Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 03:08 PM JST

PDB ID	:	7V32
EMDB ID	:	EMD-31650
Title	:	Deactive state complex I from rotenone dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-10
Resolution	:	3.20 Å(reported)

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

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

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

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

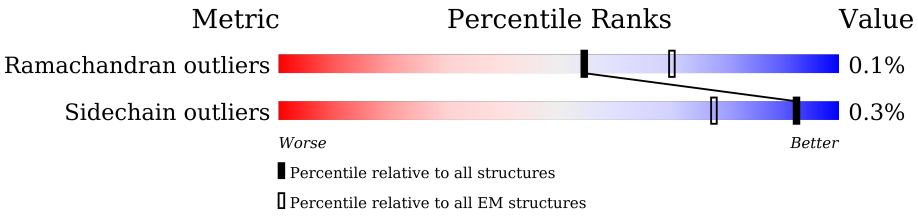
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	100%
2	B	176	100%
3	C	156	100%
4	E	115	10% 100%
5	F	86	15% 100%
6	G	88	34% 99%
6	X	88	7% 100%
7	H	112	100%
8	I	112	5% 87% 13%

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Mol	Chain	Length	Quality of chain
9	J	341	9% 87% 13%
10	K	42	26% 100%
11	L	125	6% 99%
12	M	690	100%
13	N	144	99%
14	O	217	8% 99%
15	P	208	100%
16	Q	430	97%
17	S	70	100%
18	T	96	17% 100%
19	U	83	100%
20	V	140	18% 99%
21	W	142	100%
22	Y	70	24% 99%
23	Z	84	23% 100%
24	a	140	100%
25	b	126	11% 81% 18%
26	c	156	100%
27	d	175	7% 99%
28	e	107	12% 100%
29	f	42	17% 100%
30	g	121	100%
31	h	105	100%
32	i	347	99%
33	j	113	9% 87% 12%

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Mol	Chain	Length	Quality of chain
34	k	98	6% 99%
35	l	603	99%
36	m	175	8% 74% 26%
37	n	56	18% 100%
38	o	128	100%
39	p	178	100%
40	r	459	100%
41	s	318	95% 5%
42	u	171	100%
43	v	131	18% 93% 5%
44	w	320	10% 100%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 66596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

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

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

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			664	425	102	132	5		
6	X	88	Total	C	N	O	S	0	0
			693	445	102	141	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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
			2352	1511	421	412	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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
			5293	3319	923	1012	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
			1660	1057	281	312	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	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
			567	364	104	94	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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1161	760	199	199	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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
			1315	853	213	241	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
			1461	916	265	272	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
			890	568	145	173	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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
			2710	1782	420	462	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
			4785	3173	741	820	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
			456	295	83	77	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
			1062	691	182	189		

- 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
			3631	2412	572	609	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
			1398	887	250	251	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
			992	622	180	181	9		

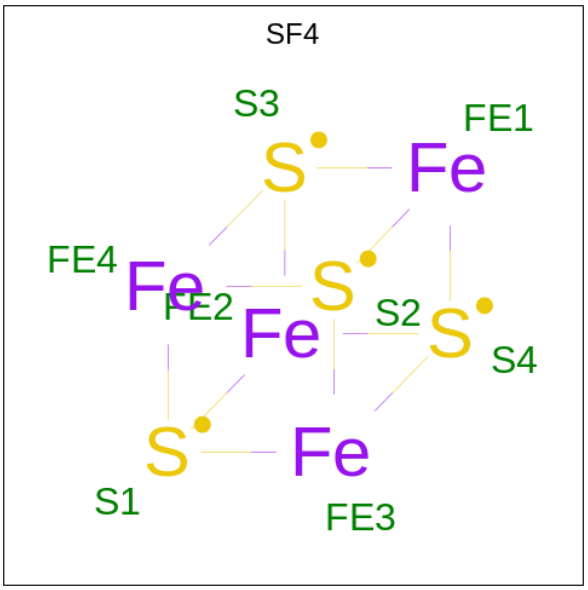
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

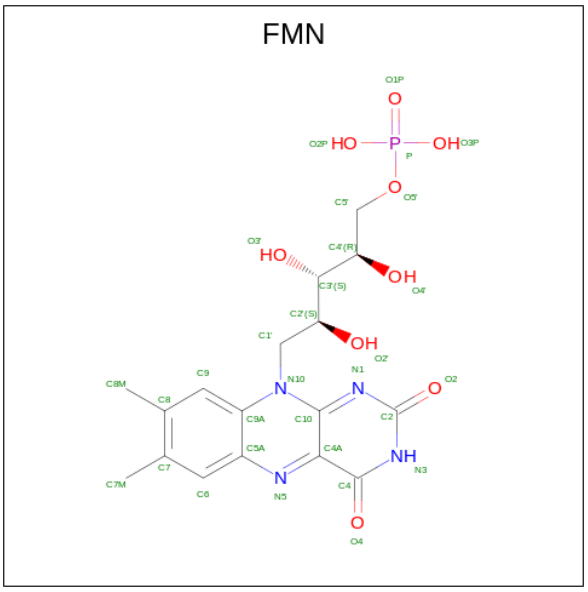
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



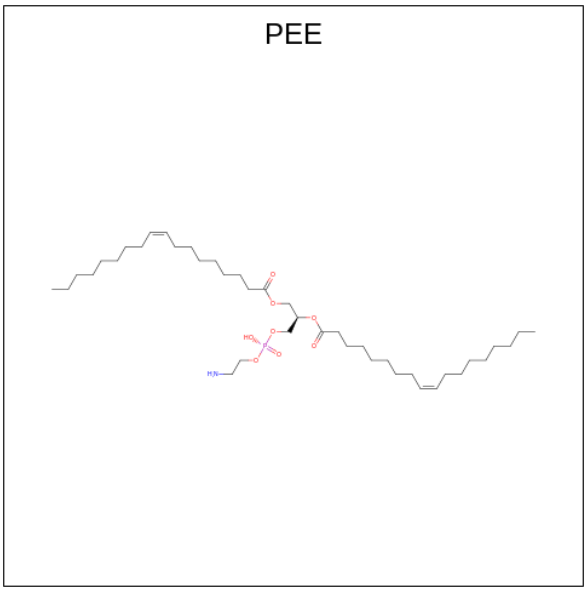
Mol	Chain	Residues	Atoms				AltConf
45	A	1	Total	Fe	S		0
			8	4	4		
45	B	1	Total	Fe	S		0
			16	8	8		
45	B	1	Total	Fe	S		0
			16	8	8		
45	C	1	Total	Fe	S		0
			8	4	4		
45	M	1	Total	Fe	S		0
			16	8	8		
45	M	1	Total	Fe	S		0
			16	8	8		

- 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 1,2-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
47	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	U	1	Total	C	N	O	P	0
			51	41	1	8	1	

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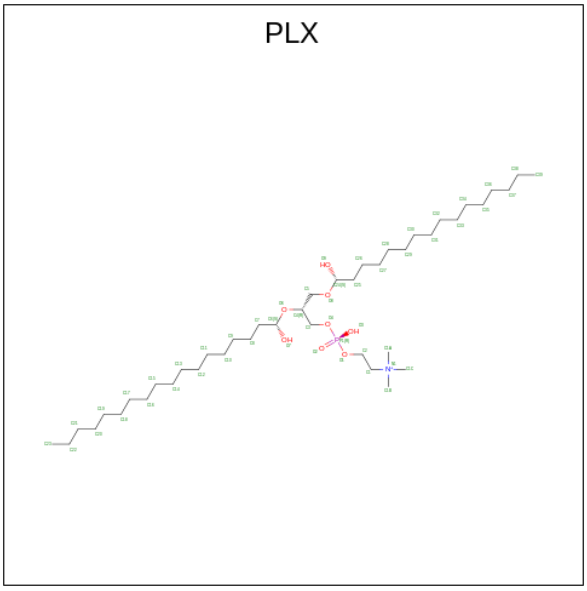
Mol	Chain	Residues	Atoms					AltConf
47	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	j	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	l	1	Total	C	N	O	P	0
			92	72	2	16	2	
47	l	1	Total	C	N	O	P	0
			92	72	2	16	2	
47	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 48 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
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	

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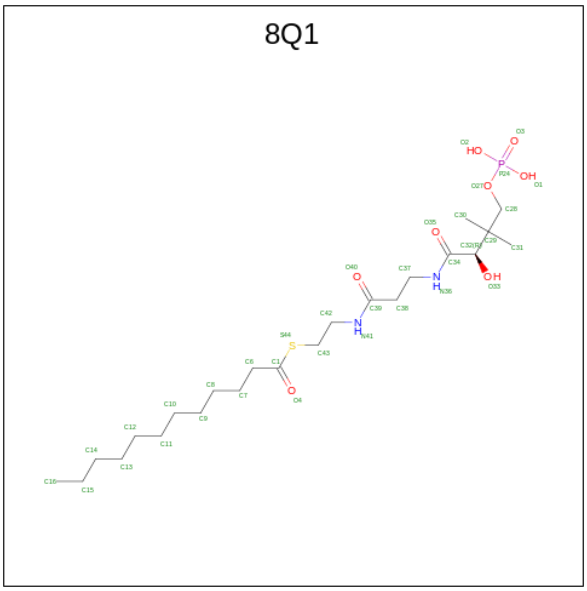
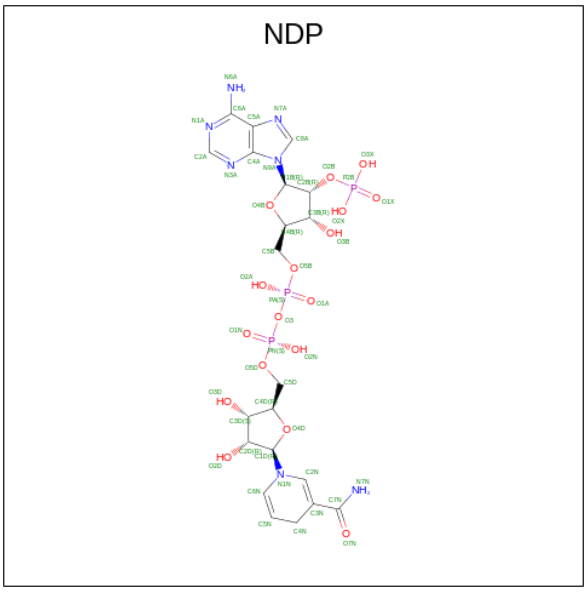
Mol	Chain	Residues	Atoms					AltConf
48	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
48	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- 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).



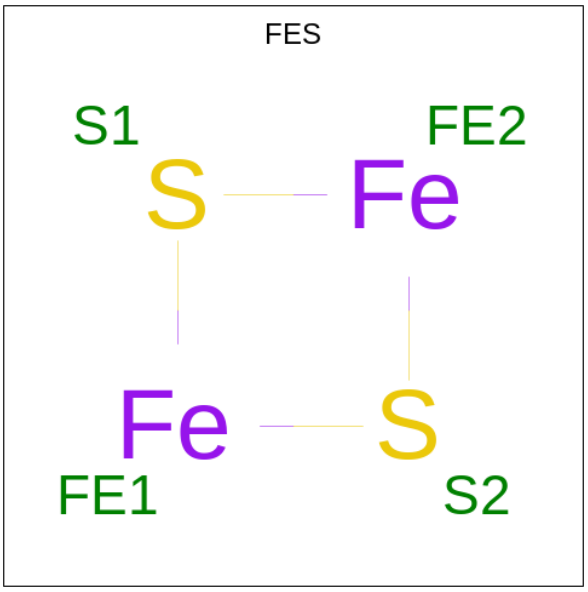
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- 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).

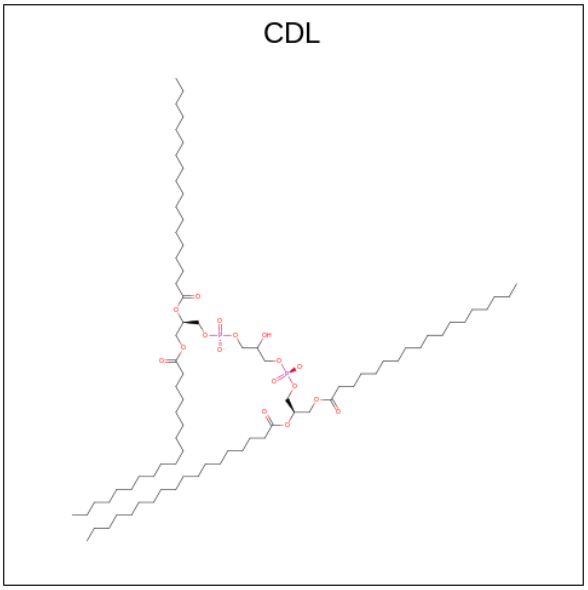


Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

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

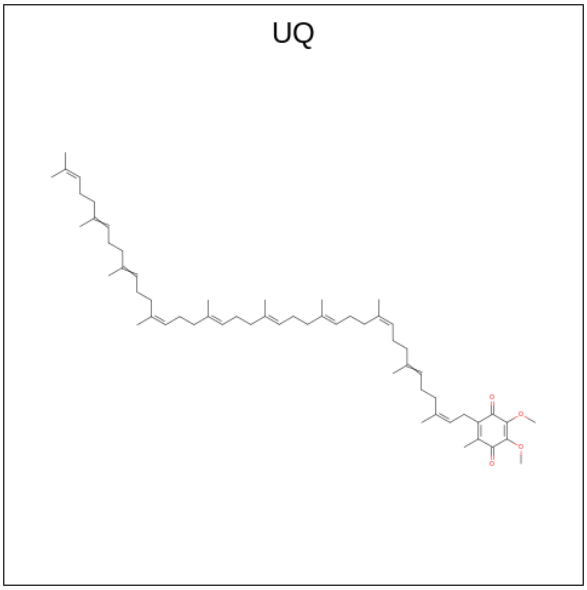


Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			51	32	17	2	
53	a	1	Total	C	O	P	0
			91	72	17	2	
53	g	1	Total	C	O	P	0
			100	81	17	2	
53	i	1	Total	C	O	P	0
			66	47	17	2	
53	l	1	Total	C	O	P	0
			199	161	34	4	
53	l	1	Total	C	O	P	0
			199	161	34	4	
53	n	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

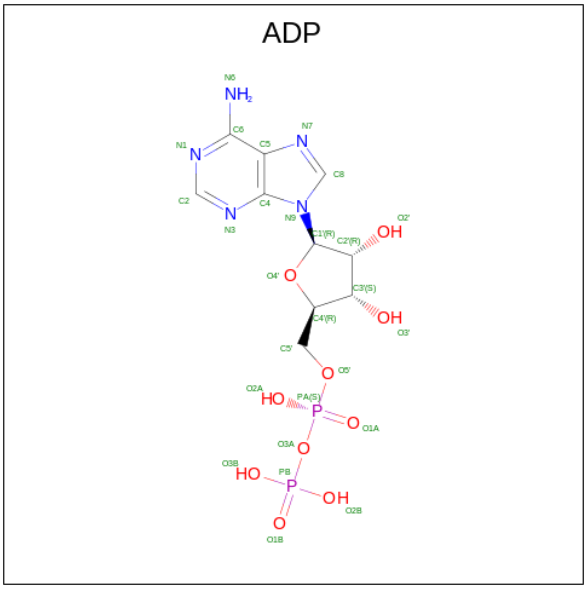
Mol	Chain	Residues	Atoms	AltConf
54	T	1	Total Zn 1 1	0

- Molecule 55 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
55	s	1	Total C O 28 24 4	0

- Molecule 56 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).



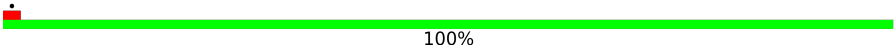
Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

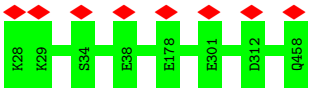
3 Residue-property plots (i)

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

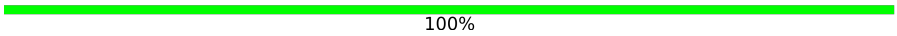
Chain A:





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

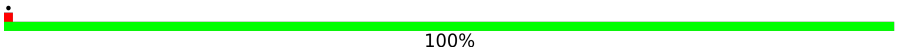
Chain B:



There are no outlier residues recorded for this chain.

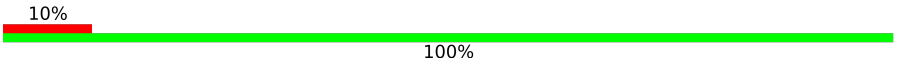
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7,mitochondrial

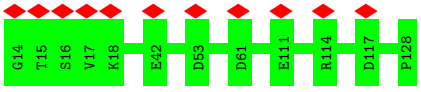
Chain C:



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

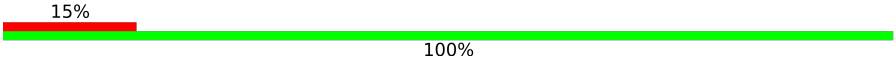
Chain E:

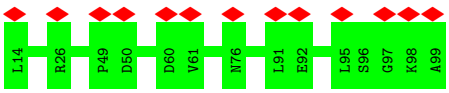




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

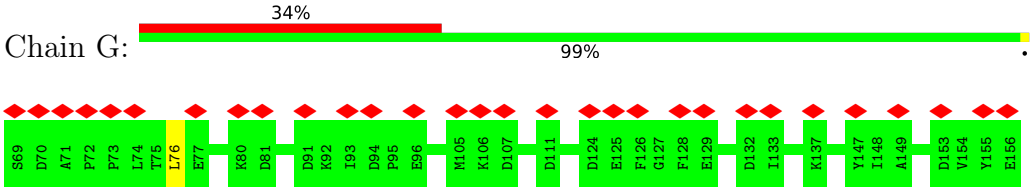
Chain F:





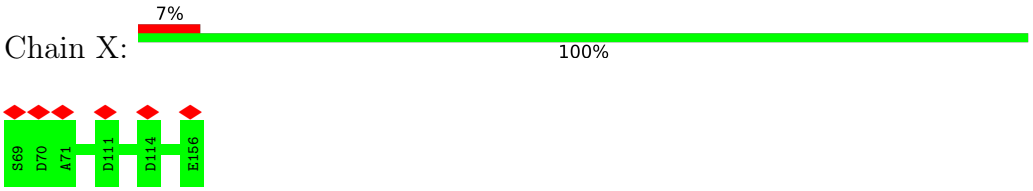
• Molecule 6: Acyl carrier protein, mitochondrial

Chain G:



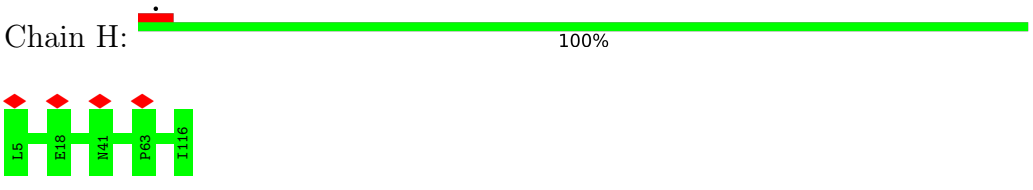
• Molecule 6: Acyl carrier protein, mitochondrial

Chain X:



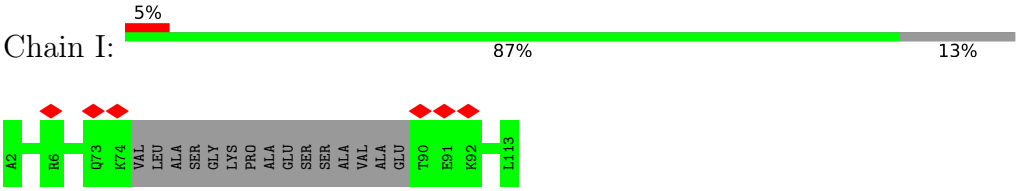
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H:



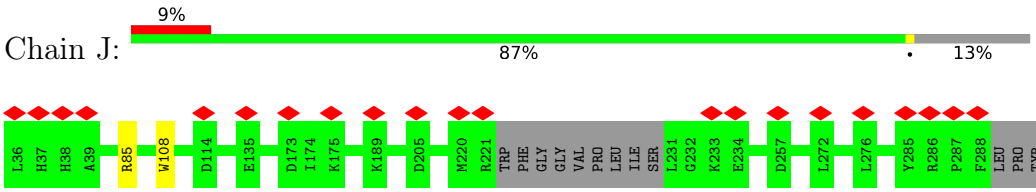
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I:



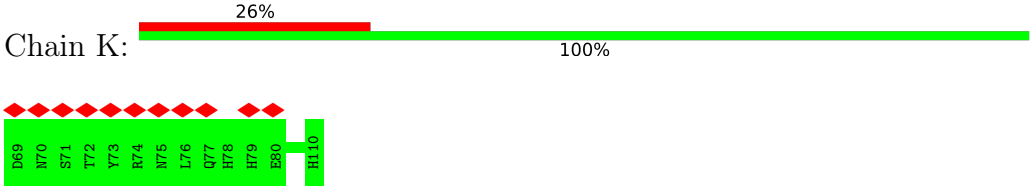
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:



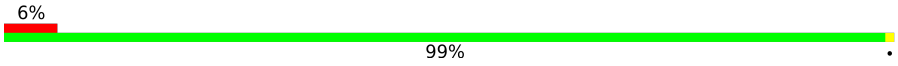
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

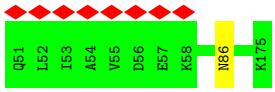
Chain K:



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

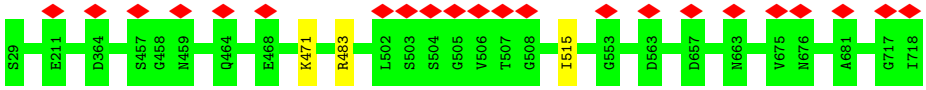
Chain L:





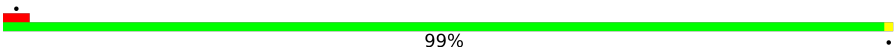
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

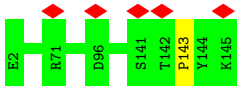
Chain M:



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

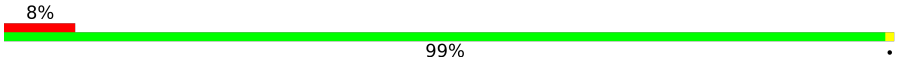
Chain N:

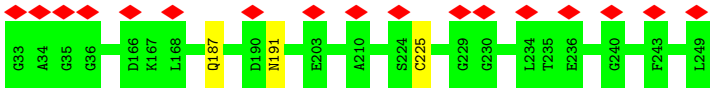




• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

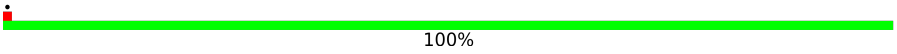
Chain O:

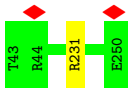




• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

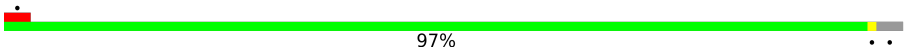
Chain P:

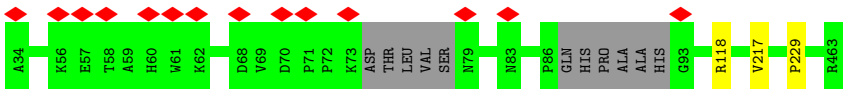




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

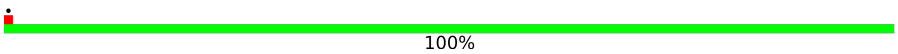
Chain Q:





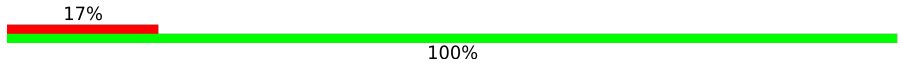
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

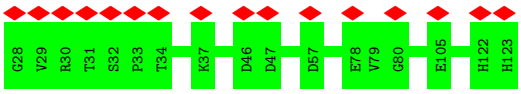
Chain S:



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

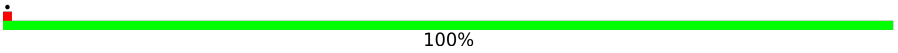
Chain T:

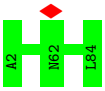




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

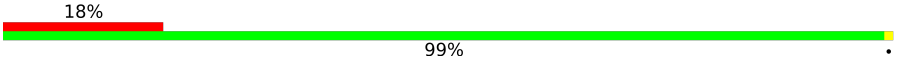
Chain U:

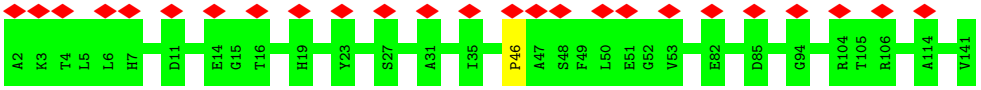




• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

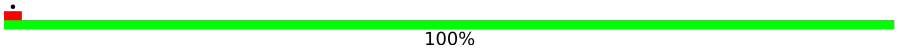
Chain V:

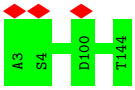




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

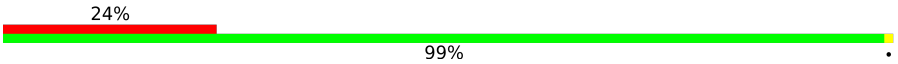
Chain W:

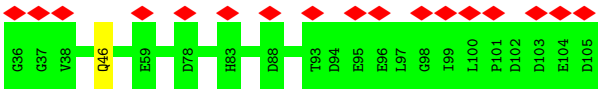




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

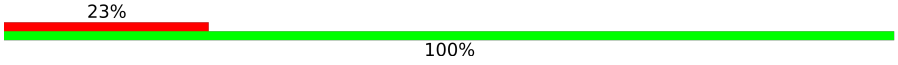
Chain Y:

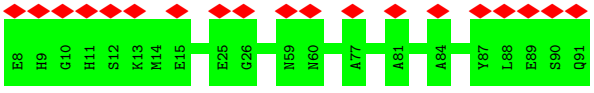




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

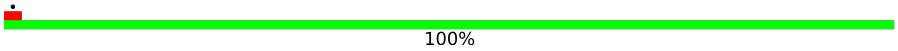
Chain Z:

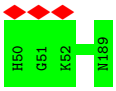




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

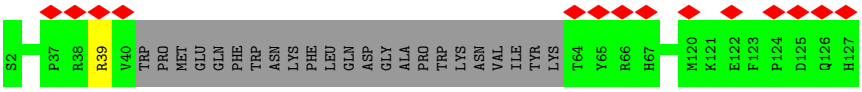
Chain a:





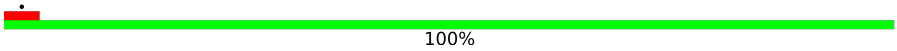
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

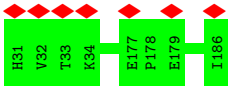
Chain b:



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

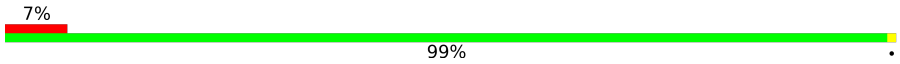
Chain c:

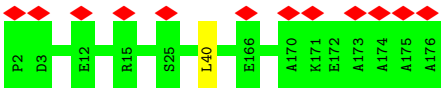




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

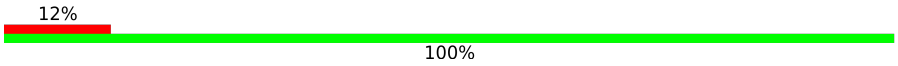
Chain d:

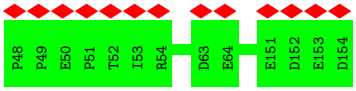




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

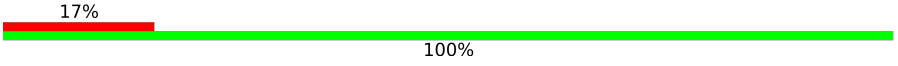
Chain e:

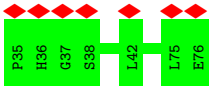




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

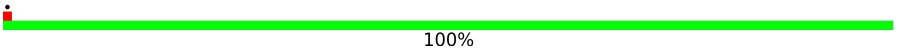
Chain f:





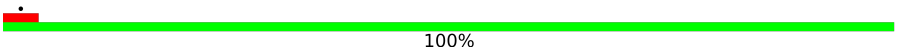
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

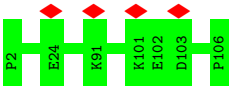
Chain g:



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

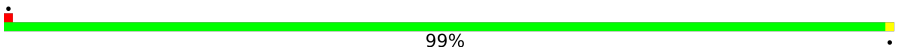
Chain h:

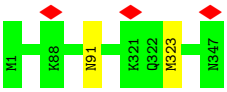




• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

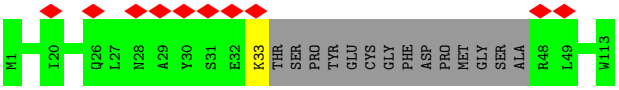
Chain i:





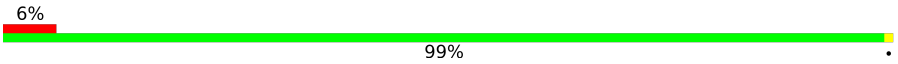
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

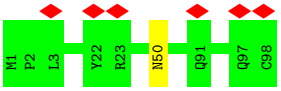
Chain j:



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

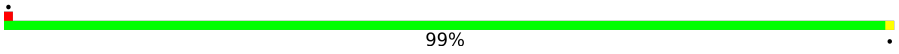
Chain k:

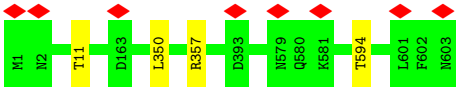




• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

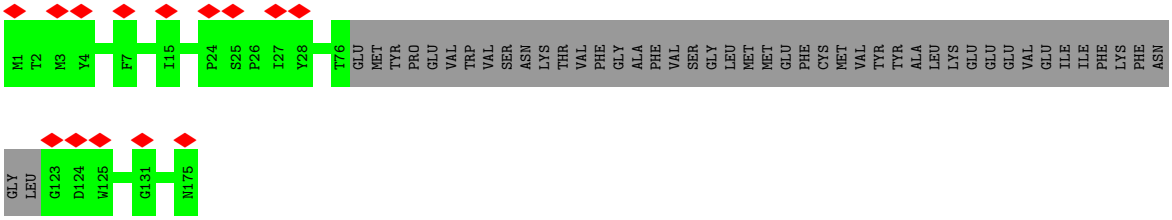
Chain l:



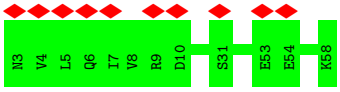


• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

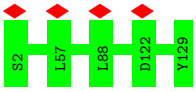
Chain m:



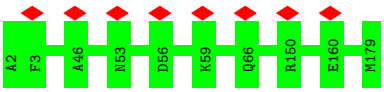
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

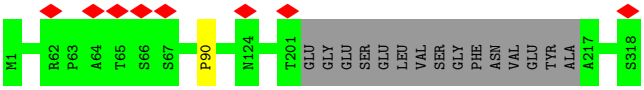


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

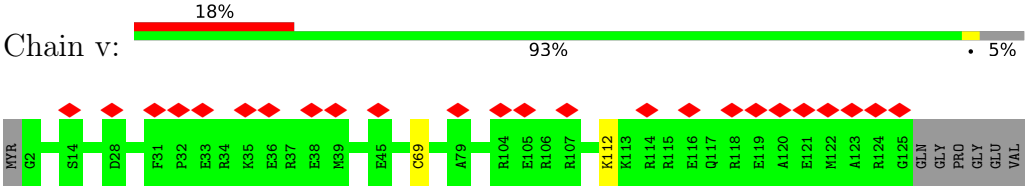
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



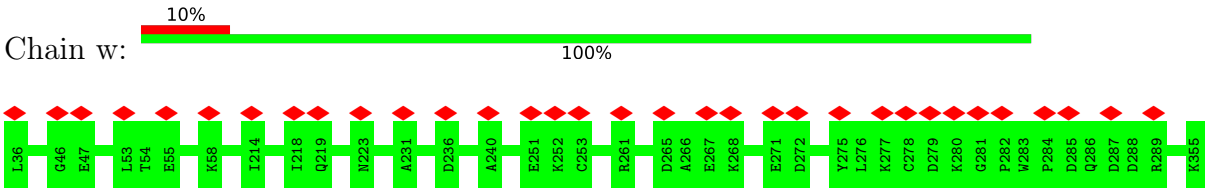
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

There are no outlier residues recorded for this chain.

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



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63623	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	0.209	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0222	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

5.1 Standard geometry

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

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	0/3393	0.50	0/4584
2	B	0.25	0/1443	0.50	0/1952
3	C	0.25	0/1279	0.54	0/1730
4	E	0.25	0/995	0.53	0/1340
5	F	0.28	0/702	0.57	0/945
6	G	0.24	0/673	0.50	0/911
6	X	0.25	0/705	0.44	0/956
7	H	0.23	0/929	0.44	0/1258
8	I	0.24	0/798	0.52	0/1079
9	J	0.25	0/2404	0.50	0/3245
10	K	0.23	0/365	0.51	0/493
11	L	0.24	0/1039	0.48	0/1403
12	M	0.24	0/5381	0.49	0/7291
13	N	0.27	0/1245	0.59	1/1694 (0.1%)
14	O	0.26	0/1699	0.48	0/2313
15	P	0.25	0/1789	0.50	0/2436
16	Q	0.26	0/3451	0.49	0/4672
17	S	0.24	0/582	0.48	0/783
18	T	0.24	0/755	0.51	0/1018
19	U	0.25	0/664	0.44	0/912
20	V	0.25	0/1042	0.48	0/1411
21	W	0.27	0/1198	0.50	0/1617
22	Y	0.25	0/626	0.46	0/857
23	Z	0.24	0/695	0.45	0/939
24	a	0.26	0/1195	0.49	0/1618
25	b	0.25	0/906	0.53	0/1232
26	c	0.25	0/1371	0.47	0/1875
27	d	0.25	0/1494	0.52	1/2015 (0.0%)
28	e	0.25	0/916	0.51	0/1246
29	f	0.23	0/350	0.42	0/473
30	g	0.26	0/1031	0.47	0/1394
31	h	0.25	0/889	0.49	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.25	0/2773	0.44	0/3768
33	j	0.26	0/819	0.46	0/1117
34	k	0.25	0/759	0.44	0/1029
35	l	0.25	0/4914	0.45	1/6683 (0.0%)
36	m	0.27	0/973	0.47	0/1320
37	n	0.23	0/468	0.53	0/633
38	o	0.27	0/1092	0.53	0/1481
39	p	0.25	0/1590	0.51	0/2155
40	r	0.25	0/3723	0.45	0/5078
41	s	0.26	0/2464	0.47	0/3369
42	u	0.25	0/1436	0.50	0/1938
43	v	0.25	0/1016	0.53	0/1370
44	w	0.25	0/2646	0.47	0/3584
All	All	0.25	0/66677	0.49	3/90407 (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})
13	N	143	PRO	CA-N-CD	-8.52	99.58	111.50
27	d	40	LEU	CA-CB-CG	5.59	128.16	115.30
35	l	350	LEU	CA-CB-CG	5.29	127.46	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	85 (99%)	0	1 (1%)	13	49
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	81 (87%)	12 (13%)	0	100	100
9	J	289/341 (85%)	278 (96%)	11 (4%)	0	100	100
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	22 (3%)	0	100	100
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	11 (3%)	1 (0%)	47	79
17	S	68/70 (97%)	68 (100%)	0	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	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%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	96 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	575 (96%)	26 (4%)	0	100	100
36	m	125/175 (71%)	113 (90%)	12 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
40	r	457/459 (100%)	446 (98%)	10 (2%)	1 (0%)	47	79
41	s	299/318 (94%)	290 (97%)	8 (3%)	1 (0%)	41	74
42	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
43	v	122/131 (93%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8315 (97%)	7732 (96%)	292 (4%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	76	LEU
40	r	48	ASN
16	Q	229	PRO
20	V	46	PRO
41	s	90	PRO

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	345/345 (100%)	345 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	66/81 (82%)	66 (100%)	0	100	100
6	X	76/81 (94%)	76 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	253/295 (86%)	251 (99%)	2 (1%)	81	93
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	91
12	M	579/580 (100%)	576 (100%)	3 (0%)	88	95
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	180/183 (98%)	177 (98%)	3 (2%)	60	83
15	P	190/190 (100%)	189 (100%)	1 (0%)	88	95
16	Q	361/370 (98%)	360 (100%)	1 (0%)	92	96
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	63/63 (100%)	62 (98%)	1 (2%)	62	84
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	121/122 (99%)	121 (100%)	0	100	100
25	b	98/119 (82%)	97 (99%)	1 (1%)	76	90
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	309 (99%)	2 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	j	88/99 (89%)	87 (99%)	1 (1%)	73 88
34	k	85/85 (100%)	84 (99%)	1 (1%)	71 88
35	l	537/537 (100%)	534 (99%)	3 (1%)	86 94
36	m	99/141 (70%)	99 (100%)	0	100 100
37	n	46/53 (87%)	46 (100%)	0	100 100
38	o	113/113 (100%)	113 (100%)	0	100 100
39	p	159/159 (100%)	159 (100%)	0	100 100
40	r	410/410 (100%)	410 (100%)	0	100 100
41	s	263/275 (96%)	263 (100%)	0	100 100
42	u	153/153 (100%)	153 (100%)	0	100 100
43	v	97/115 (84%)	95 (98%)	2 (2%)	53 79
44	w	282/283 (100%)	282 (100%)	0	100 100
All	All	7036/7238 (97%)	7014 (100%)	22 (0%)	92 96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	85	ARG
9	J	108	TRP
11	L	86	ASN
12	M	471	LYS
12	M	483	ARG
12	M	515	ILE
14	O	187	GLN
14	O	191	ASN
14	O	225	CYS
15	P	231	ARG
16	Q	217	VAL
22	Y	46	GLN
25	b	39	ARG
32	i	91	ASN
32	i	323	MET
33	j	33	LYS
34	k	50	ASN
35	l	11	THR
35	l	357	ARG
35	l	594	THR
43	v	69	CYS

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Mol	Chain	Res	Type
43	v	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
7	H	83	GLN
12	M	260	ASN
12	M	460	HIS
12	M	604	GLN
12	M	669	ASN
14	O	187	GLN
15	P	75	GLN
16	Q	60	HIS
25	b	89	HIS
26	c	132	HIS
32	i	36	ASN
32	i	91	ASN
32	i	268	GLN
37	n	14	HIS
38	o	79	ASN
40	r	26	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	1.98	1 (10%)	5,13,15	5.90	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	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	12.04	130.52	119.48
16	Q	118	2MR	CD-NE-CZ	4.31	131.49	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.11	130.74	123.86

There are no chirality outliers.

All (2) 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

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 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	SF4	C	301	3	0,12,12	-	-	-		
49	8Q1	X	201	-	31,34,34	2.16	6 (19%)	40,43,43	1.68	9 (22%)
47	PEE	j	201	-	46,46,50	1.21	6 (13%)	49,51,55	0.98	2 (4%)
48	PLX	C	302	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
48	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
47	PEE	l	704	-	45,45,50	1.21	6 (13%)	48,50,55	1.03	2 (4%)
45	SF4	M	802	12	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
53	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
47	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.01	2 (3%)
53	CDL	N	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.31	6 (10%)
51	FES	M	803	12	0,4,4	-	-	-		
53	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.19	5 (7%)
53	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
47	PEE	U	101	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
53	CDL	n	101	-	77,77,99	1.03	4 (5%)	83,89,111	1.10	4 (4%)
56	ADP	w	401	-	24,29,29	3.11	6 (25%)	29,45,45	1.34	3 (10%)
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
47	PEE	l	703	-	45,45,50	1.21	6 (13%)	48,50,55	0.99	2 (4%)
49	8Q1	G	201	-	31,34,34	2.15	6 (19%)	40,43,43	1.67	10 (25%)
48	PLX	a	202	-	51,51,51	0.62	0	55,59,59	0.68	0
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.23	8 (16%)
47	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-		
51	FES	O	301	14	0,4,4	-	-	-		
55	UQ	s	401	-	28,28,63	3.29	7 (25%)	34,37,79	2.71	10 (29%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
50	NDP	J	401	-	45,52,52	4.53	20 (44%)	53,80,80	1.99	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
53	CDL	g	202	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
48	PLX	g	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
47	PEE	m	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.00	2 (4%)
53	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.09	6 (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
45	SF4	C	301	3	-	-	0/6/5/5
49	8Q1	X	201	-	-	22/41/41/41	-
47	PEE	j	201	-	-	23/50/50/54	-
48	PLX	C	302	-	-	29/55/55/55	-
48	PLX	r	503	-	-	32/55/55/55	-
47	PEE	l	704	-	-	26/49/49/54	-
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
53	CDL	l	701	-	-	52/109/109/110	-
47	PEE	r	501	-	-	22/54/54/54	-
53	CDL	N	201	-	-	23/61/61/110	-
53	CDL	i	401	-	-	26/76/76/110	-
51	FES	M	803	12	-	-	0/1/1/1
53	CDL	l	702	-	-	62/110/110/110	-
47	PEE	U	101	-	-	23/54/54/54	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
53	CDL	n	101	-	-	32/88/88/110	-
56	ADP	w	401	-	-	4/12/32/32	0/3/3/3
47	PEE	B	303	-	-	23/54/54/54	-
47	PEE	l	703	-	-	26/49/49/54	-
49	8Q1	G	201	-	-	15/41/41/41	-
48	PLX	a	202	-	-	18/55/55/55	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
47	PEE	i	402	-	-	19/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	M	801	12	-	-	0/6/5/5
51	FES	O	301	14	-	-	0/1/1/1
55	UQ	s	401	-	-	9/21/45/87	0/1/1/1
48	PLX	r	502	-	-	21/55/55/55	-
50	NDP	J	401	-	-	9/30/77/77	0/4/5/5
48	PLX	j	202	-	-	31/55/55/55	-
53	CDL	g	202	-	-	64/110/110/110	-
48	PLX	g	201	-	-	21/55/55/55	-
47	PEE	m	201	-	-	22/44/44/54	-
53	CDL	a	201	-	-	23/101/101/110	-

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-12.42	1.25	1.52
50	J	401	NDP	C6N-C5N	12.31	1.55	1.33
50	J	401	NDP	O4D-C4D	10.67	1.68	1.45
50	J	401	NDP	C3D-C4D	-9.92	1.27	1.53
55	s	401	UQ	C13-C14	9.35	1.55	1.33
56	w	401	ADP	C3'-C4'	-9.06	1.29	1.53
55	s	401	UQ	C8-C9	8.97	1.54	1.33
50	J	401	NDP	O4B-C1B	8.28	1.52	1.41
55	s	401	UQ	C18-C19	8.24	1.56	1.32
50	J	401	NDP	O4B-C4B	-7.97	1.27	1.45
49	X	201	8Q1	P24-O27	7.97	1.85	1.60
49	G	201	8Q1	P24-O27	7.81	1.85	1.60
56	w	401	ADP	O4'-C4'	7.74	1.62	1.45
50	J	401	NDP	C2N-C3N	7.39	1.55	1.34
56	w	401	ADP	O4'-C1'	-6.55	1.31	1.41
50	J	401	NDP	P2B-O2B	5.61	1.69	1.59
50	J	401	NDP	C3B-C4B	5.36	1.66	1.53
50	J	401	NDP	O4D-C1D	-4.93	1.30	1.42
50	J	401	NDP	C6N-N1N	4.79	1.49	1.37
53	N	201	CDL	OA8-CA7	4.31	1.45	1.33
53	a	201	CDL	OA8-CA7	4.29	1.45	1.33
53	i	401	CDL	OA8-CA7	4.27	1.45	1.33
53	n	101	CDL	OA8-CA7	4.27	1.45	1.33
53	i	401	CDL	OB8-CB7	4.26	1.45	1.33
53	N	201	CDL	OB8-CB7	4.25	1.45	1.33
50	J	401	NDP	O2D-C2D	-4.22	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C7N-N7N	4.21	1.44	1.33
53	n	101	CDL	OB8-CB7	4.20	1.45	1.33
49	G	201	8Q1	C1-S44	4.17	1.86	1.76
53	i	401	CDL	OA6-CA5	4.17	1.46	1.34
53	i	401	CDL	OB6-CB5	4.16	1.46	1.34
53	n	101	CDL	OA6-CA5	4.15	1.46	1.34
53	a	201	CDL	OB8-CB7	4.15	1.45	1.33
53	a	201	CDL	OA6-CA5	4.14	1.46	1.34
53	N	201	CDL	OA6-CA5	4.13	1.45	1.34
53	a	201	CDL	OB6-CB5	4.09	1.45	1.34
50	J	401	NDP	C6A-N6A	4.07	1.48	1.34
53	N	201	CDL	OB6-CB5	4.07	1.45	1.34
53	n	101	CDL	OB6-CB5	3.95	1.45	1.34
46	A	502	FMN	C4A-N5	3.91	1.38	1.30
49	X	201	8Q1	C1-S44	3.89	1.85	1.76
56	w	401	ADP	C6-N6	3.84	1.48	1.34
47	m	201	PEE	C18-C19	3.76	1.53	1.31
47	j	201	PEE	C18-C19	3.75	1.53	1.31
47	l	703	PEE	C18-C19	3.72	1.53	1.31
47	l	704	PEE	C18-C19	3.71	1.53	1.31
47	B	303	PEE	C18-C19	3.71	1.53	1.31
47	r	501	PEE	C18-C19	3.71	1.53	1.31
47	U	101	PEE	C18-C19	3.68	1.53	1.31
47	i	402	PEE	C18-C19	3.67	1.53	1.31
47	j	201	PEE	C39-C38	3.65	1.52	1.31
49	G	201	8Q1	C34-N36	3.65	1.41	1.33
49	X	201	8Q1	C34-N36	3.63	1.41	1.33
47	r	501	PEE	C39-C38	3.63	1.52	1.31
47	B	303	PEE	C39-C38	3.62	1.52	1.31
47	i	402	PEE	C39-C38	3.62	1.52	1.31
47	l	703	PEE	C39-C38	3.62	1.52	1.31
47	U	101	PEE	C39-C38	3.62	1.52	1.31
47	l	704	PEE	C39-C38	3.61	1.52	1.31
49	X	201	8Q1	C6-C1	3.52	1.54	1.50
53	l	701	CDL	OA8-CA7	3.46	1.43	1.33
53	l	702	CDL	OA8-CA7	3.45	1.43	1.33
53	g	202	CDL	OA8-CA7	3.43	1.43	1.33
49	G	201	8Q1	C6-C1	3.37	1.54	1.50
56	w	401	ADP	O2'-C2'	-3.33	1.35	1.43
49	G	201	8Q1	O27-C28	-3.25	1.33	1.43
49	X	201	8Q1	O27-C28	-3.22	1.33	1.43
49	X	201	8Q1	C39-N41	3.21	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	G	201	8Q1	C39-N41	3.19	1.40	1.33
56	w	401	ADP	O3'-C3'	3.13	1.50	1.43
53	l	702	CDL	OB6-CB5	3.07	1.43	1.34
53	l	701	CDL	OB6-CB5	3.05	1.42	1.34
50	J	401	NDP	O3D-C3D	3.05	1.50	1.43
53	g	202	CDL	OB6-CB5	3.05	1.42	1.34
53	l	701	CDL	OB8-CB7	3.00	1.42	1.33
53	l	702	CDL	OB8-CB7	3.00	1.42	1.33
53	g	202	CDL	OB8-CB7	2.99	1.42	1.33
53	g	202	CDL	OA6-CA5	2.98	1.42	1.34
53	l	702	CDL	OA6-CA5	2.97	1.42	1.34
50	J	401	NDP	C7N-C3N	2.96	1.55	1.48
53	l	701	CDL	OA6-CA5	2.91	1.42	1.34
48	g	201	PLX	O6-C4	-2.71	1.41	1.44
48	C	302	PLX	O6-C4	-2.66	1.41	1.44
48	r	503	PLX	O6-C4	-2.65	1.41	1.44
48	j	202	PLX	O6-C4	-2.65	1.41	1.44
55	s	401	UQ	C6-C1	2.63	1.54	1.46
50	J	401	NDP	O2B-C2B	2.58	1.53	1.44
47	i	402	PEE	O3-C30	2.52	1.40	1.33
47	r	501	PEE	O2-C2	-2.49	1.40	1.46
47	r	501	PEE	O3-C30	2.48	1.40	1.33
47	B	303	PEE	O2-C2	-2.48	1.40	1.46
47	l	703	PEE	O2-C2	-2.47	1.40	1.46
46	A	502	FMN	C10-N1	2.46	1.38	1.33
47	j	201	PEE	O2-C2	-2.46	1.40	1.46
47	i	402	PEE	O2-C2	-2.46	1.40	1.46
47	B	303	PEE	O3-C30	2.46	1.40	1.33
47	l	704	PEE	O2-C2	-2.46	1.40	1.46
47	l	703	PEE	O3-C30	2.44	1.40	1.33
48	j	202	PLX	C7-C6	2.42	1.55	1.50
53	l	701	CDL	OA6-CA4	-2.41	1.40	1.46
47	j	201	PEE	O3-C30	2.41	1.40	1.33
47	l	704	PEE	O3-C30	2.40	1.40	1.33
53	l	702	CDL	OA6-CA4	-2.40	1.40	1.46
47	m	201	PEE	O2-C10	2.39	1.41	1.34
47	U	101	PEE	O3-C30	2.39	1.40	1.33
48	g	201	PLX	C7-C6	2.37	1.55	1.50
53	g	202	CDL	OA6-CA4	-2.37	1.40	1.46
48	r	502	PLX	C7-C6	2.34	1.55	1.50
47	U	101	PEE	O2-C2	-2.34	1.40	1.46
55	s	401	UQ	C7-C8	2.33	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C2D-C3D	2.32	1.59	1.53
48	C	302	PLX	C7-C6	2.31	1.55	1.50
47	U	101	PEE	O2-C10	2.30	1.40	1.34
48	r	503	PLX	C7-C6	2.29	1.55	1.50
47	j	201	PEE	O2-C10	2.29	1.40	1.34
47	m	201	PEE	O3-C30	2.29	1.40	1.33
47	i	402	PEE	O2-C10	2.26	1.40	1.34
48	r	502	PLX	O6-C4	-2.24	1.41	1.44
47	m	201	PEE	O2-C2	-2.23	1.41	1.46
53	g	202	CDL	PB2-OB2	2.23	1.68	1.59
47	m	201	PEE	O3-C3	-2.22	1.40	1.45
53	l	701	CDL	PB2-OB2	2.22	1.68	1.59
53	l	702	CDL	PB2-OB2	2.21	1.68	1.59
53	g	202	CDL	PB2-OB5	2.20	1.68	1.59
47	l	704	PEE	O3-C3	-2.20	1.40	1.45
47	r	501	PEE	O2-C10	2.19	1.40	1.34
53	l	702	CDL	PB2-OB5	2.19	1.68	1.59
47	B	303	PEE	O2-C10	2.18	1.40	1.34
53	l	701	CDL	PB2-OB5	2.17	1.68	1.59
47	l	704	PEE	O2-C10	2.17	1.40	1.34
55	s	401	UQ	O4-C4	-2.17	1.18	1.23
47	l	703	PEE	O3-C3	-2.16	1.40	1.45
50	J	401	NDP	O7N-C7N	-2.16	1.19	1.24
48	j	202	PLX	P1-O4	2.15	1.68	1.59
48	r	502	PLX	P1-O4	2.14	1.68	1.59
48	r	503	PLX	P1-O4	2.14	1.68	1.59
47	l	703	PEE	O2-C10	2.14	1.40	1.34
47	j	201	PEE	O3-C3	-2.13	1.40	1.45
53	l	701	CDL	OB6-CB4	-2.13	1.41	1.46
48	C	302	PLX	P1-O4	2.12	1.67	1.59
47	i	402	PEE	O3-C3	-2.12	1.40	1.45
55	s	401	UQ	O1-C1	-2.11	1.18	1.23
53	l	702	CDL	OB6-CB4	-2.11	1.41	1.46
48	g	201	PLX	P1-O4	2.11	1.67	1.59
53	g	202	CDL	OB6-CB4	-2.11	1.41	1.46
47	U	101	PEE	O3-C3	-2.09	1.40	1.45
47	r	501	PEE	O3-C3	-2.07	1.40	1.45
48	C	302	PLX	P1-O1	2.05	1.67	1.59
48	r	503	PLX	P1-O1	2.05	1.67	1.59
48	r	502	PLX	P1-O1	2.04	1.67	1.59
47	B	303	PEE	O3-C3	-2.04	1.40	1.45
48	j	202	PLX	P1-O1	2.03	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	g	201	PLX	P1-O1	2.01	1.67	1.59
50	J	401	NDP	PA-O5B	2.00	1.67	1.59

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	s	401	UQ	C7-C8-C9	-9.04	111.75	126.79
50	J	401	NDP	C3N-C2N-N1N	-8.29	111.27	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.58	110.16	121.11
55	s	401	UQ	C12-C13-C14	-5.87	113.52	127.66
50	J	401	NDP	C1D-N1N-C6N	-4.90	110.28	120.83
49	X	201	8Q1	C6-C1-S44	4.67	118.89	113.46
55	s	401	UQ	C11-C9-C8	-4.55	111.91	121.12
56	w	401	ADP	N3-C2-N1	-4.45	121.73	128.68
55	s	401	UQ	C10-C9-C8	-4.43	112.32	123.68
49	G	201	8Q1	C6-C1-S44	4.33	118.49	113.46
53	i	401	CDL	OA6-CA5-C11	4.32	120.80	111.50
47	B	303	PEE	O2-C10-C11	4.31	120.80	111.50
53	a	201	CDL	OB6-CB5-C51	4.26	120.68	111.50
47	r	501	PEE	O2-C10-C11	4.19	120.52	111.50
47	m	201	PEE	O2-C10-C11	4.17	120.50	111.50
50	J	401	NDP	N3A-C2A-N1A	-4.17	122.16	128.68
55	s	401	UQ	C15-C14-C13	-4.14	113.06	123.68
53	N	201	CDL	OB6-CB5-C51	4.12	120.38	111.50
53	n	101	CDL	OA6-CA5-C11	4.10	120.35	111.50
47	i	402	PEE	O2-C10-C11	4.10	120.33	111.50
53	N	201	CDL	OA6-CA5-C11	4.07	120.28	111.50
55	s	401	UQ	C17-C18-C19	-4.03	113.98	127.75
55	s	401	UQ	C16-C14-C13	-4.01	113.01	121.12
47	l	704	PEE	O2-C10-C11	4.00	120.12	111.50
47	j	201	PEE	O2-C10-C11	3.98	120.08	111.50
53	g	202	CDL	OB6-CB5-C51	3.98	120.08	111.50
53	l	701	CDL	OA6-CA5-C11	3.95	120.02	111.50
53	i	401	CDL	OB6-CB5-C51	3.95	120.02	111.50
53	l	702	CDL	OB6-CB5-C51	3.95	120.02	111.50
53	l	701	CDL	OB6-CB5-C51	3.93	119.97	111.50
47	U	101	PEE	O2-C10-C11	3.92	119.94	111.50
53	g	202	CDL	OA6-CA5-C11	3.91	119.93	111.50
53	n	101	CDL	OB6-CB5-C51	3.89	119.89	111.50
53	l	702	CDL	OA6-CA5-C11	3.89	119.88	111.50
47	l	703	PEE	O2-C10-C11	3.86	119.81	111.50
49	G	201	8Q1	C43-S44-C1	3.58	113.03	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	a	201	CDL	OA6-CA5-C11	3.53	119.10	111.50
55	s	401	UQ	C21-C19-C18	-3.33	113.03	122.65
49	G	201	8Q1	O35-C34-N36	-3.28	115.96	122.99
49	X	201	8Q1	C43-S44-C1	3.26	112.01	101.87
49	X	201	8Q1	O35-C34-N36	-3.20	116.13	122.99
46	A	502	FMN	C4-N3-C2	-3.09	119.93	125.64
55	s	401	UQ	C20-C19-C18	-3.08	113.73	122.65
53	a	201	CDL	OB8-CB7-C71	2.92	121.08	111.91
53	a	201	CDL	OA8-CA7-C31	2.92	121.06	111.91
49	G	201	8Q1	C37-C38-C39	2.90	117.18	112.36
55	s	401	UQ	CM5-C5-C6	-2.87	119.72	124.40
53	i	401	CDL	OA8-CA7-C31	2.87	120.90	111.91
50	J	401	NDP	PN-O3-PA	-2.86	123.02	132.83
49	X	201	8Q1	O2-P24-O27	-2.80	99.27	106.73
47	l	703	PEE	O3-C30-C31	2.80	120.68	111.91
49	G	201	8Q1	O2-P24-O27	-2.79	99.32	106.73
53	N	201	CDL	OA8-CA7-C31	2.79	120.65	111.91
47	r	501	PEE	O3-C30-C31	2.77	120.61	111.91
47	B	303	PEE	O3-C30-C31	2.74	120.52	111.91
53	n	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
53	a	201	CDL	CB4-OB6-CB5	-2.74	111.05	117.79
56	w	401	ADP	PA-O3A-PB	-2.72	123.48	132.83
47	l	704	PEE	O3-C30-C31	2.69	120.33	111.91
46	A	502	FMN	C4A-C4-N3	2.66	119.95	113.19
53	N	201	CDL	OB8-CB7-C71	2.66	120.25	111.91
53	l	701	CDL	OB8-CB7-C71	2.63	120.16	111.91
49	X	201	8Q1	C37-C38-C39	2.60	116.68	112.36
53	l	702	CDL	OA8-CA7-C31	2.59	120.04	111.91
53	n	101	CDL	OB8-CB7-C71	2.59	120.03	111.91
53	g	202	CDL	OB8-CB7-C71	2.58	120.02	111.91
53	l	701	CDL	OA8-CA7-C31	2.58	120.00	111.91
47	U	101	PEE	O3-C30-C31	2.57	119.97	111.91
47	m	201	PEE	O3-C30-C31	2.56	119.93	111.91
53	N	201	CDL	CB4-OB6-CB5	-2.56	111.50	117.79
53	l	702	CDL	OB8-CB7-C71	2.54	119.88	111.91
47	i	402	PEE	O3-C30-C31	2.53	119.86	111.91
47	j	201	PEE	O3-C30-C31	2.50	119.77	111.91
53	g	202	CDL	OA8-CA7-C31	2.49	119.72	111.91
48	r	503	PLX	C1A-N1-C1	2.48	120.07	109.92
49	X	201	8Q1	C32-C34-N36	2.47	121.50	116.58
46	A	502	FMN	O4-C4-C4A	-2.46	120.07	126.60
49	X	201	8Q1	O4-C1-S44	-2.46	119.42	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	A	502	FMN	C4A-C10-N10	2.44	120.04	116.48
48	r	502	PLX	C1A-N1-C1	2.42	119.81	109.92
48	j	202	PLX	C1A-N1-C1	2.41	119.79	109.92
53	i	401	CDL	OB8-CB7-C71	2.41	119.47	111.91
49	G	201	8Q1	O40-C39-N41	-2.41	118.47	123.01
49	G	201	8Q1	O1-P24-O2	2.39	116.78	107.64
49	X	201	8Q1	O1-P24-O2	2.38	116.72	107.64
49	G	201	8Q1	C32-C34-N36	2.37	121.30	116.58
48	g	201	PLX	C1A-N1-C1	2.34	119.50	109.92
46	A	502	FMN	C10-C4A-N5	-2.24	120.10	124.86
49	X	201	8Q1	O40-C39-N41	-2.23	118.80	123.01
46	A	502	FMN	C4A-C10-N1	-2.23	119.56	124.73
46	A	502	FMN	C9A-C5A-N5	-2.22	120.02	122.43
48	C	302	PLX	C1A-N1-C1	2.21	118.95	109.92
50	J	401	NDP	C4A-C5A-N7A	-2.16	107.15	109.40
56	w	401	ADP	C4-C5-N7	-2.12	107.19	109.40
46	A	502	FMN	C5A-C9A-N10	2.11	120.14	117.95
49	G	201	8Q1	O4-C1-C6	-2.07	121.54	123.99
53	a	201	CDL	OB8-CB7-OB9	-2.04	118.44	123.59
49	G	201	8Q1	O4-C1-S44	-2.04	119.96	122.61
53	i	401	CDL	CA4-OA6-CA5	-2.04	112.77	117.79
53	N	201	CDL	CA6-CA4-CA3	-2.02	107.01	111.79

There are no chirality outliers.

All (682) 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'
46	A	502	FMN	C3'-C4'-C5'-O5'
47	U	101	PEE	C19-C20-C21-C22
47	U	101	PEE	C4-O4P-P-O3P
47	U	101	PEE	C4-O4P-P-O2P
47	U	101	PEE	C4-O4P-P-O1P
47	i	402	PEE	C11-C10-O2-C2
47	j	201	PEE	C1-O3P-P-O2P
47	j	201	PEE	C1-O3P-P-O1P
47	l	703	PEE	C11-C10-O2-C2
47	l	703	PEE	C4-O4P-P-O2P
47	l	703	PEE	C4-O4P-P-O1P
47	m	201	PEE	C11-C10-O2-C2
47	m	201	PEE	C3-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
47	r	501	PEE	C15-C16-C17-C18
48	C	302	PLX	C3-O4-P1-O2
48	C	302	PLX	C3-O4-P1-O3
48	C	302	PLX	N1-C1-C2-O1
48	a	202	PLX	C3-O4-P1-O1
48	a	202	PLX	C3-O4-P1-O2
48	a	202	PLX	C3-O4-P1-O3
48	a	202	PLX	O9-C24-O8-C5
48	a	202	PLX	O9-C24-C25-C26
48	g	201	PLX	O7-C6-O6-C4
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	O7-C6-O6-C4
48	j	202	PLX	O9-C24-O8-C5
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	503	PLX	C3-O4-P1-O1
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
48	r	503	PLX	C25-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	O27-C28-C29-C31
49	G	201	8Q1	O27-C28-C29-C32
49	G	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O2
50	J	401	NDP	C5B-O5B-PA-O1A
50	J	401	NDP	C2B-O2B-P2B-O1X
53	N	201	CDL	O1-C1-CB2-OB2
53	N	201	CDL	CA2-C1-CB2-OB2
53	N	201	CDL	CA2-OA2-PA1-OA3
53	N	201	CDL	CA2-OA2-PA1-OA4
53	N	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	N	201	CDL	CA3-OA5-PA1-OA4
53	N	201	CDL	CA6-CA4-OA6-CA5
53	N	201	CDL	CB2-OB2-PB2-OB4
53	N	201	CDL	CB3-OB5-PB2-OB2
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB3-OB5-PB2-OB3
53	g	202	CDL	CA2-OA2-PA1-OA3
53	g	202	CDL	CA2-OA2-PA1-OA4
53	g	202	CDL	CA3-OA5-PA1-OA2
53	g	202	CDL	CA3-OA5-PA1-OA3
53	g	202	CDL	CA3-OA5-PA1-OA4
53	g	202	CDL	CB2-OB2-PB2-OB3
53	g	202	CDL	CB2-OB2-PB2-OB5
53	i	401	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	O1-C1-CB2-OB2
53	i	401	CDL	CA2-OA2-PA1-OA4
53	i	401	CDL	CA3-OA5-PA1-OA2
53	i	401	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	OB6-CB4-CB6-OB8
53	l	701	CDL	O1-C1-CA2-OA2
53	l	701	CDL	O1-C1-CB2-OB2
53	l	701	CDL	CA2-OA2-PA1-OA3
53	l	701	CDL	CA2-OA2-PA1-OA4
53	l	701	CDL	CA2-OA2-PA1-OA5
53	l	701	CDL	CA3-OA5-PA1-OA3
53	l	701	CDL	CB2-OB2-PB2-OB3
53	l	701	CDL	CB2-OB2-PB2-OB4
53	l	701	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	O1-C1-CA2-OA2
53	l	702	CDL	O1-C1-CB2-OB2
53	l	702	CDL	CA3-OA5-PA1-OA2
53	l	702	CDL	CA3-OA5-PA1-OA3
53	l	702	CDL	CA3-OA5-PA1-OA4
53	l	702	CDL	OA6-CA4-CA6-OA8
53	l	702	CDL	CB2-OB2-PB2-OB3
53	l	702	CDL	OB6-CB4-CB6-OB8
53	n	101	CDL	CA2-OA2-PA1-OA3
53	n	101	CDL	CA2-OA2-PA1-OA4
53	n	101	CDL	CA2-OA2-PA1-OA5
53	n	101	CDL	CA3-OA5-PA1-OA2
53	n	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
53	n	101	CDL	CA3-OA5-PA1-OA4
53	n	101	CDL	CB2-OB2-PB2-OB4
53	n	101	CDL	CB3-OB5-PB2-OB3
55	s	401	UQ	C7-C8-C9-C11
55	s	401	UQ	C12-C11-C9-C10
55	s	401	UQ	C12-C13-C14-C16
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
53	l	701	CDL	OA9-CA7-OA8-CA6
53	l	701	CDL	C31-CA7-OA8-CA6
47	i	402	PEE	O4-C10-O2-C2
47	m	201	PEE	O4-C10-O2-C2
47	r	501	PEE	O4-C10-O2-C2
53	N	201	CDL	OA7-CA5-OA6-CA4
53	g	202	CDL	C71-CB7-OB8-CB6
47	r	501	PEE	C11-C10-O2-C2
53	N	201	CDL	C11-CA5-OA6-CA4
47	B	303	PEE	C17-C18-C19-C20
47	B	303	PEE	C37-C38-C39-C40
47	U	101	PEE	C17-C18-C19-C20
55	s	401	UQ	C17-C18-C19-C21
55	s	401	UQ	C7-C8-C9-C10
47	l	703	PEE	O4-C10-O2-C2
53	l	702	CDL	OB9-CB7-OB8-CB6
47	U	101	PEE	C31-C30-O3-C3
53	l	702	CDL	C71-CB7-OB8-CB6
53	g	202	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	C11-C10-O2-C2
47	U	101	PEE	C11-C10-O2-C2
47	j	201	PEE	C11-C10-O2-C2
53	g	202	CDL	C51-CB5-OB6-CB4
48	r	503	PLX	C12-C13-C14-C15
48	C	302	PLX	C28-C29-C30-C31
48	r	502	PLX	C9-C10-C11-C12
47	U	101	PEE	C30-C31-C32-C33
53	l	702	CDL	C11-C12-C13-C14
53	l	702	CDL	C35-C36-C37-C38
47	U	101	PEE	O5-C30-O3-C3
55	s	401	UQ	C9-C11-C12-C13
48	j	202	PLX	C28-C29-C30-C31
47	m	201	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
53	l	701	CDL	C55-C56-C57-C58
48	g	201	PLX	C12-C13-C14-C15
53	g	202	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	CA2-C1-CB2-OB2
53	l	701	CDL	CA2-C1-CB2-OB2
53	l	702	CDL	CA2-C1-CB2-OB2
47	j	201	PEE	O4-C10-O2-C2
48	r	503	PLX	C2-C1-N1-C1A
53	i	401	CDL	C31-CA7-OA8-CA6
47	l	704	PEE	C10-C11-C12-C13
47	m	201	PEE	C33-C34-C35-C36
53	N	201	CDL	O1-C1-CA2-OA2
53	i	401	CDL	O1-C1-CA2-OA2
47	l	703	PEE	C31-C30-O3-C3
53	a	201	CDL	C31-C32-C33-C34
47	m	201	PEE	O5-C30-O3-C3
53	i	401	CDL	OA9-CA7-OA8-CA6
47	U	101	PEE	O4-C10-O2-C2
53	n	101	CDL	C11-CA5-OA6-CA4
47	i	402	PEE	C10-C11-C12-C13
47	r	501	PEE	C10-C11-C12-C13
53	l	701	CDL	CB7-C71-C72-C73
50	J	401	NDP	C2D-C1D-N1N-C6N
53	l	702	CDL	C59-C60-C61-C62
48	j	202	PLX	C15-C16-C17-C18
53	l	702	CDL	CB5-C51-C52-C53
47	r	501	PEE	C17-C18-C19-C20
47	r	501	PEE	C30-C31-C32-C33
53	l	702	CDL	CB7-C71-C72-C73
53	n	101	CDL	C75-C76-C77-C78
50	J	401	NDP	O4B-C4B-C5B-O5B
47	B	303	PEE	O4-C10-O2-C2
53	g	202	CDL	OB7-CB5-OB6-CB4
48	g	201	PLX	C7-C8-C9-C10
48	r	503	PLX	C2-C1-N1-C1C
53	g	202	CDL	CA7-C31-C32-C33
53	N	201	CDL	C51-CB5-OB6-CB4
47	l	703	PEE	O5-C30-O3-C3
48	r	502	PLX	C30-C31-C32-C33
47	i	402	PEE	C22-C23-C24-C25
53	g	202	CDL	O1-C1-CA2-OA2
53	l	702	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
47	j	201	PEE	C1-O3P-P-O4P
47	l	703	PEE	C4-O4P-P-O3P
47	l	704	PEE	C1-O3P-P-O4P
47	m	201	PEE	C4-O4P-P-O3P
47	r	501	PEE	C1-O3P-P-O4P
48	C	302	PLX	C3-O4-P1-O1
48	j	202	PLX	C3-O4-P1-O1
53	N	201	CDL	CA3-OA5-PA1-OA2
53	N	201	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CA2-OA2-PA1-OA5
53	a	201	CDL	CB2-OB2-PB2-OB5
53	g	202	CDL	CA2-OA2-PA1-OA5
53	g	202	CDL	CB3-OB5-PB2-OB2
53	i	401	CDL	CA2-OA2-PA1-OA5
53	i	401	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CB3-OB5-PB2-OB2
53	n	101	CDL	CB2-OB2-PB2-OB5
53	l	701	CDL	CB2-C1-CA2-OA2
53	l	702	CDL	CB2-C1-CA2-OA2
53	N	201	CDL	OB7-CB5-OB6-CB4
53	n	101	CDL	OA7-CA5-OA6-CA4
47	l	704	PEE	C31-C30-O3-C3
48	C	302	PLX	O8-C24-C25-C26
48	j	202	PLX	O6-C6-C7-C8
53	a	201	CDL	C39-C40-C41-C42
48	C	302	PLX	C25-C26-C27-C28
48	g	201	PLX	C33-C34-C35-C36
53	l	701	CDL	C52-C53-C54-C55
47	r	501	PEE	C13-C14-C15-C16
48	r	502	PLX	C27-C28-C29-C30
53	l	701	CDL	C74-C75-C76-C77
53	l	702	CDL	C33-C34-C35-C36
53	l	702	CDL	C55-C56-C57-C58
53	l	702	CDL	C72-C73-C74-C75
53	l	702	CDL	C73-C74-C75-C76
49	G	201	8Q1	O27-C28-C29-C30
47	B	303	PEE	C22-C23-C24-C25
48	g	201	PLX	C9-C10-C11-C12
48	j	202	PLX	C25-C26-C27-C28
48	r	502	PLX	C33-C34-C35-C36
48	r	503	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	C11-C12-C13-C14
53	g	202	CDL	C71-C72-C73-C74
53	l	701	CDL	C82-C83-C84-C85
53	l	702	CDL	C37-C38-C39-C40
53	l	702	CDL	C58-C59-C60-C61
53	l	702	CDL	C63-C64-C65-C66
53	n	101	CDL	CA6-CA4-OA6-CA5
47	l	703	PEE	C21-C22-C23-C24
47	r	501	PEE	C12-C13-C14-C15
49	X	201	8Q1	C11-C12-C13-C14
53	l	701	CDL	C62-C63-C64-C65
47	l	704	PEE	C17-C18-C19-C20
47	l	704	PEE	C33-C34-C35-C36
48	C	302	PLX	C14-C15-C16-C17
48	j	202	PLX	C27-C28-C29-C30
48	g	201	PLX	C25-C26-C27-C28
48	r	502	PLX	C7-C8-C9-C10
53	l	701	CDL	C35-C36-C37-C38
53	l	701	CDL	C56-C57-C58-C59
53	g	202	CDL	CB5-C51-C52-C53
47	j	201	PEE	C42-C43-C44-C45
48	r	503	PLX	C28-C29-C30-C31
53	g	202	CDL	C56-C57-C58-C59
53	g	202	CDL	C59-C60-C61-C62
47	l	703	PEE	C23-C24-C25-C26
48	g	201	PLX	C11-C10-C9-C8
48	r	503	PLX	C13-C14-C15-C16
53	g	202	CDL	C73-C74-C75-C76
48	j	202	PLX	C7-C8-C9-C10
48	r	502	PLX	C10-C11-C12-C13
48	r	503	PLX	C14-C15-C16-C17
48	r	503	PLX	C29-C30-C31-C32
53	g	202	CDL	C12-C13-C14-C15
53	g	202	CDL	C14-C15-C16-C17
53	g	202	CDL	C37-C38-C39-C40
47	U	101	PEE	C22-C23-C24-C25
47	l	704	PEE	C34-C35-C36-C37
48	C	302	PLX	C18-C19-C20-C21
49	G	201	8Q1	C6-C7-C8-C9
53	g	202	CDL	C75-C76-C77-C78
53	l	701	CDL	C75-C76-C77-C78
47	l	704	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	C	302	PLX	C16-C17-C18-C19
48	r	503	PLX	C33-C34-C35-C36
49	G	201	8Q1	C12-C13-C14-C15
53	l	701	CDL	C20-C21-C22-C23
49	G	201	8Q1	C10-C11-C12-C13
53	g	202	CDL	C33-C34-C35-C36
53	g	202	CDL	C35-C36-C37-C38
53	i	401	CDL	C36-C37-C38-C39
53	l	701	CDL	C14-C15-C16-C17
53	l	701	CDL	C73-C74-C75-C76
47	r	501	PEE	C41-C42-C43-C44
48	C	302	PLX	C17-C18-C19-C20
48	C	302	PLX	C9-C10-C11-C12
48	r	502	PLX	C14-C15-C16-C17
53	g	202	CDL	C52-C53-C54-C55
48	g	201	PLX	C31-C32-C33-C34
53	i	401	CDL	C33-C34-C35-C36
47	m	201	PEE	C11-C12-C13-C14
48	g	201	PLX	C10-C11-C12-C13
46	A	502	FMN	O4'-C4'-C5'-O5'
53	g	202	CDL	CB7-C71-C72-C73
48	r	503	PLX	C10-C11-C12-C13
53	g	202	CDL	C43-C44-C45-C46
53	l	701	CDL	C11-C12-C13-C14
47	l	704	PEE	O5-C30-O3-C3
53	a	201	CDL	C51-CB5-OB6-CB4
48	C	302	PLX	O9-C24-C25-C26
48	j	202	PLX	C10-C11-C12-C13
53	g	202	CDL	C62-C63-C64-C65
53	i	401	CDL	C11-C12-C13-C14
53	l	701	CDL	C32-C33-C34-C35
47	B	303	PEE	C30-C31-C32-C33
48	C	302	PLX	C33-C34-C35-C36
53	l	701	CDL	C61-C62-C63-C64
47	l	704	PEE	O4-C10-O2-C2
53	a	201	CDL	OB7-CB5-OB6-CB4
48	j	202	PLX	C12-C13-C14-C15
47	B	303	PEE	C14-C15-C16-C17
53	a	201	CDL	C73-C74-C75-C76
48	j	202	PLX	C2-C1-N1-C1A
48	r	503	PLX	C2-C1-N1-C1B
53	l	702	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C20-C21-C22-C23
48	j	202	PLX	C13-C14-C15-C16
53	l	702	CDL	C40-C41-C42-C43
47	l	703	PEE	C37-C38-C39-C40
53	g	202	CDL	C41-C42-C43-C44
53	n	101	CDL	C53-C54-C55-C56
47	i	402	PEE	C35-C36-C37-C38
47	l	703	PEE	C19-C20-C21-C22
47	l	703	PEE	C30-C31-C32-C33
47	B	303	PEE	C13-C14-C15-C16
47	l	703	PEE	C31-C32-C33-C34
48	r	502	PLX	C28-C29-C30-C31
48	C	302	PLX	C15-C16-C17-C18
49	G	201	8Q1	N36-C37-C38-C39
47	U	101	PEE	C42-C43-C44-C45
48	C	302	PLX	C26-C27-C28-C29
48	C	302	PLX	C30-C31-C32-C33
53	a	201	CDL	C18-C19-C20-C21
53	g	202	CDL	C17-C18-C19-C20
53	g	202	CDL	OB6-CB4-CB6-OB8
47	j	201	PEE	C20-C21-C22-C23
48	j	202	PLX	C26-C27-C28-C29
47	j	201	PEE	C11-C12-C13-C14
48	C	302	PLX	C27-C28-C29-C30
53	g	202	CDL	C82-C83-C84-C85
47	j	201	PEE	C15-C16-C17-C18
47	m	201	PEE	C19-C20-C21-C22
47	r	501	PEE	C39-C40-C41-C42
55	s	401	UQ	C12-C11-C9-C8
47	U	101	PEE	C32-C33-C34-C35
53	g	202	CDL	C61-C62-C63-C64
53	n	101	CDL	C58-C59-C60-C61
47	j	201	PEE	C34-C35-C36-C37
53	l	701	CDL	C51-C52-C53-C54
53	l	701	CDL	C60-C61-C62-C63
47	i	402	PEE	C14-C15-C16-C17
53	l	701	CDL	C58-C59-C60-C61
47	U	101	PEE	C36-C37-C38-C39
47	l	704	PEE	C18-C19-C20-C21
47	r	501	PEE	C36-C37-C38-C39
53	n	101	CDL	CB3-OB5-PB2-OB2
48	C	302	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C25-C26-C27-C28
53	l	701	CDL	C71-C72-C73-C74
47	l	703	PEE	C22-C23-C24-C25
53	i	401	CDL	C35-C36-C37-C38
53	l	702	CDL	C74-C75-C76-C77
53	l	701	CDL	C71-CB7-OB8-CB6
48	r	503	PLX	C31-C32-C33-C34
48	C	302	PLX	C13-C14-C15-C16
48	r	503	PLX	C9-C10-C11-C12
48	j	202	PLX	C9-C10-C11-C12
47	j	201	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	r	503	PLX	C3-C4-C5-O8
53	g	202	CDL	CA3-CA4-CA6-OA8
53	g	202	CDL	CB3-CB4-CB6-OB8
53	g	202	CDL	C74-C75-C76-C77
53	i	401	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	C31-C32-C33-C34
53	l	702	CDL	CB3-CB4-CB6-OB8
53	n	101	CDL	CA3-CA4-CA6-OA8
48	r	502	PLX	C15-C16-C17-C18
47	B	303	PEE	C23-C24-C25-C26
53	l	702	CDL	C14-C15-C16-C17
47	r	501	PEE	C20-C21-C22-C23
47	l	704	PEE	C15-C16-C17-C18
53	g	202	CDL	C79-C80-C81-C82
47	B	303	PEE	C21-C22-C23-C24
49	X	201	8Q1	C10-C11-C12-C13
53	n	101	CDL	C21-C22-C23-C24
53	a	201	CDL	C71-CB7-OB8-CB6
47	m	201	PEE	O3P-C1-C2-O2
48	C	302	PLX	O4-C3-C4-O6
48	j	202	PLX	C2-C1-N1-C1C
48	j	202	PLX	C2-C1-N1-C1B
53	g	202	CDL	C72-C73-C74-C75
53	i	401	CDL	C13-C14-C15-C16
53	l	702	CDL	C52-C53-C54-C55
47	m	201	PEE	C13-C14-C15-C16
49	X	201	8Q1	C13-C14-C15-C16
47	l	703	PEE	O2-C2-C3-O3
53	g	202	CDL	OA6-CA4-CA6-OA8
53	l	701	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
49	X	201	8Q1	C31-C29-C32-O33
53	g	202	CDL	C32-C33-C34-C35
47	l	704	PEE	C13-C14-C15-C16
53	g	202	CDL	C55-C56-C57-C58
47	l	704	PEE	C37-C38-C39-C40
48	r	502	PLX	C13-C14-C15-C16
53	l	702	CDL	C17-C18-C19-C20
48	g	201	PLX	C27-C28-C29-C30
48	r	503	PLX	C16-C17-C18-C19
48	r	503	PLX	C36-C37-C38-C39
49	X	201	8Q1	C29-C32-C34-O35
47	j	201	PEE	C13-C14-C15-C16
48	j	202	PLX	C33-C34-C35-C36
53	l	701	CDL	C72-C73-C74-C75
49	G	201	8Q1	N41-C42-C43-S44
48	g	201	PLX	C13-C14-C15-C16
53	g	202	CDL	C54-C55-C56-C57
53	g	202	CDL	C63-C64-C65-C66
53	l	701	CDL	C37-C38-C39-C40
48	r	502	PLX	C16-C17-C18-C19
53	g	202	CDL	C20-C21-C22-C23
47	l	704	PEE	C1-C2-C3-O3
47	m	201	PEE	C1-C2-C3-O3
48	r	502	PLX	C3-C4-C5-O8
53	l	702	CDL	CA3-CA4-CA6-OA8
48	C	302	PLX	C10-C11-C12-C13
48	r	502	PLX	C31-C32-C33-C34
53	l	701	CDL	C36-C37-C38-C39
53	l	702	CDL	C82-C83-C84-C85
48	r	503	PLX	O7-C6-C7-C8
48	r	503	PLX	C27-C28-C29-C30
48	a	202	PLX	O4-C3-C4-O6
48	r	502	PLX	O4-C3-C4-O6
47	j	201	PEE	C10-C11-C12-C13
53	l	702	CDL	CA7-C31-C32-C33
53	l	702	CDL	C16-C17-C18-C19
48	a	202	PLX	C33-C34-C35-C36
48	r	503	PLX	C11-C12-C13-C14
47	m	201	PEE	O2-C2-C3-O3
47	r	501	PEE	O2-C2-C3-O3
48	r	502	PLX	O6-C4-C5-O8
53	g	202	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
53	n	101	CDL	CB2-C1-CA2-OA2
48	r	503	PLX	C19-C20-C21-C22
47	l	703	PEE	C33-C34-C35-C36
47	l	704	PEE	C22-C23-C24-C25
53	g	202	CDL	CB4-CB3-OB5-PB2
47	B	303	PEE	C15-C16-C17-C18
48	g	201	PLX	C14-C15-C16-C17
48	g	201	PLX	C29-C30-C31-C32
48	j	202	PLX	C14-C15-C16-C17
53	i	401	CDL	C71-C72-C73-C74
49	X	201	8Q1	O4-C1-S44-C43
48	g	201	PLX	C28-C29-C30-C31
53	g	202	CDL	C57-C58-C59-C60
53	l	702	CDL	C64-C65-C66-C67
47	i	402	PEE	C24-C25-C26-C27
53	l	702	CDL	C62-C63-C64-C65
49	X	201	8Q1	O4-C1-C6-C7
49	X	201	8Q1	S44-C1-C6-C7
47	m	201	PEE	C22-C23-C24-C25
48	C	302	PLX	O4-C3-C4-C5
48	j	202	PLX	O4-C3-C4-C5
47	B	303	PEE	C38-C39-C40-C41
47	B	303	PEE	C31-C30-O3-C3
53	g	202	CDL	C13-C14-C15-C16
49	X	201	8Q1	O33-C32-C34-N36
49	X	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C6-C1-S44-C43
47	B	303	PEE	C33-C34-C35-C36
48	g	201	PLX	C3-C4-C5-O8
53	a	201	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	O3P-C1-C2-O2
53	l	702	CDL	OA5-CA3-CA4-OA6
48	g	201	PLX	C36-C37-C38-C39
47	l	704	PEE	O2-C2-C3-O3
48	g	201	PLX	O6-C4-C5-O8
48	r	503	PLX	O6-C4-C5-O8
53	n	101	CDL	OA6-CA4-CA6-OA8
47	r	501	PEE	C24-C25-C26-C27
53	l	702	CDL	C53-C54-C55-C56
53	g	202	CDL	C44-C45-C46-C47
50	J	401	NDP	C5B-O5B-PA-O3
47	i	402	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C44-C45-C46-C47
47	B	303	PEE	O5-C30-O3-C3
53	g	202	CDL	C76-C77-C78-C79
47	r	501	PEE	C22-C23-C24-C25
48	a	202	PLX	C6-C7-C8-C9
47	i	402	PEE	C1-O3P-P-O4P
53	a	201	CDL	CA3-OA5-PA1-OA2
53	a	201	CDL	CB3-OB5-PB2-OB2
53	i	401	CDL	CB3-OB5-PB2-OB2
53	l	701	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CA2-OA2-PA1-OA5
47	l	704	PEE	C21-C22-C23-C24
47	U	101	PEE	C1-O3P-P-O2P
47	i	402	PEE	C1-O3P-P-O1P
47	l	704	PEE	C1-O3P-P-O2P
47	l	704	PEE	C1-O3P-P-O1P
47	m	201	PEE	C4-O4P-P-O2P
47	m	201	PEE	C4-O4P-P-O1P
47	r	501	PEE	C1-O3P-P-O2P
47	r	501	PEE	C1-O3P-P-O1P
48	j	202	PLX	C3-O4-P1-O3
53	N	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CA2-OA2-PA1-OA4
53	a	201	CDL	CB2-OB2-PB2-OB4
53	g	202	CDL	CB2-OB2-PB2-OB4
53	g	202	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	CA3-OA5-PA1-OA4
53	i	401	CDL	CB2-OB2-PB2-OB3
53	l	701	CDL	CB3-OB5-PB2-OB4
53	l	702	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	CB3-OB5-PB2-OB4
53	n	101	CDL	CB3-OB5-PB2-OB4
48	j	202	PLX	C34-C35-C36-C37
47	m	201	PEE	O3P-C1-C2-C3
48	g	201	PLX	O4-C3-C4-C5
53	l	702	CDL	OA5-CA3-CA4-CA6
53	g	202	CDL	C64-C65-C66-C67
49	G	201	8Q1	C11-C10-C9-C8
48	r	502	PLX	C12-C13-C14-C15
53	a	201	CDL	C54-C55-C56-C57
53	n	101	CDL	CB7-C71-C72-C73
48	j	202	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
53	l	701	CDL	CA7-C31-C32-C33
53	n	101	CDL	OB5-CB3-CB4-OB6
53	i	401	CDL	C14-C15-C16-C17
48	r	503	PLX	C15-C16-C17-C18
48	r	503	PLX	C7-C8-C9-C10
53	n	101	CDL	O1-C1-CA2-OA2
47	B	303	PEE	C12-C13-C14-C15
53	l	702	CDL	C56-C57-C58-C59
47	j	201	PEE	O2-C2-C3-O3
53	n	101	CDL	C73-C74-C75-C76
53	a	201	CDL	C17-C18-C19-C20
53	l	701	CDL	C40-C41-C42-C43
48	C	302	PLX	C31-C32-C33-C34
48	C	302	PLX	O6-C6-C7-C8
48	a	202	PLX	O8-C24-C25-C26
48	r	503	PLX	O8-C24-C25-C26
47	U	101	PEE	C38-C39-C40-C41
47	l	704	PEE	C16-C17-C18-C19
48	C	302	PLX	O7-C6-C7-C8
48	j	202	PLX	C11-C12-C13-C14
48	r	502	PLX	C11-C12-C13-C14
48	r	502	PLX	C18-C19-C20-C21
47	m	201	PEE	C31-C32-C33-C34
53	a	201	CDL	CA6-CA4-OA6-CA5
48	a	202	PLX	O4-C3-C4-C5
48	r	502	PLX	O4-C3-C4-C5
46	A	502	FMN	C5'-O5'-P-O1P
47	l	704	PEE	C2-C1-O3P-P
49	G	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O3
48	g	201	PLX	O4-C3-C4-O6
47	r	501	PEE	C31-C32-C33-C34
53	g	202	CDL	C34-C35-C36-C37
50	J	401	NDP	O4D-C1D-N1N-C6N
47	U	101	PEE	C41-C42-C43-C44
48	j	202	PLX	C31-C32-C33-C34
47	B	303	PEE	C34-C35-C36-C37
47	i	402	PEE	C31-C32-C33-C34
48	a	202	PLX	C2-O1-P1-O4
48	g	201	PLX	C3-O4-P1-O1
53	n	101	CDL	C55-C56-C57-C58
47	l	703	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
48	C	302	PLX	C11-C10-C9-C8
53	l	702	CDL	C60-C61-C62-C63
53	N	201	CDL	CB7-C71-C72-C73
53	l	702	CDL	C76-C77-C78-C79
53	l	702	CDL	C31-CA7-OA8-CA6
48	a	202	PLX	C26-C27-C28-C29
47	i	402	PEE	C38-C39-C40-C41
47	l	704	PEE	C36-C37-C38-C39
47	m	201	PEE	C16-C17-C18-C19
55	s	401	UQ	C17-C18-C19-C20
53	l	701	CDL	C76-C77-C78-C79
53	l	702	CDL	OA9-CA7-OA8-CA6
47	j	201	PEE	C31-C30-O3-C3
53	l	702	CDL	C32-C33-C34-C35
53	n	101	CDL	C22-C23-C24-C25
47	j	201	PEE	O5-C30-O3-C3
53	a	201	CDL	OA5-CA3-CA4-OA6
53	n	101	CDL	OA5-CA3-CA4-OA6
47	j	201	PEE	C16-C17-C18-C19
47	l	704	PEE	C38-C39-C40-C41
48	C	302	PLX	C11-C12-C13-C14
53	l	701	CDL	C17-C18-C19-C20
48	j	202	PLX	C18-C19-C20-C21
53	g	202	CDL	C31-CA7-OA8-CA6
47	j	201	PEE	C43-C44-C45-C46
49	X	201	8Q1	C29-C32-C34-N36
48	g	201	PLX	C6-C7-C8-C9
53	i	401	CDL	CA6-CA4-OA6-CA5
53	l	701	CDL	C54-C55-C56-C57
53	l	702	CDL	C41-C42-C43-C44
47	l	703	PEE	C32-C33-C34-C35
48	j	202	PLX	C3-C4-O6-C6
53	a	201	CDL	CA7-C31-C32-C33
47	m	201	PEE	O3-C30-C31-C32
47	l	703	PEE	C24-C25-C26-C27
48	a	202	PLX	C13-C14-C15-C16
53	l	701	CDL	C44-C45-C46-C47
47	B	303	PEE	O3P-C1-C2-C3
48	r	503	PLX	C26-C27-C28-C29
53	l	701	CDL	C34-C35-C36-C37
53	g	202	CDL	CA5-C11-C12-C13
47	U	101	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
47	i	402	PEE	C32-C33-C34-C35
53	l	701	CDL	C23-C24-C25-C26
53	g	202	CDL	OA9-CA7-OA8-CA6
53	N	201	CDL	CB2-C1-CA2-OA2
55	s	401	UQ	C14-C16-C17-C18
53	g	202	CDL	C60-C61-C62-C63
48	C	302	PLX	C12-C13-C14-C15
50	J	401	NDP	PN-O3-PA-O1A
50	J	401	NDP	PN-O3-PA-O2A
53	N	201	CDL	OA9-CA7-OA8-CA6
47	i	402	PEE	C17-C18-C19-C20
47	B	303	PEE	C18-C19-C20-C21
48	a	202	PLX	C9-C10-C11-C12
53	l	701	CDL	C42-C43-C44-C45
53	n	101	CDL	C71-C72-C73-C74
47	l	704	PEE	C12-C13-C14-C15
47	m	201	PEE	C24-C25-C26-C27
47	r	501	PEE	C38-C39-C40-C41
53	l	701	CDL	OA6-CA4-CA6-OA8
53	N	201	CDL	C31-CA7-OA8-CA6
47	j	201	PEE	C44-C45-C46-C47
47	U	101	PEE	C43-C44-C45-C46
47	U	101	PEE	O3-C30-C31-C32
47	B	303	PEE	C16-C17-C18-C19
47	l	703	PEE	C18-C19-C20-C21
53	l	701	CDL	C12-C11-CA5-OA6
53	n	101	CDL	C77-C78-C79-C80
47	j	201	PEE	C38-C39-C40-C41
47	i	402	PEE	C1-C2-C3-O3
48	j	202	PLX	C7-C6-O6-C4
56	w	401	ADP	C4'-C5'-O5'-PA
47	l	703	PEE	O3P-C1-C2-O2
53	i	401	CDL	OA5-CA3-CA4-OA6
47	l	703	PEE	C17-C18-C19-C20
47	j	201	PEE	O3-C30-C31-C32
53	l	702	CDL	C12-C11-CA5-OA6
47	B	303	PEE	C24-C25-C26-C27
53	g	202	CDL	C80-C81-C82-C83
53	l	702	CDL	C71-C72-C73-C74
53	i	401	CDL	OA5-CA3-CA4-CA6
53	n	101	CDL	OB5-CB3-CB4-CB6
47	i	402	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
53	N	201	CDL	OB6-CB4-CB6-OB8
47	l	703	PEE	C36-C37-C38-C39
53	l	702	CDL	C32-C31-CA7-OA8
48	a	202	PLX	O7-C6-C7-C8
50	J	401	NDP	C2B-O2B-P2B-O2X
48	a	202	PLX	C10-C11-C12-C13
47	i	402	PEE	C2-C1-O3P-P
47	U	101	PEE	C16-C17-C18-C19
47	i	402	PEE	C36-C37-C38-C39
47	m	201	PEE	C18-C19-C20-C21
47	i	402	PEE	C18-C19-C20-C21
47	l	703	PEE	C16-C17-C18-C19
53	g	202	CDL	C83-C84-C85-C86
53	a	201	CDL	C71-C72-C73-C74
47	j	201	PEE	O5-C30-C31-C32
53	l	702	CDL	C12-C11-CA5-OA7
48	j	202	PLX	C11-C10-C9-C8
53	l	702	CDL	C32-C31-CA7-OA9
53	N	201	CDL	C31-C32-C33-C34
47	j	201	PEE	C4-O4P-P-O2P
47	l	703	PEE	C1-O3P-P-O2P
48	a	202	PLX	C2-O1-P1-O2
48	j	202	PLX	C3-O4-P1-O2
53	l	701	CDL	CB3-OB5-PB2-OB3
53	l	701	CDL	C12-C11-CA5-OA7
47	U	101	PEE	O5-C30-C31-C32
49	G	201	8Q1	C29-C32-C34-O35
47	l	703	PEE	C13-C14-C15-C16
47	l	704	PEE	C31-C32-C33-C34
53	l	702	CDL	C77-C78-C79-C80
47	l	704	PEE	C20-C21-C22-C23
53	n	101	CDL	C12-C11-CA5-OA6
47	r	501	PEE	C40-C41-C42-C43
53	g	202	CDL	C52-C51-CB5-OB6
53	l	702	CDL	C12-C13-C14-C15
48	r	503	PLX	C24-C25-C26-C27
47	U	101	PEE	O2-C10-C11-C12

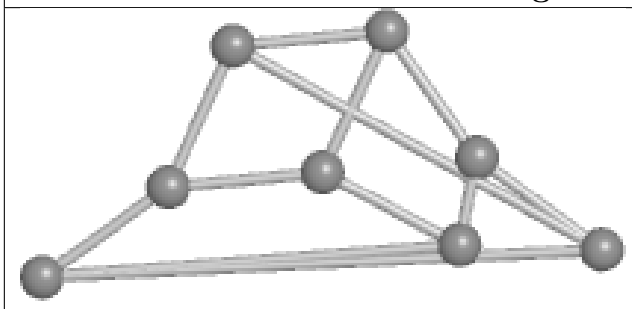
There are no ring outliers.

No monomer is involved in short contacts.

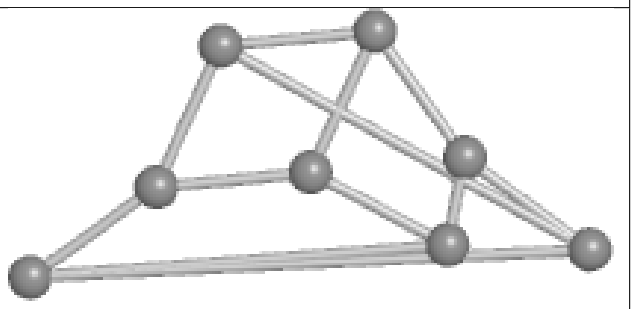
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

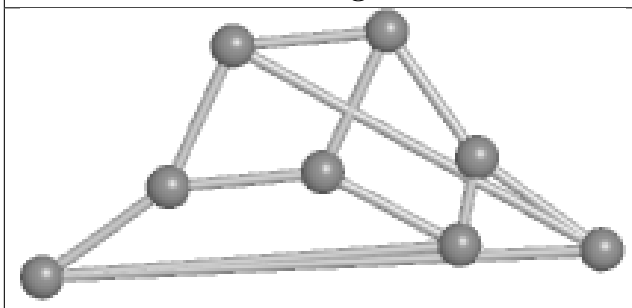
Ligand SF4 C 301



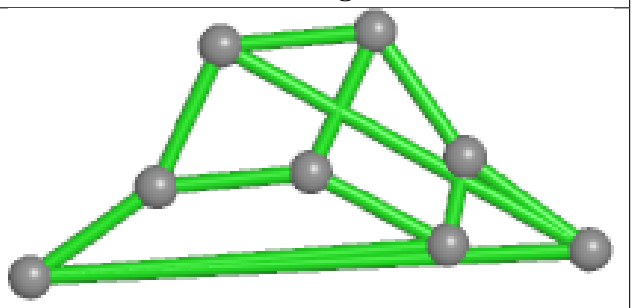
Bond lengths



Bond angles

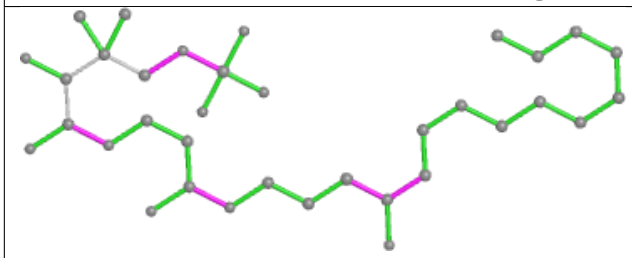


Torsions

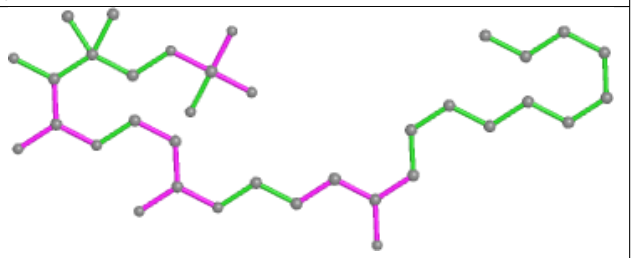


Rings

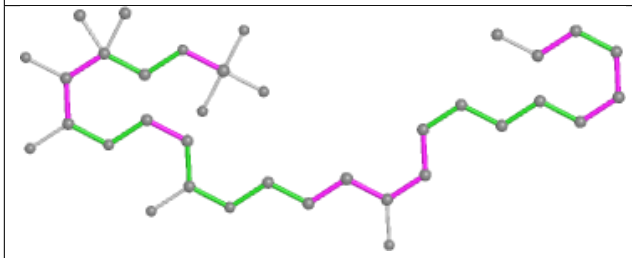
Ligand 8Q1 X 201



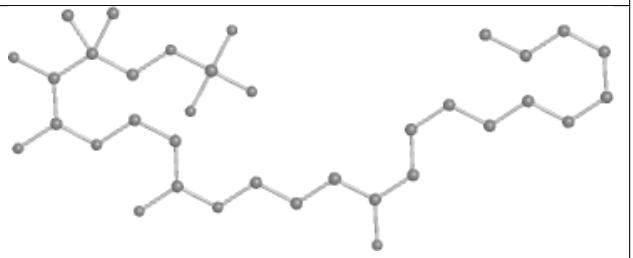
Bond lengths



Bond angles

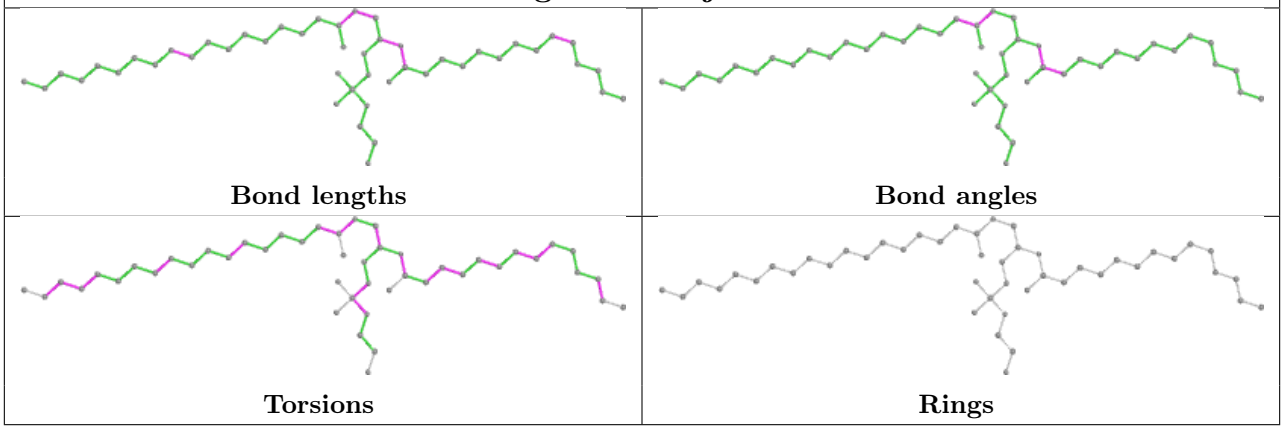


Torsions

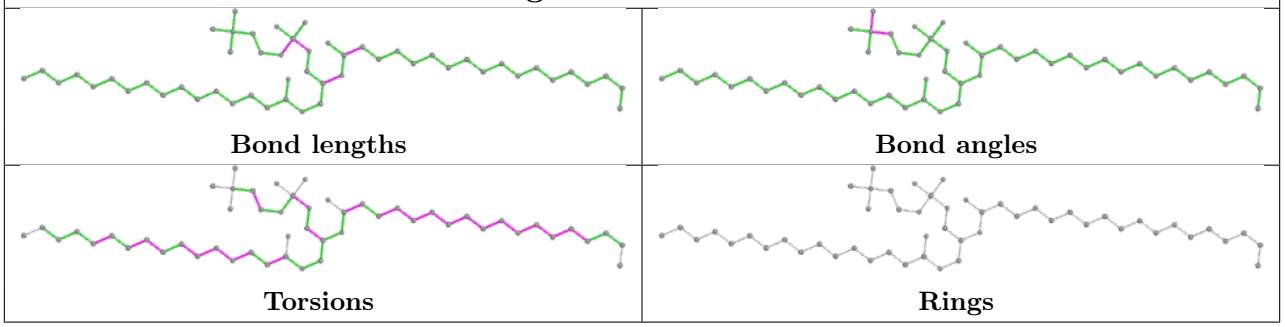


Rings

Ligand PEE j 201



Ligand PLX C 302



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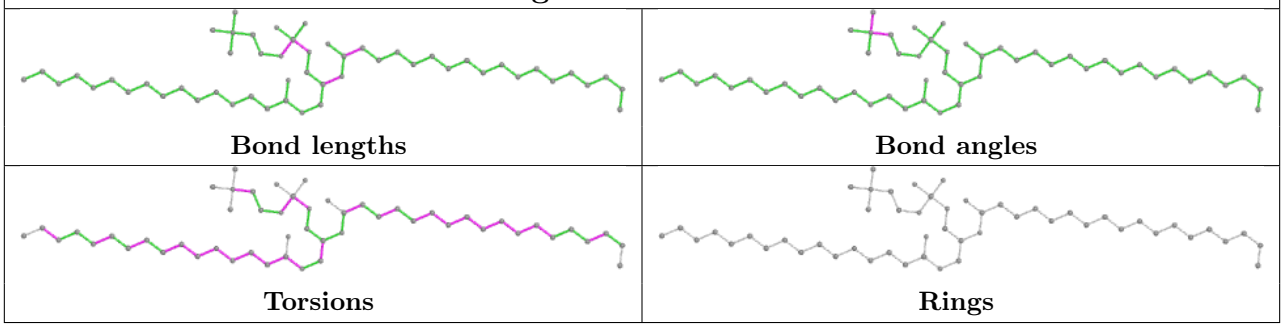
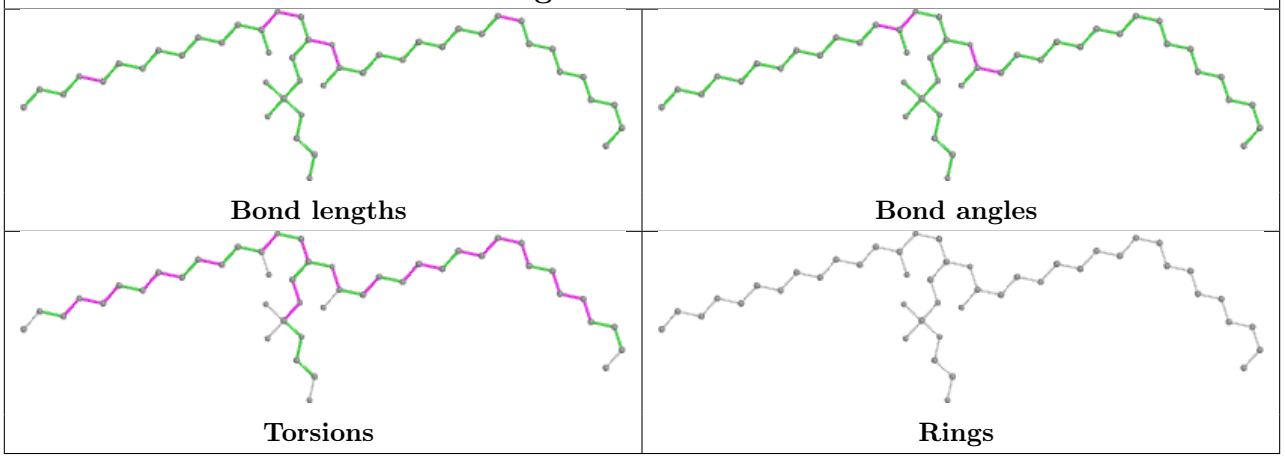
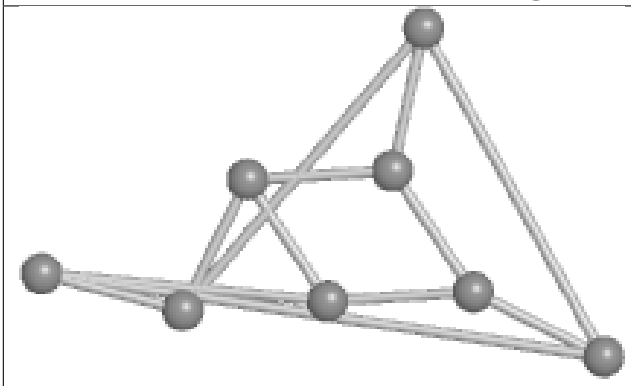


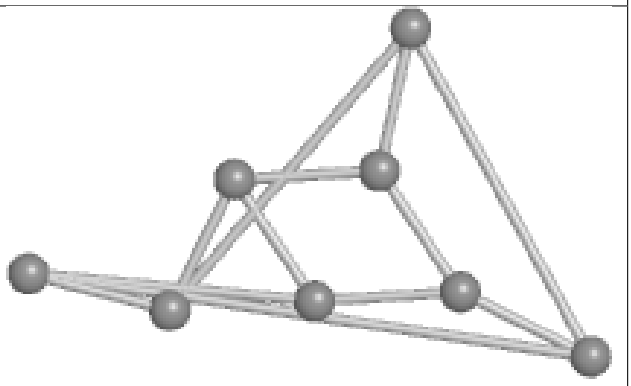
Ligand PEE l 704



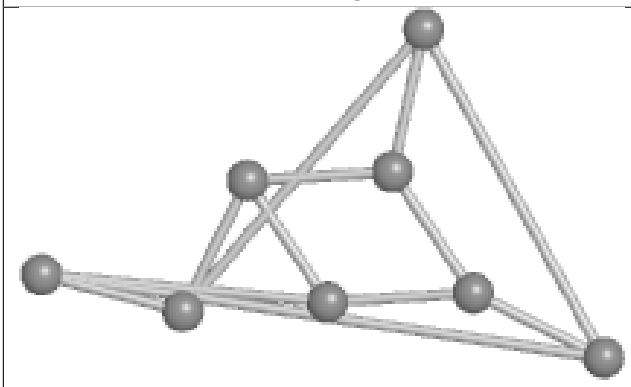
Ligand SF4 M 802



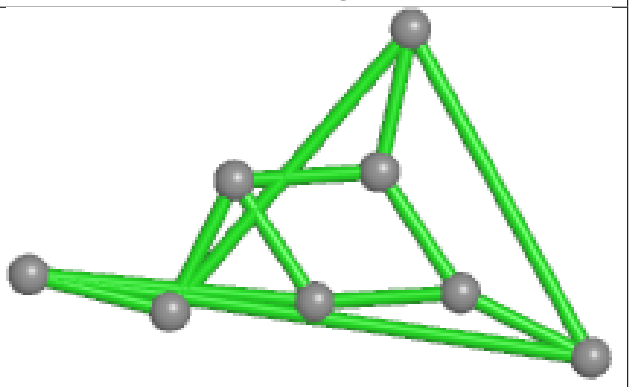
Bond lengths



Bond angles

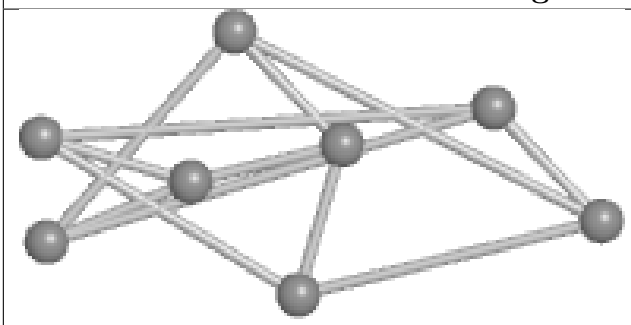


Torsions

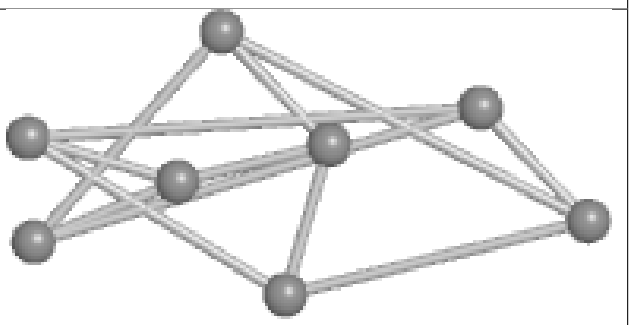


Rings

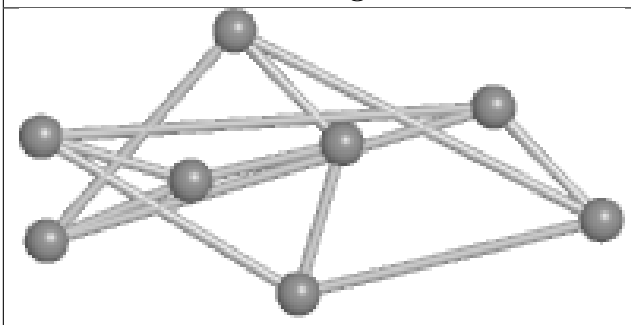
Ligand SF4 B 301



Bond lengths



Bond angles



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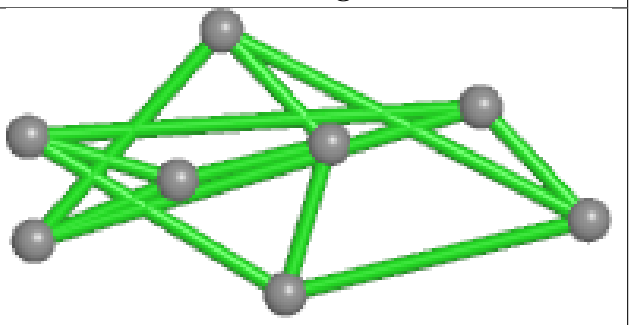
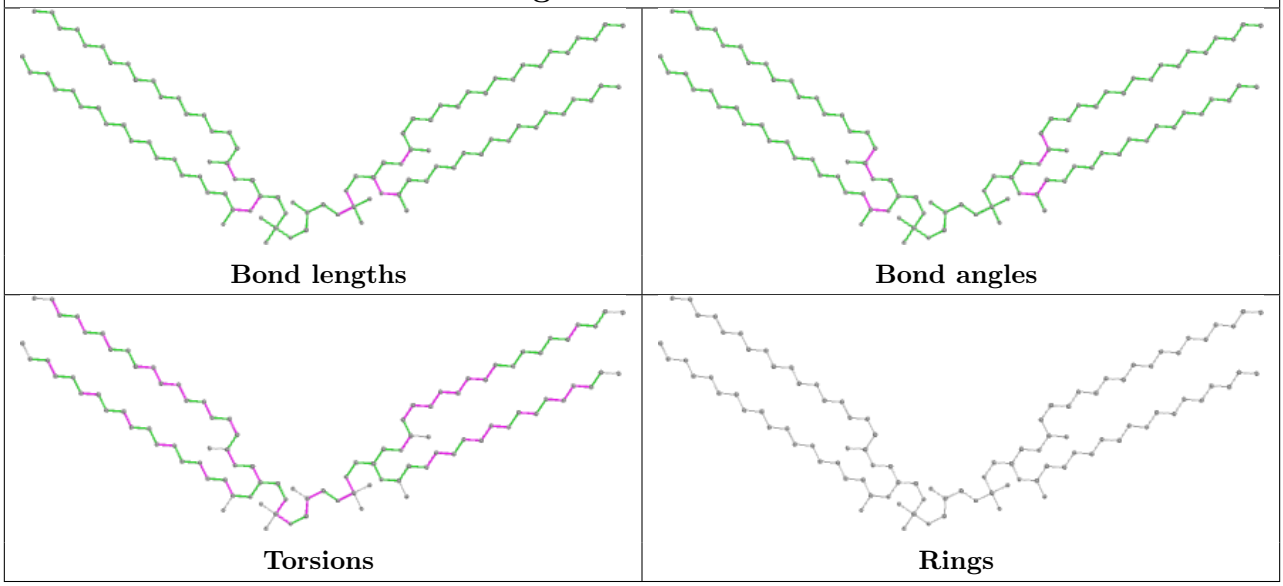
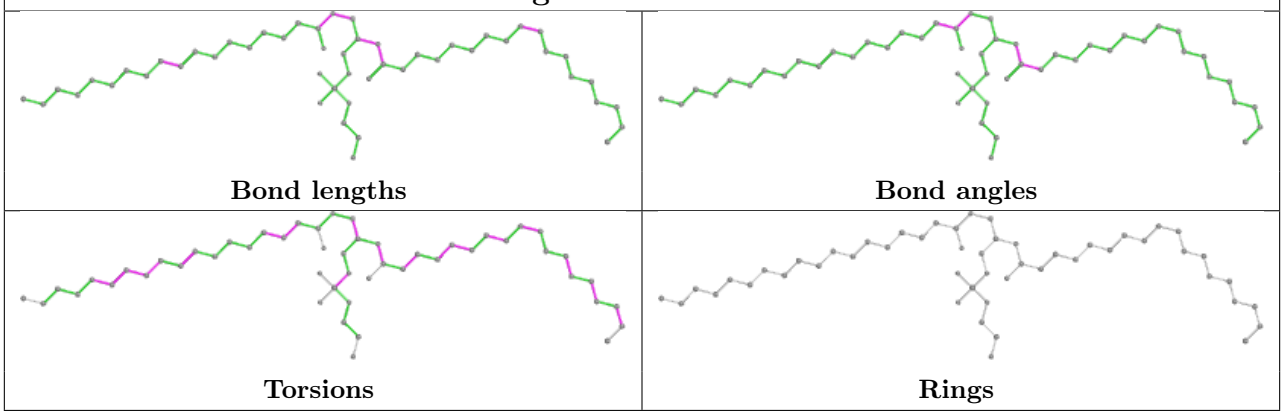


Rings

Ligand CDL l 701



Ligand PEE r 501



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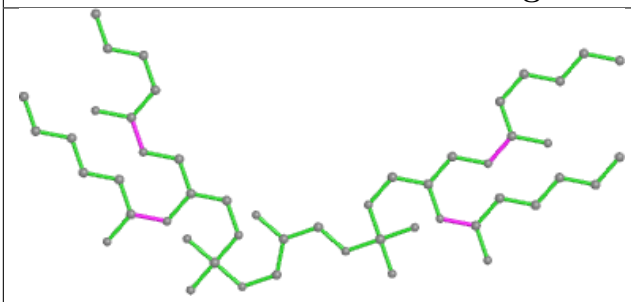

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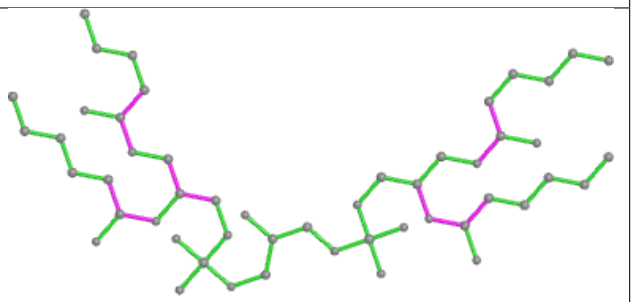
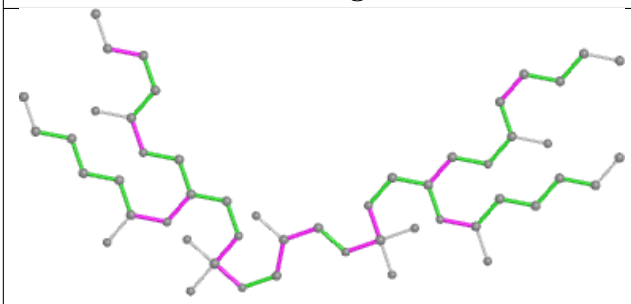
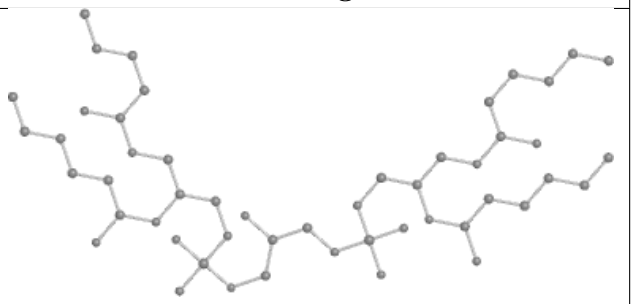


Bond angles

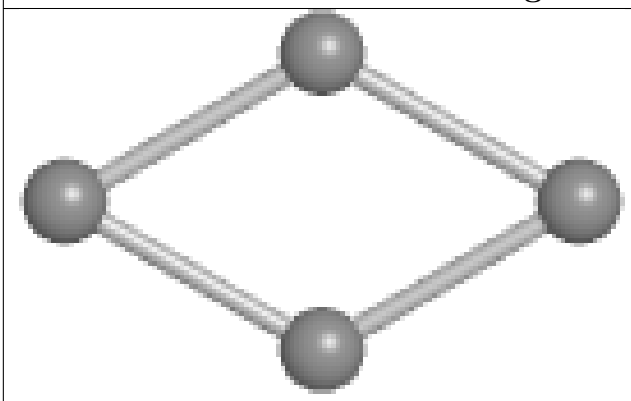


Torsions



Rings

Ligand FES M 803



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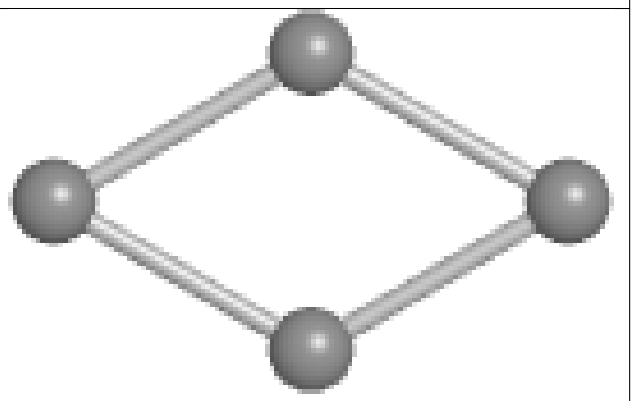
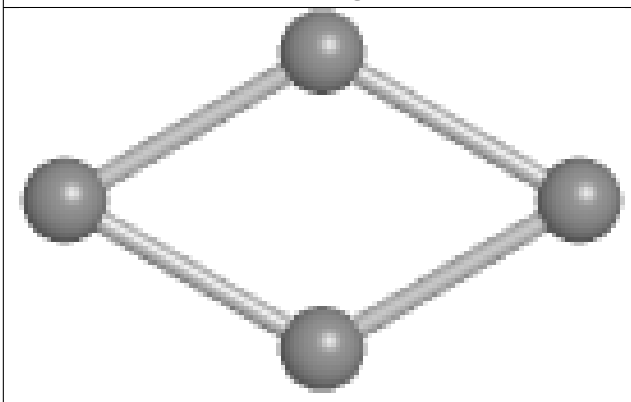


Bond angles



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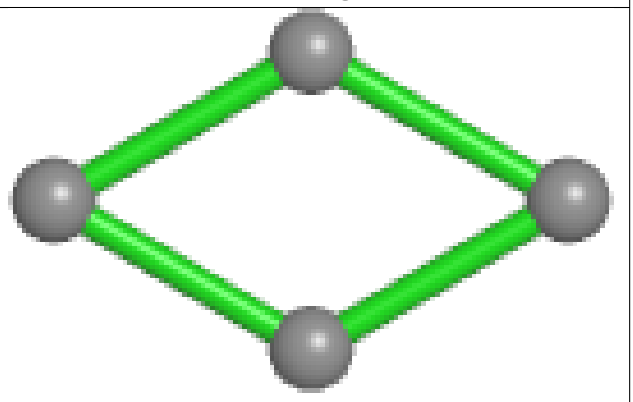
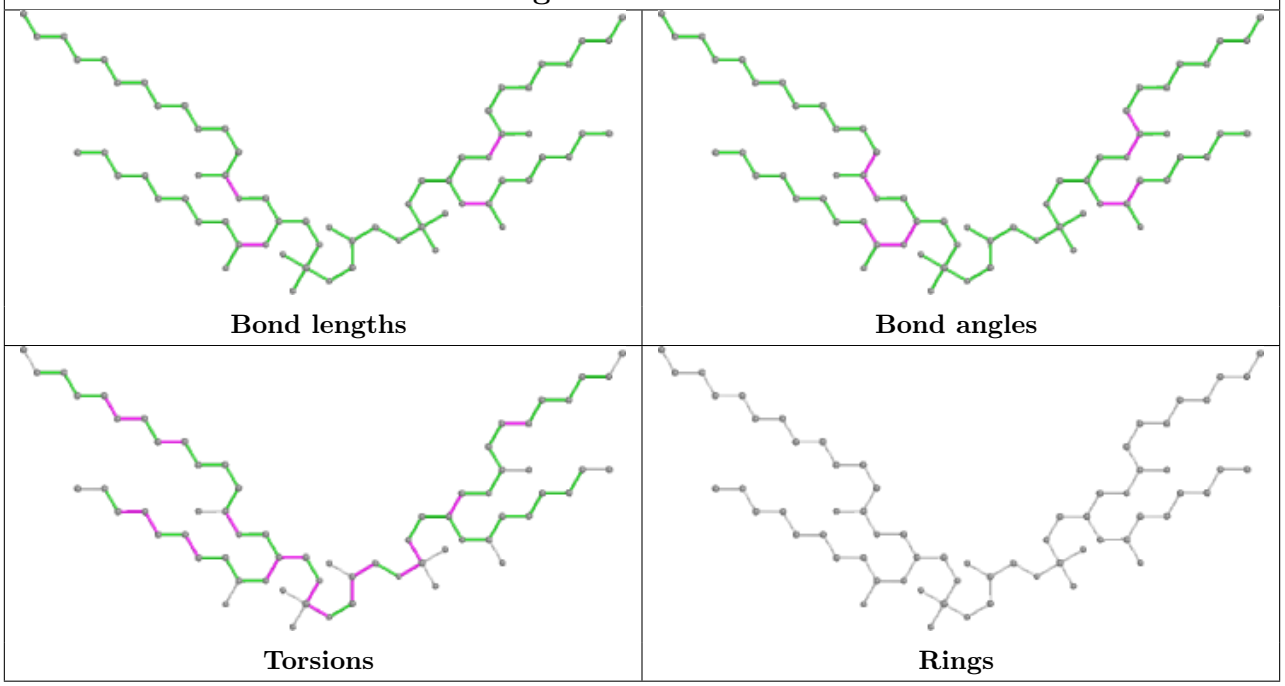
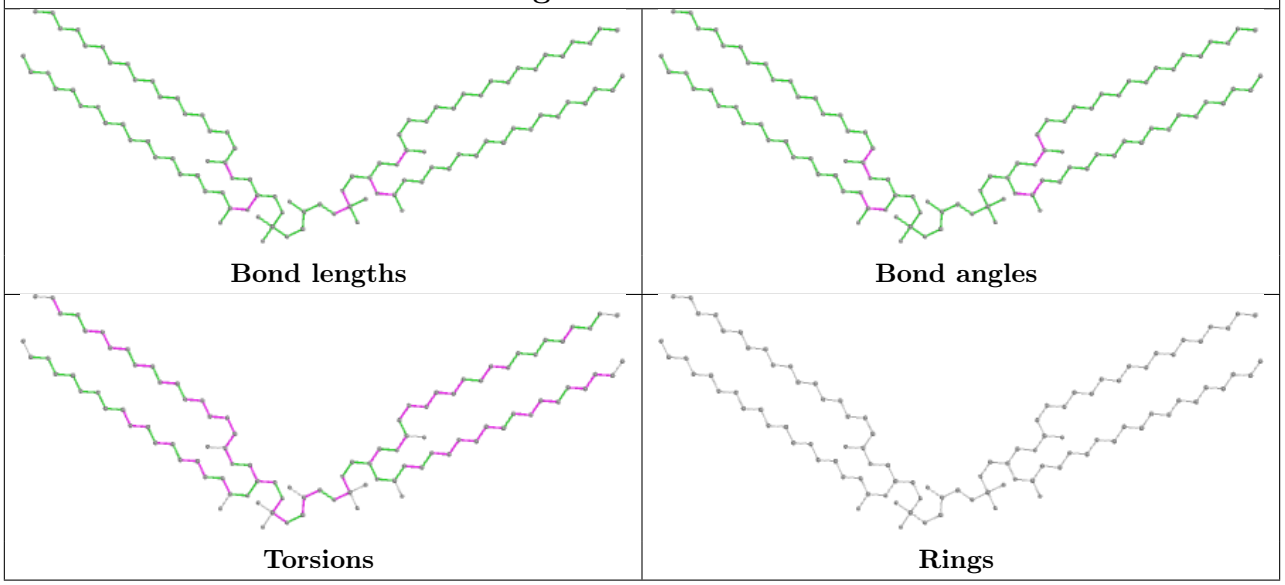


Rings

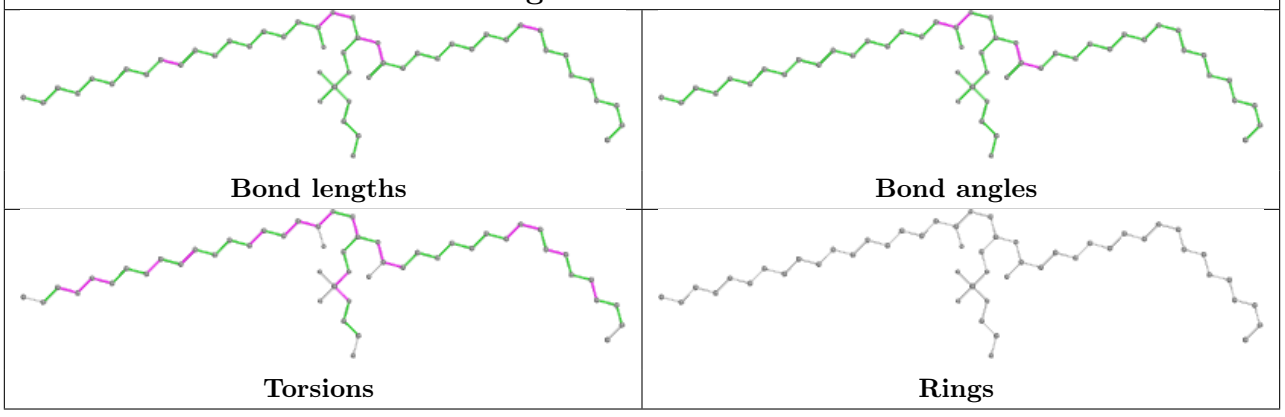
Ligand CDL i 401



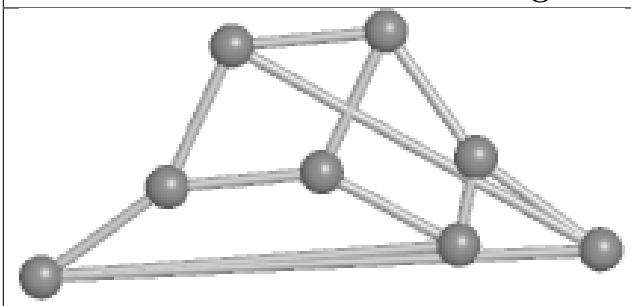
Ligand CDL l 702



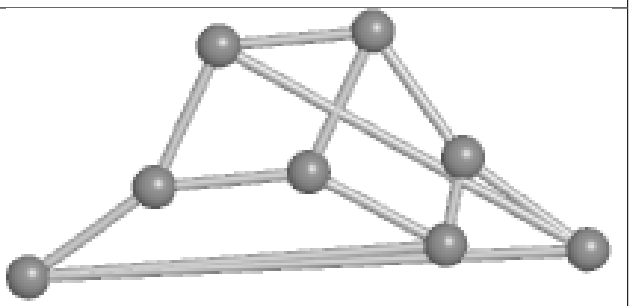
Ligand PEE U 101



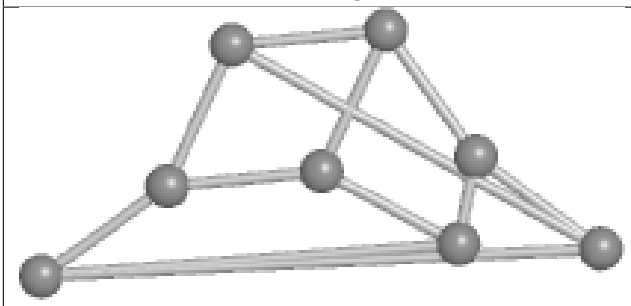
Ligand SF4 B 302



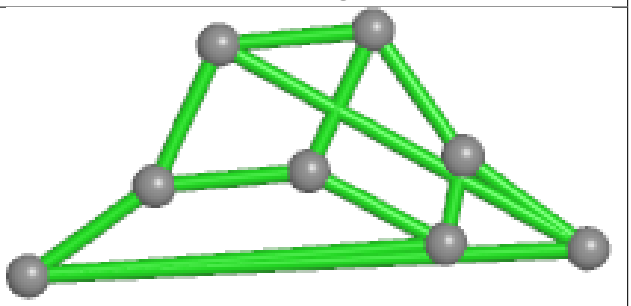
Bond lengths



Bond angles

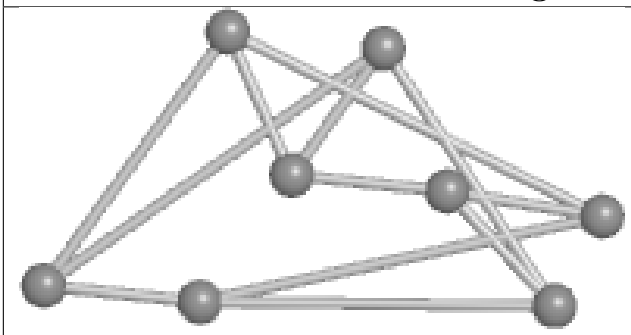


Torsions

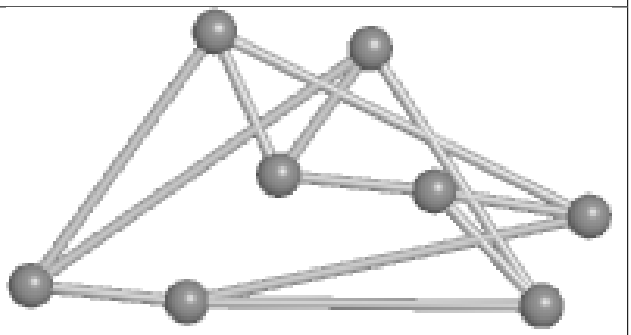


Rings

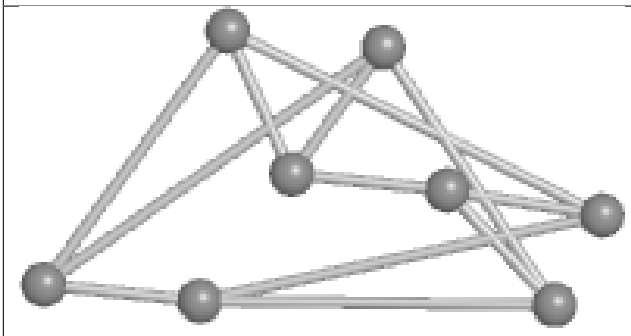
Ligand SF4 A 501



Bond lengths



Bond angles



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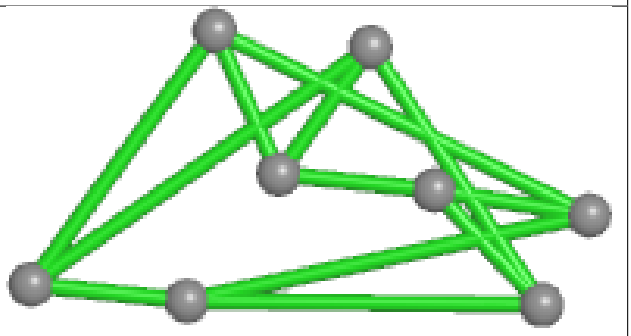
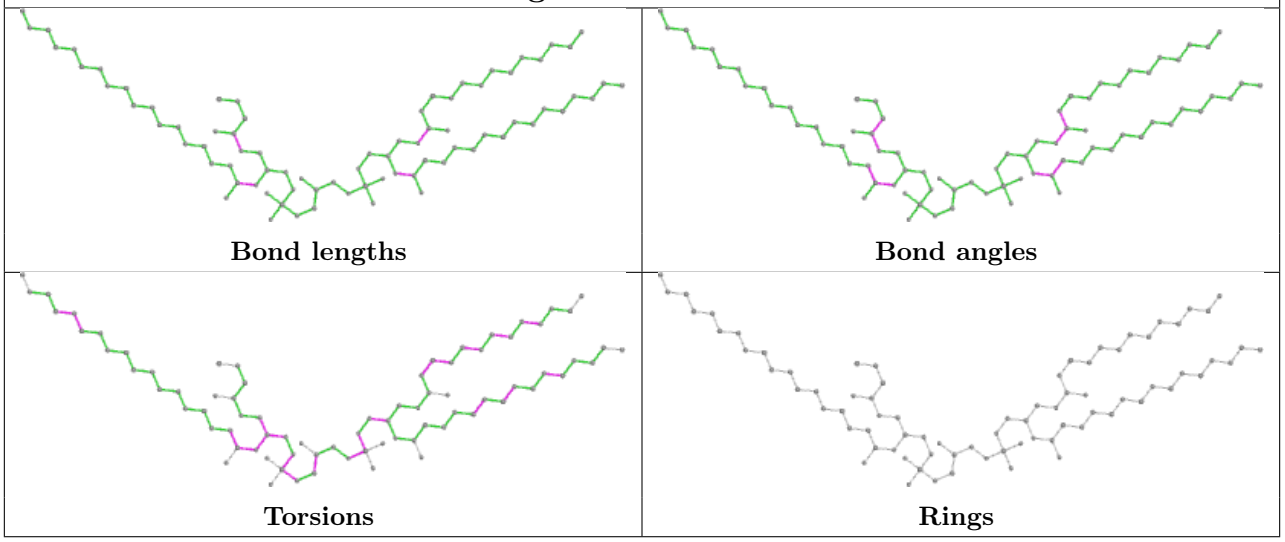
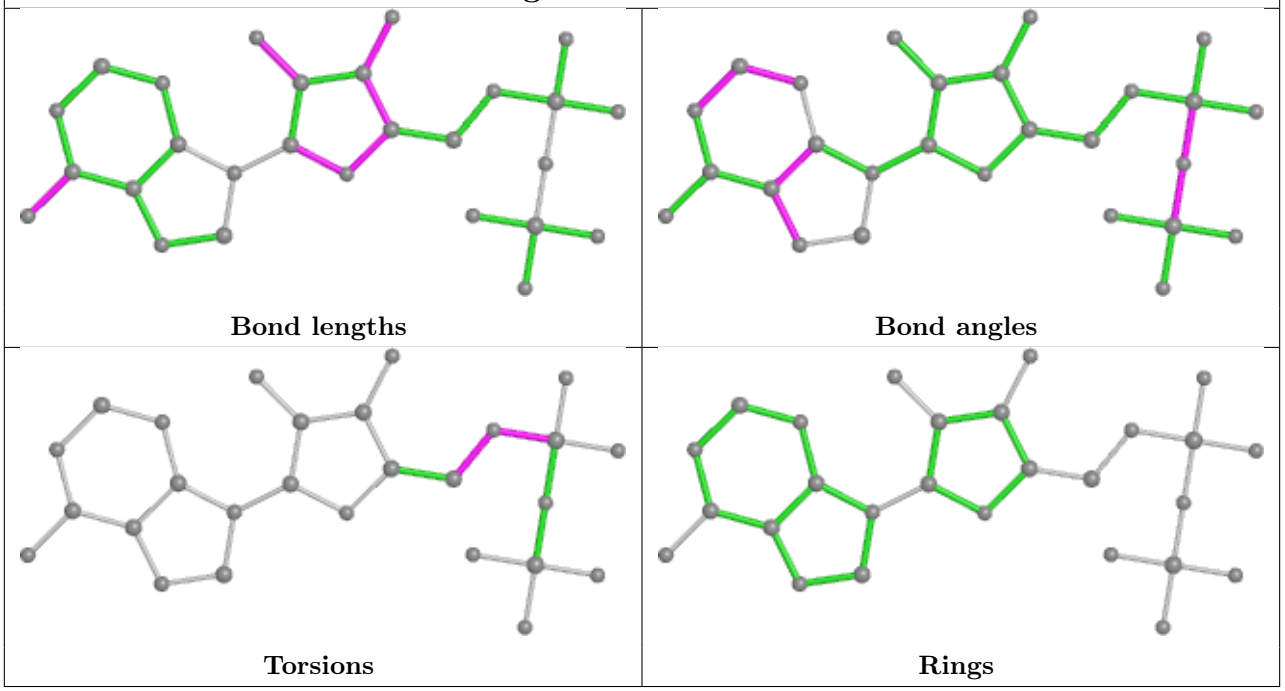


Rings

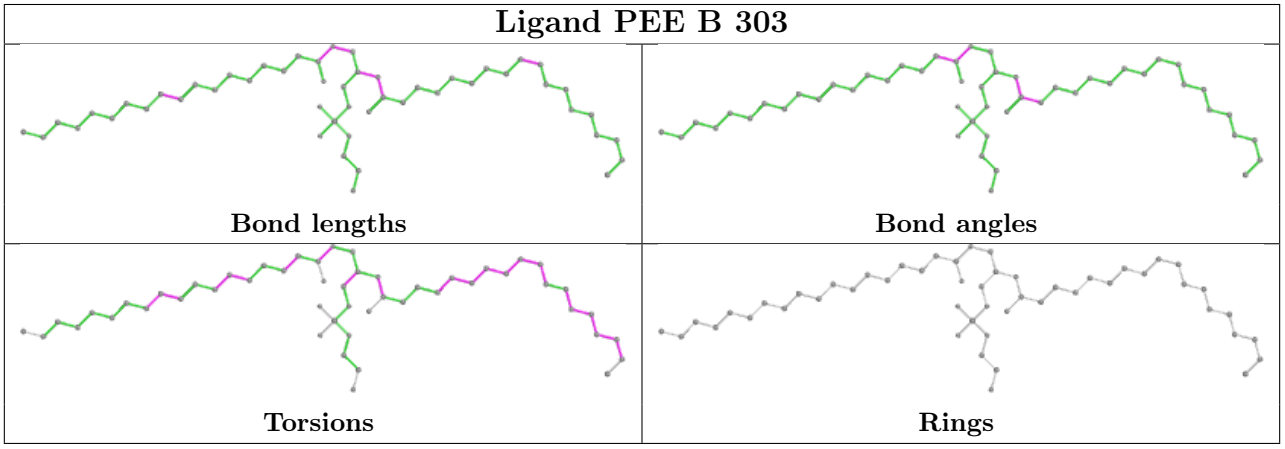
Ligand CDL n 101



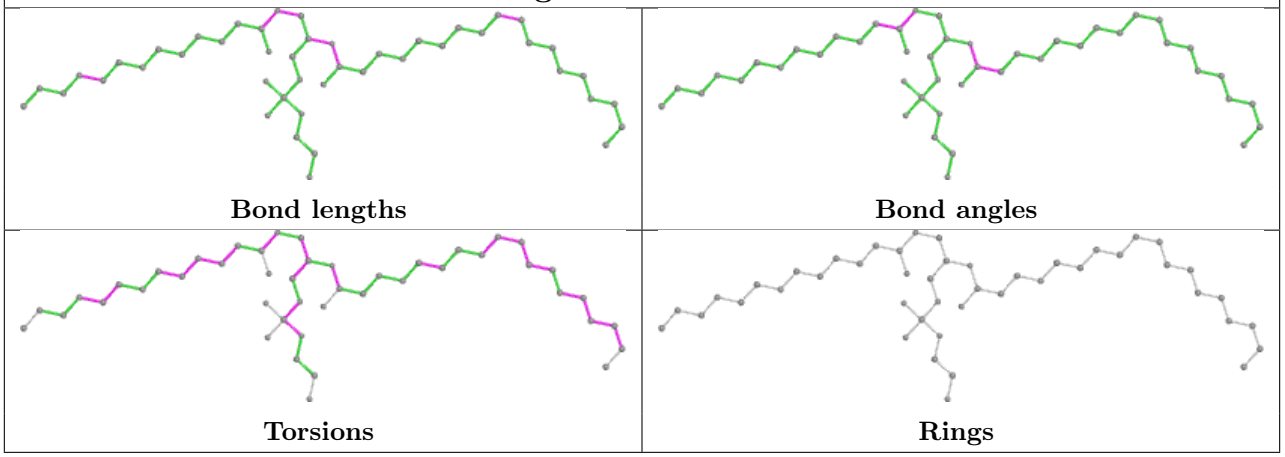
Ligand ADP w 401



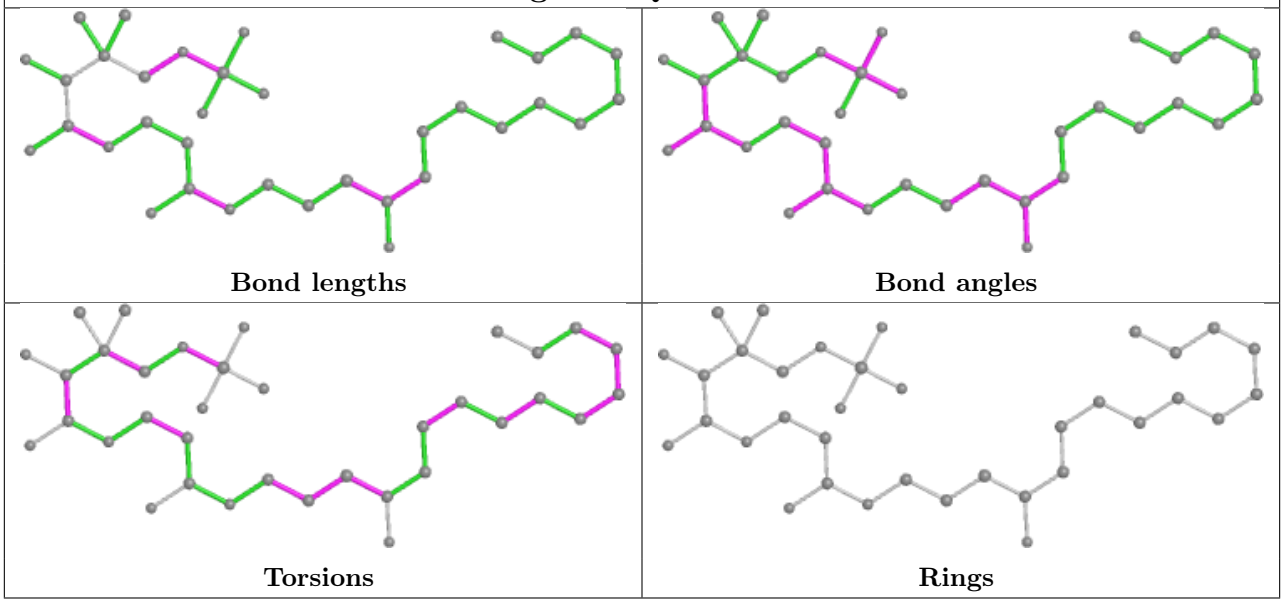
Ligand PEE B 303



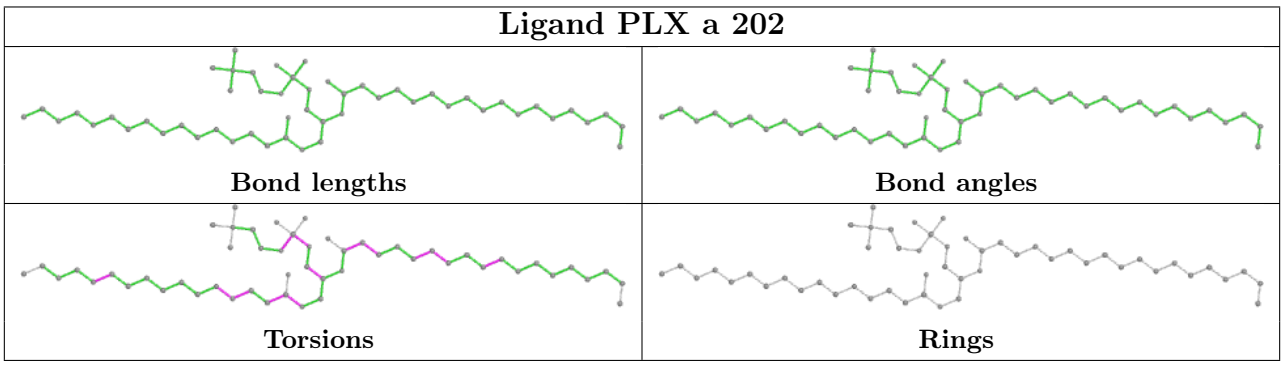
Ligand PEE l 703



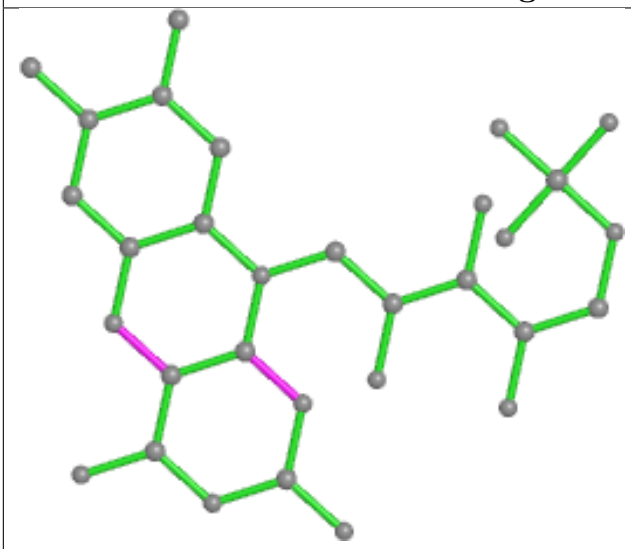
Ligand 8Q1 G 201



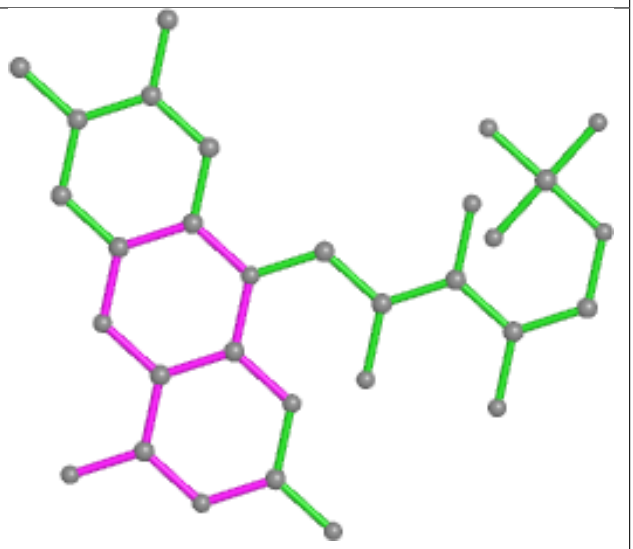
Ligand PLX a 202



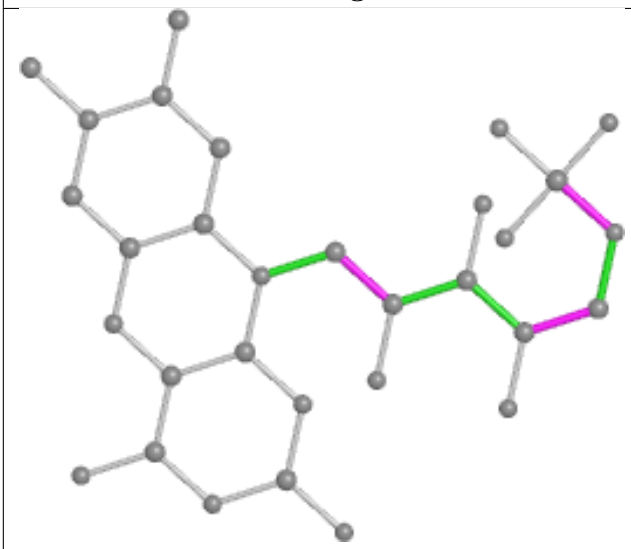
Ligand FMN A 502



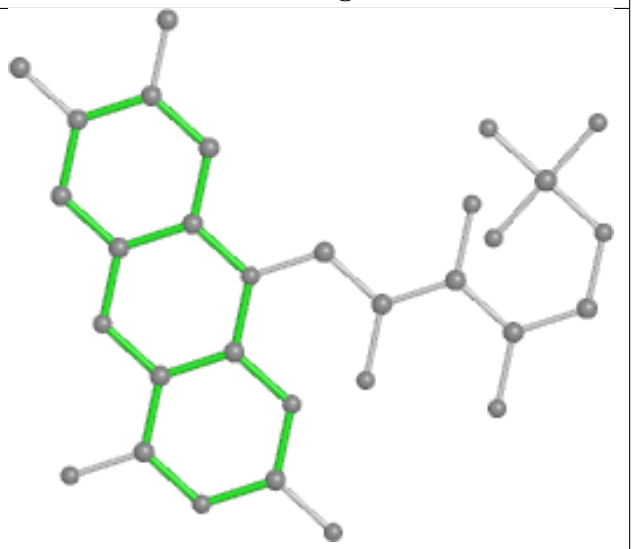
Bond lengths



Bond angles

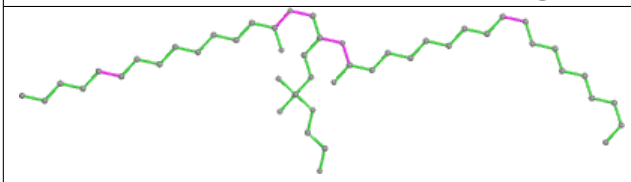


Torsions

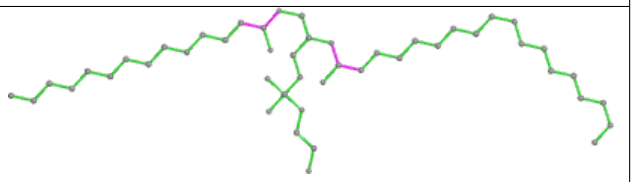


Rings

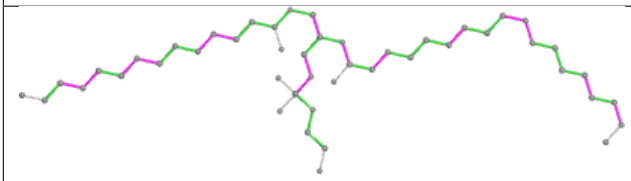
Ligand PEE i 402



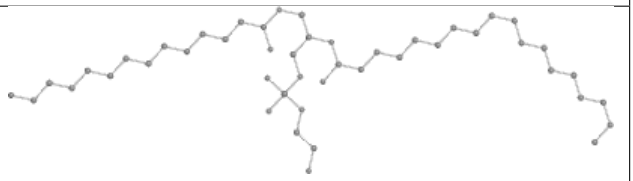
Bond lengths



Bond angles

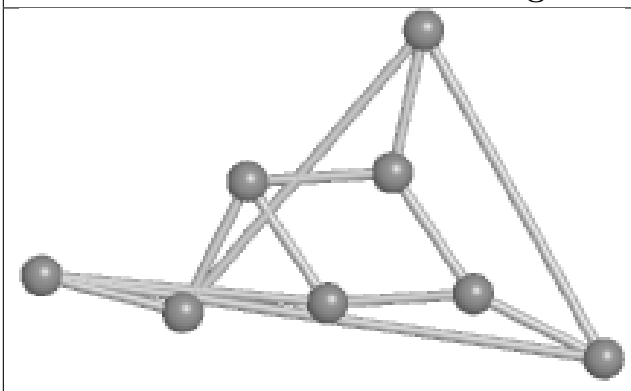


Torsions

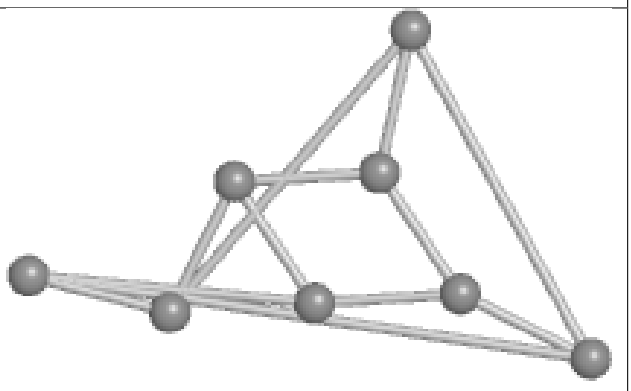


Rings

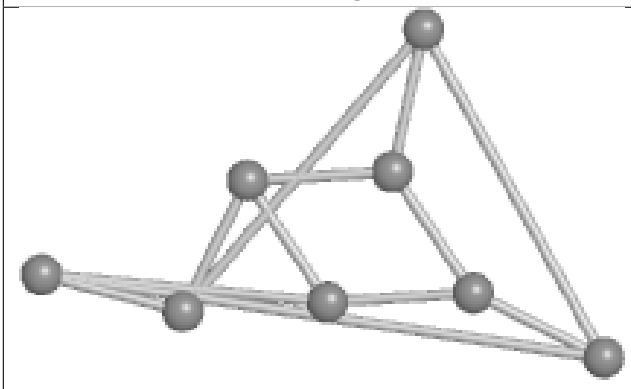
Ligand SF4 M 801



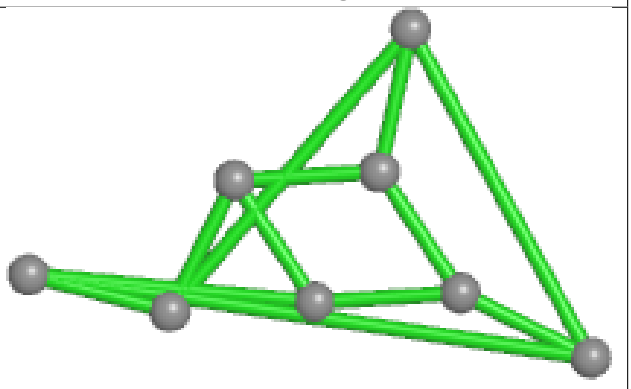
Bond lengths



Bond angles

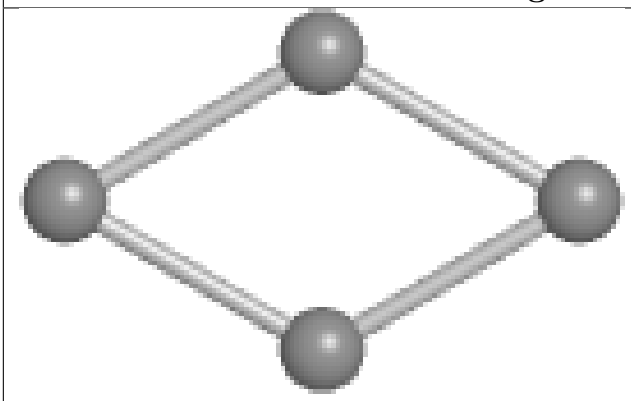


Torsions

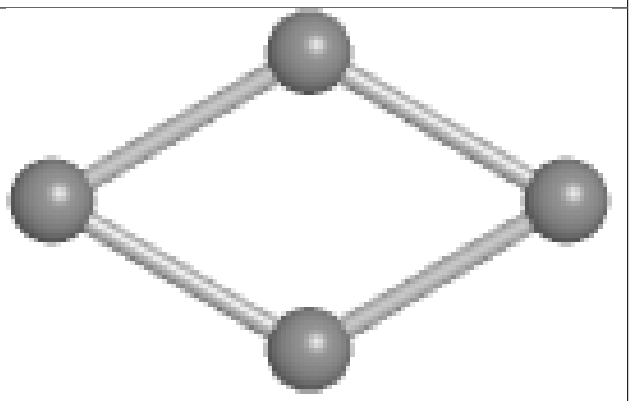


Rings

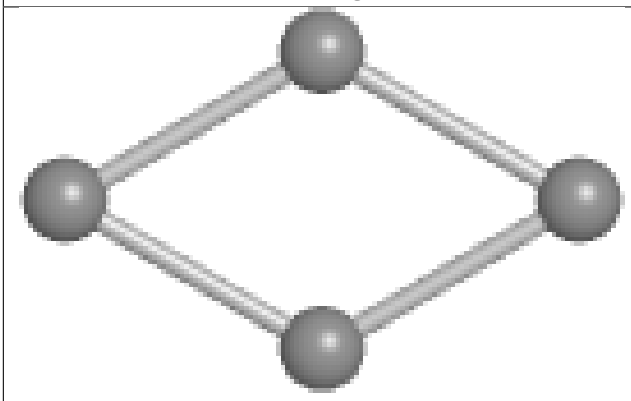
Ligand FES O 301



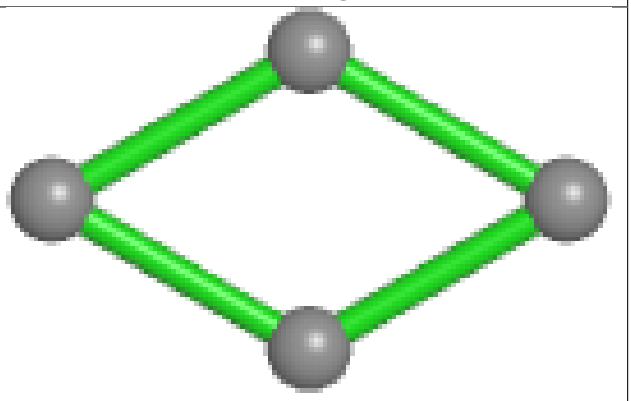
Bond lengths



Bond angles

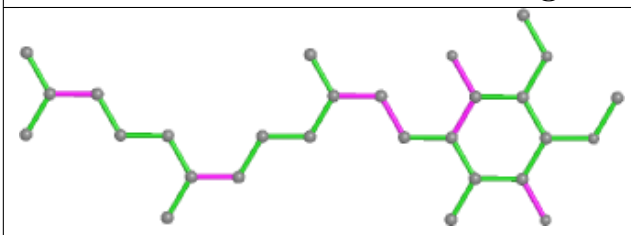


Torsions

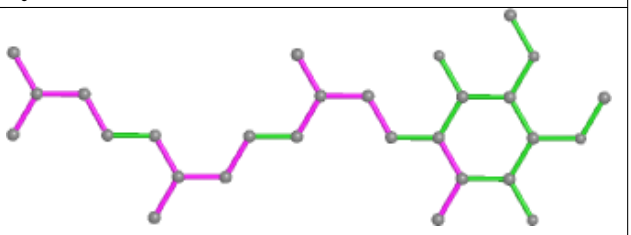


Rings

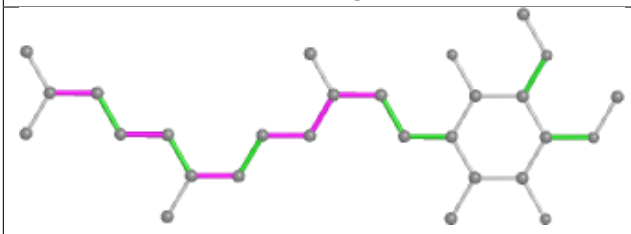
Ligand UQ s 401



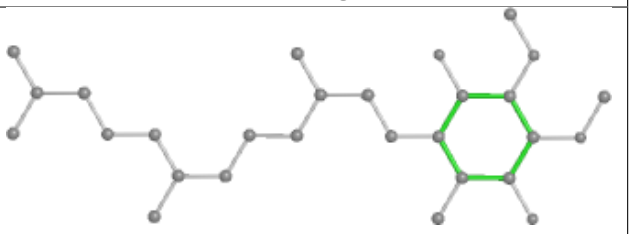
Bond lengths



Bond angles

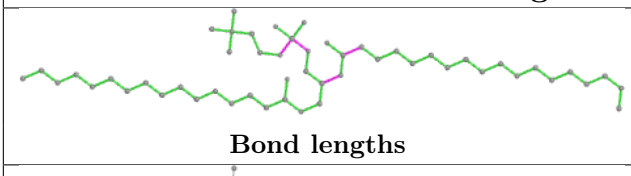


Torsions

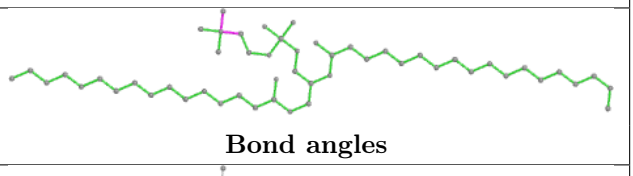


Rings

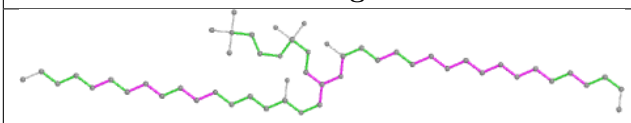
Ligand PLX r 502



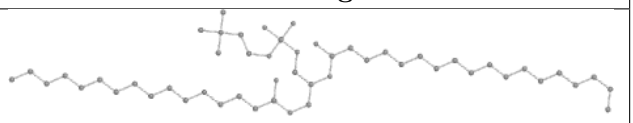
Bond lengths



Bond angles

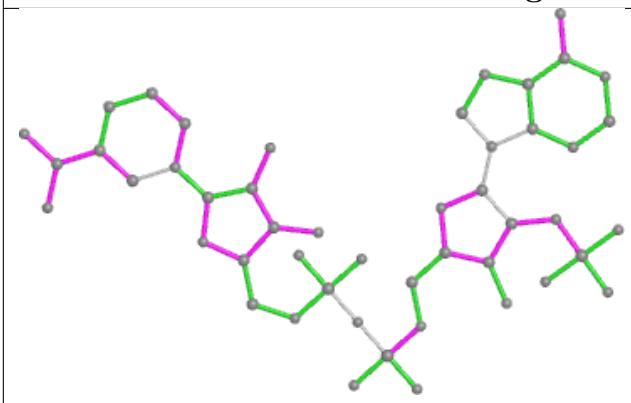


Torsions

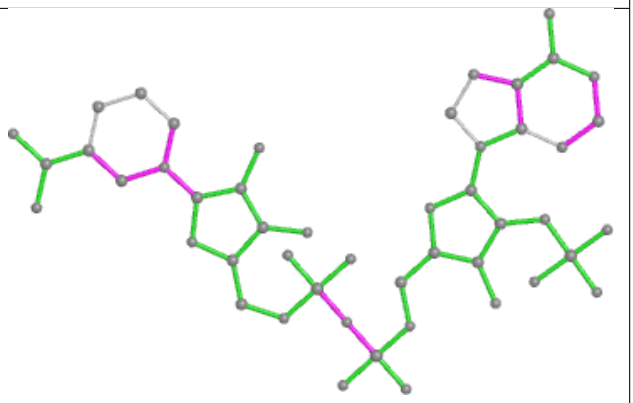


Rings

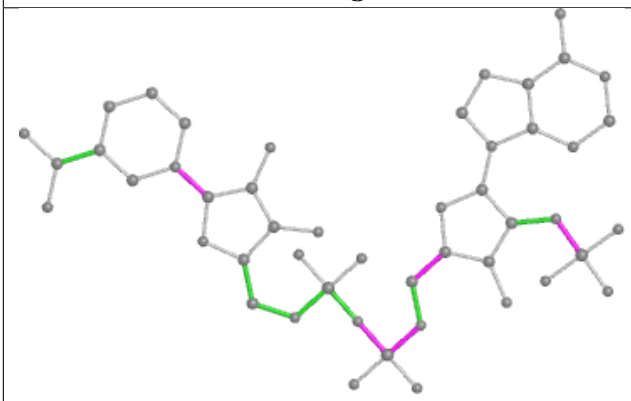
Ligand NDP J 401



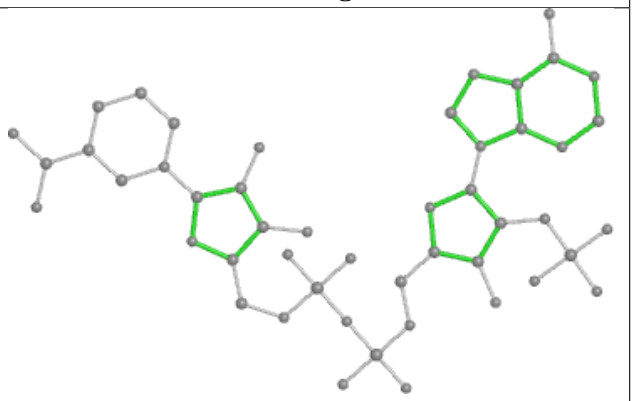
Bond lengths



Bond angles

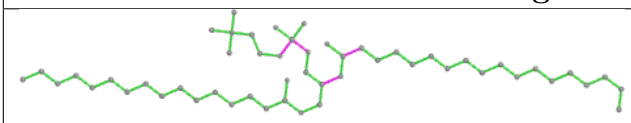


Torsions

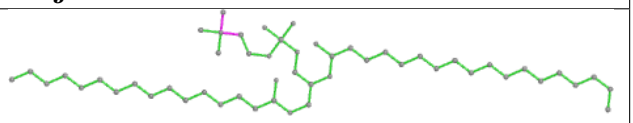


Rings

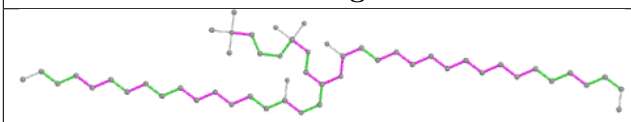
Ligand PLX j 202



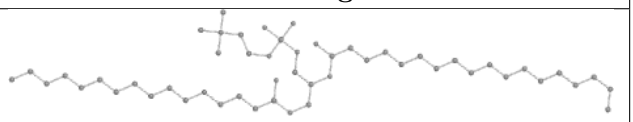
Bond lengths



Bond angles

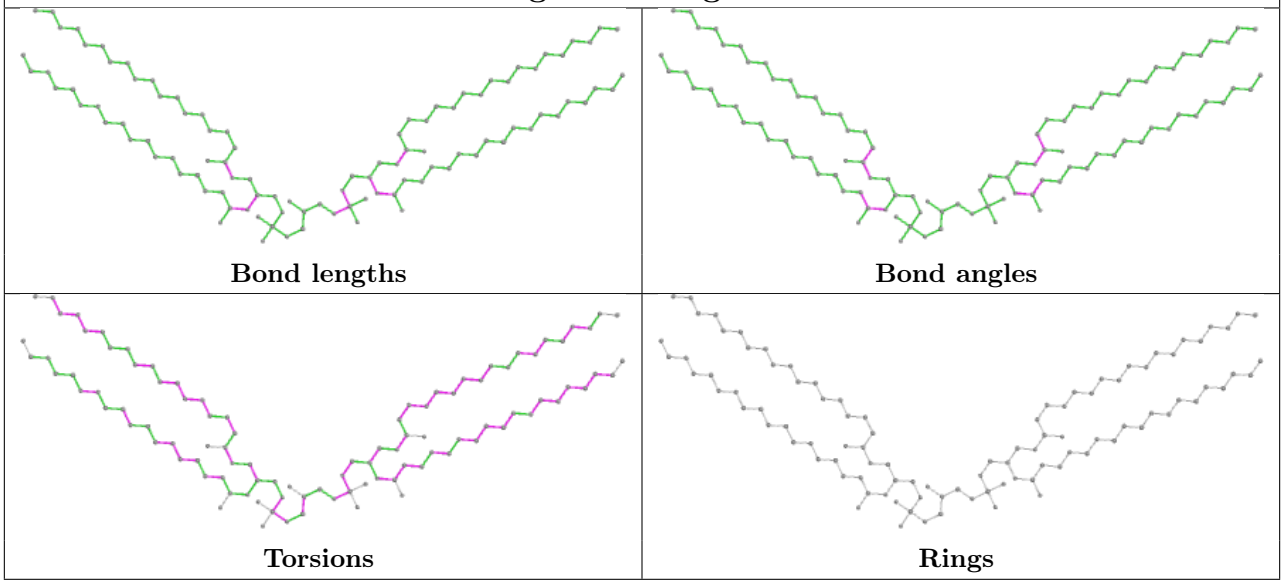


Torsions

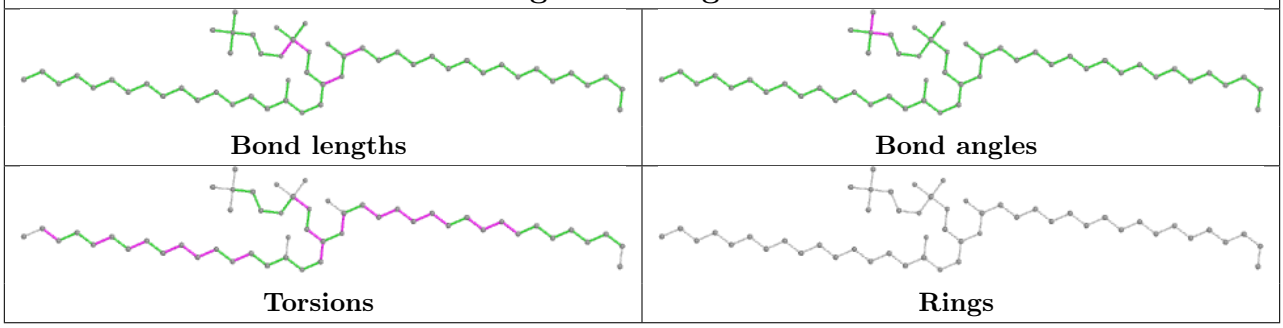


Rings

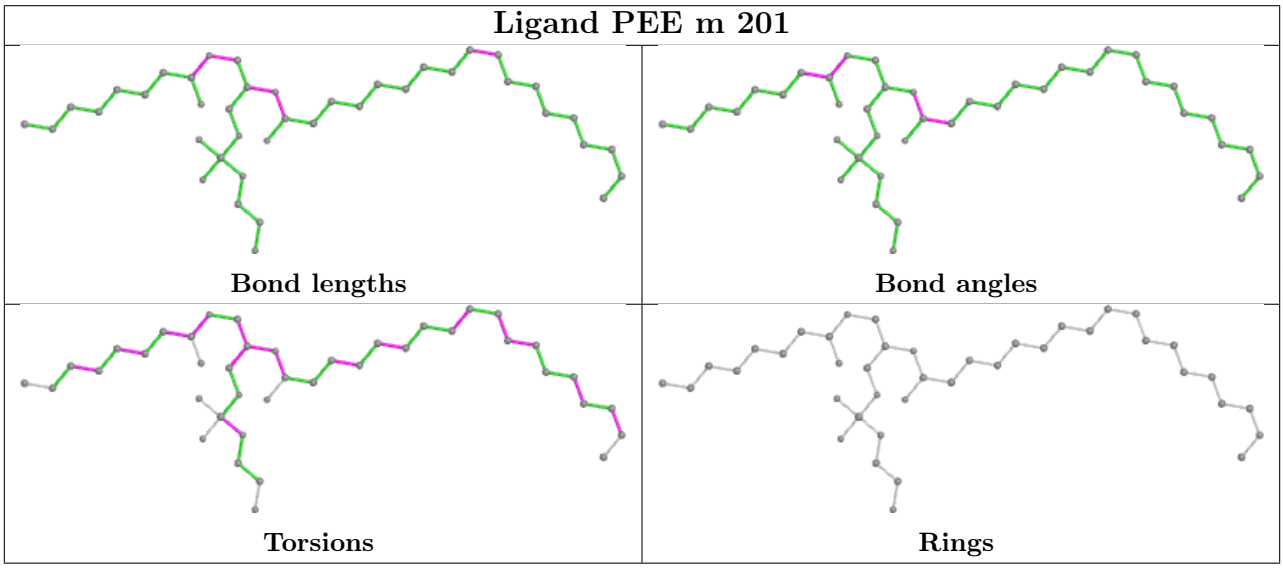
Ligand CDL g 202



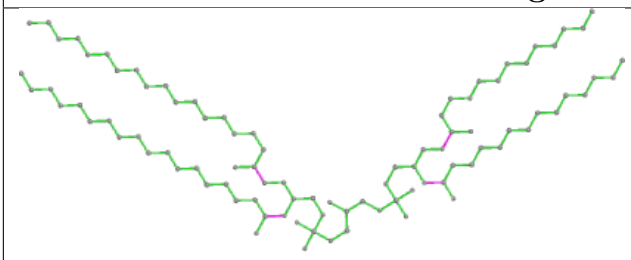
Ligand PLX g 201



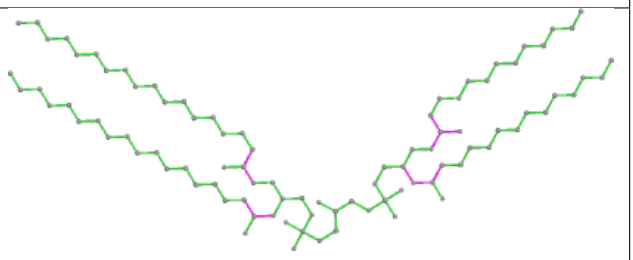
Ligand PEE m 201



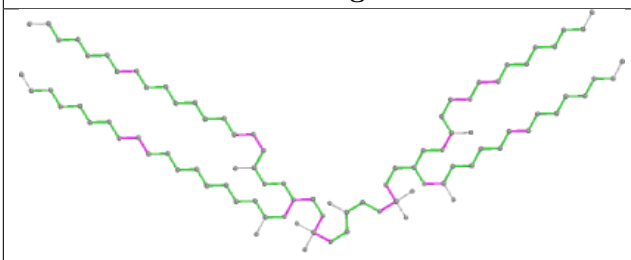
Ligand CDL a 201



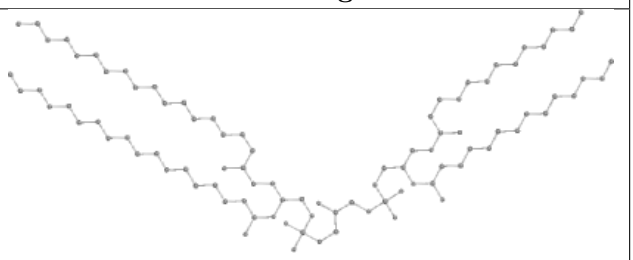
Bond lengths



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.

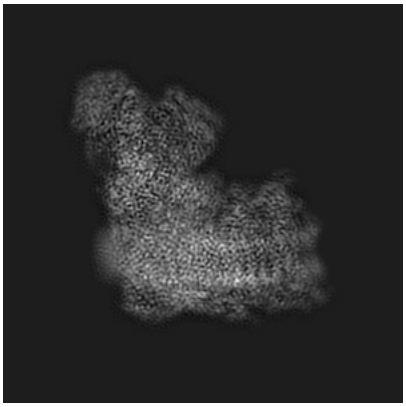
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31650. These allow visual inspection of the internal detail of the map and identification of artifacts.

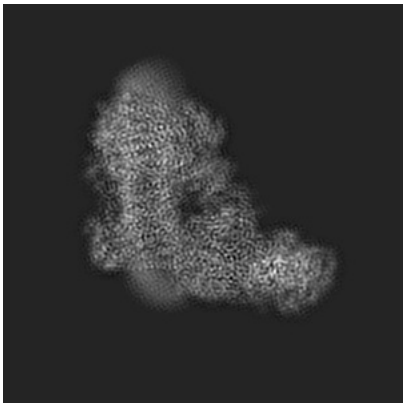
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

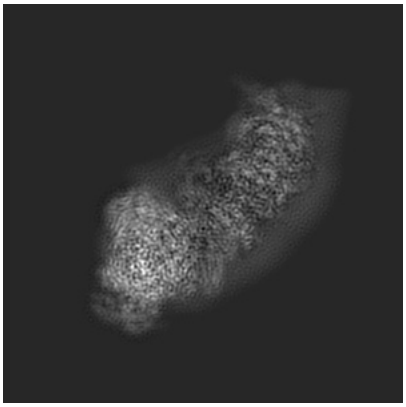
6.1.1 Primary map



X



Y

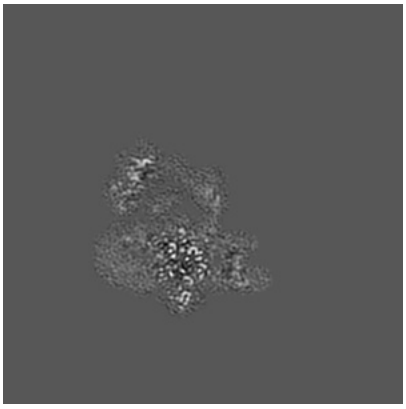


Z

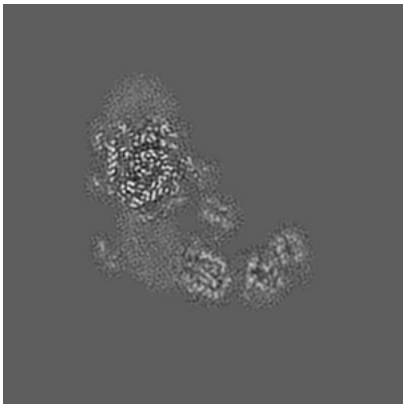
The images above show the map projected in three orthogonal directions.

6.2 Central slices

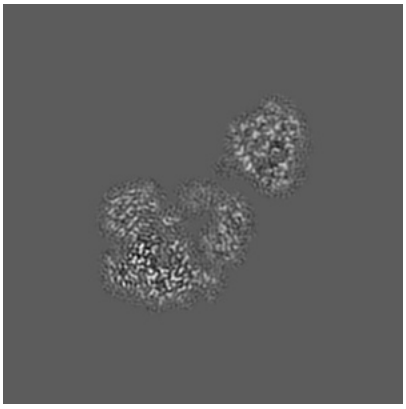
6.2.1 Primary map



X Index: 155



Y Index: 155

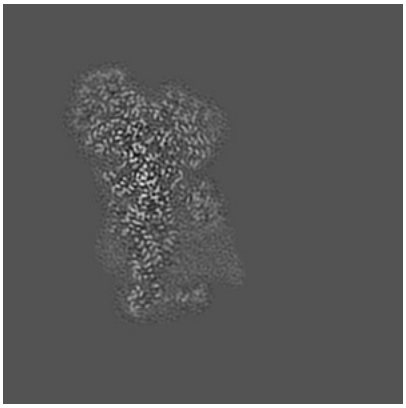


Z Index: 155

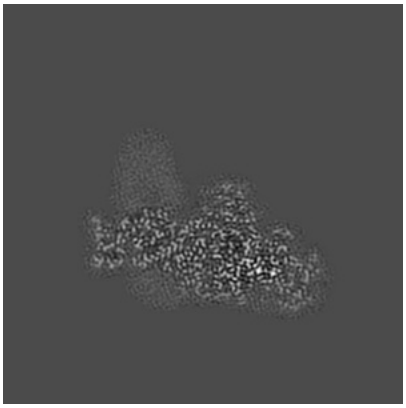
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

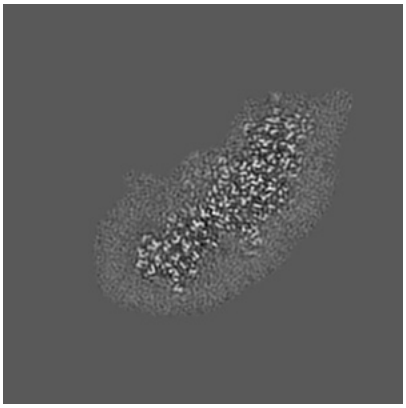
6.3.1 Primary map



X Index: 108



Y Index: 103

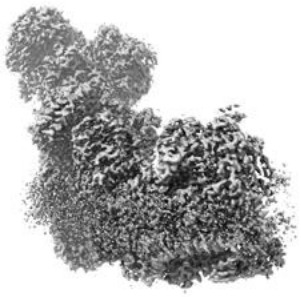


Z Index: 120

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

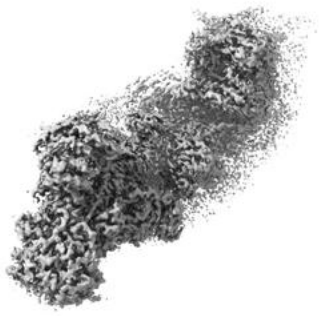
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

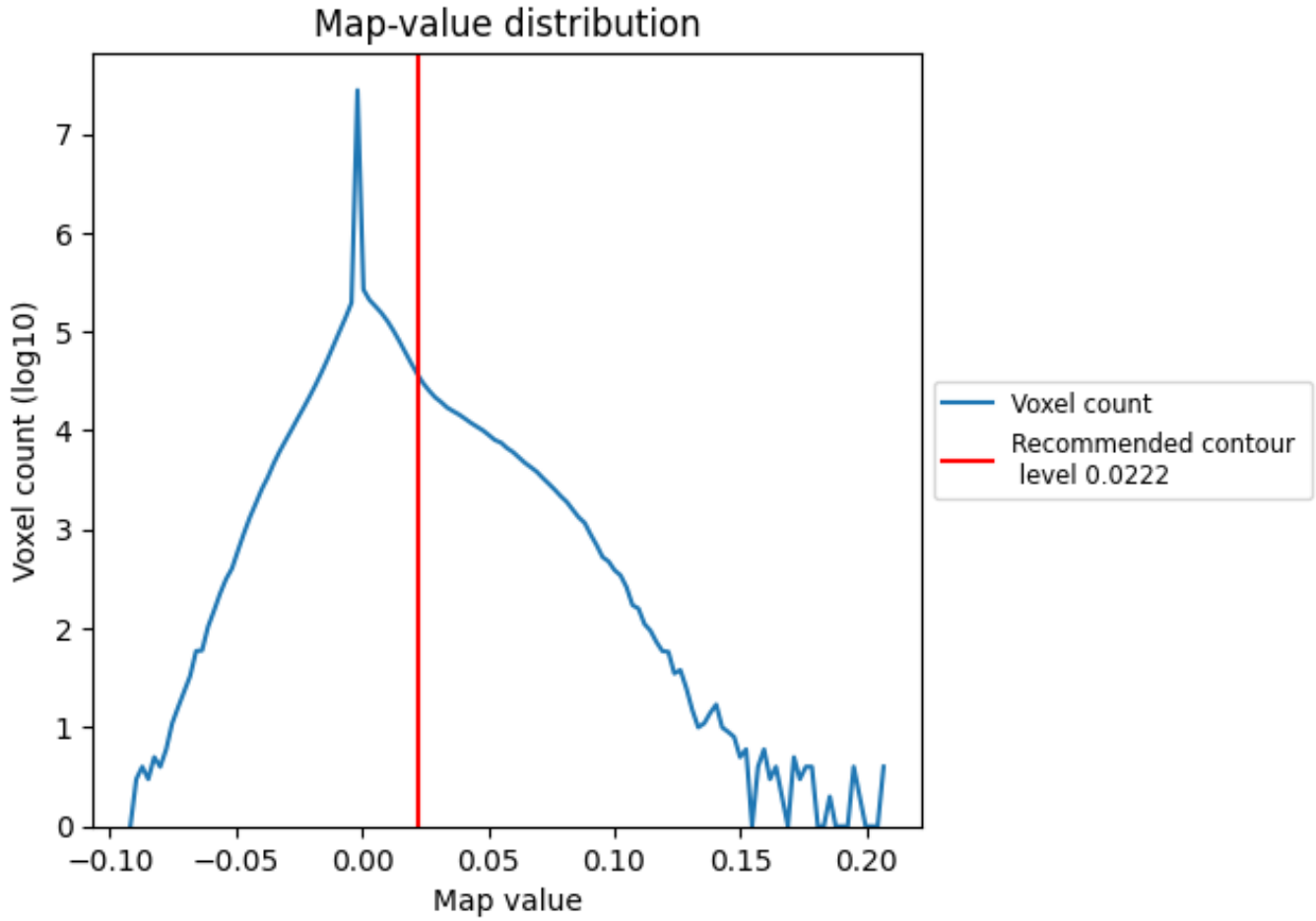
6.5 Mask visualisation (i)

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

7 Map analysis

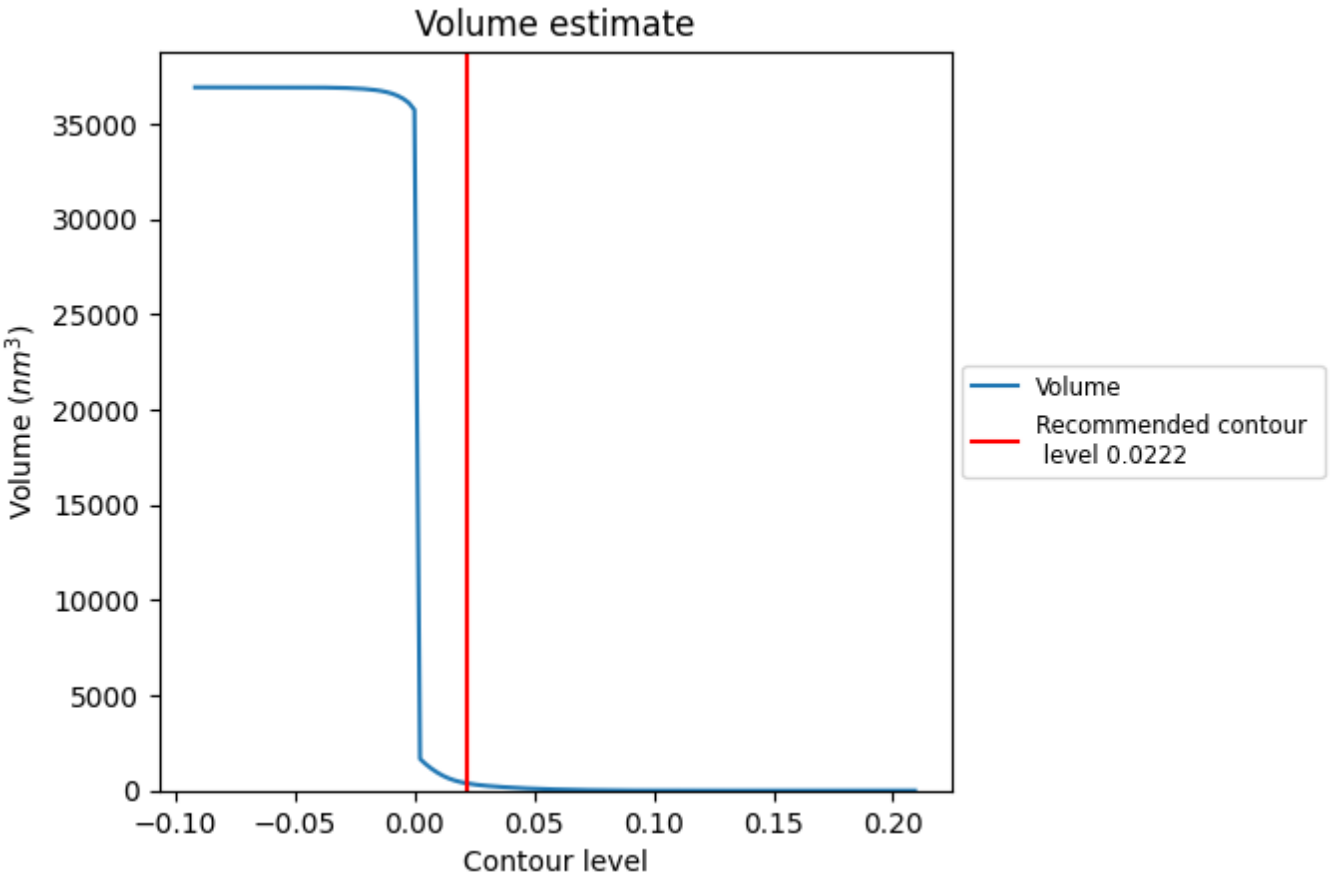
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

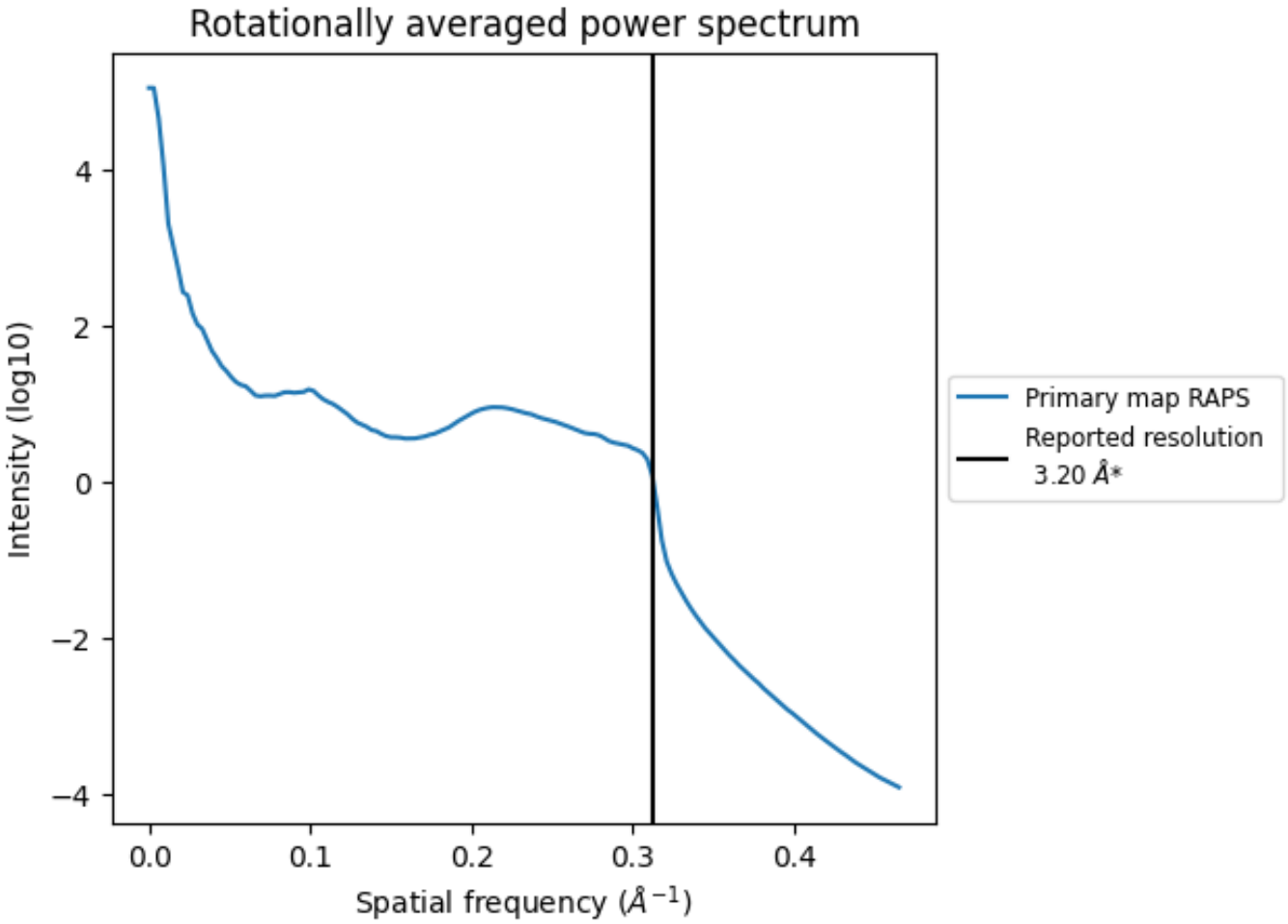
7.2 Volume estimate



The volume at the recommended contour level is 371 nm^3; this corresponds to an approximate mass of 335 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 0.312 $Å^{-1}$

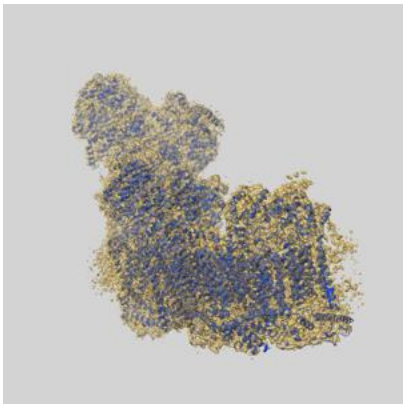
8 Fourier-Shell correlation (i)

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

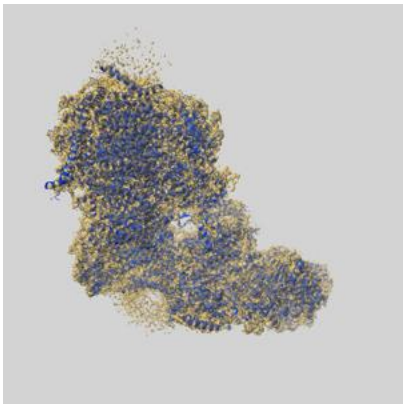
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31650 and PDB model 7V32. Per-residue inclusion information can be found in section 3 on page 20.

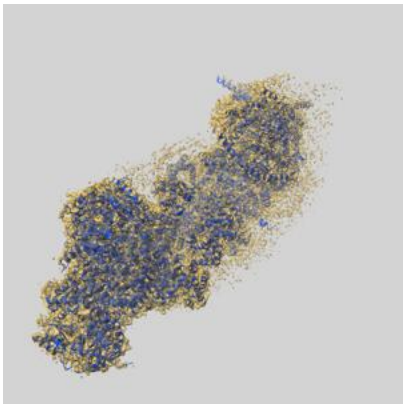
9.1 Map-model overlay



X



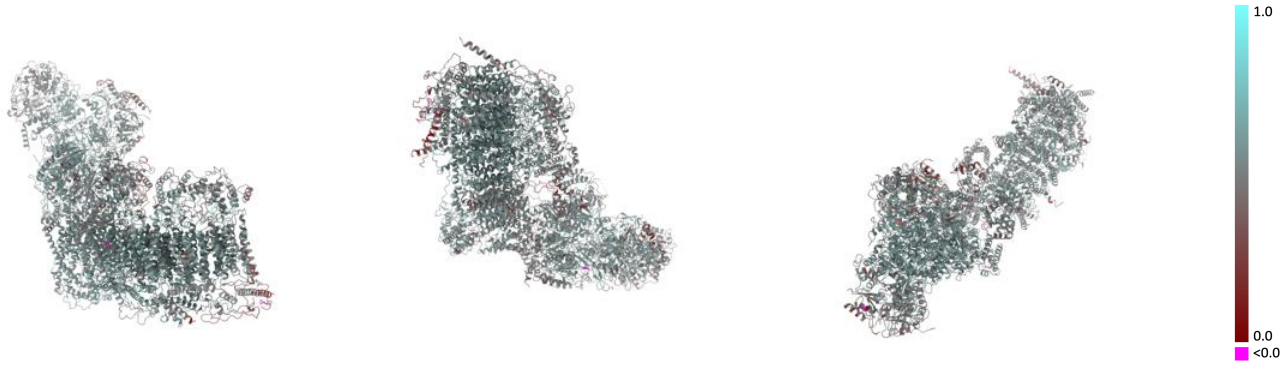
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0222 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.

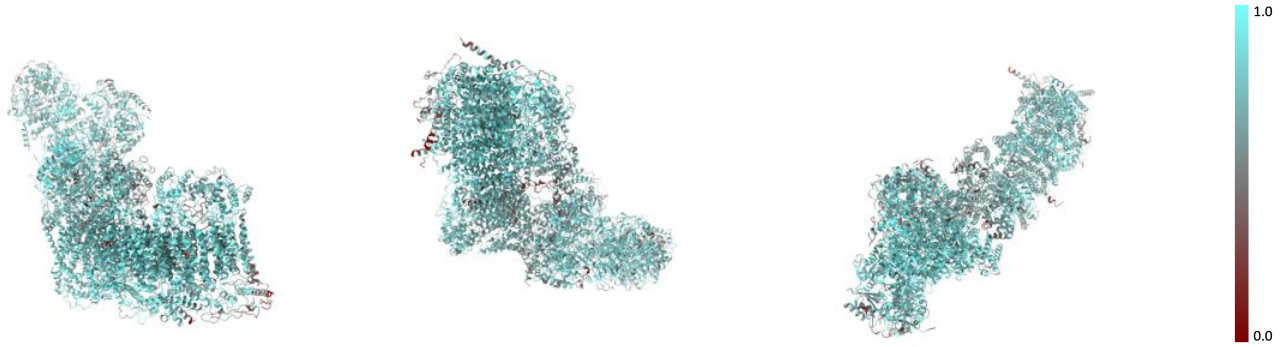
9.2 Q-score mapped to coordinate model (i)



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.

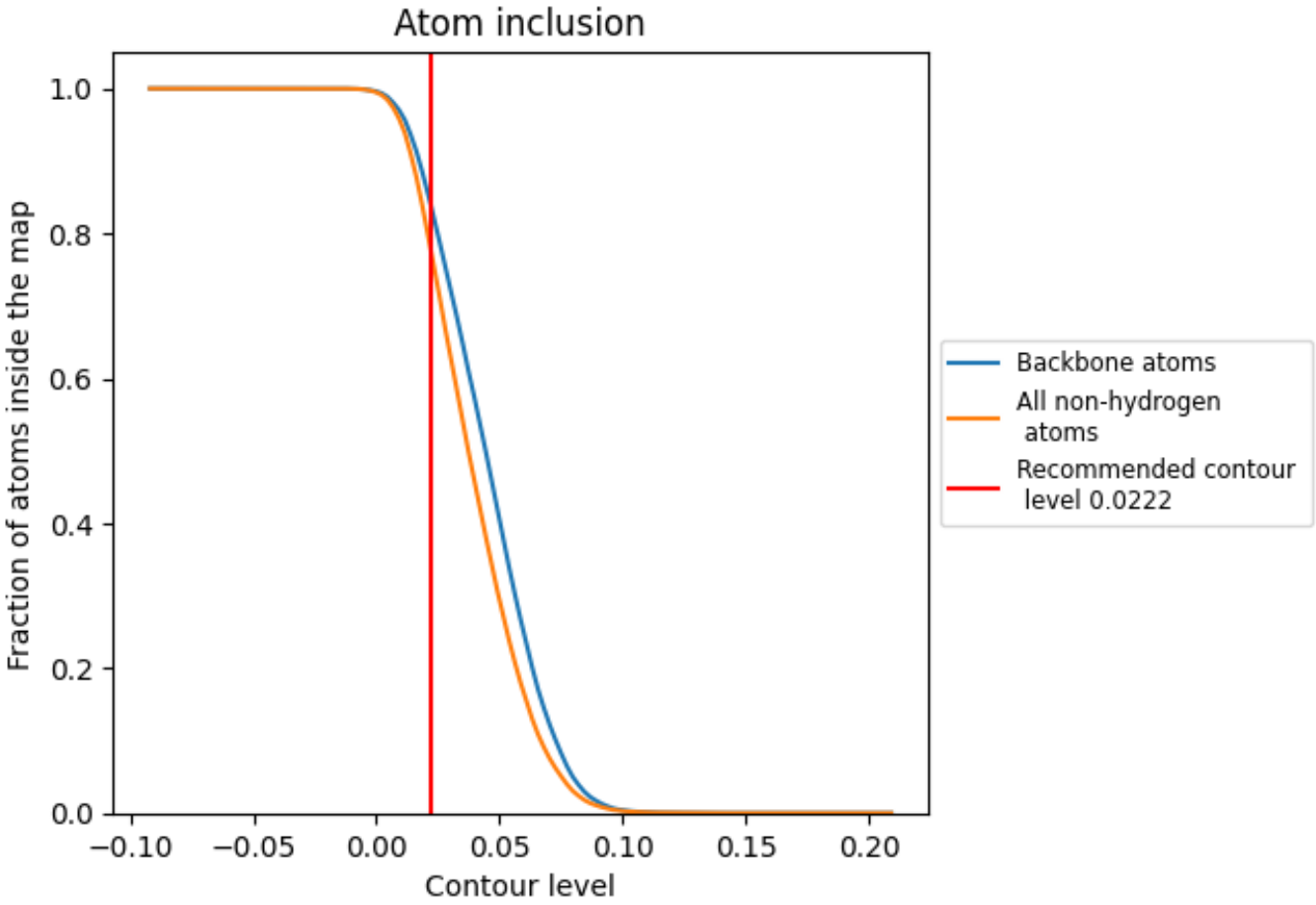
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0222).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7769	0.5330
A	0.7552	0.5080
B	0.9014	0.5870
C	0.8500	0.5650
E	0.7357	0.5190
F	0.6518	0.4320
G	0.5360	0.4160
H	0.7754	0.5150
I	0.7897	0.5470
J	0.7097	0.4950
K	0.6279	0.4300
L	0.8078	0.5620
M	0.8135	0.5450
N	0.7656	0.5430
O	0.7145	0.4900
P	0.8876	0.5840
Q	0.8507	0.5740
S	0.8571	0.5660
T	0.7050	0.5080
U	0.8088	0.5400
V	0.6124	0.4800
W	0.8285	0.5550
X	0.7050	0.4890
Y	0.6479	0.4490
Z	0.6201	0.4600
a	0.7994	0.5620
b	0.6832	0.4800
c	0.7608	0.5260
d	0.7633	0.5200
e	0.7146	0.5070
f	0.7066	0.5040
g	0.7993	0.5550
h	0.8085	0.5500
i	0.8438	0.5680
j	0.6756	0.5110

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Chain	Atom inclusion	Q-score
k	0.7520	0.5390
l	0.7856	0.5500
m	0.7197	0.5180
n	0.6756	0.5020
o	0.7794	0.5300
p	0.7806	0.5250
r	0.8547	0.5750
s	0.8252	0.5550
u	0.8294	0.5570
v	0.6352	0.4280
w	0.7121	0.4990