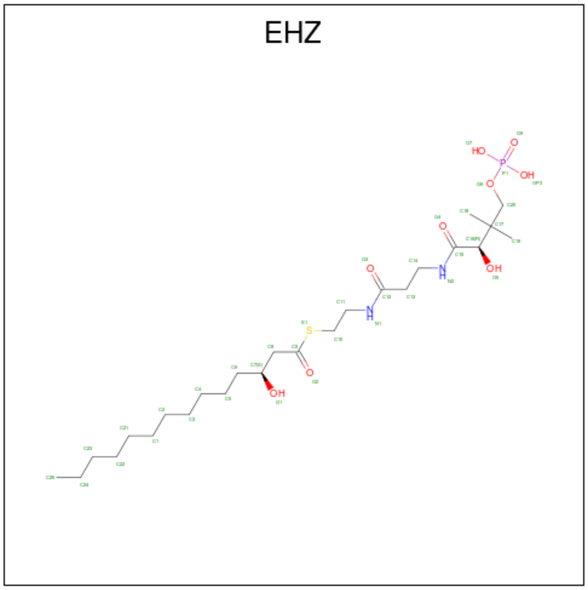


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

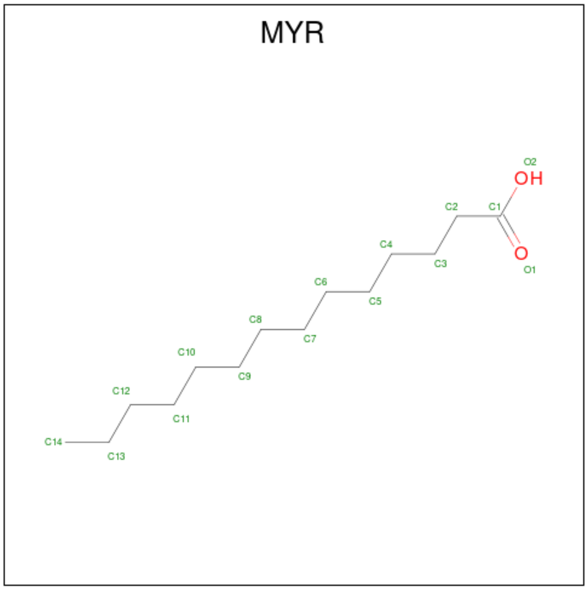
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	4	Total O 4 4	0
60	B	42	Total O 42 42	0
60	C	61	Total O 61 61	0
60	D	96	Total O 96 96	0
60	E	11	Total O 11 11	0
60	F	44	Total O 44 44	0
60	G	139	Total O 139 139	0
60	H	30	Total O 30 30	0
60	I	76	Total O 76 76	0
60	J	3	Total O 3 3	0
60	K	2	Total O 2 2	0
60	L	25	Total O 25 25	0
60	M	26	Total O 26 26	0
60	N	17	Total O 17 17	0
60	O	5	Total O 5 5	0
60	P	25	Total O 25 25	0
60	Q	51	Total O 51 51	0
60	R	18	Total O 18 18	0
60	U	2	Total O 2 2	0
60	V	10	Total O 10 10	0
60	W	3	Total O 3 3	0
60	X	10	Total O 10 10	0

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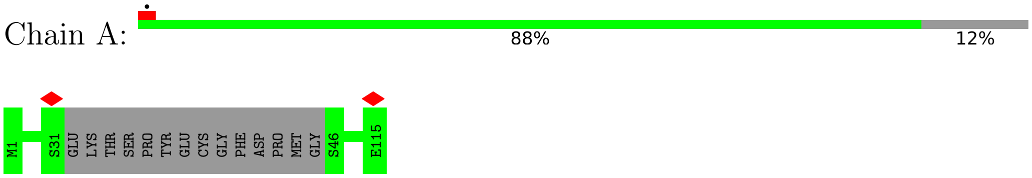
Mol	Chain	Residues	Atoms	AltConf
60	Y	1	Total O 1 1	0
60	Z	11	Total O 11 11	0
60	a	9	Total O 9 9	0
60	b	3	Total O 3 3	0
60	d	7	Total O 7 7	0
60	e	8	Total O 8 8	0
60	f	3	Total O 3 3	0
60	g	7	Total O 7 7	0
60	h	8	Total O 8 8	0
60	i	4	Total O 4 4	0
60	j	2	Total O 2 2	0
60	k	3	Total O 3 3	0
60	l	13	Total O 13 13	0
60	m	7	Total O 7 7	0
60	n	14	Total O 14 14	0
60	o	7	Total O 7 7	0
60	p	14	Total O 14 14	0
60	q	21	Total O 21 21	0
60	r	14	Total O 14 14	0
60	s	3	Total O 3 3	0

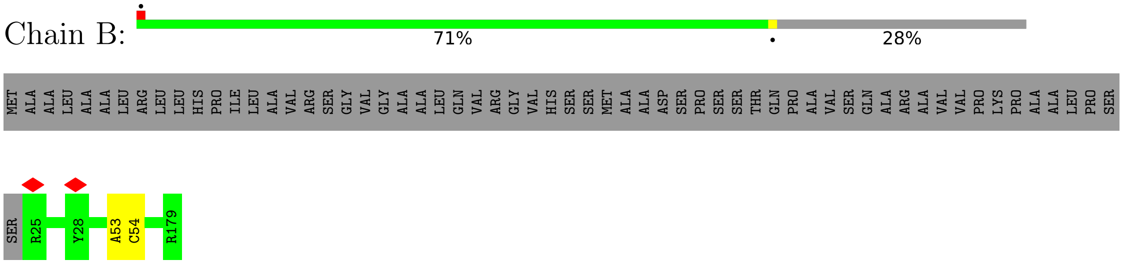
3 Residue-property plots

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.

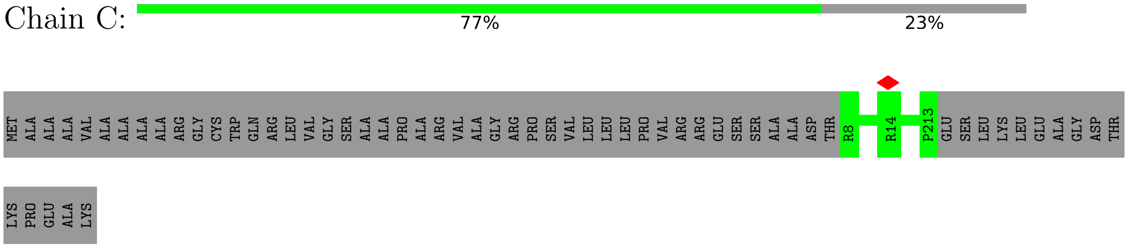
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



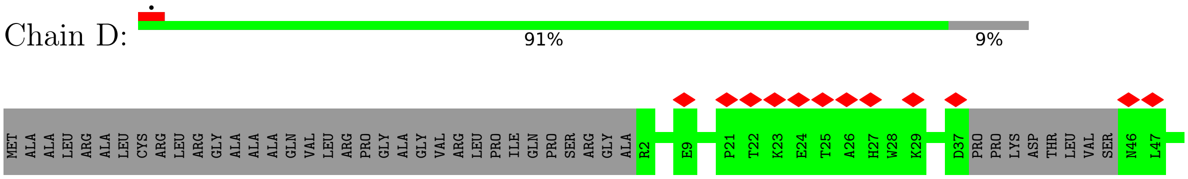
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

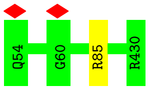


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



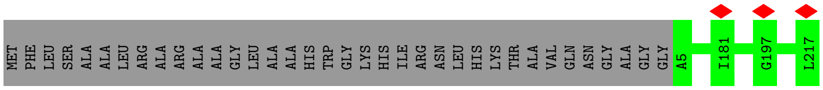
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





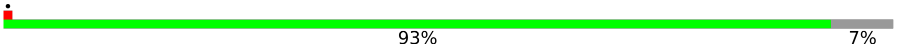
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

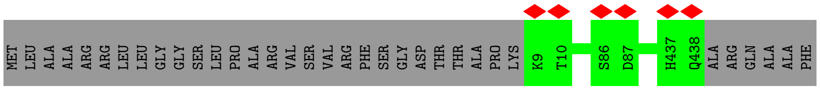
Chain E:



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

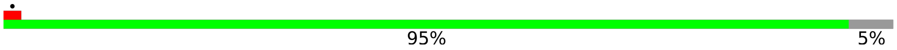
Chain F:

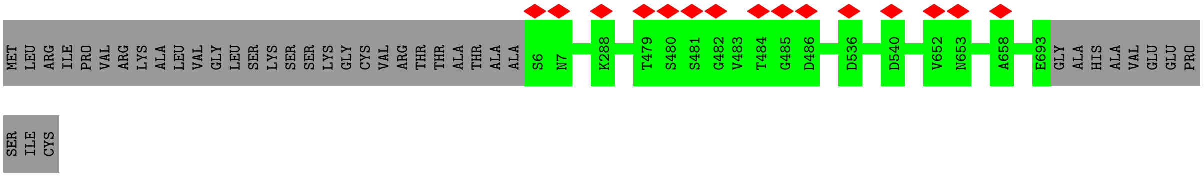




- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

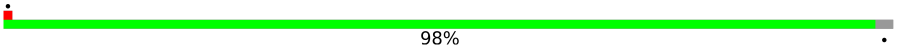
Chain G:

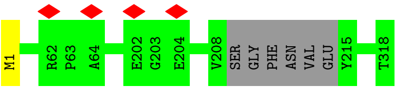




- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

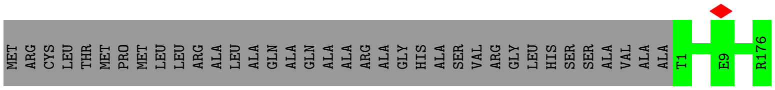
Chain H:





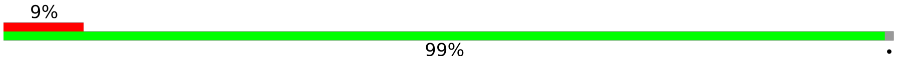
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

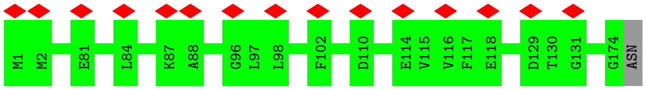
Chain I:



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

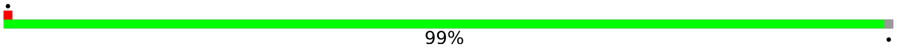
Chain J:

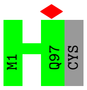




- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

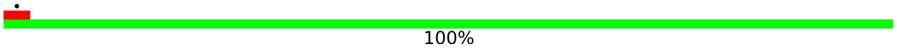
Chain K:

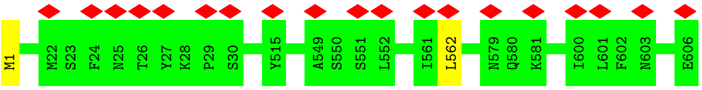




- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

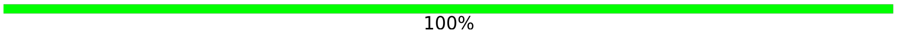
Chain L:

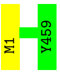




- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

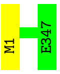
Chain M:





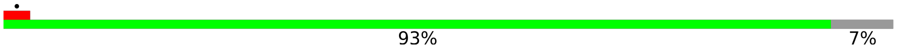
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

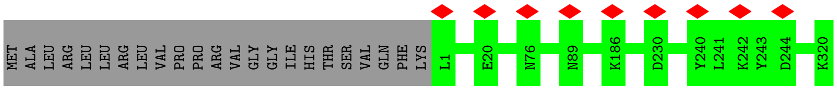
Chain N:



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

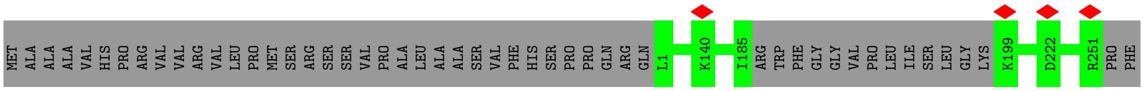
Chain O:

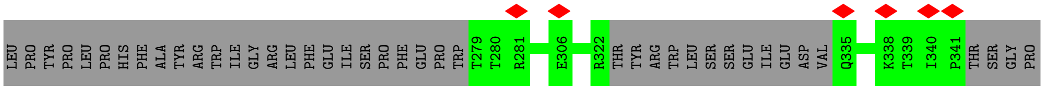




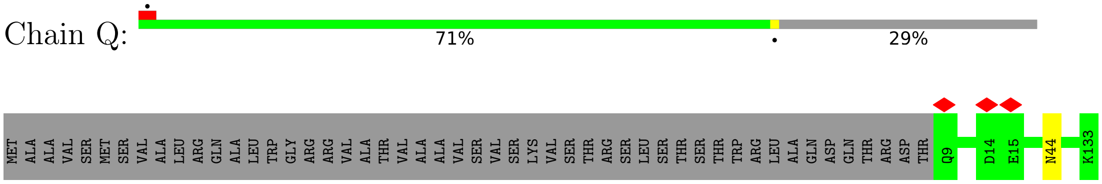
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:

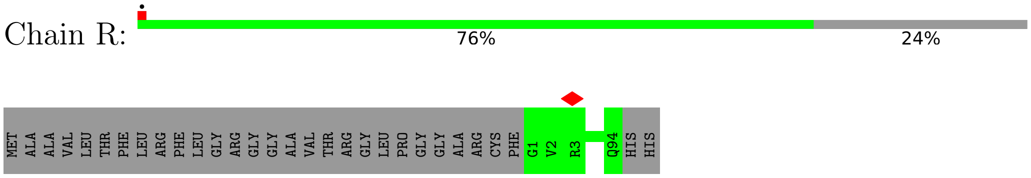




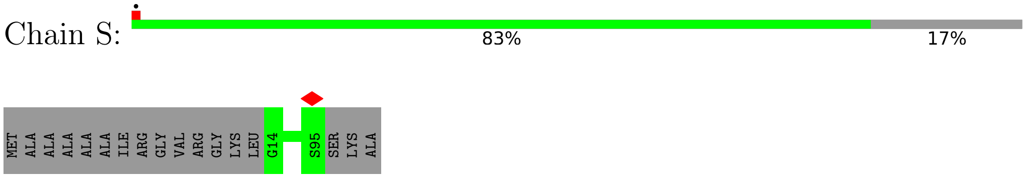
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



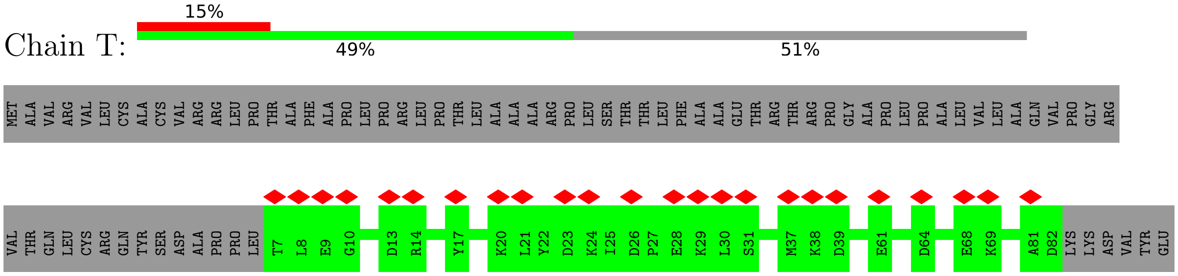
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



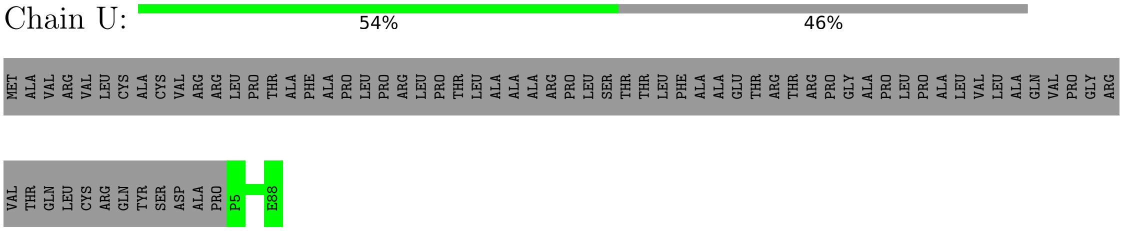
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



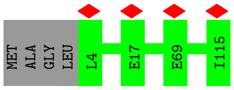
- Molecule 20: Acyl carrier protein, mitochondrial



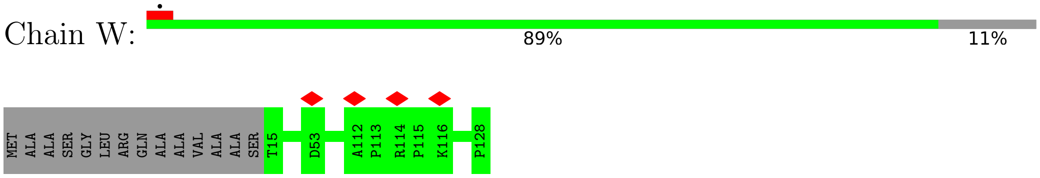
- Molecule 20: Acyl carrier protein, mitochondrial



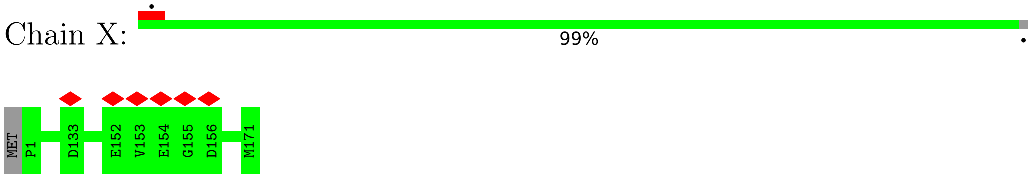
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



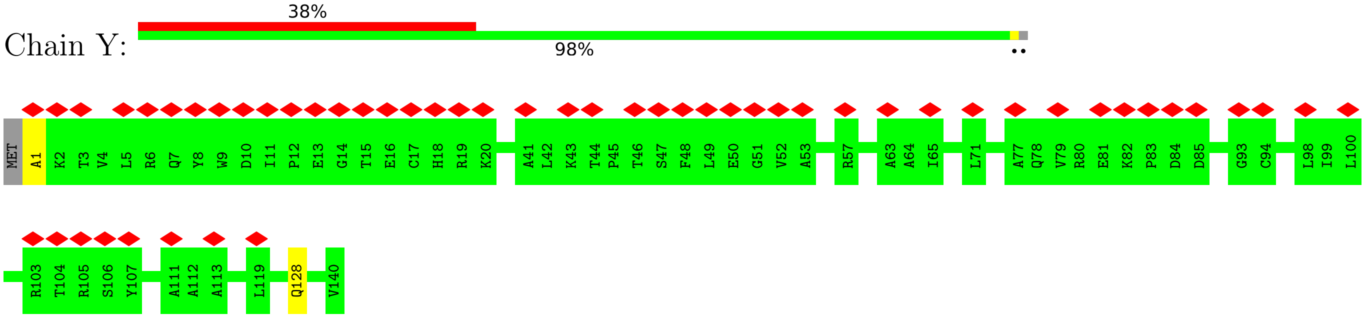
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



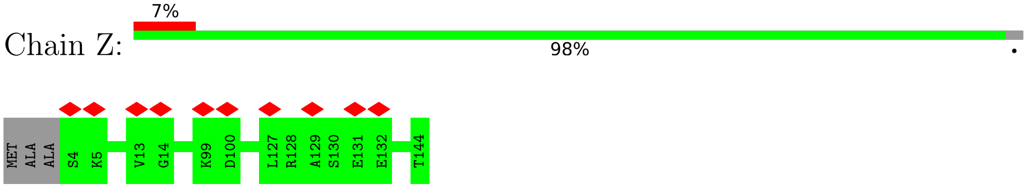
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



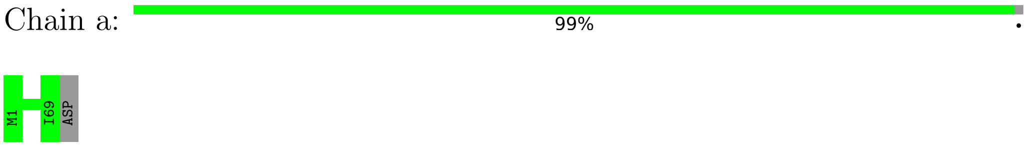
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



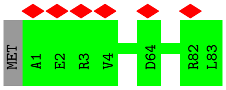
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

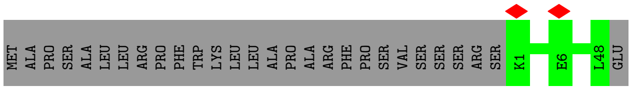


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



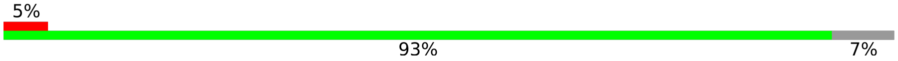
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

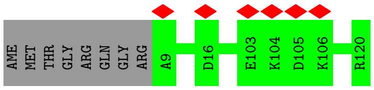
Chain c:



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

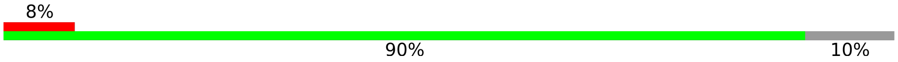
Chain d:

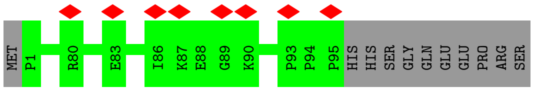




- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

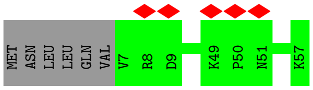
Chain e:





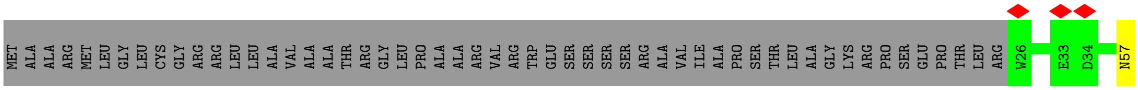
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

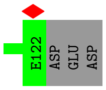
Chain f:



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

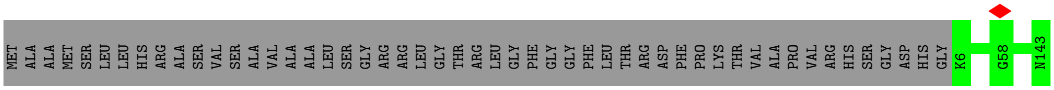
Chain g:





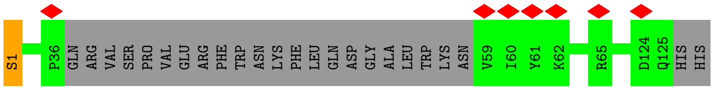
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



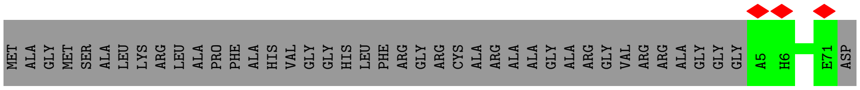
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



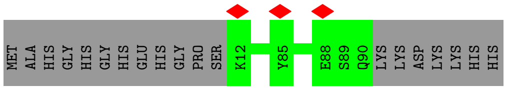
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



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

Chain k:

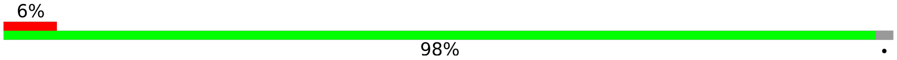


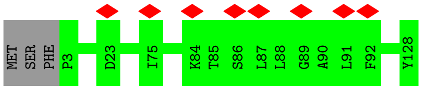
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:

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

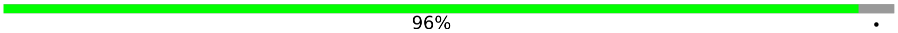
Chain m:

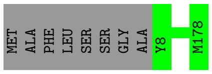




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

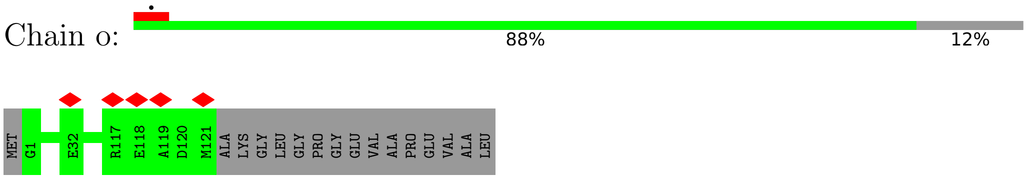
Chain n:





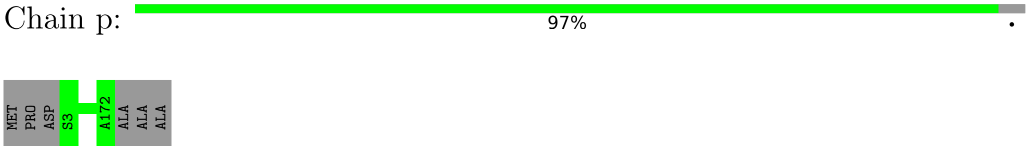
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



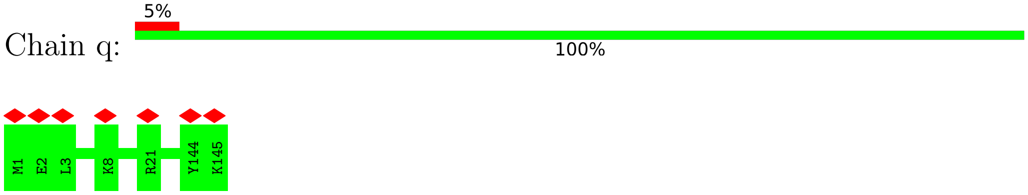
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:



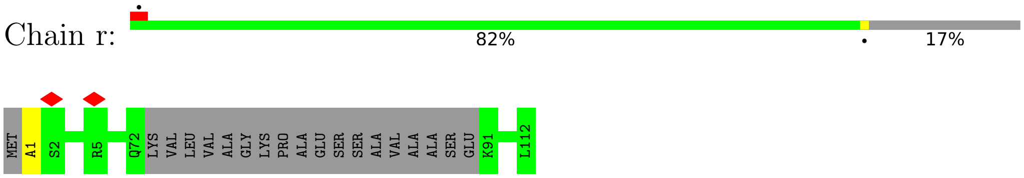
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



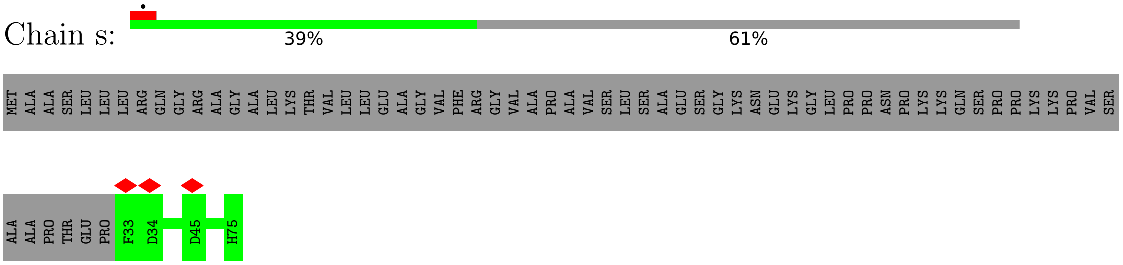
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

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, Not provided	
Number of particles used	35448	Depositor
Resolution determination method	OTHER	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	32.083	Depositor
Minimum map value	-12.979	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FES, LMT, CDL, GTP, 2MR, MYR, K, NDP, SAC, FMN, AYA, PC1, SF4, 3PE, EHZ, ZN, FME, I49

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	0.31	0/824	0.43	0/1128
2	B	0.42	1/1272 (0.1%)	0.48	0/1720
3	C	0.35	0/1765	0.45	0/2403
4	D	0.34	0/3470	0.44	0/4699
5	E	0.33	0/1695	0.44	0/2307
6	F	0.32	0/3384	0.46	0/4573
7	G	0.32	0/5367	0.47	0/7274
8	H	0.34	0/2522	0.44	0/3445
9	I	0.36	0/1445	0.47	0/1956
10	J	0.33	0/1362	0.43	0/1848
11	K	0.32	0/739	0.47	0/1000
12	L	0.33	0/4900	0.42	0/6667
13	M	0.32	0/3738	0.42	0/5097
14	N	0.31	0/2792	0.43	0/3800
15	O	0.34	0/2651	0.41	0/3587
16	P	0.31	0/2348	0.44	0/3172
17	Q	0.32	0/1039	0.45	0/1404
18	R	0.35	0/731	0.46	0/984
19	S	0.30	0/674	0.45	0/908
20	T	0.30	0/621	0.39	0/837
20	U	0.38	0/692	0.41	0/932
21	V	0.29	0/931	0.37	0/1261
22	W	0.31	0/995	0.42	0/1337
23	X	0.33	0/1439	0.41	0/1942
24	Y	0.29	0/1042	0.41	0/1414
25	Z	0.32	0/1181	0.42	0/1592
26	a	0.35	0/576	0.42	0/775
27	b	0.32	0/672	0.41	0/923
28	c	0.30	0/418	0.36	0/567
29	d	0.36	0/964	0.38	0/1305
30	e	0.30	0/818	0.42	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
31	f	0.32	0/457	0.40	0/616
32	g	0.35	0/839	0.38	0/1140
33	h	0.34	0/1188	0.41	0/1607
34	i	0.37	0/904	0.43	0/1230
35	j	0.36	0/607	0.42	0/833
36	k	0.35	0/657	0.41	0/887
37	l	0.39	0/1358	0.41	0/1858
38	m	0.36	0/1076	0.41	0/1455
39	n	0.37	0/1540	0.41	0/2085
40	o	0.39	0/1068	0.41	0/1430
41	p	0.36	0/1468	0.41	0/1979
42	q	0.33	0/1250	0.44	0/1698
43	r	0.33	0/780	0.44	0/1056
44	s	0.32	0/375	0.42	0/507
All	All	0.34	1/66634 (0.0%)	0.43	0/90331

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
34	i	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	CYS	CB-SG	-5.92	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain

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	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
2	B	153/216 (71%)	144 (94%)	8 (5%)	1 (1%)	22	32
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	416/463 (90%)	398 (96%)	18 (4%)	0	100	100
5	E	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
6	F	428/464 (92%)	419 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	661 (96%)	25 (4%)	0	100	100
8	H	308/318 (97%)	294 (96%)	14 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	157 (91%)	15 (9%)	0	100	100
11	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	580 (96%)	23 (4%)	1 (0%)	47	62
13	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	311 (98%)	7 (2%)	0	100	100
16	P	281/380 (74%)	275 (98%)	6 (2%)	0	100	100
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	92/124 (74%)	90 (98%)	2 (2%)	0	100	100
19	S	80/99 (81%)	78 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	72 (97%)	2 (3%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	132 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	139/144 (96%)	131 (94%)	8 (6%)	0	100	100
26	a	67/70 (96%)	67 (100%)	0	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
29	d	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	95/154 (62%)	89 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
38	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	119/137 (87%)	113 (95%)	6 (5%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	38 (93%)	3 (7%)	0	100	100
All	All	7993/9212 (87%)	7757 (97%)	234 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
2	B	53	ALA

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	88/100 (88%)	88 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	362/392 (92%)	362 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	344/368 (94%)	344 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	268/274 (98%)	268 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	84/85 (99%)	84 (100%)	0	100	100
12	L	529/533 (99%)	529 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	248/327 (76%)	248 (100%)	0	100	100
17	Q	112/153 (73%)	111 (99%)	1 (1%)	78	90
18	R	77/97 (79%)	77 (100%)	0	100	100
19	S	73/82 (89%)	73 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	100 (99%)	1 (1%)	76	88
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	58/59 (98%)	58 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	f	48/54 (89%)	48 (100%)	0	100	100
32	g	88/131 (67%)	87 (99%)	1 (1%)	73	87
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	98 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	61 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	112/115 (97%)	112 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	42/92 (46%)	42 (100%)	0	100	100
All	All	7059/7892 (89%)	7056 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	44	ASN
24	Y	128	GLN
32	g	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	59	HIS
4	D	157	HIS
6	F	356	HIS
15	O	190	HIS
17	Q	44	ASN
22	W	126	HIS
24	Y	128	GLN
38	m	74	ASN
39	n	12	GLN
44	s	44	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\| > 2$
10	FME	J	1	10	8,9,10	0.93	0	7,9,11	0.83	0
8	FME	H	1	8	8,9,10	0.98	1 (12%)	7,9,11	0.81	0
34	SAC	i	1	34	7,8,9	1.88	1 (14%)	8,9,11	1.78	1 (12%)
1	FME	A	1	1	8,9,10	0.95	0	7,9,11	0.96	0
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	1.21	1 (14%)
11	FME	K	1	11	8,9,10	0.91	0	7,9,11	0.78	0
14	FME	N	1	14	8,9,10	1.02	1 (12%)	7,9,11	0.86	0
43	AYA	r	1	43	6,7,8	1.77	2 (33%)	5,8,10	1.29	1 (20%)
4	2MR	D	85	4	10,12,13	2.65	4 (40%)	5,13,15	0.83	0
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	1.04	1 (14%)
24	AYA	Y	1	24	6,7,8	1.79	1 (16%)	5,8,10	1.18	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
10	FME	J	1	10	-	4/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-
34	SAC	i	1	34	-	0/7/8/10	-
1	FME	A	1	1	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	N	1	14	-	3/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	2/7/9/11	-
24	AYA	Y	1	24	-	1/4/6/8	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.97	1.44	1.33
4	D	85	2MR	CZ-NE	4.76	1.44	1.34
34	i	1	SAC	O-C	4.18	1.36	1.19
4	D	85	2MR	O-C	3.93	1.35	1.19
24	Y	1	AYA	CT-N	3.27	1.45	1.34
43	r	1	AYA	CT-N	3.10	1.45	1.34
4	D	85	2MR	CQ1-NH1	-2.09	1.42	1.46
14	N	1	FME	CA-N	-2.08	1.43	1.46
43	r	1	AYA	OT-CT	-2.03	1.18	1.23
8	H	1	FME	CA-N	-2.00	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.50	112.98	124.78
13	M	1	FME	C-CA-N	2.69	114.59	109.73
43	r	1	AYA	CM-CT-N	2.24	119.90	116.10
12	L	1	FME	C-CA-N	2.19	113.69	109.73
24	Y	1	AYA	CM-CT-N	2.07	119.61	116.10

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
12	L	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
8	H	1	FME	CB-CG-SD-CE
10	J	1	FME	C-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
24	Y	1	AYA	CB-CA-N-CT
10	J	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 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 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	X	1701	-	71,71,99	1.02	7 (9%)	77,83,111	1.19	5 (6%)
53	CDL	L	702	-	63,63,99	1.08	6 (9%)	69,75,111	1.11	4 (5%)
45	LMT	M	801	-	36,36,36	1.11	2 (5%)	47,47,47	1.21	4 (8%)
46	3PE	Z	401	-	24,24,50	1.21	4 (16%)	27,29,55	1.16	2 (7%)
45	LMT	h	1003	-	36,36,36	1.16	2 (5%)	47,47,47	0.97	2 (4%)
47	SF4	G	802	7	0,12,12	-	-	-		
46	3PE	L	703	-	44,44,50	0.91	3 (6%)	47,49,55	1.11	2 (4%)
53	CDL	d	1202	-	64,64,99	1.07	7 (10%)	70,76,111	1.14	4 (5%)
46	3PE	L	705	-	28,28,50	1.12	4 (14%)	31,33,55	1.16	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	SF4	I	202	9	0,12,12	-	-	-		
47	SF4	I	203	9	0,12,12	-	-	-		
49	FES	G	803	7	0,4,4	-	-	-		
45	LMT	A	301	-	36,36,36	1.21	2 (5%)	47,47,47	0.94	1 (2%)
53	CDL	K	401	-	49,49,99	1.01	5 (10%)	54,58,111	1.01	2 (3%)
45	LMT	N	901	-	36,36,36	1.16	3 (8%)	47,47,47	0.79	0
46	3PE	I	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.05	2 (3%)
45	LMT	M	802	-	36,36,36	1.17	3 (8%)	47,47,47	1.37	3 (6%)
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	Y	601	-	45,45,50	0.90	3 (6%)	48,50,55	1.16	3 (6%)
58	EHZ	T	101	20	29,36,37	1.66	4 (13%)	35,44,47	1.48	4 (11%)
48	PC1	B	1003	-	34,34,53	1.15	4 (11%)	40,42,61	1.13	2 (5%)
59	MYR	o	201	40	14,14,15	0.81	0	13,13,15	0.66	0
56	NDP	P	501	-	45,52,52	2.10	5 (11%)	53,80,80	1.68	10 (18%)
45	LMT	j	101	-	36,36,36	1.17	2 (5%)	47,47,47	0.81	0
54	GTP	O	401	55	26,34,34	2.92	10 (38%)	32,54,54	1.80	10 (31%)
45	LMT	h	1002	-	36,36,36	1.17	3 (8%)	47,47,47	1.31	5 (10%)
46	3PE	d	1201	-	37,37,50	0.99	4 (10%)	40,42,55	1.10	2 (5%)
48	PC1	g	1501	-	48,48,53	0.99	3 (6%)	54,56,61	0.98	2 (3%)
46	3PE	N	902	-	42,42,50	0.93	3 (7%)	45,47,55	1.13	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		
49	FES	E	301	5	0,4,4	-	-	-		
58	EHZ	U	101	20	29,36,37	1.64	5 (17%)	35,44,47	1.47	4 (11%)
45	LMT	Y	603	-	36,36,36	1.21	2 (5%)	47,47,47	1.01	1 (2%)
46	3PE	N	904	-	40,40,50	0.94	4 (10%)	43,45,55	1.13	2 (4%)
46	3PE	Y	602	-	34,34,50	1.04	4 (11%)	37,39,55	1.17	2 (5%)
45	LMT	l	201	-	36,36,36	1.22	3 (8%)	47,47,47	1.08	3 (6%)
50	FMN	F	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
46	3PE	I	204	-	30,30,50	1.08	3 (10%)	33,35,55	1.19	3 (9%)
46	3PE	H	601	-	23,23,50	1.61	4 (17%)	24,27,55	1.15	2 (8%)
53	CDL	h	1001	-	66,66,99	1.06	7 (10%)	72,78,111	1.18	4 (5%)
53	CDL	q	201	-	60,60,99	1.11	8 (13%)	66,72,111	1.11	4 (6%)
52	I49	H	602	-	15,17,17	1.53	2 (13%)	21,22,22	2.50	7 (33%)
46	3PE	B	1001	-	35,35,50	1.02	4 (11%)	38,40,55	1.11	2 (5%)
46	3PE	A	302	-	39,39,50	0.94	4 (10%)	42,44,55	1.23	2 (4%)
45	LMT	N	903	-	36,36,36	1.17	3 (8%)	47,47,47	0.90	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
45	LMT	L	704	-	36,36,36	1.18	2 (5%)	47,47,47	0.92	1 (2%)
47	SF4	B	1002	2	0,12,12	-	-	-		
46	3PE	L	701	-	48,48,50	0.87	2 (4%)	51,53,55	1.05	2 (3%)

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	X	1701	-	-	46/82/82/110	-
53	CDL	L	702	-	-	32/74/74/110	-
45	LMT	M	801	-	-	6/21/61/61	0/2/2/2
46	3PE	Z	401	-	-	13/28/28/54	-
45	LMT	h	1003	-	-	6/21/61/61	0/2/2/2
53	CDL	d	1202	-	-	36/75/75/110	-
46	3PE	L	703	-	-	25/48/48/54	-
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	L	705	-	-	15/32/32/54	-
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	I	203	9	-	-	0/6/5/5
49	FES	G	803	7	-	-	0/1/1/1
45	LMT	A	301	-	-	8/21/61/61	0/2/2/2
53	CDL	K	401	-	-	19/54/54/110	-
45	LMT	N	901	-	-	3/21/61/61	0/2/2/2
46	3PE	I	201	-	-	25/54/54/54	-
45	LMT	M	802	-	-	8/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	Y	601	-	-	26/49/49/54	-
58	EHZ	T	101	20	-	14/42/44/45	-
48	PC1	B	1003	-	-	14/38/38/57	-
59	MYR	o	201	40	-	6/11/12/13	-
56	NDP	P	501	-	-	6/30/77/77	0/5/5/5
45	LMT	j	101	-	-	5/21/61/61	0/2/2/2
54	GTP	O	401	55	-	6/18/38/38	0/3/3/3
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
46	3PE	d	1201	-	-	22/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PC1	g	1501	-	-	19/52/52/57	-
46	3PE	N	902	-	-	19/46/46/54	-
47	SF4	F	502	6	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
58	EHZ	U	101	20	-	10/42/44/45	-
45	LMT	Y	603	-	-	7/21/61/61	0/2/2/2
46	3PE	N	904	-	-	16/44/44/54	-
46	3PE	Y	602	-	-	18/38/38/54	-
45	LMT	l	201	-	-	7/21/61/61	0/2/2/2
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
46	3PE	I	204	-	-	17/34/34/54	-
46	3PE	H	601	-	-	9/26/26/54	-
53	CDL	h	1001	-	-	35/77/77/110	-
53	CDL	q	201	-	-	36/71/71/110	-
52	I49	H	602	-	-	7/10/10/10	0/1/1/1
46	3PE	B	1001	-	-	17/39/39/54	-
46	3PE	A	302	-	-	24/43/43/54	-
45	LMT	N	903	-	-	10/21/61/61	0/2/2/2
45	LMT	L	704	-	-	8/21/61/61	0/2/2/2
47	SF4	B	1002	2	-	-	0/6/5/5
46	3PE	L	701	-	-	22/52/52/54	-

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.38	1.80	1.59
54	O	401	GTP	O6-C6	8.30	1.40	1.23
58	T	101	EHZ	C15-N2	5.41	1.45	1.33
54	O	401	GTP	O4'-C1'	5.24	1.48	1.41
58	U	101	EHZ	C15-N2	5.24	1.45	1.33
46	H	601	3PE	O21-C2	-5.22	1.40	1.46
58	T	101	EHZ	C12-N1	5.03	1.44	1.33
58	U	101	EHZ	C12-N1	4.94	1.44	1.33
54	O	401	GTP	C2-N1	4.79	1.49	1.37
54	O	401	GTP	C2-N3	4.69	1.44	1.33
52	H	602	I49	C15-N02	-4.60	1.31	1.37
54	O	401	GTP	C2-N2	4.53	1.45	1.34
50	F	501	FMN	C4A-N5	3.76	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	l	201	LMT	O5B-C1B	3.60	1.51	1.41
45	Y	603	LMT	O5B-C1B	3.52	1.50	1.41
56	P	501	NDP	PN-O5D	3.48	1.73	1.59
45	j	101	LMT	O5B-C1B	3.43	1.50	1.41
45	h	1003	LMT	O5B-C1B	3.41	1.50	1.41
45	N	903	LMT	O5B-C1B	3.36	1.50	1.41
45	L	704	LMT	O5B-C1B	3.36	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.36	1.50	1.41
45	A	301	LMT	O5B-C1B	3.33	1.50	1.41
54	O	401	GTP	C2'-C1'	-3.33	1.48	1.53
45	N	901	LMT	O5B-C1B	3.28	1.50	1.41
45	A	301	LMT	O5'-C1'	3.27	1.50	1.41
45	M	801	LMT	O5B-C1B	3.21	1.50	1.41
45	Y	603	LMT	O5'-C1'	3.21	1.50	1.41
45	N	903	LMT	O5'-C1'	3.19	1.50	1.41
52	H	602	I49	C14-N03	3.19	1.38	1.29
45	M	802	LMT	O5'-C1'	3.18	1.49	1.41
56	P	501	NDP	O2B-C2B	-3.14	1.32	1.44
54	O	401	GTP	C5-C6	-3.11	1.41	1.47
45	L	704	LMT	O5'-C1'	3.09	1.49	1.41
46	H	601	3PE	O21-C21	3.05	1.40	1.33
45	j	101	LMT	O5'-C1'	3.03	1.49	1.41
45	M	802	LMT	O5B-C1B	3.00	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.95	1.49	1.41
45	l	201	LMT	O5'-C1'	2.95	1.49	1.41
45	N	901	LMT	O5'-C1'	2.91	1.49	1.41
45	h	1003	LMT	O5'-C1'	2.85	1.49	1.41
48	g	1501	PC1	O21-C2	-2.82	1.39	1.46
53	L	702	CDL	OB6-CB4	-2.80	1.39	1.46
53	X	1701	CDL	OB6-CB4	-2.80	1.39	1.46
45	M	801	LMT	O5'-C1'	2.78	1.48	1.41
46	Y	601	3PE	O21-C2	-2.74	1.39	1.46
53	d	1202	CDL	OA6-CA4	-2.72	1.39	1.46
53	h	1001	CDL	OB6-CB4	-2.71	1.39	1.46
53	K	401	CDL	OA6-CA4	-2.70	1.39	1.46
53	h	1001	CDL	OA6-CA4	-2.70	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.69	1.39	1.46
46	I	201	3PE	O21-C2	-2.69	1.39	1.46
46	L	701	3PE	O31-C3	-2.66	1.39	1.45
53	d	1202	CDL	OB6-CB4	-2.66	1.39	1.46
53	K	401	CDL	PB2-OB5	2.65	1.65	1.54
46	L	701	3PE	O21-C2	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	q	201	CDL	OB6-CB4	-2.65	1.40	1.46
53	L	702	CDL	OA6-CA4	-2.64	1.40	1.46
46	B	1001	3PE	O21-C2	-2.63	1.40	1.46
46	L	703	3PE	O21-C2	-2.62	1.40	1.46
46	N	902	3PE	O21-C2	-2.61	1.40	1.46
46	d	1201	3PE	O21-C2	-2.59	1.40	1.46
46	I	204	3PE	O21-C2	-2.56	1.40	1.46
46	Z	401	3PE	O21-C2	-2.53	1.40	1.46
46	Z	401	3PE	O31-C3	-2.51	1.39	1.45
46	N	904	3PE	O21-C2	-2.51	1.40	1.46
53	X	1701	CDL	OA6-CA4	-2.50	1.40	1.46
53	h	1001	CDL	OB8-CB6	-2.50	1.39	1.45
53	X	1701	CDL	OB8-CB7	2.50	1.40	1.33
58	T	101	EHZ	O4-C15	-2.49	1.18	1.23
46	Y	602	3PE	O21-C2	-2.49	1.40	1.46
58	U	101	EHZ	O4-C15	-2.48	1.18	1.23
46	H	601	3PE	O31-C31	2.43	1.40	1.33
46	L	703	3PE	O31-C3	-2.43	1.39	1.45
53	q	201	CDL	OB8-CB7	2.42	1.40	1.33
45	h	1002	LMT	O5B-C5B	2.41	1.50	1.44
46	L	705	3PE	O21-C2	-2.41	1.40	1.46
53	L	702	CDL	OB8-CB7	2.41	1.40	1.33
46	Y	602	3PE	O31-C31	2.40	1.40	1.33
53	d	1202	CDL	OB8-CB7	2.39	1.40	1.33
46	I	201	3PE	O31-C3	-2.38	1.39	1.45
46	N	902	3PE	O31-C31	2.38	1.40	1.33
53	q	201	CDL	OA8-CA6	-2.37	1.39	1.45
58	T	101	EHZ	O3-C12	-2.37	1.18	1.23
53	d	1202	CDL	OA8-CA6	-2.37	1.39	1.45
58	U	101	EHZ	O3-C12	-2.37	1.18	1.23
48	B	1003	PC1	O21-C2	-2.36	1.40	1.46
53	X	1701	CDL	OA8-CA7	2.35	1.40	1.33
48	B	1003	PC1	O21-C21	2.34	1.40	1.34
53	L	702	CDL	OA8-CA7	2.34	1.40	1.33
46	I	204	3PE	O31-C31	2.34	1.40	1.33
46	B	1001	3PE	O31-C3	-2.33	1.39	1.45
45	l	201	LMT	O5B-C5B	2.33	1.50	1.44
46	d	1201	3PE	O31-C31	2.33	1.40	1.33
46	L	705	3PE	O31-C31	2.31	1.40	1.33
53	K	401	CDL	OA8-CA6	-2.30	1.39	1.45
53	L	702	CDL	OA8-CA6	-2.30	1.39	1.45
48	g	1501	PC1	O31-C31	2.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	N	902	3PE	O31-C3	-2.29	1.39	1.45
53	d	1202	CDL	OB8-CB6	-2.29	1.39	1.45
46	N	904	3PE	O31-C3	-2.29	1.39	1.45
46	B	1001	3PE	O31-C31	2.27	1.40	1.33
53	q	201	CDL	OB8-CB6	-2.27	1.40	1.45
54	O	401	GTP	PG-O3G	-2.27	1.46	1.54
46	Y	602	3PE	O31-C3	-2.26	1.40	1.45
46	Y	601	3PE	O31-C31	2.25	1.39	1.33
54	O	401	GTP	PG-O2G	-2.25	1.46	1.54
53	h	1001	CDL	OA8-CA7	2.24	1.39	1.33
46	N	904	3PE	O31-C31	2.24	1.39	1.33
54	O	401	GTP	C2'-C3'	-2.23	1.47	1.53
53	K	401	CDL	OA8-CA7	2.23	1.39	1.33
56	P	501	NDP	O5D-C5D	-2.23	1.36	1.44
53	h	1001	CDL	OA8-CA6	-2.21	1.40	1.45
53	X	1701	CDL	OA6-CA5	2.21	1.40	1.34
53	X	1701	CDL	OA8-CA6	-2.21	1.40	1.45
46	A	302	3PE	O31-C31	2.20	1.39	1.33
48	B	1003	PC1	O31-C31	2.20	1.39	1.33
48	g	1501	PC1	O31-C3	-2.18	1.40	1.45
46	A	302	3PE	O31-C3	-2.18	1.40	1.45
53	h	1001	CDL	OB8-CB7	2.18	1.39	1.33
48	B	1003	PC1	O31-C3	-2.17	1.40	1.45
46	d	1201	3PE	O31-C3	-2.17	1.40	1.45
53	h	1001	CDL	OB6-CB5	2.16	1.40	1.34
53	q	201	CDL	OA8-CA7	2.16	1.39	1.33
46	Z	401	3PE	O31-C31	2.15	1.39	1.33
45	N	901	LMT	O5B-C5B	2.14	1.49	1.44
46	A	302	3PE	O21-C21	2.13	1.40	1.34
53	X	1701	CDL	OB8-CB6	-2.13	1.40	1.45
46	L	703	3PE	O31-C31	2.13	1.39	1.33
46	I	204	3PE	O31-C3	-2.13	1.40	1.45
46	B	1001	3PE	O21-C21	2.13	1.40	1.34
46	I	201	3PE	O31-C31	2.12	1.39	1.33
46	H	601	3PE	O31-C3	-2.12	1.40	1.45
53	d	1202	CDL	OA8-CA7	2.12	1.39	1.33
46	Z	401	3PE	O21-C21	2.11	1.40	1.34
53	d	1202	CDL	OB6-CB5	2.10	1.40	1.34
56	P	501	NDP	O2D-C2D	-2.09	1.38	1.43
46	L	705	3PE	O21-C21	2.09	1.40	1.34
53	q	201	CDL	OA6-CA5	2.09	1.40	1.34
46	Y	601	3PE	O31-C3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	K	401	CDL	OA6-CA5	2.07	1.40	1.34
46	Y	602	3PE	O21-C21	2.05	1.40	1.34
53	L	702	CDL	OB8-CB6	-2.05	1.40	1.45
46	N	904	3PE	O21-C21	2.04	1.40	1.34
46	A	302	3PE	O21-C2	-2.04	1.41	1.46
46	L	705	3PE	O31-C3	-2.04	1.40	1.45
45	N	903	LMT	O5B-C5B	2.04	1.49	1.44
53	q	201	CDL	OB6-CB5	2.03	1.40	1.34
50	F	501	FMN	C10-N1	2.03	1.37	1.33
46	d	1201	3PE	O21-C21	2.02	1.40	1.34
58	U	101	EHZ	O6-C20	-2.00	1.39	1.44
45	M	802	LMT	O5B-C5B	2.00	1.49	1.44

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	H	602	I49	C14-N02-C15	-7.33	113.00	125.21
56	P	501	NDP	PN-O3-PA	-7.00	108.81	132.83
58	U	101	EHZ	C8-C9-S1	5.83	120.84	113.63
58	T	101	EHZ	C8-C9-S1	5.59	120.55	113.63
45	M	802	LMT	C3B-C4B-C5B	5.20	119.51	110.24
52	H	602	I49	N01-C14-N03	4.84	129.32	120.26
53	h	1001	CDL	OB6-CB5-C51	4.49	121.17	111.50
46	A	302	3PE	O21-C21-C22	4.44	121.06	111.50
46	N	904	3PE	O21-C21-C22	4.30	120.78	111.50
48	B	1003	PC1	O21-C21-C22	4.30	120.78	111.50
46	L	705	3PE	O21-C21-C22	4.27	120.70	111.50
46	I	201	3PE	O21-C21-C22	4.17	120.49	111.50
53	X	1701	CDL	OA6-CA5-C11	4.13	120.40	111.50
46	L	703	3PE	O21-C21-C22	4.12	120.39	111.50
46	Y	602	3PE	O21-C21-C22	4.11	120.35	111.50
53	X	1701	CDL	OB6-CB5-C51	4.06	120.25	111.50
53	q	201	CDL	OA6-CA5-C11	4.06	120.24	111.50
53	d	1202	CDL	OA6-CA5-C11	4.05	120.24	111.50
46	d	1201	3PE	O21-C21-C22	4.03	120.18	111.50
46	H	601	3PE	O21-C21-O22	-4.00	120.48	125.57
46	I	204	3PE	O21-C21-C22	3.99	120.10	111.50
53	h	1001	CDL	OA6-CA5-C11	3.96	120.04	111.50
53	L	702	CDL	OB6-CB5-C51	3.92	119.95	111.50
46	N	902	3PE	O21-C21-C22	3.85	119.80	111.50
54	O	401	GTP	C3'-C2'-C1'	3.85	106.78	100.98
53	L	702	CDL	OA6-CA5-C11	3.81	119.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	Z	401	3PE	O21-C21-C22	3.79	119.66	111.50
46	L	701	3PE	O21-C21-C22	3.78	119.65	111.50
45	M	801	LMT	C1'-C2'-C3'	3.77	117.85	110.00
53	K	401	CDL	OA6-CA5-C11	3.62	119.31	111.50
54	O	401	GTP	PA-O3A-PB	-3.56	120.59	132.83
46	Y	601	3PE	O21-C21-C22	3.50	119.05	111.50
45	h	1002	LMT	O5B-C5B-C4B	3.48	116.02	109.69
48	g	1501	PC1	O21-C21-C22	3.48	119.01	111.50
56	P	501	NDP	O2B-P2B-O1X	-3.46	96.02	109.39
45	M	802	LMT	O5B-C5B-C4B	3.44	115.95	109.69
53	q	201	CDL	OB6-CB5-C51	3.37	118.77	111.50
46	B	1001	3PE	O21-C21-C22	3.37	120.20	110.80
53	d	1202	CDL	OB6-CB5-C51	3.31	120.02	110.80
46	Y	601	3PE	O31-C31-C32	3.25	122.10	111.91
45	h	1002	LMT	C2'-C3'-C4'	3.25	117.09	109.68
45	h	1002	LMT	C1'-C2'-C3'	3.24	116.75	110.00
50	F	501	FMN	C4-N3-C2	-3.22	119.70	125.64
53	X	1701	CDL	OB8-CB7-C71	3.14	121.77	111.91
54	O	401	GTP	C2-N1-C6	-3.08	119.43	125.10
54	O	401	GTP	C5-C6-N1	3.06	119.36	113.95
45	M	801	LMT	C2'-C3'-C4'	3.04	116.63	109.68
46	N	902	3PE	O31-C31-C32	3.01	121.34	111.91
46	A	302	3PE	O31-C31-C32	2.98	121.26	111.91
45	h	1003	LMT	O5'-C5'-C4'	2.97	116.01	109.75
54	O	401	GTP	O2G-PG-O3B	2.93	114.47	104.64
46	Y	602	3PE	O31-C31-C32	2.93	121.10	111.91
52	H	602	I49	N05-C15-N04	-2.87	111.42	120.26
48	B	1003	PC1	O31-C31-C32	2.86	120.89	111.91
50	F	501	FMN	C4A-C10-N10	2.86	120.66	116.48
54	O	401	GTP	O3G-PG-O3B	2.85	114.20	104.64
48	g	1501	PC1	O31-C31-C32	2.84	120.82	111.91
50	F	501	FMN	C4A-C4-N3	2.79	120.27	113.19
56	P	501	NDP	PA-O5B-C5B	-2.76	105.52	121.68
45	l	201	LMT	O5B-C5B-C4B	2.76	114.70	109.69
52	H	602	I49	C06-C07-C10	-2.75	116.03	120.54
46	I	204	3PE	O31-C31-C32	2.74	120.50	111.91
53	h	1001	CDL	OA8-CA7-C31	2.73	120.48	111.91
53	q	201	CDL	OA8-CA7-C31	2.73	120.46	111.91
46	L	703	3PE	O31-C31-C32	2.71	120.40	111.91
45	M	802	LMT	C4B-C3B-C2B	2.70	115.53	110.82
53	X	1701	CDL	OA8-CA7-C31	2.70	120.37	111.91
46	B	1001	3PE	O31-C31-C32	2.68	120.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	Y	603	LMT	C1B-O1B-C4’	-2.67	111.35	117.96
46	H	601	3PE	O31-C31-C32	2.66	120.25	111.91
45	M	801	LMT	C1’-O5’-C5’	-2.64	108.50	113.69
58	T	101	EHZ	C13-C12-N1	2.62	120.83	116.42
53	d	1202	CDL	OA8-CA7-C31	2.61	120.11	111.91
53	h	1001	CDL	OB8-CB7-C71	2.60	120.08	111.91
56	P	501	NDP	O3X-P2B-O2X	2.59	117.53	107.64
56	P	501	NDP	PN-O5D-C5D	-2.57	106.62	121.68
53	d	1202	CDL	OB8-CB7-C71	2.57	119.97	111.91
52	H	602	I49	C12-C13-I02	-2.56	119.02	121.72
52	H	602	I49	C08-C06-C07	2.55	118.79	112.87
45	h	1002	LMT	C1’-O5’-C5’	-2.54	108.70	113.69
45	l	201	LMT	C6B-C5B-C4B	-2.53	107.07	113.00
54	O	401	GTP	C2’-C3’-C4’	2.53	107.56	102.64
45	h	1002	LMT	C3B-C4B-C5B	2.53	114.75	110.24
50	F	501	FMN	O4-C4-C4A	-2.51	119.94	126.60
46	L	705	3PE	O31-C31-C32	2.50	119.77	111.91
53	K	401	CDL	OA8-CA7-C31	2.50	119.76	111.91
52	H	602	I49	N02-C14-N01	-2.44	111.80	118.08
54	O	401	GTP	PB-O3B-PG	-2.44	124.47	132.83
46	I	201	3PE	O31-C31-C32	2.43	119.54	111.91
56	P	501	NDP	C2A-N1A-C6A	-2.43	114.60	118.75
45	M	801	LMT	C1B-O5B-C5B	-2.42	108.93	113.69
46	Z	401	3PE	O31-C31-C32	2.42	119.51	111.91
53	L	702	CDL	OB8-CB7-C71	2.41	119.47	111.91
46	d	1201	3PE	O31-C31-C32	2.40	119.45	111.91
53	q	201	CDL	OB8-CB7-C71	2.36	119.32	111.91
56	P	501	NDP	O5D-PN-O1N	-2.35	99.88	109.07
46	N	904	3PE	O31-C31-C32	2.34	119.25	111.91
56	P	501	NDP	O4B-C4B-C3B	2.34	109.74	105.11
53	L	702	CDL	OA8-CA7-C31	2.33	119.22	111.91
50	F	501	FMN	C10-C4A-N5	-2.32	119.94	124.86
58	U	101	EHZ	O2-C9-S1	-2.31	119.61	122.61
54	O	401	GTP	O2A-PA-O1A	-2.28	100.95	112.24
56	P	501	NDP	O2N-PN-O1N	2.28	123.52	112.24
46	L	701	3PE	O31-C31-C32	2.28	119.06	111.91
45	A	301	LMT	O1B-C4’-C3’	2.27	113.31	107.28
58	T	101	EHZ	O2-C9-S1	-2.26	119.68	122.61
53	X	1701	CDL	CB4-OB6-CB5	-2.26	112.24	117.79
45	N	903	LMT	O1B-C4’-C3’	2.22	113.19	107.28
54	O	401	GTP	O2B-PB-O1B	-2.20	101.36	112.24
58	T	101	EHZ	C16-C15-N2	2.20	120.96	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	I	204	3PE	C2-O21-C21	-2.20	112.39	117.79
50	F	501	FMN	C4A-C10-N1	-2.11	119.82	124.73
45	L	704	LMT	C1B-O1B-C4'	-2.09	112.79	117.96
58	U	101	EHZ	C13-C12-N1	2.08	119.92	116.42
58	U	101	EHZ	C7-C8-C9	-2.08	109.14	113.89
45	h	1003	LMT	C1B-O1B-C4'	-2.07	112.84	117.96
56	P	501	NDP	O7N-C7N-N7N	-2.05	118.08	122.88
45	l	201	LMT	C2'-C3'-C4'	2.03	114.31	109.68
46	Y	601	3PE	O31-C31-O32	-2.02	118.50	123.59

There are no chirality outliers.

All (632) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C2'-C1'-O1'-C1
45	A	301	LMT	O5'-C1'-O1'-C1
45	h	1002	LMT	C2'-C1'-O1'-C1
45	h	1002	LMT	O5'-C1'-O1'-C1
45	h	1003	LMT	C2-C1-O1'-C1'
45	j	101	LMT	O5'-C1'-O1'-C1
46	A	302	3PE	O21-C2-C3-O31
46	A	302	3PE	O22-C21-O21-C2
46	A	302	3PE	C22-C21-O21-C2
46	B	1001	3PE	C1-O11-P-O12
46	B	1001	3PE	C1-O11-P-O14
46	B	1001	3PE	C11-O13-P-O14
46	B	1001	3PE	O13-C11-C12-N
46	B	1001	3PE	C22-C21-O21-C2
46	H	601	3PE	O13-C11-C12-N
46	H	601	3PE	C1-C2-O21-C21
46	H	601	3PE	C3-C2-O21-C21
46	H	601	3PE	O22-C21-O21-C2
46	I	201	3PE	O13-C11-C12-N
46	I	201	3PE	O22-C21-O21-C2
46	I	201	3PE	C22-C21-O21-C2
46	I	204	3PE	C11-O13-P-O11
46	I	204	3PE	C11-O13-P-O12
46	I	204	3PE	C11-O13-P-O14
46	I	204	3PE	O13-C11-C12-N
46	L	701	3PE	O13-C11-C12-N
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	L	703	3PE	C1-O11-P-O14
46	L	703	3PE	C11-O13-P-O11
46	L	703	3PE	C11-O13-P-O12
46	L	703	3PE	C11-O13-P-O14
46	L	705	3PE	C1-O11-P-O12
46	L	705	3PE	C1-O11-P-O13
46	L	705	3PE	C1-O11-P-O14
46	L	705	3PE	O22-C21-O21-C2
46	N	902	3PE	O13-C11-C12-N
46	N	904	3PE	C1-O11-P-O14
46	N	904	3PE	O13-C11-C12-N
46	Y	601	3PE	C11-O13-P-O11
46	Y	601	3PE	C11-O13-P-O12
46	Y	601	3PE	C11-O13-P-O14
46	Y	602	3PE	O13-C11-C12-N
46	Y	602	3PE	C22-C21-O21-C2
46	Z	401	3PE	C1-O11-P-O12
46	Z	401	3PE	C1-O11-P-O13
46	Z	401	3PE	C1-O11-P-O14
46	Z	401	3PE	O13-C11-C12-N
46	d	1201	3PE	C22-C21-O21-C2
52	H	602	I49	C07-C06-C08-N01
52	H	602	I49	N04-C15-N02-C14
52	H	602	I49	N05-C15-N02-C14
53	K	401	CDL	CB2-OB2-PB2-OB4
53	K	401	CDL	CB2-OB2-PB2-OB5
53	L	702	CDL	CB2-C1-CA2-OA2
53	L	702	CDL	CA2-OA2-PA1-OA4
53	L	702	CDL	CA2-OA2-PA1-OA5
53	L	702	CDL	CA3-OA5-PA1-OA3
53	X	1701	CDL	OA7-CA5-OA6-CA4
53	X	1701	CDL	CB2-OB2-PB2-OB3
53	d	1202	CDL	CA2-OA2-PA1-OA3
53	d	1202	CDL	CA2-OA2-PA1-OA4
53	d	1202	CDL	CA3-OA5-PA1-OA2
53	d	1202	CDL	CA3-OA5-PA1-OA3
53	d	1202	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	CA2-OA2-PA1-OA3
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CA3-OA5-PA1-OA2
53	h	1001	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	CB2-OB2-PB2-OB3
53	h	1001	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA4
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	OB5-CB3-CB4-OB6
54	O	401	GTP	PB-O3B-PG-O2G
54	O	401	GTP	C5'-O5'-PA-O3A
56	P	501	NDP	C2B-O2B-P2B-O1X
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-C17
58	T	101	EHZ	N2-C15-C16-O5
58	T	101	EHZ	O4-C15-C16-C17
58	U	101	EHZ	C16-C17-C20-O6
45	A	301	LMT	C3'-C4'-O1B-C1B
53	X	1701	CDL	OB9-CB7-OB8-CB6
45	M	802	LMT	O5B-C1B-O1B-C4'
53	X	1701	CDL	C71-CB7-OB8-CB6
46	N	902	3PE	O32-C31-O31-C3
46	Y	602	3PE	O32-C31-O31-C3
46	Z	401	3PE	O32-C31-O31-C3
53	X	1701	CDL	OA9-CA7-OA8-CA6
53	d	1202	CDL	OB9-CB7-OB8-CB6
53	h	1001	CDL	OB9-CB7-OB8-CB6
46	L	701	3PE	O22-C21-O21-C2
46	L	703	3PE	O22-C21-O21-C2
46	Y	602	3PE	O22-C21-O21-C2
46	d	1201	3PE	O22-C21-O21-C2
53	d	1202	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	OA7-CA5-OA6-CA4
45	M	802	LMT	C2B-C1B-O1B-C4'
46	N	902	3PE	C32-C31-O31-C3
46	Z	401	3PE	C32-C31-O31-C3
46	d	1201	3PE	C32-C31-O31-C3
53	h	1001	CDL	C71-CB7-OB8-CB6
45	l	201	LMT	C4'-C5'-C6'-O6'
46	L	701	3PE	C22-C21-O21-C2
46	L	703	3PE	C22-C21-O21-C2
46	L	705	3PE	C22-C21-O21-C2
53	X	1701	CDL	C11-CA5-OA6-CA4
53	h	1001	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	C11-CA5-OA6-CA4
45	N	903	LMT	C3'-C4'-O1B-C1B
46	Y	602	3PE	C32-C31-O31-C3
53	X	1701	CDL	C31-CA7-OA8-CA6
53	d	1202	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	C31-CA7-OA8-CA6
45	j	101	LMT	O5'-C5'-C6'-O6'
46	B	1001	3PE	O22-C21-O21-C2
46	d	1201	3PE	O32-C31-O31-C3
45	A	301	LMT	O5'-C5'-C6'-O6'
53	d	1202	CDL	O1-C1-CA2-OA2
45	h	1002	LMT	O5B-C5B-C6B-O6B
46	Y	601	3PE	C22-C21-O21-C2
48	B	1003	PC1	C22-C21-O21-C2
53	d	1202	CDL	C11-CA5-OA6-CA4
45	h	1002	LMT	O5B-C1B-O1B-C4'
45	h	1003	LMT	O5'-C5'-C6'-O6'
45	h	1003	LMT	C4'-C5'-C6'-O6'
45	j	101	LMT	C4'-C5'-C6'-O6'
56	P	501	NDP	O4D-C4D-C5D-O5D
45	Y	603	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	CB4-CB3-OB5-PB2
45	l	201	LMT	O5'-C5'-C6'-O6'
53	q	201	CDL	OA9-CA7-OA8-CA6
45	L	704	LMT	O5'-C1'-O1'-C1
45	N	903	LMT	O5'-C1'-O1'-C1
45	M	801	LMT	C4B-C5B-C6B-O6B
53	h	1001	CDL	CA2-C1-CB2-OB2
46	Y	601	3PE	O22-C21-O21-C2
48	B	1003	PC1	O22-C21-O21-C2
53	d	1202	CDL	OA7-CA5-OA6-CA4
45	N	903	LMT	C4'-C5'-C6'-O6'
46	N	904	3PE	O32-C31-O31-C3
45	h	1002	LMT	C3'-C4'-O1B-C1B
46	L	701	3PE	C32-C31-O31-C3
46	L	703	3PE	C32-C31-O31-C3
46	N	904	3PE	C32-C31-O31-C3
48	B	1003	PC1	C32-C31-O31-C3
48	g	1501	PC1	C32-C31-O31-C3
45	Y	603	LMT	C4B-C5B-C6B-O6B
46	B	1001	3PE	O11-C1-C2-O21
45	L	704	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
48	g	1501	PC1	O32-C31-O31-C3
45	N	901	LMT	C4B-C5B-C6B-O6B
45	N	901	LMT	O5B-C5B-C6B-O6B
53	L	702	CDL	C71-CB7-OB8-CB6
46	N	902	3PE	C31-C32-C33-C34
46	d	1201	3PE	C31-C32-C33-C34
45	M	802	LMT	C3'-C4'-O1B-C1B
46	I	204	3PE	C21-C22-C23-C24
46	L	701	3PE	C31-C32-C33-C34
46	L	701	3PE	C21-C22-C23-C24
48	B	1003	PC1	C21-C22-C23-C24
53	X	1701	CDL	CB7-C71-C72-C73
53	h	1001	CDL	CB5-C51-C52-C53
45	M	801	LMT	O5B-C5B-C6B-O6B
58	U	101	EHZ	C5-C6-C7-O1
46	Z	401	3PE	C31-C32-C33-C34
53	L	702	CDL	CB5-C51-C52-C53
48	B	1003	PC1	O32-C31-O31-C3
46	L	701	3PE	O32-C31-O31-C3
45	A	301	LMT	C4'-C5'-C6'-O6'
46	L	703	3PE	C21-C22-C23-C24
53	L	702	CDL	O1-C1-CA2-OA2
53	h	1001	CDL	O1-C1-CB2-OB2
45	h	1002	LMT	C5'-C4'-O1B-C1B
46	L	703	3PE	O32-C31-O31-C3
46	Y	602	3PE	C31-C32-C33-C34
53	L	702	CDL	OB9-CB7-OB8-CB6
46	B	1001	3PE	C1-O11-P-O13
46	H	601	3PE	C11-O13-P-O11
53	K	401	CDL	CA3-OA5-PA1-OA2
53	d	1202	CDL	CA2-OA2-PA1-OA5
53	d	1202	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	CA2-OA2-PA1-OA5
53	q	201	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	CB3-OB5-PB2-OB2
53	d	1202	CDL	CB2-C1-CA2-OA2
48	g	1501	PC1	C31-C32-C33-C34
45	M	802	LMT	C5'-C4'-O1B-C1B
59	o	201	MYR	C2-C3-C4-C5
46	I	204	3PE	C22-C21-O21-C2
46	N	902	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
46	N	904	3PE	C22-C23-C24-C25
46	N	904	3PE	C23-C24-C25-C26
46	d	1201	3PE	C33-C34-C35-C36
53	L	702	CDL	C54-C55-C56-C57
53	X	1701	CDL	C57-C58-C59-C60
53	d	1202	CDL	C33-C34-C35-C36
58	U	101	EHZ	C3-C4-C5-C6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
46	A	302	3PE	C2A-C2B-C2C-C2D
48	g	1501	PC1	C24-C25-C26-C27
53	q	201	CDL	C59-C60-C61-C62
46	I	204	3PE	O22-C21-O21-C2
46	d	1201	3PE	C21-C22-C23-C24
48	g	1501	PC1	C21-C22-C23-C24
53	X	1701	CDL	C56-C57-C58-C59
53	h	1001	CDL	C71-C72-C73-C74
48	g	1501	PC1	C2A-C2B-C2C-C2D
46	A	302	3PE	C26-C27-C28-C29
53	h	1001	CDL	C17-C18-C19-C20
53	h	1001	CDL	C20-C21-C22-C23
59	o	201	MYR	C11-C10-C9-C8
46	I	201	3PE	C21-C22-C23-C24
53	K	401	CDL	CA5-C11-C12-C13
53	d	1202	CDL	CB7-C71-C72-C73
46	I	204	3PE	C32-C31-O31-C3
45	Y	603	LMT	C2-C3-C4-C5
46	A	302	3PE	C28-C29-C2A-C2B
45	N	903	LMT	O5’-C5’-C6’-O6’
45	N	903	LMT	C11-C10-C9-C8
46	Y	601	3PE	C2A-C2B-C2C-C2D
48	g	1501	PC1	C28-C29-C2A-C2B
53	X	1701	CDL	C72-C73-C74-C75
46	I	204	3PE	C23-C24-C25-C26
46	N	904	3PE	C32-C33-C34-C35
53	L	702	CDL	C51-C52-C53-C54
59	o	201	MYR	C4-C5-C6-C7
46	L	703	3PE	C3C-C3D-C3E-C3F
53	X	1701	CDL	C11-C12-C13-C14
53	X	1701	CDL	CA5-C11-C12-C13
53	d	1202	CDL	CA7-C31-C32-C33
46	d	1201	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	C31-CA7-OA8-CA6
53	h	1001	CDL	C12-C13-C14-C15
45	Y	603	LMT	C2-C1-O1'-C1'
53	X	1701	CDL	C19-C20-C21-C22
46	Y	602	3PE	C1-C2-C3-O31
53	L	702	CDL	C34-C35-C36-C37
53	K	401	CDL	C31-C32-C33-C34
45	N	903	LMT	C1-C2-C3-C4
53	d	1202	CDL	C32-C33-C34-C35
58	U	101	EHZ	C1-C2-C3-C4
48	B	1003	PC1	C32-C33-C34-C35
45	Y	603	LMT	C3-C4-C5-C6
46	I	201	3PE	C33-C34-C35-C36
53	X	1701	CDL	C20-C21-C22-C23
46	H	601	3PE	C32-C33-C34-C35
53	q	201	CDL	C51-C52-C53-C54
45	L	704	LMT	C5-C6-C7-C8
46	I	204	3PE	O32-C31-O31-C3
45	A	301	LMT	O5B-C5B-C6B-O6B
53	h	1001	CDL	OA9-CA7-OA8-CA6
53	X	1701	CDL	OB7-CB5-OB6-CB4
58	T	101	EHZ	C5-C6-C7-C8
45	A	301	LMT	C1-C2-C3-C4
46	L	705	3PE	C33-C34-C35-C36
45	h	1002	LMT	C4B-C5B-C6B-O6B
46	N	902	3PE	C33-C34-C35-C36
46	N	902	3PE	C37-C38-C39-C3A
53	L	702	CDL	C31-C32-C33-C34
46	L	703	3PE	C31-C32-C33-C34
53	X	1701	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	C11-CA5-OA6-CA4
53	K	401	CDL	C36-C37-C38-C39
53	L	702	CDL	C35-C36-C37-C38
46	A	302	3PE	C27-C28-C29-C2A
53	q	201	CDL	C52-C53-C54-C55
53	X	1701	CDL	O1-C1-CB2-OB2
46	N	904	3PE	C33-C34-C35-C36
48	g	1501	PC1	C2C-C2D-C2E-C2F
56	P	501	NDP	C3D-C4D-C5D-O5D
46	B	1001	3PE	C35-C36-C37-C38
48	B	1003	PC1	C24-C25-C26-C27
45	Y	603	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	CB2-OB2-PB2-OB5
46	H	601	3PE	C2-C1-O11-P
46	d	1201	3PE	C2-C1-O11-P
46	B	1001	3PE	O11-C1-C2-C3
53	X	1701	CDL	OB5-CB3-CB4-CB6
46	A	302	3PE	C2C-C2D-C2E-C2F
53	q	201	CDL	C57-C58-C59-C60
46	Z	401	3PE	C32-C33-C34-C35
46	L	703	3PE	C34-C35-C36-C37
46	N	904	3PE	C26-C27-C28-C29
46	I	204	3PE	C35-C36-C37-C38
45	N	903	LMT	O5B-C5B-C6B-O6B
46	L	701	3PE	C1-C2-C3-O31
46	d	1201	3PE	C1-C2-C3-O31
48	B	1003	PC1	C1-C2-C3-O31
53	L	702	CDL	CA3-CA4-CA6-OA8
46	Y	602	3PE	C3B-C3C-C3D-C3E
46	d	1201	3PE	C3F-C3G-C3H-C3I
53	d	1202	CDL	C31-C32-C33-C34
53	h	1001	CDL	C15-C16-C17-C18
58	T	101	EHZ	O4-C15-C16-O5
46	I	204	3PE	C25-C26-C27-C28
46	A	302	3PE	C35-C36-C37-C38
46	Y	602	3PE	C23-C24-C25-C26
53	L	702	CDL	C11-CA5-OA6-CA4
58	T	101	EHZ	C5-C6-C7-O1
53	h	1001	CDL	C16-C17-C18-C19
46	L	703	3PE	C22-C23-C24-C25
53	X	1701	CDL	C21-C22-C23-C24
46	A	302	3PE	C1-C2-O21-C21
46	B	1001	3PE	C34-C35-C36-C37
53	q	201	CDL	CA5-C11-C12-C13
46	N	902	3PE	C2E-C2F-C2G-C2H
46	Y	601	3PE	C33-C34-C35-C36
53	L	702	CDL	C38-C39-C40-C41
53	K	401	CDL	CB2-OB2-PB2-OB3
46	I	201	3PE	C3A-C3B-C3C-C3D
59	o	201	MYR	C7-C8-C9-C10
46	L	701	3PE	O21-C2-C3-O31
53	L	702	CDL	OB6-CB4-CB6-OB8
53	X	1701	CDL	OA6-CA4-CA6-OA8
53	X	1701	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C22-C23-C24-C25
48	g	1501	PC1	C2E-C2F-C2G-C2H
46	I	201	3PE	C2B-C2C-C2D-C2E
53	h	1001	CDL	C51-C52-C53-C54
53	X	1701	CDL	CB2-C1-CA2-OA2
53	X	1701	CDL	CA2-C1-CB2-OB2
53	h	1001	CDL	OA7-CA5-OA6-CA4
53	K	401	CDL	C18-C19-C20-C21
46	A	302	3PE	C32-C31-O31-C3
45	l	201	LMT	C3'-C4'-O1B-C1B
46	I	204	3PE	C24-C25-C26-C27
45	l	201	LMT	C5'-C4'-O1B-C1B
46	L	701	3PE	C28-C29-C2A-C2B
46	A	302	3PE	O11-C1-C2-C3
46	L	703	3PE	O11-C1-C2-C3
53	X	1701	CDL	OA5-CA3-CA4-CA6
53	q	201	CDL	OB5-CB3-CB4-CB6
46	L	705	3PE	C31-C32-C33-C34
46	Y	601	3PE	O13-C11-C12-N
46	d	1201	3PE	O13-C11-C12-N
53	X	1701	CDL	O1-C1-CA2-OA2
53	L	702	CDL	OA7-CA5-OA6-CA4
53	K	401	CDL	C16-C17-C18-C19
48	g	1501	PC1	C22-C21-O21-C2
53	q	201	CDL	C1-CA2-OA2-PA1
45	l	201	LMT	C4-C5-C6-C7
45	M	801	LMT	C2-C1-O1'-C1'
52	H	602	I49	C08-C06-C07-C09
53	X	1701	CDL	CB3-CB4-CB6-OB8
45	l	201	LMT	O1'-C1-C2-C3
48	B	1003	PC1	C34-C35-C36-C37
46	L	701	3PE	C3B-C3C-C3D-C3E
46	L	703	3PE	C29-C2A-C2B-C2C
46	Y	601	3PE	C32-C33-C34-C35
46	B	1001	3PE	C32-C33-C34-C35
53	L	702	CDL	C60-C61-C62-C63
46	N	904	3PE	C1-O11-P-O13
53	X	1701	CDL	CA2-OA2-PA1-OA5
46	I	201	3PE	C29-C2A-C2B-C2C
53	h	1001	CDL	C24-C25-C26-C27
46	A	302	3PE	O11-C1-C2-O21
46	Z	401	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
46	I	204	3PE	O21-C2-C3-O31
48	B	1003	PC1	O21-C2-C3-O31
53	X	1701	CDL	OB6-CB4-CB6-OB8
53	q	201	CDL	OB6-CB4-CB6-OB8
52	H	602	I49	C08-C06-C07-C10
46	N	902	3PE	C38-C39-C3A-C3B
46	I	201	3PE	C37-C38-C39-C3A
46	A	302	3PE	C2-C1-O11-P
48	g	1501	PC1	C2-C1-O11-P
48	g	1501	PC1	C29-C2A-C2B-C2C
46	Y	601	3PE	C28-C29-C2A-C2B
48	g	1501	PC1	C3A-C3B-C3C-C3D
53	K	401	CDL	OA7-CA5-OA6-CA4
53	K	401	CDL	C11-CA5-OA6-CA4
58	T	101	EHZ	C21-C22-C23-C24
46	Y	601	3PE	C29-C2A-C2B-C2C
53	h	1001	CDL	C72-C73-C74-C75
53	q	201	CDL	OA5-CA3-CA4-CA6
48	g	1501	PC1	C23-C24-C25-C26
48	g	1501	PC1	O22-C21-O21-C2
45	M	802	LMT	C7-C8-C9-C10
46	H	601	3PE	C33-C34-C35-C36
53	L	702	CDL	C51-CB5-OB6-CB4
48	B	1003	PC1	C31-C32-C33-C34
53	d	1202	CDL	C41-C42-C43-C44
46	L	701	3PE	C2C-C2D-C2E-C2F
53	d	1202	CDL	C38-C39-C40-C41
46	A	302	3PE	C1-C2-C3-O31
52	H	602	I49	N01-C14-N02-C15
53	L	702	CDL	CB3-CB4-CB6-OB8
53	X	1701	CDL	CA3-CA4-CA6-OA8
53	q	201	CDL	CA4-CA3-OA5-PA1
53	q	201	CDL	CB3-CB4-CB6-OB8
46	L	705	3PE	O11-C1-C2-O21
53	X	1701	CDL	OA5-CA3-CA4-OA6
53	q	201	CDL	OA5-CA3-CA4-OA6
46	I	201	3PE	C32-C33-C34-C35
58	T	101	EHZ	O1-C7-C8-C9
46	A	302	3PE	O32-C31-O31-C3
46	d	1201	3PE	O21-C2-C3-O31
53	L	702	CDL	CB7-C71-C72-C73
53	h	1001	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	C32-C33-C34-C35
46	L	701	3PE	C33-C34-C35-C36
53	L	702	CDL	OB7-CB5-OB6-CB4
45	A	301	LMT	C3-C4-C5-C6
53	h	1001	CDL	C31-C32-C33-C34
45	L	704	LMT	C9-C10-C11-C12
46	L	705	3PE	C21-C22-C23-C24
46	N	904	3PE	C22-C21-O21-C2
46	d	1201	3PE	C3A-C3B-C3C-C3D
46	B	1001	3PE	C11-O13-P-O11
46	Y	602	3PE	C1-O11-P-O13
56	P	501	NDP	O4D-C1D-N1N-C6N
45	L	704	LMT	O1'-C1-C2-C3
45	N	903	LMT	C5'-C4'-O1B-C1B
46	A	302	3PE	C11-O13-P-O14
46	B	1001	3PE	C11-O13-P-O12
46	H	601	3PE	C11-O13-P-O12
46	I	201	3PE	C1-O11-P-O14
46	L	701	3PE	C1-O11-P-O12
53	K	401	CDL	CA3-OA5-PA1-OA3
53	K	401	CDL	CA3-OA5-PA1-OA4
53	L	702	CDL	CA2-OA2-PA1-OA3
53	d	1202	CDL	CB2-OB2-PB2-OB3
53	d	1202	CDL	CB2-OB2-PB2-OB4
53	h	1001	CDL	CA3-OA5-PA1-OA3
53	h	1001	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CA2-OA2-PA1-OA3
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB3-OB5-PB2-OB3
53	q	201	CDL	CB3-OB5-PB2-OB4
54	O	401	GTP	C5'-O5'-PA-O1A
54	O	401	GTP	C5'-O5'-PA-O2A
58	T	101	EHZ	C6-C7-C8-C9
46	Z	401	3PE	O11-C1-C2-C3
46	L	701	3PE	C27-C28-C29-C2A
53	q	201	CDL	C56-C57-C58-C59
46	I	201	3PE	C12-C11-O13-P
46	N	902	3PE	C12-C11-O13-P
46	Y	601	3PE	C12-C11-O13-P
46	N	902	3PE	C36-C37-C38-C39
46	Y	601	3PE	C26-C27-C28-C29
58	U	101	EHZ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
46	L	703	3PE	O11-C1-C2-O21
53	X	1701	CDL	OB5-CB3-CB4-OB6
53	d	1202	CDL	OB5-CB3-CB4-OB6
46	L	703	3PE	C27-C28-C29-C2A
53	q	201	CDL	C15-C16-C17-C18
46	Y	601	3PE	C34-C35-C36-C37
46	Y	601	3PE	C36-C37-C38-C39
48	g	1501	PC1	C39-C3A-C3B-C3C
58	T	101	EHZ	C16-C17-C20-O6
46	Y	602	3PE	O21-C2-C3-O31
53	L	702	CDL	OA6-CA4-CA6-OA8
58	U	101	EHZ	C1-C21-C22-C23
46	L	701	3PE	C2F-C2G-C2H-C2I
46	N	902	3PE	C22-C23-C24-C25
46	B	1001	3PE	O31-C31-C32-C33
46	I	201	3PE	C24-C25-C26-C27
53	d	1202	CDL	C71-C72-C73-C74
45	N	903	LMT	C3-C4-C5-C6
46	I	201	3PE	C23-C24-C25-C26
53	X	1701	CDL	C52-C51-CB5-OB6
46	L	701	3PE	C2D-C2E-C2F-C2G
58	T	101	EHZ	C18-C17-C20-O6
46	I	201	3PE	C25-C26-C27-C28
46	Y	601	3PE	O21-C21-C22-C23
53	h	1001	CDL	CA6-CA4-OA6-CA5
53	d	1202	CDL	OB5-CB3-CB4-CB6
46	N	904	3PE	O22-C21-O21-C2
45	M	801	LMT	C1-C2-C3-C4
46	d	1201	3PE	C3E-C3F-C3G-C3H
46	L	703	3PE	C25-C26-C27-C28
46	I	201	3PE	C2D-C2E-C2F-C2G
50	F	501	FMN	C5'-O5'-P-O1P
46	N	902	3PE	C26-C27-C28-C29
46	Y	601	3PE	C23-C24-C25-C26
45	N	903	LMT	C5-C6-C7-C8
53	X	1701	CDL	C54-C55-C56-C57
46	Y	601	3PE	C35-C36-C37-C38
53	L	702	CDL	C32-C31-CA7-OA8
46	A	302	3PE	C11-O13-P-O11
46	Y	601	3PE	C1-O11-P-O13
46	Y	602	3PE	C11-O13-P-O11
53	L	702	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	CB3-OB5-PB2-OB2
53	h	1001	CDL	CB3-OB5-PB2-OB2
46	L	701	3PE	C2E-C2F-C2G-C2H
46	I	204	3PE	C1-C2-C3-O31
53	d	1202	CDL	C44-C45-C46-C47
46	L	703	3PE	C3B-C3C-C3D-C3E
46	Y	601	3PE	C37-C38-C39-C3A
54	O	401	GTP	PG-O3B-PB-O2B
45	M	802	LMT	C4'-C5'-C6'-O6'
59	o	201	MYR	C11-C12-C13-C14
46	N	904	3PE	C2-C1-O11-P
46	Y	601	3PE	C2-C1-O11-P
46	I	204	3PE	C33-C34-C35-C36
46	A	302	3PE	C2B-C2C-C2D-C2E
46	d	1201	3PE	C3B-C3C-C3D-C3E
46	L	703	3PE	C39-C3A-C3B-C3C
46	N	902	3PE	C2A-C2B-C2C-C2D
48	g	1501	PC1	C33-C34-C35-C36
53	d	1202	CDL	C76-C77-C78-C79
53	K	401	CDL	O1-C1-CB2-OB2
46	B	1001	3PE	C36-C37-C38-C39
46	N	902	3PE	O21-C2-C3-O31
46	L	703	3PE	C2-C1-O11-P
45	h	1002	LMT	C5-C6-C7-C8
45	l	201	LMT	C11-C10-C9-C8
46	Y	602	3PE	C33-C34-C35-C36
58	U	101	EHZ	C22-C23-C24-C25
46	L	701	3PE	C1-O11-P-O13
53	X	1701	CDL	C1-CB2-OB2-PB2
46	N	902	3PE	O11-C1-C2-O21
46	Y	601	3PE	C27-C28-C29-C2A
45	L	704	LMT	C4B-C5B-C6B-O6B
46	I	201	3PE	C3B-C3C-C3D-C3E
46	N	904	3PE	C27-C28-C29-C2A
53	q	201	CDL	CA2-C1-CB2-OB2
46	N	904	3PE	C3A-C3B-C3C-C3D
56	P	501	NDP	PN-O3-PA-O1A
46	L	701	3PE	C3C-C3D-C3E-C3F
46	Y	602	3PE	C34-C35-C36-C37
46	Y	602	3PE	C39-C3A-C3B-C3C
46	I	201	3PE	C2E-C2F-C2G-C2H
59	o	201	MYR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
45	Y	603	LMT	O5'-C1'-O1'-C1
46	L	705	3PE	O11-C1-C2-C3
46	L	703	3PE	C33-C34-C35-C36
53	X	1701	CDL	C16-C17-C18-C19
45	M	801	LMT	C2'-C1'-O1'-C1
46	A	302	3PE	C23-C24-C25-C26
46	N	902	3PE	C23-C24-C25-C26
46	L	705	3PE	C24-C25-C26-C27
46	I	204	3PE	C32-C33-C34-C35
48	g	1501	PC1	C38-C39-C3A-C3B
46	d	1201	3PE	C35-C36-C37-C38
53	d	1202	CDL	C11-C12-C13-C14
53	X	1701	CDL	C53-C54-C55-C56
46	A	302	3PE	C22-C23-C24-C25
46	I	201	3PE	C27-C28-C29-C2A
53	h	1001	CDL	C32-C33-C34-C35
58	T	101	EHZ	C22-C23-C24-C25
53	L	702	CDL	C52-C51-CB5-OB6
46	Y	601	3PE	C38-C39-C3A-C3B
46	Z	401	3PE	O22-C21-O21-C2
48	B	1003	PC1	O21-C21-C22-C23
58	T	101	EHZ	C12-C13-C14-N2
58	U	101	EHZ	C10-C11-N1-C12
53	K	401	CDL	C12-C11-CA5-OA6
46	N	902	3PE	C1-C2-C3-O31
53	d	1202	CDL	CA3-CA4-CA6-OA8
53	d	1202	CDL	OA5-CA3-CA4-OA6
53	K	401	CDL	C32-C31-CA7-OA8
53	K	401	CDL	C33-C34-C35-C36
46	B	1001	3PE	C37-C38-C39-C3A
53	L	702	CDL	C55-C56-C57-C58
53	d	1202	CDL	C40-C41-C42-C43
53	d	1202	CDL	CA5-C11-C12-C13
53	X	1701	CDL	C12-C11-CA5-OA6
46	Y	602	3PE	O11-C1-C2-C3
53	X	1701	CDL	C59-C60-C61-C62
46	I	201	3PE	O21-C2-C3-O31
53	d	1202	CDL	OA6-CA4-CA6-OA8
53	q	201	CDL	OA6-CA4-CA6-OA8
46	L	703	3PE	C38-C39-C3A-C3B
46	I	201	3PE	C32-C31-O31-C3
46	d	1201	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	C32-C31-CA7-OA8
53	X	1701	CDL	C77-C78-C79-C80
46	Y	602	3PE	C2-C1-O11-P
53	d	1202	CDL	C72-C71-CB7-OB8
53	q	201	CDL	C52-C51-CB5-OB6
46	N	902	3PE	C27-C28-C29-C2A
48	B	1003	PC1	C35-C36-C37-C38
53	h	1001	CDL	C22-C23-C24-C25
46	I	201	3PE	O32-C31-O31-C3
45	M	801	LMT	C4'-C5'-C6'-O6'
45	L	704	LMT	O5B-C5B-C6B-O6B
53	K	401	CDL	C12-C11-CA5-OA7
52	H	602	I49	N03-C14-N02-C15
53	X	1701	CDL	C12-C11-CA5-OA7
46	A	302	3PE	C33-C34-C35-C36
46	I	201	3PE	C26-C27-C28-C29
53	K	401	CDL	C32-C31-CA7-OA9
53	q	201	CDL	C52-C51-CB5-OB7
45	M	802	LMT	C5-C6-C7-C8
46	L	701	3PE	C11-O13-P-O12
46	L	705	3PE	C11-O13-P-O14
46	d	1201	3PE	C11-O13-P-O14
53	X	1701	CDL	CA2-OA2-PA1-OA4
56	P	501	NDP	O4B-C4B-C5B-O5B
53	L	702	CDL	C52-C51-CB5-OB7
45	h	1003	LMT	C7-C8-C9-C10
45	j	101	LMT	O5B-C5B-C6B-O6B
46	L	705	3PE	C32-C33-C34-C35
54	O	401	GTP	PB-O3B-PG-O1G
48	B	1003	PC1	O22-C21-C22-C23
48	g	1501	PC1	C2F-C2G-C2H-C2I
46	Y	601	3PE	C3A-C3B-C3C-C3D
46	L	705	3PE	C12-C11-O13-P
46	Z	401	3PE	C12-C11-O13-P
53	d	1202	CDL	C72-C71-CB7-OB9
46	A	302	3PE	C25-C26-C27-C28
45	N	901	LMT	C4'-C5'-C6'-O6'
45	h	1003	LMT	C6-C7-C8-C9
46	d	1201	3PE	C36-C37-C38-C39
45	j	101	LMT	C1-C2-C3-C4
45	L	704	LMT	C6-C7-C8-C9
46	I	201	3PE	C28-C29-C2A-C2B

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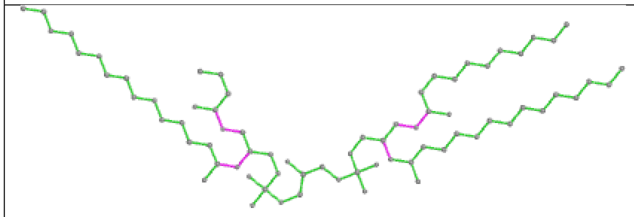
Mol	Chain	Res	Type	Atoms
45	h	1003	LMT	C11-C10-C9-C8
46	I	201	3PE	C2C-C2D-C2E-C2F
46	d	1201	3PE	O22-C21-C22-C23
53	q	201	CDL	C32-C31-CA7-OA9
46	Y	601	3PE	C25-C26-C27-C28
46	Y	602	3PE	O11-C1-C2-O21
50	F	501	FMN	N10-C1'-C2'-O2'
46	L	705	3PE	O21-C21-C22-C23
45	M	802	LMT	C2-C1-O1'-C1'
53	X	1701	CDL	C32-C31-CA7-OA8
53	X	1701	CDL	C32-C31-CA7-OA9
46	A	302	3PE	O21-C21-C22-C23
46	N	904	3PE	O21-C21-C22-C23
46	Y	601	3PE	C2C-C2D-C2E-C2F
46	d	1201	3PE	C34-C35-C36-C37
46	Z	401	3PE	O31-C31-C32-C33

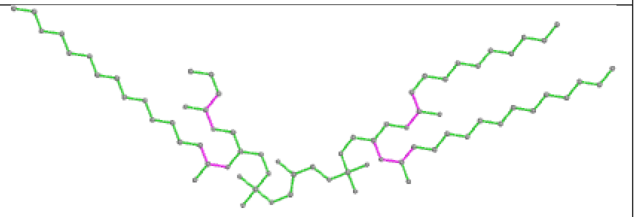
There are no ring outliers.

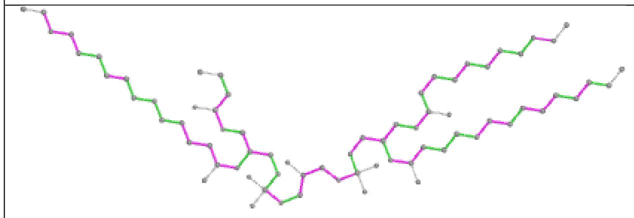
No monomer is involved in short contacts.

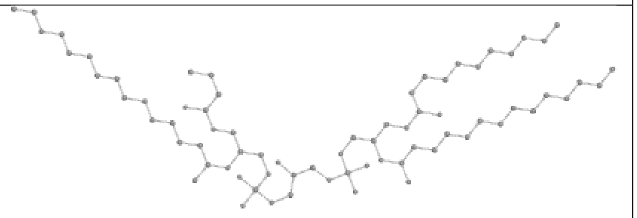
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 X 1701

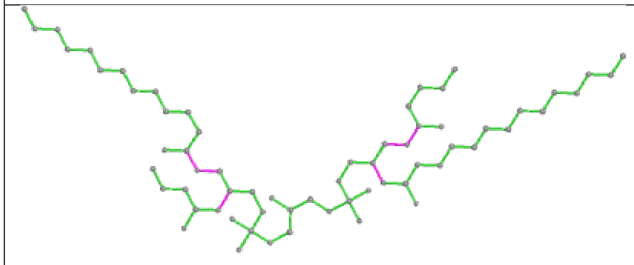

Bond lengths

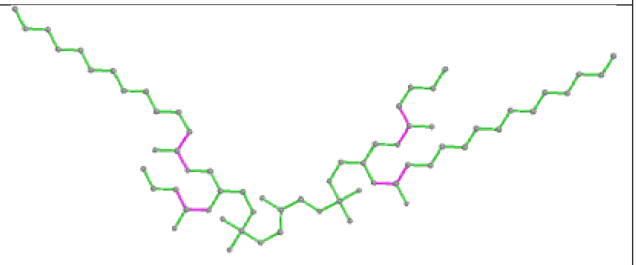

Bond angles

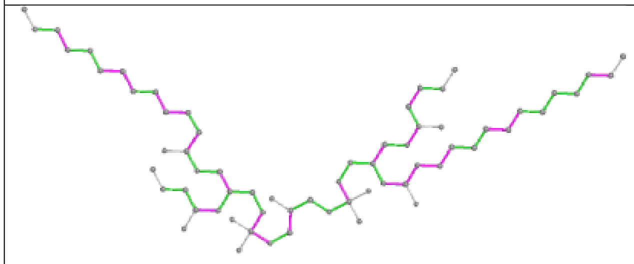

Torsions

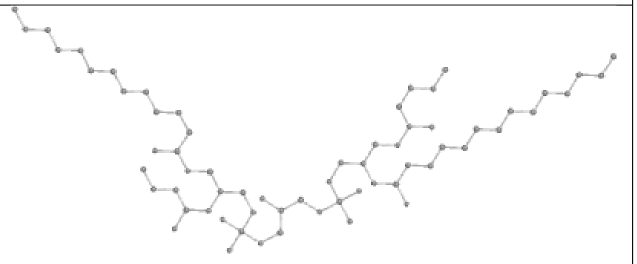

Rings

Ligand CDL L 702

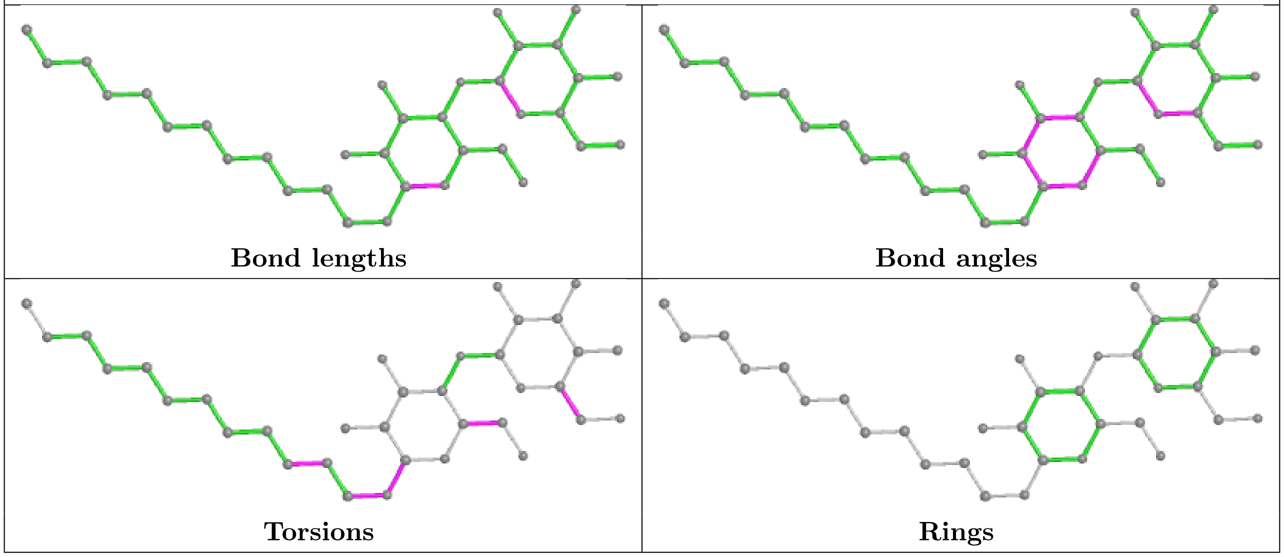

Bond lengths


Bond angles

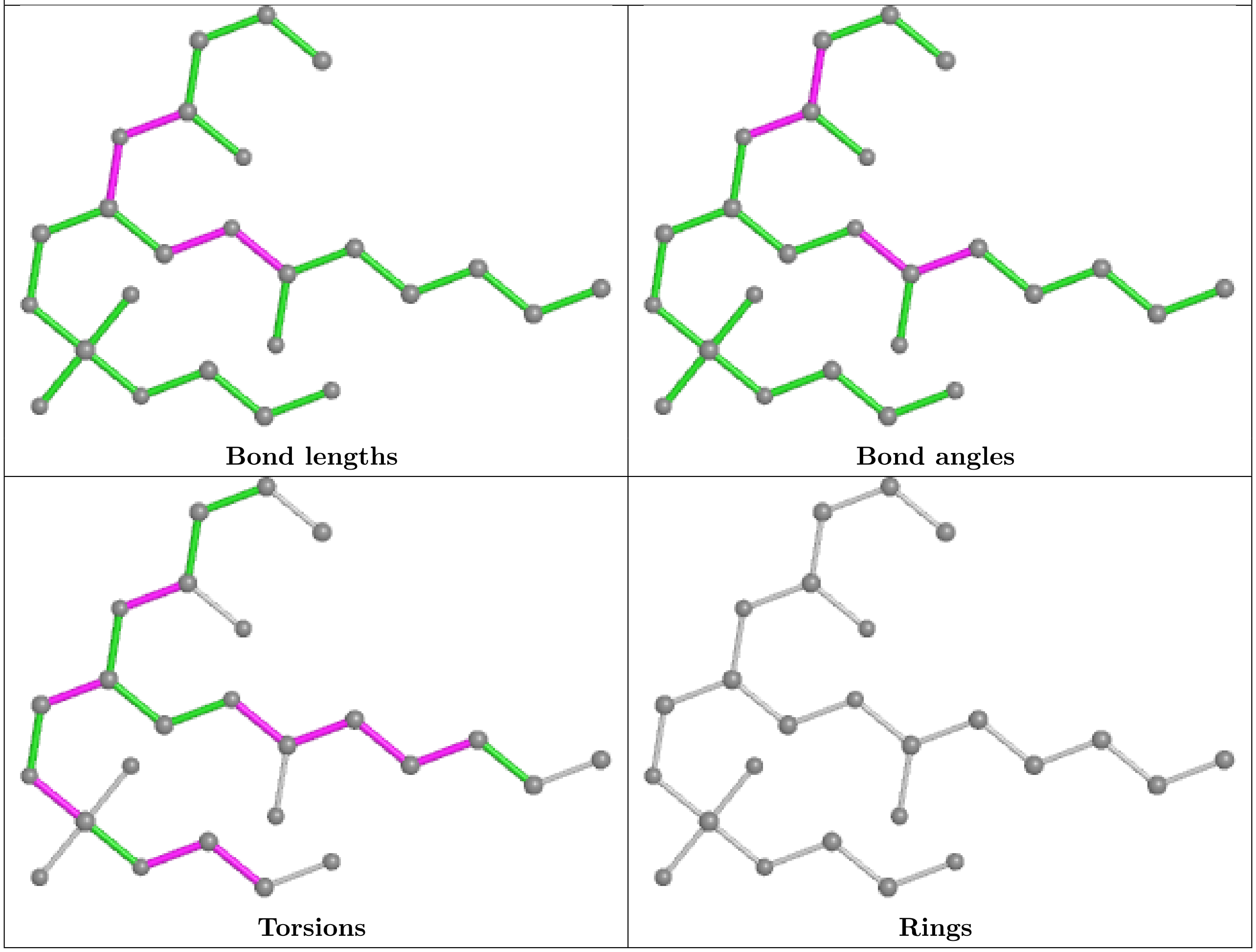

Torsions


Rings

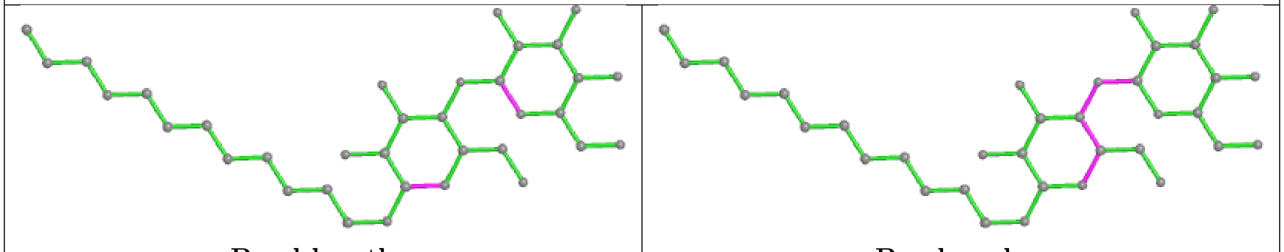
Ligand LMT M 801



Ligand 3PE Z 401

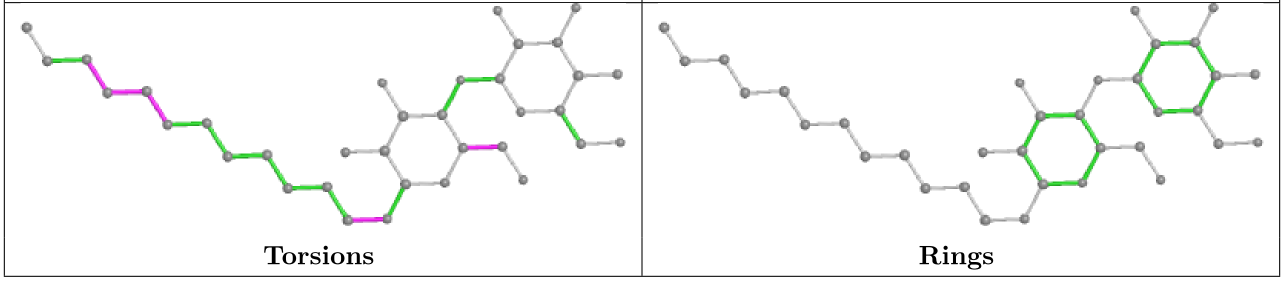


Ligand LMT h 1003



Bond lengths

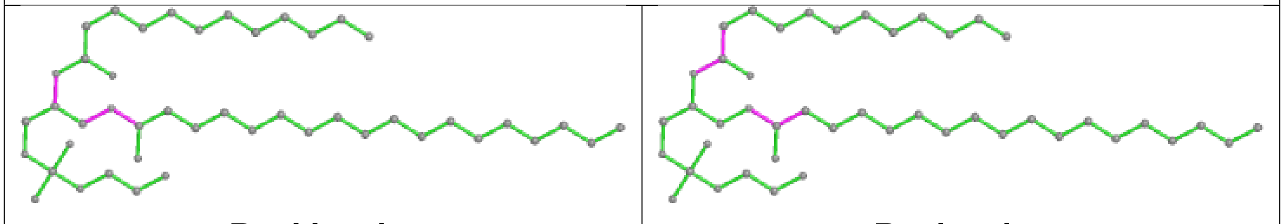
Bond angles



Torsions

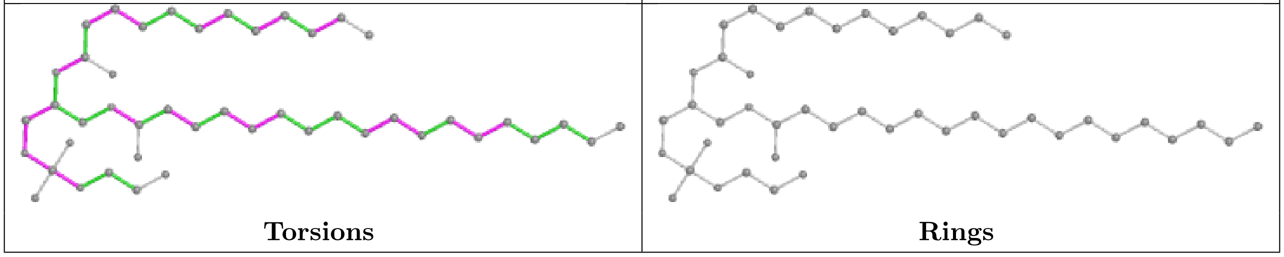
Rings

Ligand 3PE L 703



Bond lengths

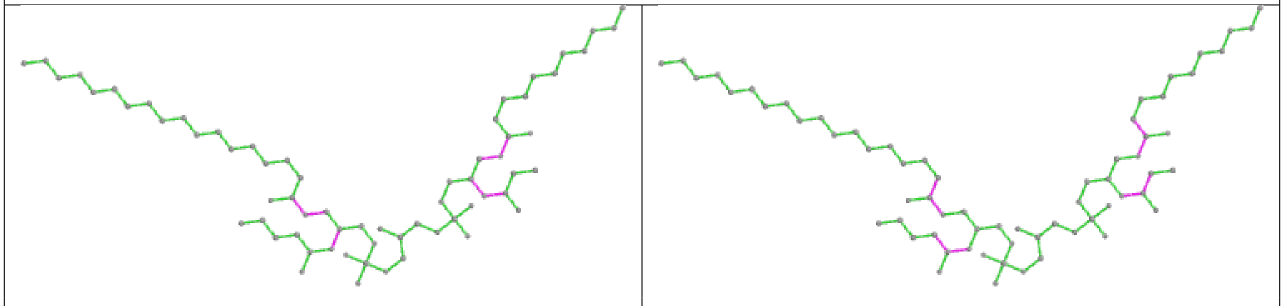
Bond angles



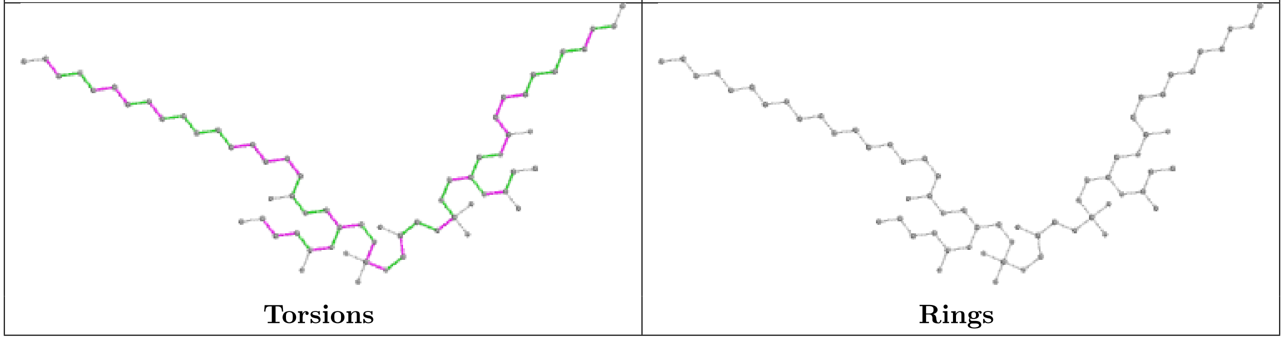
Torsions

Rings

Ligand CDL d 1202

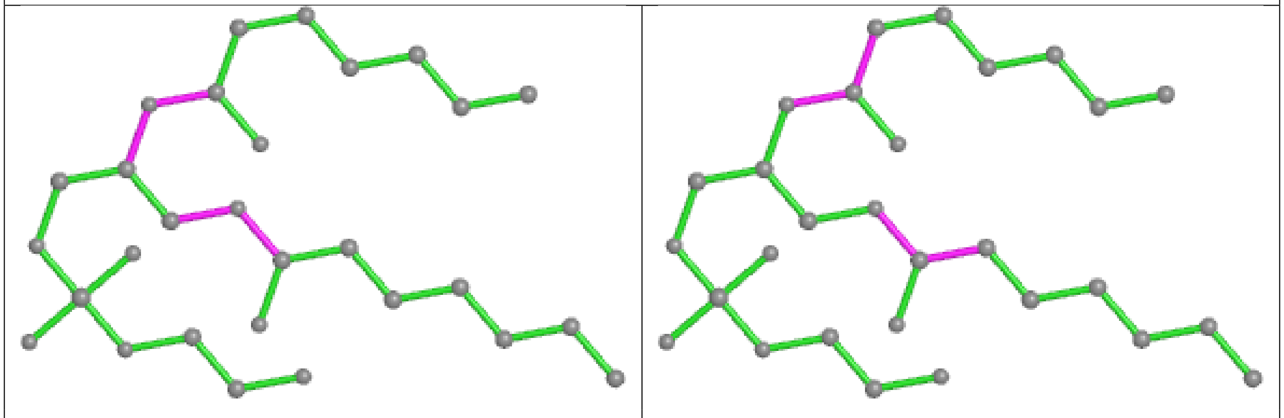


Bond lengths Bond angles

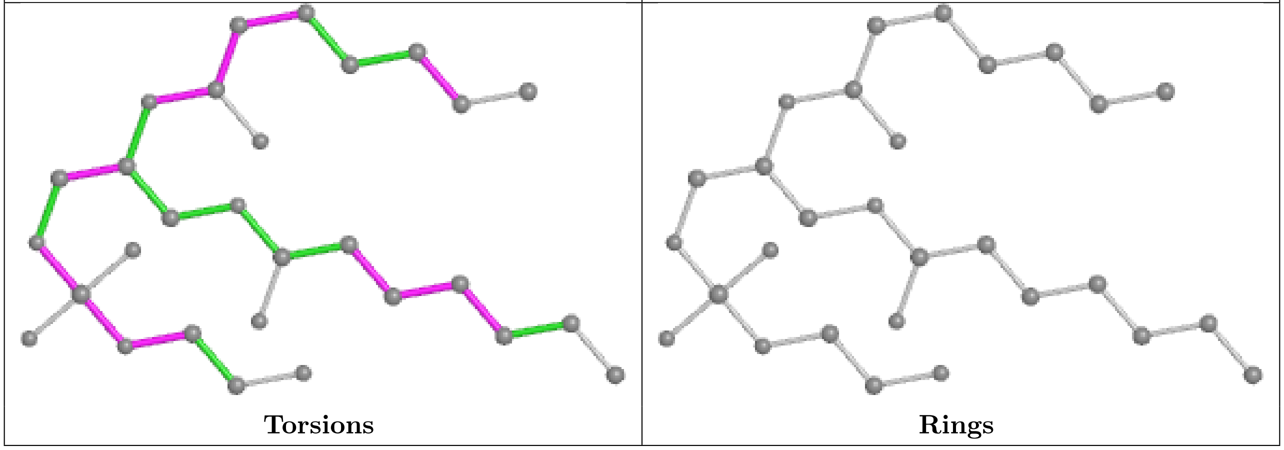


Torsions Rings

Ligand 3PE L 705

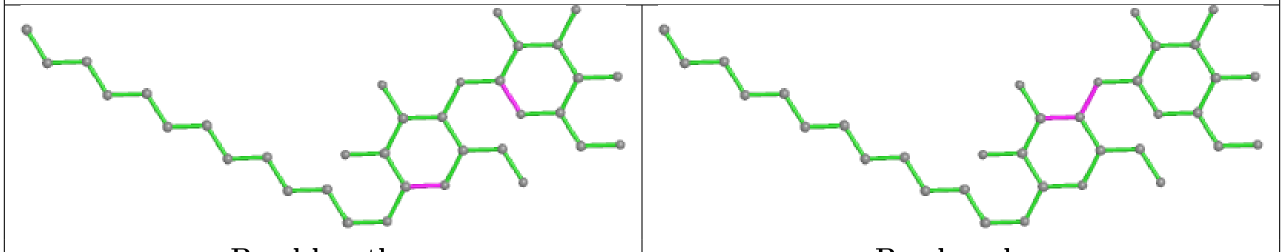


Bond lengths Bond angles



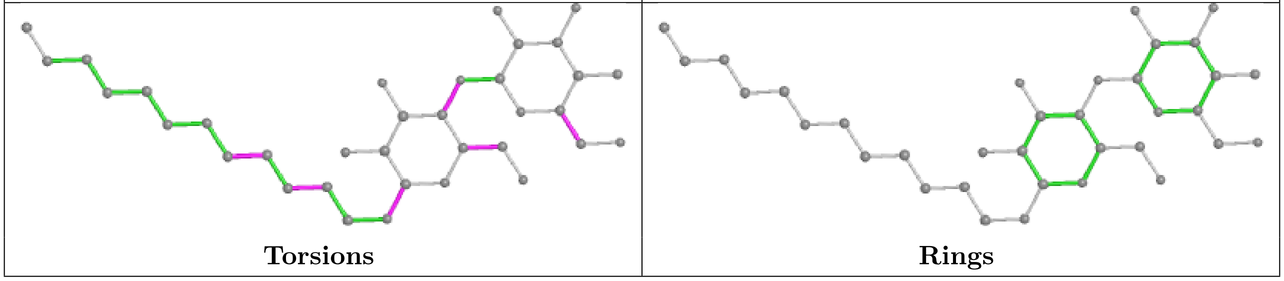
Torsions Rings

Ligand LMT A 301



Bond lengths

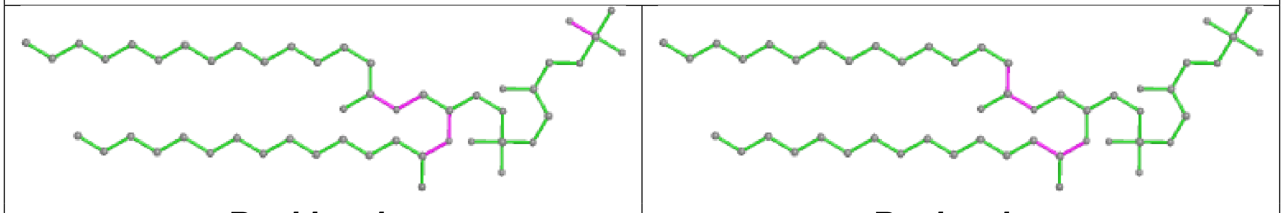
Bond angles



Torsions

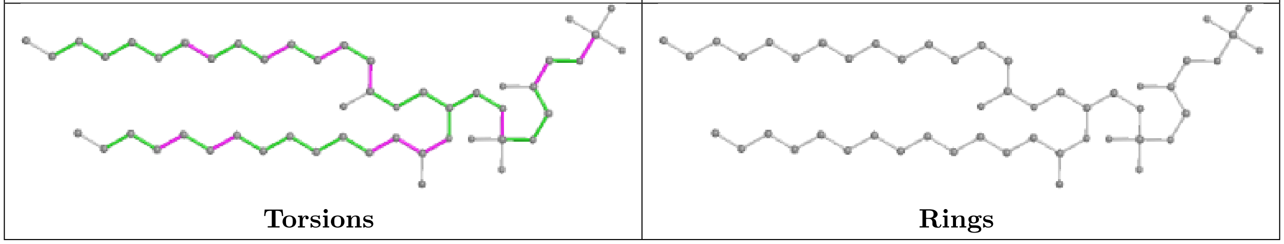
Rings

Ligand CDL K 401



Bond lengths

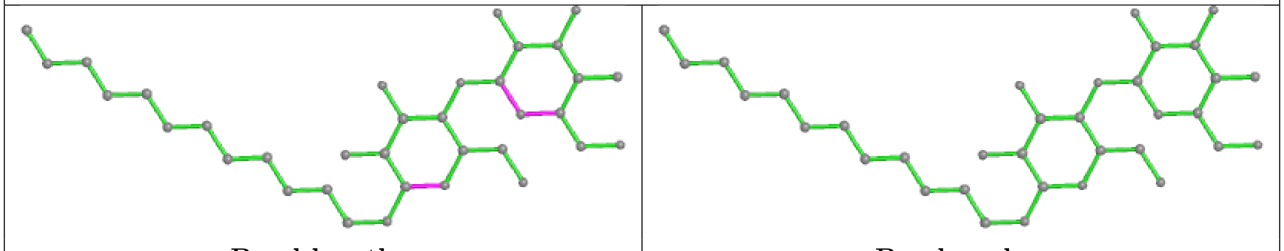
Bond angles



Torsions

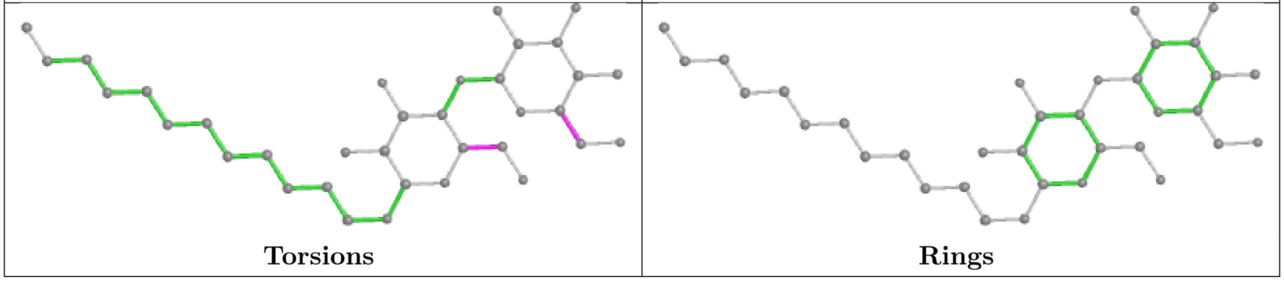
Rings

Ligand LMT N 901



Bond lengths

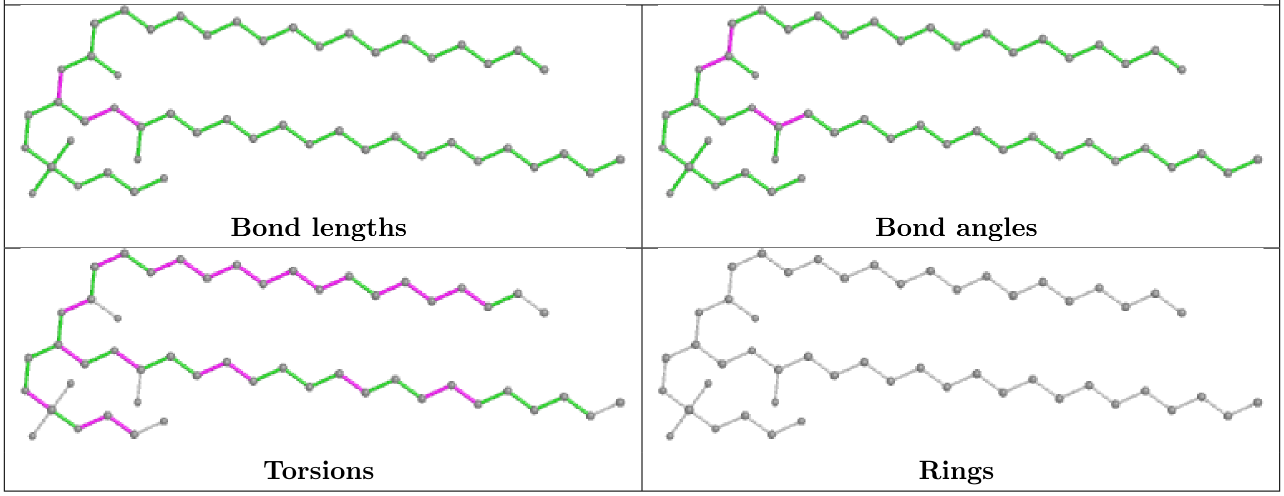
Bond angles



Torsions

Rings

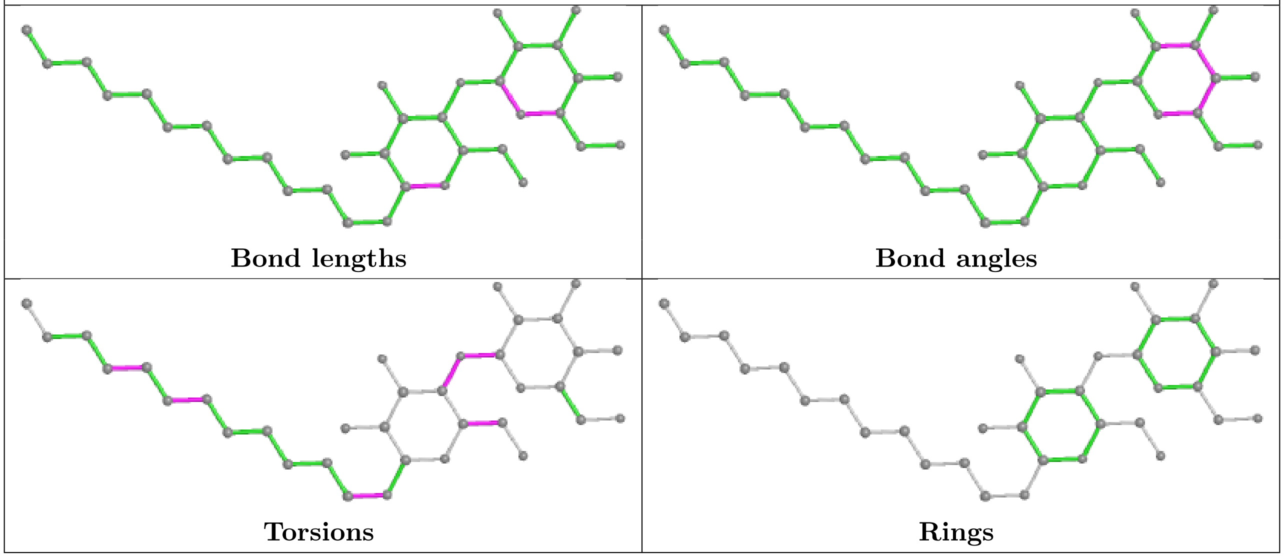
Ligand 3PE I 201



Bond lengths Bond angles

Torsions Rings

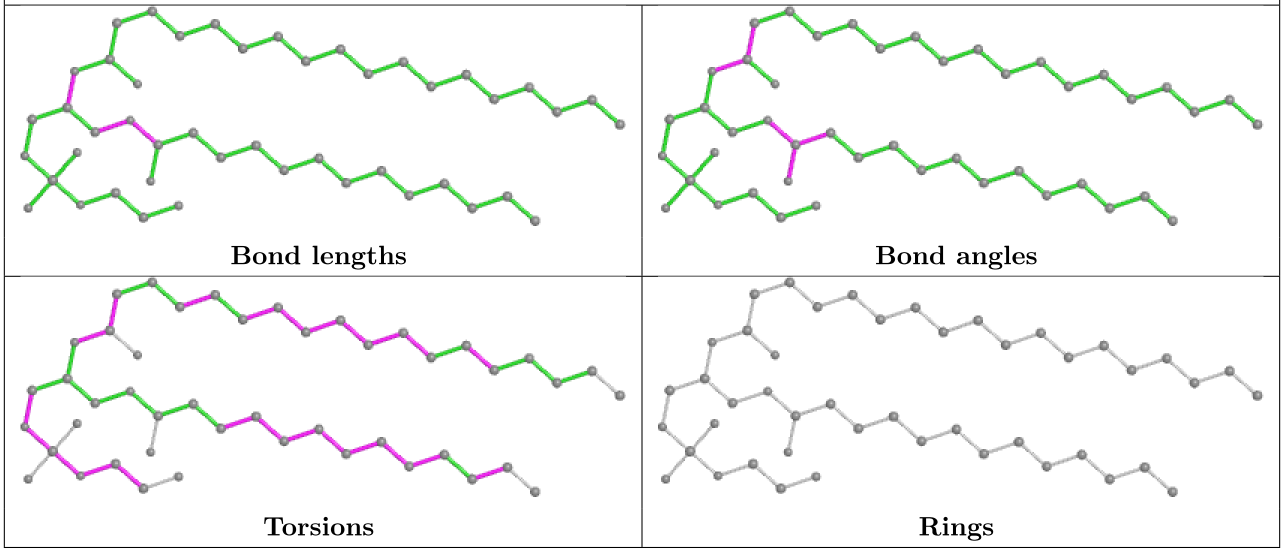
Ligand LMT M 802



Bond lengths Bond angles

Torsions Rings

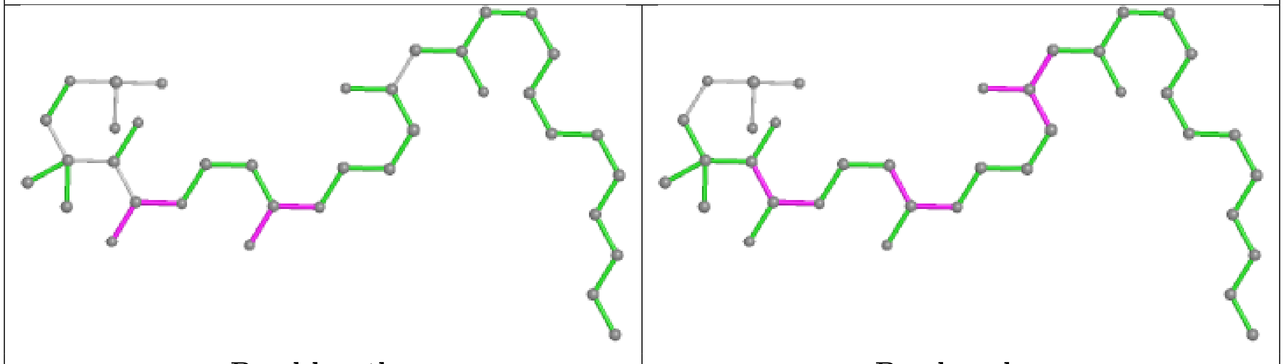
Ligand 3PE Y 601



Bond lengths Bond angles

Torsions Rings

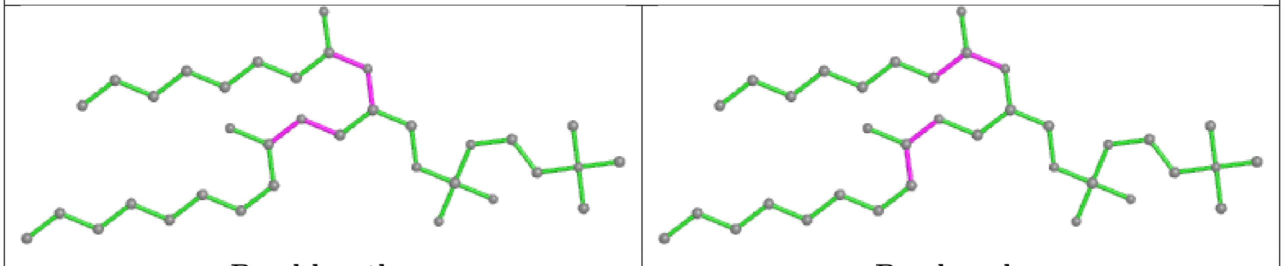
Ligand EHZ T 101



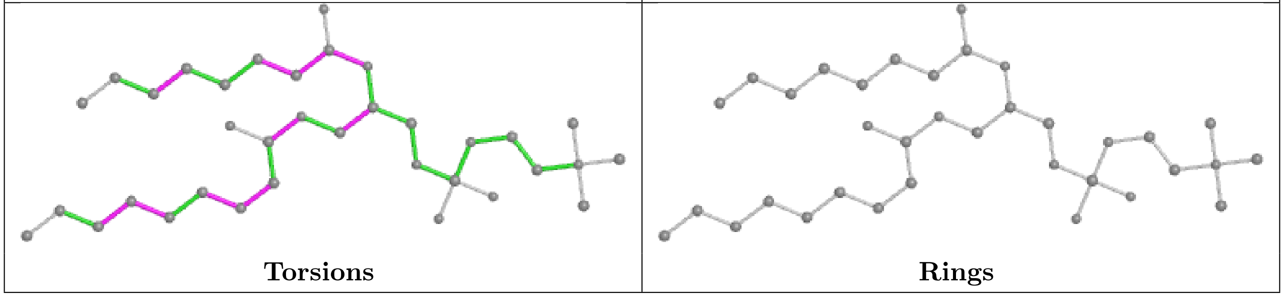
Bond lengths **Bond angles**

Torsions **Rings**

Ligand PC1 B 1003

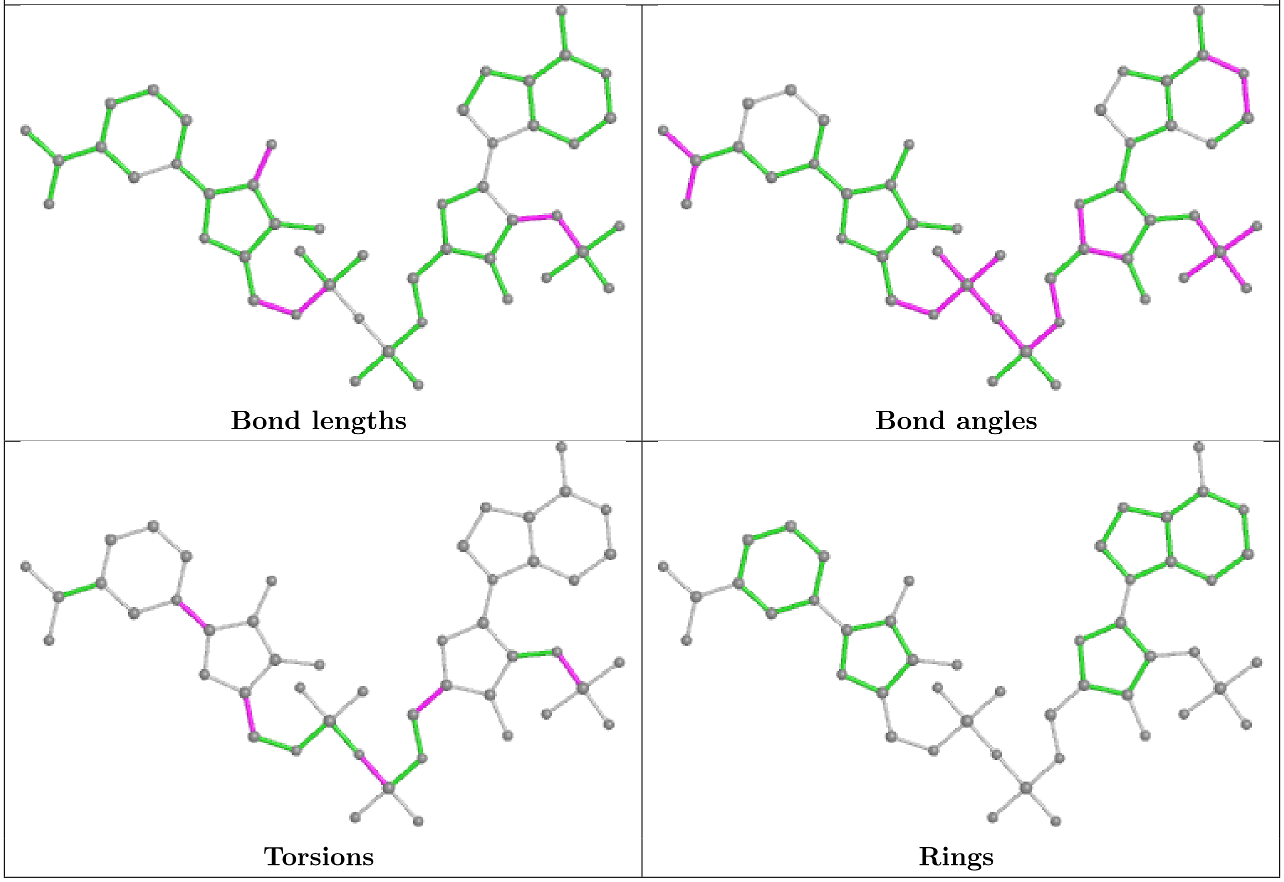


Bond lengths **Bond angles**



Torsions **Rings**

Ligand NDP P 501



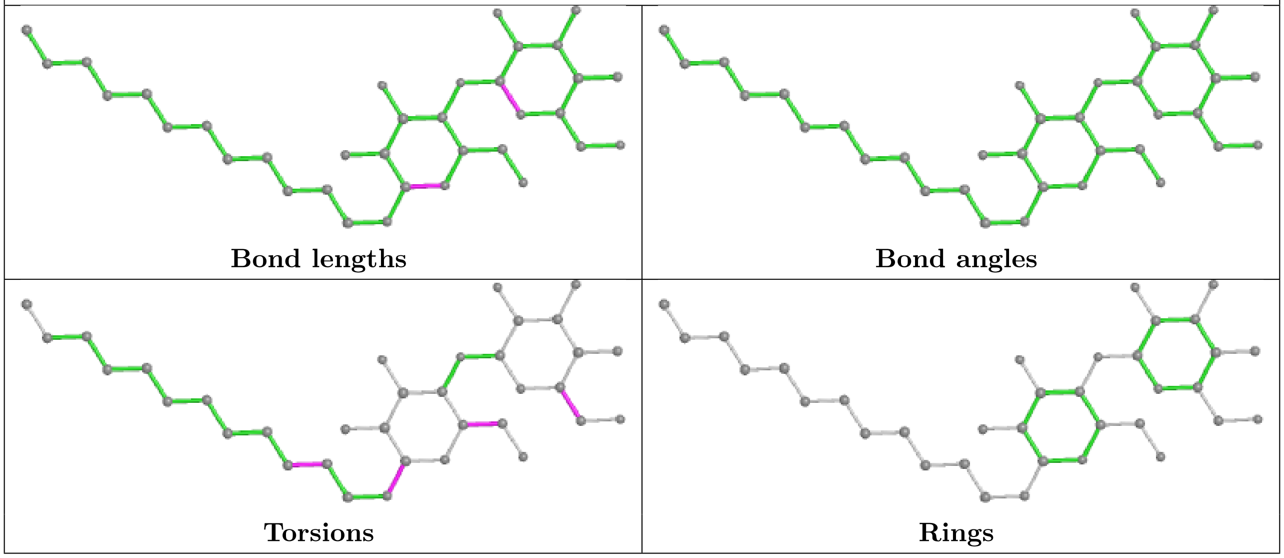
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT j 101



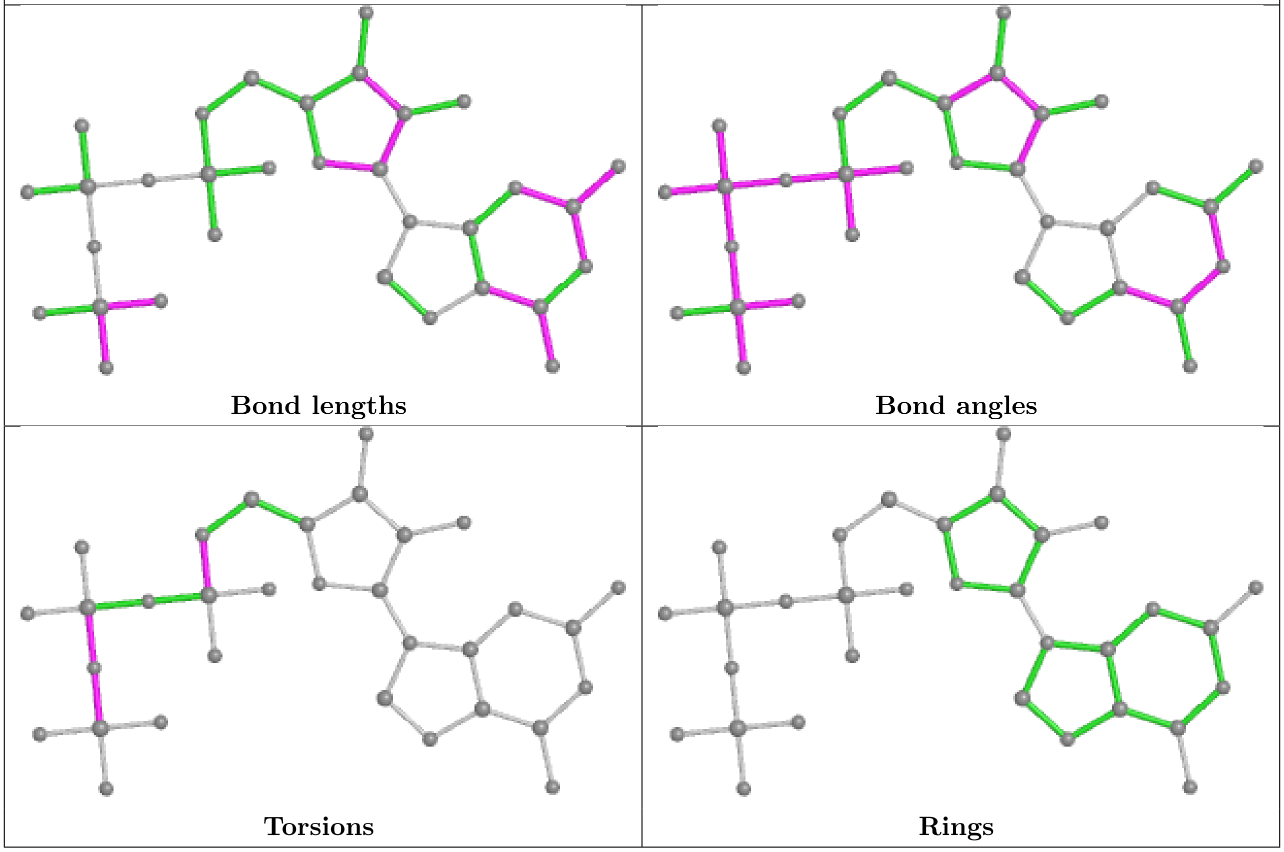
Bond lengths

Bond angles

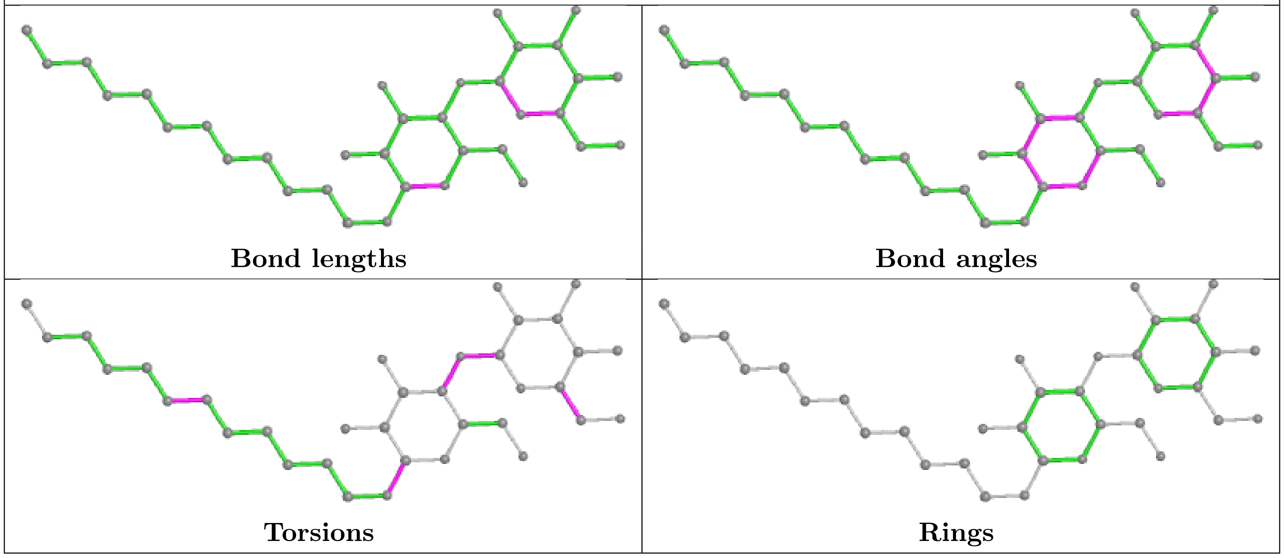
Torsions

Rings

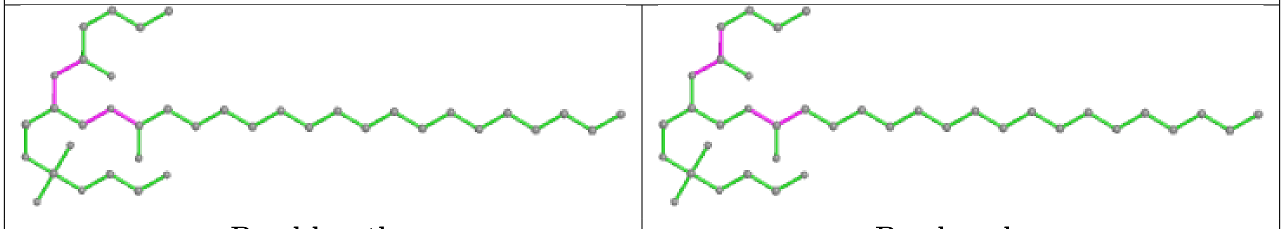
Ligand GTP O 401

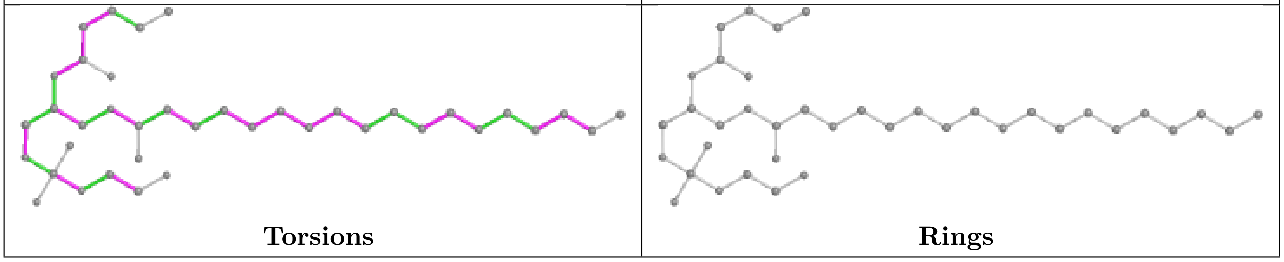


Ligand LMT h 1002

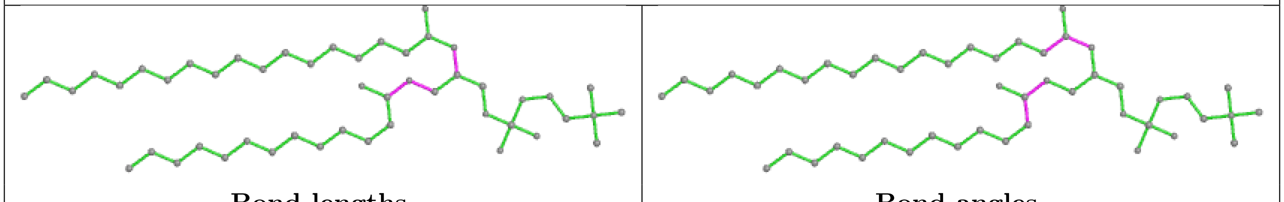


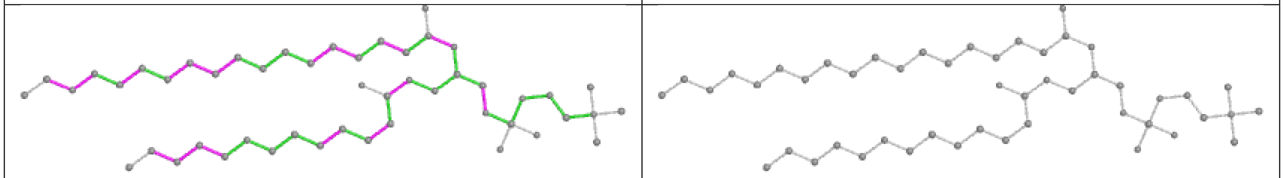
Ligand 3PE d 1201


Bond lengths Bond angles

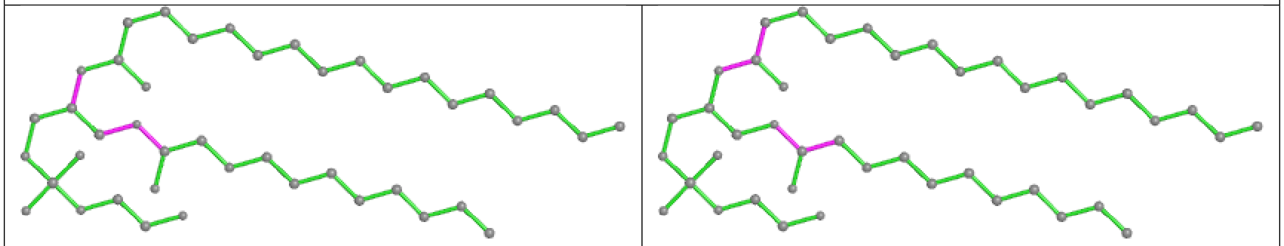

Torsions Rings

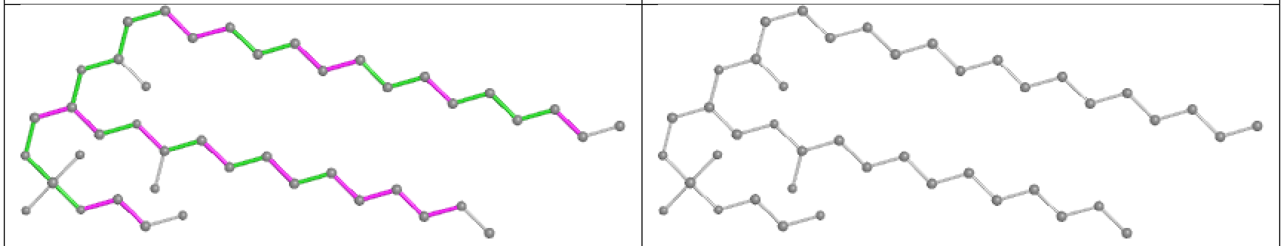
Ligand PC1 g 1501


Bond lengths Bond angles

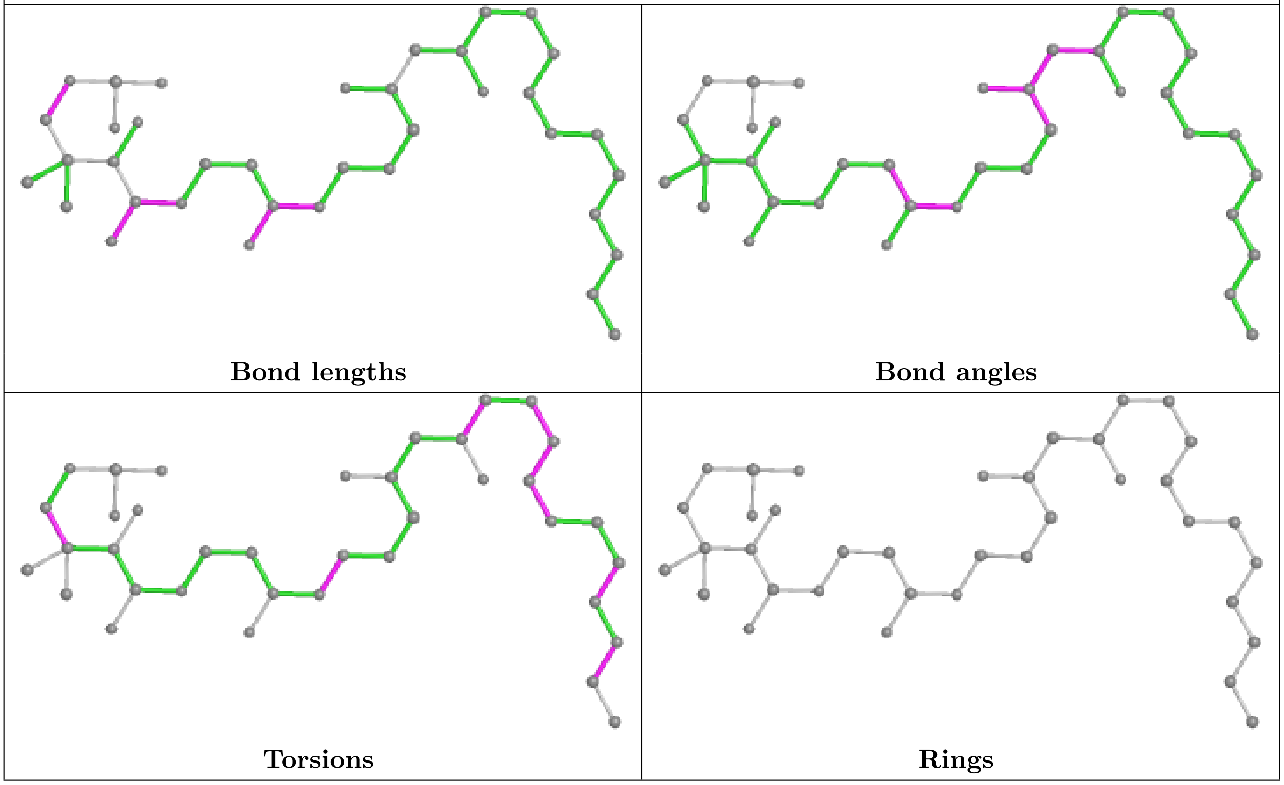

Torsions Rings

Ligand 3PE N 902


Bond lengths Bond angles


Torsions Rings

Ligand EHZ U 101



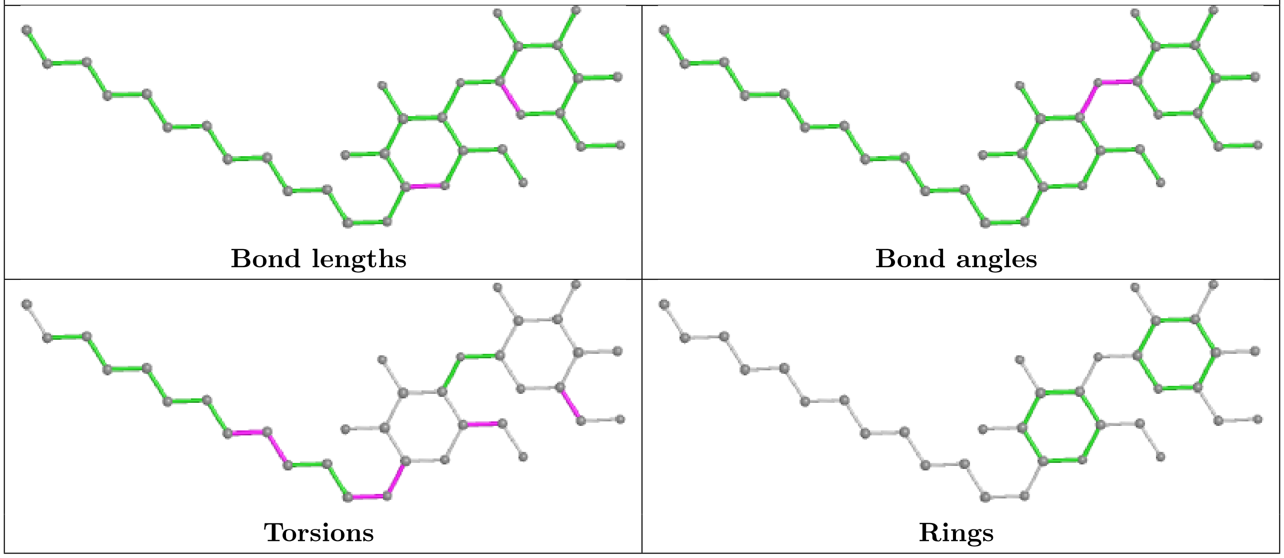
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT Y 603



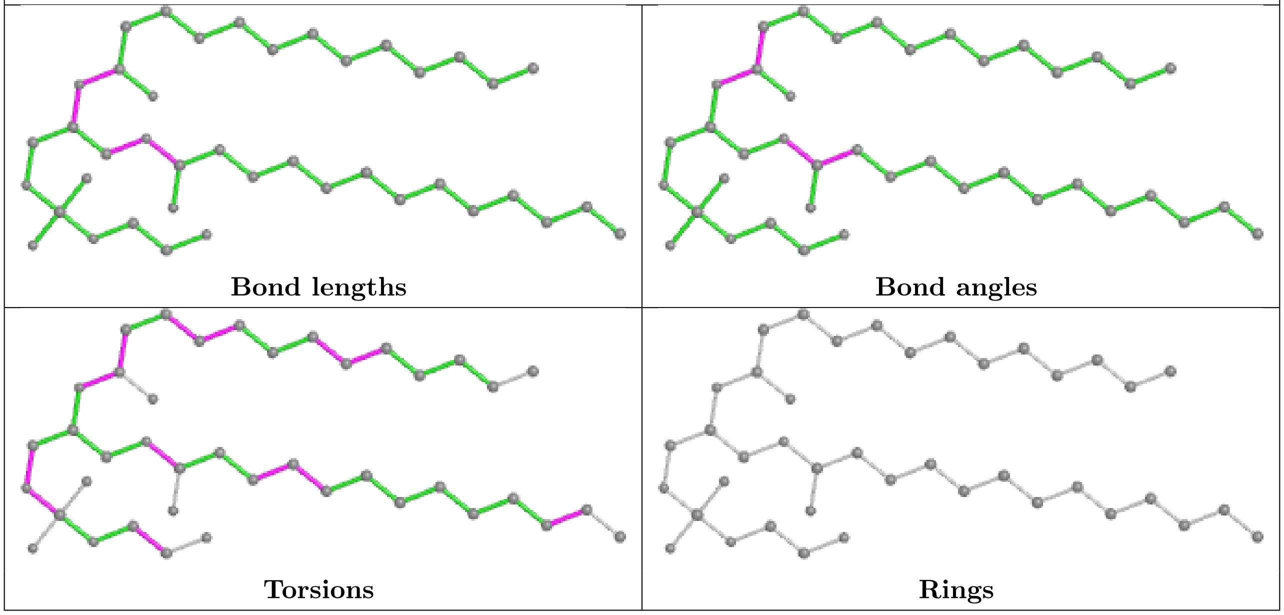
Bond lengths

Bond angles

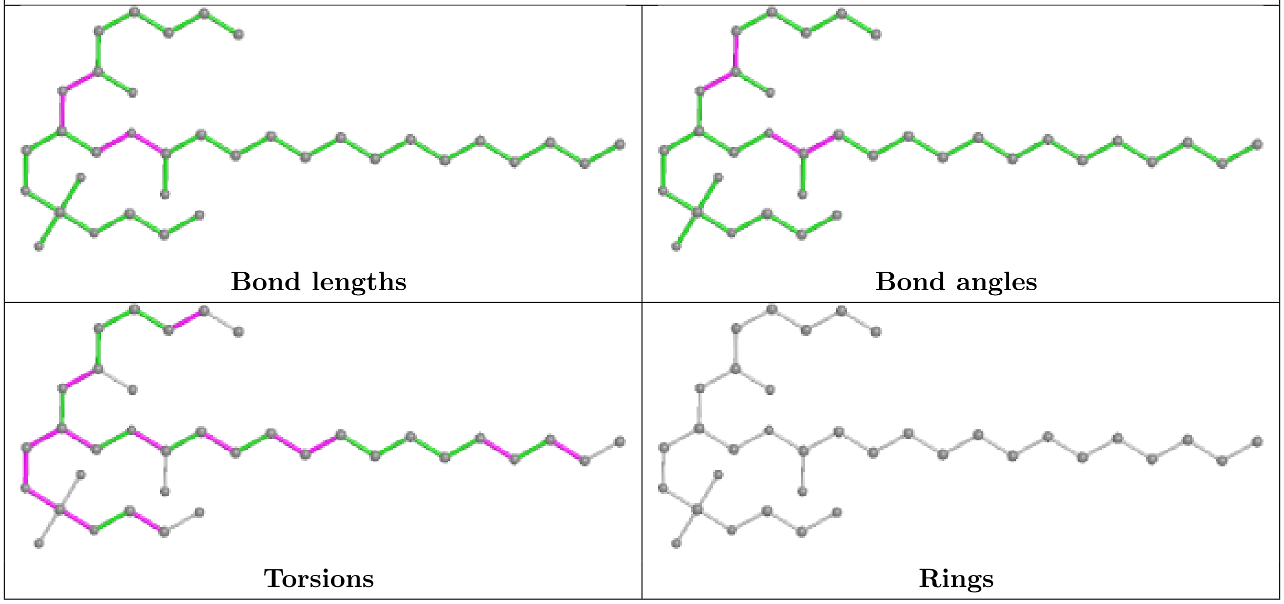
Torsions

Rings

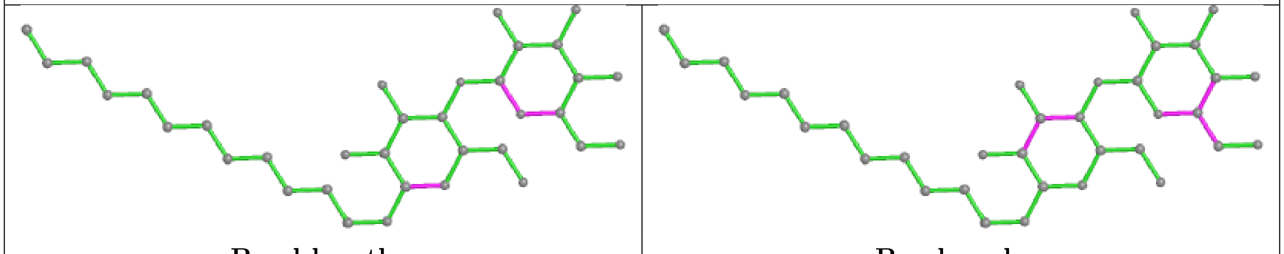
Ligand 3PE N 904



Ligand 3PE Y 602

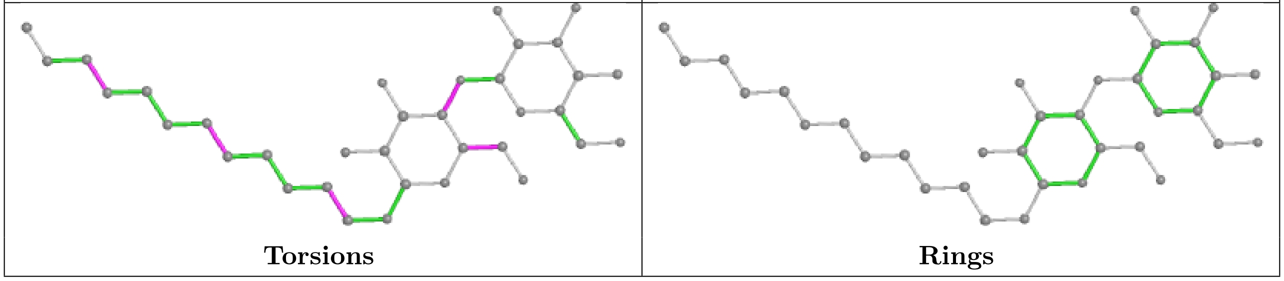


Ligand LMT l 201



Bond lengths

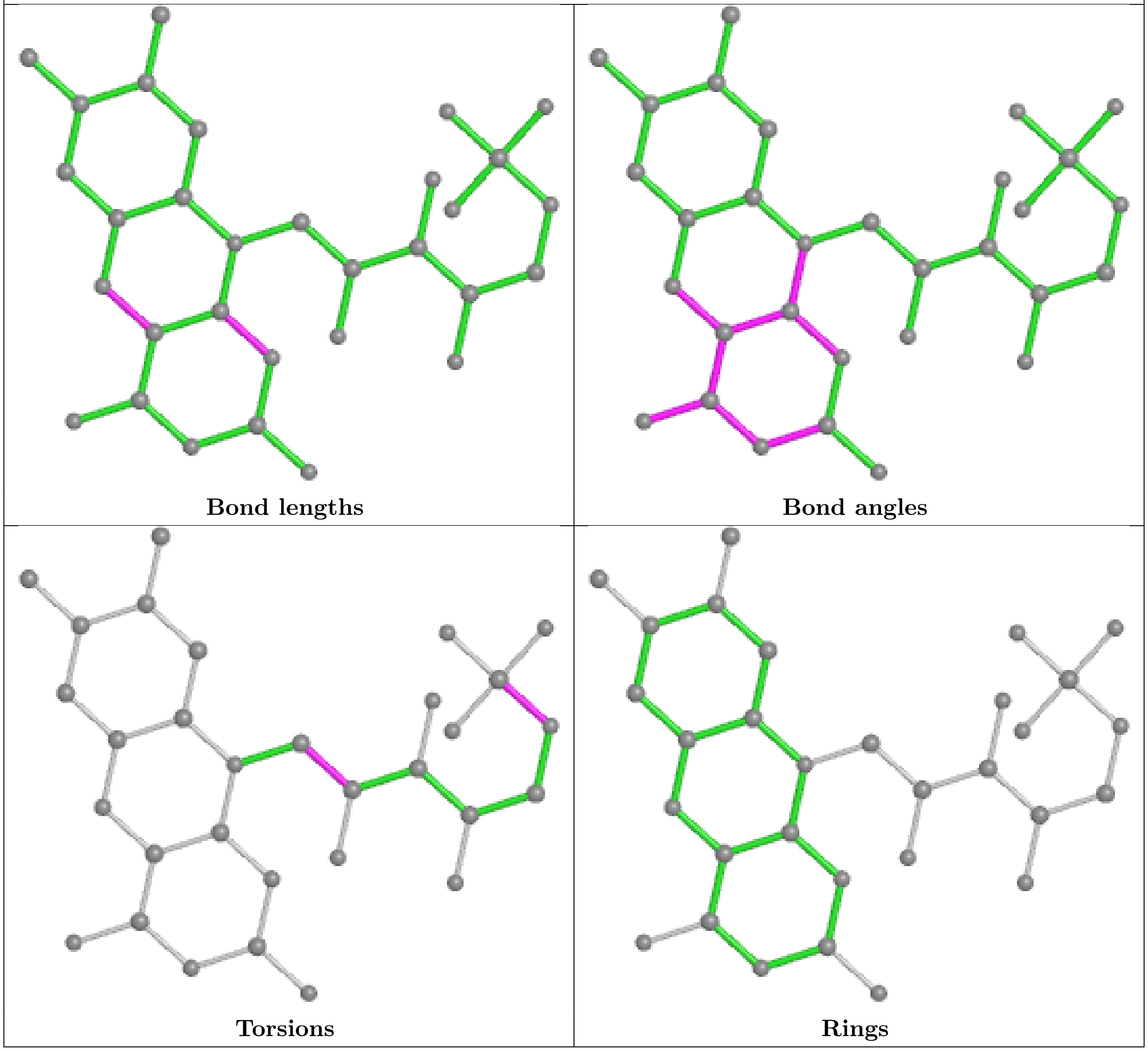
Bond angles



Torsions

Rings

Ligand FMN F 501



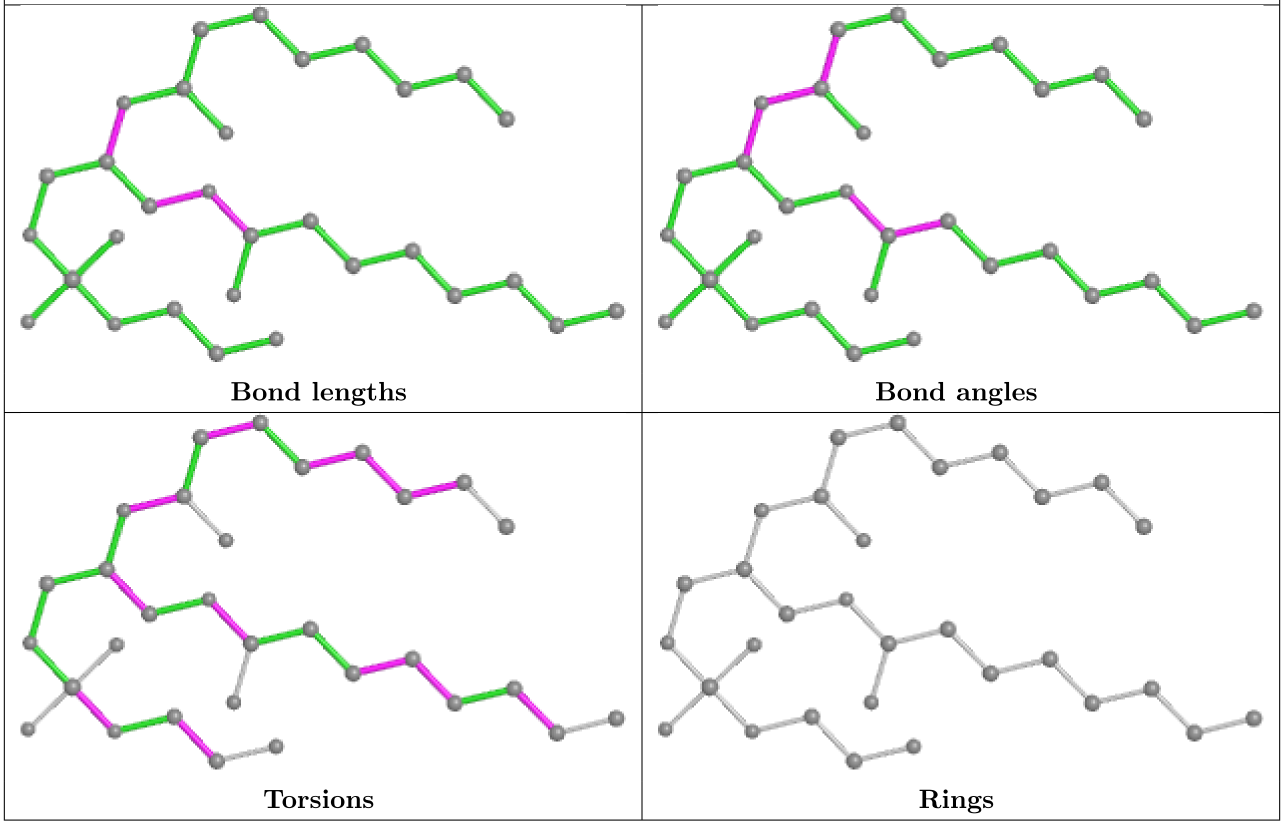
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE I 204



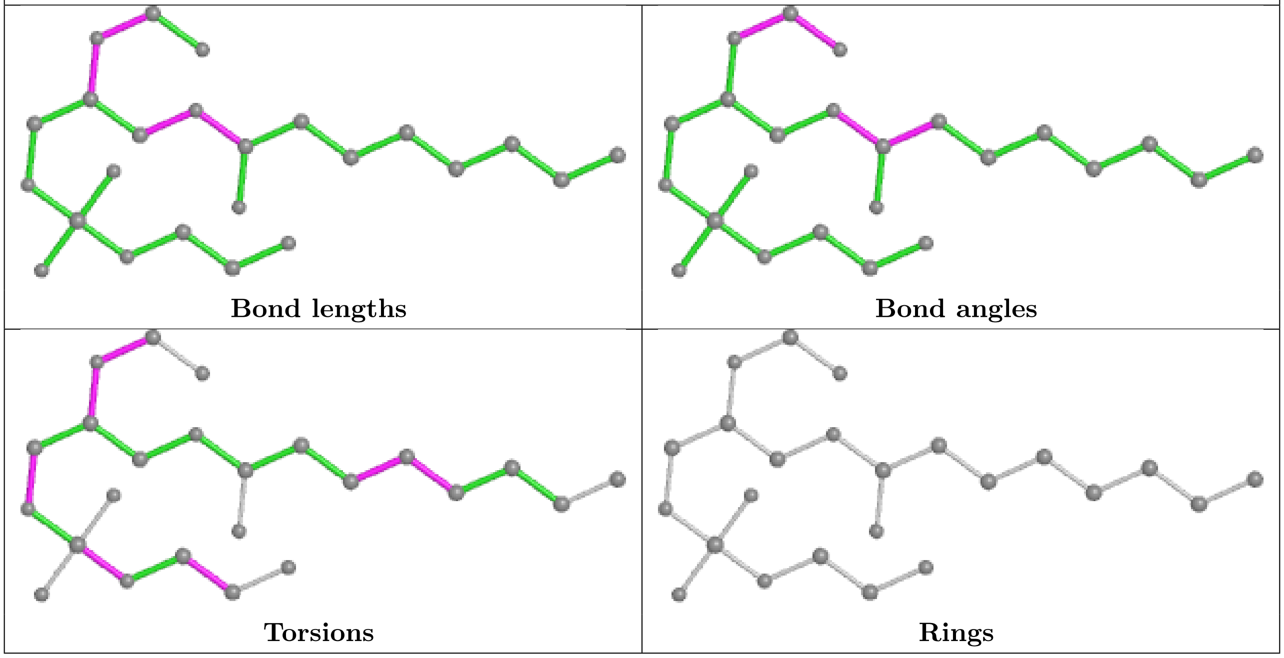
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE H 601



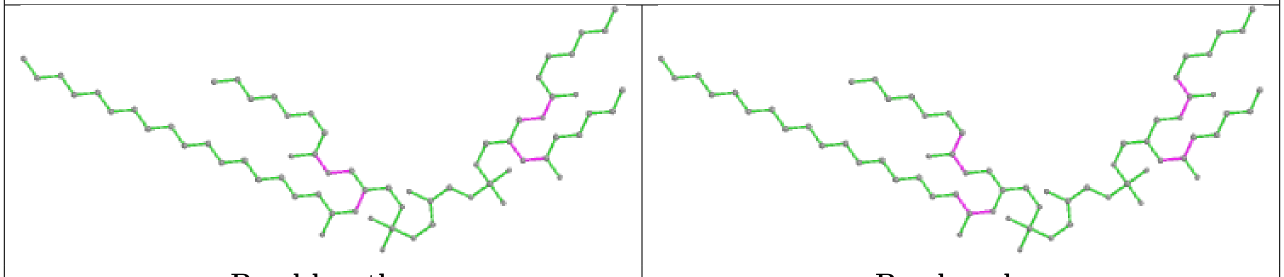
Bond lengths

Bond angles

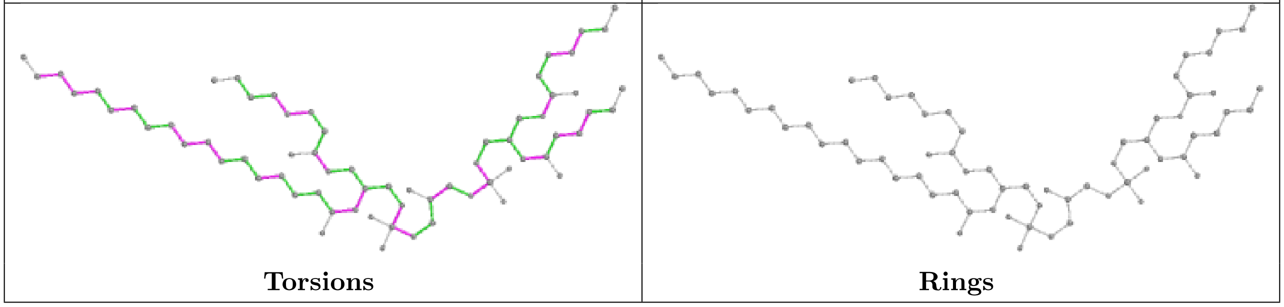
Torsions

Rings

Ligand CDL h 1001

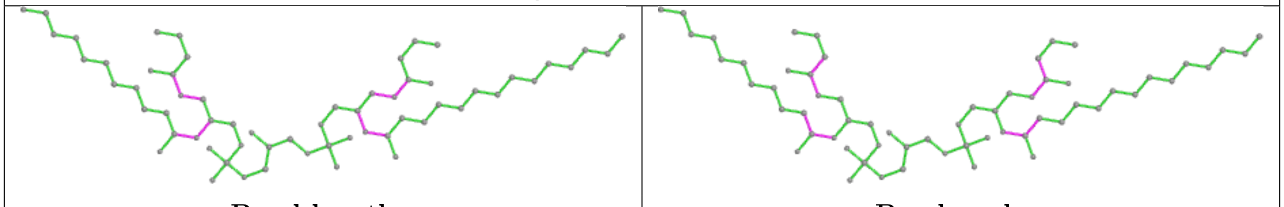


Bond lengths Bond angles

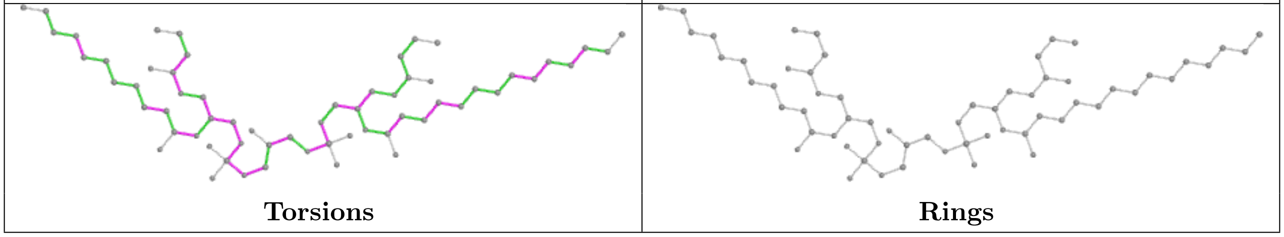


Torsions Rings

Ligand CDL q 201

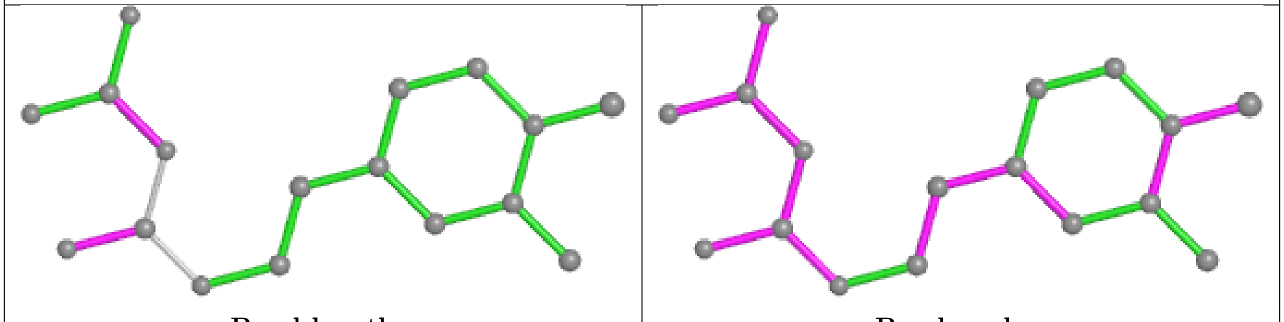


Bond lengths Bond angles



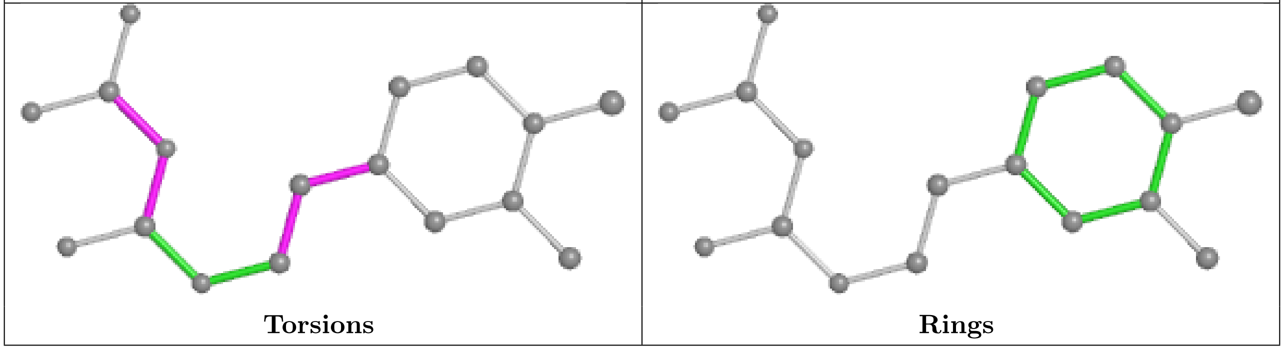
Torsions Rings

Ligand I49 H 602



Bond lengths

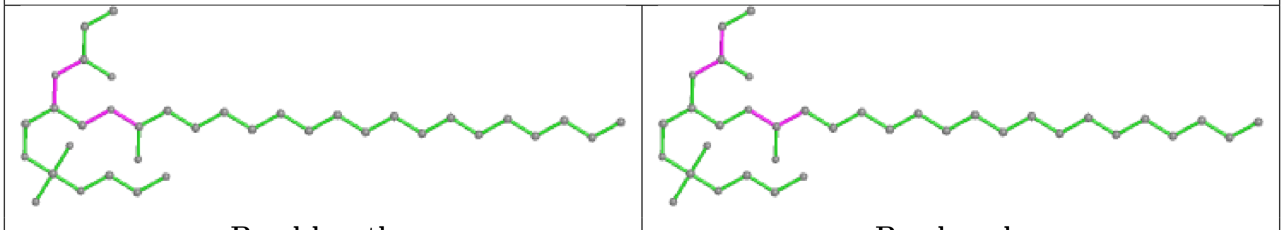
Bond angles



Torsions

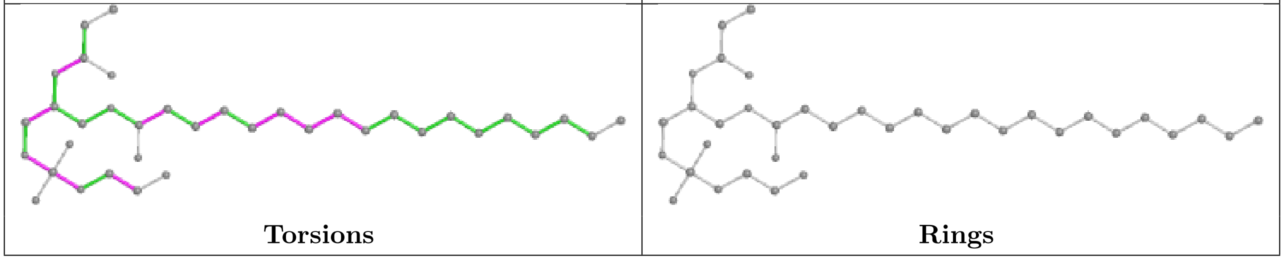
Rings

Ligand 3PE B 1001



Bond lengths

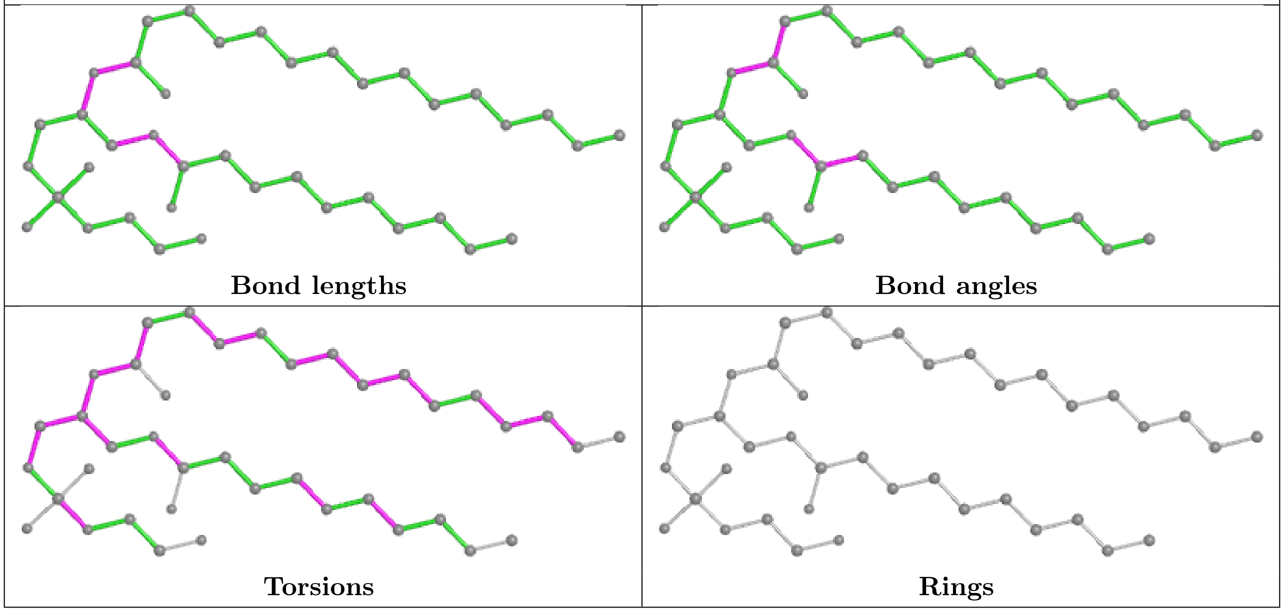
Bond angles



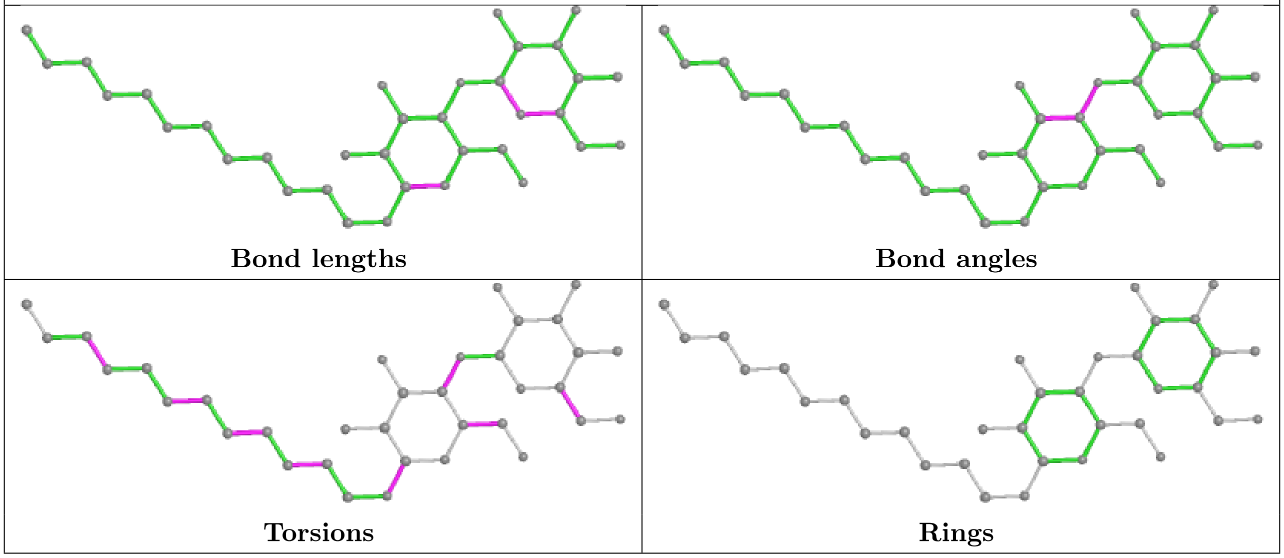
Torsions

Rings

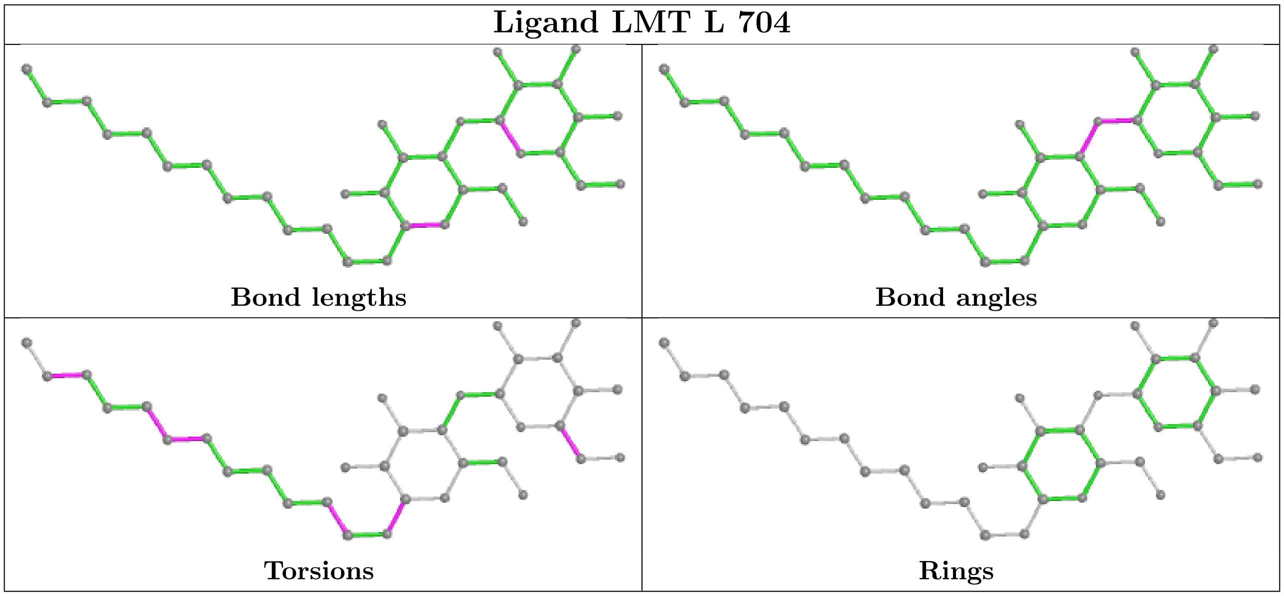
Ligand 3PE A 302



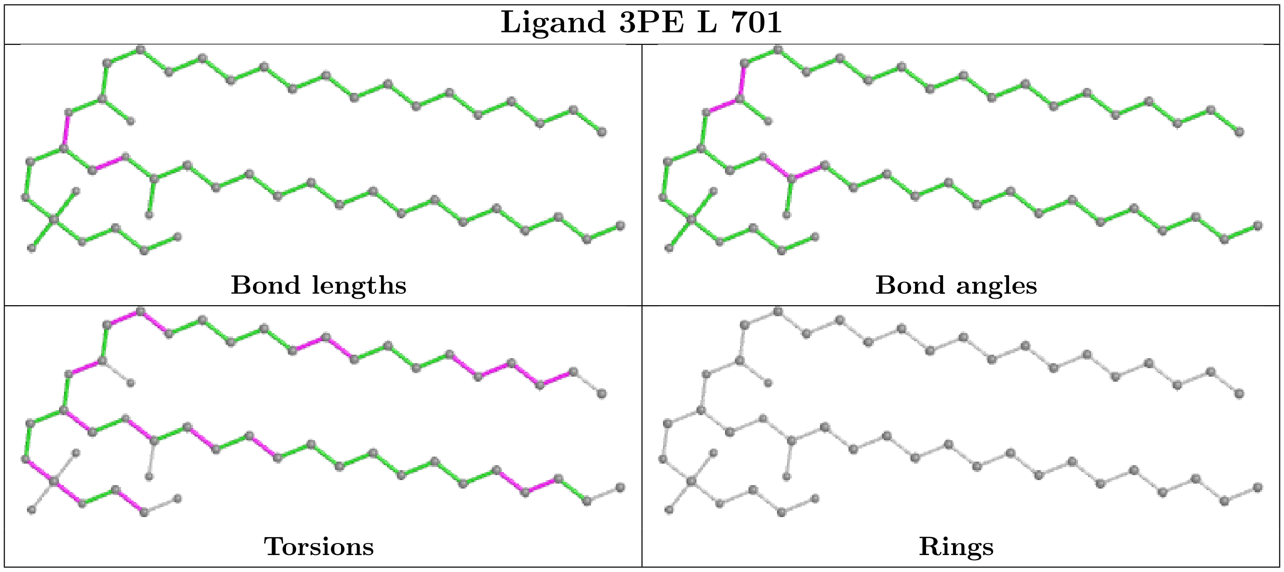
Ligand LMT N 903



Ligand LMT L 704



Ligand 3PE L 701



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.

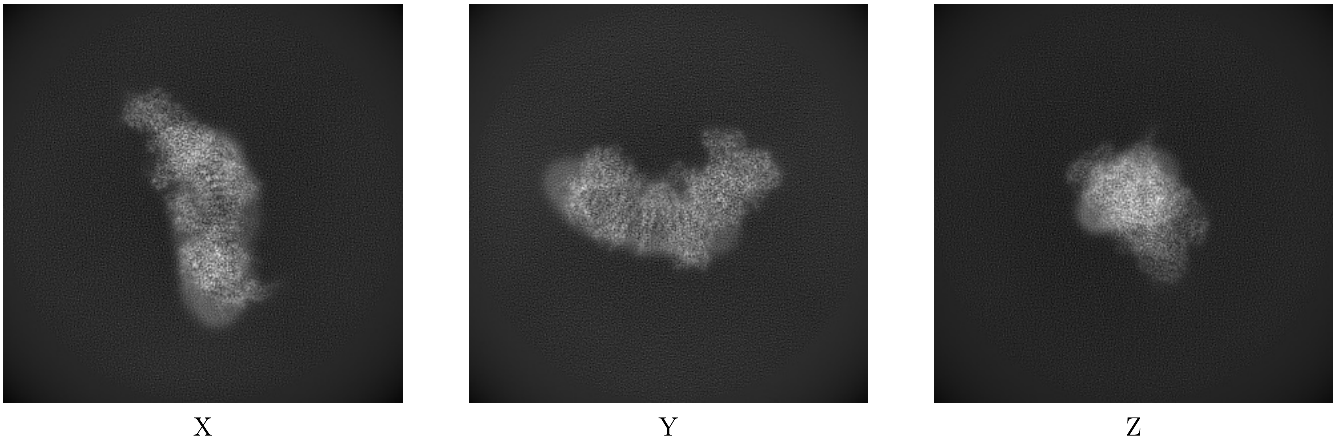
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-14277. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

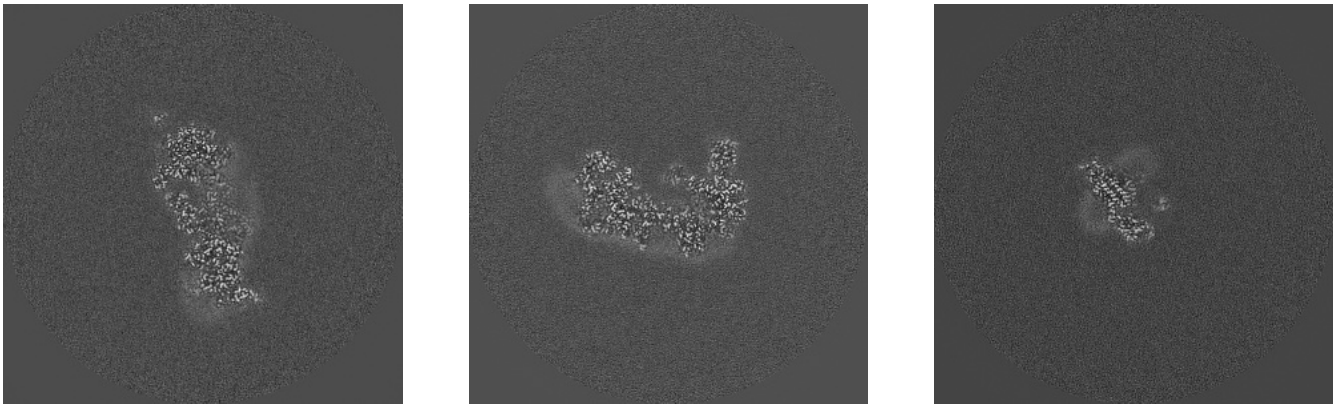
6.1.1 Primary map



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

6.2 Central slices ⓘ

6.2.1 Primary map



X Index: 330

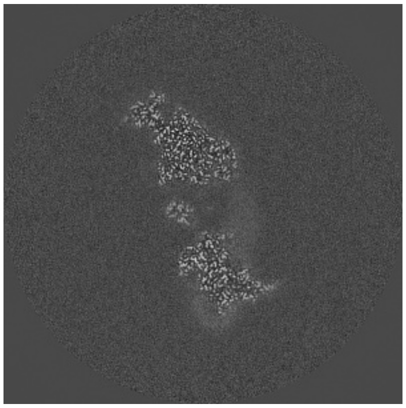
Y Index: 330

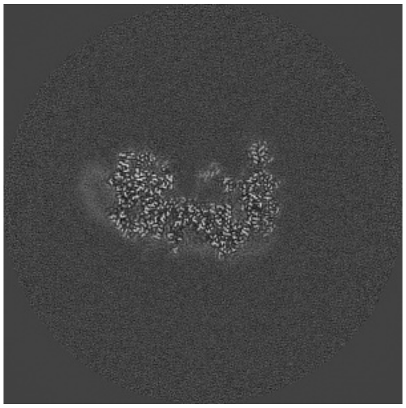
Z Index: 330

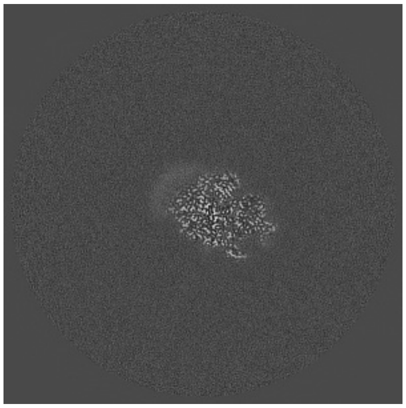
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map


X Index: 358


Y Index: 337


Z Index: 421

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map


X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

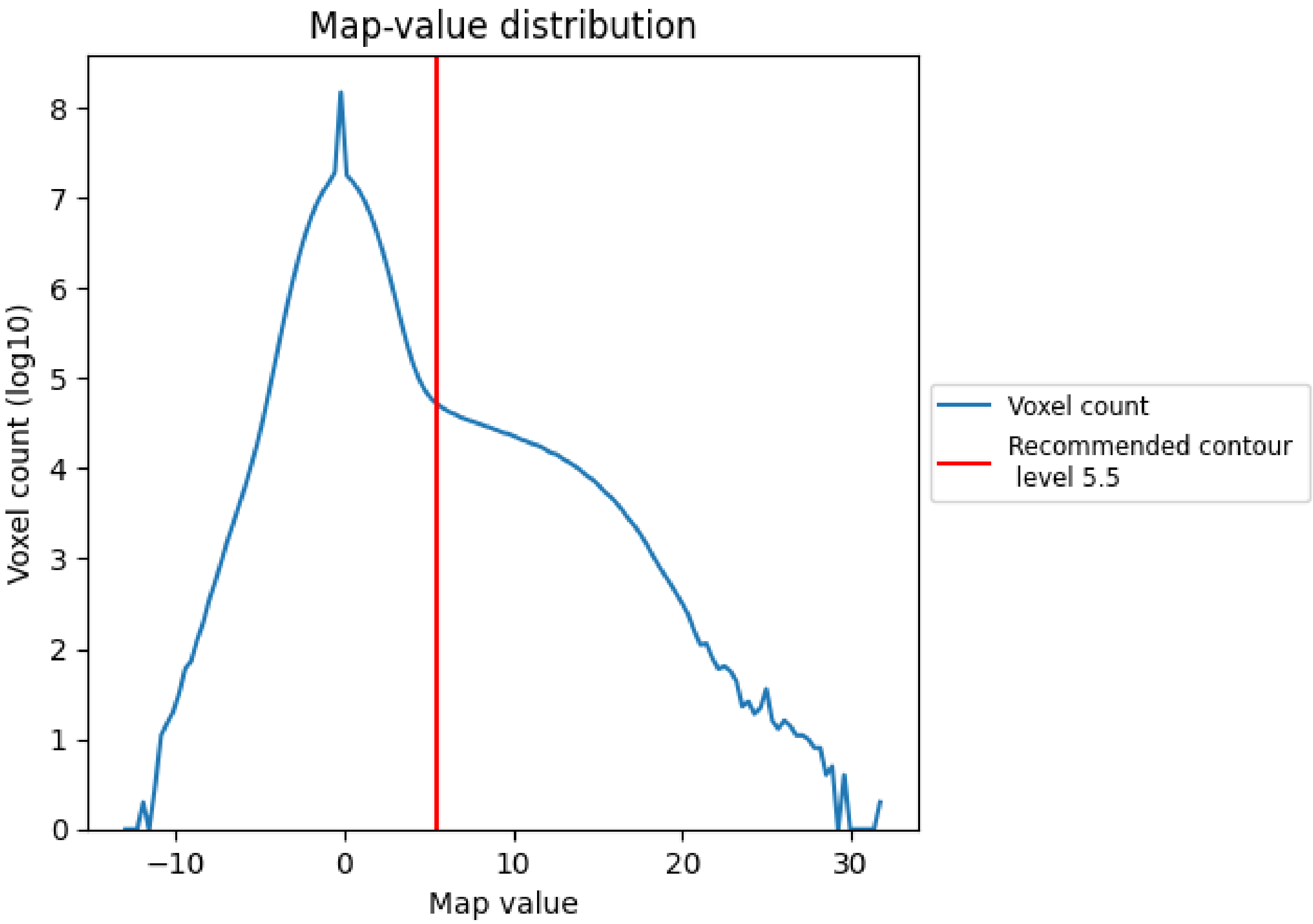
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

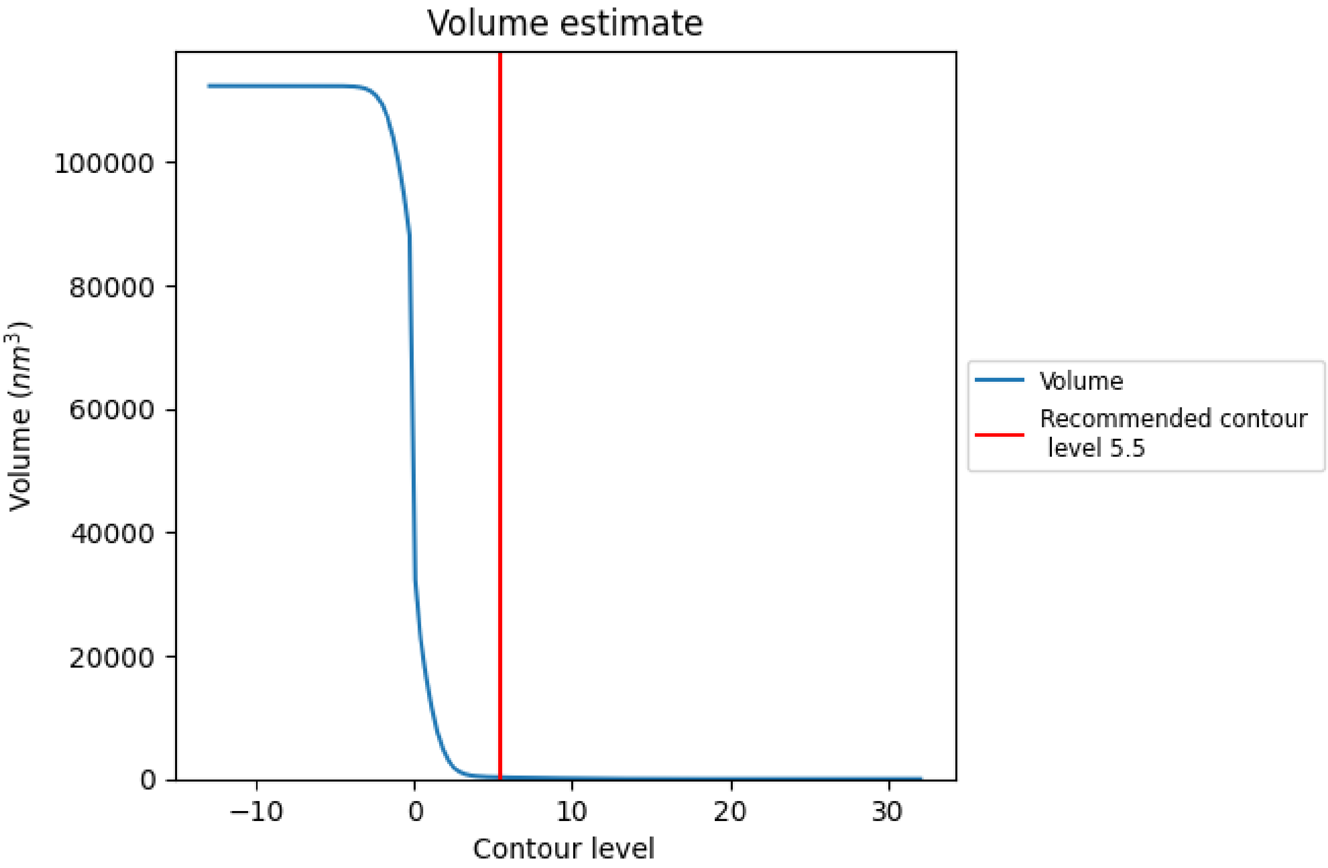
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

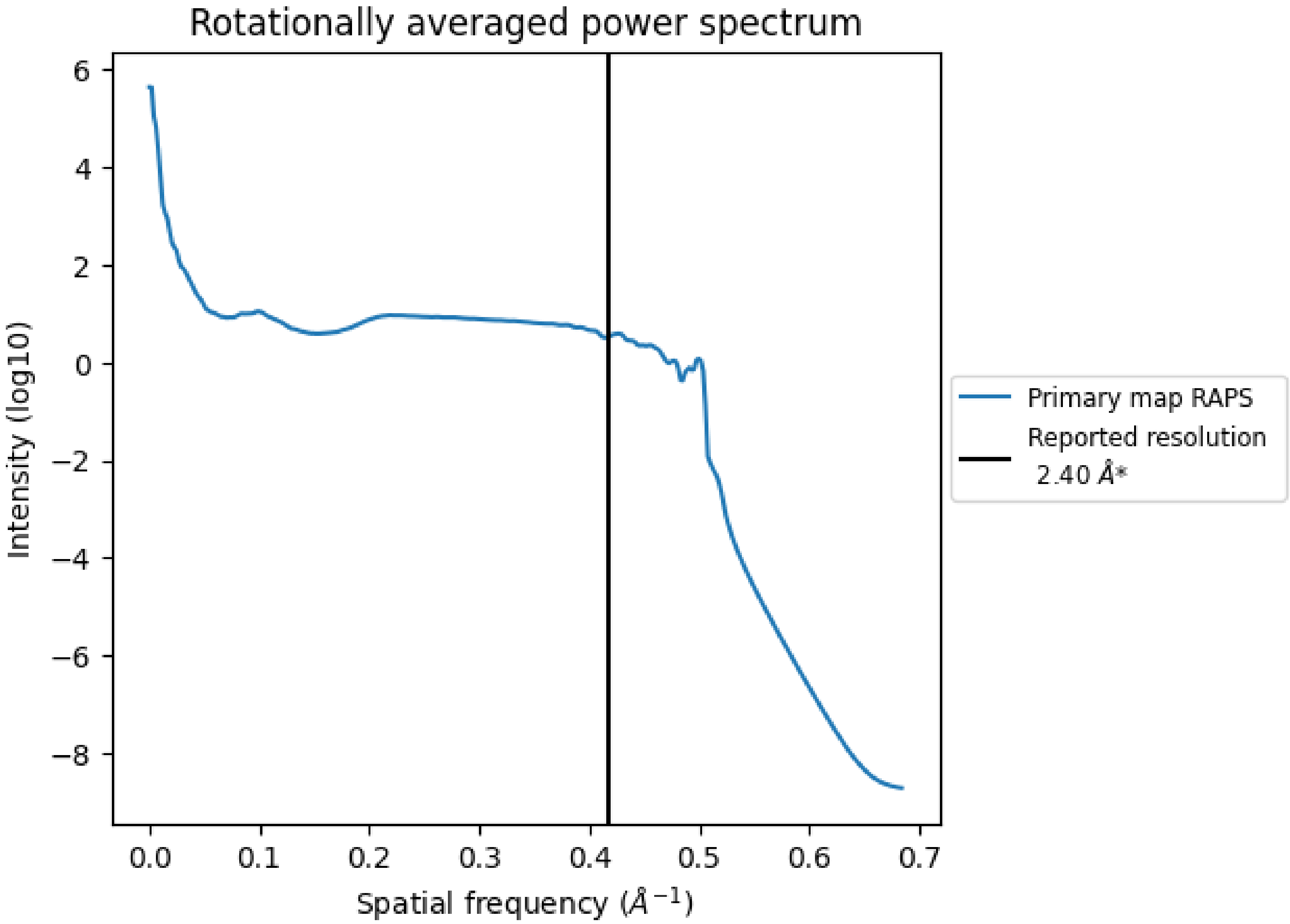
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 270 nm^3; this corresponds to an approximate mass of 244 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 0.417 Å^{-1}

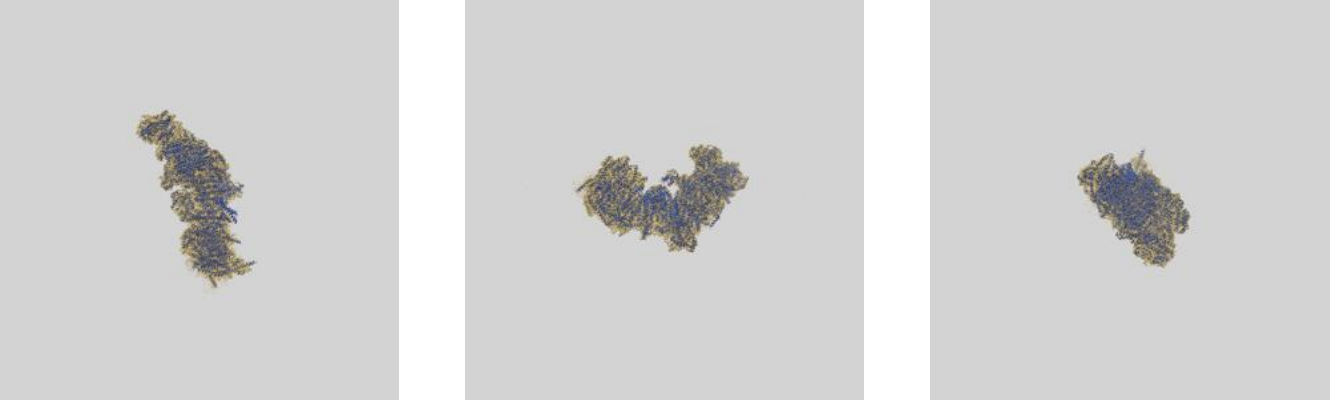
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14277 and PDB model 7R46. Per-residue inclusion information can be found in section 3 on page 23.

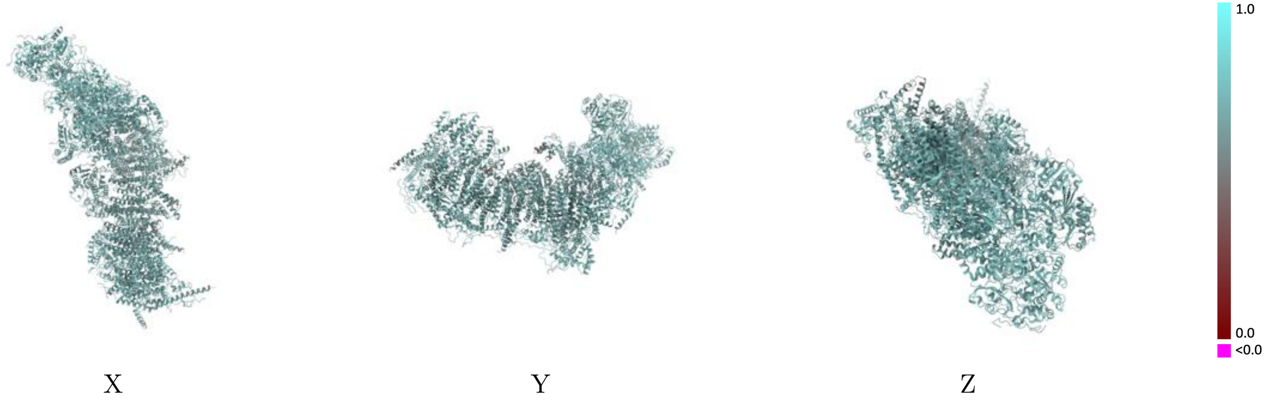
9.1 Map-model overlay



X Y Z

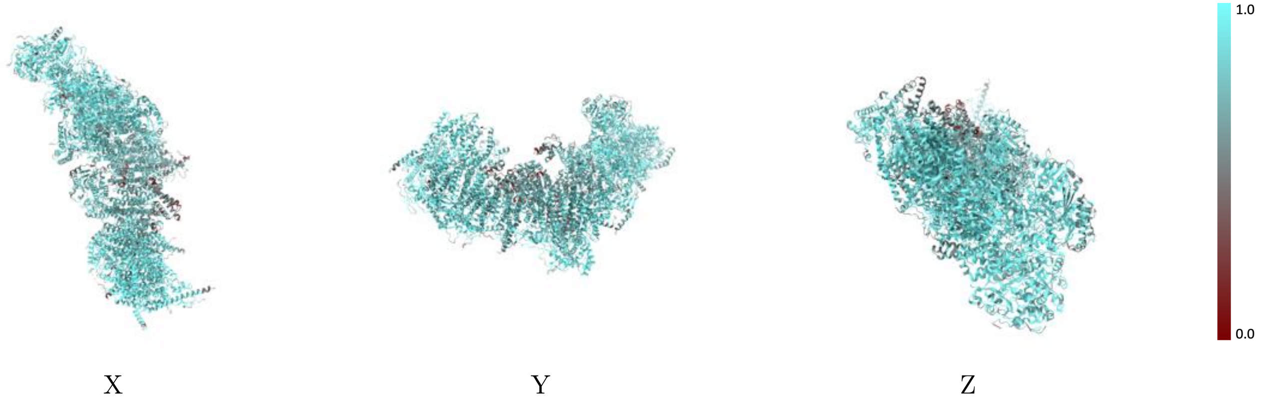
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



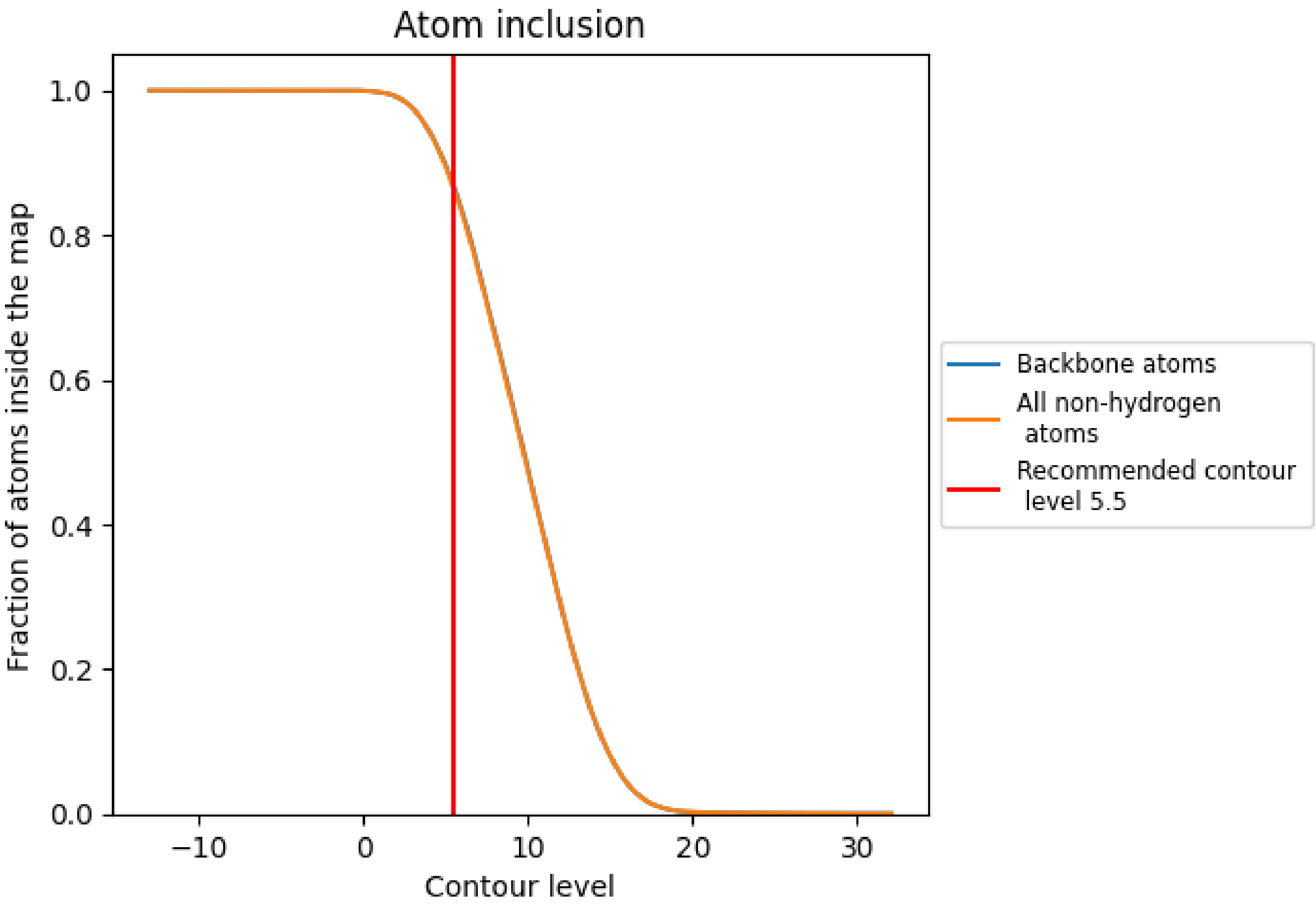
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8636	0.6720
A	0.8218	0.6570
B	0.8892	0.6930
C	0.9496	0.7160
D	0.9076	0.7050
E	0.8556	0.6700
F	0.9004	0.6840
G	0.8947	0.6920
H	0.9230	0.6800
I	0.9408	0.7170
J	0.7926	0.6490
K	0.8506	0.6780
L	0.8857	0.6640
M	0.9464	0.6890
N	0.9224	0.6890
O	0.8196	0.6420
P	0.8444	0.6720
Q	0.8943	0.6970
R	0.8962	0.6970
S	0.8121	0.6520
T	0.5699	0.5870
U	0.9003	0.6620
V	0.8326	0.6780
W	0.8386	0.6730
X	0.8373	0.6570
Y	0.4884	0.6040
Z	0.8253	0.6570
a	0.9113	0.6800
b	0.8320	0.6530
c	0.7045	0.6200
d	0.8198	0.6650
e	0.8054	0.6480
f	0.8005	0.6360
g	0.8549	0.6590
h	0.8611	0.6670

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Chain	Atom inclusion	Q-score
i	0.8452	0.6350
j	0.8417	0.6310
k	0.8473	0.6310
l	0.8803	0.6570
m	0.8168	0.6370
n	0.9044	0.6580
o	0.8584	0.6380
p	0.8855	0.6590
q	0.8309	0.6810
r	0.8504	0.6860
s	0.8338	0.6650