wwPDB EM Validation Summary Report (i)

Jun 22, 2023 – 10:36 AM JST

PDB ID	:	7W1O
EMDB ID	:	EMD-32253
Title	:	Deactive state CI from Q10-NADH dataset, Subclass 1
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-19
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

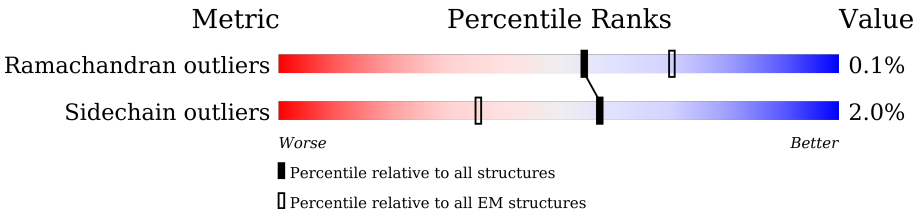
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	14% 100%
2	B	176	98%
3	C	156	98%
4	E	115	13% 99%
5	F	86	24% 97%
6	G	88	57% 98%
6	X	88	25% 95% 5%
7	H	112	16% 97%
8	I	112	17% 84% 13%

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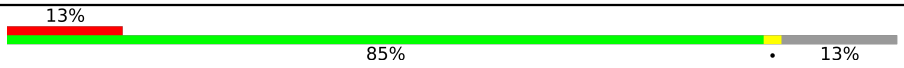
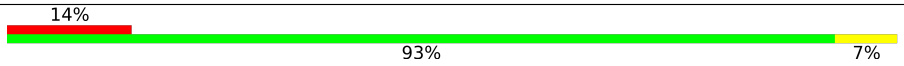
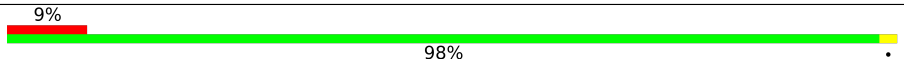
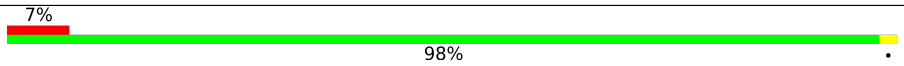
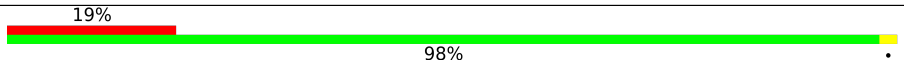
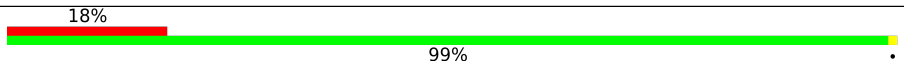
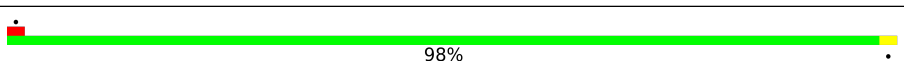
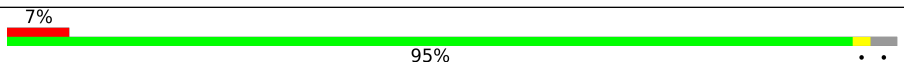
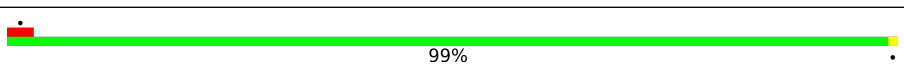
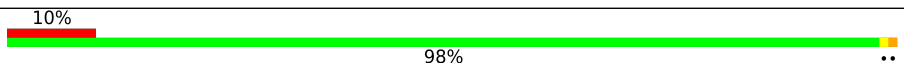
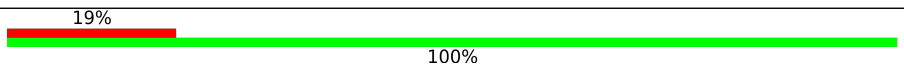
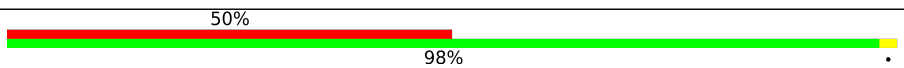
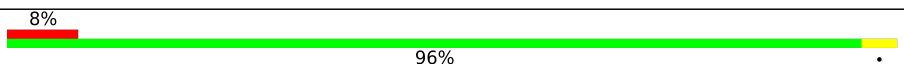
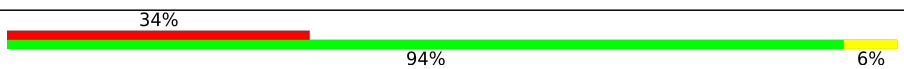
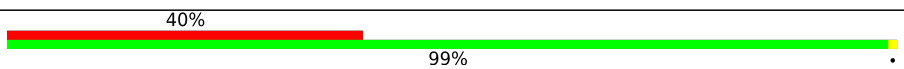
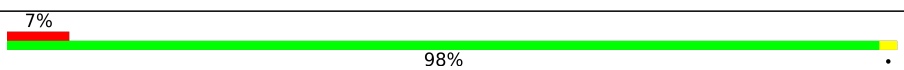
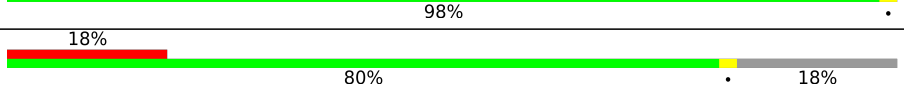
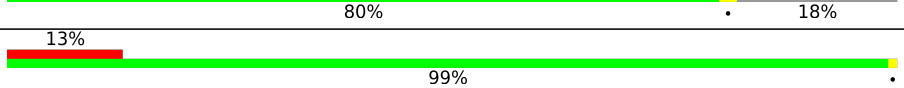
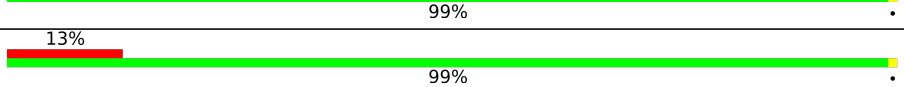
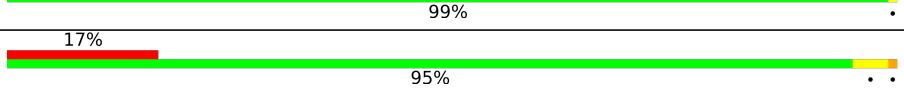
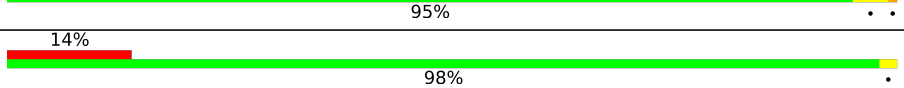
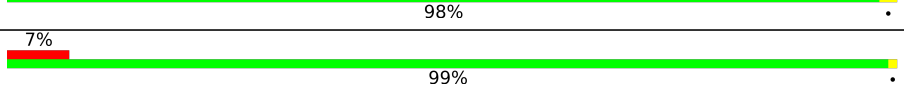
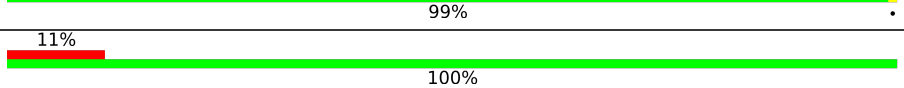
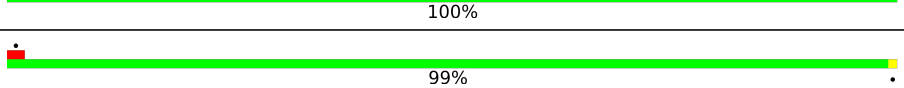
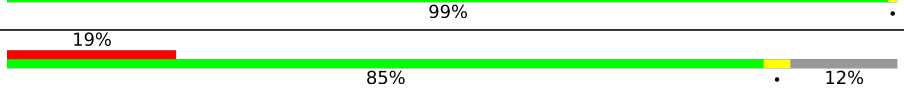
Mol	Chain	Length	Quality of chain
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	

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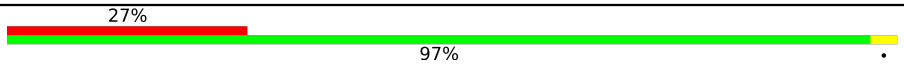
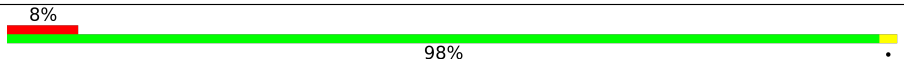
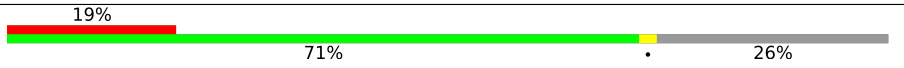
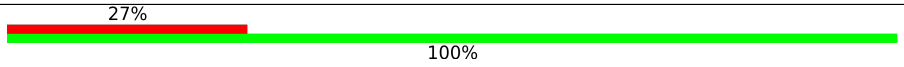
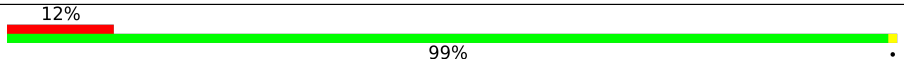
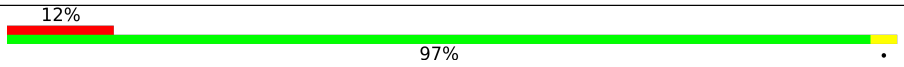
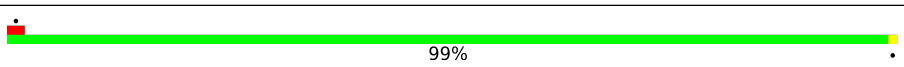
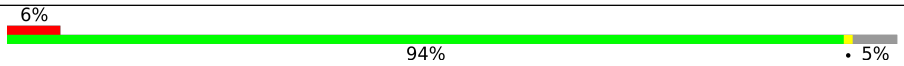
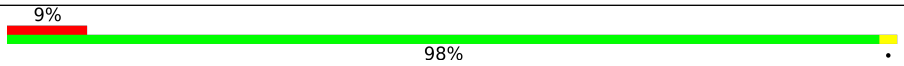
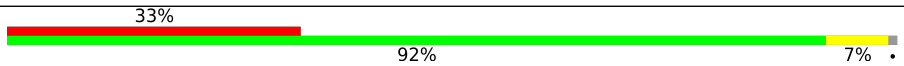
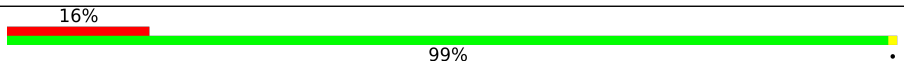
Mol	Chain	Length	Quality of chain
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3315	2094	590	611	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1405	881	243	268	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1239	790	224	211	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			959	614	176	164	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			697	448	103	141	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2337	1502	419	408	8		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1668	1064	280	314	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1731	1121	298	310	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3362	2155	578	605	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			560	359	104	92	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	1		

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1311	851	213	239	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1441	903	260	270	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			889	568	145	172	4		

- Molecule 29 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2707	1781	419	461	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4784	3173	741	819	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1045	679	182	184		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3628	2411	571	608	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1378	878	244	246	10		

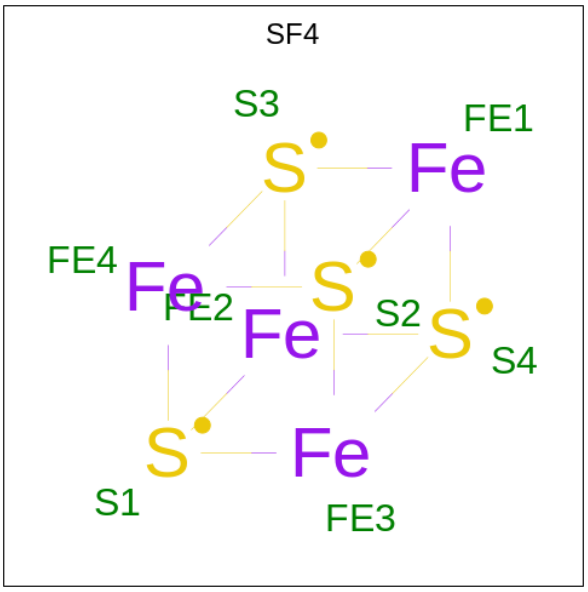
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1012	633	188	182	9		

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

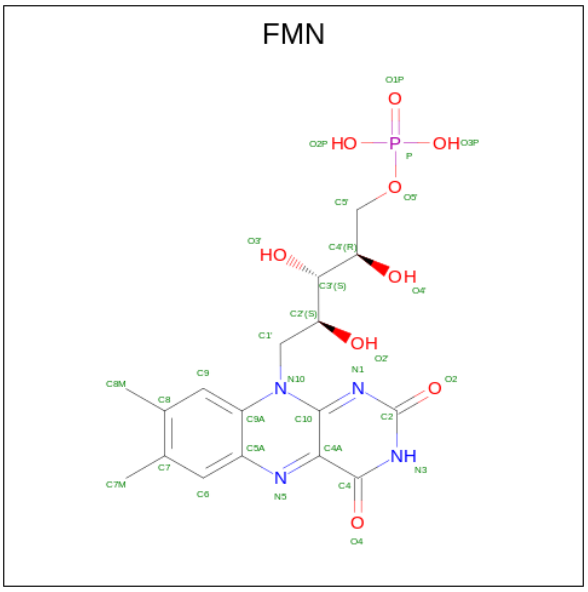
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2583	1646	437	491	9		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



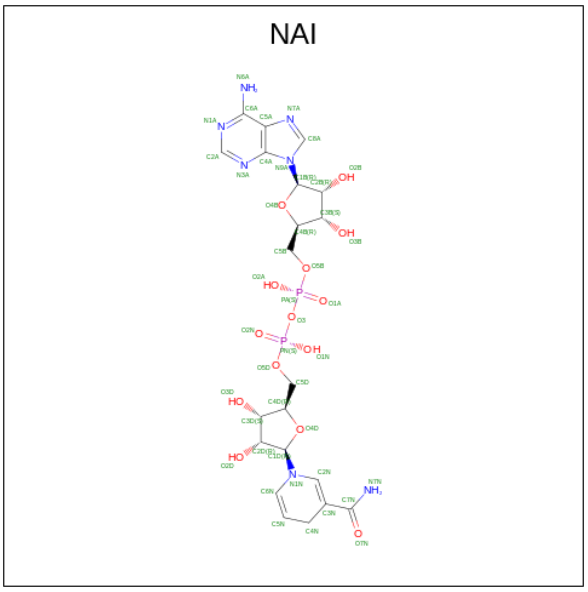
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



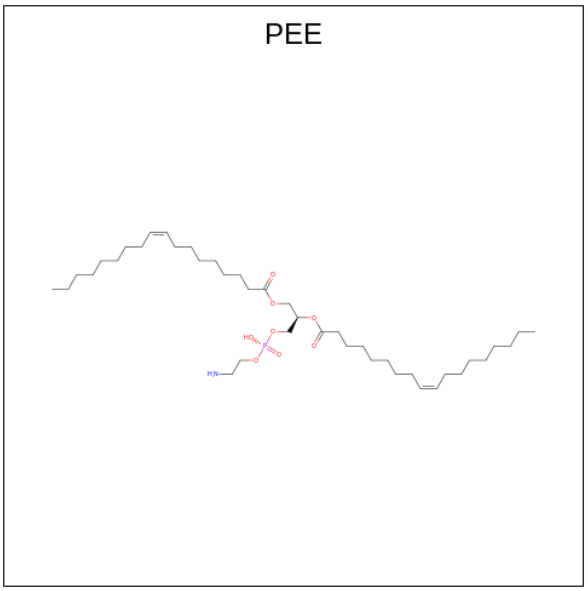
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



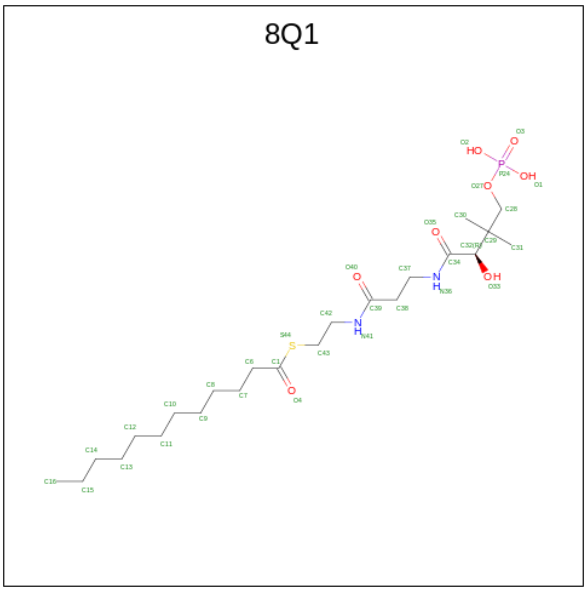
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



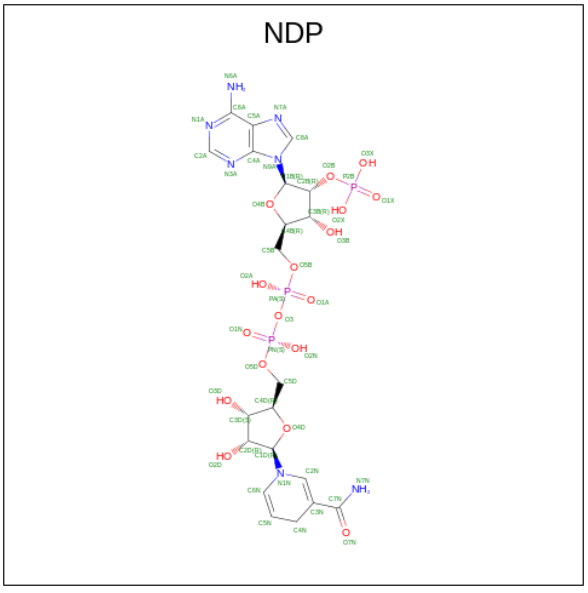
Mol	Chain	Residues	Atoms	AltConf
48	B	1	Total C N O P 51 41 1 8 1	0
48	Q	1	Total N 1 1	0
48	V	1	Total C N O P 40 30 1 8 1	0
48	j	1	Total N 1 1	0
48	j	1	Total C N O P 51 41 1 8 1	0
48	l	1	Total C N O P 46 36 1 8 1	0
48	l	1	Total C N O P 46 36 1 8 1	0
48	m	1	Total C N O P 41 31 1 8 1	0
48	r	1	Total C N O P 51 41 1 8 1	0

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



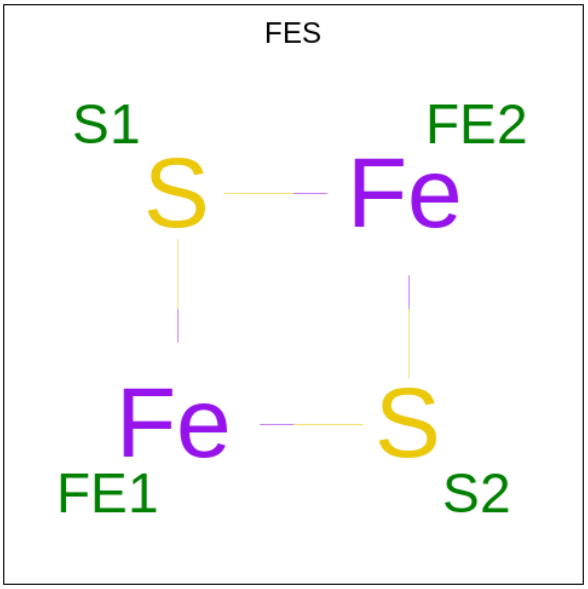
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

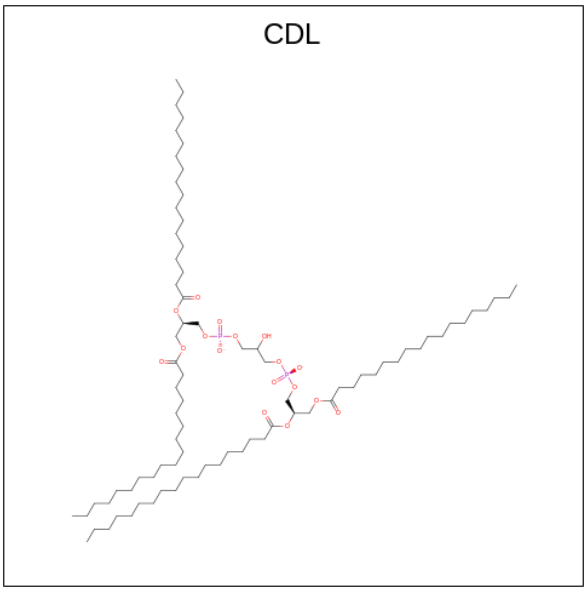
- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
52	M	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

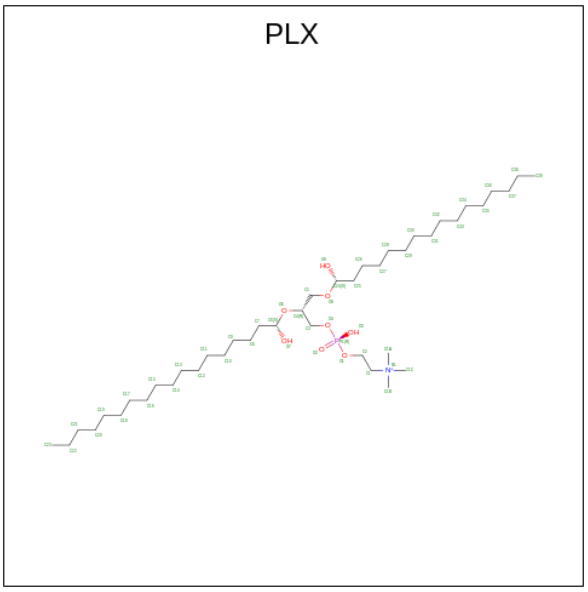
Mol	Chain	Residues	Atoms		AltConf
53	T	1	Total	Zn	0
			1	1	

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



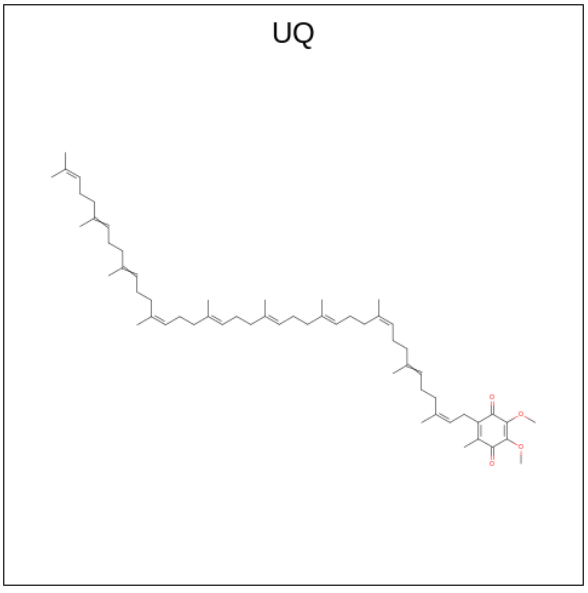
Mol	Chain	Residues	Atoms				AltConf
54	V	1	Total	C	O	P	0
			94	75	17	2	
54	V	1	Total	C	O	P	0
			68	49	17	2	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	g	1	Total	C	O	P	0
			97	78	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	l	1	Total	C	O	P	0
			99	80	17	2	
54	l	1	Total	C	O	P	0
			100	81	17	2	
54	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 55 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



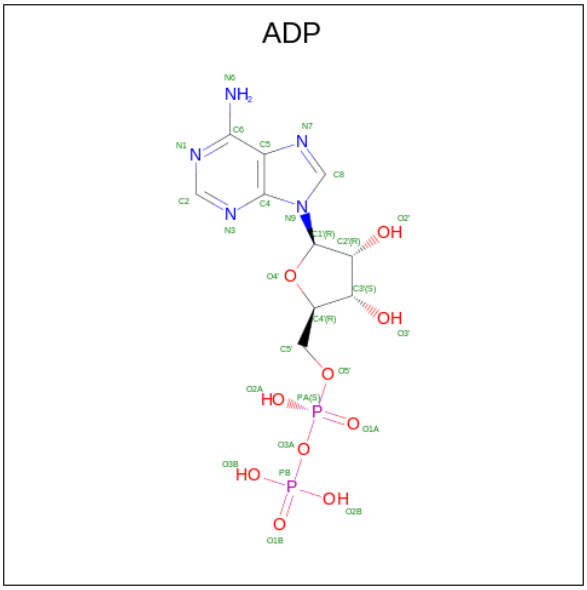
Mol	Chain	Residues	Atoms					AltConf
55	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
55	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
55	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
55	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			28	24	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

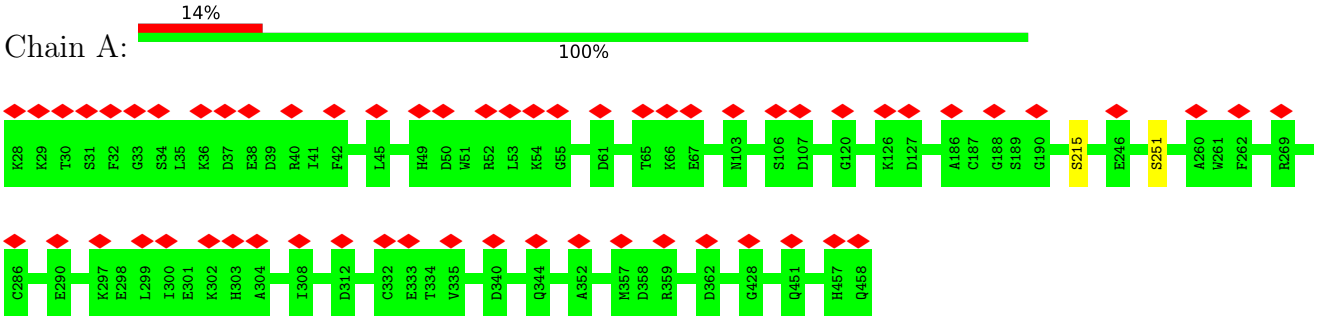


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

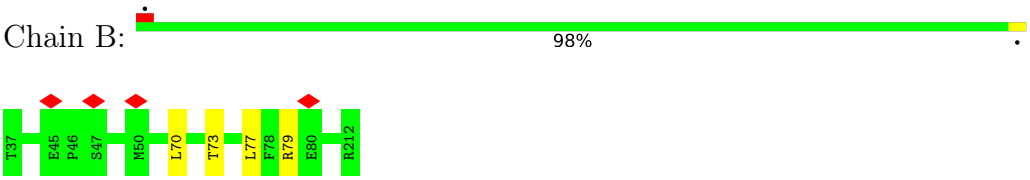
3 Residue-property plots (i)

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.

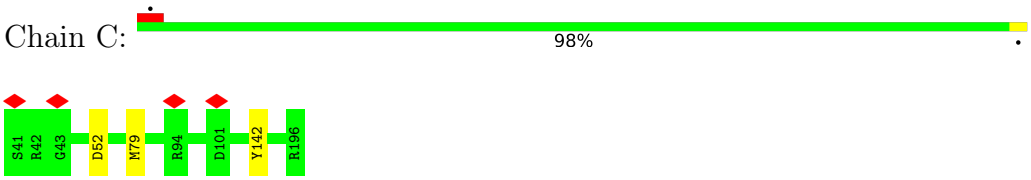
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



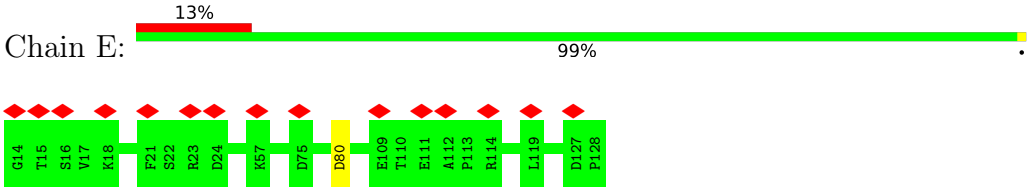
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



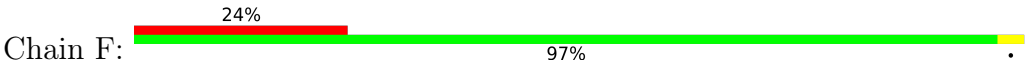
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

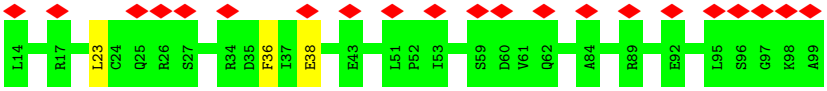


• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

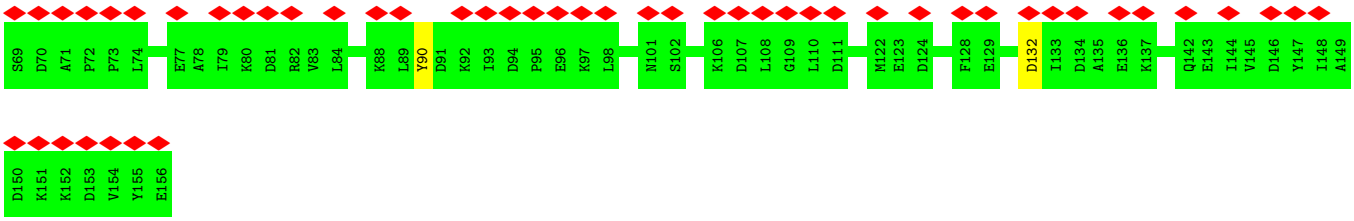


• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

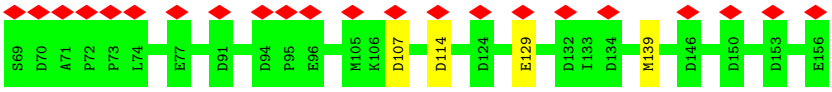




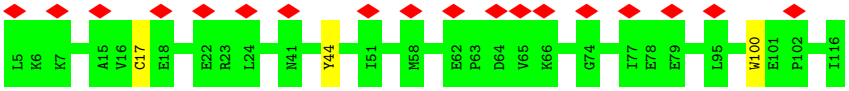
• Molecule 6: Acyl carrier protein



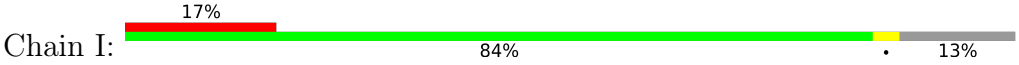
• Molecule 6: Acyl carrier protein

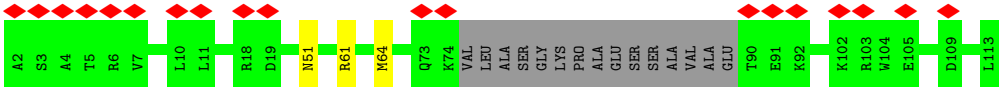


• Molecule 7: Complex I subunit B13

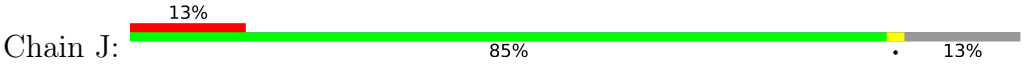


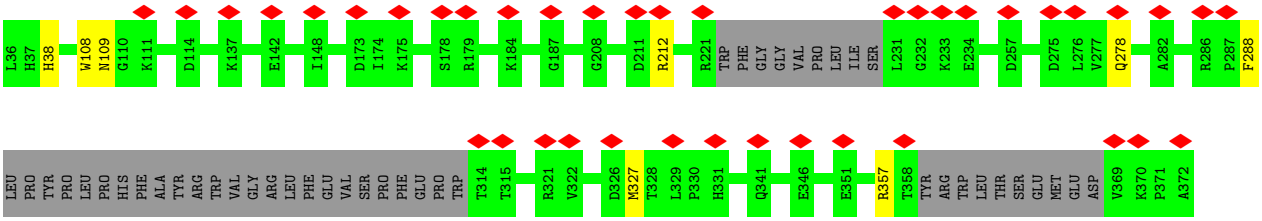
• Molecule 8: Complex I-B14.5a





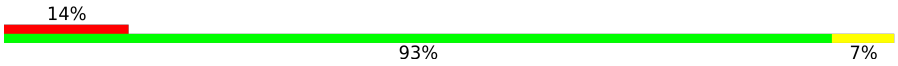
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

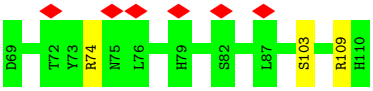




• Molecule 10: Complex I-9kD

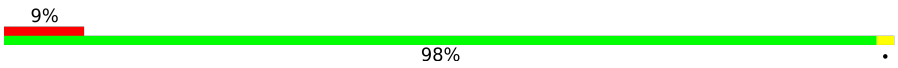
Chain K:

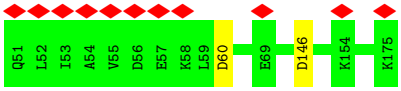




• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

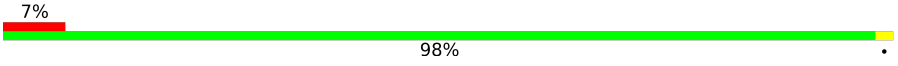
Chain L:

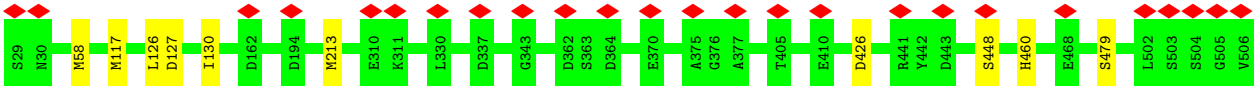


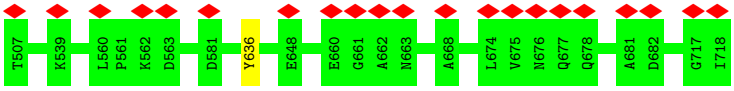


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:

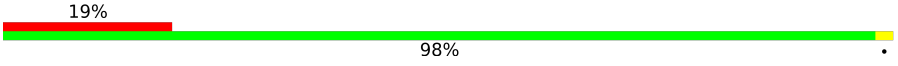


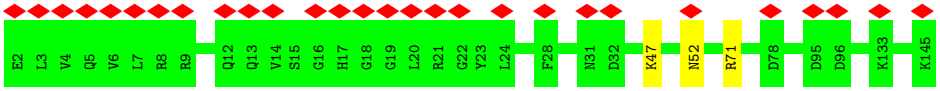




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

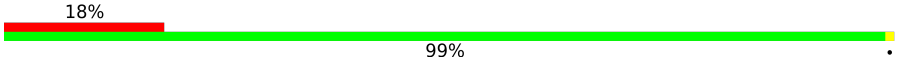
Chain N:

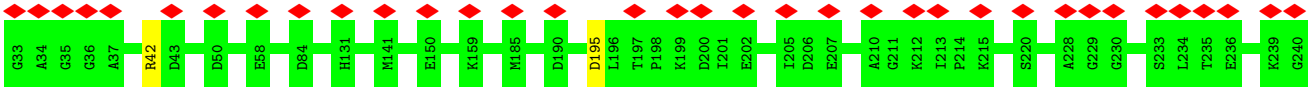


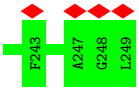


• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:

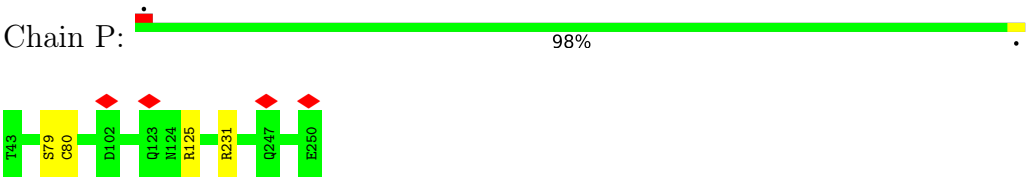






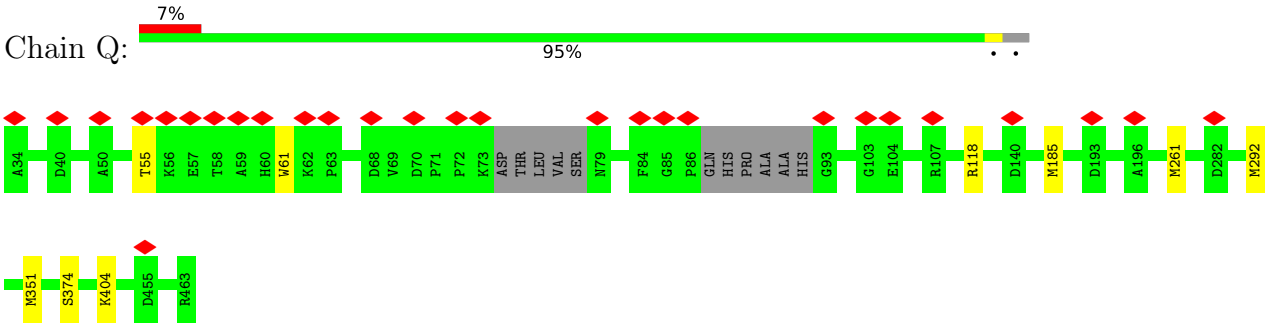
• Molecule 15: Complex I-30kD

Chain P:



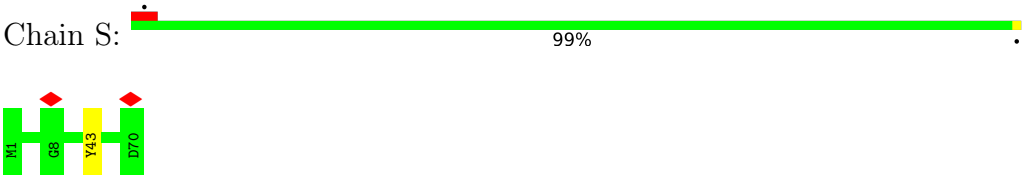
• Molecule 16: Complex I-49kD

Chain Q:



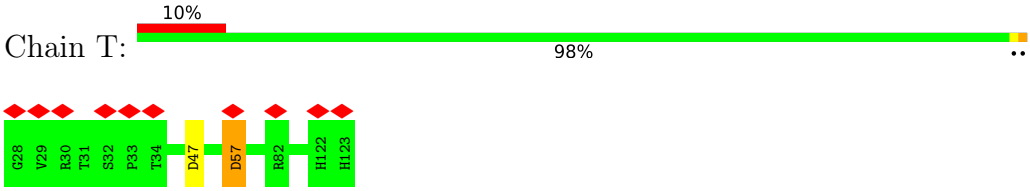
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:



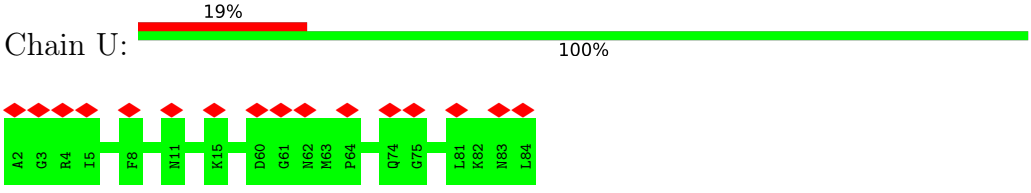
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:



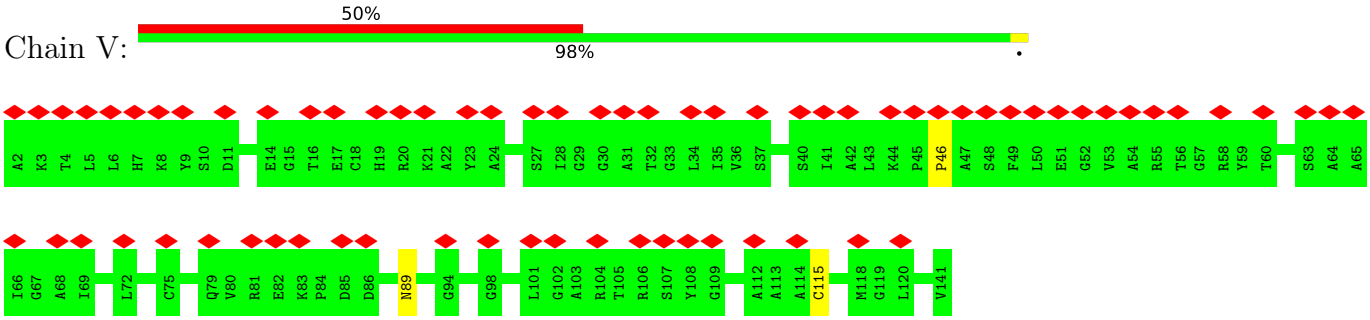
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:



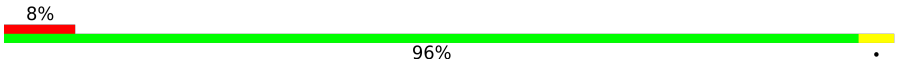
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

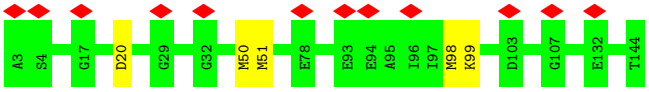
Chain V:



• Molecule 21: Complex I-B16.6

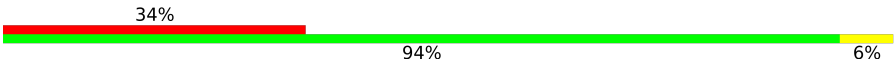
Chain W:

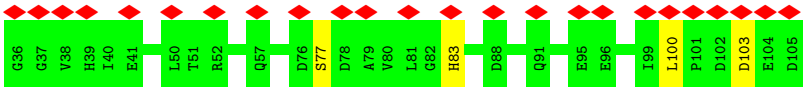




• Molecule 22: Complex I-AGGG

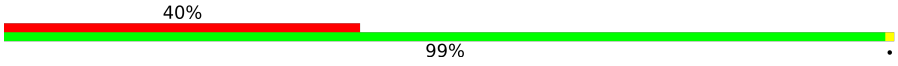
Chain Y:

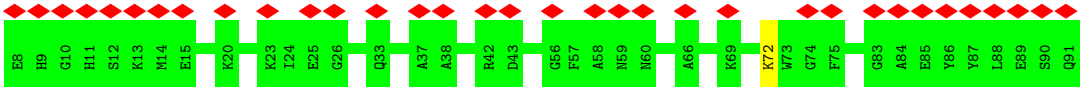




• Molecule 23: Complex I-B12

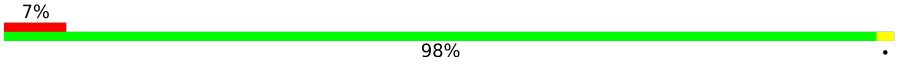
Chain Z:

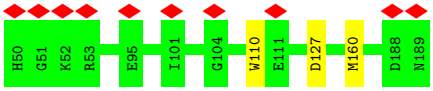




• Molecule 24: Complex I-SGDH

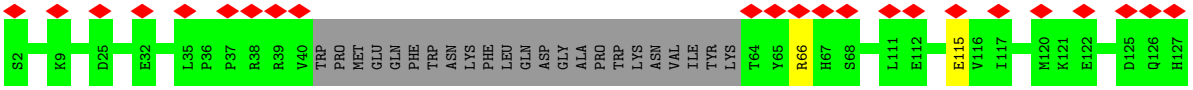
Chain a:





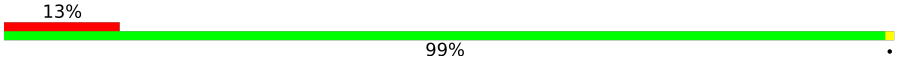
• Molecule 25: Complex I-B17

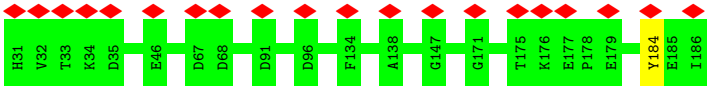
Chain b:



• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

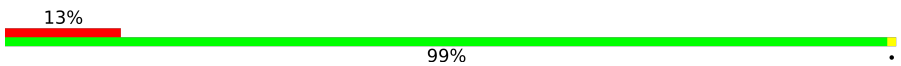
Chain c:

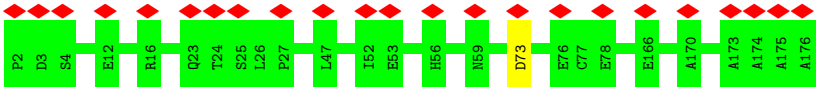




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

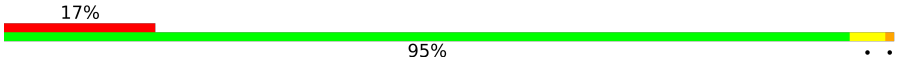
Chain d:

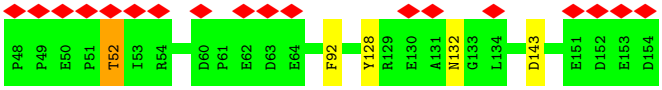




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

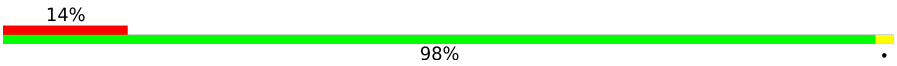
Chain e:

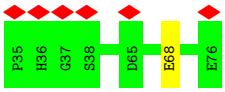




• Molecule 29: Complex I-KFYI

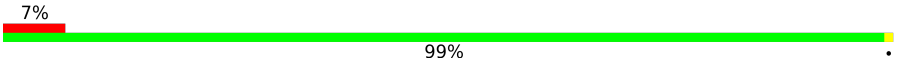
Chain f:

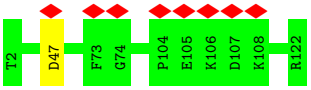




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

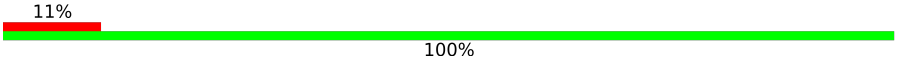
Chain g:

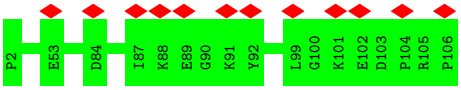




• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

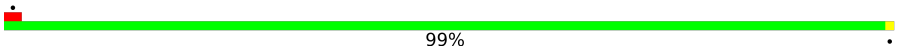
Chain h:

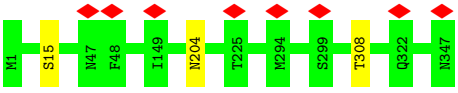




• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

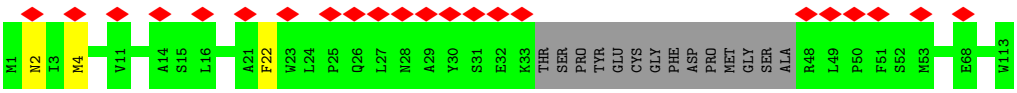
Chain i:





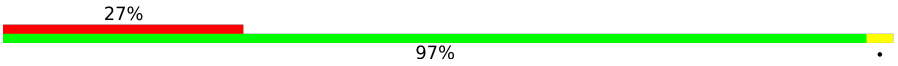
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

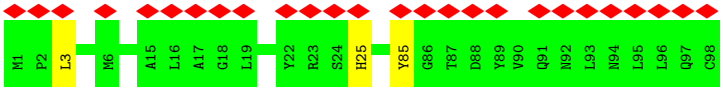
Chain j:



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

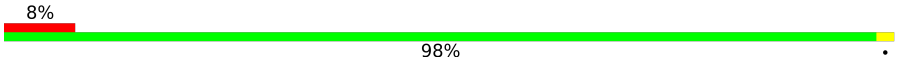
Chain k:

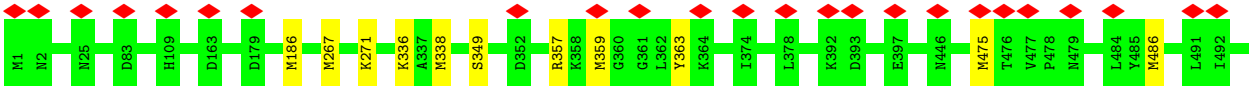


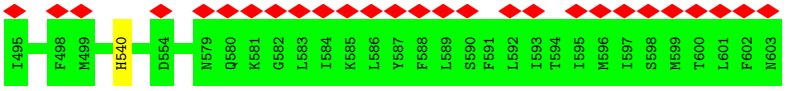


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:

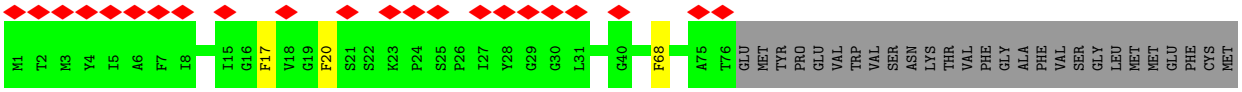


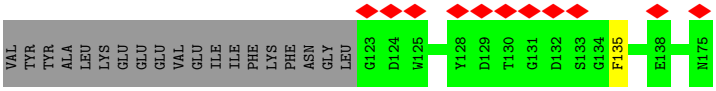




• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

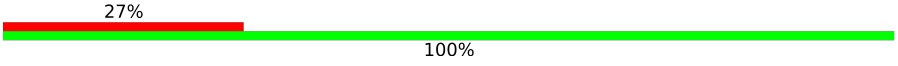
Chain m:

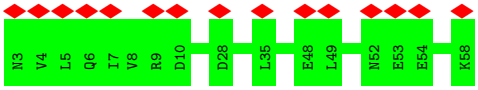




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

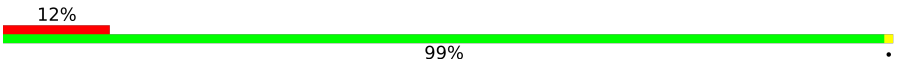
Chain n:

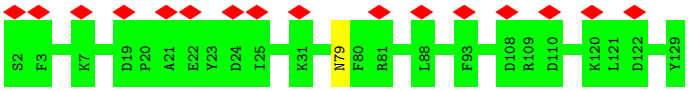




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

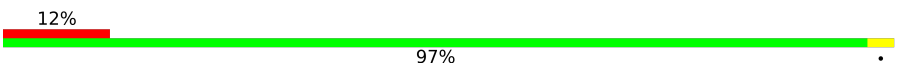
Chain o:

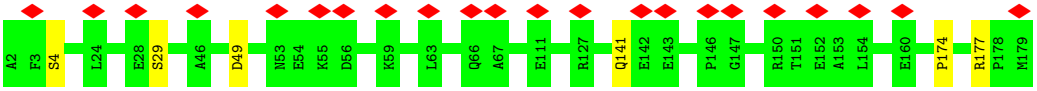




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

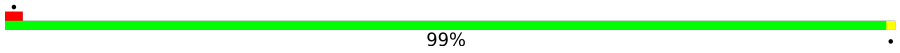
Chain p:

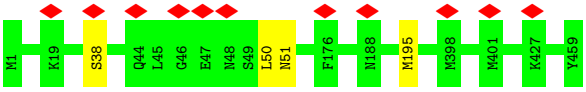




• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

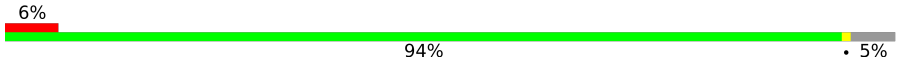
Chain r:

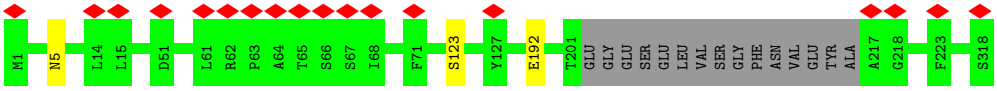




• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

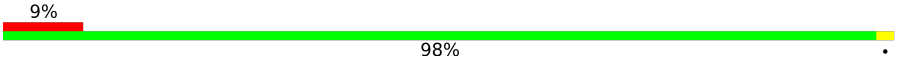
Chain s:

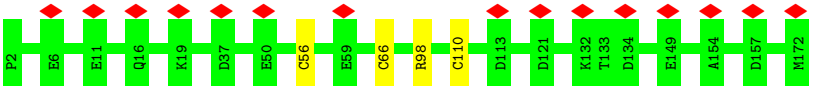




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

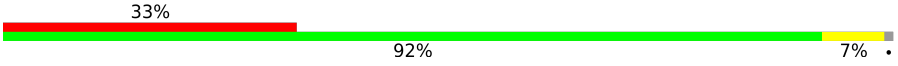
Chain u:

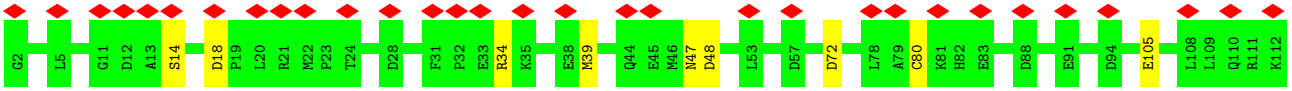


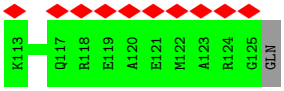


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:

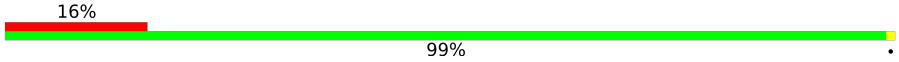


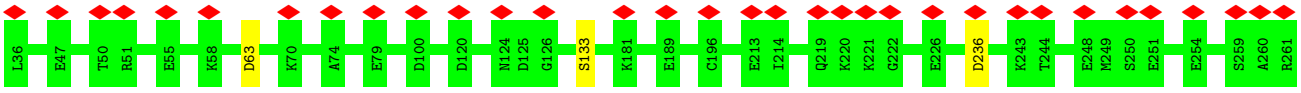


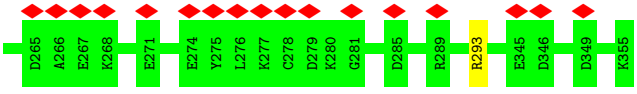


• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24886	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.239	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0267	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, ZN, UQ, MG, ADP, PEE, FMN, PLX, SF4, NAI, CDL, FES, NDP, 8Q1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/3390	0.52	0/4580
2	B	0.27	0/1435	0.53	0/1941
3	C	0.28	0/1270	0.53	0/1719
4	E	0.26	0/983	0.54	0/1325
5	F	0.30	0/702	0.61	0/945
6	G	0.28	0/705	0.53	0/956
6	X	0.30	0/709	0.52	0/960
7	H	0.30	0/929	0.53	0/1258
8	I	0.27	0/798	0.55	0/1079
9	J	0.26	0/2388	0.53	0/3225
10	K	0.25	0/365	0.52	0/493
11	L	0.27	0/1039	0.55	0/1403
12	M	0.26	0/5384	0.52	0/7295
13	N	0.26	0/1245	0.53	0/1694
14	O	0.27	0/1708	0.51	0/2324
15	P	0.28	0/1782	0.54	0/2427
16	Q	0.28	0/3436	0.52	0/4653
17	S	0.27	0/575	0.53	0/774
18	T	0.26	0/755	0.55	1/1018 (0.1%)
19	U	0.28	0/664	0.51	0/912
20	V	0.28	0/1042	0.50	0/1411
21	W	0.28	0/1198	0.52	0/1617
22	Y	0.30	0/626	0.59	0/857
23	Z	0.28	0/695	0.51	0/939
24	a	0.28	0/1199	0.52	0/1623
25	b	0.30	0/906	0.57	0/1232
26	c	0.29	0/1367	0.53	0/1870
27	d	0.27	0/1473	0.55	0/1989
28	e	0.29	0/915	0.55	0/1245
29	f	0.26	0/350	0.43	0/473
30	g	0.29	0/1031	0.53	1/1394 (0.1%)
31	h	0.27	0/889	0.52	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	i	0.27	0/2770	0.49	0/3764
33	j	0.30	0/819	0.55	0/1117
34	k	0.27	0/759	0.52	1/1029 (0.1%)
35	l	0.28	0/4913	0.50	0/6682
36	m	0.29	0/973	0.48	0/1320
37	n	0.25	0/491	0.53	0/663
38	o	0.28	0/1074	0.55	0/1457
39	p	0.28	0/1590	0.55	0/2155
40	r	0.27	0/3720	0.50	0/5074
41	s	0.28	0/2464	0.49	0/3369
42	u	0.26	0/1416	0.50	0/1913
43	v	0.29	0/1036	0.56	0/1393
44	w	0.27	0/2643	0.50	0/3580
All	All	0.28	0/66621	0.52	3/90337 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	k	3	LEU	CA-CB-CG	5.37	127.65	115.30
18	T	57	ASP	CB-CG-OD1	5.32	123.08	118.30
30	g	47	ASP	CB-CG-OD1	5.27	123.04	118.30

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	A	429/431 (100%)	414 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	267 (92%)	20 (7%)	2 (1%)	22	61
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
12	M	688/690 (100%)	663 (96%)	24 (4%)	1 (0%)	51	84
13	N	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	186 (90%)	19 (9%)	1 (0%)	29	68
16	Q	412/430 (96%)	399 (97%)	11 (3%)	2 (0%)	29	68
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	61
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	97 (98%)	2 (2%)	0	100	100
26	c	154/156 (99%)	141 (92%)	13 (8%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	98 (93%)	6 (6%)	1 (1%)	15	54
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	i	345/347 (99%)	328 (95%)	17 (5%)	0	100 100
33	j	95/113 (84%)	91 (96%)	4 (4%)	0	100 100
34	k	96/98 (98%)	88 (92%)	8 (8%)	0	100 100
35	l	601/603 (100%)	567 (94%)	34 (6%)	0	100 100
36	m	125/175 (71%)	109 (87%)	16 (13%)	0	100 100
37	n	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100 100
39	p	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	25 64
40	r	457/459 (100%)	445 (97%)	12 (3%)	0	100 100
41	s	299/318 (94%)	279 (93%)	20 (7%)	0	100 100
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100 100
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100 100
44	w	318/320 (99%)	301 (95%)	17 (5%)	0	100 100
All	All	8029/8309 (97%)	7637 (95%)	383 (5%)	9 (0%)	54 84

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	357	ARG
28	e	52	THR
15	P	125	ARG
12	M	126	LEU
16	Q	61	TRP

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	A	344/345 (100%)	342 (99%)	2 (1%)	86 94
2	B	150/151 (99%)	146 (97%)	4 (3%)	44 73
3	C	130/132 (98%)	127 (98%)	3 (2%)	50 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	103/107 (96%)	102 (99%)	1 (1%)	76	88
5	F	76/76 (100%)	73 (96%)	3 (4%)	32	64
6	G	76/81 (94%)	74 (97%)	2 (3%)	46	74
6	X	76/81 (94%)	72 (95%)	4 (5%)	22	55
7	H	99/99 (100%)	96 (97%)	3 (3%)	41	71
8	I	87/97 (90%)	84 (97%)	3 (3%)	37	68
9	J	248/295 (84%)	242 (98%)	6 (2%)	49	76
10	K	41/41 (100%)	38 (93%)	3 (7%)	14	45
11	L	113/113 (100%)	111 (98%)	2 (2%)	59	81
12	M	580/580 (100%)	570 (98%)	10 (2%)	60	82
13	N	130/130 (100%)	127 (98%)	3 (2%)	50	77
14	O	182/183 (100%)	180 (99%)	2 (1%)	73	88
15	P	188/190 (99%)	185 (98%)	3 (2%)	62	83
16	Q	357/370 (96%)	351 (98%)	6 (2%)	60	82
17	S	56/58 (97%)	55 (98%)	1 (2%)	59	81
18	T	79/79 (100%)	77 (98%)	2 (2%)	47	75
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	99 (98%)	2 (2%)	55	79
21	W	122/123 (99%)	117 (96%)	5 (4%)	30	63
22	Y	63/63 (100%)	59 (94%)	4 (6%)	18	51
23	Z	65/65 (100%)	64 (98%)	1 (2%)	65	84
24	a	122/122 (100%)	119 (98%)	3 (2%)	47	75
25	b	98/119 (82%)	96 (98%)	2 (2%)	55	79
26	c	140/141 (99%)	139 (99%)	1 (1%)	84	93
27	d	151/155 (97%)	150 (99%)	1 (1%)	84	93
28	e	98/99 (99%)	93 (95%)	5 (5%)	24	57
29	f	35/38 (92%)	34 (97%)	1 (3%)	42	71
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	307 (99%)	3 (1%)	76	88
33	j	88/99 (89%)	85 (97%)	3 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	k	85/85 (100%)	83 (98%)	2 (2%)	49 76
35	l	536/537 (100%)	524 (98%)	12 (2%)	52 78
36	m	99/141 (70%)	95 (96%)	4 (4%)	31 64
37	n	53/53 (100%)	53 (100%)	0	100 100
38	o	109/113 (96%)	108 (99%)	1 (1%)	78 90
39	p	159/159 (100%)	154 (97%)	5 (3%)	40 70
40	r	409/410 (100%)	405 (99%)	4 (1%)	76 88
41	s	263/275 (96%)	260 (99%)	3 (1%)	73 88
42	u	148/153 (97%)	144 (97%)	4 (3%)	44 73
43	v	101/112 (90%)	92 (91%)	9 (9%)	9 37
44	w	281/283 (99%)	277 (99%)	4 (1%)	67 85
All	All	7021/7235 (97%)	6879 (98%)	142 (2%)	57 79

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	p	49	ASP
40	r	50	LEU
43	v	18	ASP
15	P	80	CYS
15	P	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
41	s	5	ASN
40	r	51	ASN
26	c	183	HIS
40	r	44	GLN
26	c	154	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	6.32	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.61	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	13.00	131.40	119.48
16	Q	118	2MR	CD-NE-CZ	4.76	132.32	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.73	129.91	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

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 38 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
56	UQ	s	401	-	28,28,63	3.30	7 (25%)	34,37,79	2.99	11 (32%)
54	CDL	u	201	-	77,77,99	1.19	8 (10%)	83,89,111	0.94	4 (4%)
47	NAI	A	503	-	42,48,48	4.97	19 (45%)	47,73,73	1.29	5 (10%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.46	4 (13%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.02	2 (3%)
54	CDL	l	701	-	98,98,99	1.08	8 (8%)	104,110,111	0.93	5 (4%)
48	PEE	V	203	-	39,39,50	1.31	6 (15%)	41,44,55	1.02	2 (4%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.22	8 (16%)
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
50	NDP	J	401	-	45,52,52	4.58	20 (44%)	53,80,80	1.93	9 (16%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.56	8 (20%)
54	CDL	V	202	-	67,67,99	1.25	9 (13%)	73,79,111	1.00	4 (5%)
55	PLX	r	502	-	51,51,51	1.14	3 (5%)	55,59,59	0.65	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	PLX	j	203	-	51,51,51	1.16	4 (7%)	55,59,59	0.58	1 (1%)
54	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.91	4 (4%)
54	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
54	CDL	i	401	-	65,65,99	1.27	8 (12%)	71,77,111	1.03	5 (7%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.96	2 (4%)
55	PLX	a	202	-	51,51,51	1.16	5 (9%)	55,59,59	0.62	1 (1%)
51	FES	M	803	12	0,4,4	-	-	-		
45	SF4	C	301	3,16	0,12,12	-	-	-		
54	CDL	a	201	-	90,90,99	1.12	8 (8%)	96,102,111	0.94	4 (4%)
54	CDL	g	202	-	96,96,99	1.10	8 (8%)	102,108,111	0.85	4 (3%)
51	FES	O	301	14	0,4,4	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
49	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.60	5 (12%)
55	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
48	PEE	j	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
48	PEE	m	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.04	3 (6%)

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
56	UQ	s	401	-	-	12/21/45/87	0/1/1/1
54	CDL	u	201	-	-	42/88/88/110	-
47	NAI	A	503	-	-	7/25/72/72	0/5/5/5
57	ADP	w	401	-	-	2/12/32/32	0/3/3/3
48	PEE	B	303	-	-	28/54/54/54	-
54	CDL	l	701	-	-	56/109/109/110	-
48	PEE	V	203	-	-	19/43/43/54	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
48	PEE	l	703	-	-	27/49/49/54	-
50	NDP	J	401	-	-	10/30/77/77	0/4/5/5
49	8Q1	X	201	-	-	7/41/41/41	-
45	SF4	B	301	2	-	-	0/6/5/5
54	CDL	V	202	-	-	45/78/78/110	-
55	PLX	r	502	-	-	35/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	r	501	-	-	22/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
55	PLX	j	203	-	-	26/55/55/55	-
54	CDL	V	201	-	-	62/104/104/110	-
54	CDL	l	702	-	-	69/110/110/110	-
54	CDL	i	401	-	-	45/76/76/110	-
48	PEE	l	704	-	-	31/49/49/54	-
55	PLX	a	202	-	-	25/55/55/55	-
51	FES	M	803	12	-	-	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
54	CDL	a	201	-	-	50/101/101/110	-
45	SF4	C	301	3,16	-	-	0/6/5/5
54	CDL	g	202	-	-	60/107/107/110	-
51	FES	O	301	14	-	-	0/1/1/1
48	PEE	m	201	-	-	22/44/44/54	-
49	8Q1	G	201	6	-	18/41/41/41	-
55	PLX	g	201	-	-	21/55/55/55	-
48	PEE	j	202	-	-	28/54/54/54	-

The worst 5 of 188 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.29	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.56	1.30	1.53
50	J	401	NDP	C3B-C2B	-12.80	1.24	1.52
50	J	401	NDP	C6N-C5N	12.50	1.55	1.33
50	J	401	NDP	O4D-C4D	10.56	1.68	1.45

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-10.56	109.22	126.79
50	J	401	NDP	C3N-C2N-N1N	-7.77	112.01	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.35	110.54	121.11
49	G	201	8Q1	C6-C1-S44	6.05	120.50	113.46
49	X	201	8Q1	C6-C1-S44	5.82	120.23	113.46

There are no chirality outliers.

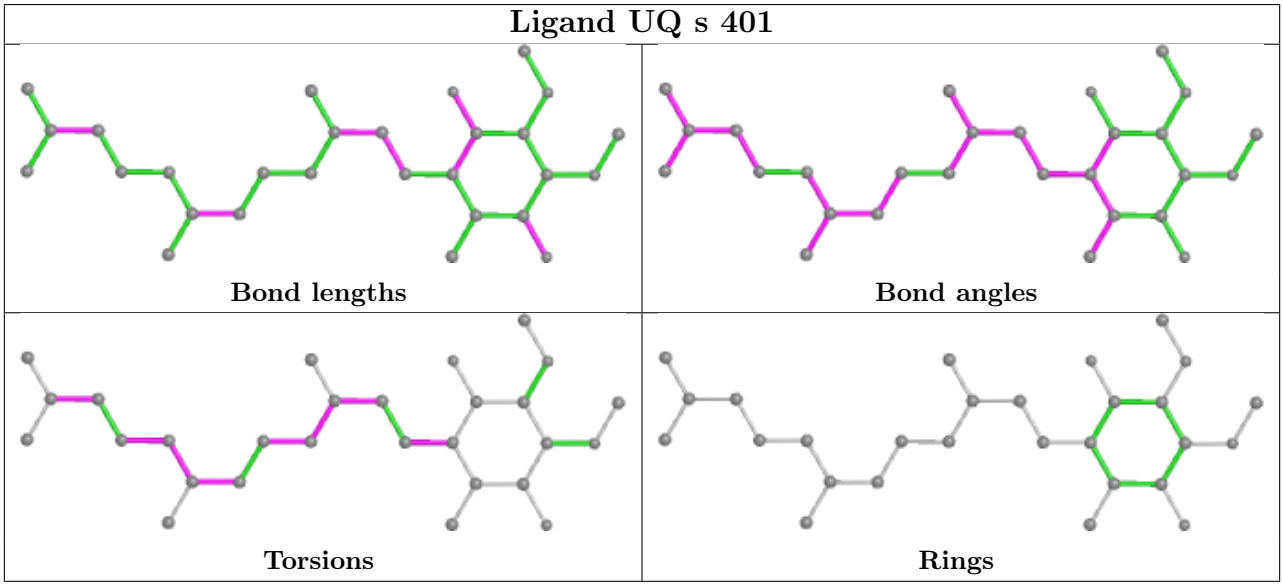
5 of 774 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	PN-O3-PA-O5B
47	A	503	NAI	C5D-O5D-PN-O3
47	A	503	NAI	O4D-C4D-C5D-O5D

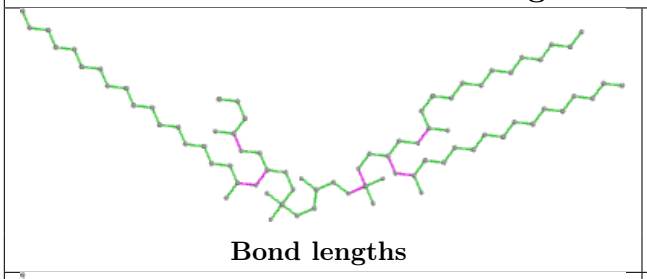
There are no ring outliers.

No monomer is involved in short contacts.

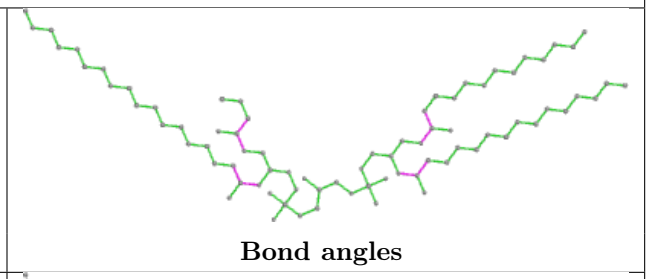
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



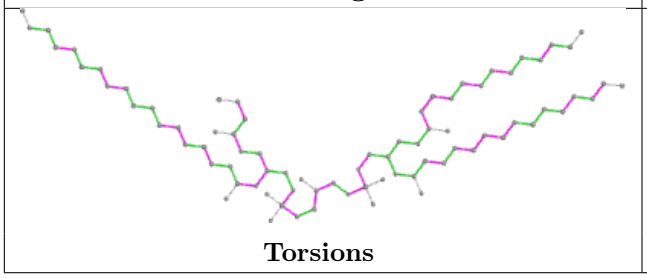
Ligand CDL u 201



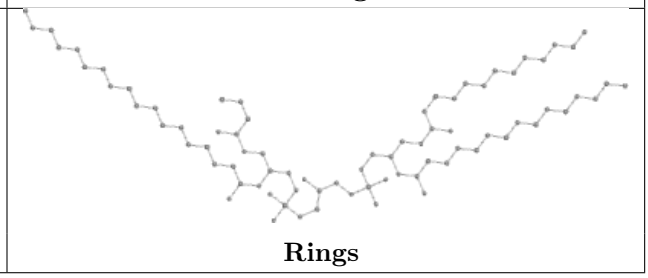
Bond lengths



Bond angles

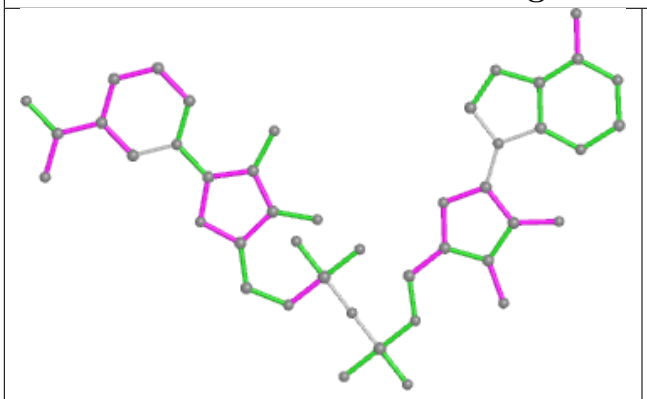


Torsions

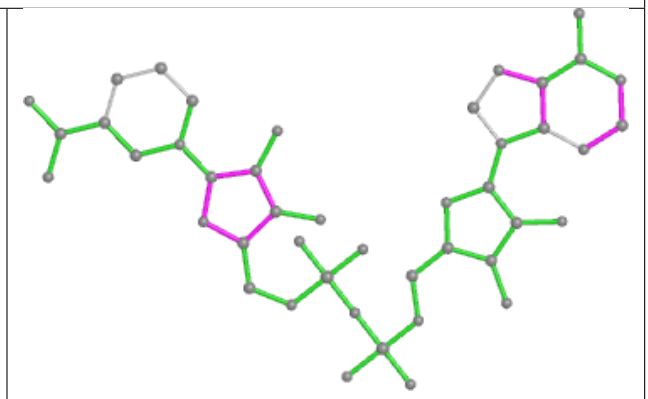


Rings

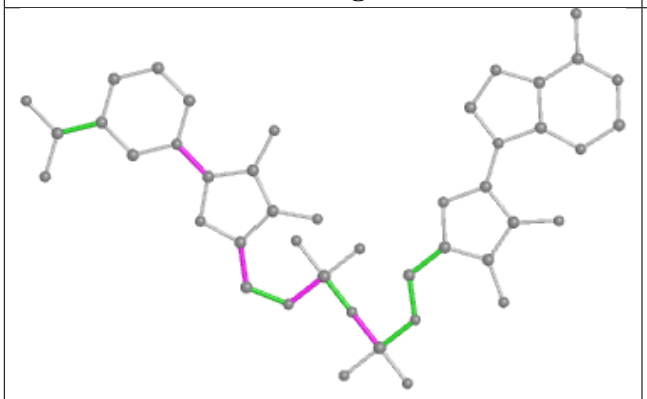
Ligand NAI A 503



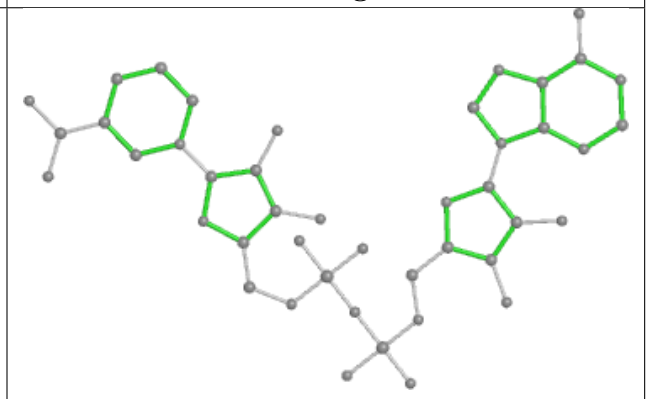
Bond lengths



Bond angles

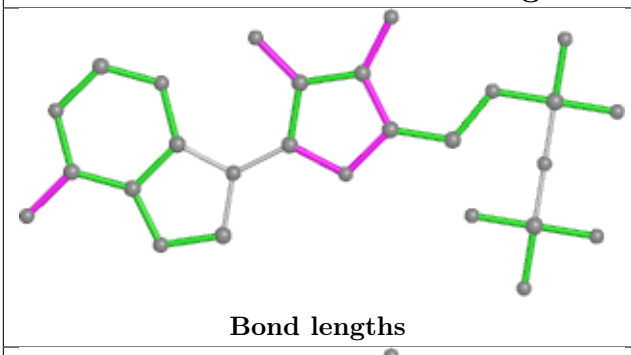


Torsions

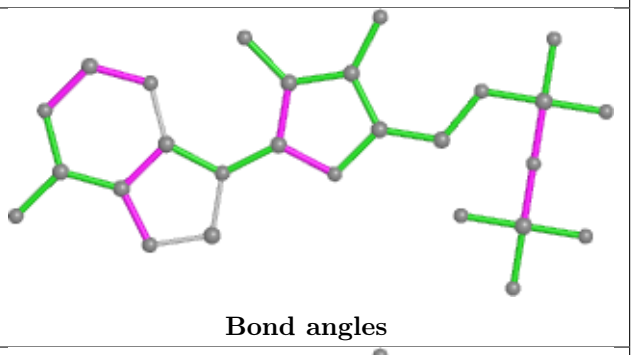


Rings

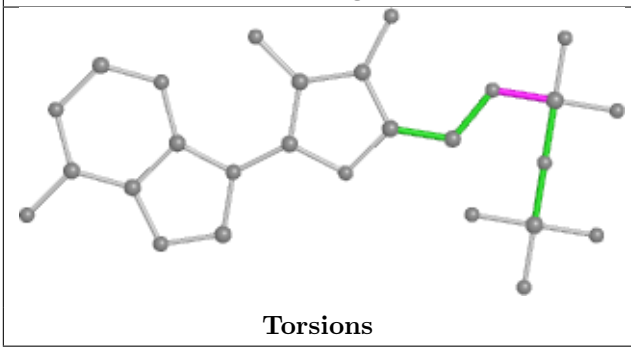
Ligand ADP w 401



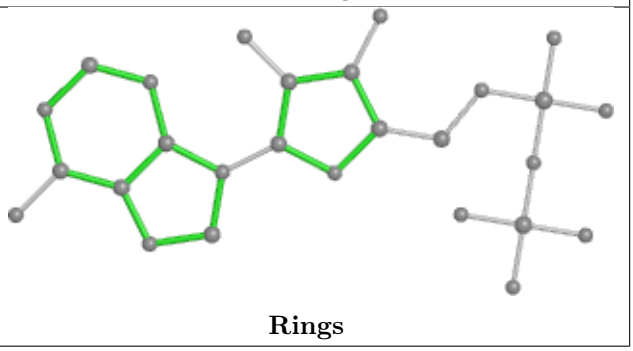
Bond lengths



Bond angles

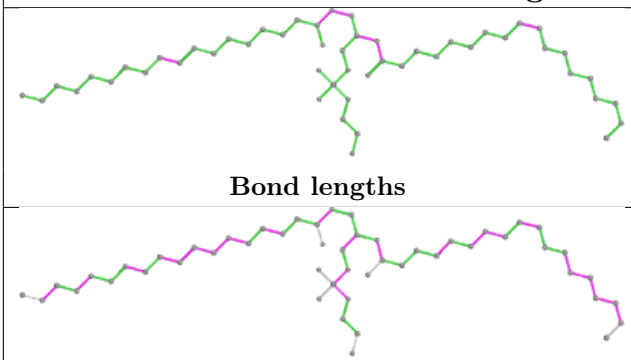


Torsions

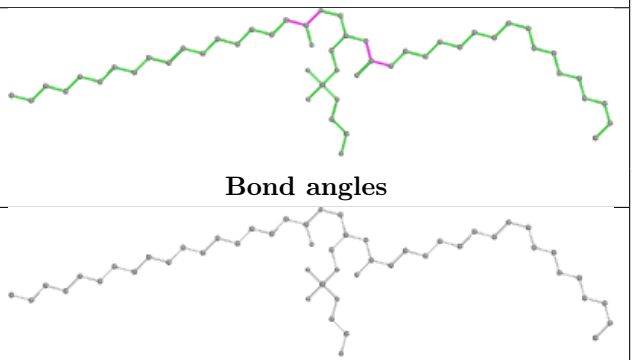


Rings

Ligand PEE B 303



Bond lengths

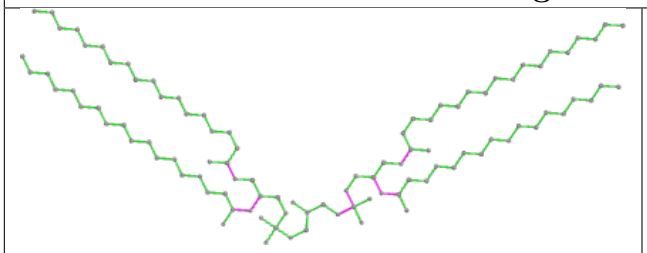


Bond angles

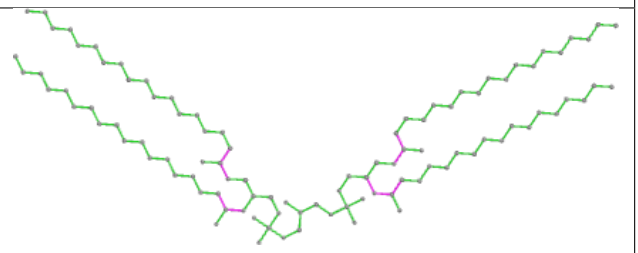
Torsions

Rings

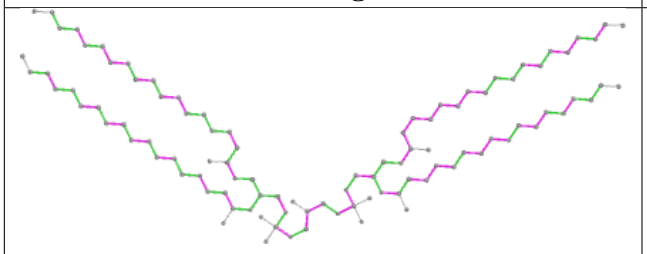
Ligand CDL l 701



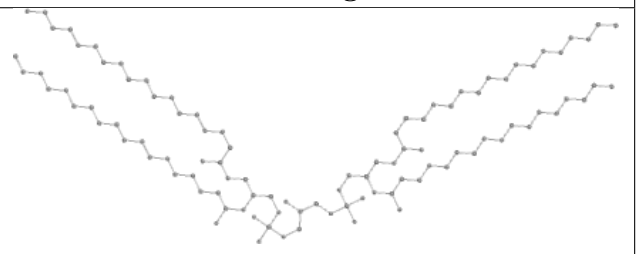
Bond lengths



Bond angles

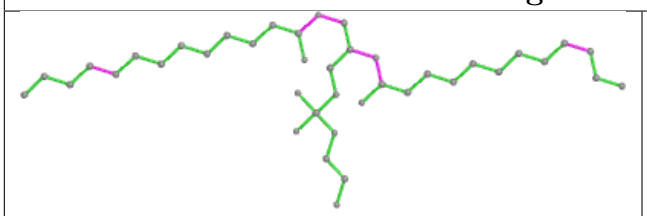


Torsions



Rings

Ligand PEE V 203



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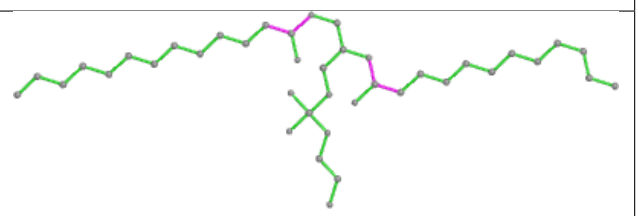

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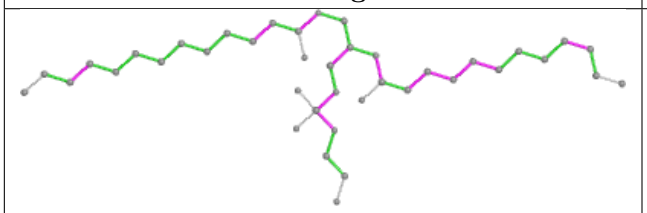
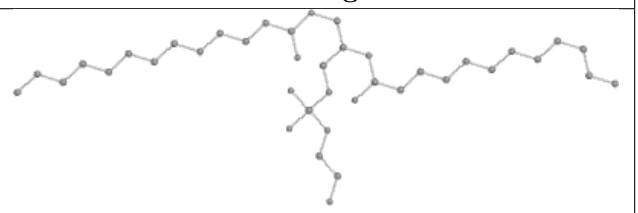
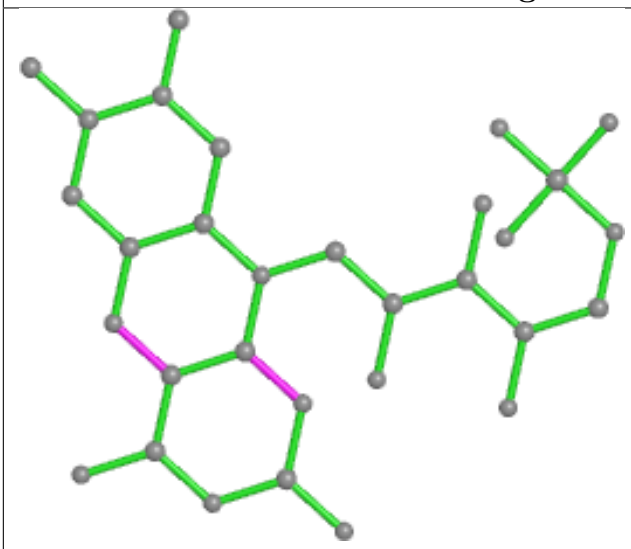


Torsions



Rings

Ligand FMN A 502



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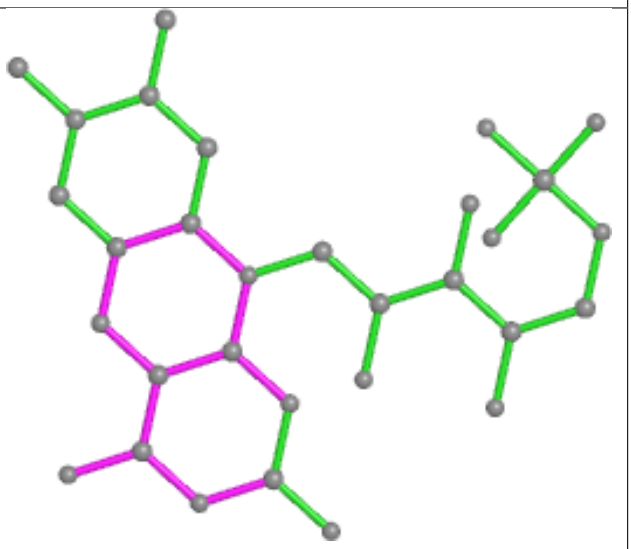
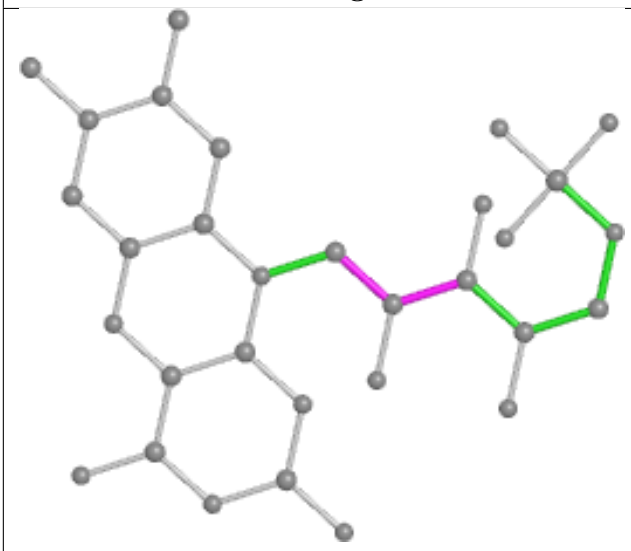
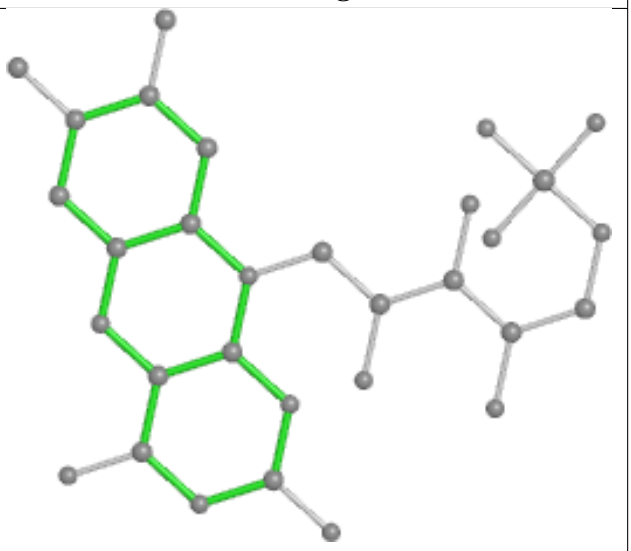


Bond angles

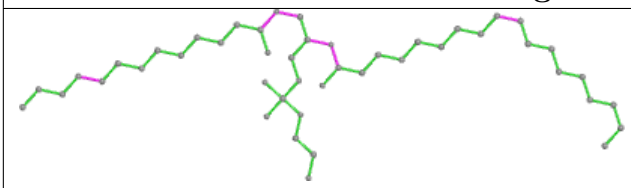


Torsions



Rings

Ligand PEE l 703



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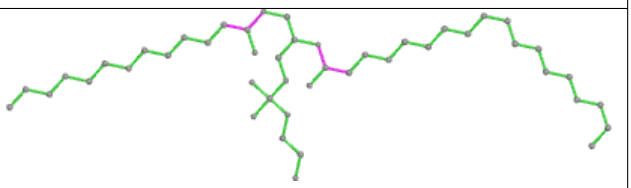
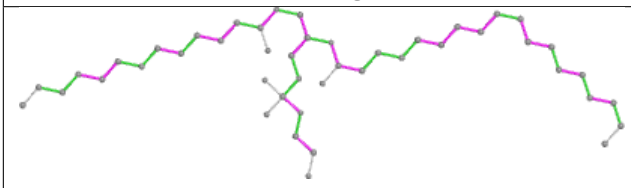


Bond angles



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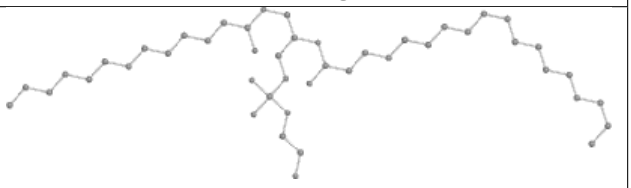
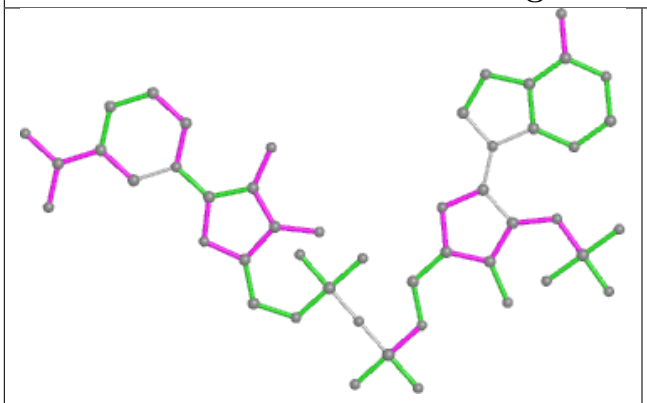
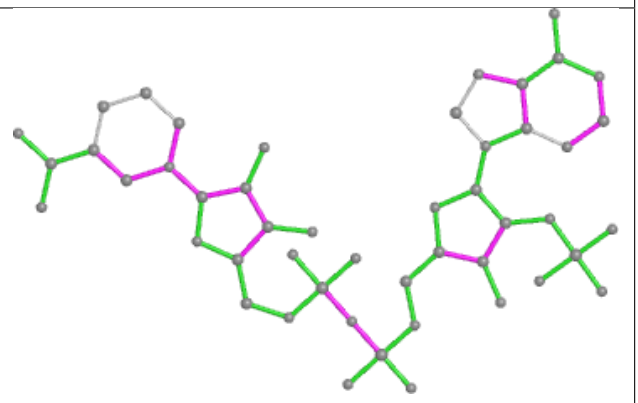


Rings

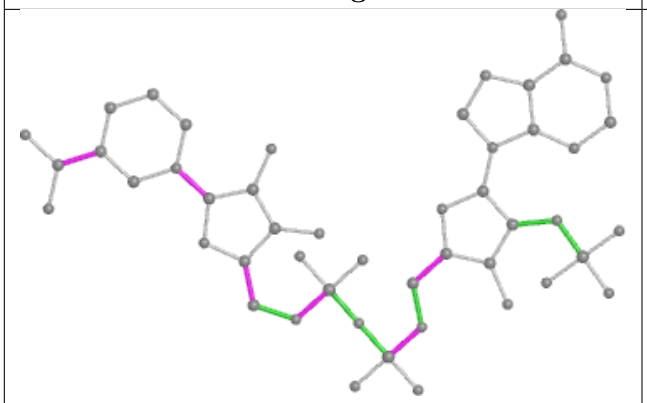
Ligand NDP J 401



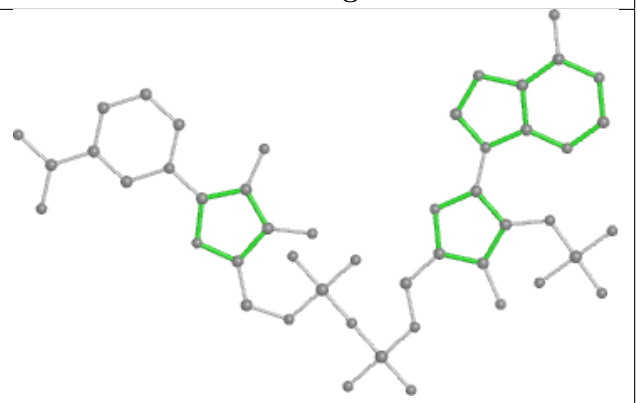
Bond lengths



Bond angles

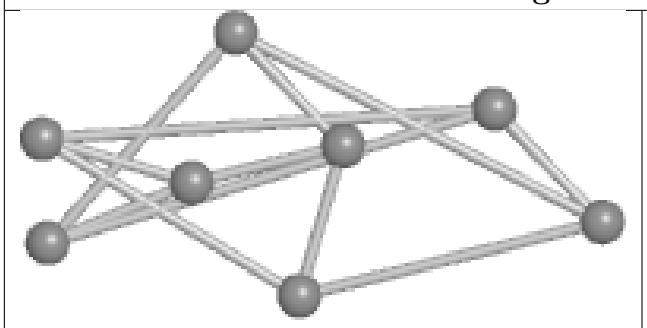


Torsions

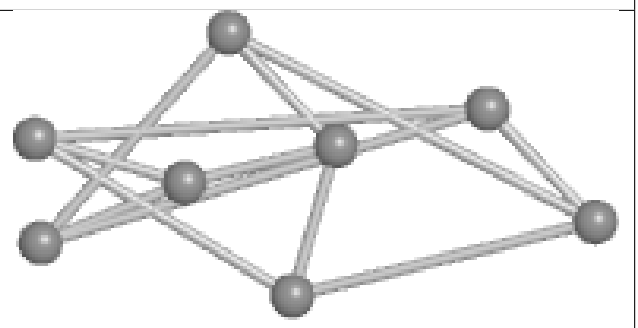


Rings

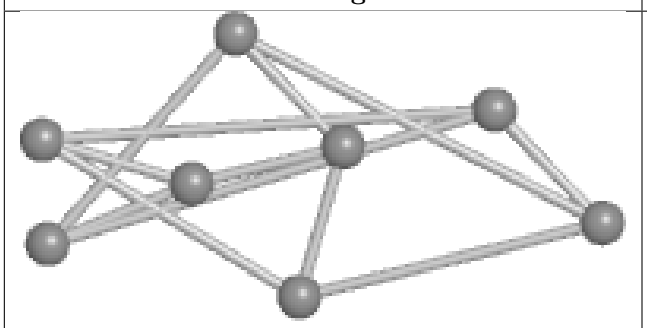
Ligand SF4 B 301



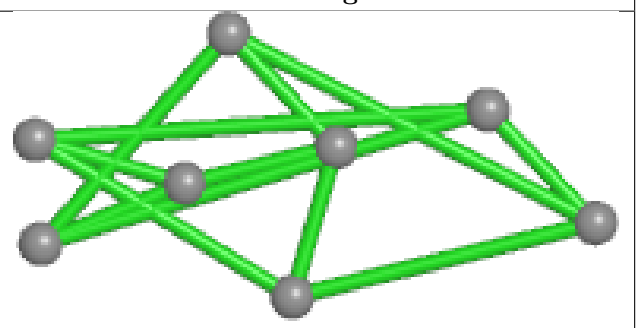
Bond lengths



Bond angles

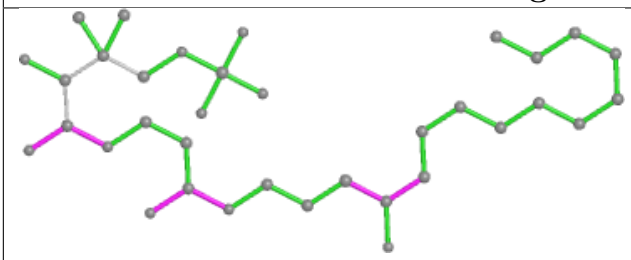


Torsions

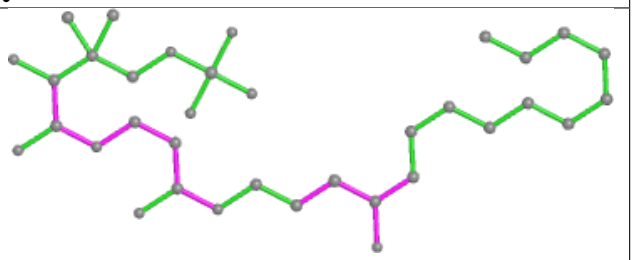


Rings

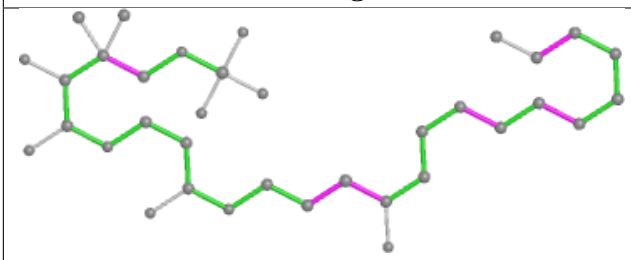
Ligand 8Q1 X 201



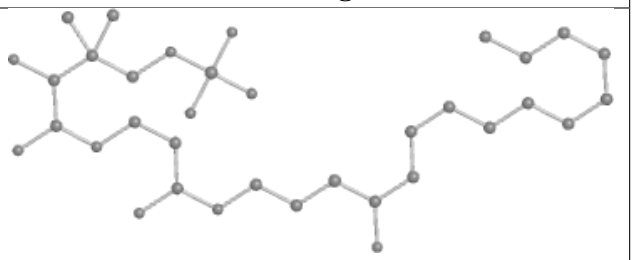
Bond lengths



Bond angles

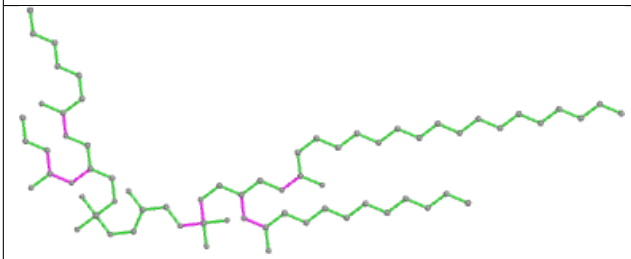


Torsions

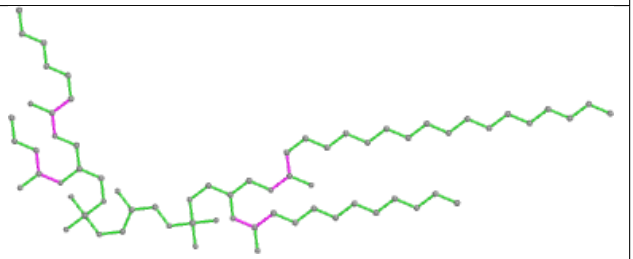


Rings

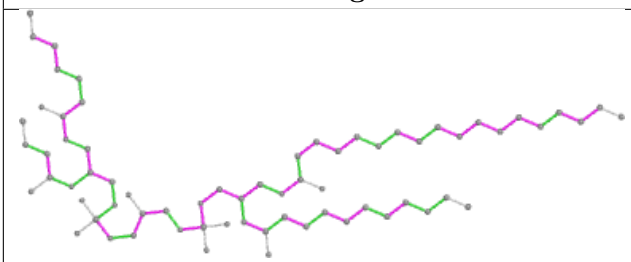
Ligand CDL V 202



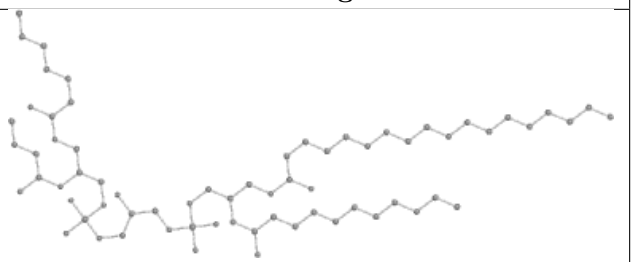
Bond lengths



Bond angles

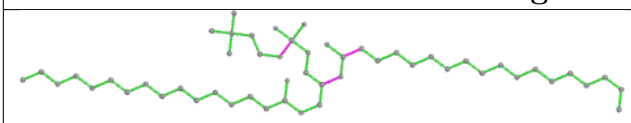


Torsions

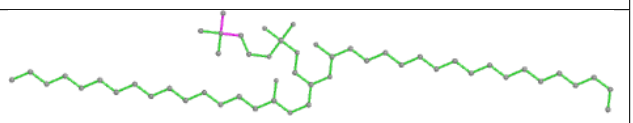


Rings

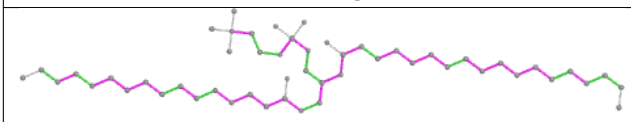
Ligand PLX r 502



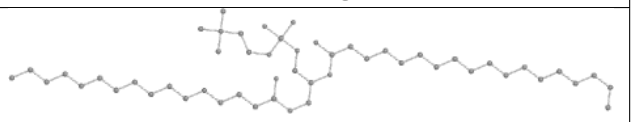
Bond lengths



Bond angles

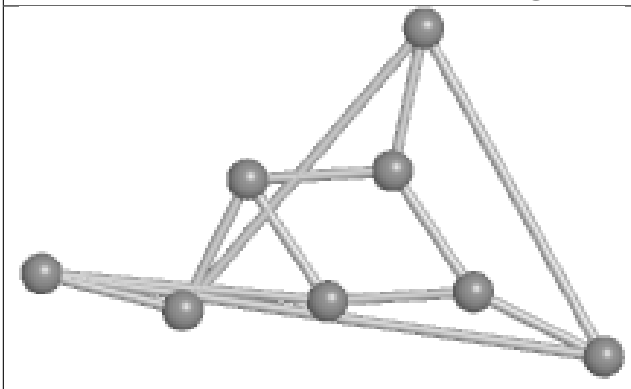


Torsions

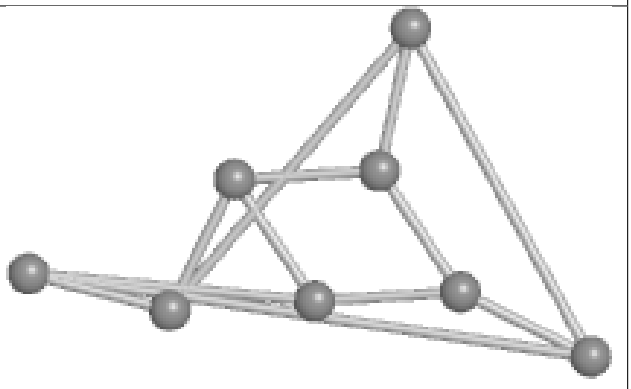


Rings

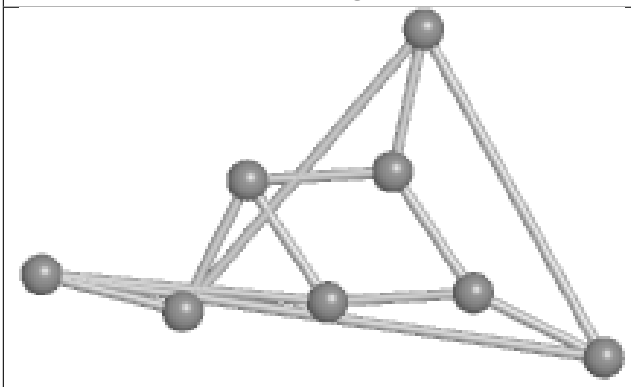
Ligand SF4 M 801



Bond lengths



Bond angles



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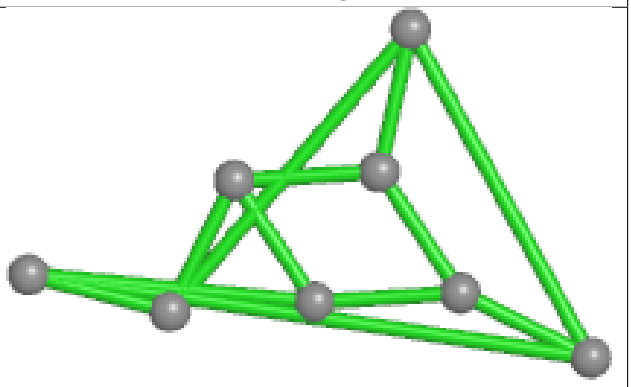
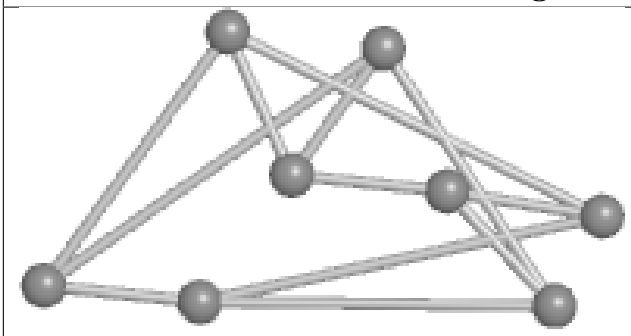


Rings

Ligand SF4 A 501



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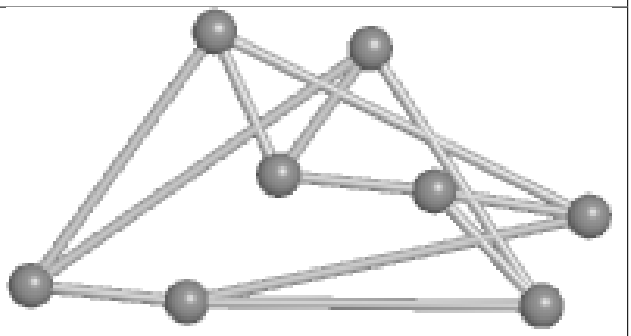
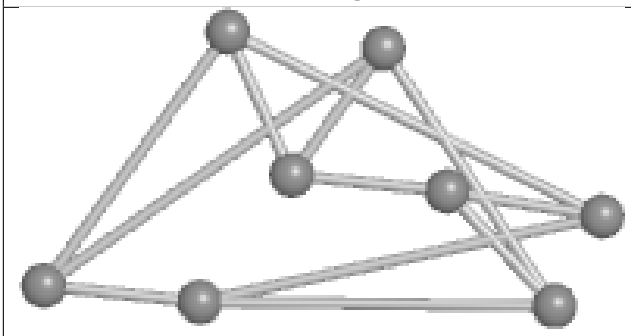
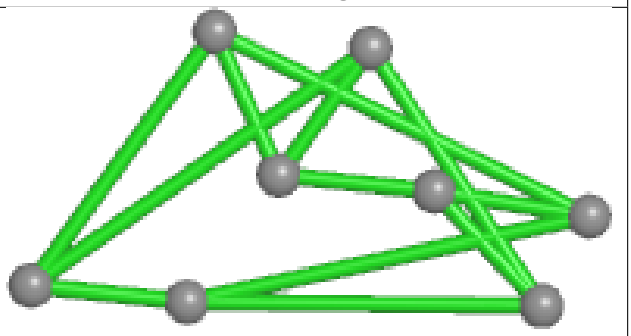


Bond angles

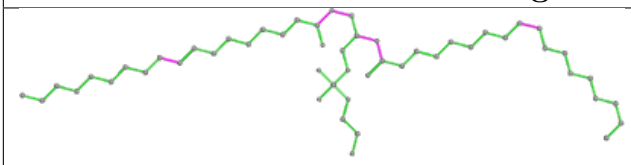


Torsions



Rings

Ligand PEE r 501



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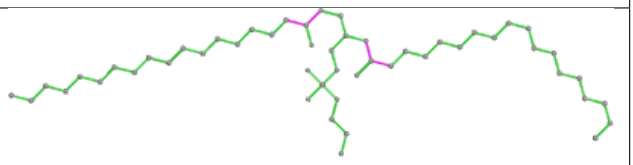
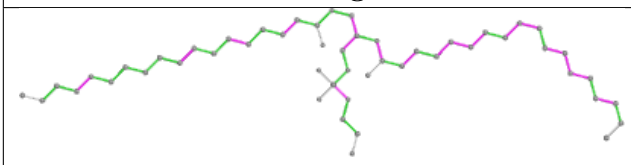
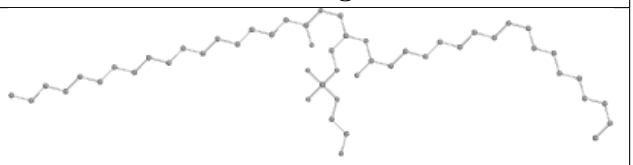


Bond angles

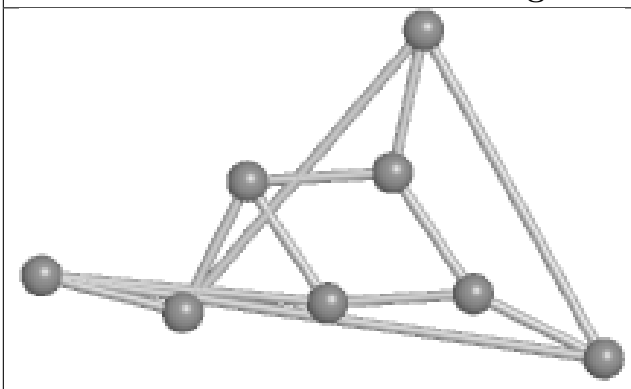


Torsions



Rings

Ligand SF4 M 802



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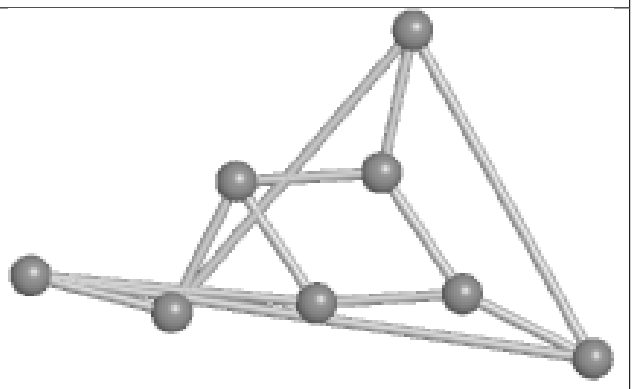
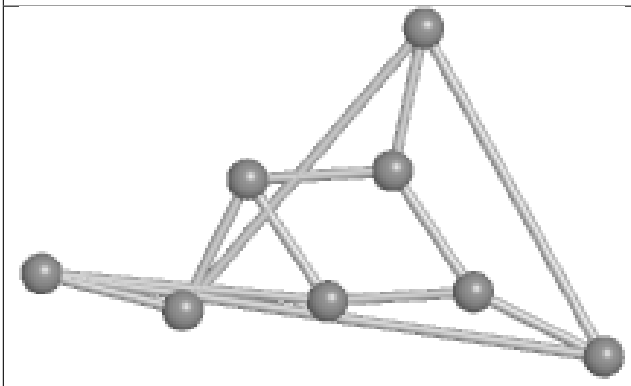
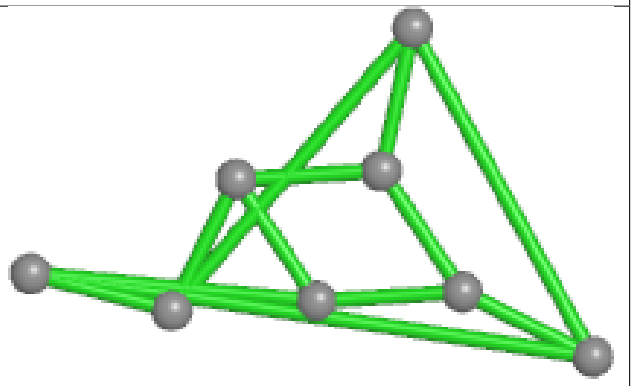


Bond angles

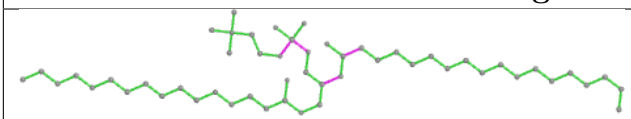


Torsions



Rings

Ligand PLX j 203



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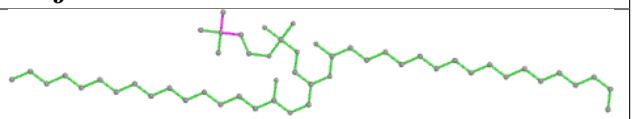
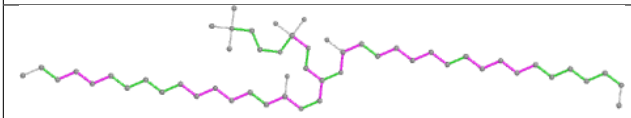
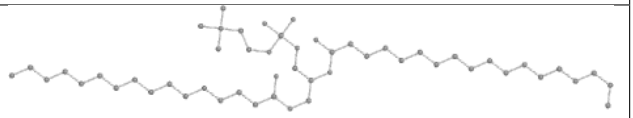


Bond angles

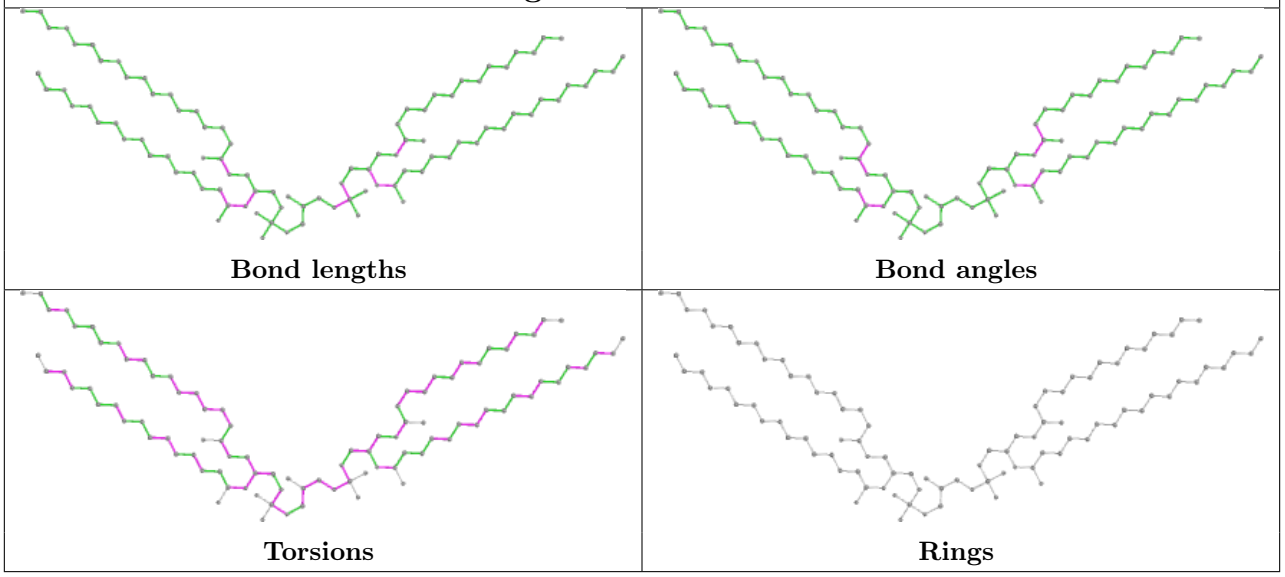


Torsions

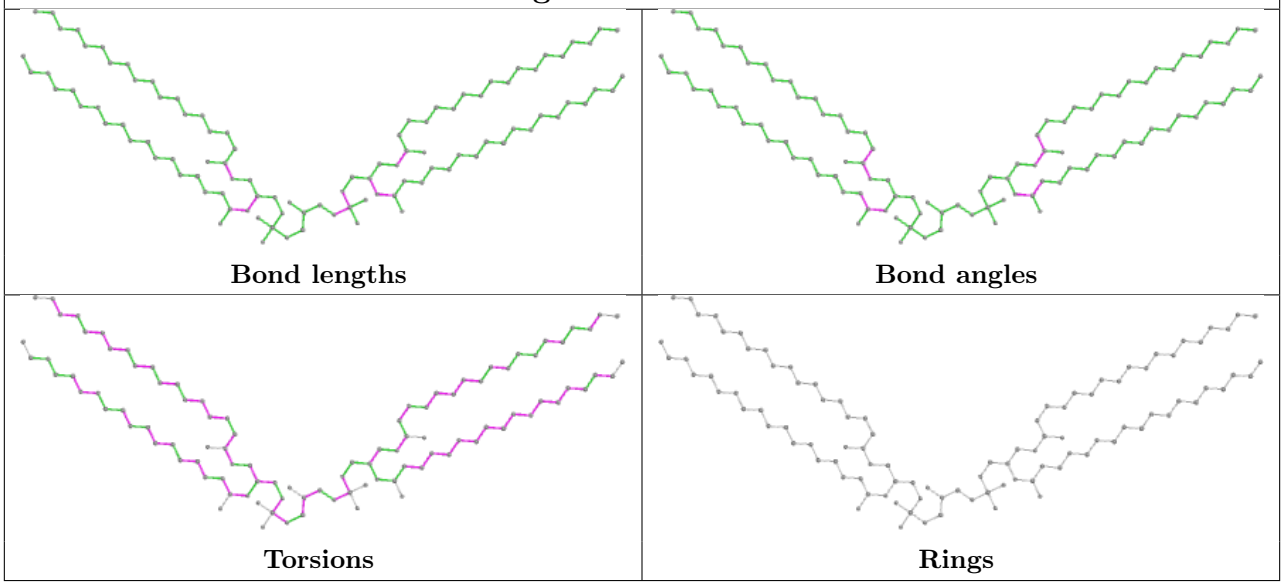


Rings

Ligand CDL V 201



Ligand CDL l 702



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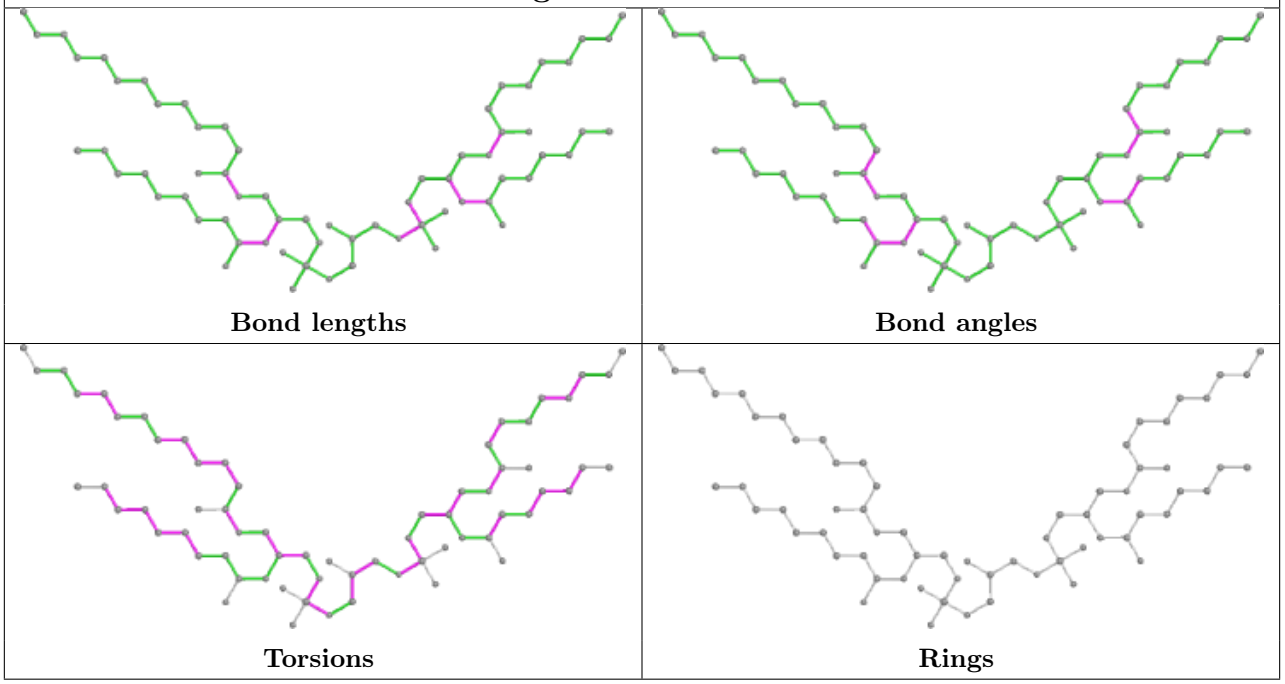
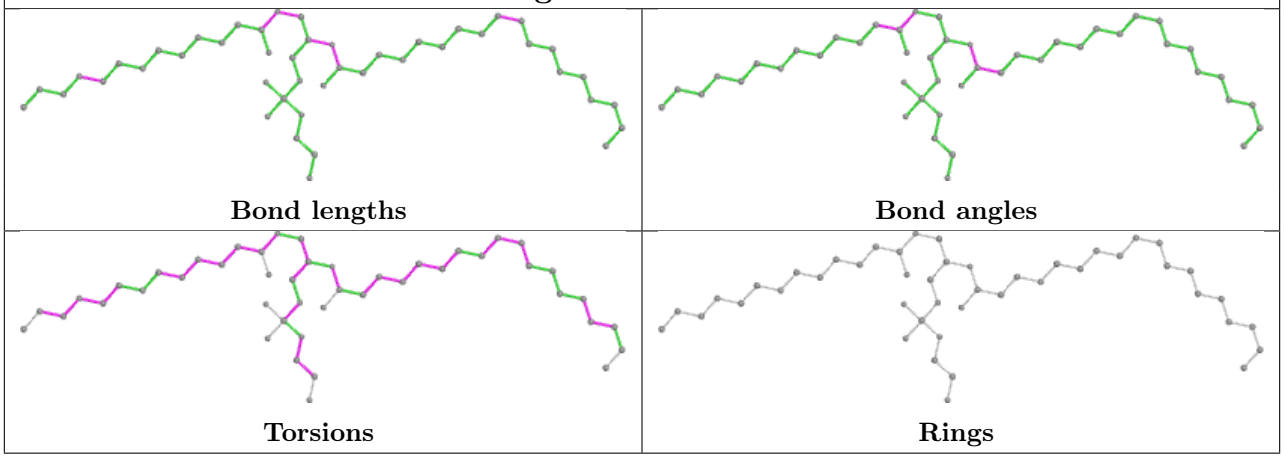
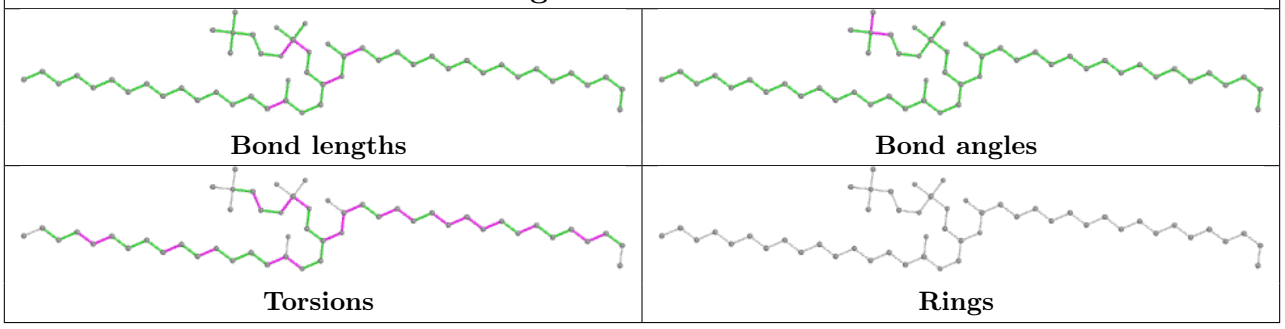


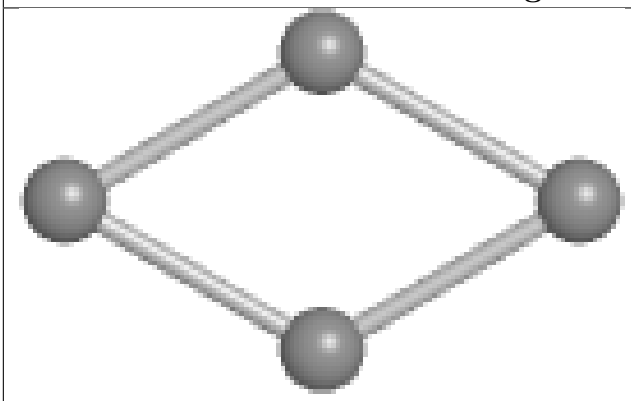
Ligand PEE l 704



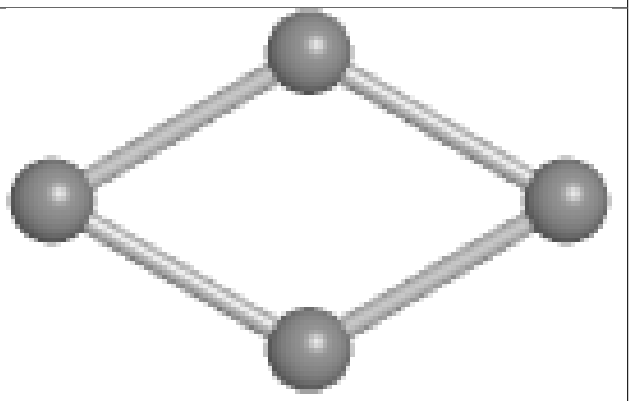
Ligand PLX a 202



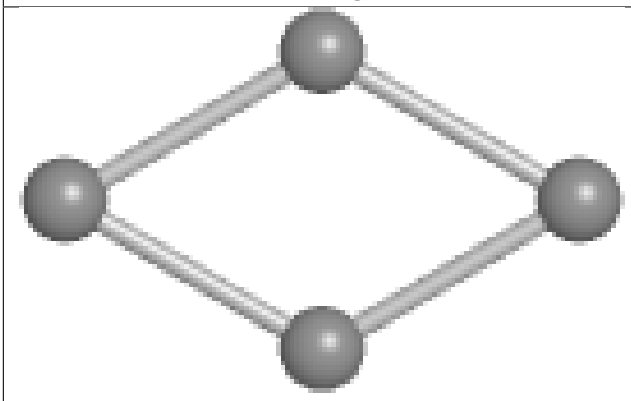
Ligand FES M 803



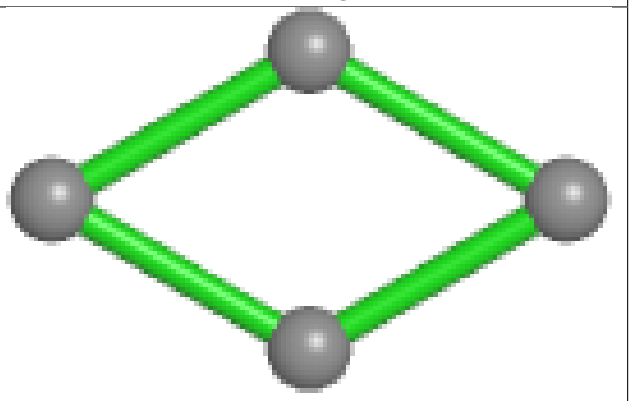
Bond lengths



Bond angles

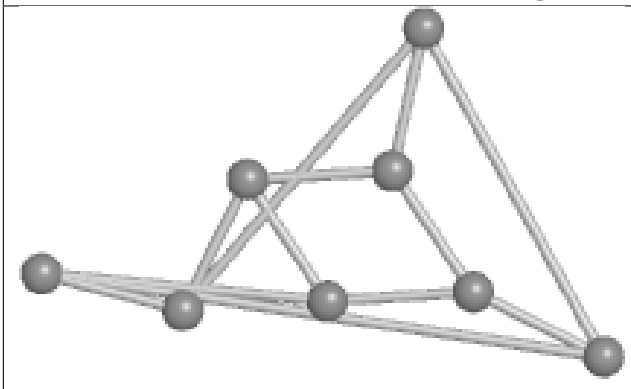


Torsions



Rings

Ligand SF4 C 301



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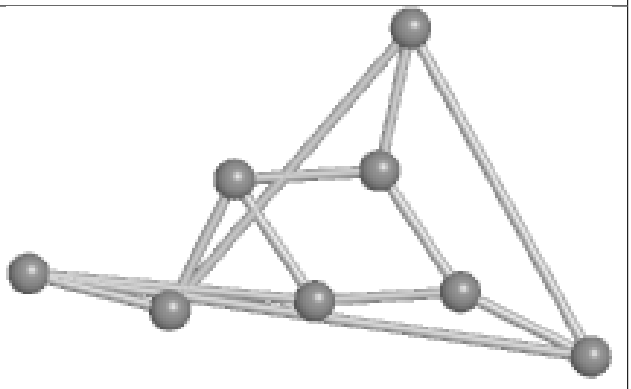
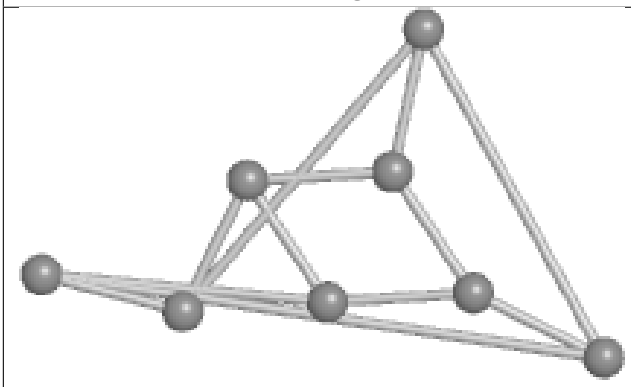
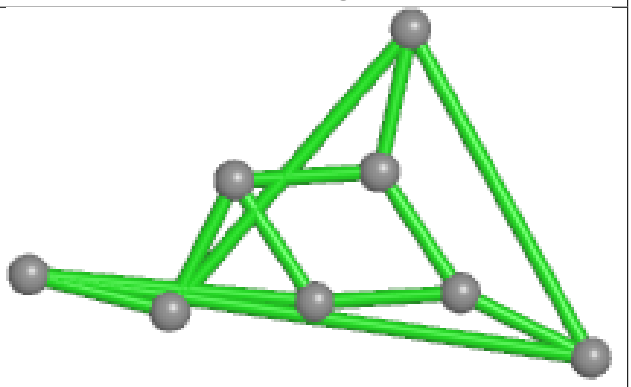


Bond angles

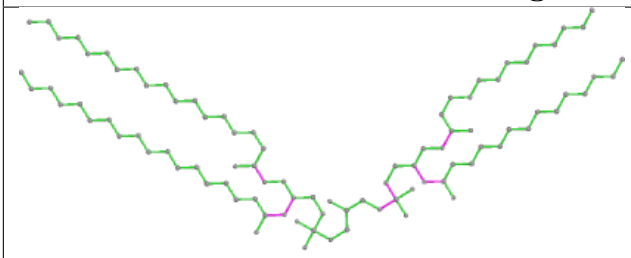


Torsions

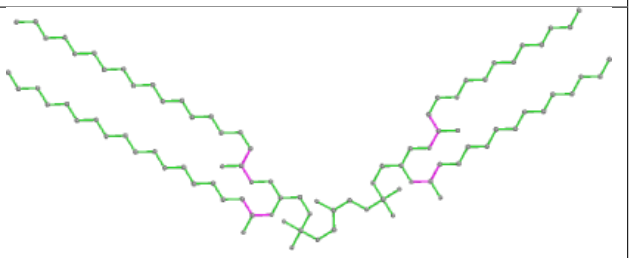


Rings

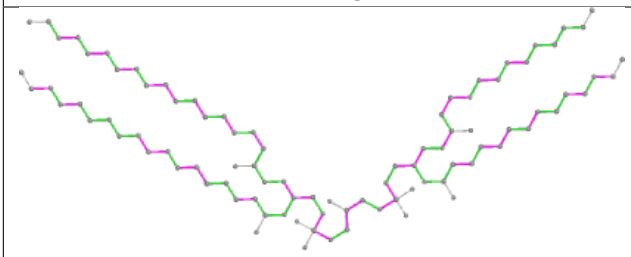
Ligand CDL a 201



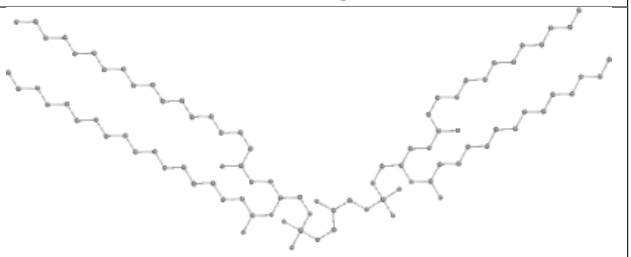
Bond lengths



Bond angles

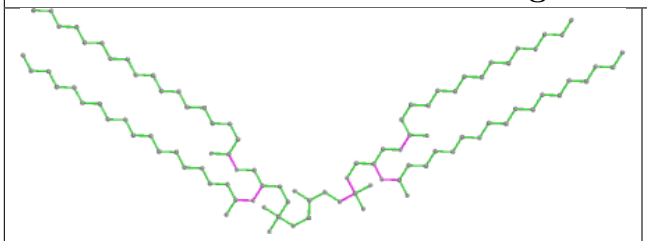


Torsions



Rings

Ligand CDL g 202



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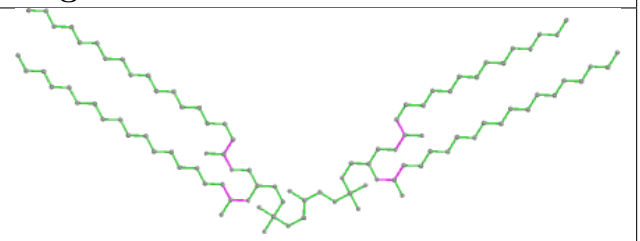
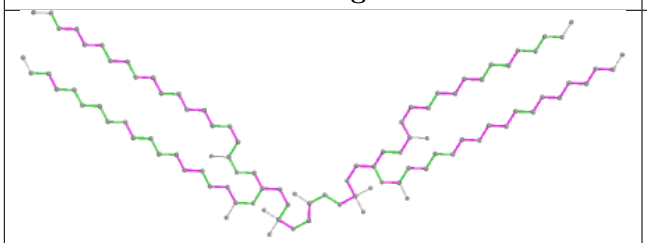
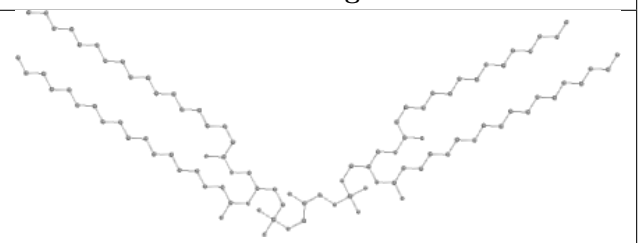


Bond angles

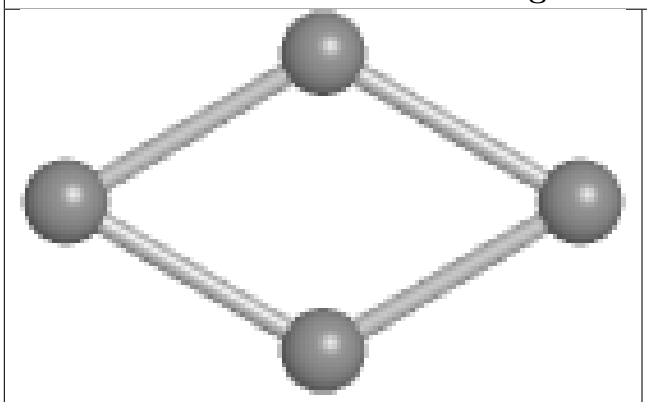


Torsions

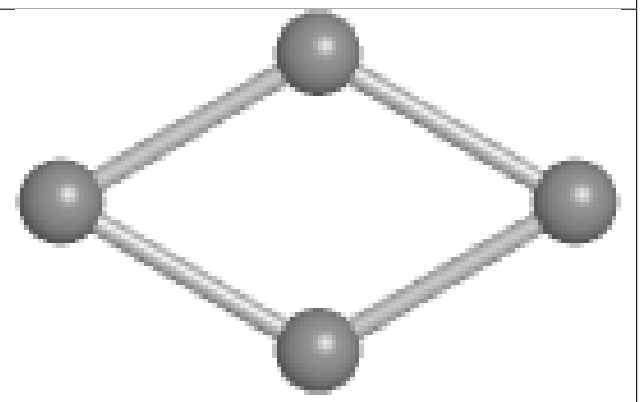


Rings

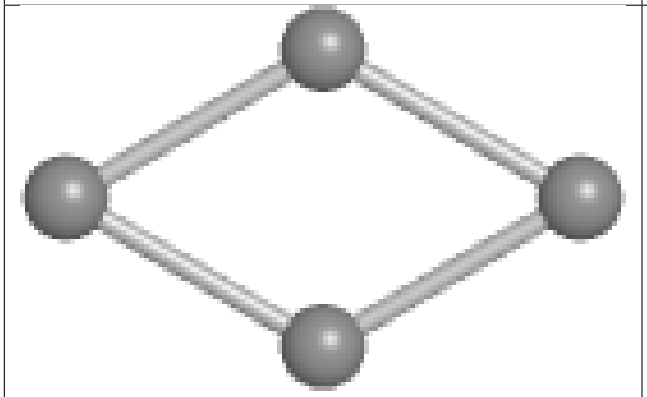
Ligand FES O 301



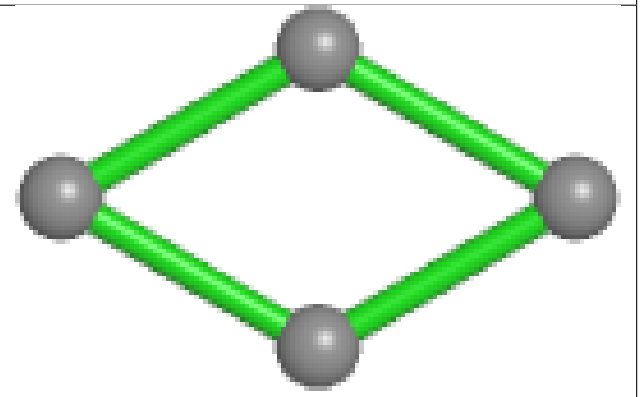
Bond lengths



Bond angles

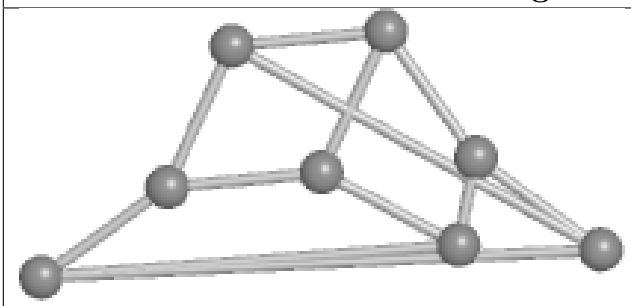


Torsions

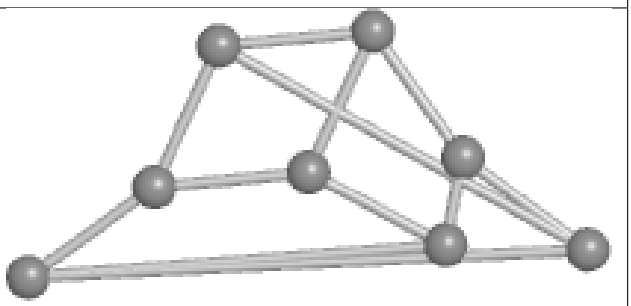


Rings

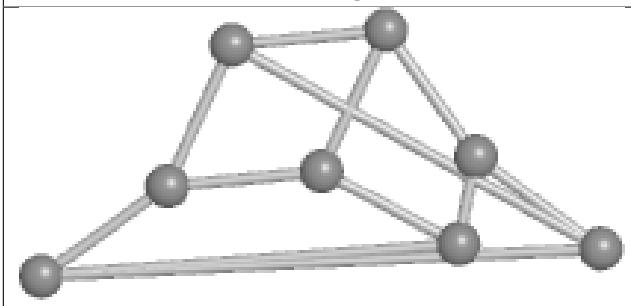
Ligand SF4 B 302



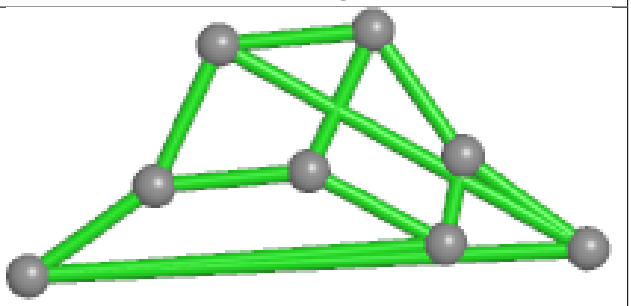
Bond lengths



Bond angles

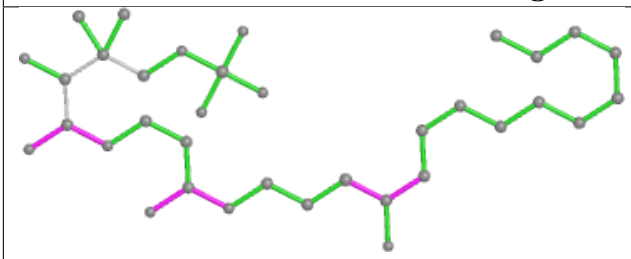


Torsions

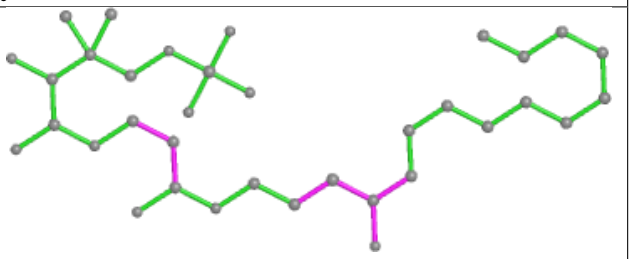


Rings

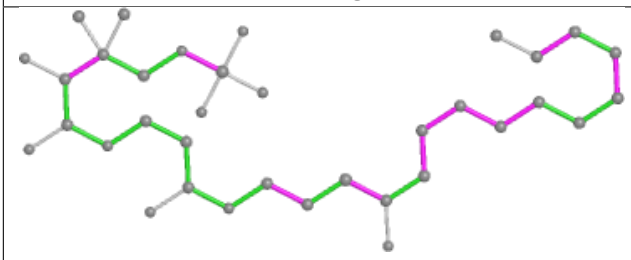
Ligand 8Q1 G 201



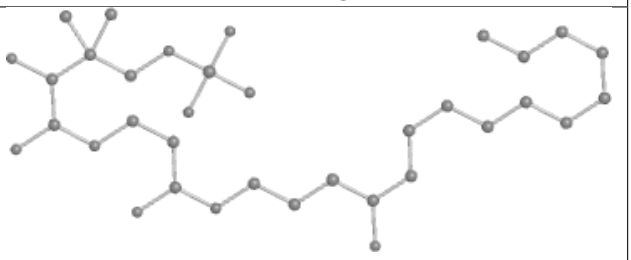
Bond lengths



Bond angles

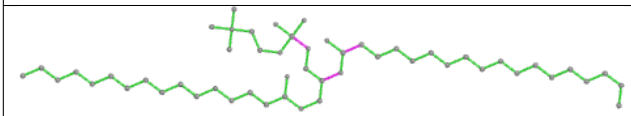


Torsions

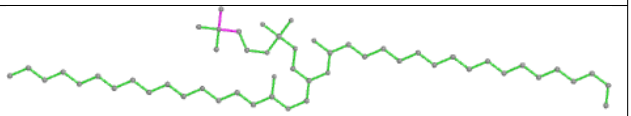


Rings

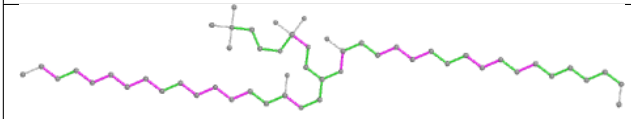
Ligand PLX g 201



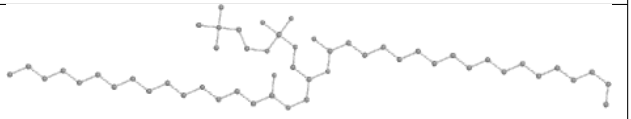
Bond lengths



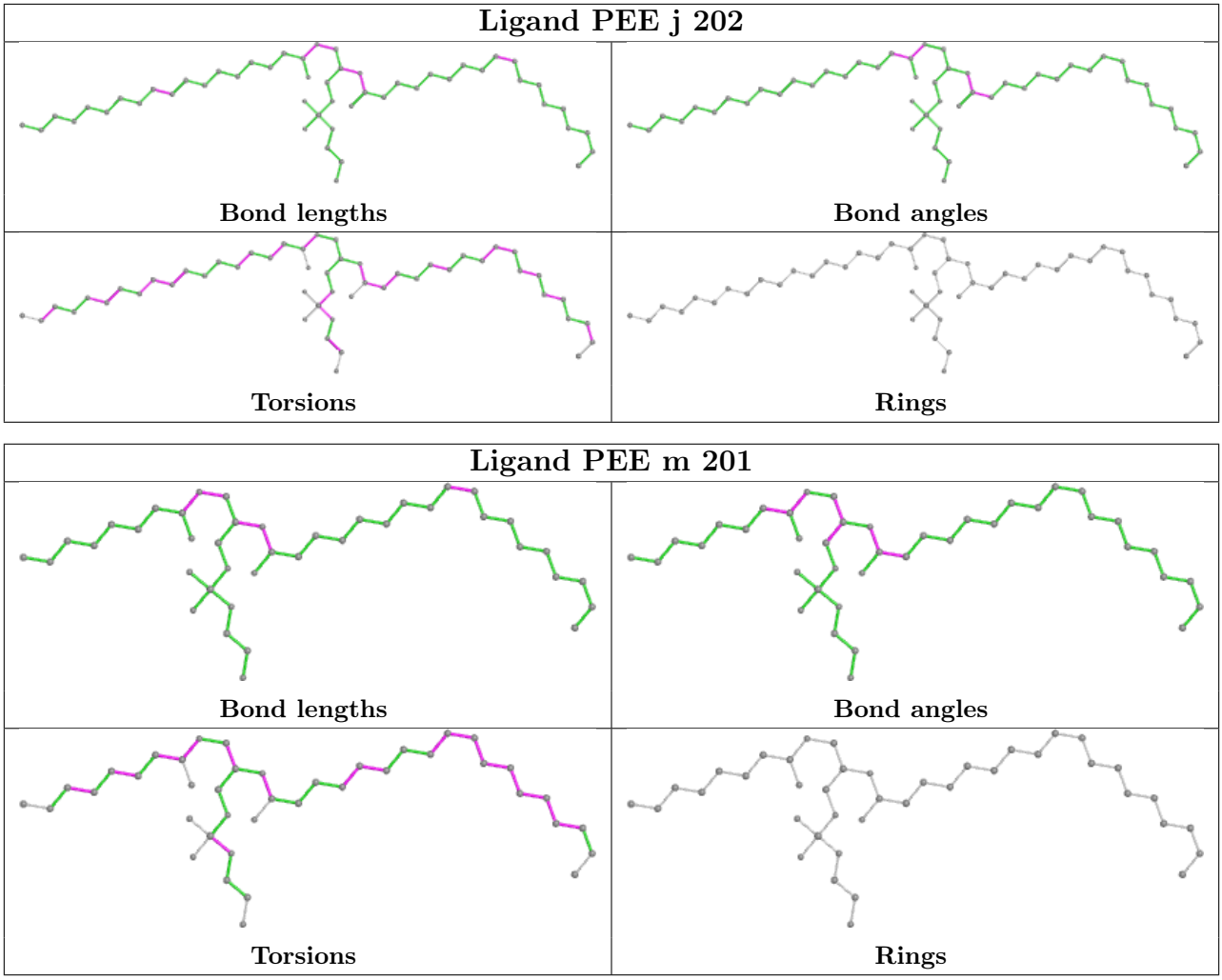
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

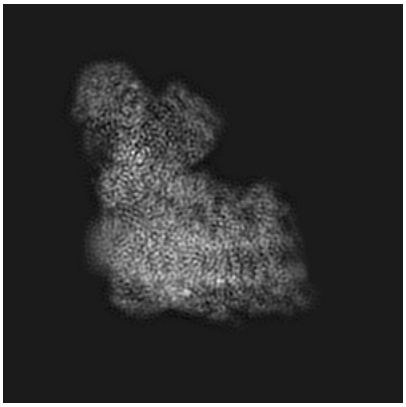
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32253. These allow visual inspection of the internal detail of the map and identification of artifacts.

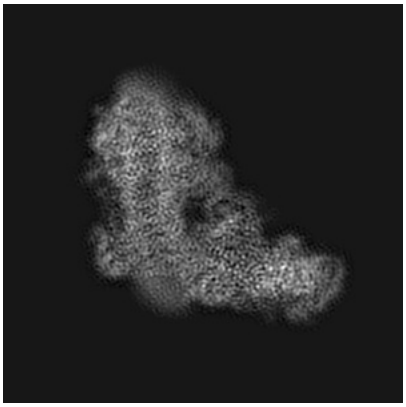
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

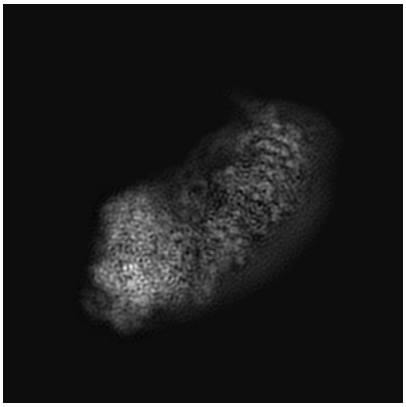
6.1.1 Primary map



X



Y

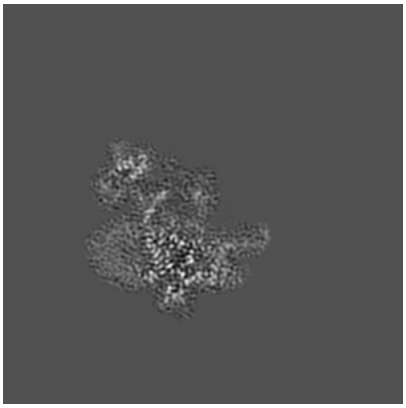


Z

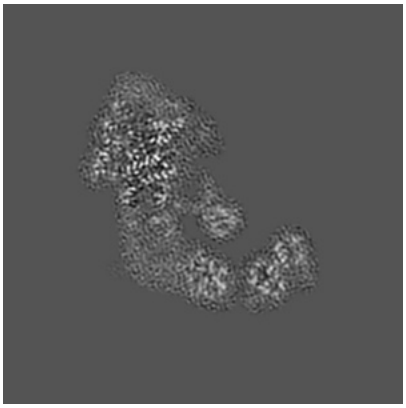
The images above show the map projected in three orthogonal directions.

6.2 Central slices

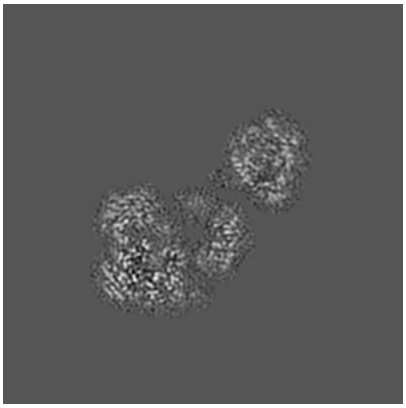
6.2.1 Primary map



X Index: 155



Y Index: 155



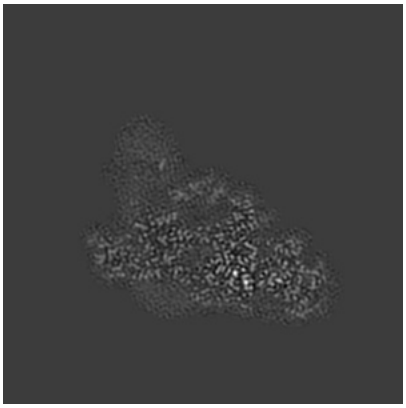
Z Index: 155

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

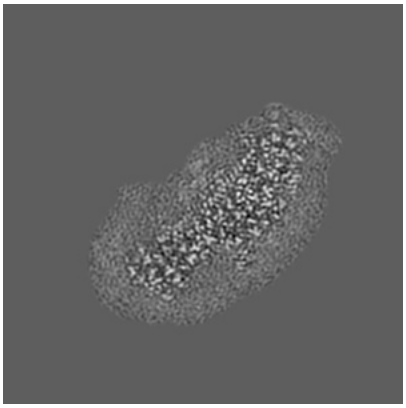
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 101



Y Index: 105

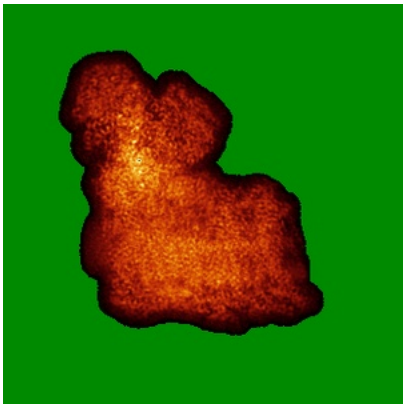


Z Index: 121

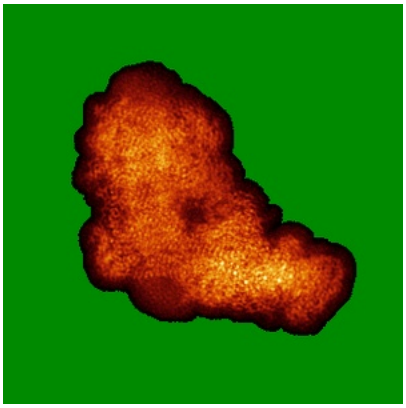
The images above show the largest variance slices of the map in three orthogonal directions.

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

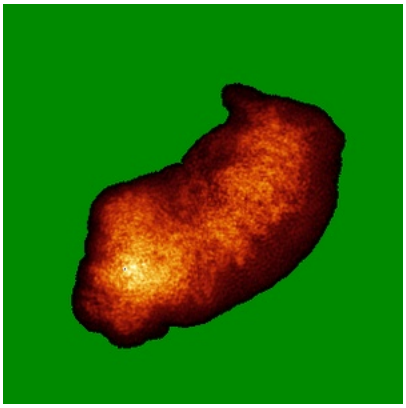
6.4.1 Primary map



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 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

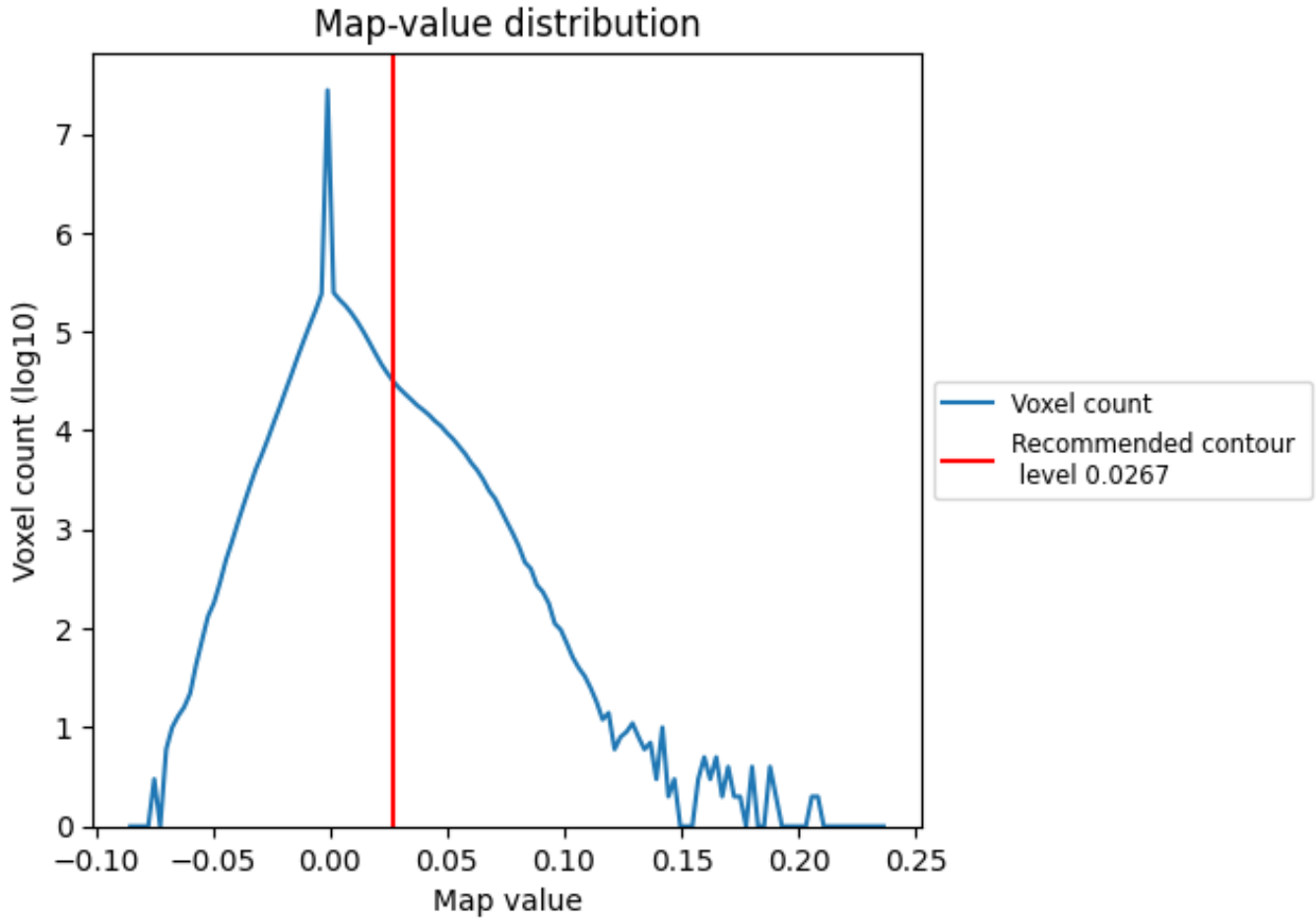
6.6 Mask visualisation (i)

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

7 Map analysis

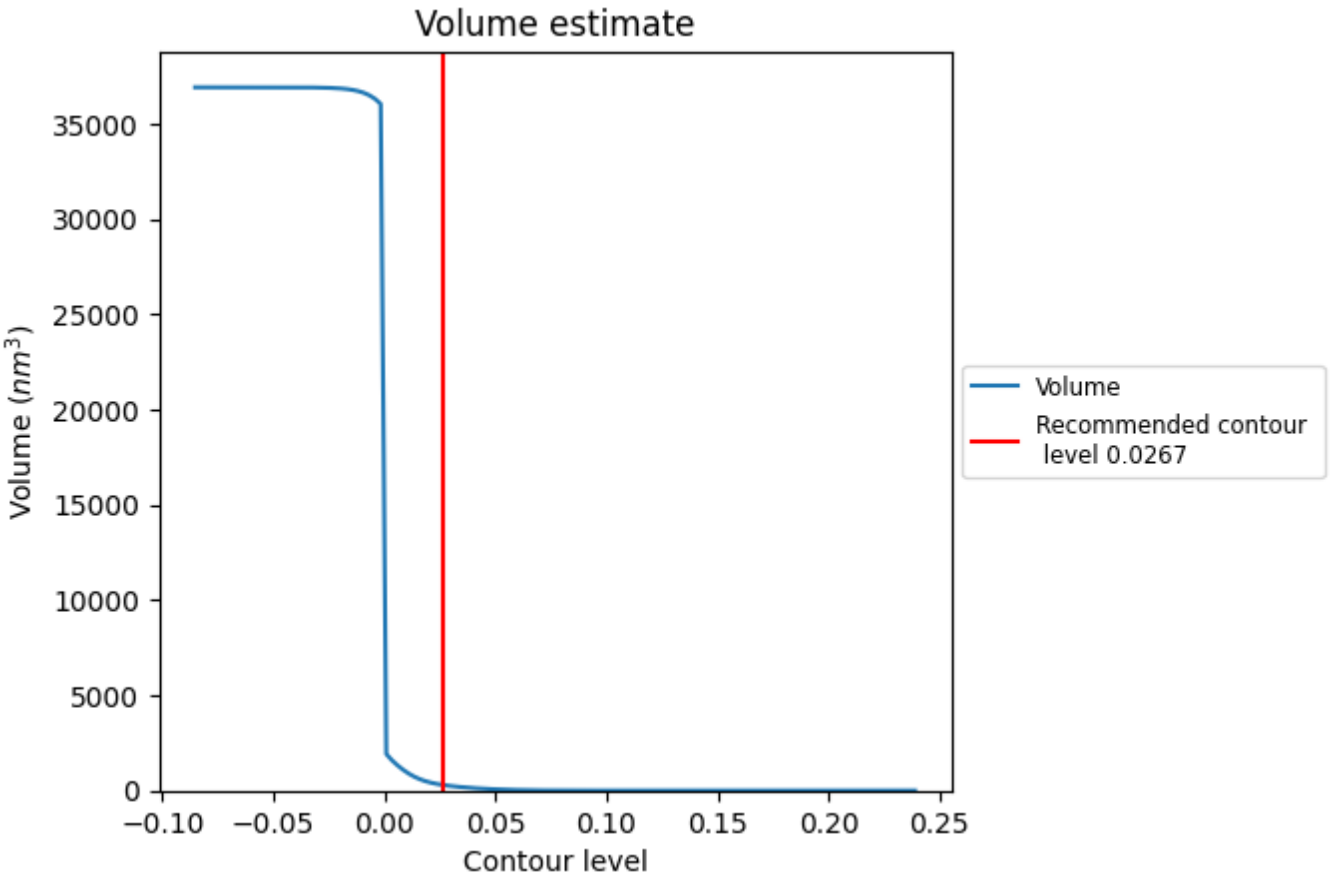
This section contains the results of statistical analysis of the map.

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.

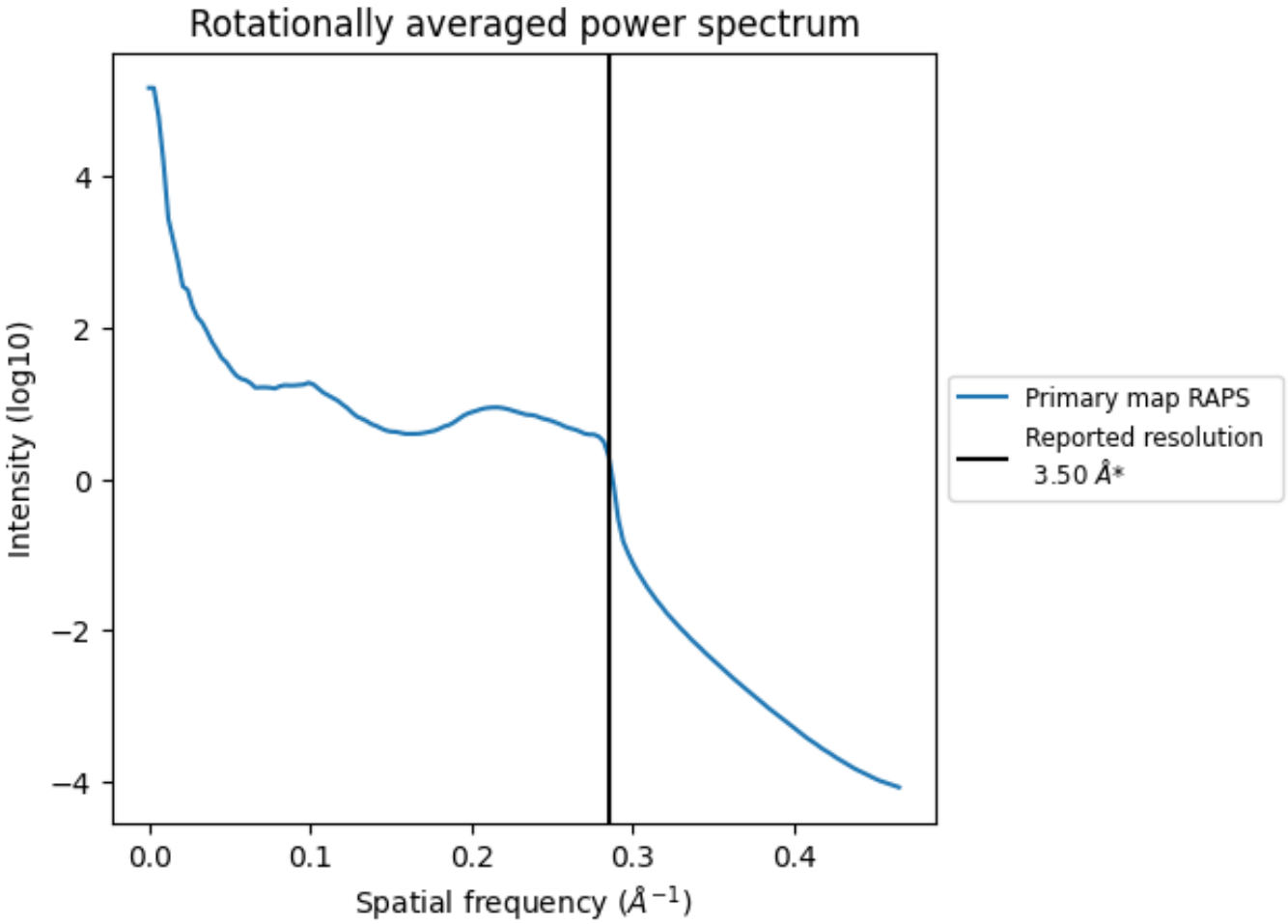
7.2 Volume estimate (i)



The volume at the recommended contour level is 289 nm^3; this corresponds to an approximate mass of 261 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 (i)



*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

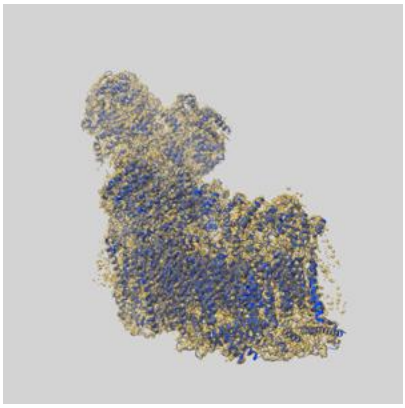
8 Fourier-Shell correlation (i)

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

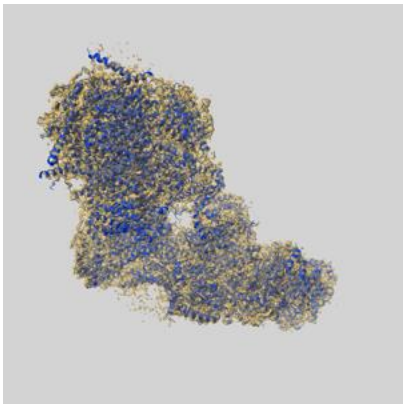
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32253 and PDB model 7W1O. Per-residue inclusion information can be found in section 3 on page 20.

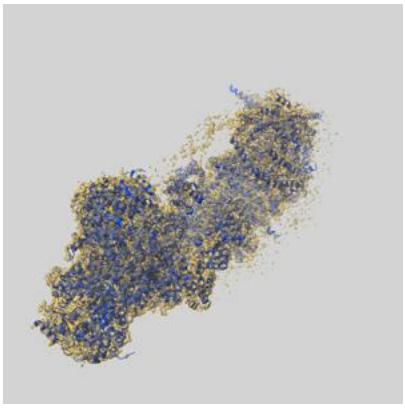
9.1 Map-model overlay



X



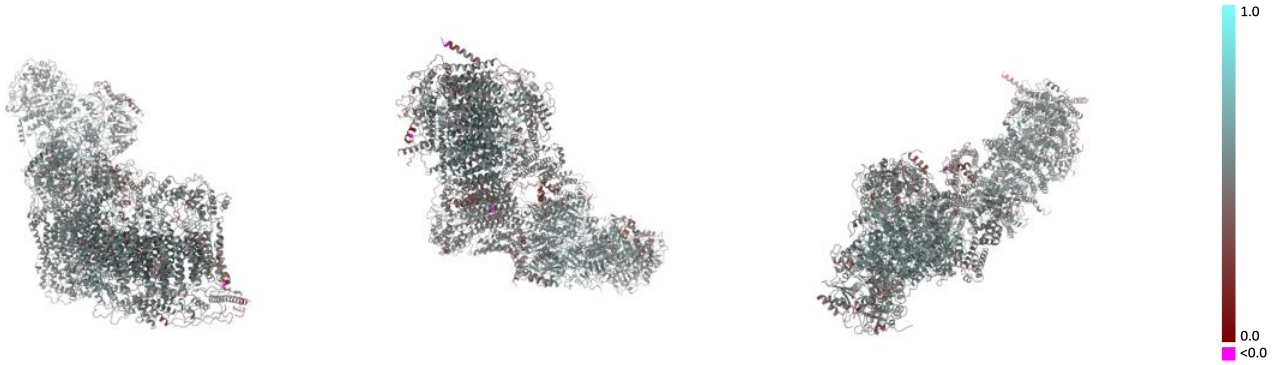
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0267 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.

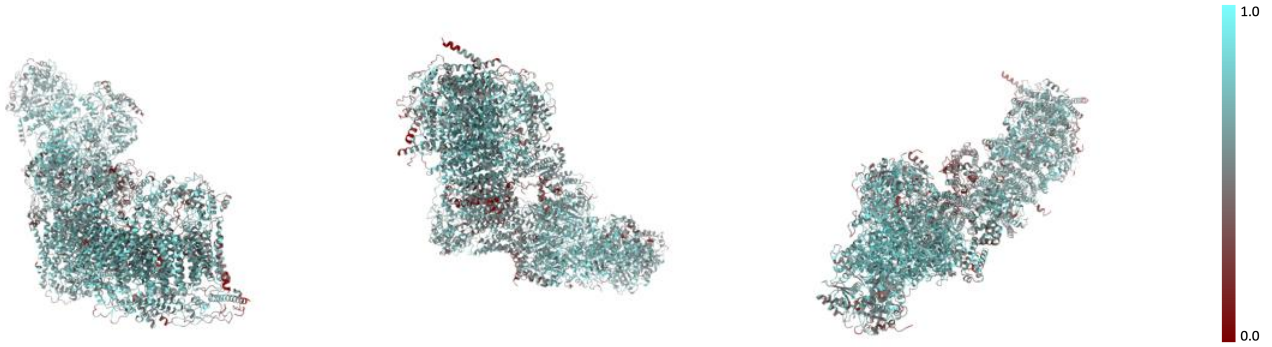
9.2 Q-score mapped to coordinate model (i)



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.

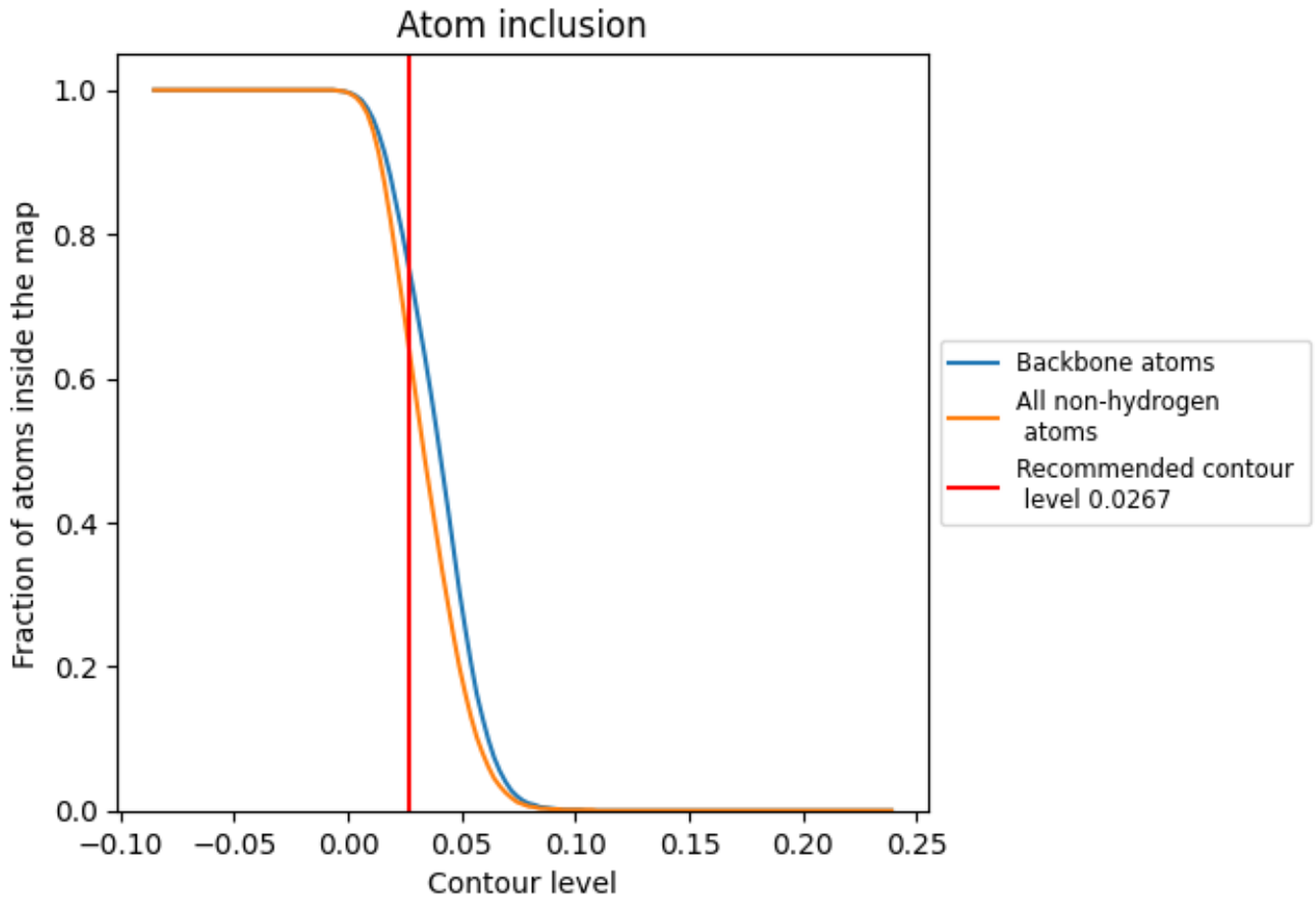
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0267).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6440	0.5020
A	0.6230	0.4850
B	0.7710	0.5530
C	0.7660	0.5350
E	0.6670	0.5000
F	0.5370	0.4390
G	0.3860	0.3860
H	0.6160	0.4880
I	0.6390	0.5110
J	0.6210	0.4870
K	0.6160	0.4970
L	0.6980	0.5360
M	0.7020	0.5200
N	0.6460	0.5080
O	0.6160	0.4840
P	0.7670	0.5420
Q	0.7420	0.5390
S	0.7030	0.5140
T	0.6870	0.5260
U	0.6250	0.4820
V	0.3520	0.4240
W	0.6730	0.5070
X	0.5500	0.4730
Y	0.4960	0.4390
Z	0.4620	0.3890
a	0.6520	0.5090
b	0.5710	0.4670
c	0.6520	0.5010
d	0.6270	0.4840
e	0.5990	0.4880
f	0.5810	0.4700
g	0.6470	0.5170
h	0.6430	0.4920
i	0.7130	0.5320
j	0.5140	0.4740

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Chain	Atom inclusion	Q-score
k	0.5460	0.4780
l	0.6250	0.5070
m	0.5370	0.4710
n	0.5520	0.4760
o	0.6400	0.5010
p	0.6410	0.4980
r	0.7070	0.5340
s	0.6800	0.5120
u	0.6440	0.5040
v	0.5440	0.4520
w	0.6140	0.4850