Full wwPDB EM Validation Report ⓘ

Jul 20, 2024 – 08:38 am BST

PDB ID	:	8RGQ
EMDB ID	:	EMD-19146
Title	:	Open Complex I from murine liver
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2023-12-14
Resolution	:	3.00 Å(reported)
Based on initial model	:	6g2j

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

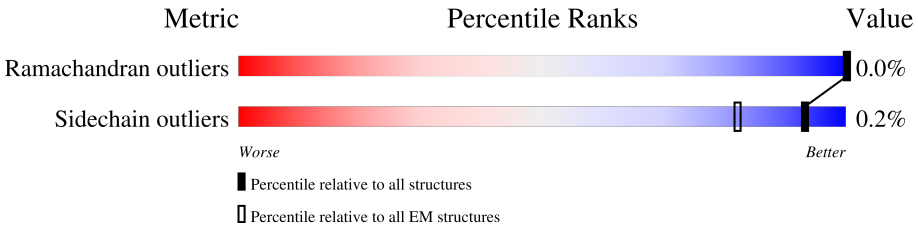
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	6	224	70% 30%
2	C	263	79% 21%
3	D	463	5% 90% 10%
4	2	248	86% 14%
5	1	464	93% 7%
6	3	727	95% 5%
7	9	212	83% 16%
8	P	377	6% 83% 17%
9	Q	175	72% 28%

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Mol	Chain	Length	Quality of chain
10	7	116	82% 17%
11	S	99	84% 15%
12	T	156	51% 49%
12	U	156	56% 44%
13	V	116	97%
14	W	131	86% 13%
15	q	145	100%
16	r	113	84% 14%
17	s	104	40% 60%
18	A	115	79% 19%
19	H	318	96%
20	J	172	11% 96%
21	K	98	98%
22	L	607	100%
23	M	459	100%
24	N	345	100%
25	O	355	90% 10%
26	X	172	99%
27	Y	141	99%
28	Z	144	96%
29	a	70	100%
30	b	84	98%
31	c	76	63% 37%
32	d	120	100%
33	e	106	99%

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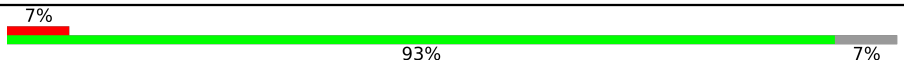
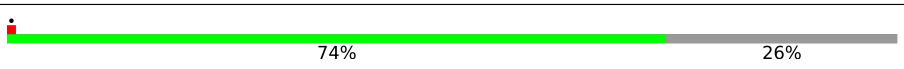
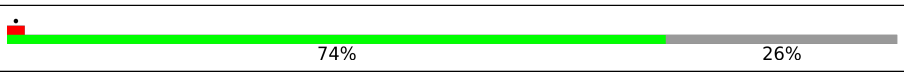
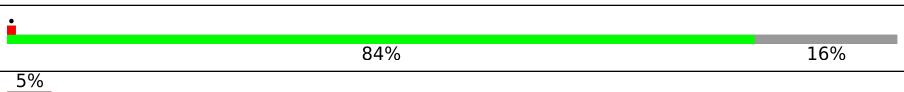
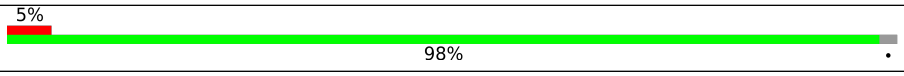
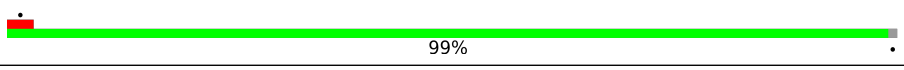
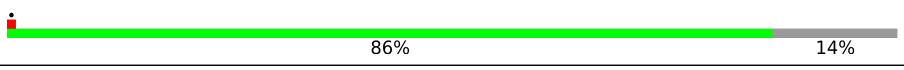
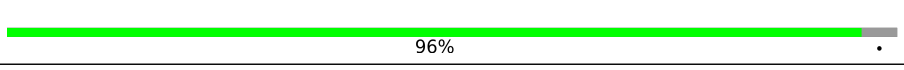
Mol	Chain	Length	Quality of chain
34	f	57	
35	g	151	
36	h	189	
37	i	128	
38	j	105	
39	k	104	
40	l	186	
41	m	129	
42	n	179	
43	o	137	
44	p	176	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 67118 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	157	1258	802	227	215	14	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	208	1730	1116	297	314	3	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	418	3371	2156	577	614	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	214	1660	1056	279	314	11	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1	430	3321	2092	596	611	22	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	314	Total	C	N	O	S	0	0
			2513	1611	453	442	7		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	79	Total	C	N	O	S	0	0
			637	410	95	127	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	97	Total	C	N	O	S	0	0
			781	493	146	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	s	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	93	Total	C	N	O	S	0	0
			760	527	104	124	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	306	Total	C	N	O	S	0	0
			2452	1652	371	407	22		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	165	Total	C	N	O	S	0	0
			1246	837	178	216	15		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	82	Total	C	N	O	S	0	0
			643	422	104	113	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

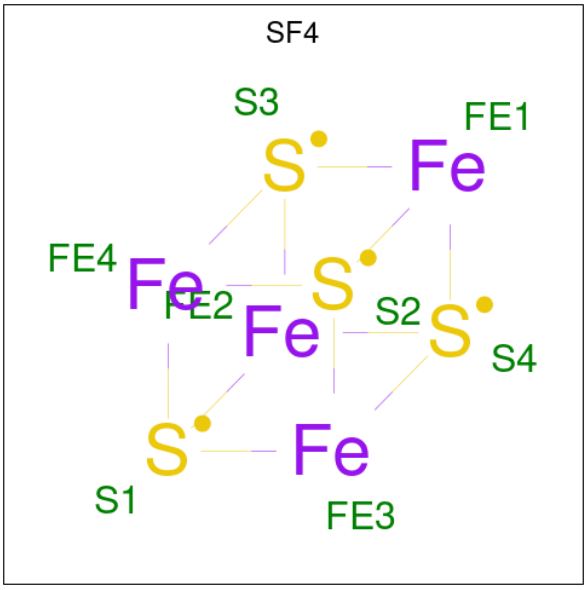
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

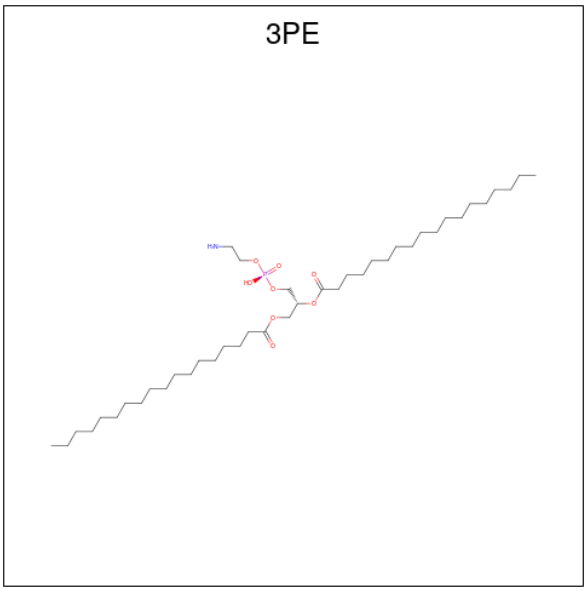
Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	169	Total	C	N	O	S	0	0
			1430	899	257	266	8		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				AltConf
45	6	1	Total	Fe	S		0
			8	4	4		
45	1	1	Total	Fe	S		0
			8	4	4		
45	3	1	Total	Fe	S		0
			8	4	4		
45	3	1	Total	Fe	S		0
			8	4	4		
45	9	1	Total	Fe	S		0
			8	4	4		
45	9	1	Total	Fe	S		0
			8	4	4		

- 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	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	r	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	Y	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	d	1	Total	C	N	O	P	0
			31	21	1	8	1	

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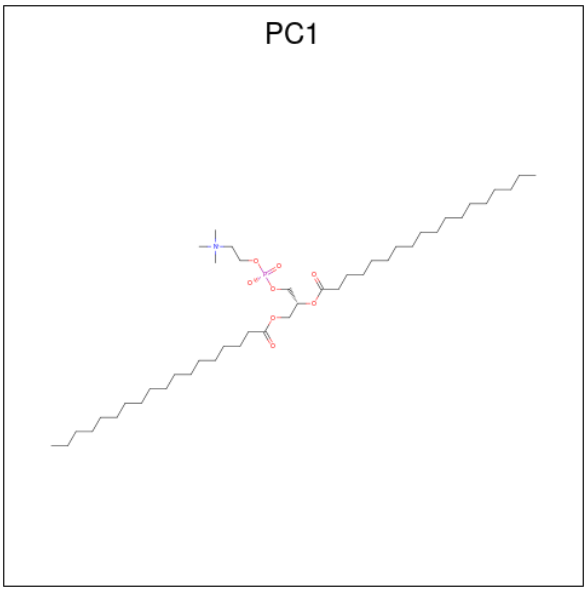
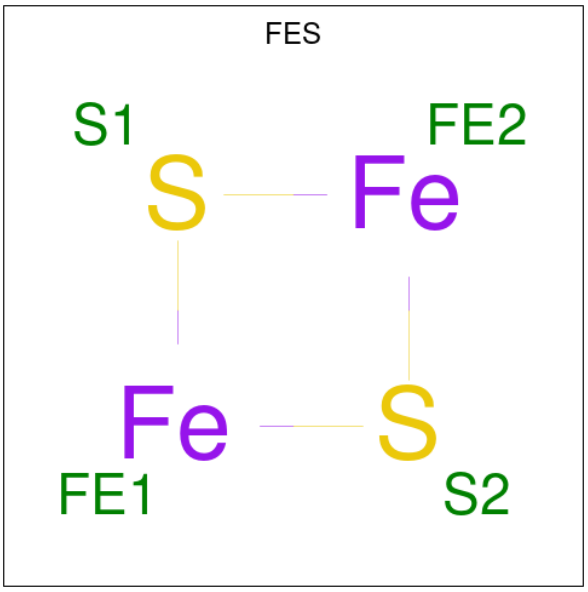
Mol	Chain	Residues	Atoms					AltConf
46	d	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	m	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



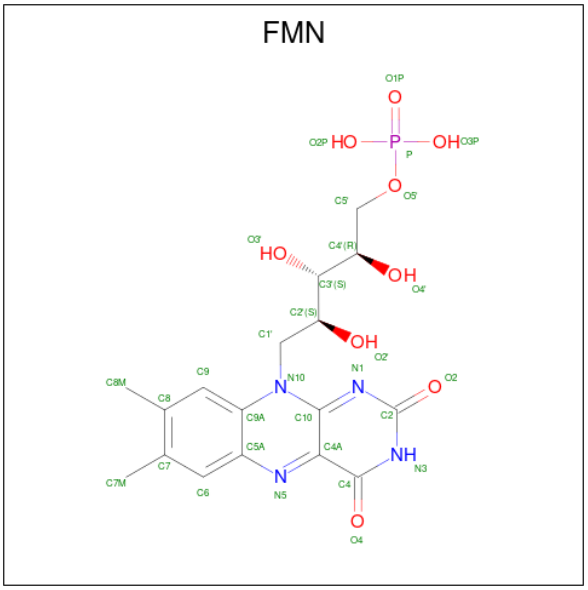
Mol	Chain	Residues	Atoms					AltConf
47	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

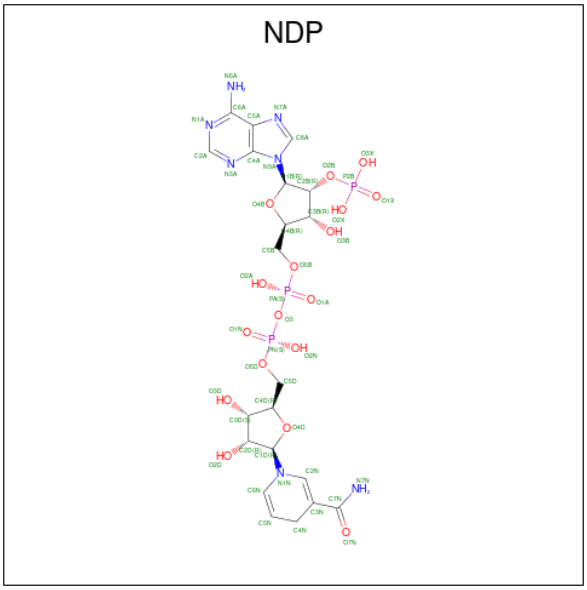


Mol	Chain	Residues	Atoms					AltConf
49	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
50	3	1	Total K 1 1	0

- Molecule 51 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
51	P	1	Total C N O P 48 21 7 17 3	0

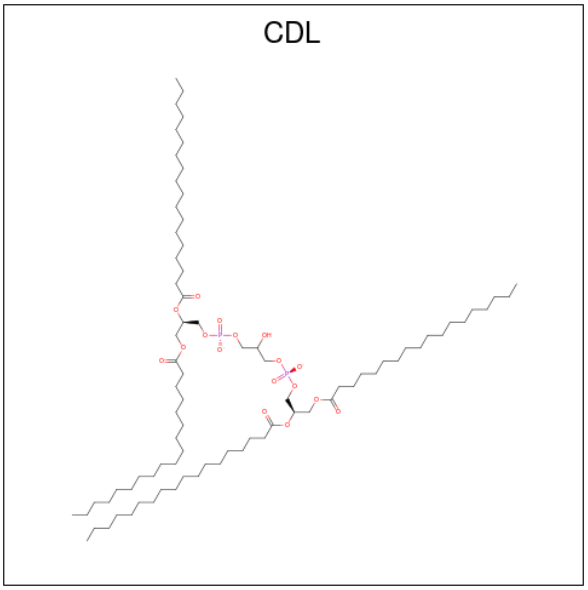
- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
52	7	1	Total Zn 1 1	0

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

Mol	Chain	Residues	Atoms						AltConf
53	W	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
53	n	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
54	r	1	Total	C	O	P	0
			57	38	17	2	
54	L	1	Total	C	O	P	0
			78	59	17	2	

Continued on next page...

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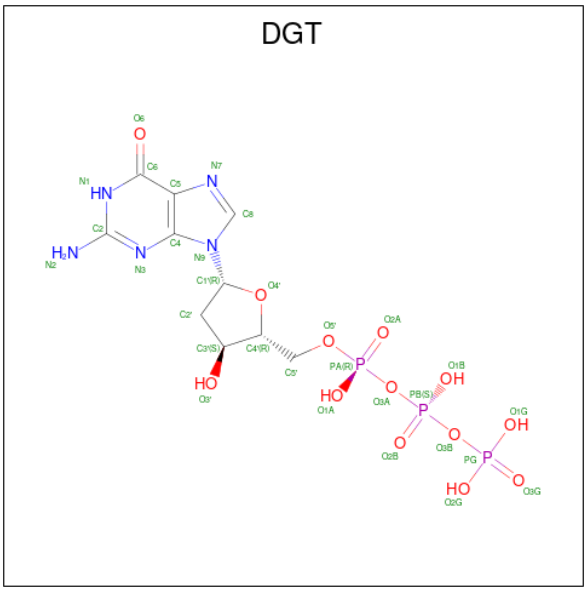
Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			90	71	17	2	
54	d	1	Total	C	O	P	0
			67	48	17	2	
54	h	1	Total	C	O	P	0
			70	51	17	2	
54	m	1	Total	C	O	P	0
			72	53	17	2	

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



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

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

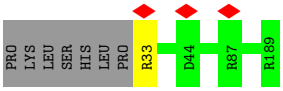
Mol	Chain	Residues	Atoms		AltConf
56	O	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

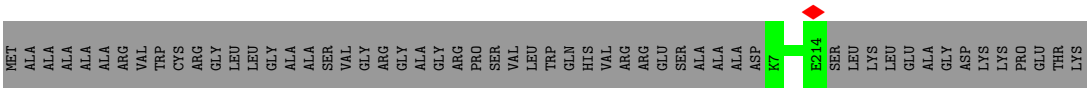
• Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:



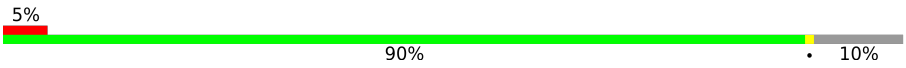
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

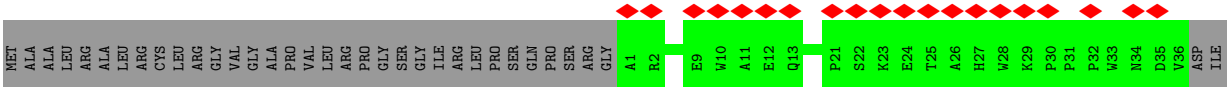
Chain C:

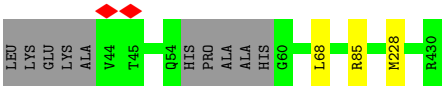


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:





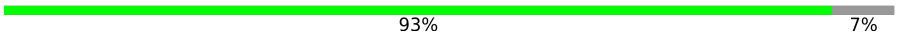


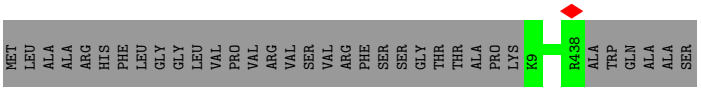
• Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2:

• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

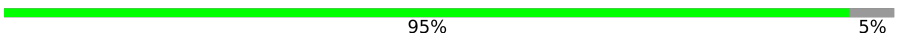
Chain 1:

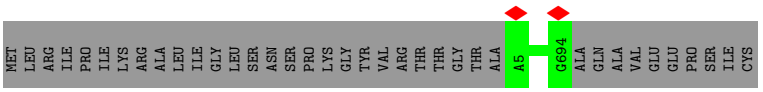




• Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

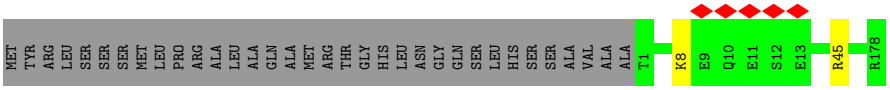
Chain 3:





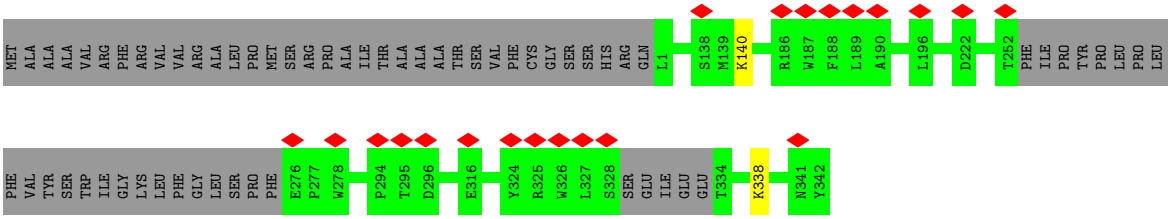
• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:



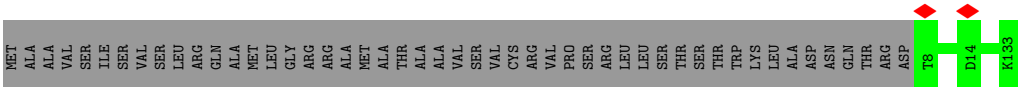
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



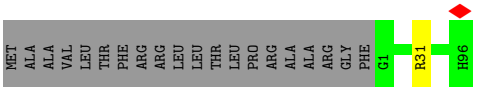
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



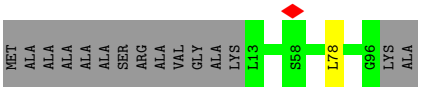
• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7:



• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:

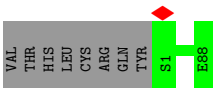


• Molecule 12: Acyl carrier protein, mitochondrial

Chain T:

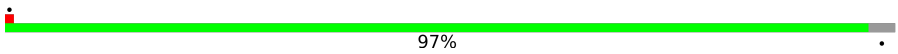
• Molecule 12: Acyl carrier protein, mitochondrial

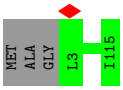
Chain U:



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

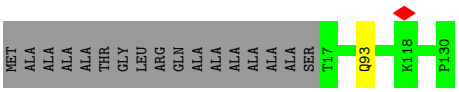
Chain V:





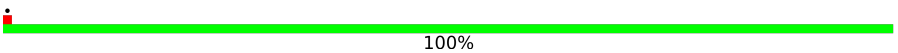
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



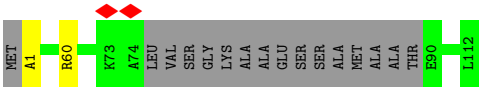
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



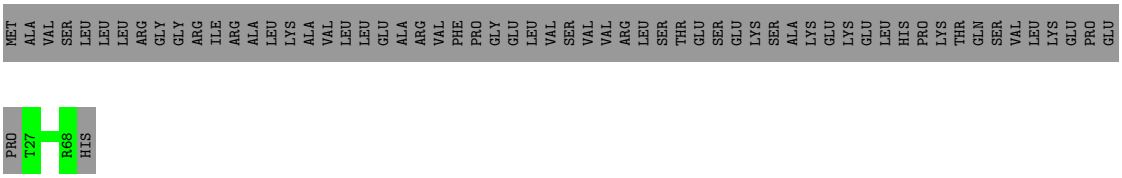
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



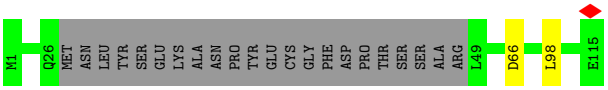
• Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:



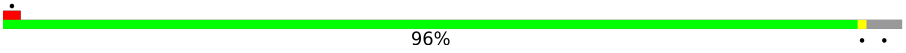
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

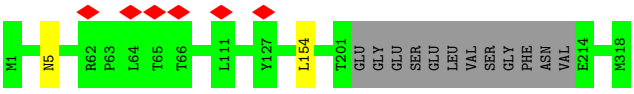
Chain A:



• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

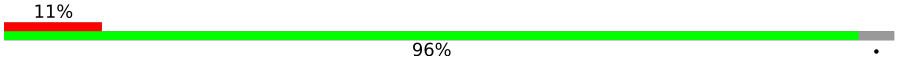
Chain H:

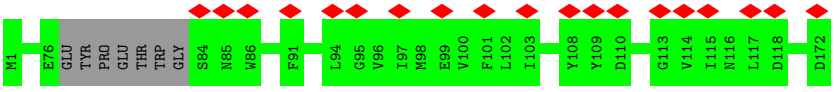




• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

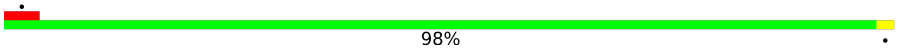
Chain J:

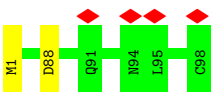




• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

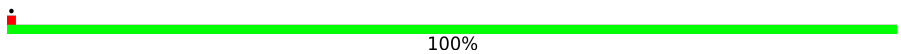
Chain K:

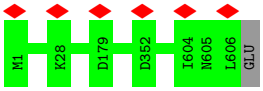




• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain L:



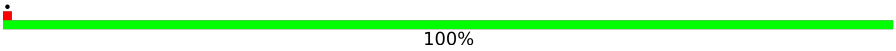


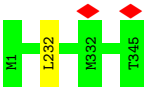
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain M:

• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

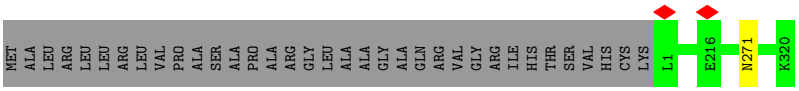
Chain N:





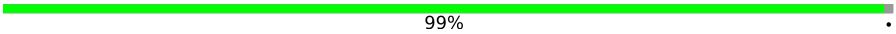
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



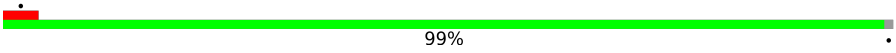
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

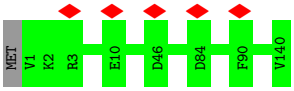
Chain X:



• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

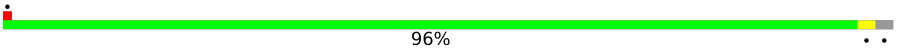
Chain Y:

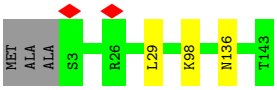




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

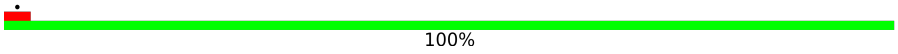
Chain Z:

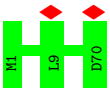




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

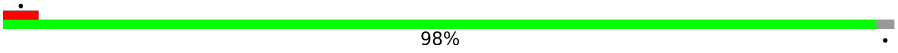
Chain a:

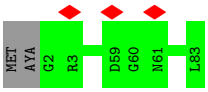




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

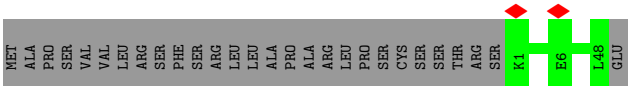
Chain b:





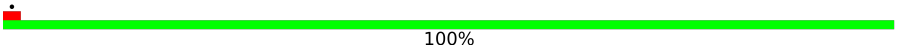
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

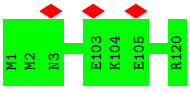
Chain c:



• Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2

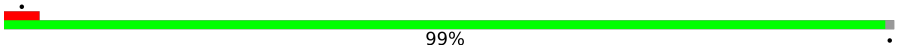
Chain d:

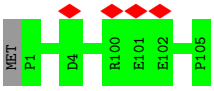




• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

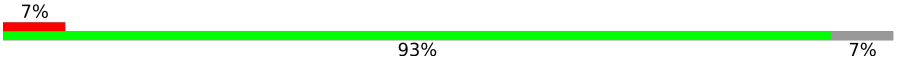
Chain e:

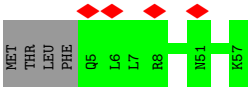




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

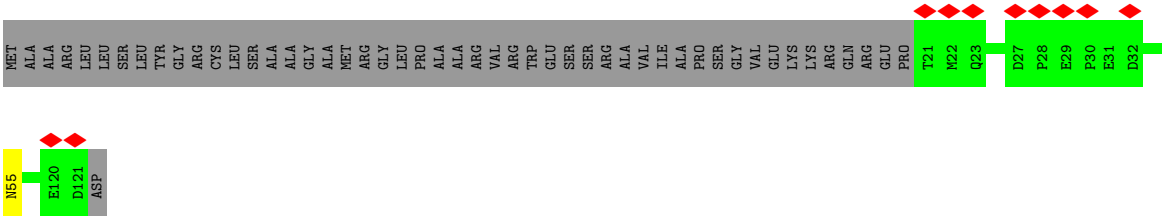
Chain f:





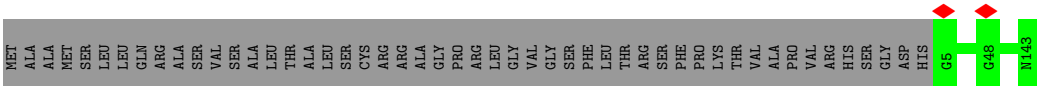
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



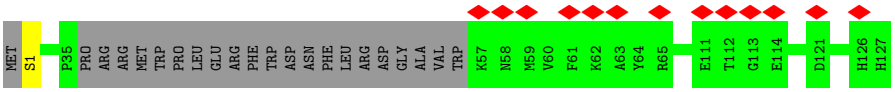
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



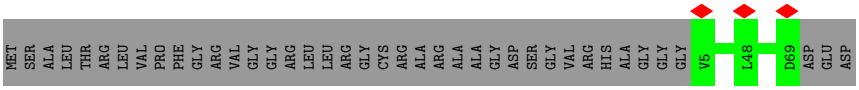
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



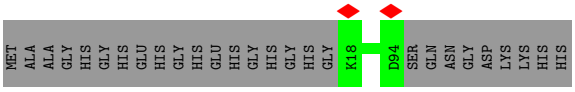
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



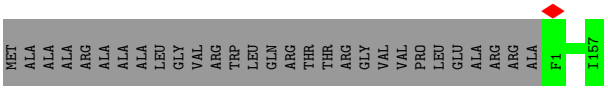
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



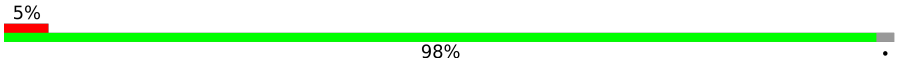
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

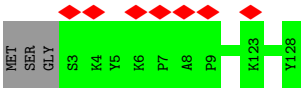
Chain l:



• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

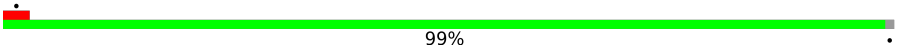
Chain m:

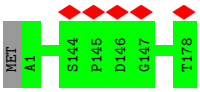




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

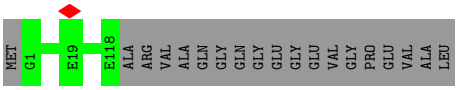
Chain n:





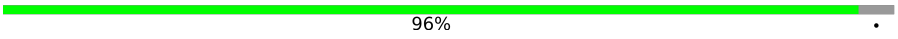
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

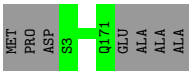
Chain o:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	317317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	232.13998, 207.76, 207.76	wwPDB
Map dimensions	219, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	6	0.31	0/1289	0.61	0/1744
2	C	0.28	0/1780	0.55	0/2424
3	D	0.29	0/3442	0.55	1/4659 (0.0%)
4	2	0.29	0/1700	0.52	0/2316
5	1	0.29	0/3396	0.55	0/4586
6	3	0.28	0/5392	0.52	0/7305
7	9	0.30	0/1461	0.60	0/1974
8	P	0.27	0/2574	0.55	0/3483
9	Q	0.28	0/1045	0.52	0/1411
10	7	0.27	0/773	0.49	0/1041
11	S	0.28	0/682	0.65	1/920 (0.1%)
12	T	0.29	0/646	0.64	0/869
12	U	0.30	0/718	0.46	0/970
13	V	0.25	0/945	0.44	0/1281
14	W	0.27	0/993	0.55	0/1335
15	q	0.28	0/1251	0.56	0/1702
16	r	0.27	0/791	0.52	0/1069
17	s	0.25	0/360	0.52	0/489
18	A	0.30	0/770	0.60	2/1052 (0.2%)
19	H	0.33	0/2517	0.60	1/3441 (0.0%)
20	J	0.32	0/1263	0.62	0/1715
21	K	0.30	0/738	0.62	1/1002 (0.1%)
22	L	0.30	0/4913	0.53	0/6686
23	M	0.29	0/3709	0.59	2/5052 (0.0%)
24	N	0.30	0/2755	0.58	1/3751 (0.0%)
25	O	0.28	0/2674	0.51	0/3626
26	X	0.27	0/1434	0.52	0/1937
27	Y	0.31	0/1061	0.58	0/1439
28	Z	0.27	0/1198	0.56	1/1616 (0.1%)
29	a	0.31	0/585	0.60	0/788
30	b	0.26	0/666	0.50	0/914
31	c	0.25	0/409	0.50	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	d	0.28	0/1028	0.50	0/1387
33	e	0.26	0/900	0.50	0/1199
34	f	0.25	0/468	0.55	0/630
35	g	0.28	0/878	0.51	0/1196
36	h	0.28	0/1201	0.49	0/1626
37	i	0.27	0/917	0.55	0/1243
38	j	0.26	0/587	0.54	0/804
39	k	0.27	0/646	0.49	0/873
40	l	0.27	0/1379	0.51	0/1882
41	m	0.28	0/1079	0.57	0/1463
42	n	0.27	0/1596	0.52	0/2162
43	o	0.28	0/1039	0.57	0/1394
44	p	0.28	0/1463	0.52	0/1977
All	All	0.29	0/67111	0.55	10/90988 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	174	LEU	CA-CB-CG	6.50	130.24	115.30
21	K	88	ASP	CB-CG-OD1	6.36	124.02	118.30
18	A	66	ASP	CB-CG-OD1	6.14	123.83	118.30
23	M	281	ASP	CB-CG-OD1	5.85	123.57	118.30
18	A	98	LEU	CA-CB-CG	5.84	128.72	115.30
24	N	232	LEU	CA-CB-CG	5.54	128.04	115.30
19	H	154	LEU	CB-CG-CD2	-5.47	101.70	111.00
28	Z	29	LEU	CA-CB-CG	5.45	127.83	115.30
3	D	68	LEU	CA-CB-CG	5.13	127.10	115.30
11	S	78	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	155/224 (69%)	145 (94%)	10 (6%)	0	100	100
2	C	206/263 (78%)	198 (96%)	8 (4%)	0	100	100
3	D	411/463 (89%)	391 (95%)	20 (5%)	0	100	100
4	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	29	68
5	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
6	3	688/727 (95%)	660 (96%)	28 (4%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	308/377 (82%)	296 (96%)	12 (4%)	0	100	100
9	Q	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
10	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
11	S	82/99 (83%)	78 (95%)	4 (5%)	0	100	100
12	T	77/156 (49%)	75 (97%)	2 (3%)	0	100	100
12	U	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
13	V	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
14	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
15	q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
16	r	93/113 (82%)	91 (98%)	2 (2%)	0	100	100
17	s	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
18	A	89/115 (77%)	86 (97%)	3 (3%)	0	100	100
19	H	302/318 (95%)	290 (96%)	12 (4%)	0	100	100
20	J	161/172 (94%)	151 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
22	L	604/607 (100%)	571 (94%)	33 (6%)	0	100	100
23	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
24	N	343/345 (99%)	327 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	O	318/355 (90%)	305 (96%)	13 (4%)	0	100	100
26	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
27	Y	138/141 (98%)	138 (100%)	0	0	100	100
28	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
29	a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
30	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
31	c	46/76 (60%)	46 (100%)	0	0	100	100
32	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
33	e	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
34	f	51/57 (90%)	51 (100%)	0	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	133 (97%)	4 (3%)	0	100	100
37	i	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
38	j	63/105 (60%)	59 (94%)	4 (6%)	0	100	100
39	k	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
40	l	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
41	m	124/129 (96%)	124 (100%)	0	0	100	100
42	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
43	o	116/137 (85%)	108 (93%)	8 (7%)	0	100	100
44	p	167/176 (95%)	165 (99%)	2 (1%)	0	100	100
All	All	8042/9212 (87%)	7742 (96%)	299 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	183	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	6	133/185 (72%)	132 (99%)	1 (1%)	81 93
2	C	190/227 (84%)	190 (100%)	0	100 100
3	D	361/394 (92%)	360 (100%)	1 (0%)	92 97
4	2	184/206 (89%)	184 (100%)	0	100 100
5	1	345/370 (93%)	345 (100%)	0	100 100
6	3	580/610 (95%)	580 (100%)	0	100 100
7	9	152/178 (85%)	150 (99%)	2 (1%)	69 89
8	P	273/325 (84%)	271 (99%)	2 (1%)	84 94
9	Q	113/153 (74%)	113 (100%)	0	100 100
10	7	81/96 (84%)	80 (99%)	1 (1%)	71 90
11	S	74/80 (92%)	74 (100%)	0	100 100
12	T	73/135 (54%)	73 (100%)	0	100 100
12	U	81/135 (60%)	81 (100%)	0	100 100
13	V	101/102 (99%)	101 (100%)	0	100 100
14	W	108/114 (95%)	107 (99%)	1 (1%)	78 92
15	q	131/131 (100%)	131 (100%)	0	100 100
16	r	86/96 (90%)	85 (99%)	1 (1%)	71 90
17	s	41/95 (43%)	41 (100%)	0	100 100
18	A	84/103 (82%)	84 (100%)	0	100 100
19	H	269/279 (96%)	268 (100%)	1 (0%)	91 97
20	J	131/137 (96%)	131 (100%)	0	100 100
21	K	87/87 (100%)	87 (100%)	0	100 100
22	L	548/549 (100%)	548 (100%)	0	100 100
23	M	414/414 (100%)	414 (100%)	0	100 100
24	N	307/307 (100%)	307 (100%)	0	100 100
25	O	284/309 (92%)	283 (100%)	1 (0%)	91 97
26	X	153/154 (99%)	153 (100%)	0	100 100
27	Y	105/106 (99%)	105 (100%)	0	100 100
28	Z	122/123 (99%)	120 (98%)	2 (2%)	62 86
29	a	60/60 (100%)	60 (100%)	0	100 100
30	b	72/73 (99%)	72 (100%)	0	100 100
31	c	42/67 (63%)	42 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	d	107/107 (100%)	107 (100%)	0	100 100
33	e	93/94 (99%)	93 (100%)	0	100 100
34	f	49/53 (92%)	49 (100%)	0	100 100
35	g	92/129 (71%)	91 (99%)	1 (1%)	73 90
36	h	123/162 (76%)	123 (100%)	0	100 100
37	i	99/119 (83%)	99 (100%)	0	100 100
38	j	61/87 (70%)	61 (100%)	0	100 100
39	k	60/78 (77%)	60 (100%)	0	100 100
40	l	142/161 (88%)	142 (100%)	0	100 100
41	m	112/114 (98%)	112 (100%)	0	100 100
42	n	163/164 (99%)	163 (100%)	0	100 100
43	o	109/121 (90%)	109 (100%)	0	100 100
44	p	154/158 (98%)	154 (100%)	0	100 100
All	All	7149/7947 (90%)	7135 (100%)	14 (0%)	93 98

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

Mol	Chain	Res	Type
1	6	33	ARG
3	D	228	MET
7	9	8	LYS
7	9	45	ARG
8	P	140	LYS
8	P	338	LYS
10	7	31	ARG
14	W	93	GLN
16	r	60	ARG
19	H	5	ASN
25	O	271	ASN
28	Z	98	LYS
28	Z	136	ASN
35	g	55	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
14	W	93	GLN
22	L	332	HIS
24	N	125	HIS
24	N	172	GLN
41	m	85	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 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	$\#\|Z\| > 2$
24	FME	N	1	24	8,9,10	0.94	0	7,9,11	0.93	0
3	2MR	D	85	3	10,12,13	2.61	2 (20%)	5,13,15	3.03	2 (40%)
37	SAC	i	1	37	7,8,9	1.00	0	8,9,11	0.87	1 (12%)
22	FME	L	1	22	8,9,10	0.92	0	7,9,11	0.93	0
18	FME	A	1	18	8,9,10	0.92	0	7,9,11	0.88	0
19	FME	H	1	19	8,9,10	0.94	0	7,9,11	0.90	0
16	AYA	r	1	16	6,7,8	1.27	1 (16%)	5,8,10	1.27	1 (20%)
21	FME	K	1	21	8,9,10	0.91	0	7,9,11	2.05	2 (28%)
20	FME	J	1	20	8,9,10	0.94	0	7,9,11	0.95	0
23	FME	M	1	23	8,9,10	0.97	0	7,9,11	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	FME	N	1	24	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2MR	D	85	3	-	3/10/13/15	-
37	SAC	i	1	37	-	0/7/8/10	-
22	FME	L	1	22	-	3/7/9/11	-
18	FME	A	1	18	-	2/7/9/11	-
19	FME	H	1	19	-	3/7/9/11	-
16	AYA	r	1	16	-	0/4/6/8	-
21	FME	K	1	21	-	3/7/9/11	-
20	FME	J	1	20	-	4/7/9/11	-
23	FME	M	1	23	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.92	1.47	1.34
3	D	85	2MR	CZ-NH2	5.12	1.44	1.33
16	r	1	AYA	CA-N	-2.47	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	85	2MR	CD-NE-CZ	5.73	134.13	123.41
21	K	1	FME	C-CA-N	4.68	118.17	109.73
3	D	85	2MR	NE-CZ-NH2	-3.45	116.32	119.48
16	r	1	AYA	CB-CA-N	2.63	112.53	109.61
21	K	1	FME	O-C-CA	-2.20	119.02	124.78
37	i	1	SAC	OG-CB-CA	-2.05	105.73	110.97

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	C-CA-CB-CG
18	A	1	FME	N-CA-CB-CG
19	H	1	FME	N-CA-CB-CG
19	H	1	FME	O-C-CA-CB
20	J	1	FME	CB-CA-N-CN
20	J	1	FME	CA-CB-CG-SD
21	K	1	FME	O1-CN-N-CA
21	K	1	FME	N-CA-CB-CG
22	L	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
24	N	1	FME	N-CA-CB-CG
24	N	1	FME	C-CA-CB-CG
3	D	85	2MR	NE-CD-CG-CB
23	M	1	FME	N-CA-CB-CG
3	D	85	2MR	CA-CB-CG-CD
20	J	1	FME	C-CA-CB-CG
21	K	1	FME	CA-CB-CG-SD
24	N	1	FME	CB-CG-SD-CE
18	A	1	FME	C-CA-CB-CG
19	H	1	FME	C-CA-CB-CG
22	L	1	FME	C-CA-CB-CG
20	J	1	FME	CB-CG-SD-CE
22	L	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 3 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
45	SF4	3	801	6	0,12,12	-	-	-		
46	3PE	i	201	-	41,41,50	0.33	0	44,46,55	0.31	0
45	SF4	9	201	7	0,12,12	-	-	-		
54	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.30	0
46	3PE	d	202	-	30,30,50	0.37	0	33,35,55	0.32	0
46	3PE	M	502	-	50,50,50	0.30	0	53,55,55	0.29	0
47	PC1	M	501	-	53,53,53	0.29	0	59,61,61	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	SF4	1	502	5	0,12,12	-	-	-		
49	FMN	1	501	-	33,33,33	0.27	0	48,50,50	0.49	1 (2%)
54	CDL	N	401	-	89,89,99	0.32	0	95,101,111	0.39	1 (1%)
47	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
54	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.31	0
46	3PE	A	201	-	42,42,50	0.33	0	45,47,55	0.33	0
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.46	0
45	SF4	9	202	7	0,12,12	-	-	-		
46	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
55	DGT	O	401	56	26,33,33	0.78	1 (3%)	32,52,52	0.47	0
53	ZMP	n	201	-	25,31,36	0.75	1 (4%)	30,38,45	0.92	1 (3%)
54	CDL	h	201	-	69,69,99	0.35	0	75,81,111	0.42	0
46	3PE	N	402	-	37,37,50	0.35	0	40,42,55	0.32	0
48	FES	3	803	6	0,4,4	-	-	-		
47	PC1	6	203	-	42,42,53	0.35	0	48,50,61	0.49	1 (2%)
46	3PE	r	201	-	45,45,50	0.32	0	48,50,55	0.28	0
46	3PE	M	503	-	50,50,50	0.30	0	53,55,55	0.27	0
46	3PE	M	504	-	35,35,50	0.35	0	38,40,55	0.30	0
46	3PE	Y	201	-	27,27,50	0.40	0	30,32,55	0.36	0
45	SF4	3	802	6	0,12,12	-	-	-		
45	SF4	6	201	1	0,12,12	-	-	-		
48	FES	2	301	4	0,4,4	-	-	-		
54	CDL	r	202	-	56,56,99	0.39	0	62,68,111	0.47	0
46	3PE	d	203	-	31,31,50	0.37	0	34,36,55	0.33	0
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.31	0
47	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.44	0
46	3PE	L	703	-	50,50,50	0.31	0	53,55,55	0.31	0
46	3PE	m	202	-	29,29,50	0.38	0	32,34,55	0.33	0
53	ZMP	W	201	-	27,33,36	0.62	1 (3%)	32,40,45	1.13	2 (6%)
46	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.30	0
46	3PE	Y	202	-	41,41,50	0.33	0	44,46,55	0.31	0
54	CDL	m	201	-	71,71,99	0.36	0	77,83,111	0.42	1 (1%)
51	NDP	P	501	-	45,52,52	0.53	0	53,80,80	0.59	1 (1%)

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
45	SF4	3	801	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	i	201	-	-	7/45/45/54	-
45	SF4	9	201	7	-	-	0/6/5/5
54	CDL	L	702	-	-	15/88/88/110	-
46	3PE	d	202	-	-	9/34/34/54	-
46	3PE	M	502	-	-	13/54/54/54	-
47	PC1	M	501	-	-	11/57/57/57	-
45	SF4	1	502	5	-	-	0/6/5/5
49	FMN	1	501	-	-	5/18/18/18	0/3/3/3
54	CDL	N	401	-	-	16/100/100/110	-
47	PC1	9	204	-	-	13/50/50/57	-
54	CDL	d	201	-	-	11/77/77/110	-
46	3PE	A	201	-	-	8/46/46/54	-
46	3PE	L	701	-	-	8/54/54/54	-
46	3PE	H	401	-	-	14/54/54/54	-
45	SF4	9	202	7	-	-	0/6/5/5
55	DGT	O	401	56	-	9/18/34/34	0/3/3/3
53	ZMP	n	201	-	-	12/36/38/43	-
54	CDL	h	201	-	-	20/80/80/110	-
46	3PE	N	402	-	-	7/41/41/54	-
48	FES	3	803	6	-	-	0/1/1/1
47	PC1	6	203	-	-	10/46/46/57	-
46	3PE	r	201	-	-	7/49/49/54	-
46	3PE	M	503	-	-	13/54/54/54	-
46	3PE	M	504	-	-	9/39/39/54	-
46	3PE	Y	201	-	-	4/31/31/54	-
45	SF4	3	802	6	-	-	0/6/5/5
45	SF4	6	201	1	-	-	0/6/5/5
54	CDL	r	202	-	-	15/67/67/110	-
48	FES	2	301	4	-	-	0/1/1/1
46	3PE	d	203	-	-	6/35/35/54	-
46	3PE	K	201	-	-	12/44/44/54	-
47	PC1	9	203	-	-	11/57/57/57	-
46	3PE	L	703	-	-	8/54/54/54	-
46	3PE	m	202	-	-	12/33/33/54	-
53	ZMP	W	201	-	-	8/38/40/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	6	202	-	-	4/35/35/54	-
46	3PE	Y	202	-	-	9/45/45/54	-
54	CDL	m	201	-	-	21/82/82/110	-
51	NDP	P	501	-	-	6/30/77/77	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	n	201	ZMP	C9-C10	2.60	1.53	1.50
55	O	401	DGT	C5-C6	-2.20	1.42	1.47
53	W	201	ZMP	C9-C10	2.10	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	W	201	ZMP	O1-C10-C9	-3.12	120.30	123.99
53	n	201	ZMP	O1-C10-C9	-2.49	121.05	123.99
53	W	201	ZMP	C15-C14-C13	-2.31	108.51	112.36
51	P	501	NDP	C5A-C6A-N6A	2.30	123.85	120.35
49	1	501	FMN	P-O5'-C5'	2.18	124.31	118.30
47	6	203	PC1	C2-O21-C21	2.09	122.94	117.79
46	H	401	3PE	C2-O21-C21	2.08	122.91	117.79
54	N	401	CDL	CB4-OB6-CB5	2.03	122.78	117.79
54	m	201	CDL	CA4-OA6-CA5	2.01	122.73	117.79

There are no chirality outliers.

All (333) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O14
46	6	202	3PE	O13-C11-C12-N
46	r	201	3PE	O13-C11-C12-N
46	A	201	3PE	C11-O13-P-O11
46	A	201	3PE	C11-O13-P-O14
46	A	201	3PE	O13-C11-C12-N
46	H	401	3PE	C1-O11-P-O14
46	H	401	3PE	C11-O13-P-O12
46	H	401	3PE	C11-O13-P-O14
46	K	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C1-O11-P-O14
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	O13-C11-C12-N
46	M	502	3PE	C1-O11-P-O13
46	M	503	3PE	C1-O11-P-O14
46	M	503	3PE	C11-O13-P-O12
46	M	504	3PE	C1-O11-P-O14
46	M	504	3PE	C11-O13-P-O12
46	M	504	3PE	C11-O13-P-O14
46	N	402	3PE	C1-O11-P-O12
46	Y	201	3PE	C1-O11-P-O12
46	Y	201	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O14
46	Y	201	3PE	O13-C11-C12-N
46	Y	202	3PE	O13-C11-C12-N
46	d	202	3PE	C1-O11-P-O12
46	d	202	3PE	C1-O11-P-O13
46	d	202	3PE	C1-O11-P-O14
46	d	202	3PE	C11-O13-P-O11
46	d	202	3PE	C11-O13-P-O12
46	d	202	3PE	C11-O13-P-O14
46	d	202	3PE	O13-C11-C12-N
46	d	203	3PE	C1-O11-P-O12
46	d	203	3PE	C1-O11-P-O14
46	d	203	3PE	C11-O13-P-O12
46	i	201	3PE	C1-O11-P-O12
46	i	201	3PE	C1-O11-P-O14
46	i	201	3PE	C11-O13-P-O14
46	i	201	3PE	O13-C11-C12-N
46	m	202	3PE	C1-O11-P-O14
46	m	202	3PE	C11-O13-P-O11
46	m	202	3PE	C11-O13-P-O12
46	m	202	3PE	C11-O13-P-O14
46	m	202	3PE	O13-C11-C12-N
47	6	203	PC1	C1-O11-P-O12
47	6	203	PC1	C1-O11-P-O14
47	M	501	PC1	C11-O13-P-O12
47	M	501	PC1	C11-O13-P-O14
47	M	501	PC1	C11-O13-P-O11
49	1	501	FMN	N10-C1'-C2'-O2'
49	1	501	FMN	N10-C1'-C2'-C3'
49	1	501	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
49	1	501	FMN	C5'-O5'-P-O3P
53	W	201	ZMP	C17-C18-C21-O5
53	W	201	ZMP	S1-C11-C12-N1
53	W	201	ZMP	O1-C10-S1-C11
53	W	201	ZMP	C9-C10-S1-C11
53	n	201	ZMP	C16-C17-C18-C21
53	n	201	ZMP	C17-C16-N2-C15
54	r	202	CDL	CA2-OA2-PA1-OA3
54	r	202	CDL	CA2-OA2-PA1-OA4
54	r	202	CDL	CA3-OA5-PA1-OA3
54	r	202	CDL	CA3-OA5-PA1-OA4
54	r	202	CDL	CB2-OB2-PB2-OB3
54	L	702	CDL	CA2-OA2-PA1-OA3
54	L	702	CDL	CA2-OA2-PA1-OA4
54	L	702	CDL	CA3-OA5-PA1-OA3
54	L	702	CDL	CB2-OB2-PB2-OB3
54	L	702	CDL	CB2-OB2-PB2-OB5
54	N	401	CDL	OA6-CA4-CA6-OA8
54	N	401	CDL	CB2-OB2-PB2-OB3
54	d	201	CDL	CB2-OB2-PB2-OB3
54	d	201	CDL	CB2-OB2-PB2-OB5
54	h	201	CDL	CA2-OA2-PA1-OA3
54	h	201	CDL	CB3-OB5-PB2-OB2
54	h	201	CDL	CB3-OB5-PB2-OB3
54	h	201	CDL	CB3-OB5-PB2-OB4
54	m	201	CDL	CA2-OA2-PA1-OA3
54	m	201	CDL	CA2-OA2-PA1-OA5
54	m	201	CDL	CA3-OA5-PA1-OA2
54	m	201	CDL	CA3-OA5-PA1-OA3
54	m	201	CDL	CB2-OB2-PB2-OB3
54	m	201	CDL	CB2-OB2-PB2-OB4
54	m	201	CDL	CB2-OB2-PB2-OB5
54	m	201	CDL	CB3-OB5-PB2-OB2
54	m	201	CDL	CB3-OB5-PB2-OB3
54	m	201	CDL	CB3-OB5-PB2-OB4
54	m	201	CDL	OB5-CB3-CB4-OB6
55	O	401	DGT	PB-O3B-PG-O1G
55	O	401	DGT	C5'-O5'-PA-O3A
55	O	401	DGT	C5'-O5'-PA-O1A
55	O	401	DGT	C5'-O5'-PA-O2A
53	n	201	ZMP	O3-C16-N2-C15
46	L	701	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
46	M	502	3PE	C21-C22-C23-C24
47	6	203	PC1	C11-C12-N-C14
47	9	204	PC1	C11-C12-N-C15
46	r	201	3PE	C1-O11-P-O13
46	r	201	3PE	C11-O13-P-O11
46	H	401	3PE	C11-O13-P-O11
46	K	201	3PE	C11-O13-P-O11
46	L	701	3PE	C1-O11-P-O13
46	L	703	3PE	C1-O11-P-O13
46	M	503	3PE	C1-O11-P-O13
46	M	504	3PE	C1-O11-P-O13
46	M	504	3PE	C11-O13-P-O11
46	Y	202	3PE	C11-O13-P-O11
46	d	203	3PE	C1-O11-P-O13
46	i	201	3PE	C1-O11-P-O13
46	i	201	3PE	C11-O13-P-O11
47	6	203	PC1	C1-O11-P-O13
47	9	204	PC1	C11-O13-P-O11
54	r	202	CDL	CA2-OA2-PA1-OA5
54	r	202	CDL	CA3-OA5-PA1-OA2
54	r	202	CDL	CB3-OB5-PB2-OB2
54	L	702	CDL	CA2-OA2-PA1-OA5
54	L	702	CDL	CA3-OA5-PA1-OA2
54	N	401	CDL	CA2-OA2-PA1-OA5
54	N	401	CDL	CB2-OB2-PB2-OB5
54	d	201	CDL	CA3-OA5-PA1-OA2
54	h	201	CDL	CA2-OA2-PA1-OA5
54	h	201	CDL	CB2-OB2-PB2-OB5
54	L	702	CDL	CA5-C11-C12-C13
53	W	201	ZMP	C19-C18-C21-O5
53	W	201	ZMP	C20-C18-C21-O5
53	n	201	ZMP	C6-C7-C8-C9
46	L	703	3PE	C38-C39-C3A-C3B
54	N	401	CDL	C81-C82-C83-C84
54	d	201	CDL	C63-C64-C65-C66
47	M	501	PC1	C37-C38-C39-C3A
46	H	401	3PE	C21-C22-C23-C24
46	M	503	3PE	C26-C27-C28-C29
47	9	204	PC1	C11-C12-N-C13
46	N	402	3PE	O13-C11-C12-N
46	M	503	3PE	C22-C23-C24-C25
46	A	201	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
47	6	203	PC1	C11-C12-N-C13
47	6	203	PC1	C11-C12-N-C15
47	9	204	PC1	C11-C12-N-C14
46	L	703	3PE	C32-C33-C34-C35
54	d	201	CDL	C55-C56-C57-C58
47	9	204	PC1	C29-C2A-C2B-C2C
54	d	201	CDL	OB5-CB3-CB4-OB6
46	H	401	3PE	C31-C32-C33-C34
46	N	402	3PE	O21-C2-C3-O31
46	M	502	3PE	C22-C23-C24-C25
46	M	502	3PE	O11-C1-C2-C3
54	m	201	CDL	OB5-CB3-CB4-CB6
46	A	201	3PE	C34-C35-C36-C37
46	M	502	3PE	C36-C37-C38-C39
46	N	402	3PE	C1-C2-C3-O31
46	Y	202	3PE	C1-C2-C3-O31
53	n	201	ZMP	O3-C16-C17-O4
47	6	203	PC1	C35-C36-C37-C38
49	1	501	FMN	C5'-O5'-P-O1P
54	L	702	CDL	OB5-CB3-CB4-OB6
54	h	201	CDL	OB6-CB4-CB6-OB8
54	d	201	CDL	OB5-CB3-CB4-CB6
47	M	501	PC1	C21-C22-C23-C24
46	M	503	3PE	C34-C35-C36-C37
54	d	201	CDL	CA3-CA4-CA6-OA8
54	m	201	CDL	CB3-CB4-CB6-OB8
46	N	402	3PE	C32-C33-C34-C35
47	9	204	PC1	C34-C35-C36-C37
46	M	503	3PE	C11-O13-P-O11
46	M	502	3PE	O11-C1-C2-O21
46	Y	202	3PE	O21-C2-C3-O31
47	6	203	PC1	O21-C2-C3-O31
46	A	201	3PE	C2-C1-O11-P
46	L	701	3PE	C2-C1-O11-P
46	M	504	3PE	C2-C1-O11-P
47	9	203	PC1	C28-C29-C2A-C2B
47	6	203	PC1	C33-C34-C35-C36
46	L	701	3PE	O11-C1-C2-C3
46	m	202	3PE	O11-C1-C2-C3
53	n	201	ZMP	N2-C16-C17-O4
47	9	203	PC1	C35-C36-C37-C38
53	n	201	ZMP	C13-C14-C15-N2

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Mol	Chain	Res	Type	Atoms
46	M	503	3PE	C1-C2-C3-O31
54	N	401	CDL	CA3-CA4-CA6-OA8
54	h	201	CDL	C1-CA2-OA2-PA1
46	m	202	3PE	O11-C1-C2-O21
54	d	201	CDL	OA6-CA4-CA6-OA8
47	9	203	PC1	C11-C12-N-C13
51	P	501	NDP	C5B-O5B-PA-O3
51	P	501	NDP	PN-O3-PA-O2A
55	O	401	DGT	PB-O3A-PA-O1A
54	r	202	CDL	CB2-OB2-PB2-OB5
46	K	201	3PE	C2-C1-O11-P
54	h	201	CDL	CA4-CA3-OA5-PA1
46	r	201	3PE	C1-O11-P-O12
46	r	201	3PE	C1-O11-P-O14
46	r	201	3PE	C11-O13-P-O12
46	K	201	3PE	C11-O13-P-O14
46	L	701	3PE	C1-O11-P-O12
46	M	502	3PE	C1-O11-P-O12
46	M	503	3PE	C1-O11-P-O12
46	M	503	3PE	C11-O13-P-O14
46	M	504	3PE	C1-O11-P-O12
46	Y	202	3PE	C11-O13-P-O14
46	d	203	3PE	C11-O13-P-O14
46	i	201	3PE	C11-O13-P-O12
47	9	203	PC1	C11-C12-N-C14
54	r	202	CDL	CB3-OB5-PB2-OB3
54	L	702	CDL	CA3-OA5-PA1-OA4
54	N	401	CDL	CA2-OA2-PA1-OA3
54	N	401	CDL	CA2-OA2-PA1-OA4
54	N	401	CDL	CB2-OB2-PB2-OB4
54	d	201	CDL	CA3-OA5-PA1-OA3
54	h	201	CDL	CA2-OA2-PA1-OA4
54	h	201	CDL	CB2-OB2-PB2-OB4
54	L	702	CDL	OB5-CB3-CB4-CB6
54	h	201	CDL	OB5-CB3-CB4-CB6
46	H	401	3PE	O13-C11-C12-N
47	9	204	PC1	C35-C36-C37-C38
54	h	201	CDL	OB5-CB3-CB4-OB6
46	L	703	3PE	C31-C32-C33-C34
47	M	501	PC1	O13-C11-C12-N
54	m	201	CDL	OB6-CB4-CB6-OB8
46	M	502	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
53	n	201	ZMP	C5-C6-C7-C8
46	A	201	3PE	C38-C39-C3A-C3B
46	H	401	3PE	C33-C34-C35-C36
46	M	502	3PE	C37-C38-C39-C3A
46	N	402	3PE	C2-C1-O11-P
47	9	203	PC1	C11-C12-N-C15
46	M	503	3PE	O21-C2-C3-O31
46	A	201	3PE	C1-O11-P-O13
46	H	401	3PE	C1-O11-P-O13
46	K	201	3PE	C1-O11-P-O13
46	m	202	3PE	C1-O11-P-O13
47	M	501	PC1	C1-O11-P-O13
54	N	401	CDL	CA3-OA5-PA1-OA2
46	r	201	3PE	O31-C31-C32-C33
53	W	201	ZMP	C22-C1-C2-C3
54	m	201	CDL	C72-C73-C74-C75
51	P	501	NDP	O4D-C1D-N1N-C6N
46	L	703	3PE	O21-C21-C22-C23
46	L	703	3PE	C3D-C3E-C3F-C3G
54	N	401	CDL	CB4-CB3-OB5-PB2
46	H	401	3PE	O31-C31-C32-C33
53	n	201	ZMP	C19-C18-C21-O5
47	M	501	PC1	C34-C35-C36-C37
46	H	401	3PE	C3-C2-O21-C21
47	9	203	PC1	C3-C2-O21-C21
46	d	203	3PE	C11-O13-P-O11
46	M	502	3PE	C3D-C3E-C3F-C3G
54	m	201	CDL	C1-CB2-OB2-PB2
54	L	702	CDL	O1-C1-CB2-OB2
54	d	201	CDL	C59-C60-C61-C62
53	n	201	ZMP	C12-C11-S1-C10
54	N	401	CDL	OB6-CB4-CB6-OB8
51	P	501	NDP	C2D-C1D-N1N-C6N
46	H	401	3PE	C2A-C2B-C2C-C2D
46	Y	202	3PE	O11-C1-C2-O21
46	M	502	3PE	O21-C21-C22-C23
47	9	204	PC1	O11-C1-C2-C3
46	K	201	3PE	O31-C31-C32-C33
55	O	401	DGT	PB-O3B-PG-O3G
54	r	202	CDL	C52-C51-CB5-OB6
47	M	501	PC1	C23-C24-C25-C26
46	M	504	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C3-C2-O21-C21
54	h	201	CDL	CB6-CB4-OB6-CB5
47	9	204	PC1	O31-C31-C32-C33
54	m	201	CDL	C12-C11-CA5-OA6
54	r	202	CDL	C1-CB2-OB2-PB2
54	h	201	CDL	CB3-CB4-CB6-OB8
53	n	201	ZMP	C16-C17-C18-C20
55	O	401	DGT	PB-O3B-PG-O2G
46	m	202	3PE	O31-C31-C32-C33
46	m	202	3PE	O21-C21-C22-C23
53	n	201	ZMP	C3-C4-C5-C6
46	H	401	3PE	O11-C1-C2-C3
46	K	201	3PE	O21-C21-C22-C23
54	h	201	CDL	C32-C31-CA7-OA8
47	M	501	PC1	O21-C2-C3-O31
53	W	201	ZMP	C2-C1-C22-C23
46	M	502	3PE	O31-C31-C32-C33
46	d	202	3PE	O31-C31-C32-C33
51	P	501	NDP	C2B-O2B-P2B-O3X
54	h	201	CDL	C12-C11-CA5-OA6
54	h	201	CDL	C72-C71-CB7-OB8
54	L	702	CDL	C11-C12-C13-C14
55	O	401	DGT	PB-O3A-PA-O2A
54	m	201	CDL	C12-C11-CA5-OA7
46	K	201	3PE	O32-C31-C32-C33
46	M	502	3PE	O32-C31-C32-C33
47	9	203	PC1	C27-C28-C29-C2A
46	K	201	3PE	C2A-C2B-C2C-C2D
55	O	401	DGT	C4'-C5'-O5'-PA
54	N	401	CDL	C80-C81-C82-C83
46	6	202	3PE	C1-O11-P-O14
46	N	402	3PE	C1-O11-P-O14
47	9	204	PC1	C11-O13-P-O14
51	P	501	NDP	C2N-C3N-C7N-N7N
54	r	202	CDL	CB3-OB5-PB2-OB4
54	N	401	CDL	CA3-OA5-PA1-OA3
46	m	202	3PE	O32-C31-C32-C33
54	h	201	CDL	C32-C31-CA7-OA9
54	h	201	CDL	C72-C71-CB7-OB9
46	L	701	3PE	O31-C31-C32-C33
46	K	201	3PE	O22-C21-C22-C23
54	m	201	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
46	d	202	3PE	O32-C31-C32-C33
47	9	204	PC1	O32-C31-C32-C33
47	M	501	PC1	C3B-C3C-C3D-C3E
46	M	503	3PE	O21-C21-C22-C23
54	N	401	CDL	CA5-C11-C12-C13
46	M	504	3PE	O22-C21-C22-C23
46	m	202	3PE	O22-C21-C22-C23
46	K	201	3PE	C12-C11-O13-P
47	6	203	PC1	C3-C2-O21-C21
47	9	204	PC1	C12-C11-O13-P
54	r	202	CDL	CA3-CA4-OA6-CA5
54	N	401	CDL	CB6-CB4-OB6-CB5
54	m	201	CDL	CA6-CA4-OA6-CA5
47	9	203	PC1	C2D-C2E-C2F-C2G
47	9	204	PC1	O21-C21-C22-C23
54	r	202	CDL	C1-CA2-OA2-PA1
54	L	702	CDL	C1-CA2-OA2-PA1
46	Y	202	3PE	O31-C31-C32-C33
47	9	203	PC1	O21-C21-C22-C23
46	K	201	3PE	C25-C26-C27-C28
54	L	702	CDL	C52-C51-CB5-OB6
54	m	201	CDL	C52-C51-CB5-OB7
46	Y	202	3PE	O21-C21-C22-C23
46	M	503	3PE	O22-C21-C22-C23
46	H	401	3PE	C23-C24-C25-C26
47	9	203	PC1	C3D-C3E-C3F-C3G
46	Y	202	3PE	O32-C31-C32-C33
47	9	203	PC1	O22-C21-C22-C23

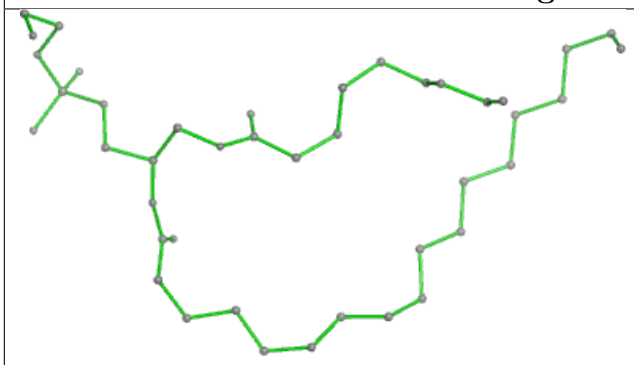
There are no ring outliers.

No monomer is involved in short contacts.

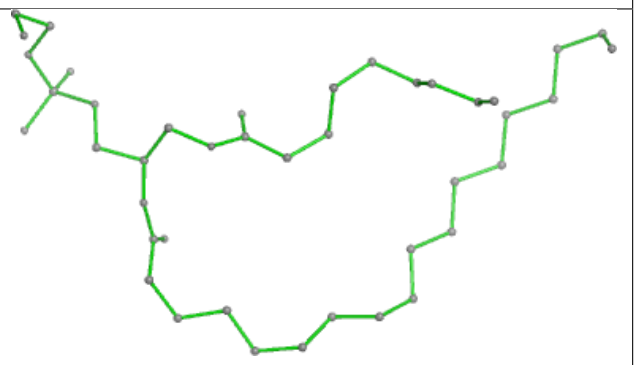
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

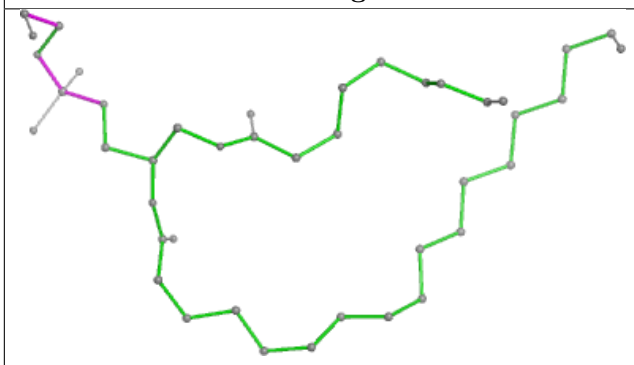
Ligand 3PE i 201



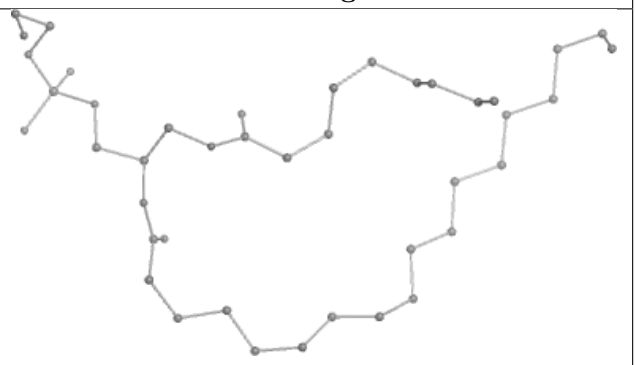
Bond lengths



Bond angles

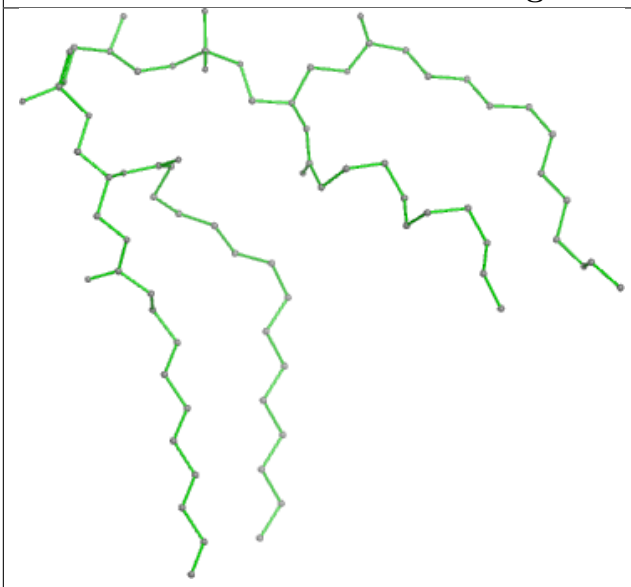


Torsions

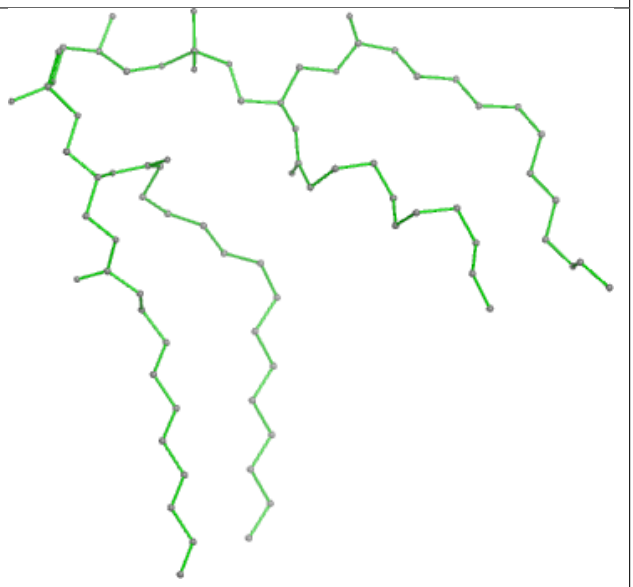


Rings

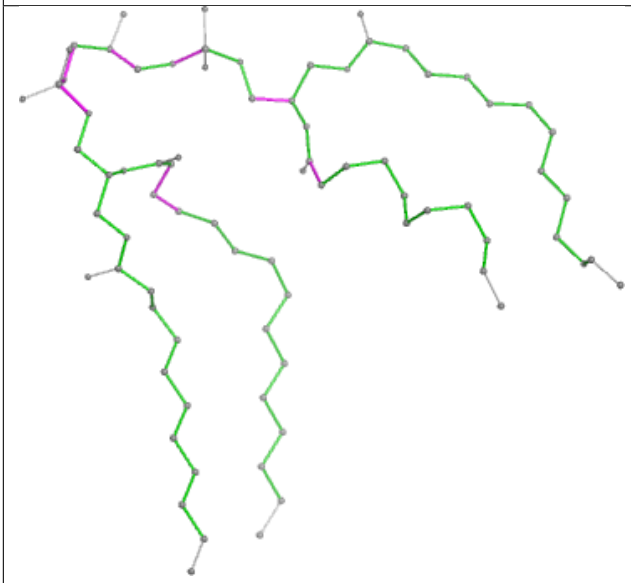
Ligand CDL L 702



Bond lengths



Bond angles



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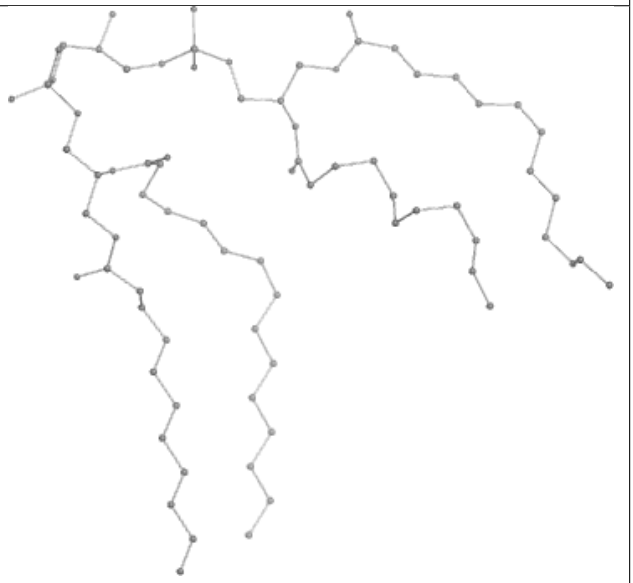
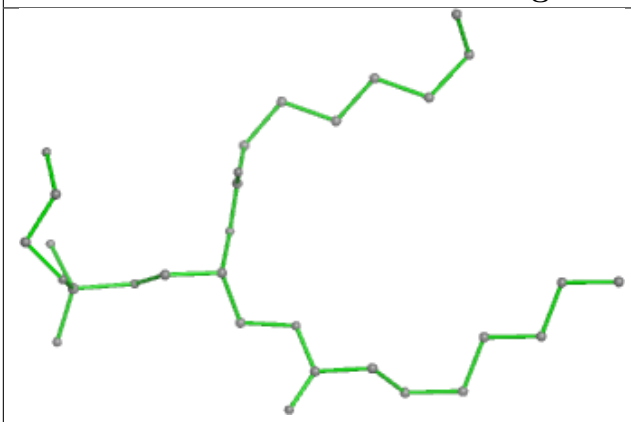
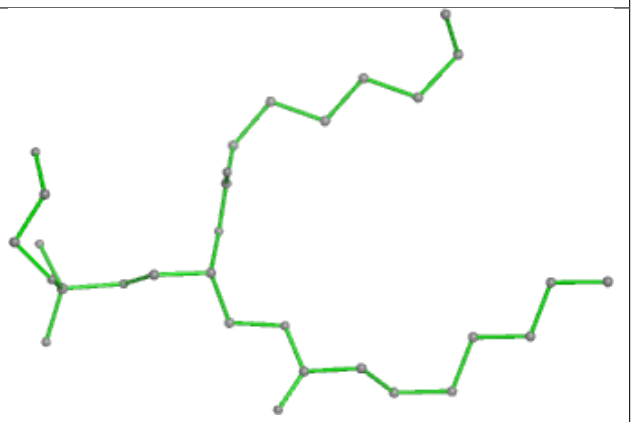


Rings

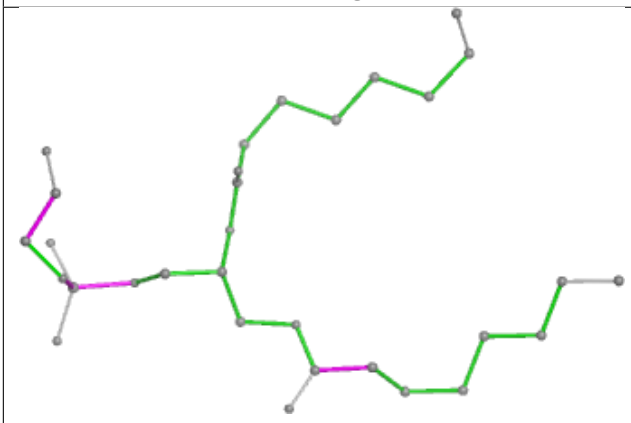
Ligand 3PE d 202



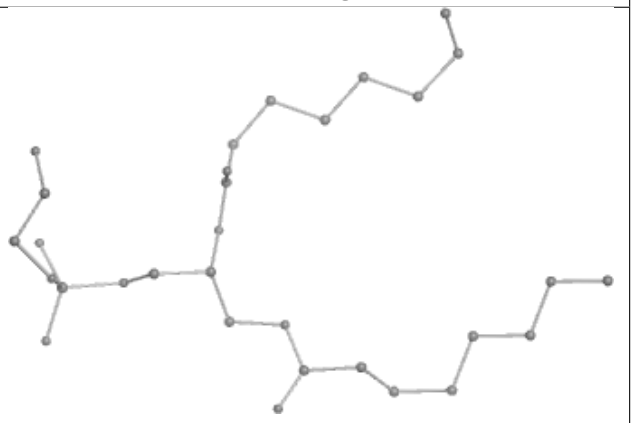
Bond lengths



Bond angles

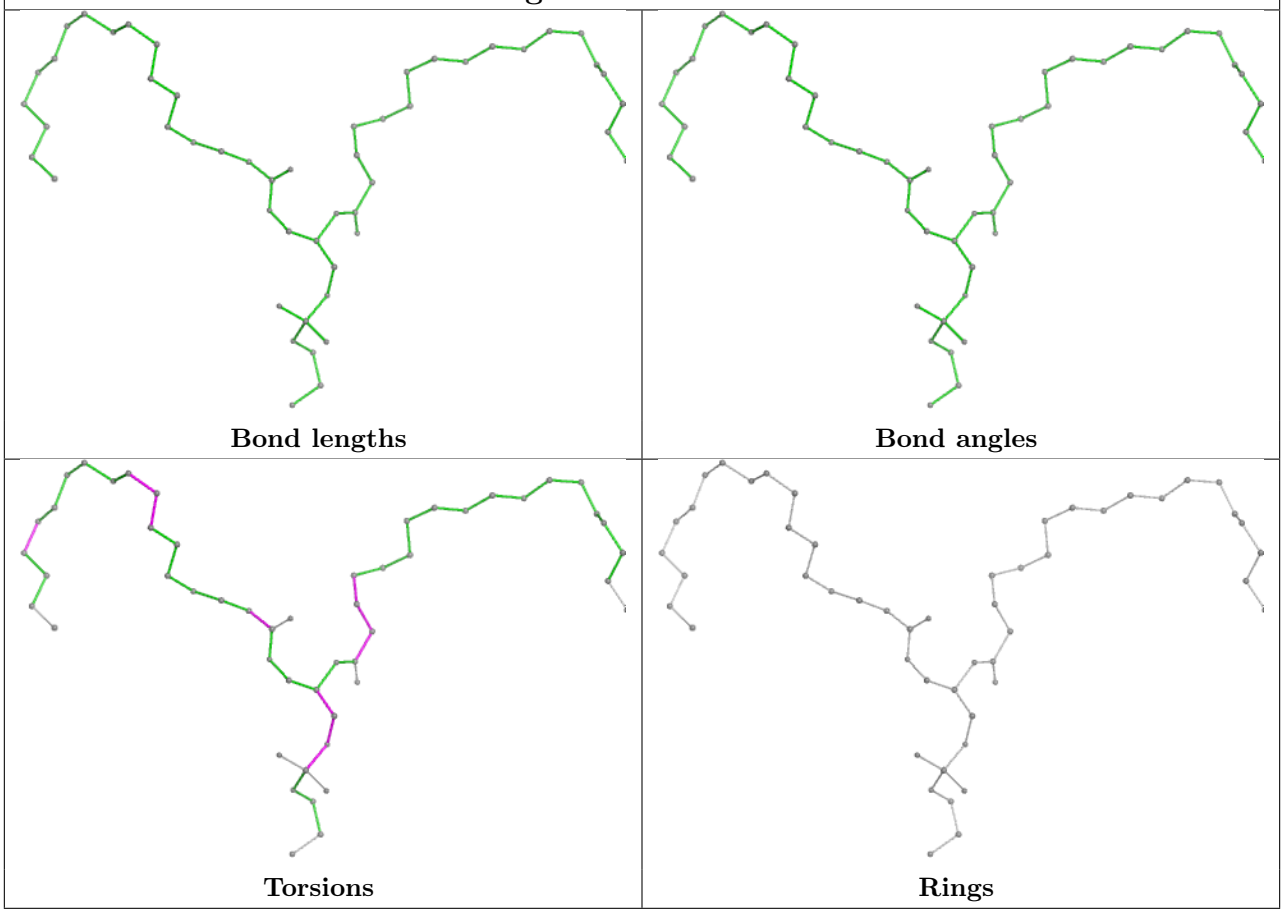


Torsions



Rings

Ligand 3PE M 502



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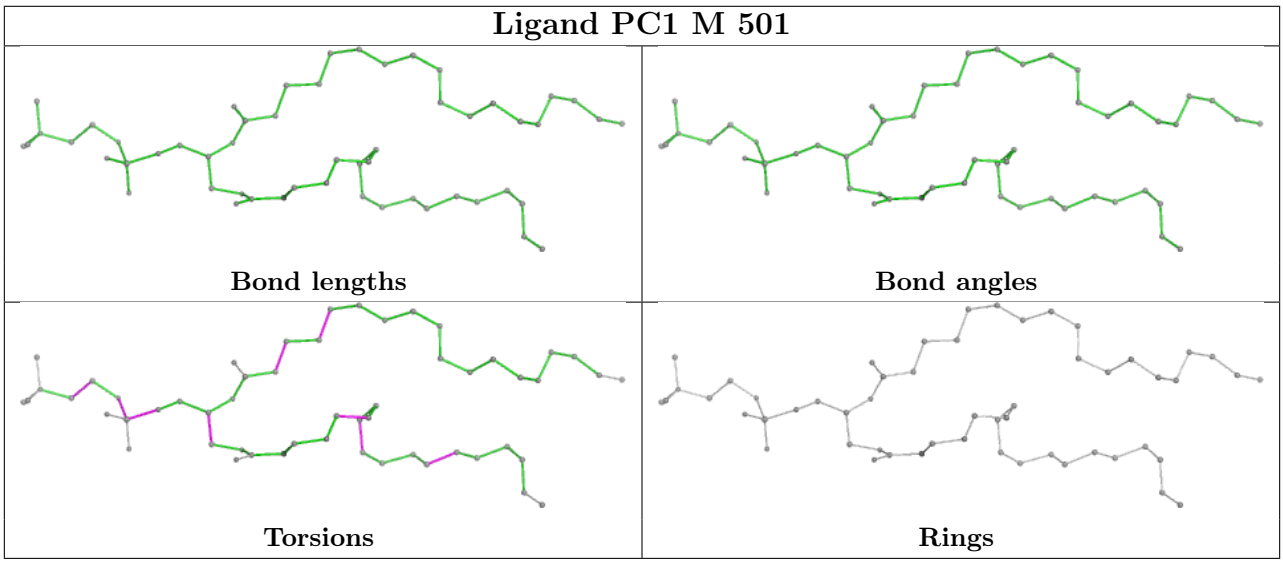

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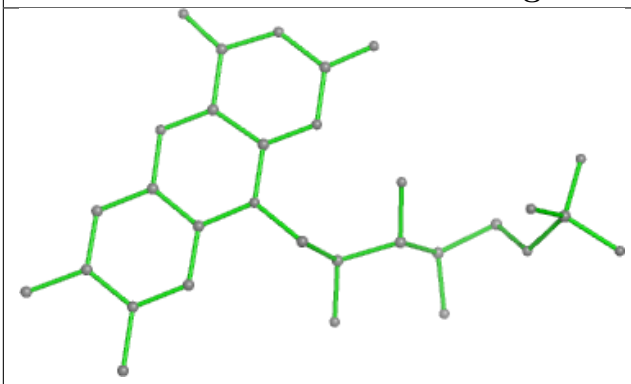
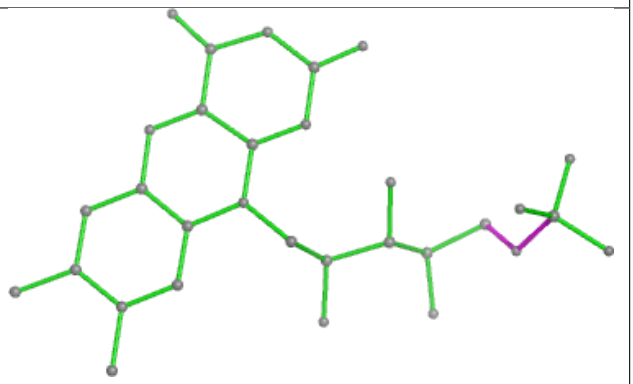
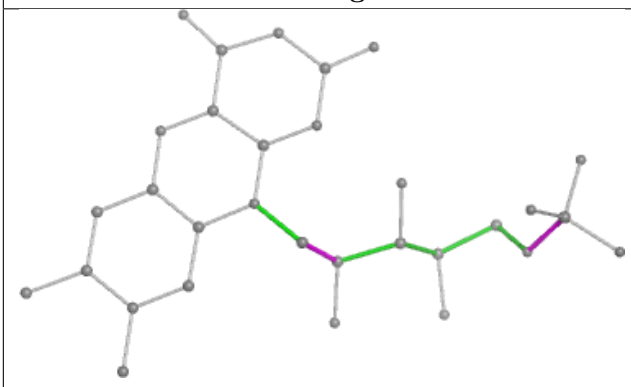


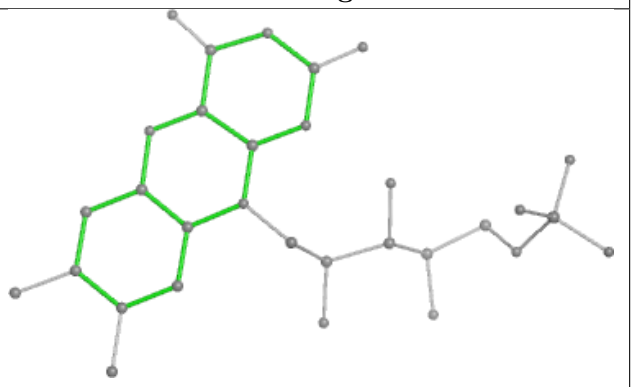
Bond lengths



Bond angles



Torsions



Rings

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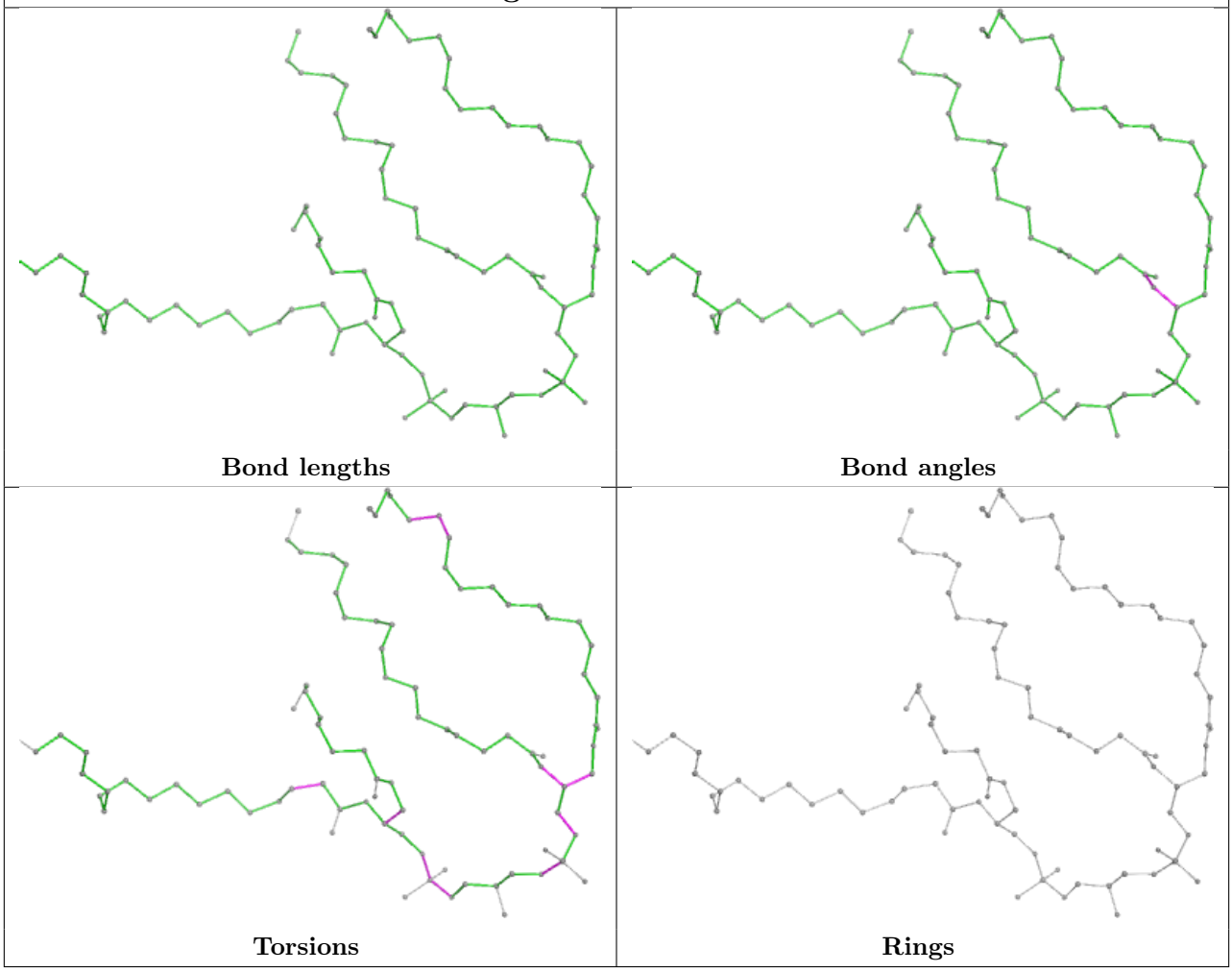
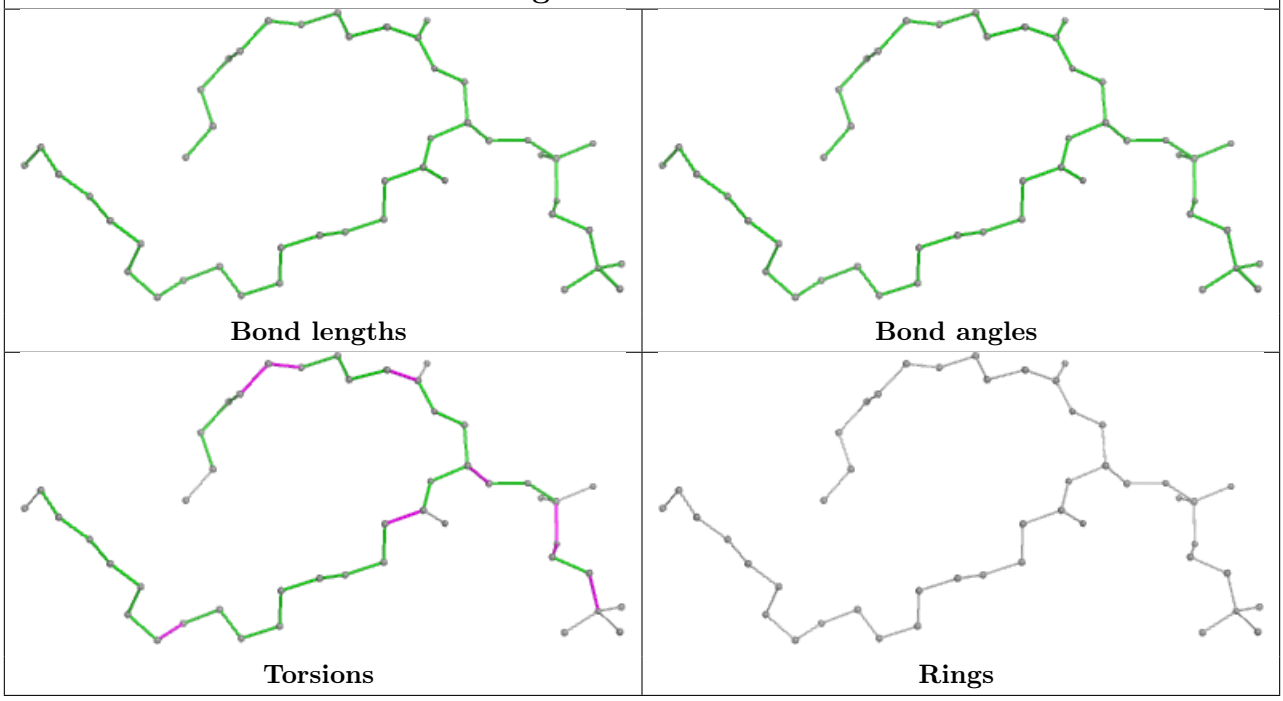
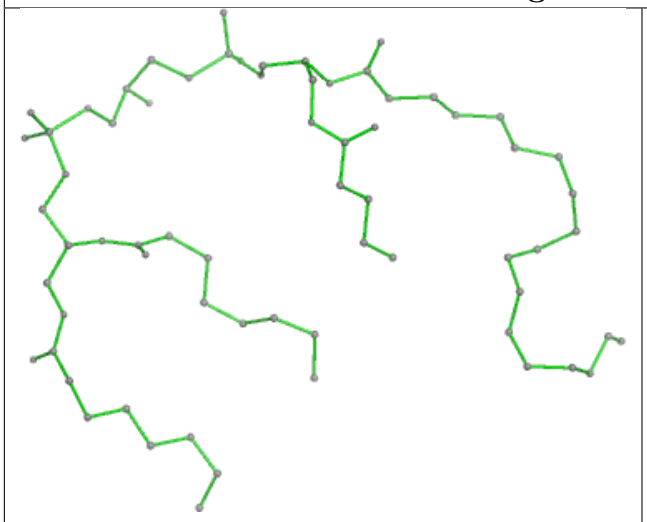


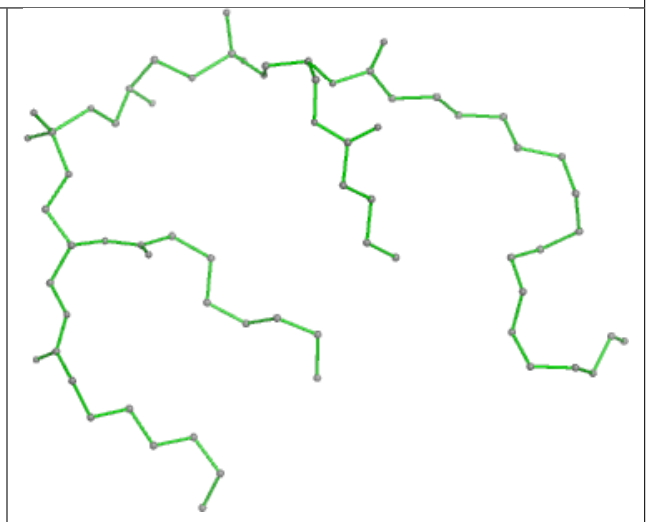
Ligand PC1 9 204



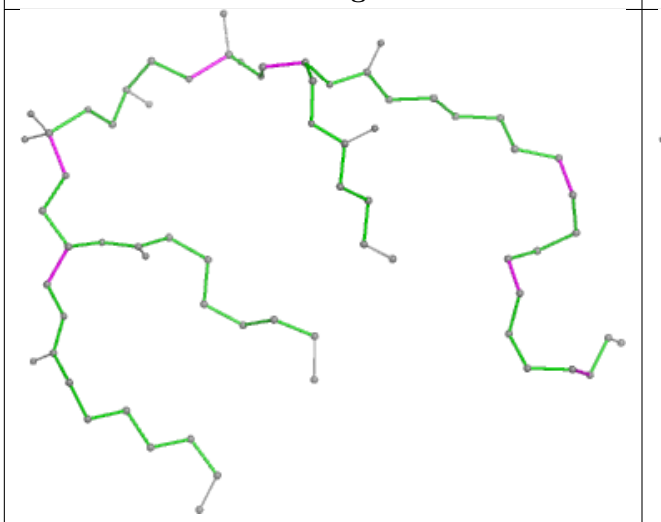
Ligand CDL d 201



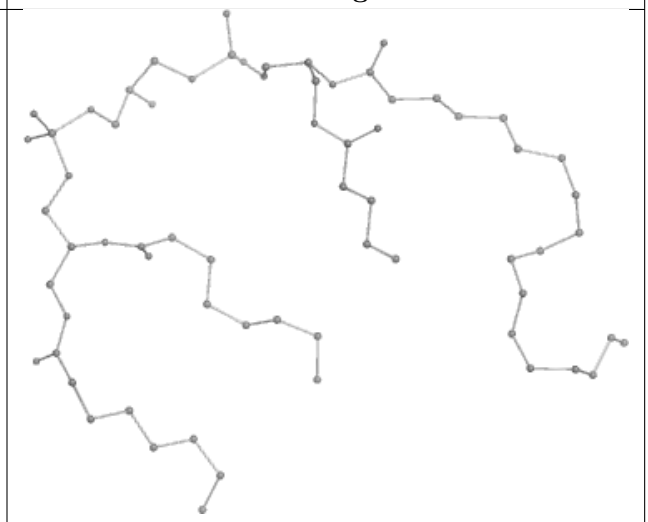
Bond lengths



Bond angles

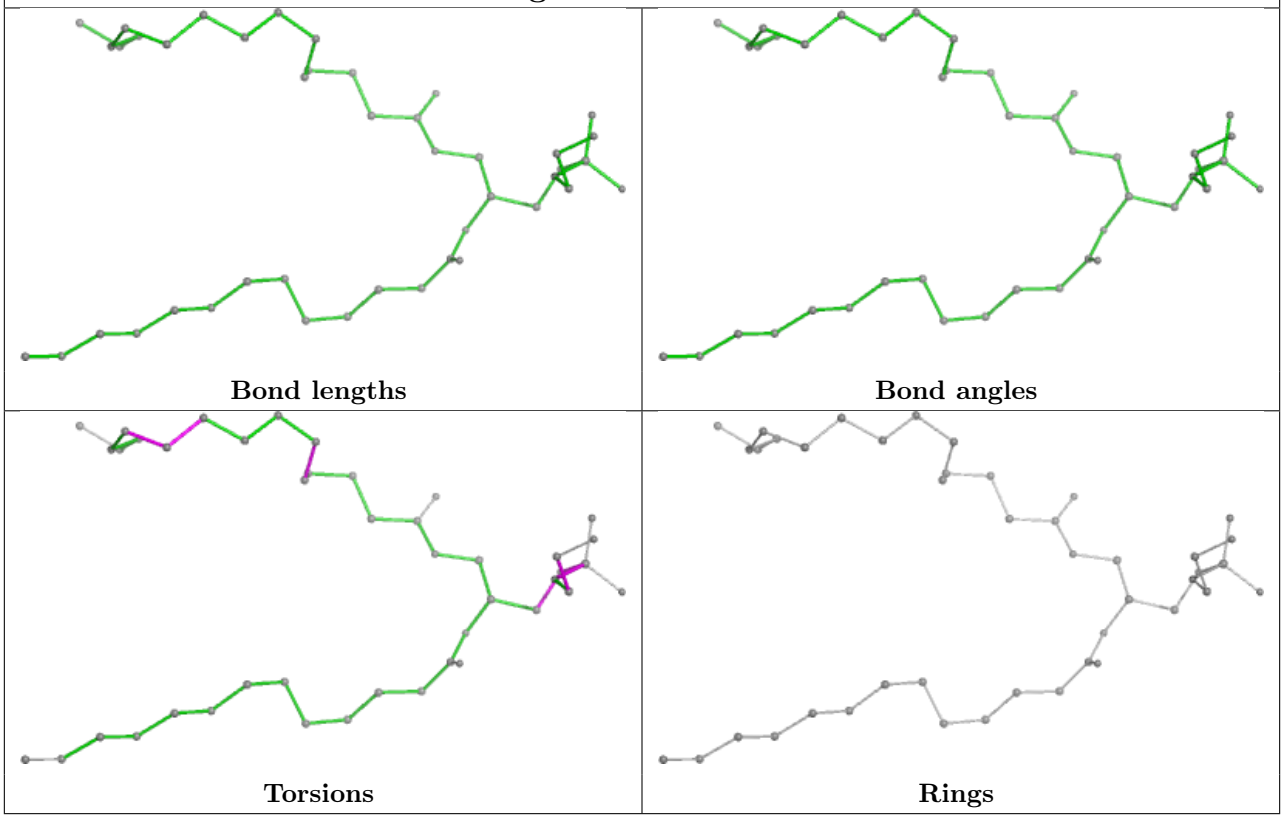


Torsions

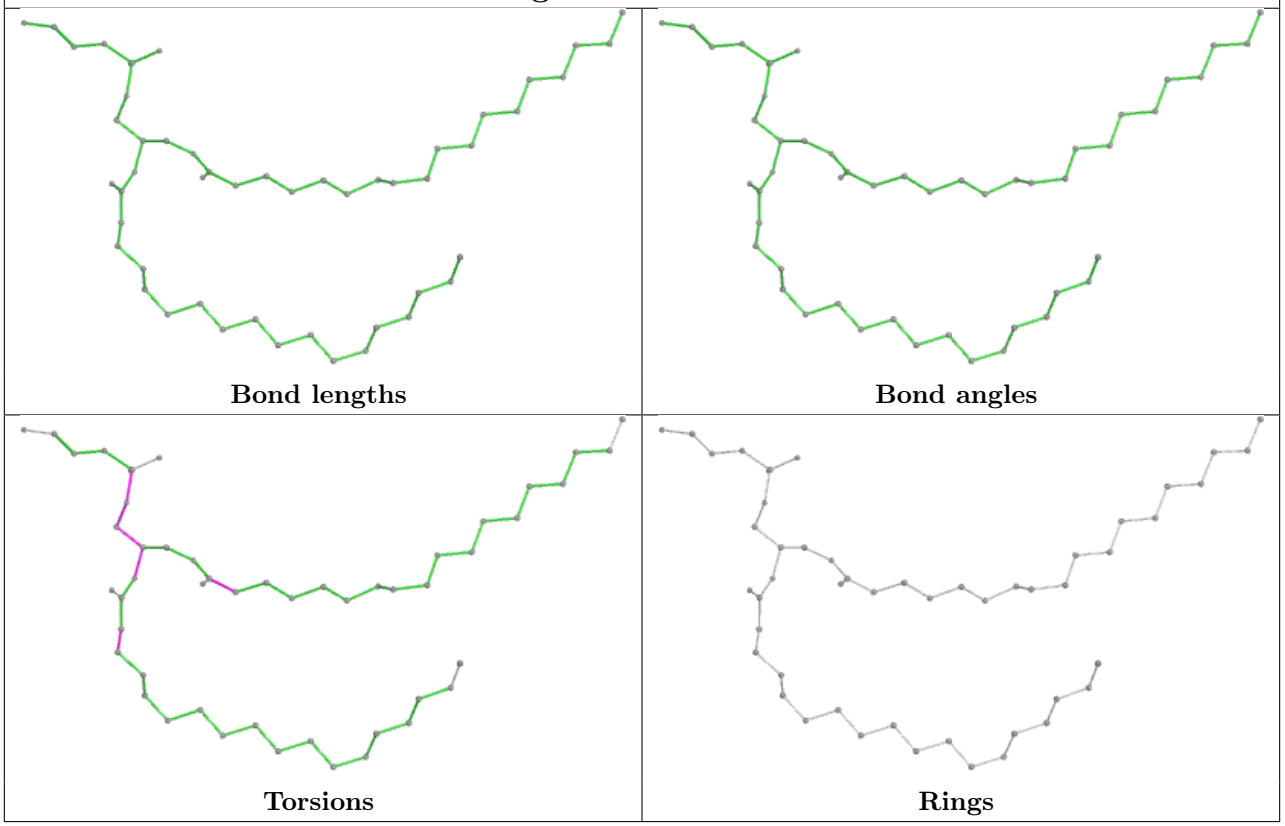


Rings

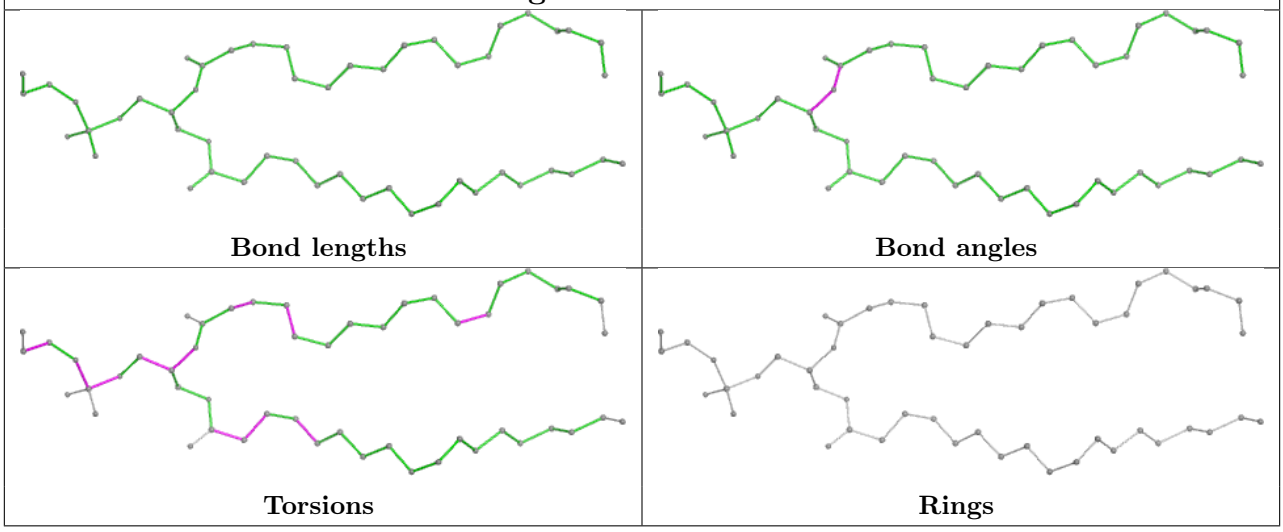
Ligand 3PE A 201



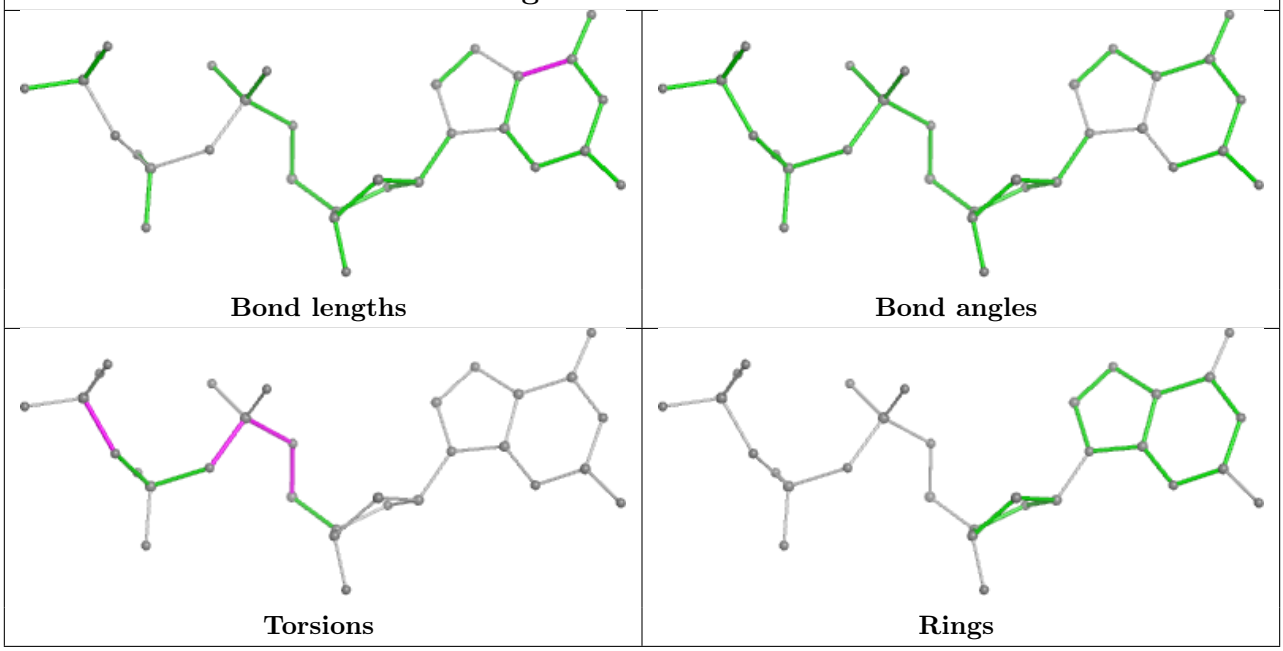
Ligand 3PE L 701



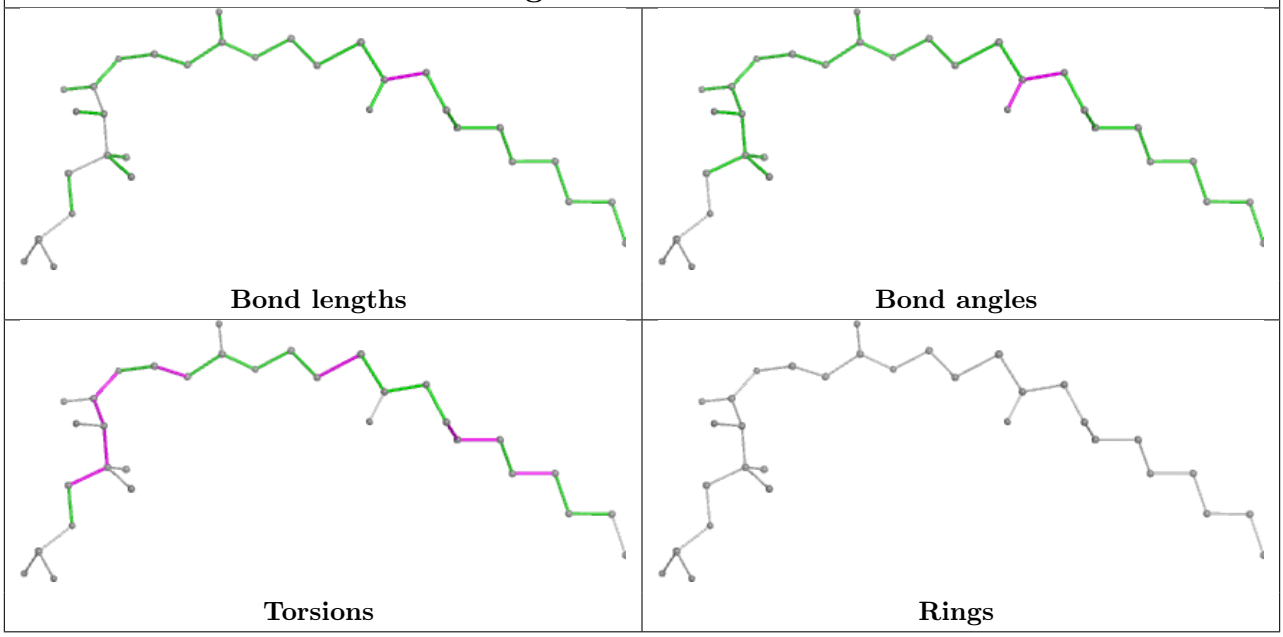
Ligand 3PE H 401



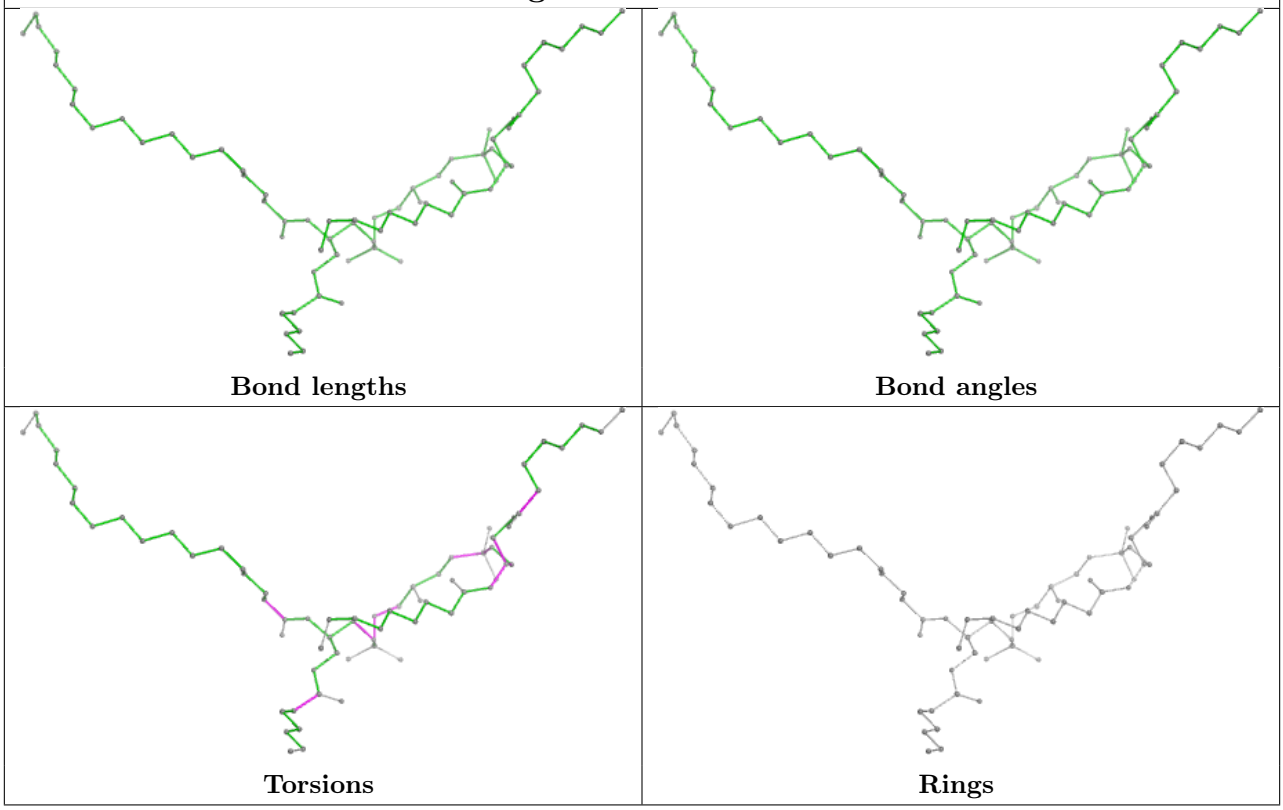
Ligand DGT O 401



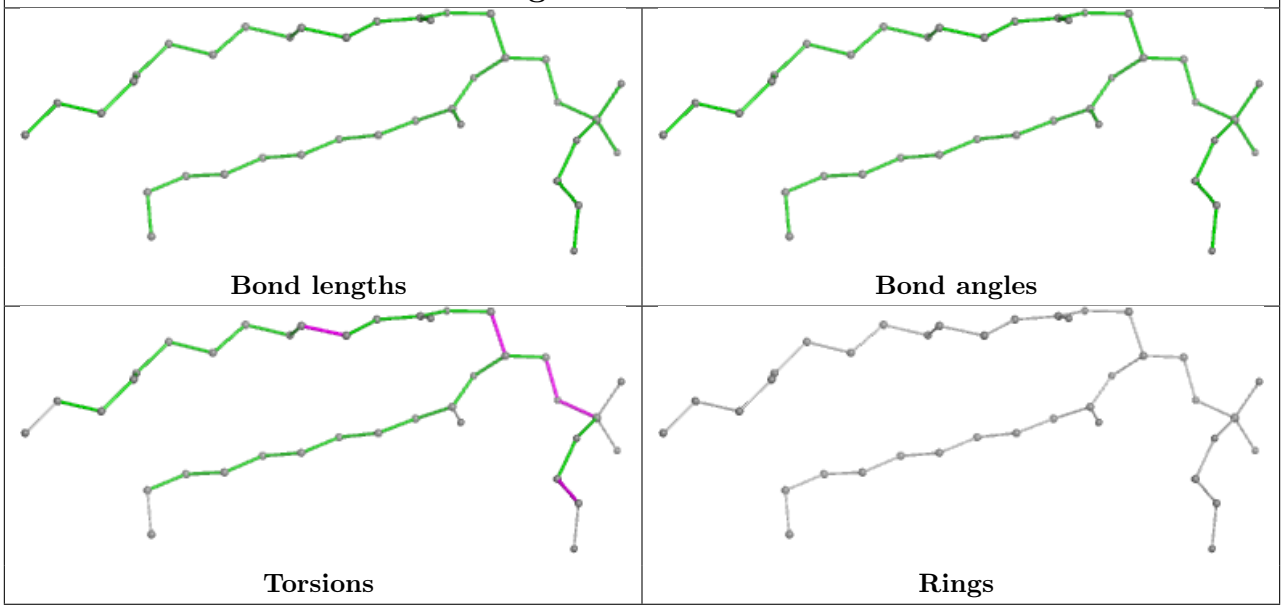
Ligand ZMP n 201



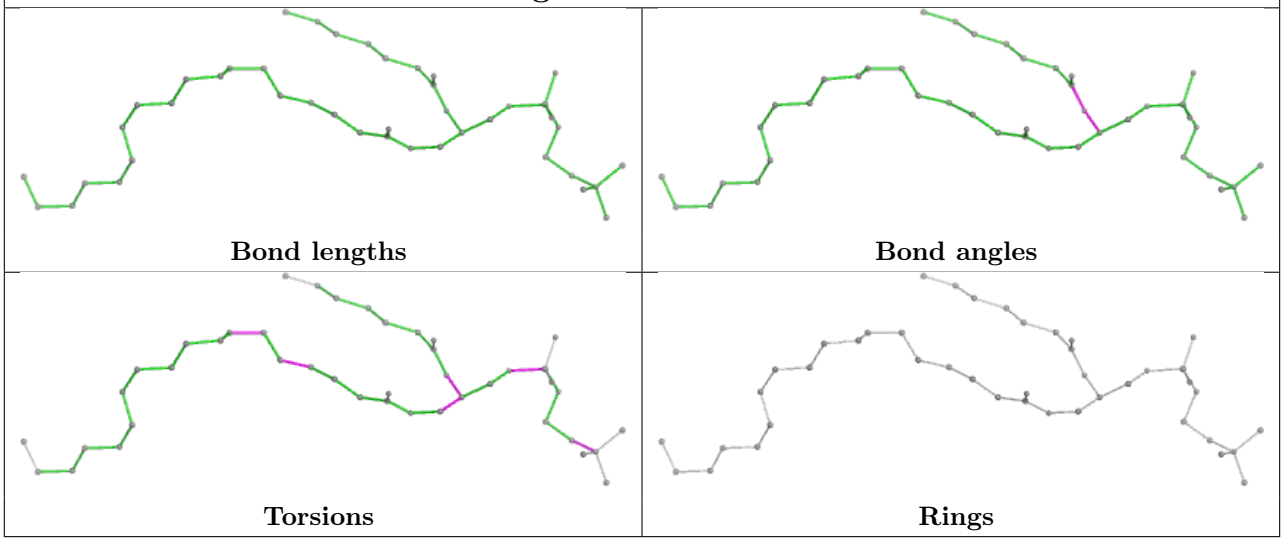
Ligand CDL h 201



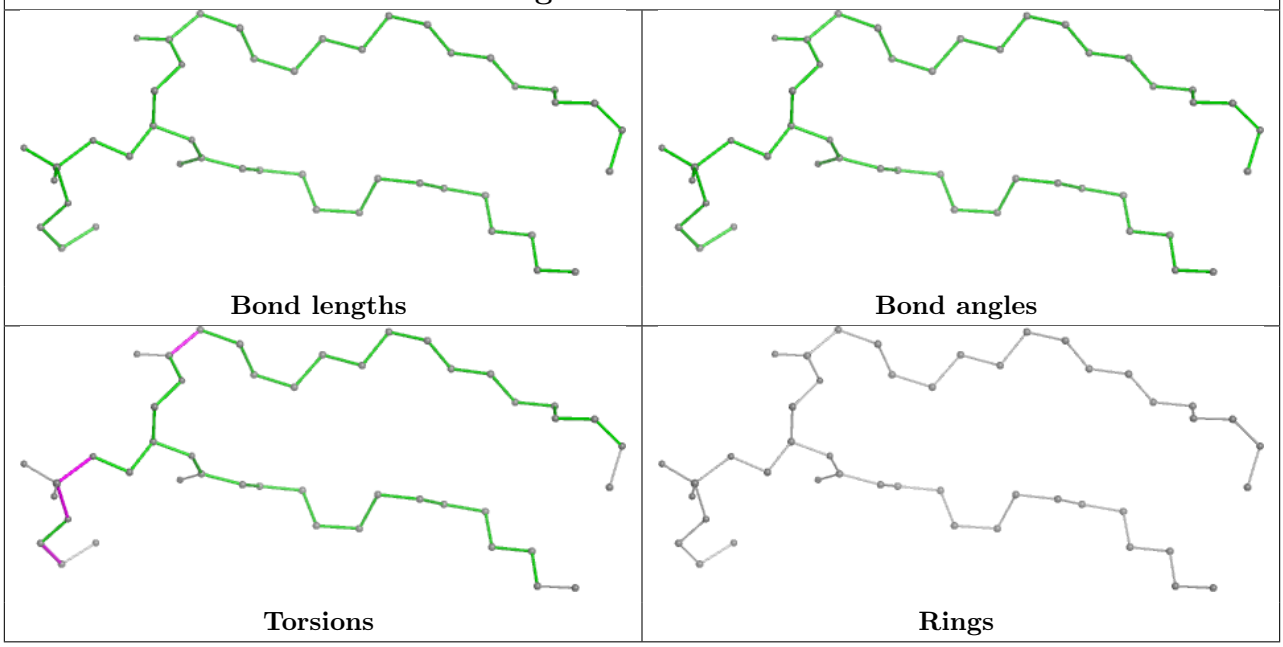
Ligand 3PE N 402



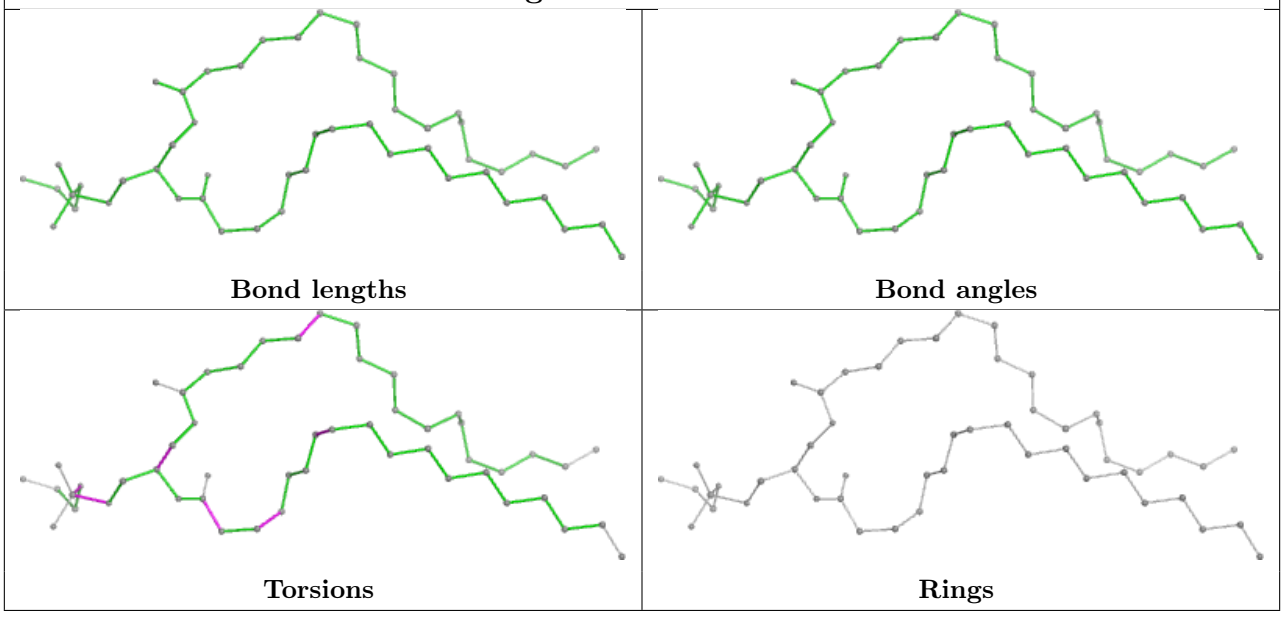
Ligand PC1 6 203



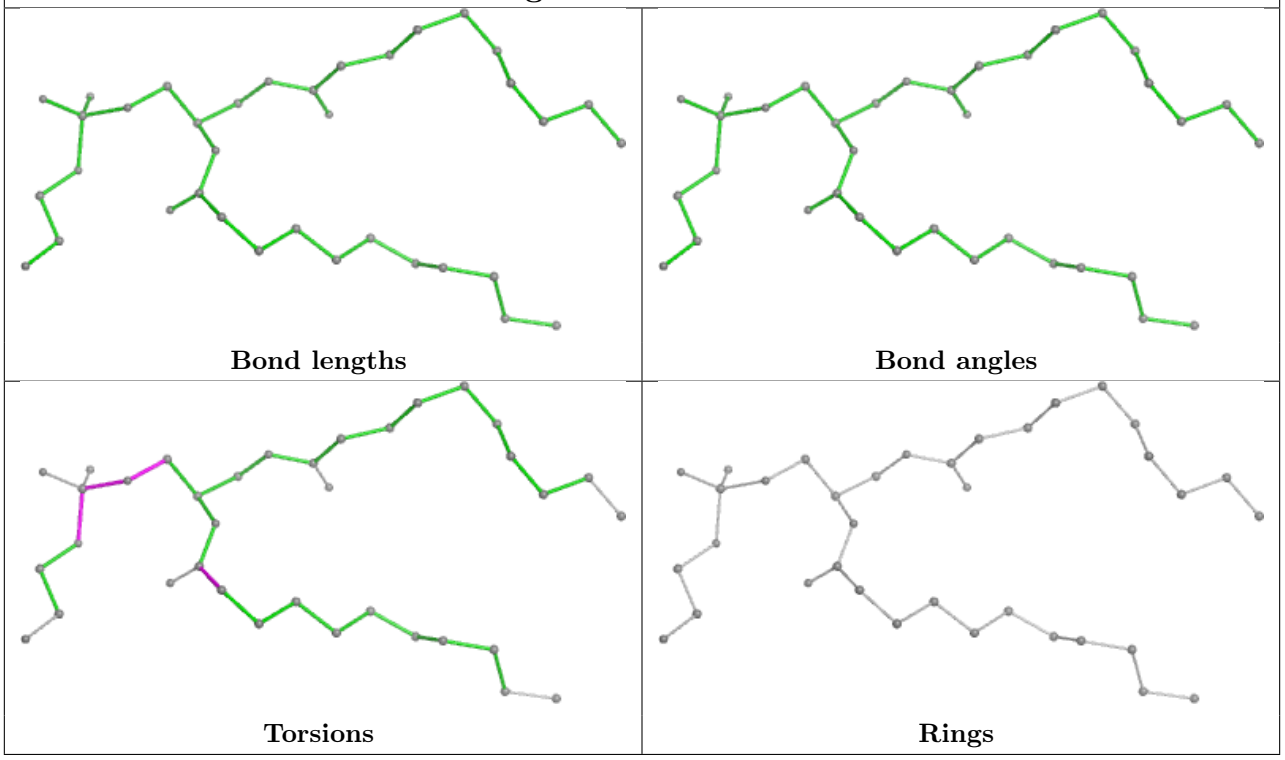
Ligand 3PE r 201



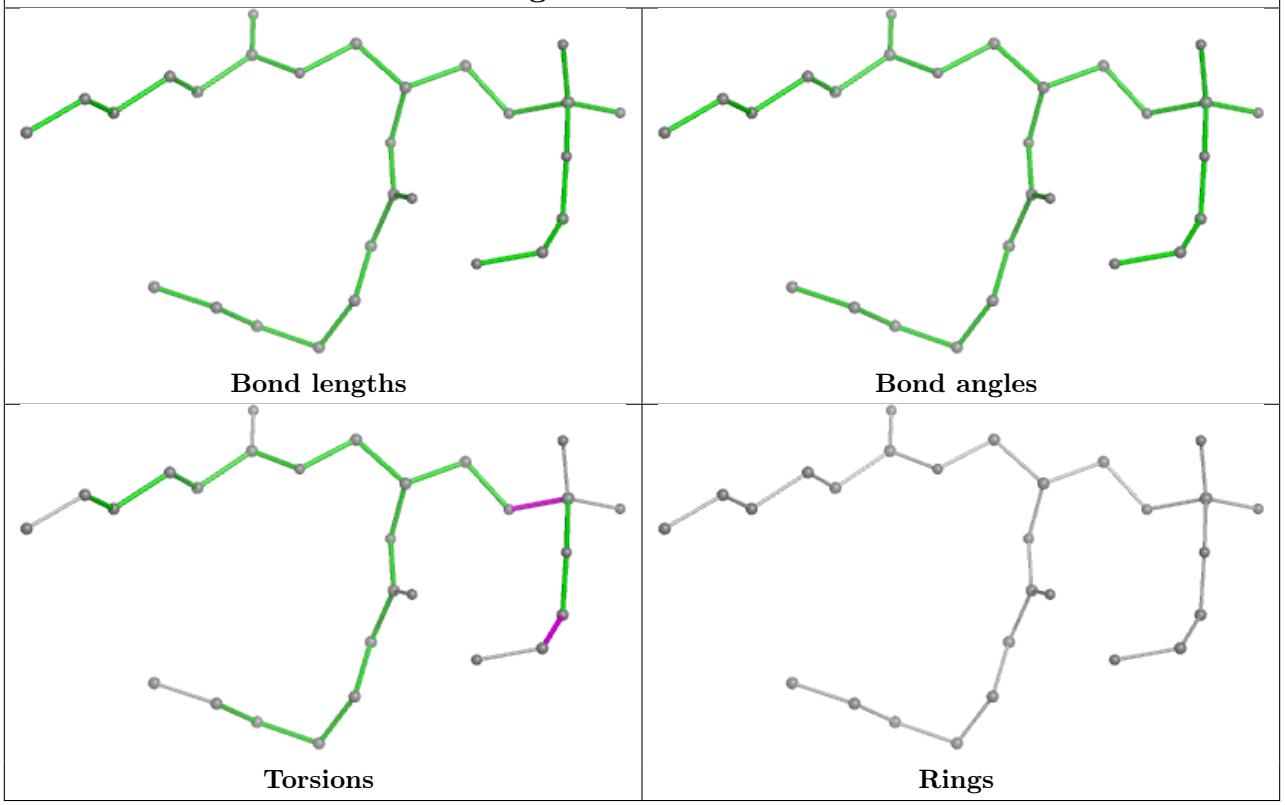
Ligand 3PE M 503



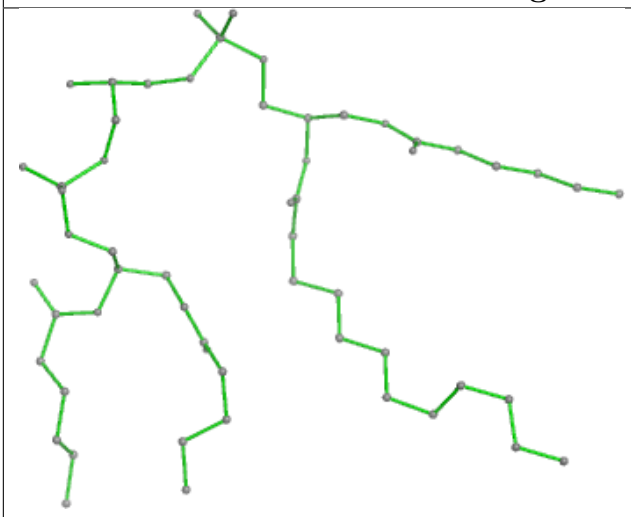
Ligand 3PE M 504



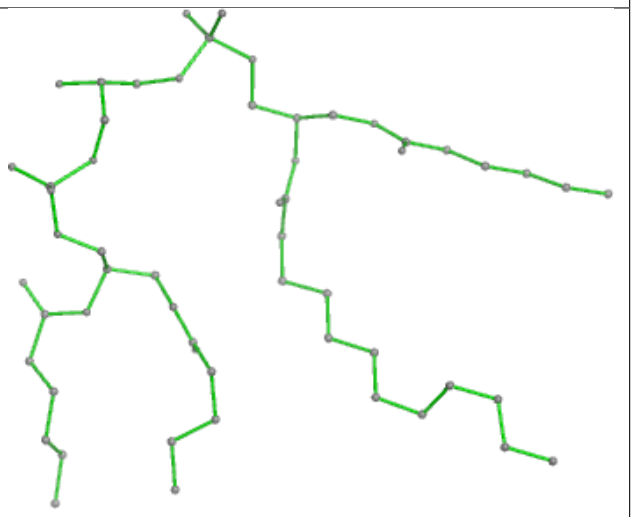
Ligand 3PE Y 201



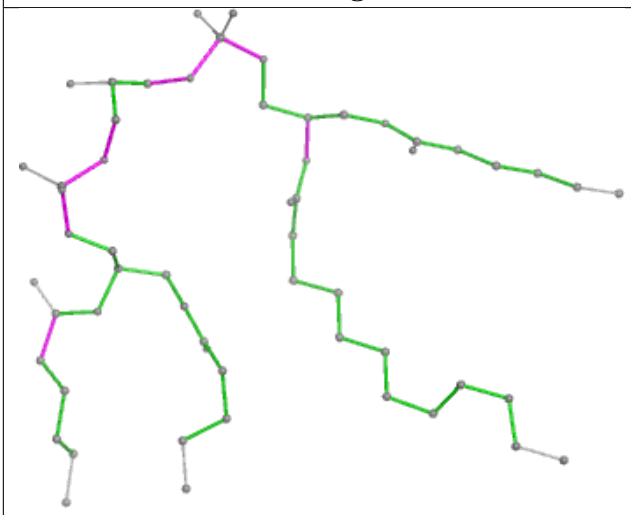
Ligand CDL r 202



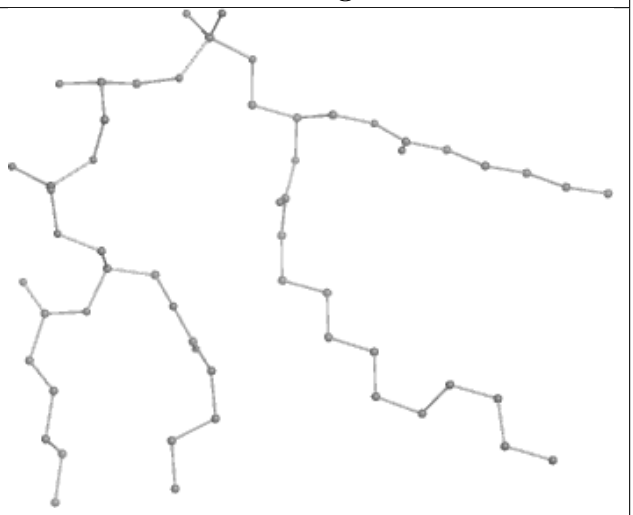
Bond lengths



Bond angles

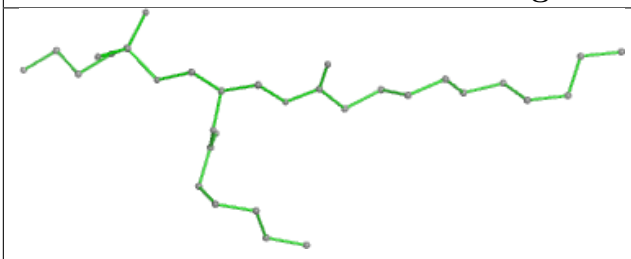


Torsions

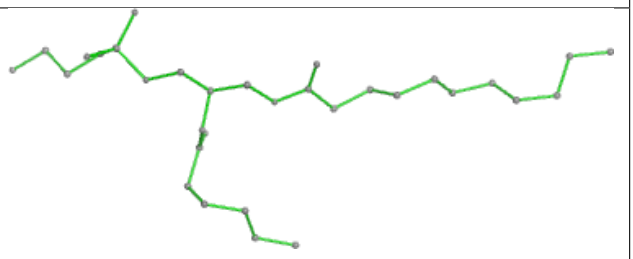


Rings

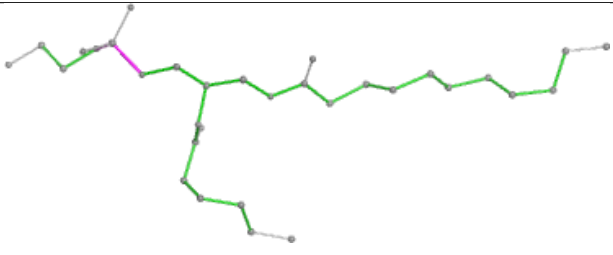
Ligand 3PE d 203



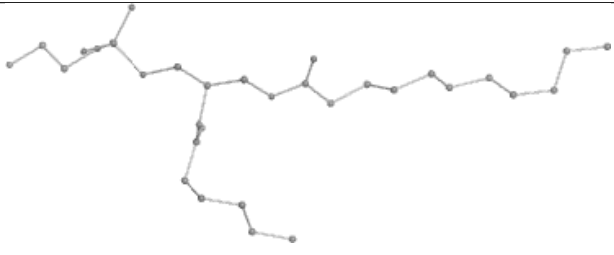
Bond lengths



Bond angles

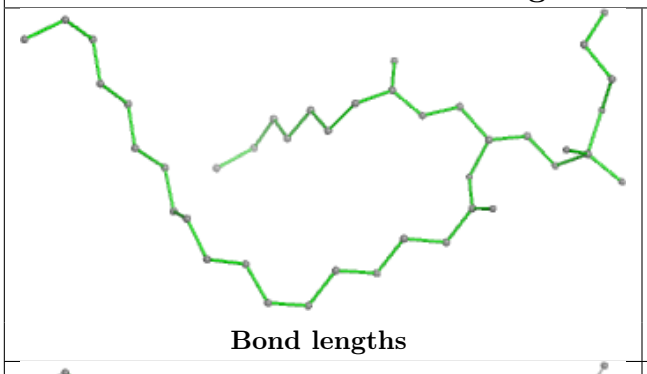


Torsions

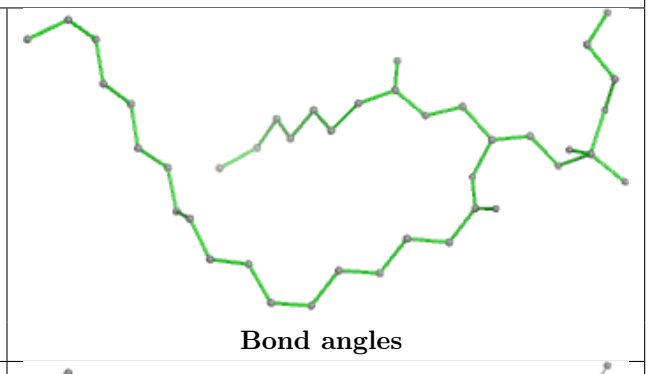


Rings

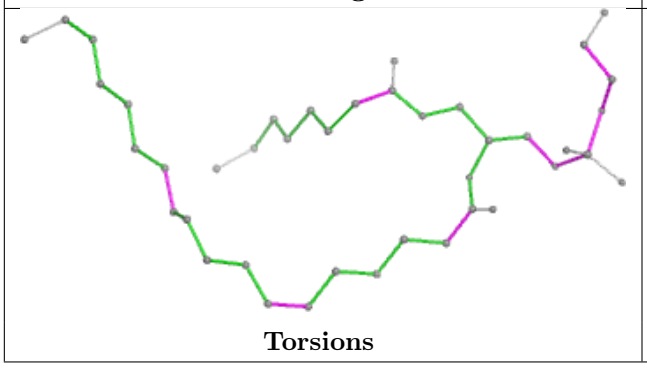
Ligand 3PE K 201



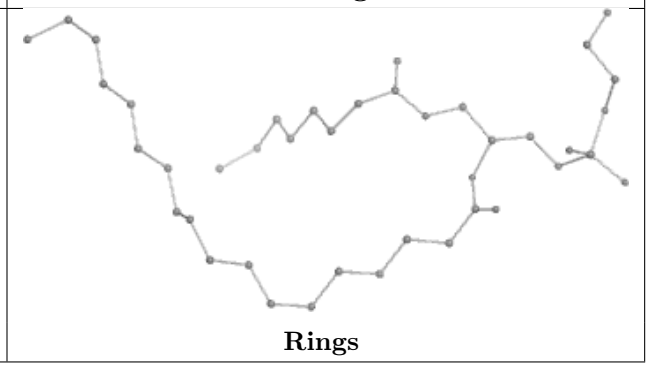
Bond lengths



Bond angles

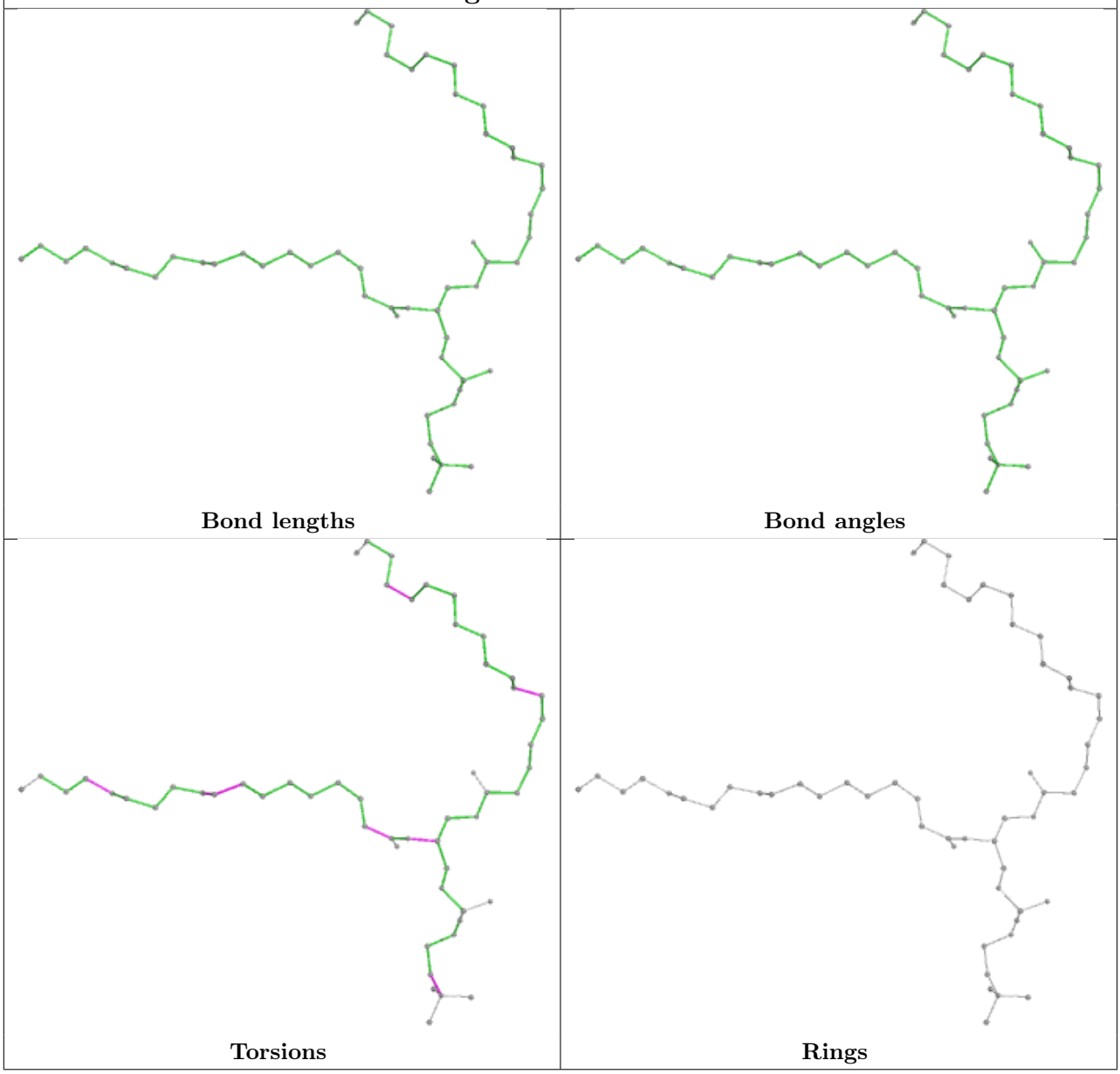


Torsions

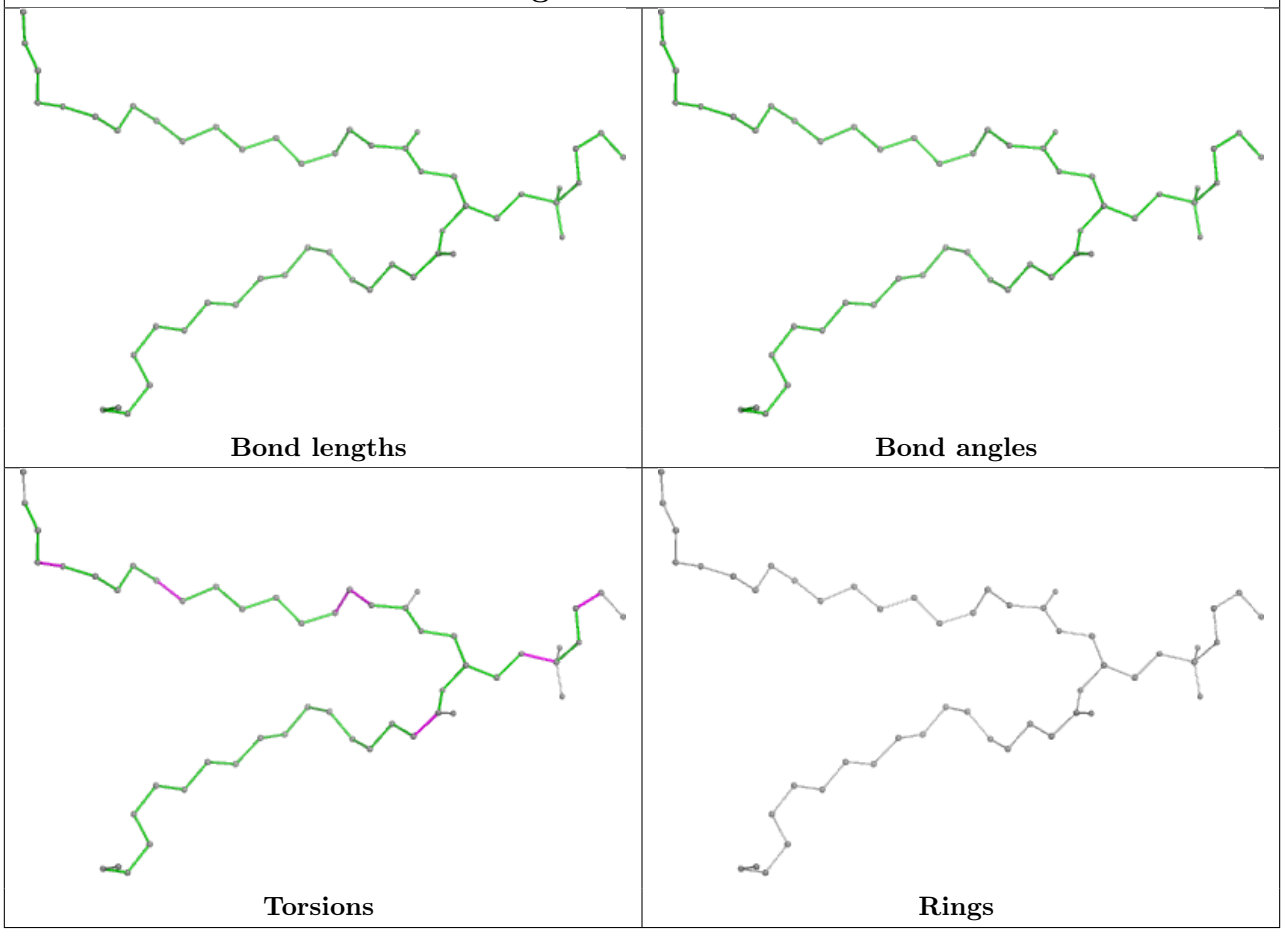


Rings

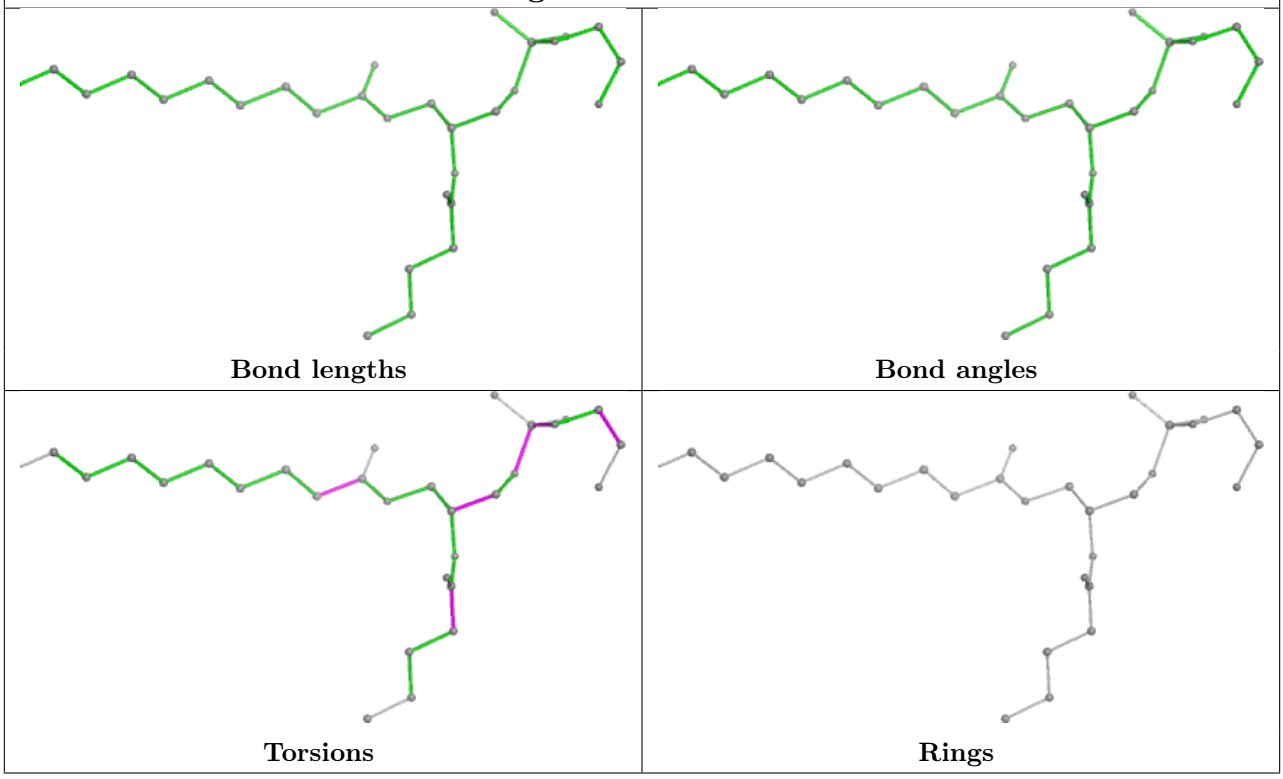
Ligand PC1 9 203



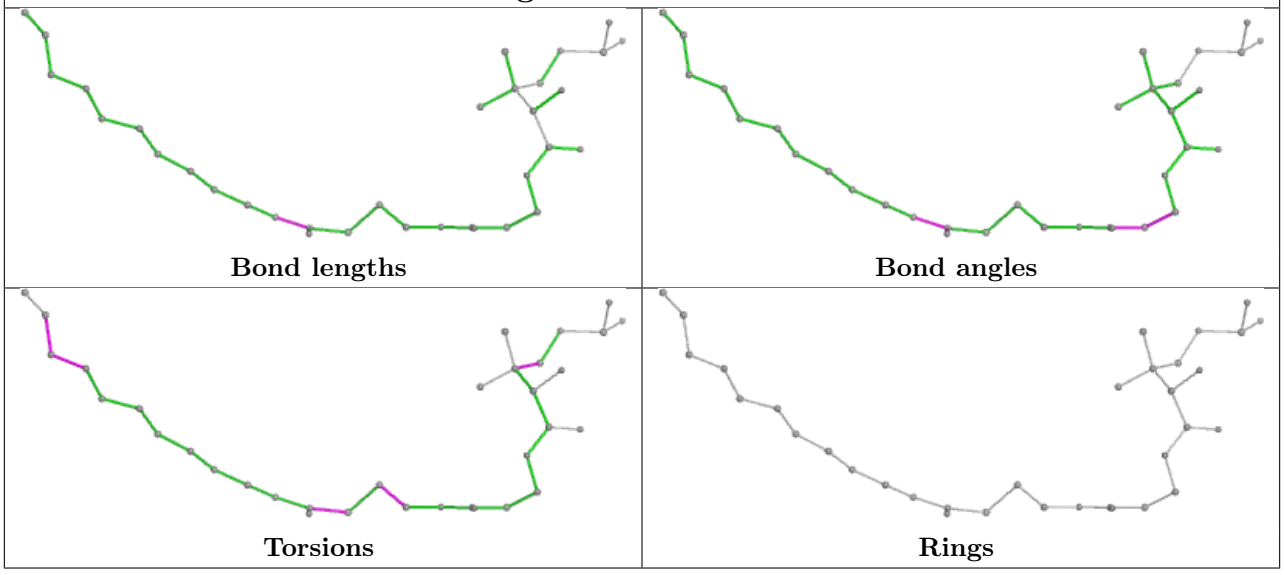
Ligand 3PE L 703



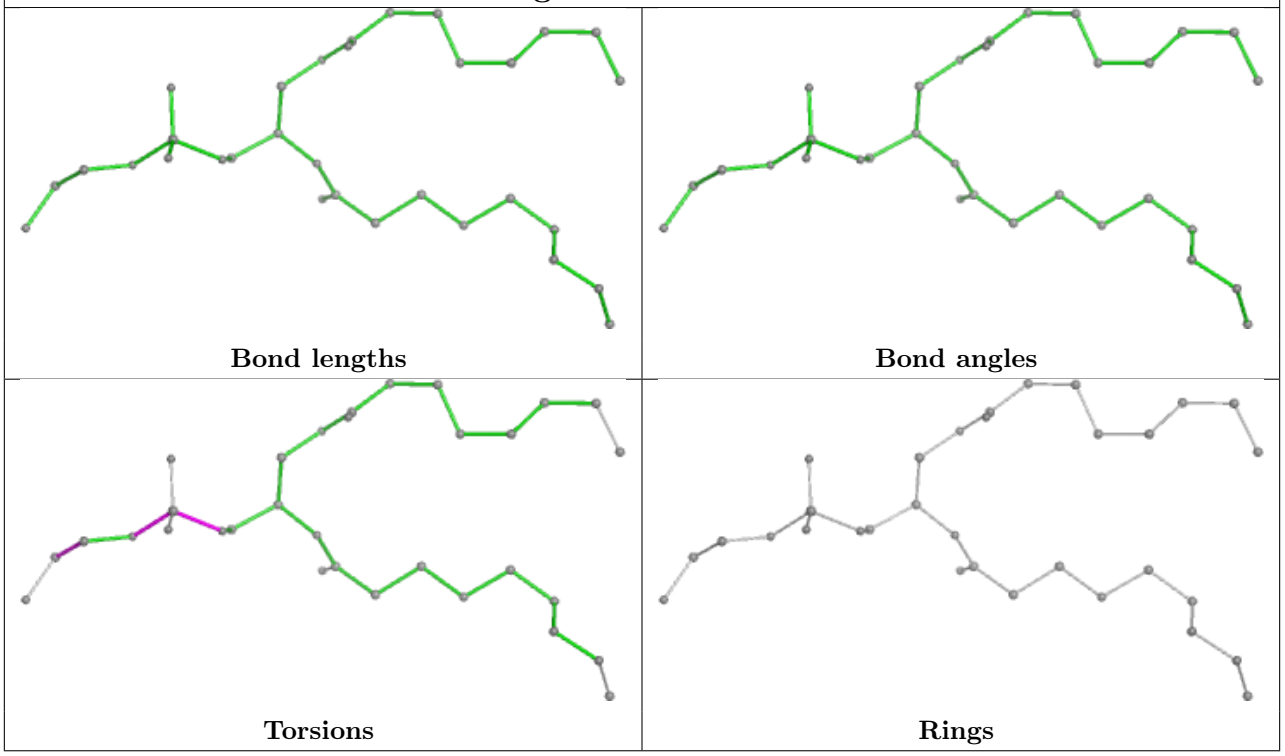
Ligand 3PE m 202



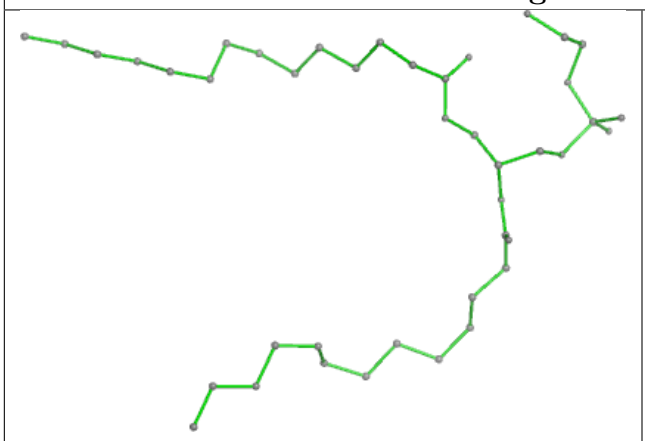
Ligand ZMP W 201



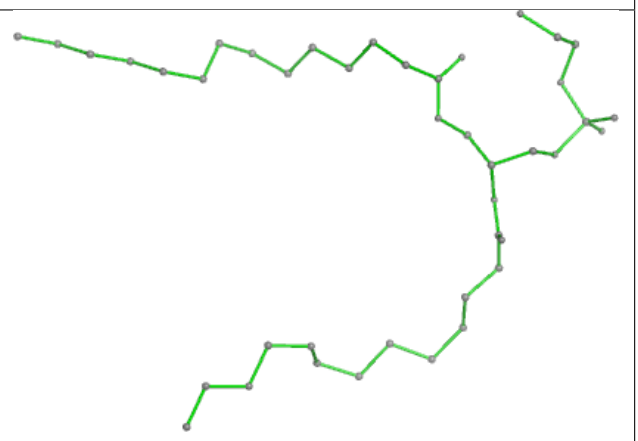
Ligand 3PE 6 202



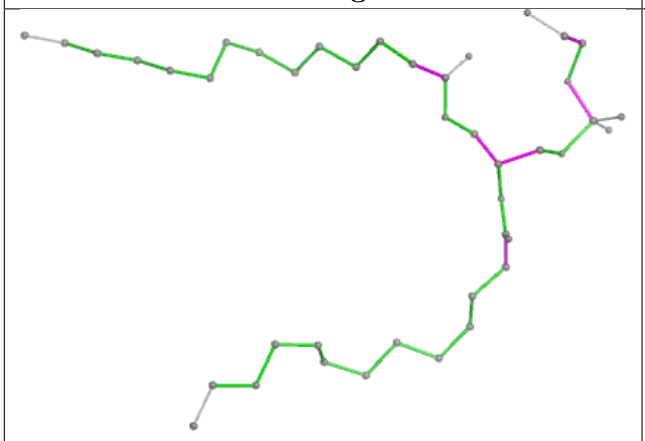
Ligand 3PE Y 202



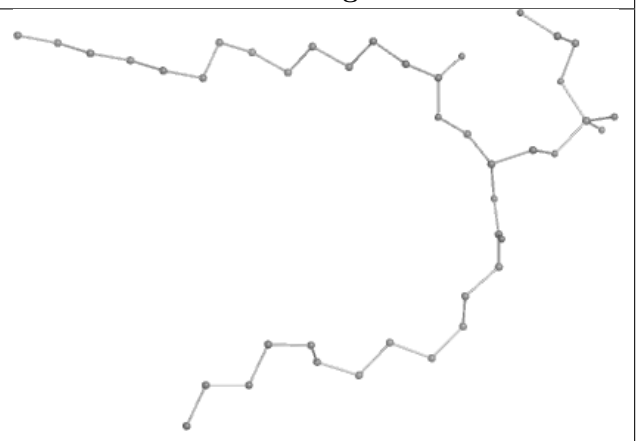
Bond lengths



Bond angles

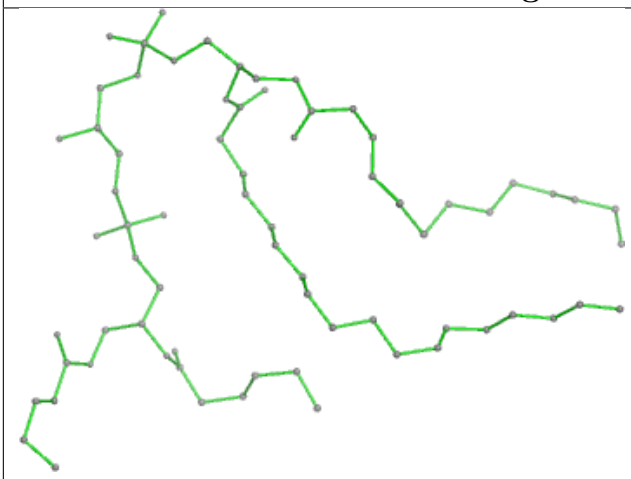


Torsions

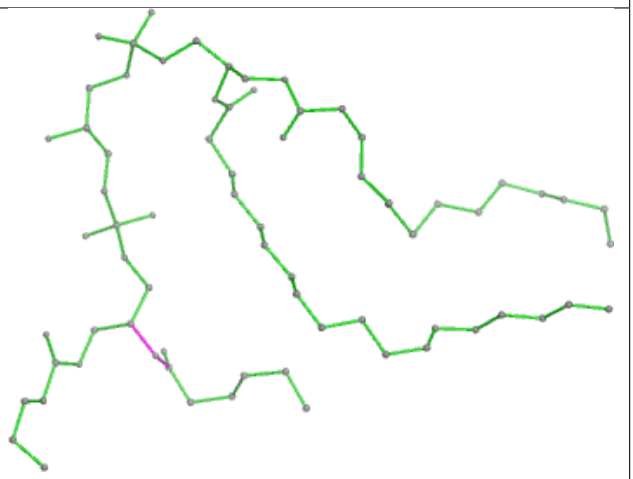


Rings

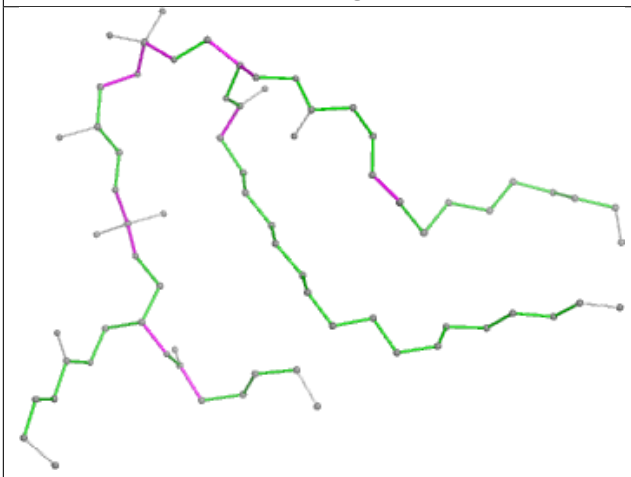
Ligand CDL m 201



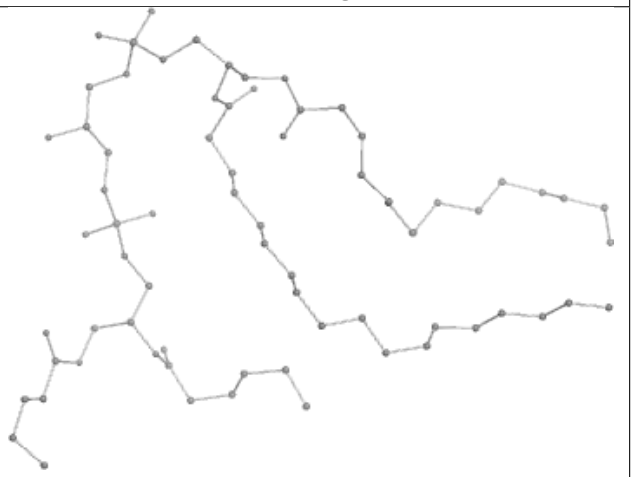
Bond lengths



Bond angles

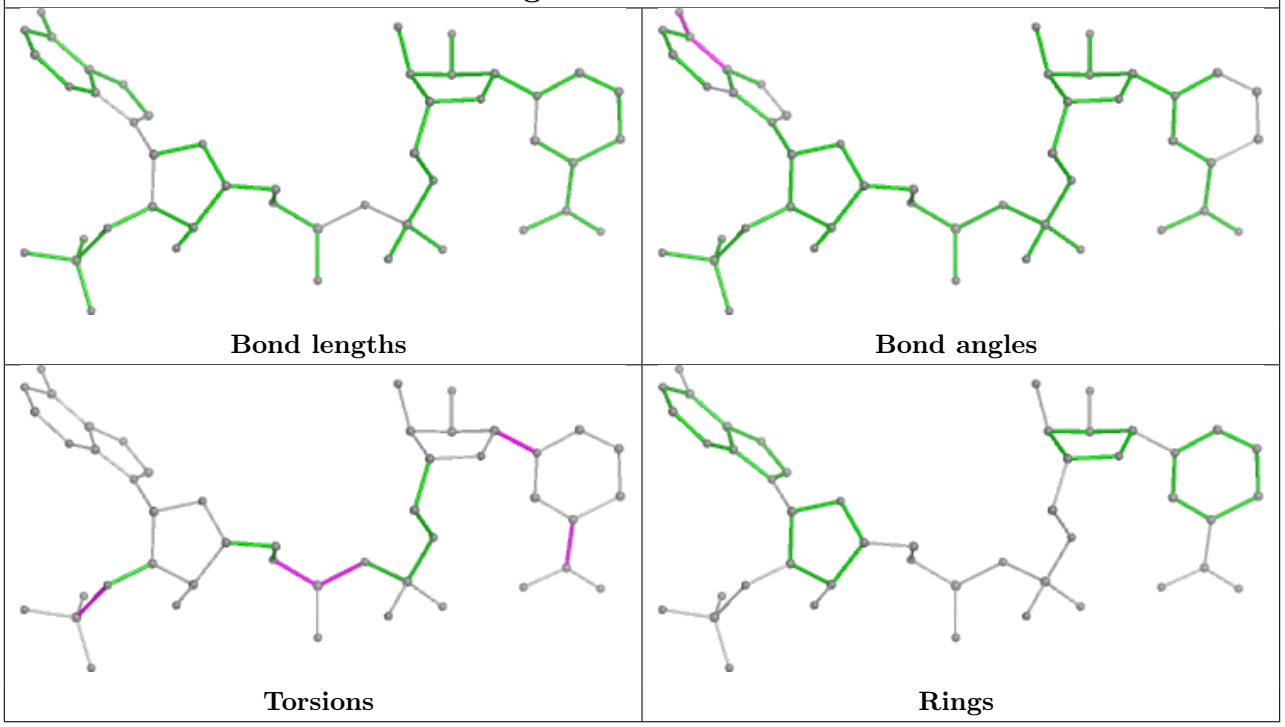


Torsions



Rings

Ligand NDP P 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

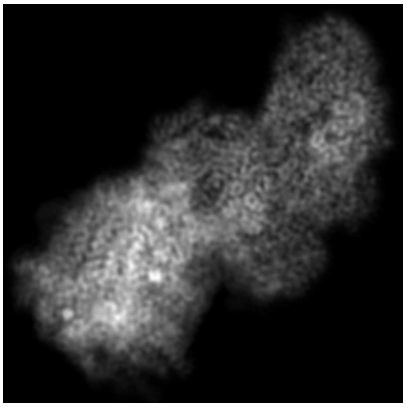
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19146. These allow visual inspection of the internal detail of the map and identification of artifacts.

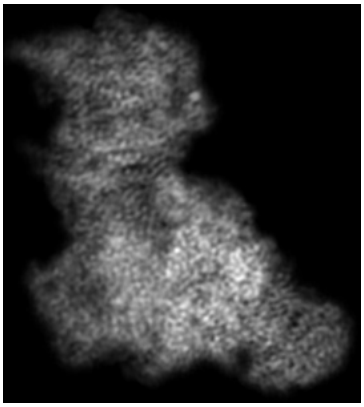
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

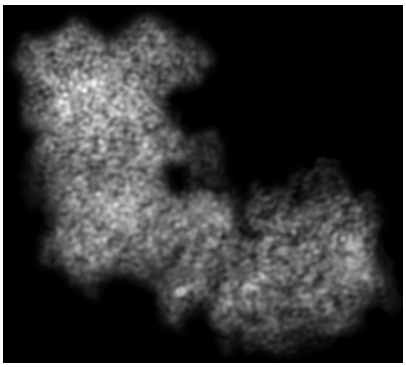
6.1.1 Primary map



X



Y

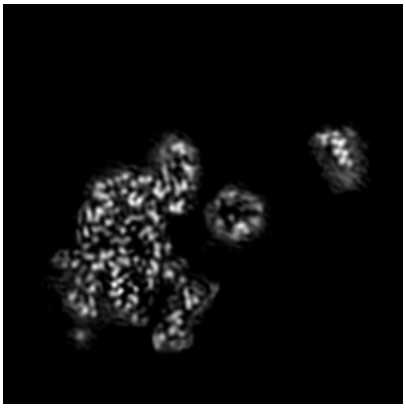


Z

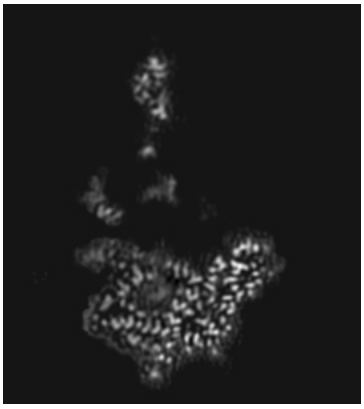
The images above show the map projected in three orthogonal directions.

6.2 Central slices

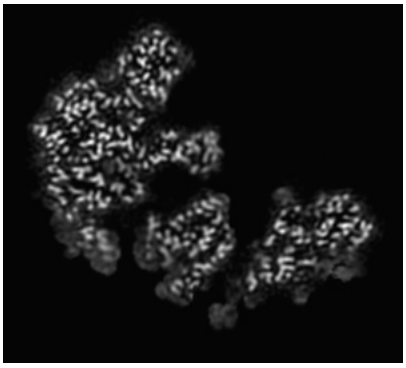
6.2.1 Primary map



X Index: 109



Y Index: 98

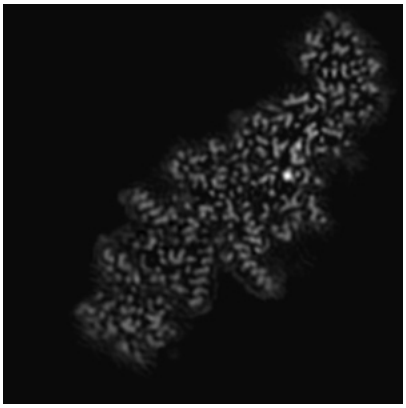


Z Index: 98

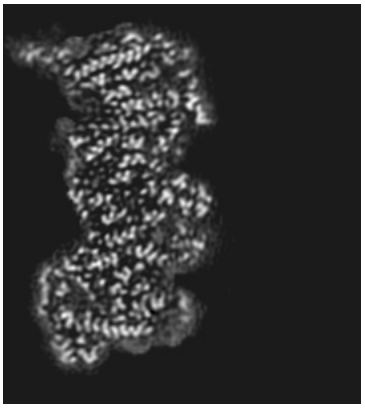
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

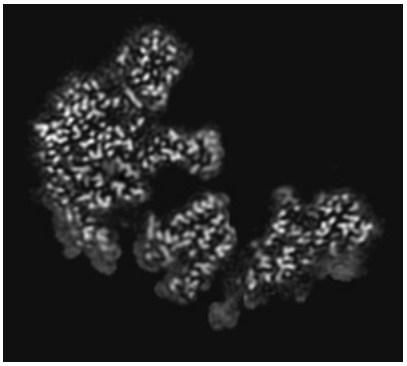
6.3.1 Primary map



X Index: 45



Y Index: 63

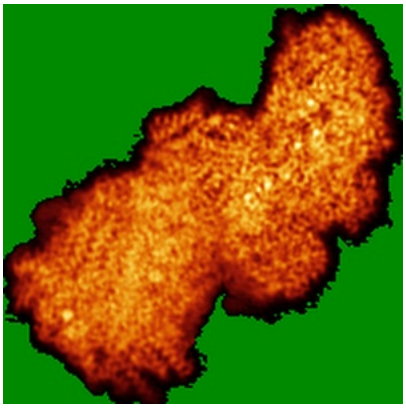


Z Index: 97

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

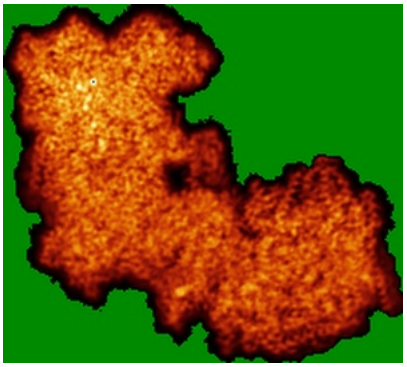
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X

Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

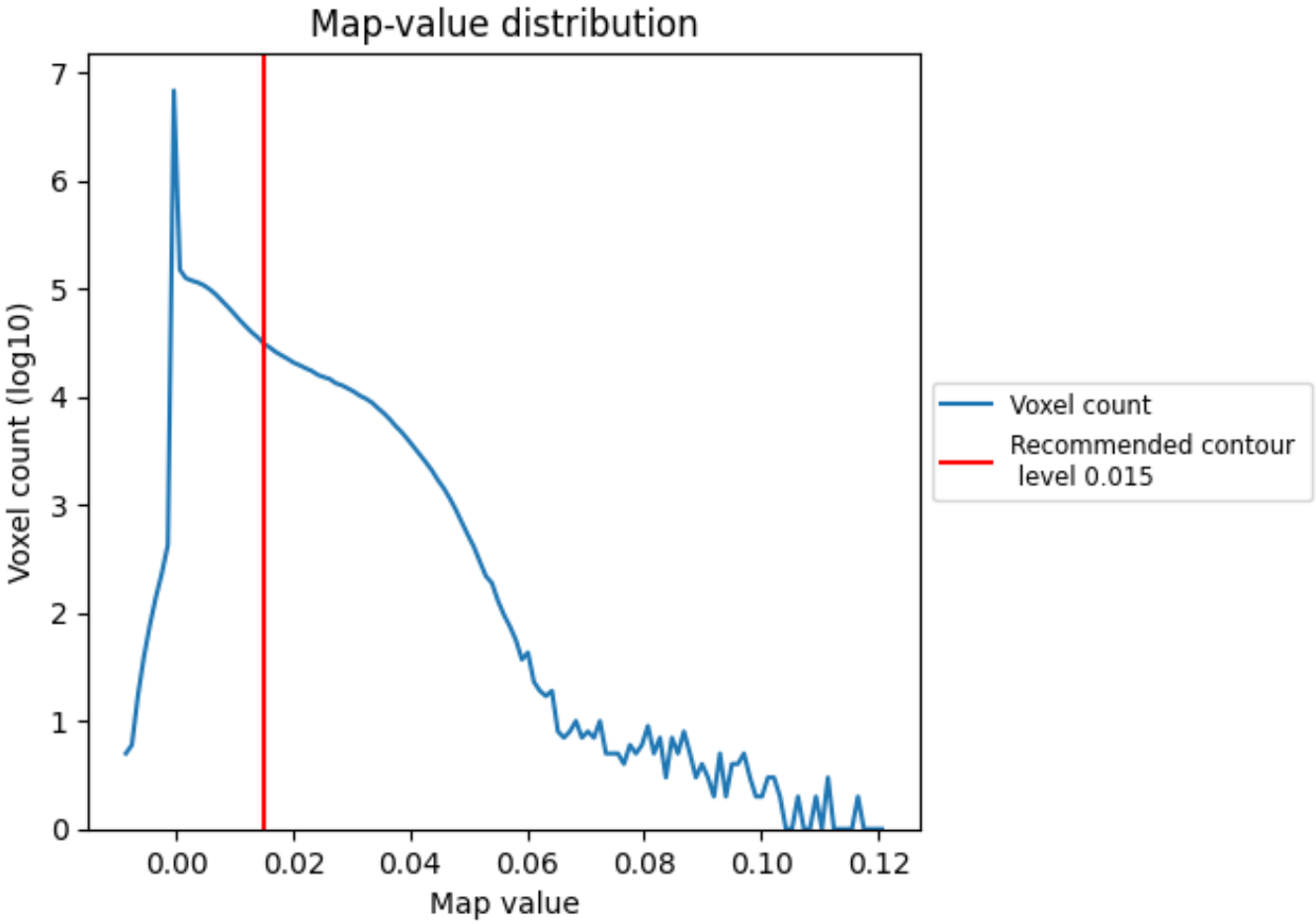
6.6 Mask visualisation (i)

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

7 Map analysis

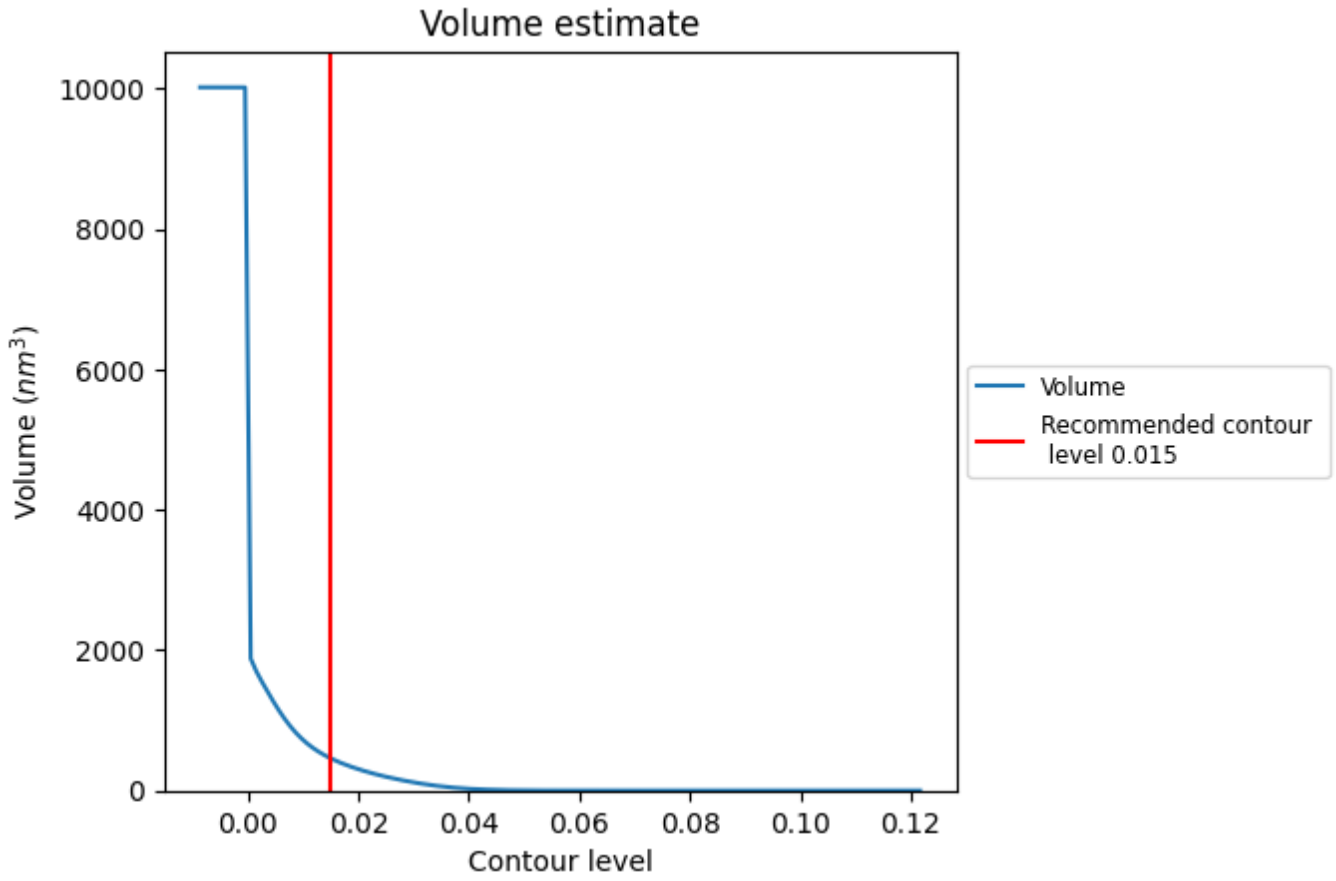
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 460 nm^3; this corresponds to an approximate mass of 416 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.

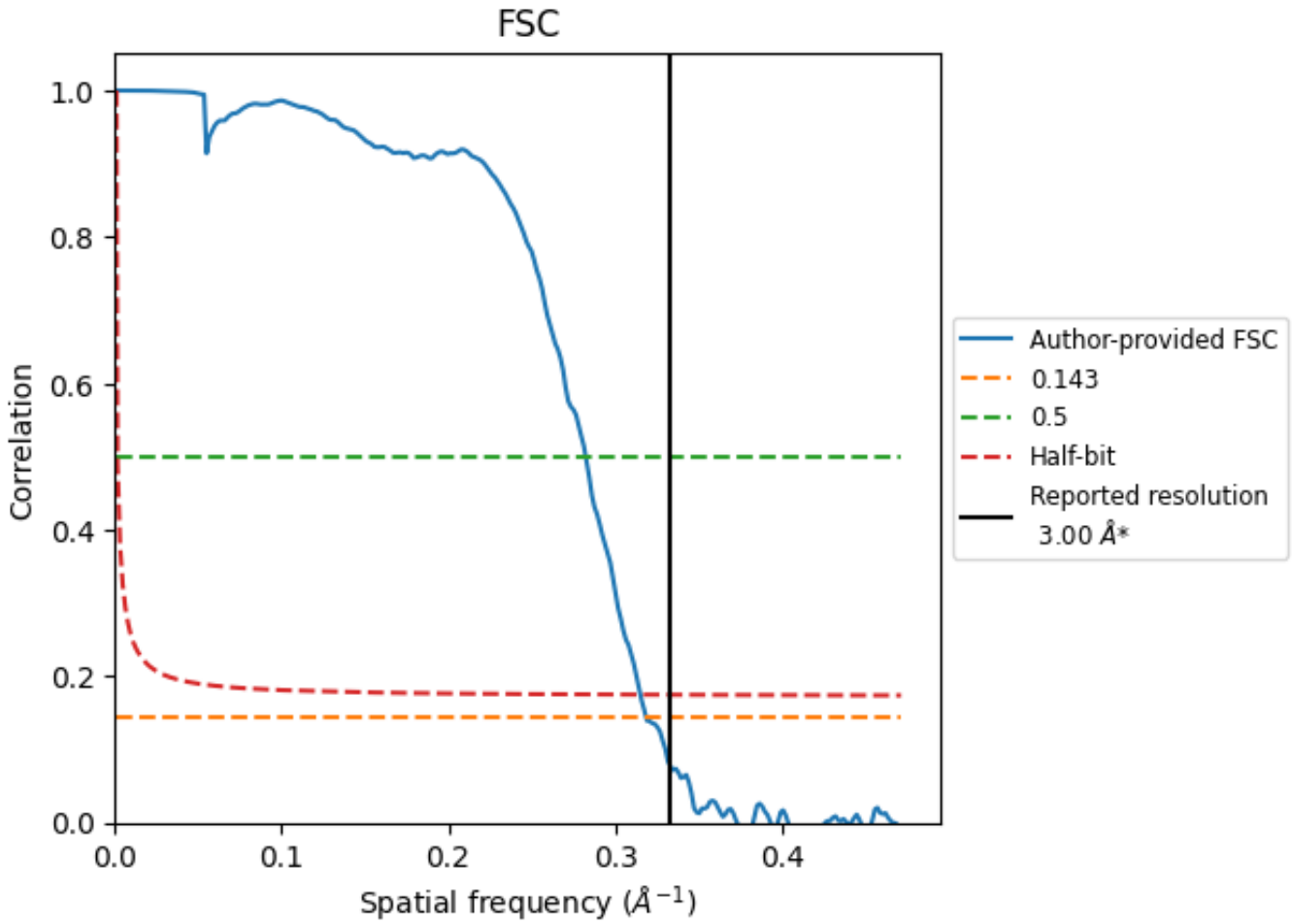
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

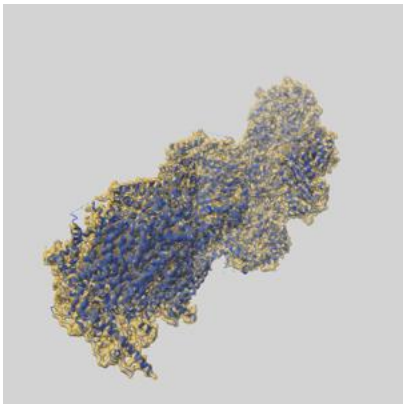
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.14	3.54	3.17
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

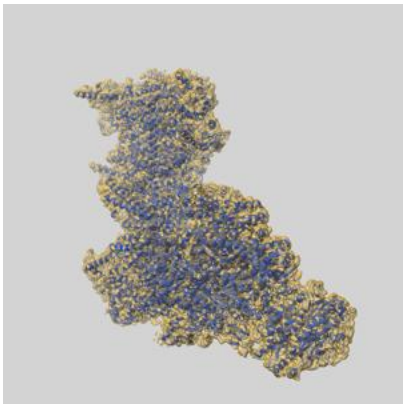
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19146 and PDB model 8RGQ. Per-residue inclusion information can be found in section 3 on page 19.

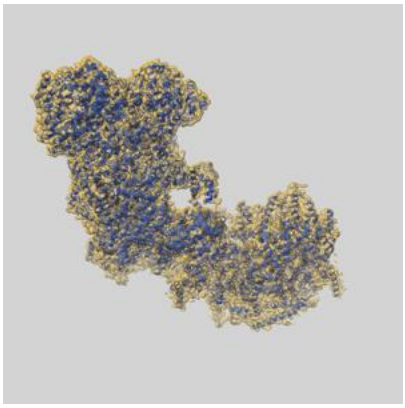
9.1 Map-model overlay



X



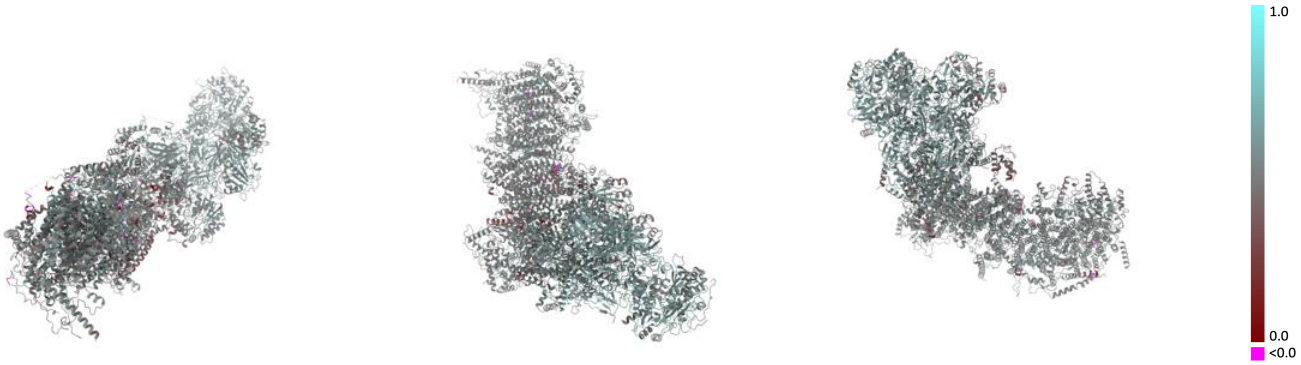
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

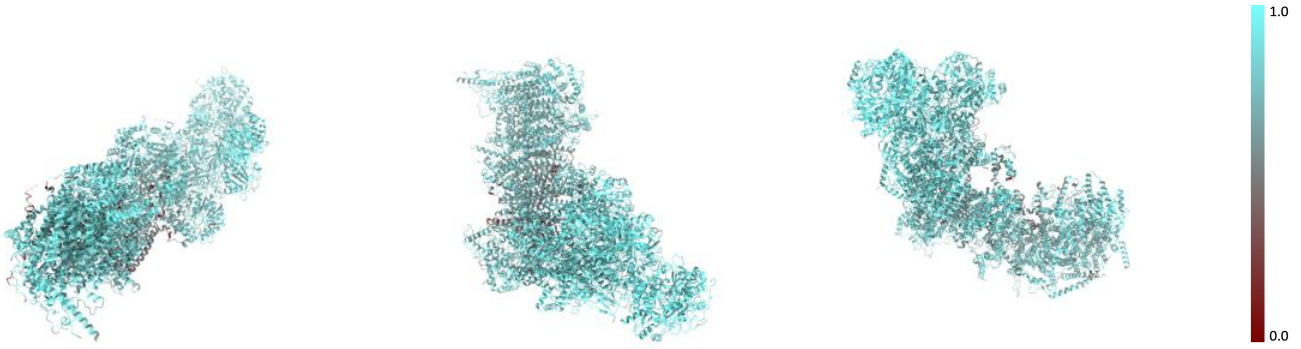
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

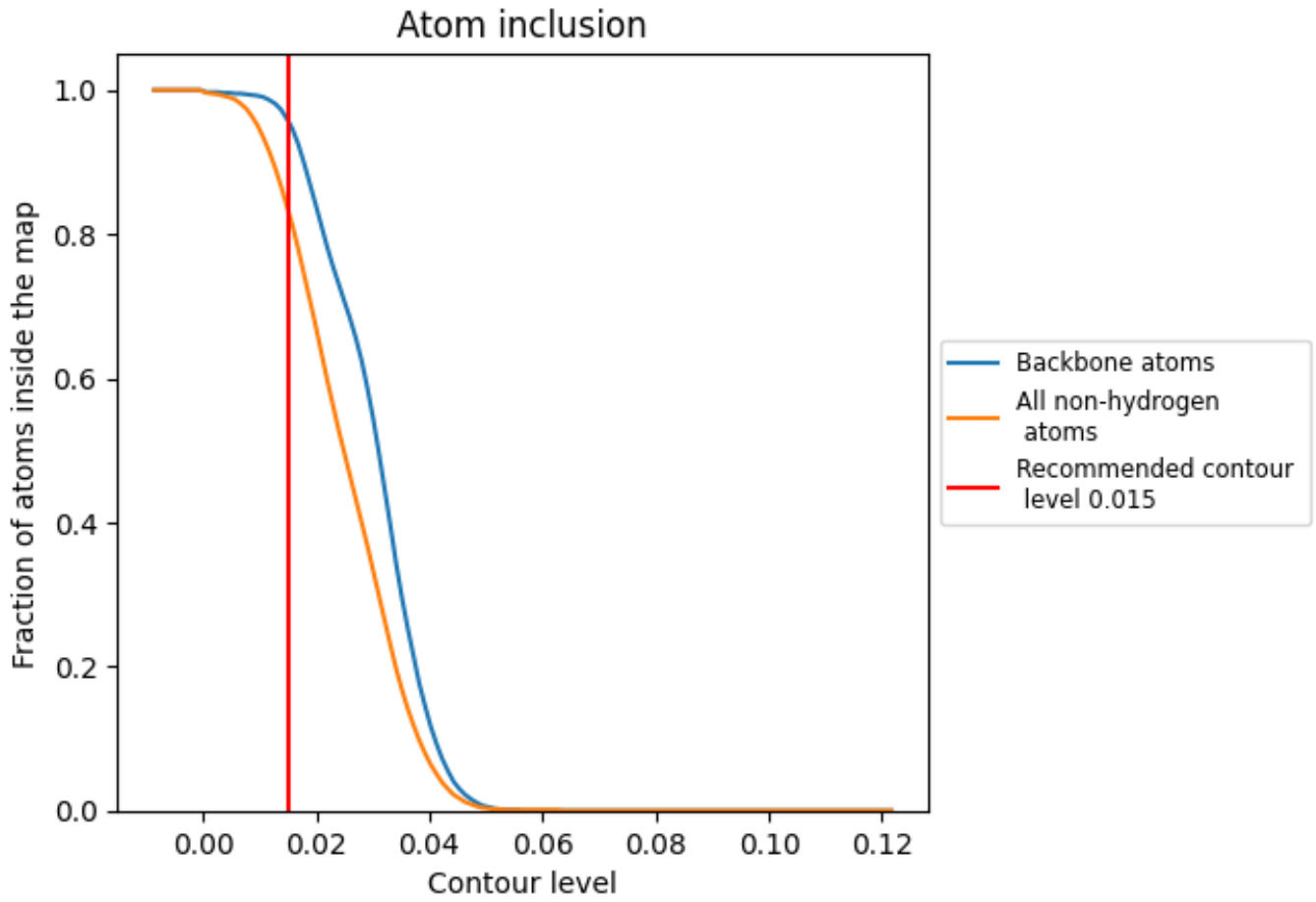
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5150
1	0.9300	0.5540
2	0.9220	0.5480
3	0.9120	0.5550
6	0.8500	0.5210
7	0.9190	0.5580
9	0.8890	0.5510
A	0.7160	0.4950
C	0.9140	0.5670
D	0.8470	0.5240
H	0.7960	0.4970
J	0.6600	0.4530
K	0.7030	0.4900
L	0.7970	0.5080
M	0.7900	0.5170
N	0.7750	0.5120
O	0.8510	0.5030
P	0.8070	0.5000
Q	0.8800	0.5670
S	0.8790	0.4970
T	0.7180	0.3940
U	0.8400	0.5000
V	0.8740	0.5270
W	0.8870	0.5350
X	0.8630	0.5020
Y	0.7090	0.4690
Z	0.8650	0.5080
a	0.8450	0.5090
b	0.8310	0.4760
c	0.7930	0.4890
d	0.7680	0.5080
e	0.8120	0.5070
f	0.7700	0.4850
g	0.7820	0.4840
h	0.8430	0.5010

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Chain	Atom inclusion	Q-score
i	0.7480	0.4570
j	0.8360	0.4780
k	0.8410	0.4970
l	0.8500	0.5170
m	0.7190	0.4480
n	0.8550	0.5090
o	0.8330	0.4820
p	0.8710	0.5110
q	0.9170	0.5540
r	0.8510	0.5470
s	0.8920	0.5290