Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 02:58 PM JST

PDB ID	:	7V33
EMDB ID	:	EMD-31651
Title	:	Active state complex I from rotenone-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-10
Resolution	:	2.60 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:

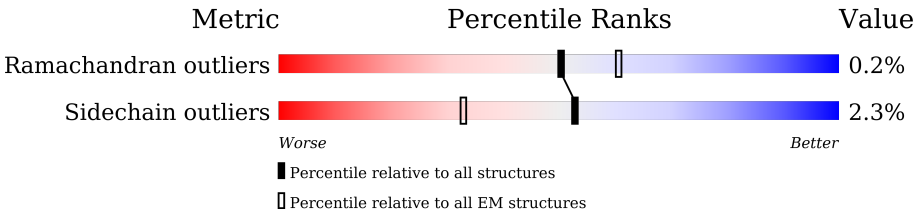
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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	433	97%
2	B	176	99%
3	C	156	99%
4	E	115	99%
5	F	86	94% 6%
6	G	88	17% 95% 5%
6	X	88	97%
7	H	112	99%
8	I	112	6% 79% 7% 13%

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Mol	Chain	Length	Quality of chain
9	J	342	97%
10	K	43	7% 95% 5%
11	L	125	99%
12	M	690	99%
13	N	144	97%
14	O	217	98%
15	P	208	99%
16	Q	430	98%
17	S	70	100%
18	T	96	5% 97%
19	U	83	95% 5%
20	V	140	96%
21	W	142	98%
22	Y	67	9% 97%
23	Z	80	14% 96%
24	a	138	99%
25	b	126	6% 76% 22%
26	c	156	97%
27	d	175	6% 100%
28	e	104	7% 96%
29	f	49	22% 100%
30	g	122	99%
31	h	105	97%
32	i	347	99%
33	j	115	97%

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Mol	Chain	Length	Quality of chain
34	k	98	98%
35	l	606	98%
36	m	175	10% 98%
37	n	56	16% 98%
38	o	128	98%
39	p	178	97%
40	r	459	98%
41	s	318	100%
42	u	171	95% 5%
43	v	125	14% 96%
44	w	320	97%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68246 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	433	3330	2103	593	614	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	684	431	129	122	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
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	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	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	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
			1671	1065	281	315	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	430	Total	C	N	O	S	0	0
			3459	2212	594	629	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
			566	364	103	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
			1161	749	197	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	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	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	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			377	246	65	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	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	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- 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	606	Total	C	N	O	S	0	0
			4797	3181	743	822	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1276	850	187	226	13		

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

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

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			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
			3624	2406	572	608	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	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
			1036	646	196	185	9		

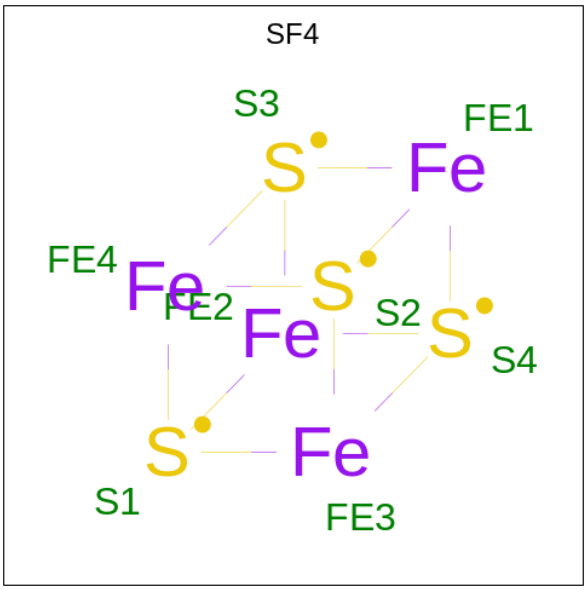
There is a discrepancy between the modelled and reference sequences:

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.

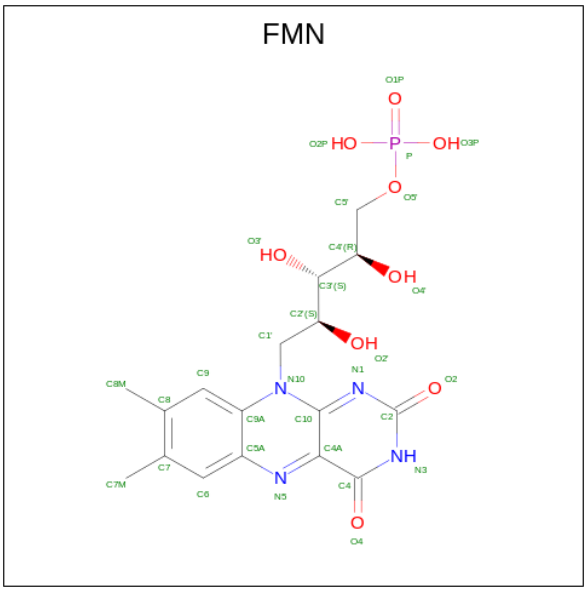
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



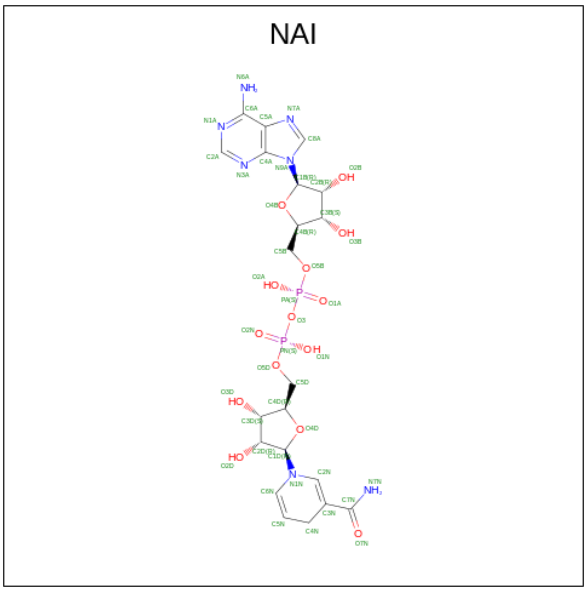
Mol	Chain	Residues	Atoms				AltConf
45	A	1	Total	Fe	S		0
			8	4	4		
45	B	1	Total	Fe	S		0
			16	8	8		
45	B	1	Total	Fe	S		0
			16	8	8		
45	C	1	Total	Fe	S		0
			8	4	4		
45	M	1	Total	Fe	S		0
			16	8	8		
45	M	1	Total	Fe	S		0
			16	8	8		

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



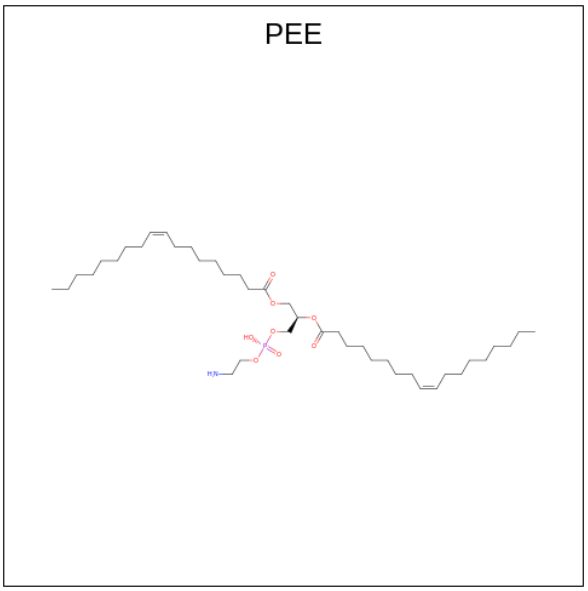
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



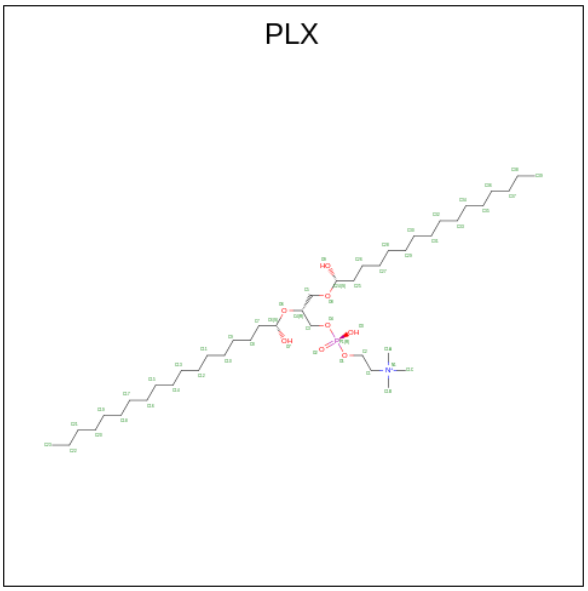
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



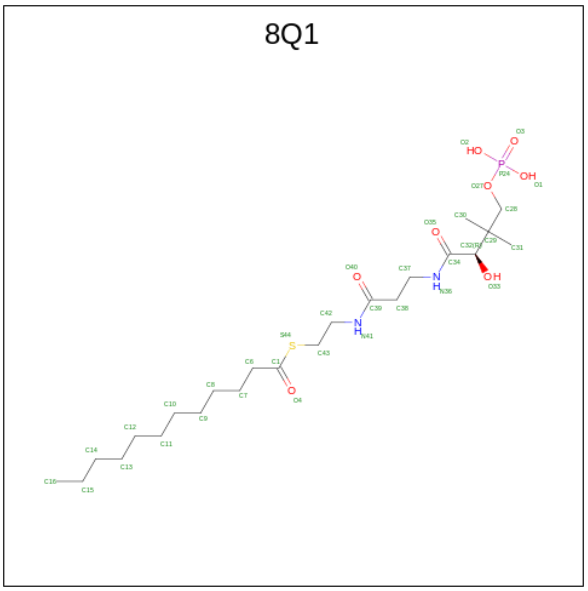
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	N				0
			1	1				
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			143	113	3	24	3	
48	l	1	Total	C	N	O	P	0
			143	113	3	24	3	
48	l	1	Total	C	N	O	P	0
			143	113	3	24	3	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 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).



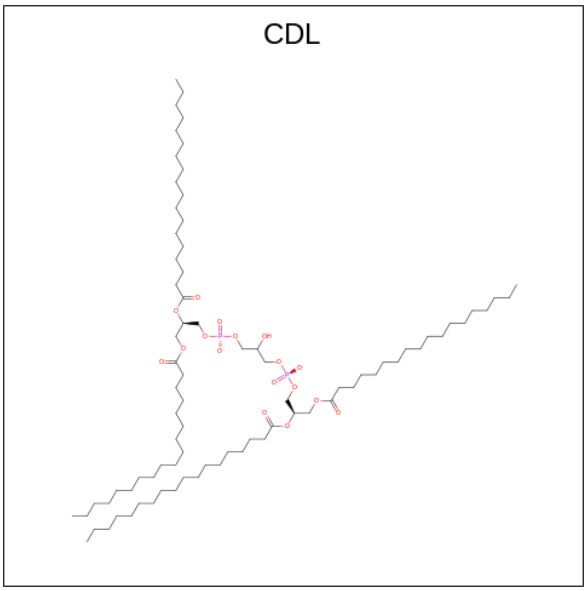
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
49	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- Molecule 50 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
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 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
51	I	1	Total	C	O	P	0
			51	32	17	2	

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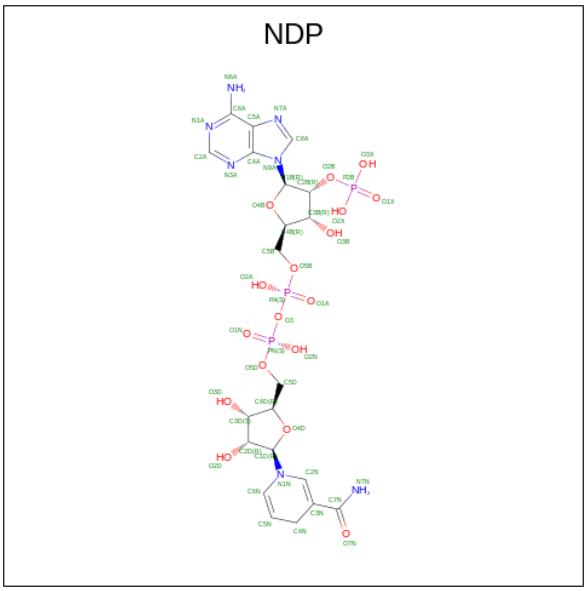
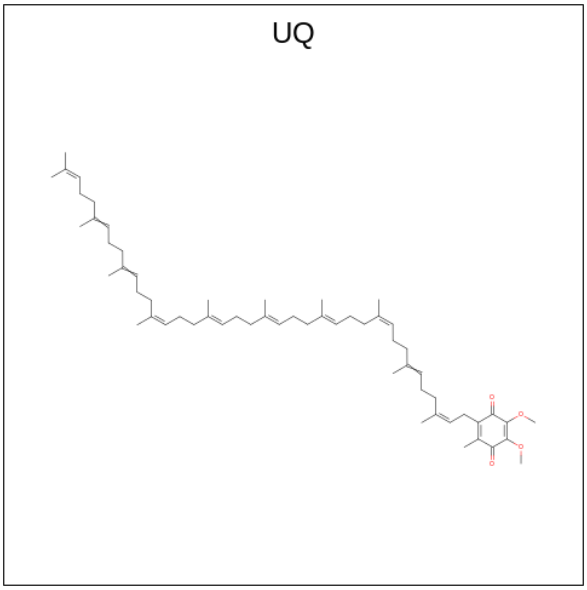
Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			94	75	17	2	
51	a	1	Total	C	O	P	0
			100	81	17	2	
51	i	1	Total	C	O	P	0
			100	81	17	2	
51	k	1	Total	C	O	P	0
			78	59	17	2	
51	l	1	Total	C	O	P	0
			199	161	34	4	
51	l	1	Total	C	O	P	0
			199	161	34	4	
51	m	1	Total	C	O	P	0
			89	70	17	2	
51	o	1	Total	C	O	P	0
			100	81	17	2	
51	r	1	Total	C	O	P	0
			99	80	17	2	
51	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 52 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).



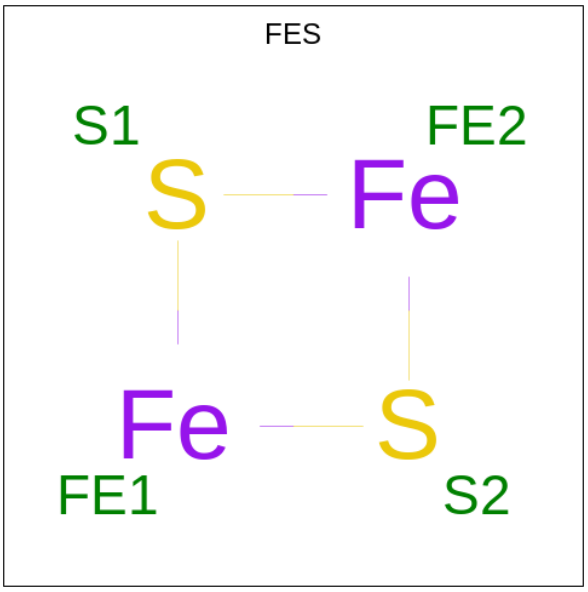
Mol	Chain	Residues	Atoms					AltConf
52	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 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
53	J	1	Total	C	O	0
			33	29	4	
53	s	1	Total	C	O	0
			38	34	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

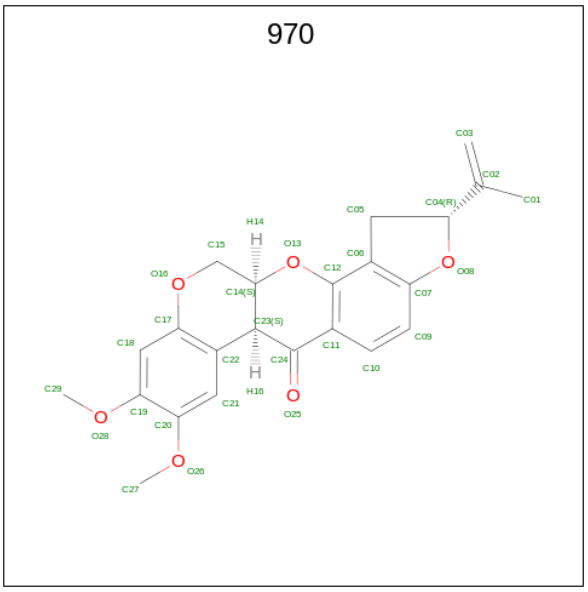


Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total 4	Fe 2	S 2	0
54	O	1	Total 4	Fe 2	S 2	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (three-letter code: 970) (formula: $C_{23}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).

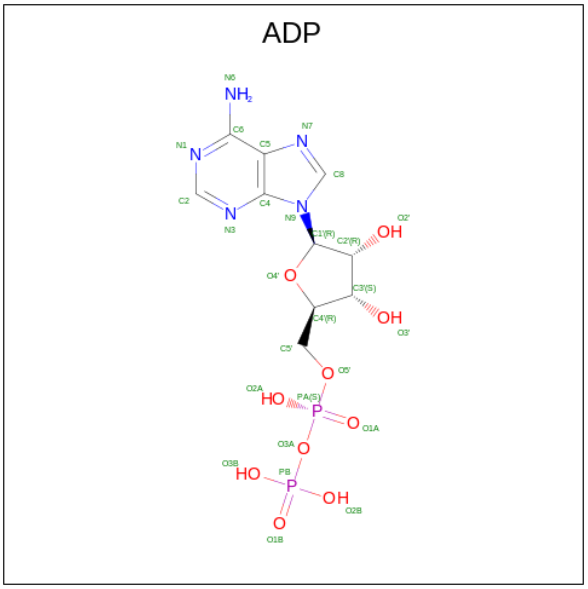


Mol	Chain	Residues	Atoms	AltConf
56	Q	1	Total C O 29 23 6	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 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).



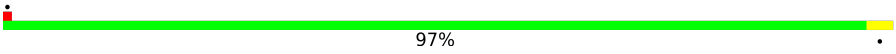
Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

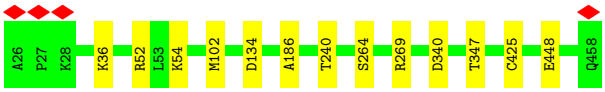
3 Residue-property plots (i)

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

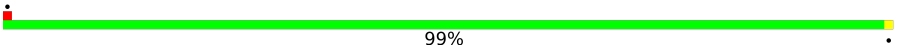
Chain A:

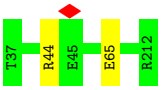




• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

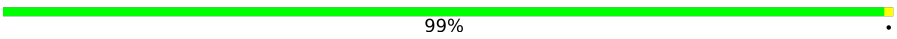
Chain B:





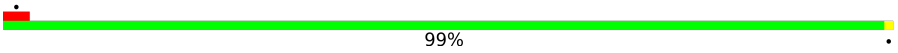
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7,mitochondrial

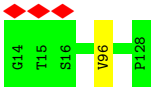
Chain C:



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

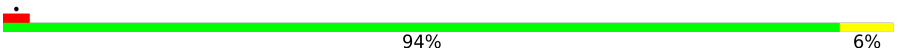
Chain E:

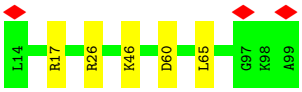




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

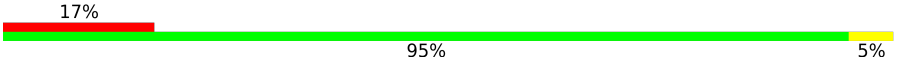
Chain F:

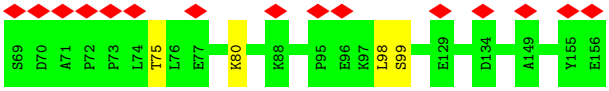




• Molecule 6: Acyl carrier protein, mitochondrial

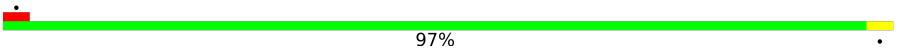
Chain G:





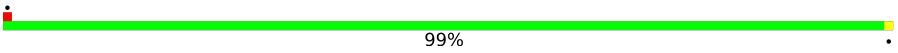
• Molecule 6: Acyl carrier protein, mitochondrial

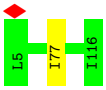
Chain X:



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

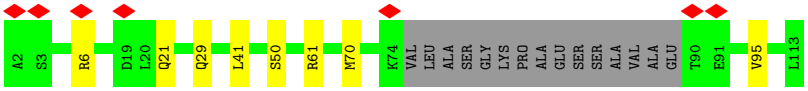
Chain H:





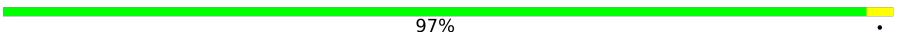
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

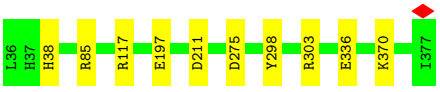
Chain I:



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

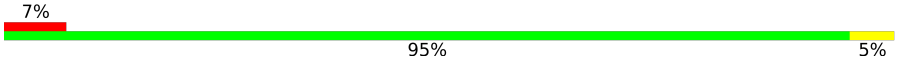
Chain J:

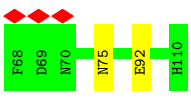




• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

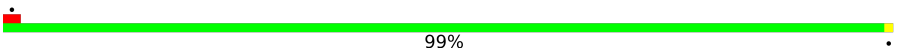
Chain K:

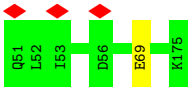




• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

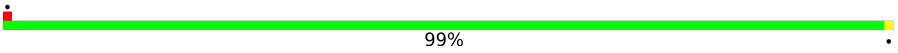
Chain L:

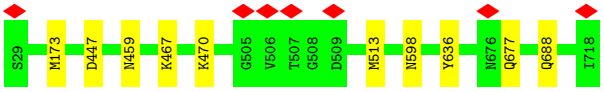




• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

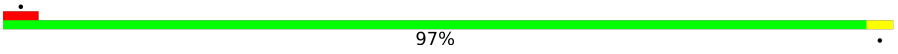
Chain M:

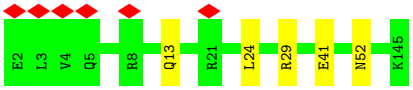




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

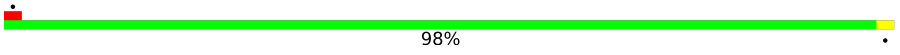
Chain N:

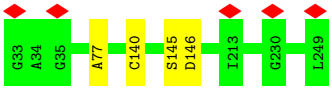




• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

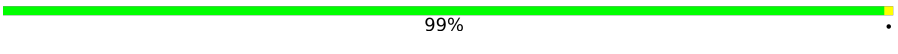
Chain O:

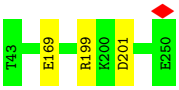




• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

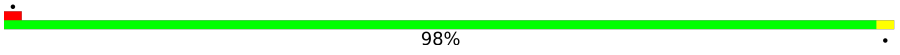
Chain P:

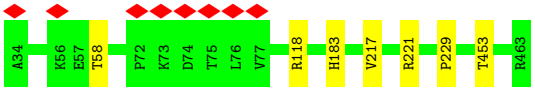




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

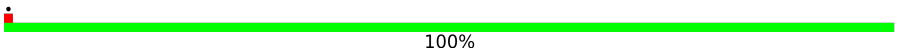
Chain Q:





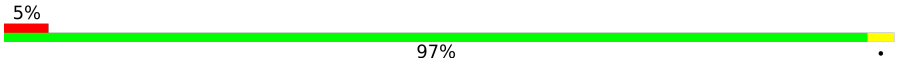
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

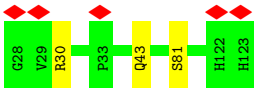
Chain S:



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

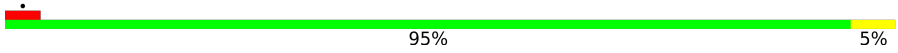
Chain T:

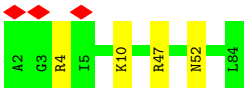




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

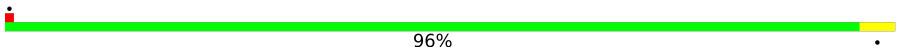
Chain U:

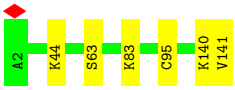




• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

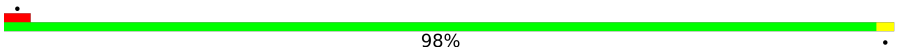
Chain V:

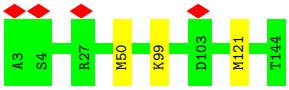




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

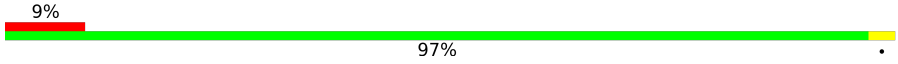
Chain W:

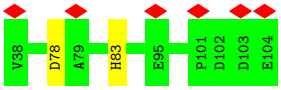




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

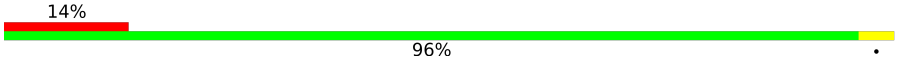
Chain Y:

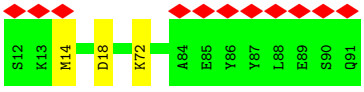




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

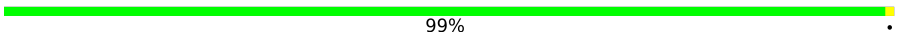
Chain Z:

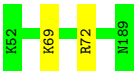




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

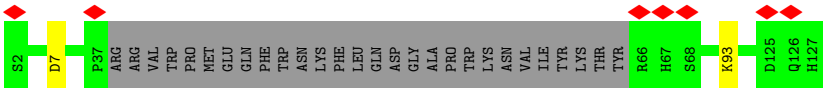
Chain a:





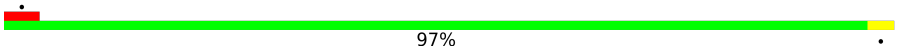
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:



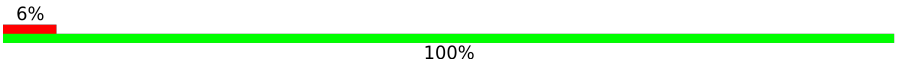
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:



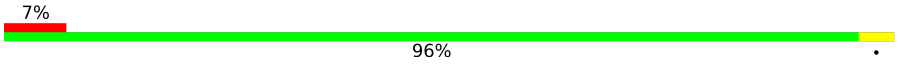
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

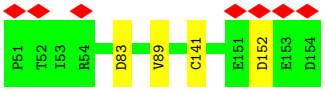
Chain d:



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

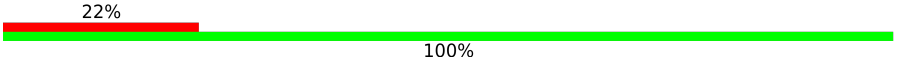
Chain e:

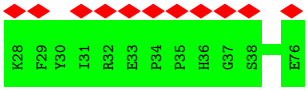




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

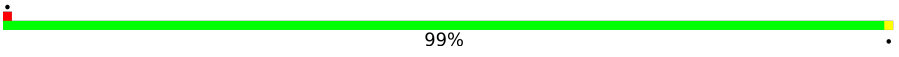
Chain f:

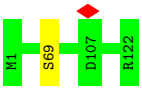




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

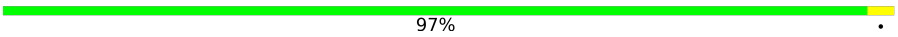
Chain g:

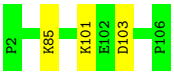




• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

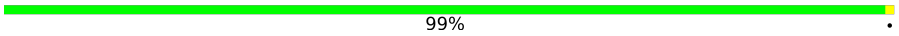
Chain h:





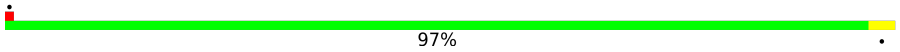
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

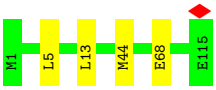
Chain i:



• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

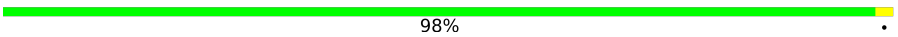
Chain j:

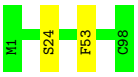




• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

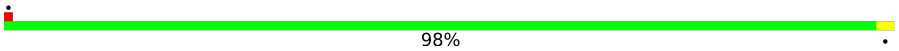
Chain k:

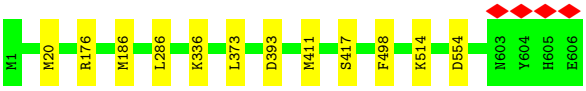




• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

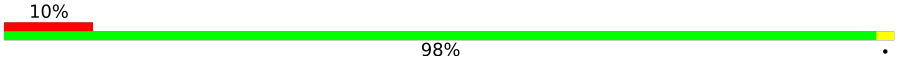
Chain l:

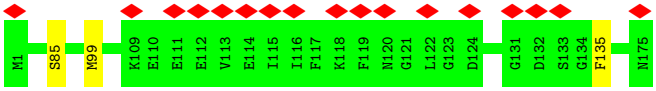




• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

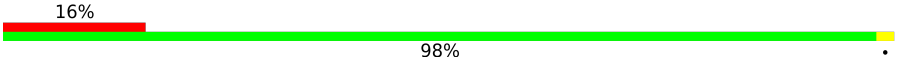
Chain m:

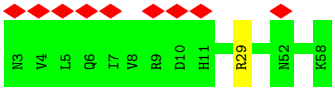




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

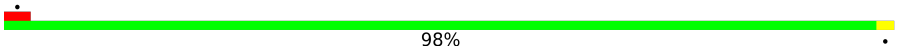
Chain n:

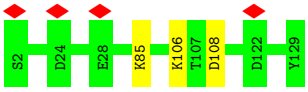




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

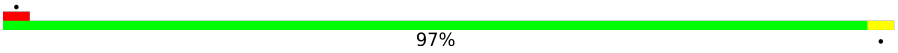
Chain o:

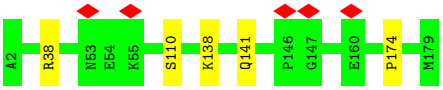




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

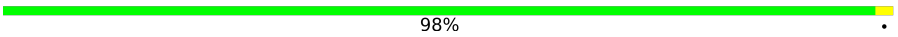
Chain p:





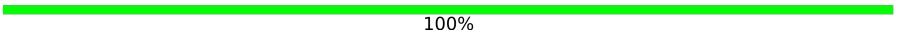
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

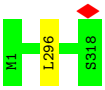
Chain r:



• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

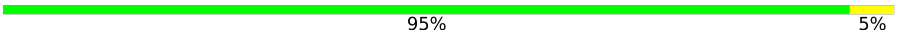
Chain s:

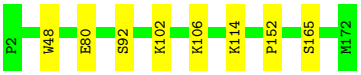




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

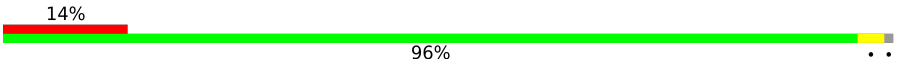
Chain u:





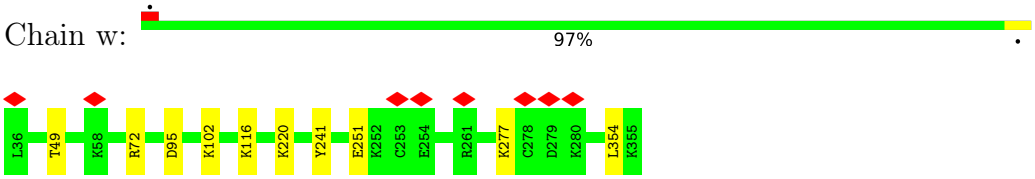
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:



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

Chain w:


97%
L36
T49
K58
R72
D95
K102
K116
K220
Y241
E251
K252
C253
E254
R261
K277
C278
D279
K280
L354
K355

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326044	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	0.248	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0271	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 970, MG, NDP, ZN, 8Q1, PEE, CDL, PLX, SF4, FES, UQ, 2MR, FMN, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/3406	0.50	0/4603
2	B	0.34	0/1443	0.53	0/1952
3	C	0.37	0/1279	0.52	0/1730
4	E	0.30	0/995	0.54	0/1340
5	F	0.29	0/695	0.54	0/936
6	G	0.28	0/705	0.49	0/956
6	X	0.28	0/708	0.49	0/959
7	H	0.28	0/929	0.49	0/1258
8	I	0.30	0/798	0.57	0/1079
9	J	0.31	0/2828	0.52	0/3834
10	K	0.30	0/377	0.53	0/509
11	L	0.30	0/1039	0.50	0/1403
12	M	0.31	0/5381	0.55	0/7291
13	N	0.32	0/1245	0.55	0/1694
14	O	0.29	0/1711	0.50	0/2328
15	P	0.35	0/1789	0.56	0/2436
16	Q	0.37	0/3538	0.55	0/4796
17	S	0.30	0/581	0.53	0/781
18	T	0.31	0/755	0.54	0/1018
19	U	0.28	0/664	0.46	0/912
20	V	0.34	1/1042 (0.1%)	0.50	0/1411
21	W	0.32	0/1192	0.53	0/1610
22	Y	0.29	0/610	0.50	0/836
23	Z	0.28	0/660	0.48	0/892
24	a	0.32	0/1184	0.51	0/1603
25	b	0.29	0/844	0.49	0/1149
26	c	0.32	0/1371	0.52	0/1875
27	d	0.31	0/1494	0.52	0/2015
28	e	0.29	0/891	0.50	0/1210
29	f	0.29	0/385	0.45	0/522
30	g	0.32	0/1036	0.49	0/1401
31	h	0.29	0/889	0.52	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.31	0/2773	0.50	0/3768
33	j	0.29	0/938	0.44	0/1281
34	k	0.29	0/759	0.49	0/1029
35	l	0.30	0/4926	0.47	0/6700
36	m	0.32	0/1307	0.50	0/1777
37	n	0.26	0/491	0.51	0/663
38	o	0.30	0/1092	0.49	0/1481
39	p	0.30	0/1590	0.50	0/2155
40	r	0.30	0/3715	0.49	0/5067
41	s	0.32	0/2581	0.51	0/3529
42	u	0.29	0/1436	0.49	0/1938
43	v	0.28	0/1060	0.52	0/1421
44	w	0.30	0/2646	0.49	0/3584
All	All	0.31	1/67778 (0.0%)	0.51	0/91922

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	95	CYS	CB-SG	-5.21	1.73	1.81

There are no bond angle outliers.

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	431/433 (100%)	414 (96%)	15 (4%)	2 (0%)	29	52
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
4	E	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	17	35
5	F	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	13	27
6	G	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	17	35
8	I	93/112 (83%)	84 (90%)	7 (8%)	2 (2%)	6	12
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	41	64
10	K	41/43 (95%)	39 (95%)	1 (2%)	1 (2%)	6	10
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	665 (97%)	23 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	29	52
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	410 (96%)	16 (4%)	1 (0%)	47	71
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
21	W	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	143 (93%)	10 (6%)	1 (1%)	25	47
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	i	345/347 (99%)	332 (96%)	12 (4%)	1 (0%)	41 64
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100 100
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100 100
35	l	604/606 (100%)	587 (97%)	17 (3%)	0	100 100
36	m	173/175 (99%)	154 (89%)	19 (11%)	0	100 100
37	n	54/56 (96%)	54 (100%)	0	0	100 100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100 100
39	p	176/178 (99%)	171 (97%)	4 (2%)	1 (1%)	25 47
40	r	457/459 (100%)	451 (99%)	6 (1%)	0	100 100
41	s	316/318 (99%)	305 (96%)	11 (4%)	0	100 100
42	u	169/171 (99%)	163 (96%)	5 (3%)	1 (1%)	25 47
43	v	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	19 39
44	w	318/320 (99%)	309 (97%)	9 (3%)	0	100 100
All	All	8175/8314 (98%)	7857 (96%)	302 (4%)	16 (0%)	50 71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	60	ASP
10	K	75	ASN
1	A	264	SER
8	I	29	GLN
9	J	38	HIS
7	H	77	ILE
14	O	77	ALA
16	Q	229	PRO
43	v	58	TYR
8	I	41	LEU
26	c	127	ASN
32	i	50	PRO
42	u	152	PRO
1	A	186	ALA
4	E	96	VAL
39	p	174	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	346/346 (100%)	335 (97%)	11 (3%)	39	65
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	86
3	C	132/132 (100%)	131 (99%)	1 (1%)	81	92
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	74/76 (97%)	70 (95%)	4 (5%)	22	44
6	G	76/81 (94%)	72 (95%)	4 (5%)	22	45
6	X	77/81 (95%)	74 (96%)	3 (4%)	32	58
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	81 (93%)	6 (7%)	15	31
9	J	296/296 (100%)	287 (97%)	9 (3%)	41	67
10	K	42/42 (100%)	41 (98%)	1 (2%)	49	74
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	91
12	M	579/580 (100%)	569 (98%)	10 (2%)	60	81
13	N	130/130 (100%)	125 (96%)	5 (4%)	33	59
14	O	183/183 (100%)	180 (98%)	3 (2%)	62	82
15	P	190/190 (100%)	187 (98%)	3 (2%)	62	82
16	Q	370/370 (100%)	365 (99%)	5 (1%)	67	85
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	76 (96%)	3 (4%)	33	59
19	U	69/69 (100%)	65 (94%)	4 (6%)	20	40
20	V	101/101 (100%)	96 (95%)	5 (5%)	24	47
21	W	121/123 (98%)	118 (98%)	3 (2%)	47	73
22	Y	62/62 (100%)	60 (97%)	2 (3%)	39	65
23	Z	62/62 (100%)	59 (95%)	3 (5%)	25	49
24	a	121/121 (100%)	119 (98%)	2 (2%)	60	81
25	b	90/119 (76%)	88 (98%)	2 (2%)	52	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	c	141/141 (100%)	137 (97%)	4 (3%)	43 69
27	d	155/155 (100%)	155 (100%)	0	100 100
28	e	96/96 (100%)	92 (96%)	4 (4%)	30 55
29	f	35/45 (78%)	35 (100%)	0	100 100
30	g	108/109 (99%)	107 (99%)	1 (1%)	78 91
31	h	93/93 (100%)	90 (97%)	3 (3%)	39 65
32	i	311/311 (100%)	307 (99%)	4 (1%)	69 86
33	j	100/100 (100%)	96 (96%)	4 (4%)	31 57
34	k	85/85 (100%)	83 (98%)	2 (2%)	49 74
35	l	536/540 (99%)	524 (98%)	12 (2%)	52 76
36	m	127/141 (90%)	124 (98%)	3 (2%)	49 74
37	n	53/53 (100%)	52 (98%)	1 (2%)	57 79
38	o	113/113 (100%)	110 (97%)	3 (3%)	44 71
39	p	159/159 (100%)	155 (98%)	4 (2%)	47 73
40	r	409/410 (100%)	399 (98%)	10 (2%)	49 74
41	s	275/275 (100%)	274 (100%)	1 (0%)	91 97
42	u	153/153 (100%)	146 (95%)	7 (5%)	27 51
43	v	106/111 (96%)	103 (97%)	3 (3%)	43 69
44	w	282/283 (100%)	272 (96%)	10 (4%)	36 62
All	All	7151/7241 (99%)	6983 (98%)	168 (2%)	53 75

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	52	ARG
1	A	54	LYS
1	A	102	MET
1	A	134	ASP
1	A	240	THR
1	A	269	ARG
1	A	340	ASP
1	A	347	THR
1	A	425	CYS
1	A	448	GLU

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Mol	Chain	Res	Type
2	B	44	ARG
2	B	65	GLU
3	C	142	TYR
5	F	17	ARG
5	F	26	ARG
5	F	46	LYS
5	F	65	LEU
6	G	75	THR
6	G	80	LYS
6	G	98	LEU
6	G	99	SER
8	I	6	ARG
8	I	21	GLN
8	I	50	SER
8	I	61	ARG
8	I	70	MET
8	I	95	VAL
9	J	85	ARG
9	J	117	ARG
9	J	197	GLU
9	J	211	ASP
9	J	275	ASP
9	J	298	TYR
9	J	303	ARG
9	J	336	GLU
9	J	370	LYS
10	K	92	GLU
11	L	69	GLU
12	M	173	MET
12	M	447	ASP
12	M	459	ASN
12	M	467	LYS
12	M	470	LYS
12	M	513	MET
12	M	598	ASN
12	M	636	TYR
12	M	677	GLN
12	M	688	GLN
13	N	13	GLN
13	N	24	LEU
13	N	29	ARG
13	N	41	GLU

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Mol	Chain	Res	Type
13	N	52	ASN
14	O	140	CYS
14	O	145	SER
14	O	146	ASP
15	P	169	GLU
15	P	199	ARG
15	P	201	ASP
16	Q	58	THR
16	Q	183	HIS
16	Q	217	VAL
16	Q	221	ARG
16	Q	453	THR
18	T	30	ARG
18	T	43	GLN
18	T	81	SER
19	U	4	ARG
19	U	10	LYS
19	U	47	ARG
19	U	52	ASN
20	V	44	LYS
20	V	63	SER
20	V	83	LYS
20	V	140	LYS
20	V	141	VAL
21	W	50	MET
21	W	99	LYS
21	W	121	MET
6	X	77	GLU
6	X	105	MET
6	X	140	CYS
22	Y	78	ASP
22	Y	83	HIS
23	Z	14	MET
23	Z	18	ASP
23	Z	72	LYS
24	a	69	LYS
24	a	72	ARG
25	b	7	ASP
25	b	93	LYS
26	c	36	MET
26	c	53	LYS
26	c	82	SER

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Mol	Chain	Res	Type
26	c	159	LYS
28	e	83	ASP
28	e	89	VAL
28	e	141	CYS
28	e	152	ASP
30	g	69	SER
31	h	85	LYS
31	h	101	LYS
31	h	103	ASP
32	i	147	GLN
32	i	171	ASN
32	i	223	SER
32	i	336	VAL
33	j	5	LEU
33	j	13	LEU
33	j	44	MET
33	j	68	GLU
34	k	24	SER
34	k	53	PHE
35	l	20	MET
35	l	176	ARG
35	l	186	MET
35	l	286	LEU
35	l	336	LYS
35	l	373	LEU
35	l	393	ASP
35	l	411	MET
35	l	417	SER
35	l	498	PHE
35	l	514	LYS
35	l	554	ASP
36	m	85	SER
36	m	99	MET
36	m	135	PHE
37	n	29	ARG
38	o	85	LYS
38	o	106	LYS
38	o	108	ASP
39	p	38	ARG
39	p	110	SER
39	p	138	LYS
39	p	141	GLN

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Mol	Chain	Res	Type
40	r	90	THR
40	r	114	GLU
40	r	122	PHE
40	r	183	SER
40	r	209	LEU
40	r	212	LEU
40	r	243	MET
40	r	273	SER
40	r	401	MET
40	r	420	THR
41	s	296	LEU
42	u	48	TRP
42	u	80	GLU
42	u	92	SER
42	u	102	LYS
42	u	106	LYS
42	u	114	LYS
42	u	165	SER
43	v	21	ARG
43	v	85	HIS
43	v	113	LYS
44	w	49	THR
44	w	72	ARG
44	w	95	ASP
44	w	102	LYS
44	w	116	LYS
44	w	220	LYS
44	w	241	TYR
44	w	251	GLU
44	w	277	LYS
44	w	354	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	25	GLN
8	I	21	GLN
8	I	25	GLN
8	I	29	GLN
9	J	138	ASN
10	K	79	HIS
12	M	278	HIS

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Mol	Chain	Res	Type
12	M	300	GLN
12	M	336	ASN
12	M	540	ASN
12	M	598	ASN
13	N	52	ASN
16	Q	88	HIS
17	S	31	ASN
18	T	123	HIS
19	U	62	ASN
32	i	144	GLN
32	i	171	ASN
32	i	273	ASN
35	l	2	ASN
35	l	59	GLN
35	l	192	HIS
40	r	81	GLN
40	r	180	HIS
40	r	304	GLN

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	2.02	2 (20%)	5,13,15	6.11	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.59	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.05	1.41	1.45

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	12.39	130.84	119.48
16	Q	118	2MR	CD-NE-CZ	4.45	131.74	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.23	131.01	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
48	PEE	l	704	-	49,49,50	1.16	6 (12%)	52,54,55	0.95	2 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
53	UQ	J	402	-	33,33,63	3.42	9 (27%)	40,43,79	2.87	13 (32%)
46	FMN	A	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.27	9 (18%)
51	CDL	V	201	-	93,93,99	1.12	8 (8%)	99,105,111	0.86	4 (4%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	PLX	J	403	-	51,51,51	1.12	2 (3%)	55,59,59	0.62	1 (1%)
51	CDL	o	201	-	99,99,99	1.07	9 (9%)	105,111,111	0.88	5 (4%)
48	PEE	C	302	-	46,46,50	1.19	6 (13%)	49,51,55	0.99	2 (4%)
50	8Q1	X	201	-	31,34,34	2.10	6 (19%)	40,43,43	1.69	11 (27%)
48	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
49	PLX	C	303	-	51,51,51	0.62	0	55,59,59	0.74	1 (1%)
51	CDL	l	702	-	99,99,99	0.91	4 (4%)	105,111,111	1.10	7 (6%)
48	PEE	j	201	-	40,40,50	1.16	4 (10%)	43,45,55	1.04	2 (4%)
53	UQ	s	401	-	38,38,63	3.55	10 (26%)	46,49,79	2.84	16 (34%)
47	NAI	A	503	-	42,48,48	4.93	18 (42%)	47,73,73	1.30	6 (12%)
45	SF4	A	501	1	0,12,12	-	-	-		
49	PLX	r	503	-	51,51,51	1.13	3 (5%)	55,59,59	0.55	0
51	CDL	a	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.89	4 (3%)
51	CDL	i	401	-	99,99,99	0.93	4 (4%)	105,111,111	1.01	4 (3%)
52	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.08	3 (5%)
54	FES	M	803	12	0,4,4	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
48	PEE	l	705	-	45,45,50	1.22	5 (11%)	48,50,55	0.98	2 (4%)
54	FES	O	301	14	0,4,4	-	-	-		
51	CDL	k	101	-	77,77,99	1.18	6 (7%)	83,89,111	0.94	4 (4%)
58	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.36	3 (10%)
51	CDL	m	201	-	88,88,99	0.97	4 (4%)	94,100,111	1.10	6 (6%)
51	CDL	r	504	-	98,98,99	1.07	8 (8%)	104,110,111	0.86	4 (3%)
48	PEE	B	303	-	50,50,50	1.15	6 (12%)	53,55,55	0.99	2 (3%)
49	PLX	g	201	-	51,51,51	1.12	3 (5%)	55,59,59	0.67	1 (1%)
51	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.09	8 (7%)
48	PEE	l	703	-	46,46,50	1.19	6 (13%)	49,51,55	1.03	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	CDL	I	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.35	6 (10%)
51	CDL	u	201	-	54,54,99	1.22	4 (7%)	60,66,111	1.25	5 (8%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.62	1 (1%)
56	970	Q	501	-	33,33,33	4.84	14 (42%)	48,50,50	2.41	21 (43%)
45	SF4	M	802	12	0,12,12	-	-	-		
49	PLX	r	502	-	51,51,51	1.14	5 (9%)	55,59,59	0.62	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
50	8Q1	G	201	-	31,34,34	2.12	6 (19%)	40,43,43	1.81	12 (30%)
48	PEE	U	101	-	50,50,50	1.15	5 (10%)	53,55,55	0.93	2 (3%)
49	PLX	j	202	-	51,51,51	1.13	4 (7%)	55,59,59	0.59	1 (1%)
48	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	l	704	-	-	22/53/53/54	-
45	SF4	B	302	2	-	-	0/6/5/5
53	UQ	J	402	-	-	14/27/51/87	0/1/1/1
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
51	CDL	V	201	-	-	58/104/104/110	-
45	SF4	B	301	2	-	-	0/6/5/5
49	PLX	J	403	-	-	27/55/55/55	-
51	CDL	o	201	-	-	56/110/110/110	-
48	PEE	C	302	-	-	28/50/50/54	-
50	8Q1	X	201	-	-	27/41/41/41	-
48	PEE	W	201	-	-	23/44/44/54	-
49	PLX	C	303	-	-	20/55/55/55	-
51	CDL	l	702	-	-	40/110/110/110	-
48	PEE	j	201	-	-	17/44/44/54	-
53	UQ	s	401	-	-	13/33/57/87	0/1/1/1
47	NAI	A	503	-	-	6/25/72/72	0/5/5/5
49	PLX	r	503	-	-	37/55/55/55	-
51	CDL	a	201	-	-	60/110/110/110	-
51	CDL	i	401	-	-	35/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	NDP	J	401	-	-	8/30/77/77	0/5/5/5
45	SF4	A	501	1	-	-	0/6/5/5
54	FES	M	803	12	-	-	0/1/1/1
45	SF4	C	301	3	-	-	0/6/5/5
48	PEE	l	705	-	-	22/49/49/54	-
54	FES	O	301	14	-	-	0/1/1/1
51	CDL	k	101	-	-	41/88/88/110	-
58	ADP	w	401	-	-	6/12/32/32	0/3/3/3
51	CDL	m	201	-	-	35/99/99/110	-
51	CDL	r	504	-	-	58/109/109/110	-
48	PEE	B	303	-	-	26/54/54/54	-
49	PLX	g	201	-	-	36/55/55/55	-
51	CDL	l	701	-	-	39/109/109/110	-
48	PEE	l	703	-	-	26/50/50/54	-
51	CDL	I	201	-	-	28/61/61/110	-
51	CDL	u	201	-	-	19/65/65/110	-
49	PLX	a	202	-	-	34/55/55/55	-
56	970	Q	501	-	-	7/8/41/41	0/5/5/5
45	SF4	M	802	12	-	-	0/6/5/5
49	PLX	r	502	-	-	30/55/55/55	-
50	8Q1	G	201	-	-	17/41/41/41	-
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	U	101	-	-	30/54/54/54	-
49	PLX	j	202	-	-	33/55/55/55	-
48	PEE	r	501	-	-	34/54/54/54	-

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Q	501	970	O16-C17	19.03	1.58	1.37
47	A	503	NAI	O4B-C1B	16.13	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.48	1.30	1.53
56	Q	501	970	C14-C23	-11.88	1.41	1.52
47	A	503	NAI	C3D-C4D	-10.45	1.26	1.53
53	s	401	UQ	C18-C19	9.61	1.56	1.33
53	J	402	UQ	C18-C19	9.55	1.55	1.33
53	s	401	UQ	C13-C14	9.29	1.55	1.33
53	J	402	UQ	C13-C14	9.18	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	s	401	UQ	C23-C24	9.08	1.54	1.33
58	w	401	ADP	C3'-C4'	-9.07	1.29	1.53
53	s	401	UQ	C8-C9	8.98	1.54	1.33
53	J	402	UQ	C8-C9	8.90	1.54	1.33
56	Q	501	970	O13-C12	8.28	1.50	1.37
47	A	503	NAI	O4B-C4B	-8.23	1.26	1.45
53	J	402	UQ	C23-C24	7.81	1.54	1.32
58	w	401	ADP	O4'-C4'	7.77	1.62	1.45
53	s	401	UQ	C28-C29	7.69	1.54	1.32
50	X	201	8Q1	P24-O27	7.68	1.84	1.60
47	A	503	NAI	C2D-C1D	-7.63	1.29	1.53
50	G	201	8Q1	P24-O27	7.57	1.84	1.60
47	A	503	NAI	O4D-C4D	6.78	1.60	1.45
56	Q	501	970	O08-C07	6.74	1.47	1.37
58	w	401	ADP	O4'-C1'	-6.56	1.31	1.41
47	A	503	NAI	C2D-C3D	5.85	1.69	1.53
47	A	503	NAI	C7N-N7N	5.75	1.48	1.33
56	Q	501	970	C23-C24	-5.50	1.46	1.52
56	Q	501	970	C22-C23	-5.37	1.43	1.51
47	A	503	NAI	O4D-C1D	5.33	1.54	1.42
47	A	503	NAI	C4N-C3N	-5.02	1.40	1.49
47	A	503	NAI	O2B-C2B	4.49	1.53	1.43
51	I	201	CDL	OB8-CB7	4.35	1.46	1.33
51	l	701	CDL	OA8-CA7	4.33	1.46	1.33
51	m	201	CDL	OA8-CA7	4.32	1.46	1.33
51	i	401	CDL	OA8-CA7	4.30	1.45	1.33
51	l	702	CDL	OB8-CB7	4.27	1.45	1.33
51	l	701	CDL	OB8-CB7	4.26	1.45	1.33
51	I	201	CDL	OA8-CA7	4.26	1.45	1.33
51	m	201	CDL	OA6-CA5	4.25	1.46	1.34
51	i	401	CDL	OB8-CB7	4.21	1.45	1.33
51	u	201	CDL	OA8-CA7	4.18	1.45	1.33
51	i	401	CDL	OB6-CB5	4.16	1.46	1.34
51	l	702	CDL	OA8-CA7	4.14	1.45	1.33
51	i	401	CDL	OA6-CA5	4.13	1.46	1.34
51	u	201	CDL	OB8-CB7	4.12	1.45	1.33
51	u	201	CDL	OA6-CA5	4.10	1.45	1.34
47	A	503	NAI	C6N-C5N	4.10	1.40	1.33
51	m	201	CDL	OB8-CB7	4.09	1.45	1.33
51	l	701	CDL	OA6-CA5	4.09	1.45	1.34
51	u	201	CDL	OB6-CB5	4.09	1.45	1.34
51	I	201	CDL	OA6-CA5	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	I	201	CDL	OB6-CB5	4.03	1.45	1.34
51	l	702	CDL	OA6-CA5	3.99	1.45	1.34
51	m	201	CDL	OB6-CB5	3.97	1.45	1.34
50	G	201	8Q1	C1-S44	3.94	1.85	1.76
51	l	702	CDL	OB6-CB5	3.91	1.45	1.34
51	l	701	CDL	OB6-CB5	3.89	1.45	1.34
50	G	201	8Q1	C6-C1	3.86	1.54	1.50
50	X	201	8Q1	C1-S44	3.85	1.85	1.76
56	Q	501	970	C05-C04	-3.85	1.48	1.54
58	w	401	ADP	C6-N6	3.84	1.48	1.34
48	l	705	PEE	C18-C19	3.73	1.53	1.31
48	l	704	PEE	C18-C19	3.72	1.53	1.31
48	C	302	PEE	C18-C19	3.72	1.53	1.31
48	j	201	PEE	C18-C19	3.72	1.53	1.31
48	B	303	PEE	C18-C19	3.70	1.53	1.31
48	W	201	PEE	C18-C19	3.70	1.53	1.31
48	r	501	PEE	C18-C19	3.69	1.53	1.31
48	l	703	PEE	C18-C19	3.68	1.53	1.31
48	U	101	PEE	C18-C19	3.68	1.53	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
48	U	101	PEE	C39-C38	3.62	1.52	1.31
48	l	705	PEE	C39-C38	3.62	1.52	1.31
48	l	703	PEE	C39-C38	3.62	1.52	1.31
48	C	302	PEE	C39-C38	3.61	1.52	1.31
48	l	704	PEE	C39-C38	3.60	1.52	1.31
56	Q	501	970	O13-C14	3.59	1.49	1.45
47	A	503	NAI	C6A-N6A	3.59	1.47	1.34
46	A	502	FMN	C4A-N5	3.59	1.37	1.30
47	A	503	NAI	C7N-C3N	3.52	1.56	1.48
51	V	201	CDL	OA8-CA7	3.49	1.43	1.33
50	G	201	8Q1	C34-N36	3.48	1.41	1.33
51	o	201	CDL	OA8-CA7	3.42	1.43	1.33
50	G	201	8Q1	O27-C28	-3.41	1.32	1.43
51	a	201	CDL	OA8-CA7	3.39	1.43	1.33
50	X	201	8Q1	C34-N36	3.37	1.41	1.33
52	J	401	NDP	C6N-C5N	3.35	1.39	1.33
51	r	504	CDL	OA8-CA7	3.35	1.43	1.33
58	w	401	ADP	O2'-C2'	-3.35	1.35	1.43
51	k	101	CDL	OA8-CA7	3.34	1.43	1.33
56	Q	501	970	O16-C15	3.33	1.52	1.44
47	A	503	NAI	C4N-C5N	-3.32	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	X	201	8Q1	O27-C28	-3.26	1.33	1.43
51	k	101	CDL	OA6-CA5	3.25	1.43	1.34
50	X	201	8Q1	C39-N41	3.17	1.40	1.33
50	X	201	8Q1	C6-C1	3.15	1.54	1.50
58	w	401	ADP	O3'-C3'	3.15	1.50	1.43
51	a	201	CDL	OB6-CB5	3.11	1.43	1.34
51	V	201	CDL	OA6-CA5	3.03	1.42	1.34
51	r	504	CDL	OB8-CB7	3.03	1.42	1.33
51	V	201	CDL	OB6-CB5	2.98	1.42	1.34
51	o	201	CDL	OA6-CA5	2.95	1.42	1.34
49	a	202	PLX	O6-C4	-2.93	1.40	1.44
51	V	201	CDL	OB8-CB7	2.93	1.41	1.33
50	G	201	8Q1	C39-N41	2.92	1.40	1.33
51	k	101	CDL	OB8-CB7	2.91	1.41	1.33
51	k	101	CDL	OB6-CB5	2.89	1.42	1.34
51	a	201	CDL	OB8-CB7	2.89	1.41	1.33
51	o	201	CDL	OB6-CB5	2.86	1.42	1.34
49	g	201	PLX	O6-C4	-2.83	1.40	1.44
51	r	504	CDL	OB6-CB5	2.83	1.42	1.34
51	a	201	CDL	OA6-CA5	2.79	1.42	1.34
56	Q	501	970	O25-C24	-2.78	1.18	1.22
51	r	504	CDL	OA6-CA5	2.76	1.42	1.34
56	Q	501	970	C10-C11	2.75	1.44	1.39
51	o	201	CDL	OB8-CB7	2.75	1.41	1.33
53	s	401	UQ	C6-C1	2.73	1.54	1.46
49	r	503	PLX	O6-C4	-2.71	1.41	1.44
53	J	402	UQ	C6-C1	2.66	1.54	1.46
48	U	101	PEE	O3-C30	2.65	1.41	1.33
51	a	201	CDL	OA6-CA4	-2.58	1.40	1.46
48	j	201	PEE	O3-C30	2.57	1.40	1.33
56	Q	501	970	C12-C06	2.56	1.43	1.39
47	A	503	NAI	O3B-C3B	-2.55	1.37	1.43
53	s	401	UQ	C7-C8	2.54	1.54	1.50
48	C	302	PEE	O2-C2	-2.54	1.40	1.46
49	j	202	PLX	O6-C4	-2.52	1.41	1.44
48	l	703	PEE	O2-C2	-2.51	1.40	1.46
48	l	705	PEE	O3-C30	2.49	1.40	1.33
48	l	704	PEE	O3-C30	2.49	1.40	1.33
48	W	201	PEE	O2-C2	-2.47	1.40	1.46
51	r	504	CDL	OA6-CA4	-2.47	1.40	1.46
49	r	502	PLX	O6-C4	-2.47	1.41	1.44
49	j	202	PLX	C7-C6	2.43	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	U	101	PEE	O2-C2	-2.43	1.40	1.46
48	l	704	PEE	O2-C2	-2.42	1.40	1.46
48	j	201	PEE	O2-C2	-2.41	1.40	1.46
51	o	201	CDL	OA6-CA4	-2.41	1.40	1.46
48	r	501	PEE	O2-C2	-2.39	1.40	1.46
48	l	705	PEE	O2-C2	-2.39	1.40	1.46
49	r	502	PLX	C7-C6	2.39	1.55	1.50
51	k	101	CDL	OB6-CB4	-2.38	1.40	1.46
48	B	303	PEE	O2-C2	-2.38	1.40	1.46
49	J	403	PLX	C7-C6	2.37	1.55	1.50
48	l	703	PEE	O3-C30	2.34	1.40	1.33
51	r	504	CDL	OB6-CB4	-2.33	1.40	1.46
48	W	201	PEE	O3-C30	2.33	1.40	1.33
53	J	402	UQ	C7-C8	2.33	1.54	1.50
48	C	302	PEE	O3-C30	2.33	1.40	1.33
49	a	202	PLX	C7-C6	2.32	1.55	1.50
48	B	303	PEE	O3-C30	2.29	1.40	1.33
48	l	705	PEE	O2-C10	2.28	1.40	1.34
49	r	503	PLX	C7-C6	2.28	1.55	1.50
51	o	201	CDL	OB6-CB4	-2.28	1.40	1.46
46	A	502	FMN	C10-N1	2.28	1.37	1.33
48	j	201	PEE	O2-C10	2.28	1.40	1.34
48	W	201	PEE	O3-C3	-2.27	1.40	1.45
51	V	201	CDL	OA6-CA4	-2.27	1.40	1.46
48	r	501	PEE	O3-C30	2.27	1.40	1.33
49	J	403	PLX	O6-C4	-2.27	1.41	1.44
51	V	201	CDL	PB2-OB2	2.27	1.68	1.59
56	Q	501	970	C05-C06	-2.27	1.48	1.51
49	g	201	PLX	C7-C6	2.25	1.55	1.50
51	V	201	CDL	PB2-OB5	2.25	1.68	1.59
48	l	703	PEE	O2-C10	2.23	1.40	1.34
51	V	201	CDL	OB6-CB4	-2.23	1.41	1.46
53	s	401	UQ	O4-C4	-2.22	1.18	1.23
48	W	201	PEE	O2-C10	2.22	1.40	1.34
51	o	201	CDL	PB2-OB2	2.21	1.68	1.59
53	J	402	UQ	O4-C4	-2.21	1.18	1.23
48	U	101	PEE	O2-C10	2.19	1.40	1.34
51	a	201	CDL	OB6-CB4	-2.19	1.41	1.46
51	a	201	CDL	PB2-OB5	2.19	1.68	1.59
48	r	501	PEE	O3-C3	-2.18	1.40	1.45
51	a	201	CDL	PB2-OB2	2.18	1.68	1.59
48	C	302	PEE	O3-C3	-2.17	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C5B-C4B	2.16	1.58	1.51
47	A	503	NAI	PN-O5D	2.16	1.68	1.59
48	r	501	PEE	O2-C10	2.16	1.40	1.34
49	r	502	PLX	P1-O4	2.15	1.68	1.59
48	l	704	PEE	O3-C3	-2.14	1.40	1.45
48	B	303	PEE	O2-C10	2.14	1.40	1.34
48	l	704	PEE	O2-C10	2.14	1.40	1.34
52	J	401	NDP	C5A-C4A	2.13	1.46	1.40
49	j	202	PLX	P1-O4	2.12	1.67	1.59
51	o	201	CDL	PB2-OB5	2.11	1.67	1.59
49	a	202	PLX	P1-O4	2.10	1.67	1.59
51	r	504	CDL	PB2-OB2	2.10	1.67	1.59
48	B	303	PEE	O3-C3	-2.10	1.40	1.45
48	C	302	PEE	O2-C10	2.09	1.40	1.34
49	r	502	PLX	P1-O1	2.09	1.67	1.59
53	s	401	UQ	C21-C19	2.07	1.55	1.51
53	s	401	UQ	O1-C1	-2.06	1.18	1.23
49	g	201	PLX	P1-O4	2.05	1.67	1.59
51	o	201	CDL	C11-CA5	2.05	1.56	1.50
49	r	503	PLX	P1-O4	2.05	1.67	1.59
51	k	101	CDL	PB2-OB5	2.05	1.67	1.59
48	l	703	PEE	O3-C3	-2.05	1.40	1.45
49	r	502	PLX	C25-C24	2.05	1.55	1.50
51	r	504	CDL	PB2-OB5	2.05	1.67	1.59
56	Q	501	970	C04-C02	2.02	1.52	1.50
49	a	202	PLX	P1-O1	2.02	1.67	1.59
49	j	202	PLX	P1-O1	2.02	1.67	1.59
53	J	402	UQ	O1-C1	-2.01	1.19	1.23
53	J	402	UQ	O3-CM3	-2.00	1.40	1.45

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	J	402	UQ	C7-C8-C9	-8.19	113.16	126.79
53	s	401	UQ	C7-C8-C9	-7.84	113.74	126.79
56	Q	501	970	O08-C07-C06	-7.63	108.35	113.00
53	J	402	UQ	C12-C13-C14	-6.42	112.19	127.66
53	J	402	UQ	C17-C18-C19	-6.32	112.44	127.66
53	s	401	UQ	C22-C23-C24	-5.96	113.30	127.66
56	Q	501	970	C15-C14-C23	5.78	115.31	110.62
53	s	401	UQ	C12-C13-C14	-5.78	113.75	127.66
53	s	401	UQ	C17-C18-C19	-5.72	113.89	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	G	201	8Q1	C6-C1-S44	5.24	119.56	113.46
51	l	702	CDL	OA6-CA5-C11	4.66	121.55	111.50
51	l	701	CDL	OA6-CA5-C11	4.59	121.38	111.50
58	w	401	ADP	N3-C2-N1	-4.56	121.56	128.68
51	a	201	CDL	OB6-CB5-C51	4.56	121.32	111.50
56	Q	501	970	C05-C04-C02	-4.52	109.00	115.62
53	s	401	UQ	C10-C9-C8	-4.47	112.20	123.68
53	J	402	UQ	C22-C23-C24	-4.43	112.61	127.75
50	X	201	8Q1	C6-C1-S44	4.43	118.61	113.46
47	A	503	NAI	N3A-C2A-N1A	-4.37	121.85	128.68
48	j	201	PEE	O2-C10-C11	4.37	120.91	111.50
53	J	402	UQ	C20-C19-C18	-4.35	112.51	123.68
53	J	402	UQ	C10-C9-C8	-4.30	112.65	123.68
53	s	401	UQ	C21-C19-C18	-4.27	112.47	121.12
53	s	401	UQ	C25-C24-C23	-4.26	112.74	123.68
51	m	201	CDL	OB6-CB5-C51	4.26	120.68	111.50
53	J	402	UQ	C11-C9-C8	-4.26	112.50	121.12
53	s	401	UQ	C27-C28-C29	-4.25	113.23	127.75
48	B	303	PEE	O2-C10-C11	4.24	120.64	111.50
53	J	402	UQ	C15-C14-C13	-4.24	112.81	123.68
51	i	401	CDL	OA6-CA5-C11	4.23	120.63	111.50
53	J	402	UQ	C21-C19-C18	-4.23	112.55	121.12
51	m	201	CDL	OA6-CA5-C11	4.21	120.58	111.50
53	s	401	UQ	C11-C9-C8	-4.19	112.65	121.12
51	r	504	CDL	OA6-CA5-C11	4.16	120.46	111.50
53	s	401	UQ	C16-C14-C13	-4.15	112.71	121.12
48	l	705	PEE	O2-C10-C11	4.11	120.35	111.50
51	l	702	CDL	OB6-CB5-C51	4.11	120.35	111.50
48	r	501	PEE	O2-C10-C11	4.07	120.28	111.50
53	J	402	UQ	C16-C14-C13	-4.04	112.95	121.12
51	u	201	CDL	OA6-CA5-C11	4.03	120.19	111.50
51	I	201	CDL	OA6-CA5-C11	4.01	120.14	111.50
51	o	201	CDL	OB6-CB5-C51	3.98	120.08	111.50
51	u	201	CDL	OB6-CB5-C51	3.98	120.07	111.50
51	l	701	CDL	OB6-CB5-C51	3.97	120.06	111.50
56	Q	501	970	O08-C07-C09	3.94	131.89	123.89
51	i	401	CDL	OB6-CB5-C51	3.93	119.98	111.50
48	W	201	PEE	O2-C10-C11	3.93	119.96	111.50
53	s	401	UQ	C20-C19-C18	-3.92	113.61	123.68
53	s	401	UQ	C26-C24-C23	-3.91	113.21	121.12
51	I	201	CDL	OB6-CB5-C51	3.90	119.91	111.50
53	s	401	UQ	C15-C14-C13	-3.89	113.70	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	C	302	PEE	O2-C10-C11	3.88	119.86	111.50
50	X	201	8Q1	C43-S44-C1	3.87	113.92	101.87
51	V	201	CDL	OB6-CB5-C51	3.82	119.74	111.50
48	l	703	PEE	O2-C10-C11	3.81	119.70	111.50
51	o	201	CDL	OA6-CA5-C11	3.80	119.70	111.50
51	r	504	CDL	OB6-CB5-C51	3.79	119.67	111.50
51	V	201	CDL	OA6-CA5-C11	3.76	119.61	111.50
51	a	201	CDL	OA6-CA5-C11	3.75	119.59	111.50
50	G	201	8Q1	C43-S44-C1	3.74	113.53	101.87
51	k	101	CDL	OB6-CB5-C51	3.74	119.56	111.50
56	Q	501	970	C22-C23-C14	3.67	114.69	109.56
48	U	101	PEE	O2-C10-C11	3.65	119.36	111.50
48	l	704	PEE	O2-C10-C11	3.61	119.29	111.50
56	Q	501	970	O28-C19-C20	3.56	120.37	115.41
51	k	101	CDL	OA6-CA5-C11	3.52	119.08	111.50
50	X	201	8Q1	O35-C34-N36	-3.46	115.57	122.99
53	s	401	UQ	C30-C29-C28	-3.42	112.76	122.65
53	J	402	UQ	C25-C24-C23	-3.39	112.85	122.65
53	J	402	UQ	C26-C24-C23	-3.39	112.85	122.65
56	Q	501	970	C06-C05-C04	3.33	104.44	101.45
50	G	201	8Q1	O35-C34-N36	-3.25	116.02	122.99
53	s	401	UQ	C31-C29-C28	-3.25	113.26	122.65
52	J	401	NDP	N3A-C2A-N1A	-3.23	123.63	128.68
46	A	502	FMN	C4-N3-C2	-3.23	119.68	125.64
56	Q	501	970	C09-C07-C06	-3.21	119.76	123.20
47	A	503	NAI	C4D-O4D-C1D	-3.09	102.66	109.47
51	l	701	CDL	OB8-CB7-C71	3.06	121.52	111.91
51	u	201	CDL	OB8-CB7-C71	3.04	121.46	111.91
51	l	701	CDL	OA8-CA7-C31	3.01	121.35	111.91
51	I	201	CDL	CA6-CA4-CA3	-2.99	104.71	111.79
51	u	201	CDL	OA8-CA7-C31	2.98	119.19	111.38
56	Q	501	970	C07-C06-C12	2.98	121.66	118.74
51	l	702	CDL	OB8-CB7-C71	2.95	121.16	111.91
51	k	101	CDL	OB8-CB7-C71	2.94	121.12	111.91
51	l	702	CDL	CA4-OA6-CA5	-2.92	110.60	117.79
56	Q	501	970	O26-C20-C19	2.91	119.46	115.41
50	G	201	8Q1	O2-P24-O27	-2.88	99.06	106.73
50	G	201	8Q1	C37-C38-C39	2.88	117.15	112.36
48	l	704	PEE	O3-C30-C31	2.87	120.93	111.91
50	X	201	8Q1	C37-C38-C39	2.84	117.09	112.36
48	U	101	PEE	O3-C30-C31	2.83	120.79	111.91
47	A	503	NAI	C3D-C2D-C1D	2.83	106.80	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	G	201	8Q1	O4-C1-S44	-2.82	118.95	122.61
51	a	201	CDL	OB8-CB7-C71	2.79	120.66	111.91
51	l	702	CDL	CB4-OB6-CB5	-2.77	110.97	117.79
51	I	201	CDL	OB8-CB7-C71	2.76	120.57	111.91
58	w	401	ADP	PA-O3A-PB	-2.74	123.42	132.83
46	A	502	FMN	C4A-C4-N3	2.74	120.14	113.19
48	B	303	PEE	O3-C30-C31	2.74	120.50	111.91
56	Q	501	970	O28-C19-C18	-2.74	119.41	124.12
51	I	201	CDL	OA8-CA7-C31	2.72	120.45	111.91
51	I	201	CDL	CB4-OB6-CB5	-2.71	111.11	117.79
51	m	201	CDL	OB8-CB7-C71	2.71	120.42	111.91
51	l	701	CDL	CA4-OA6-CA5	-2.69	111.17	117.79
47	A	503	NAI	C2D-C3D-C4D	2.68	107.84	102.64
48	l	703	PEE	O3-C30-C31	2.67	120.30	111.91
52	J	401	NDP	C4A-C5A-N7A	-2.67	106.61	109.40
51	V	201	CDL	OB8-CB7-C71	2.67	120.28	111.91
56	Q	501	970	C29-O28-C19	-2.67	113.50	117.53
51	o	201	CDL	OA8-CA7-C31	2.67	120.27	111.91
51	m	201	CDL	OA8-CA7-C31	2.64	120.21	111.91
48	j	201	PEE	O3-C30-C31	2.64	120.19	111.91
51	o	201	CDL	OB8-CB7-C71	2.63	120.16	111.91
50	G	201	8Q1	O40-C39-N41	-2.63	118.05	123.01
51	i	401	CDL	OA8-CA7-C31	2.61	120.10	111.91
46	A	502	FMN	O4-C4-C4A	-2.59	119.72	126.60
51	i	401	CDL	OB8-CB7-C71	2.59	120.03	111.91
53	J	402	UQ	CM5-C5-C6	-2.59	120.18	124.40
51	k	101	CDL	OA8-CA7-C31	2.59	120.03	111.91
50	G	201	8Q1	C32-C34-N36	2.58	121.72	116.58
47	A	503	NAI	C4A-C5A-N7A	-2.57	106.72	109.40
56	Q	501	970	C11-C24-C23	2.56	119.61	115.92
51	a	201	CDL	OA8-CA7-C31	2.55	119.92	111.91
51	r	504	CDL	OB8-CB7-C71	2.55	119.90	111.91
48	r	501	PEE	O3-C30-C31	2.53	119.84	111.91
50	X	201	8Q1	O2-P24-O27	-2.52	100.02	106.73
51	l	702	CDL	OA8-CA7-C31	2.52	119.80	111.91
52	J	401	NDP	PN-O3-PA	-2.51	124.20	132.83
49	g	201	PLX	C1A-N1-C1	2.50	120.14	109.92
48	W	201	PEE	O3-C30-C31	2.50	119.75	111.91
48	C	302	PEE	O3-C30-C31	2.50	119.74	111.91
48	l	703	PEE	C2-O2-C10	-2.49	111.67	117.79
51	r	504	CDL	OA8-CA7-C31	2.45	119.60	111.91
56	Q	501	970	C11-C12-C06	-2.43	119.22	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	V	201	CDL	OA8-CA7-C31	2.43	119.54	111.91
50	X	201	8Q1	O27-P24-O3	-2.41	99.70	106.47
46	A	502	FMN	C4A-C10-N1	-2.41	119.14	124.73
49	a	202	PLX	C1A-N1-C1	2.40	119.75	109.92
48	l	705	PEE	O3-C30-C31	2.40	119.43	111.91
49	r	502	PLX	C1A-N1-C1	2.38	119.66	109.92
50	X	201	8Q1	C32-C34-N36	2.35	121.26	116.58
49	J	403	PLX	C1A-N1-C1	2.34	119.47	109.92
51	l	702	CDL	OA6-CA5-OA7	-2.33	118.08	123.70
50	G	201	8Q1	O1-P24-O2	2.31	116.45	107.64
49	j	202	PLX	C1A-N1-C1	2.30	119.32	109.92
46	A	502	FMN	C9A-C5A-N5	-2.27	119.96	122.43
46	A	502	FMN	C4A-C10-N10	2.27	119.80	116.48
56	Q	501	970	C27-O26-C20	-2.26	114.11	117.53
56	Q	501	970	C05-C06-C12	-2.26	127.24	131.59
50	X	201	8Q1	O1-P24-O2	2.26	116.28	107.64
56	Q	501	970	C15-O16-C17	-2.26	110.59	115.30
56	Q	501	970	O26-C20-C21	-2.25	120.25	124.12
50	X	201	8Q1	O40-C39-N41	-2.25	118.78	123.01
51	l	701	CDL	CB4-OB6-CB5	-2.24	112.27	117.79
56	Q	501	970	C12-O13-C14	-2.22	112.26	116.06
47	A	503	NAI	PN-O3-PA	-2.22	125.22	132.83
51	u	201	CDL	OB8-CB7-OB9	-2.21	118.00	123.59
50	G	201	8Q1	C38-C39-N41	2.21	120.14	116.42
53	s	401	UQ	CM5-C5-C6	-2.20	120.80	124.40
50	X	201	8Q1	O4-C1-S44	-2.15	119.82	122.61
56	Q	501	970	C05-C06-C07	2.14	111.10	108.54
56	Q	501	970	O13-C14-C23	2.14	114.56	112.40
51	m	201	CDL	CB4-OB6-CB5	-2.13	112.55	117.79
50	G	201	8Q1	O27-P24-O3	-2.12	100.52	106.47
50	G	201	8Q1	O4-C1-C6	-2.12	121.49	123.99
51	m	201	CDL	OB8-CB7-OB9	-2.11	118.26	123.59
46	A	502	FMN	C5A-C9A-N10	2.11	120.13	117.95
46	A	502	FMN	C10-C4A-N5	-2.11	120.39	124.86
58	w	401	ADP	C4-C5-N7	-2.07	107.24	109.40
51	l	701	CDL	OB8-CB7-OB9	-2.07	118.37	123.59
50	X	201	8Q1	O4-C1-C6	-2.05	121.57	123.99
51	l	701	CDL	OA6-CA5-OA7	-2.04	118.78	123.70
49	C	303	PLX	C6-O6-C4	-2.04	111.13	115.20
46	A	502	FMN	C4-C4A-C10	2.04	120.21	116.79
51	o	201	CDL	CB4-OB6-CB5	-2.00	112.86	117.79

There are no chirality outliers.

All (1019) 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'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	O4P-C4-C5-N
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	O4P-C4-C5-N
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C1-O3P-P-O1P
48	l	703	PEE	C4-O4P-P-O3P
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O1P
48	l	703	PEE	C5-C4-O4P-P
48	l	703	PEE	O4P-C4-C5-N
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	O4P-C4-C5-N
48	l	705	PEE	C1-O3P-P-O2P
48	l	705	PEE	C1-O3P-P-O1P
48	l	705	PEE	O4P-C4-C5-N
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C2-O1-P1-O2
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C2-O1-P1-O4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	O9-C24-O8-C5
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C3-O4-P1-O3
49	j	202	PLX	O9-C24-O8-C5
49	r	502	PLX	O6-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	O9-C24-C25-C26
50	G	201	8Q1	C1-C6-C7-C8
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C29-C32-C34-N36
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C43-C42-N41-C39

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	I	201	CDL	CA2-OA2-PA1-OA3
51	I	201	CDL	CA3-OA5-PA1-OA4
51	I	201	CDL	CB3-OB5-PB2-OB4
51	V	201	CDL	CA2-OA2-PA1-OA3
51	V	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CB2-C1-CA2-OA2
51	a	201	CDL	CA2-OA2-PA1-OA3
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	OB7-CB5-OB6-CB4
51	a	201	CDL	C51-CB5-OB6-CB4
51	i	401	CDL	CA2-OA2-PA1-OA4
51	i	401	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CA3-OA5-PA1-OA3
51	i	401	CDL	CA3-OA5-PA1-OA4
51	i	401	CDL	CB3-OB5-PB2-OB3
51	k	101	CDL	CA2-OA2-PA1-OA4
51	k	101	CDL	OA5-CA3-CA4-OA6
51	k	101	CDL	CB2-OB2-PB2-OB3
51	l	701	CDL	CB3-OB5-PB2-OB2
51	l	701	CDL	CB3-OB5-PB2-OB3
51	l	701	CDL	CB3-OB5-PB2-OB4
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CA3-OA5-PA1-OA3
51	l	702	CDL	CA3-OA5-PA1-OA4
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	C51-CB5-OB6-CB4
51	m	201	CDL	CA2-OA2-PA1-OA3
51	m	201	CDL	CA3-OA5-PA1-OA3
51	m	201	CDL	CB2-OB2-PB2-OB3
51	m	201	CDL	CB2-OB2-PB2-OB4
51	m	201	CDL	CB2-OB2-PB2-OB5
51	m	201	CDL	C51-CB5-OB6-CB4
51	o	201	CDL	CA2-OA2-PA1-OA3
51	o	201	CDL	CA2-OA2-PA1-OA4
51	o	201	CDL	CA3-OA5-PA1-OA3
51	o	201	CDL	CB3-OB5-PB2-OB3
51	o	201	CDL	CB3-OB5-PB2-OB4
51	o	201	CDL	C51-CB5-OB6-CB4
51	r	504	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	CA3-OA5-PA1-OA3
51	r	504	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB4
51	r	504	CDL	C51-CB5-OB6-CB4
51	u	201	CDL	CA2-OA2-PA1-OA3
51	u	201	CDL	CB3-OB5-PB2-OB3
52	J	401	NDP	C5D-O5D-PN-O1N
53	J	402	UQ	C1-C6-C7-C8
53	J	402	UQ	C5-C6-C7-C8
53	J	402	UQ	C7-C8-C9-C11
53	J	402	UQ	C12-C13-C14-C16
53	s	401	UQ	C7-C8-C9-C10
53	s	401	UQ	C7-C8-C9-C11
56	Q	501	970	C03-C02-C04-C05
56	Q	501	970	C03-C02-C04-O08
58	w	401	ADP	C5'-O5'-PA-O2A
58	w	401	ADP	C5'-O5'-PA-O3A
48	U	101	PEE	O5-C30-O3-C3
48	l	703	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
51	l	702	CDL	OB7-CB5-OB6-CB4
51	m	201	CDL	OB7-CB5-OB6-CB4
51	o	201	CDL	OB7-CB5-OB6-CB4
51	r	504	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C31-C30-O3-C3
53	J	402	UQ	C22-C23-C24-C26
53	s	401	UQ	C18-C19-C21-C22
48	l	705	PEE	C2-C3-O3-C30
49	r	502	PLX	C9-C10-C11-C12
51	V	201	CDL	C11-C12-C13-C14
51	V	201	CDL	C31-CA7-OA8-CA6
53	J	402	UQ	C7-C8-C9-C10
49	J	403	PLX	C25-C26-C27-C28
48	j	201	PEE	O4-C10-O2-C2
51	V	201	CDL	OA7-CA5-OA6-CA4
53	J	402	UQ	C17-C18-C19-C21
53	s	401	UQ	C17-C18-C19-C21
53	s	401	UQ	C22-C23-C24-C26
51	V	201	CDL	OA9-CA7-OA8-CA6
51	l	702	CDL	OB9-CB7-OB8-CB6
49	J	403	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	O1-C1-CB2-OB2
51	l	701	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CA2-OA2
51	m	201	CDL	O1-C1-CA2-OA2
51	o	201	CDL	O1-C1-CA2-OA2
51	o	201	CDL	O1-C1-CB2-OB2
51	r	504	CDL	O1-C1-CA2-OA2
51	u	201	CDL	O1-C1-CB2-OB2
51	i	401	CDL	C31-CA7-OA8-CA6
51	l	702	CDL	C71-CB7-OB8-CB6
51	i	401	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	C11-C10-O2-C2
51	I	201	CDL	C11-CA5-OA6-CA4
51	V	201	CDL	C11-CA5-OA6-CA4
51	k	101	CDL	C73-C74-C75-C76
49	r	502	PLX	C7-C8-C9-C10
51	V	201	CDL	C62-C63-C64-C65
48	l	705	PEE	C34-C35-C36-C37
49	r	502	PLX	C11-C12-C13-C14
48	B	303	PEE	C34-C35-C36-C37
49	j	202	PLX	C13-C14-C15-C16
48	l	704	PEE	C31-C30-O3-C3
53	J	402	UQ	C12-C11-C9-C8
48	l	704	PEE	O5-C30-O3-C3
51	a	201	CDL	C34-C35-C36-C37
51	r	504	CDL	C83-C84-C85-C86
51	l	701	CDL	C31-CA7-OA8-CA6
51	r	504	CDL	C71-CB7-OB8-CB6
51	V	201	CDL	C32-C33-C34-C35
53	s	401	UQ	C27-C28-C29-C31
53	s	401	UQ	C22-C23-C24-C25
51	a	201	CDL	CA2-C1-CB2-OB2
51	l	701	CDL	CB2-C1-CA2-OA2
51	o	201	CDL	CA2-C1-CB2-OB2
51	l	701	CDL	OA9-CA7-OA8-CA6
51	r	504	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C2-C1-N1-C1A
48	W	201	PEE	C31-C30-O3-C3
51	I	201	CDL	C31-CA7-OA8-CA6
51	a	201	CDL	C31-CA7-OA8-CA6
51	r	504	CDL	C51-C52-C53-C54
49	a	202	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	OB5-CB3-CB4-OB6
51	l	702	CDL	O1-C1-CB2-OB2
51	V	201	CDL	OB6-CB4-CB6-OB8
51	i	401	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C31-C30-O3-C3
48	r	501	PEE	C33-C34-C35-C36
49	g	201	PLX	C7-C8-C9-C10
51	I	201	CDL	OA9-CA7-OA8-CA6
51	a	201	CDL	OA9-CA7-OA8-CA6
51	i	401	CDL	CA7-C31-C32-C33
51	u	201	CDL	CB7-C71-C72-C73
51	a	201	CDL	C36-C37-C38-C39
51	l	701	CDL	CB5-C51-C52-C53
51	l	701	CDL	CB7-C71-C72-C73
51	r	504	CDL	CA5-C11-C12-C13
48	B	303	PEE	C17-C18-C19-C20
48	r	501	PEE	C10-C11-C12-C13
51	a	201	CDL	CA5-C11-C12-C13
48	l	705	PEE	C21-C22-C23-C24
51	l	702	CDL	C75-C76-C77-C78
48	C	302	PEE	O4-C10-O2-C2
51	I	201	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C2-C1-N1-C1B
51	l	702	CDL	CB7-C71-C72-C73
48	W	201	PEE	C22-C23-C24-C25
53	J	402	UQ	C9-C11-C12-C13
53	s	401	UQ	C14-C16-C17-C18
51	r	504	CDL	CB7-C71-C72-C73
51	a	201	CDL	O1-C1-CA2-OA2
51	k	101	CDL	O1-C1-CA2-OA2
51	V	201	CDL	C71-CB7-OB8-CB6
49	j	202	PLX	C19-C20-C21-C22
48	W	201	PEE	O5-C30-O3-C3
48	W	201	PEE	C17-C18-C19-C20
48	B	303	PEE	O5-C30-O3-C3
51	V	201	CDL	C51-CB5-OB6-CB4
49	g	201	PLX	C9-C10-C11-C12
51	I	201	CDL	C51-C52-C53-C54
51	o	201	CDL	C11-C12-C13-C14
48	B	303	PEE	C4-O4P-P-O3P
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C1-O3P-P-O4P
48	l	705	PEE	C1-O3P-P-O4P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
49	J	403	PLX	C2-O1-P1-O4
49	a	202	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O1
49	g	201	PLX	C2-O1-P1-O4
51	I	201	CDL	CA2-OA2-PA1-OA5
51	I	201	CDL	CA3-OA5-PA1-OA2
51	I	201	CDL	CB3-OB5-PB2-OB2
51	a	201	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CA2-OA2-PA1-OA5
51	i	401	CDL	CB3-OB5-PB2-OB2
51	k	101	CDL	CA2-OA2-PA1-OA5
51	k	101	CDL	CB2-OB2-PB2-OB5
51	l	701	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	CA3-OA5-PA1-OA2
51	o	201	CDL	CA2-OA2-PA1-OA5
51	o	201	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CB3-OB5-PB2-OB2
51	u	201	CDL	CA2-OA2-PA1-OA5
51	u	201	CDL	CA3-OA5-PA1-OA2
51	u	201	CDL	CB3-OB5-PB2-OB2
51	m	201	CDL	CA5-C11-C12-C13
51	k	101	CDL	CB2-C1-CA2-OA2
51	l	702	CDL	CB2-C1-CA2-OA2
51	o	201	CDL	CB2-C1-CA2-OA2
51	r	504	CDL	CB2-C1-CA2-OA2
51	V	201	CDL	OB7-CB5-OB6-CB4
48	j	201	PEE	C31-C30-O3-C3
49	J	403	PLX	C34-C35-C36-C37
48	B	303	PEE	C35-C36-C37-C38
48	U	101	PEE	C19-C20-C21-C22
49	j	202	PLX	C33-C34-C35-C36
50	G	201	8Q1	C10-C11-C12-C13
51	o	201	CDL	C14-C15-C16-C17
48	l	705	PEE	C11-C10-O2-C2
51	l	702	CDL	C11-CA5-OA6-CA4
48	U	101	PEE	C22-C23-C24-C25
48	W	201	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C14-C15-C16-C17
49	J	403	PLX	C31-C32-C33-C34
49	a	202	PLX	C10-C11-C12-C13
49	a	202	PLX	C9-C10-C11-C12
49	j	202	PLX	C27-C28-C29-C30
51	o	201	CDL	C59-C60-C61-C62
48	C	302	PEE	C34-C35-C36-C37
48	r	501	PEE	C11-C12-C13-C14
49	J	403	PLX	C28-C29-C30-C31
49	a	202	PLX	C33-C34-C35-C36
49	a	202	PLX	C34-C35-C36-C37
49	g	201	PLX	C11-C10-C9-C8
49	g	201	PLX	C30-C31-C32-C33
51	V	201	CDL	C56-C57-C58-C59
51	o	201	CDL	C60-C61-C62-C63
48	l	705	PEE	O4-C10-O2-C2
48	B	303	PEE	C13-C14-C15-C16
48	j	201	PEE	C12-C13-C14-C15
49	r	503	PLX	C34-C35-C36-C37
51	V	201	CDL	C31-C32-C33-C34
51	a	201	CDL	C35-C36-C37-C38
51	a	201	CDL	C39-C40-C41-C42
51	a	201	CDL	C62-C63-C64-C65
51	i	401	CDL	C38-C39-C40-C41
48	l	705	PEE	C37-C38-C39-C40
48	l	704	PEE	C21-C22-C23-C24
49	J	403	PLX	C13-C14-C15-C16
51	l	701	CDL	C73-C74-C75-C76
51	o	201	CDL	C37-C38-C39-C40
51	o	201	CDL	C54-C55-C56-C57
48	r	501	PEE	C40-C41-C42-C43
49	j	202	PLX	C11-C12-C13-C14
49	r	502	PLX	C11-C10-C9-C8
49	r	502	PLX	C25-C26-C27-C28
49	r	503	PLX	C10-C11-C12-C13
48	W	201	PEE	C13-C14-C15-C16
49	J	403	PLX	C33-C34-C35-C36
49	j	202	PLX	C25-C26-C27-C28
51	V	201	CDL	C71-C72-C73-C74
51	o	201	CDL	C74-C75-C76-C77
51	r	504	CDL	C80-C81-C82-C83
48	j	201	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C23-C24-C25-C26
48	C	302	PEE	C13-C14-C15-C16
49	J	403	PLX	C30-C31-C32-C33
49	g	201	PLX	C14-C15-C16-C17
49	g	201	PLX	C13-C14-C15-C16
49	r	503	PLX	C32-C33-C34-C35
51	V	201	CDL	C34-C35-C36-C37
53	s	401	UQ	C23-C24-C26-C27
48	l	705	PEE	C20-C21-C22-C23
48	r	501	PEE	C21-C22-C23-C24
49	a	202	PLX	C7-C8-C9-C10
49	r	503	PLX	C7-C8-C9-C10
51	V	201	CDL	C35-C36-C37-C38
51	V	201	CDL	C75-C76-C77-C78
51	a	201	CDL	C75-C76-C77-C78
51	k	101	CDL	C11-C12-C13-C14
49	C	303	PLX	C25-C26-C27-C28
49	j	202	PLX	C10-C11-C12-C13
51	l	702	CDL	OA7-CA5-OA6-CA4
51	I	201	CDL	C51-CB5-OB6-CB4
49	r	503	PLX	C25-C26-C27-C28
51	V	201	CDL	C58-C59-C60-C61
51	a	201	CDL	C60-C61-C62-C63
51	k	101	CDL	C71-C72-C73-C74
51	o	201	CDL	C82-C83-C84-C85
48	l	704	PEE	C15-C16-C17-C18
51	u	201	CDL	CB5-C51-C52-C53
48	j	201	PEE	C23-C24-C25-C26
48	l	704	PEE	C31-C32-C33-C34
49	j	202	PLX	C16-C17-C18-C19
50	G	201	8Q1	C12-C13-C14-C15
51	V	201	CDL	C78-C79-C80-C81
51	a	201	CDL	C73-C74-C75-C76
51	o	201	CDL	C17-C18-C19-C20
49	J	403	PLX	C7-C8-C9-C10
49	a	202	PLX	C30-C31-C32-C33
49	g	201	PLX	C28-C29-C30-C31
49	j	202	PLX	C14-C15-C16-C17
51	V	201	CDL	C72-C73-C74-C75
51	a	201	CDL	C17-C18-C19-C20
51	o	201	CDL	C75-C76-C77-C78
49	g	201	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C59-C60-C61-C62
51	a	201	CDL	C22-C23-C24-C25
51	a	201	CDL	C80-C81-C82-C83
48	r	501	PEE	C13-C14-C15-C16
49	g	201	PLX	C27-C28-C29-C30
49	r	502	PLX	C12-C13-C14-C15
48	U	101	PEE	C21-C22-C23-C24
51	I	201	CDL	C11-C12-C13-C14
51	m	201	CDL	C16-C17-C18-C19
51	r	504	CDL	C43-C44-C45-C46
51	r	504	CDL	C55-C56-C57-C58
51	o	201	CDL	C35-C36-C37-C38
51	r	504	CDL	C14-C15-C16-C17
51	r	504	CDL	C31-C32-C33-C34
51	V	201	CDL	OB9-CB7-OB8-CB6
49	C	303	PLX	C15-C16-C17-C18
49	C	303	PLX	C9-C10-C11-C12
49	r	502	PLX	C28-C29-C30-C31
51	o	201	CDL	C83-C84-C85-C86
48	r	501	PEE	C1-C2-C3-O3
51	o	201	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	C17-C18-C19-C20
49	r	503	PLX	C16-C17-C18-C19
51	a	201	CDL	C11-C12-C13-C14
51	k	101	CDL	C17-C18-C19-C20
48	U	101	PEE	C41-C42-C43-C44
51	i	401	CDL	C14-C15-C16-C17
48	B	303	PEE	C11-C10-O2-C2
51	l	702	CDL	C33-C34-C35-C36
49	C	303	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	a	202	PLX	C19-C20-C21-C22
49	r	502	PLX	C33-C34-C35-C36
51	V	201	CDL	C73-C74-C75-C76
51	a	201	CDL	C52-C53-C54-C55
51	r	504	CDL	C41-C42-C43-C44
48	l	705	PEE	C15-C16-C17-C18
51	V	201	CDL	C40-C41-C42-C43
51	l	701	CDL	C11-C12-C13-C14
48	U	101	PEE	C30-C31-C32-C33
51	V	201	CDL	CB5-C51-C52-C53
51	l	702	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C26-C27-C28-C29
51	l	702	CDL	C12-C13-C14-C15
51	r	504	CDL	C21-C22-C23-C24
51	I	201	CDL	OB7-CB5-OB6-CB4
51	r	504	CDL	C13-C14-C15-C16
51	r	504	CDL	C17-C18-C19-C20
49	a	202	PLX	C13-C14-C15-C16
51	i	401	CDL	C77-C78-C79-C80
51	r	504	CDL	C32-C33-C34-C35
49	g	201	PLX	C2-C1-N1-C1C
49	g	201	PLX	C10-C11-C12-C13
51	V	201	CDL	C43-C44-C45-C46
51	o	201	CDL	C51-C52-C53-C54
48	r	501	PEE	C11-C10-O2-C2
48	r	501	PEE	C20-C21-C22-C23
49	r	502	PLX	C27-C28-C29-C30
48	l	705	PEE	C30-C31-C32-C33
49	r	502	PLX	C18-C19-C20-C21
51	l	701	CDL	C81-C82-C83-C84
53	s	401	UQ	C27-C28-C29-C30
48	j	201	PEE	C13-C14-C15-C16
48	r	501	PEE	C34-C35-C36-C37
49	g	201	PLX	C25-C26-C27-C28
49	r	502	PLX	C19-C20-C21-C22
51	r	504	CDL	C82-C83-C84-C85
48	B	303	PEE	C38-C39-C40-C41
48	B	303	PEE	O4-C10-O2-C2
48	W	201	PEE	O4-C10-O2-C2
48	W	201	PEE	C24-C25-C26-C27
48	W	201	PEE	C21-C22-C23-C24
51	o	201	CDL	C12-C13-C14-C15
48	l	703	PEE	C10-C11-C12-C13
51	a	201	CDL	CB5-C51-C52-C53
49	r	503	PLX	C17-C18-C19-C20
49	r	503	PLX	C29-C30-C31-C32
51	V	201	CDL	C79-C80-C81-C82
51	k	101	CDL	C23-C24-C25-C26
56	Q	501	970	C20-C19-O28-C29
48	l	705	PEE	C13-C14-C15-C16
49	g	201	PLX	C12-C13-C14-C15
49	j	202	PLX	C11-C10-C9-C8
51	o	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	o	201	CDL	C72-C73-C74-C75
48	W	201	PEE	C11-C10-O2-C2
51	i	401	CDL	C11-CA5-OA6-CA4
51	o	201	CDL	OB5-CB3-CB4-OB6
49	r	503	PLX	C13-C14-C15-C16
51	r	504	CDL	C52-C53-C54-C55
48	r	501	PEE	O4-C10-O2-C2
51	i	401	CDL	OA7-CA5-OA6-CA4
51	r	504	CDL	CB5-C51-C52-C53
48	W	201	PEE	C20-C21-C22-C23
51	o	201	CDL	OA6-CA4-CA6-OA8
51	o	201	CDL	OB6-CB4-CB6-OB8
49	r	503	PLX	C28-C29-C30-C31
49	r	502	PLX	C13-C14-C15-C16
49	r	503	PLX	C11-C10-C9-C8
48	C	302	PEE	C19-C20-C21-C22
48	l	703	PEE	C35-C36-C37-C38
48	U	101	PEE	C17-C18-C19-C20
48	j	201	PEE	C11-C12-C13-C14
51	m	201	CDL	C12-C13-C14-C15
48	r	501	PEE	C30-C31-C32-C33
51	o	201	CDL	C36-C37-C38-C39
48	W	201	PEE	C4-O4P-P-O3P
51	a	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CB2-OB2-PB2-OB5
48	l	703	PEE	C32-C33-C34-C35
51	r	504	CDL	C59-C60-C61-C62
51	V	201	CDL	OB5-CB3-CB4-CB6
49	j	202	PLX	C7-C8-C9-C10
51	V	201	CDL	C61-C62-C63-C64
49	C	303	PLX	C10-C11-C12-C13
51	l	701	CDL	C35-C36-C37-C38
51	i	401	CDL	C13-C14-C15-C16
51	k	101	CDL	C81-C82-C83-C84
48	U	101	PEE	C35-C36-C37-C38
48	C	302	PEE	C44-C45-C46-C47
48	l	703	PEE	C31-C30-O3-C3
51	u	201	CDL	CA2-C1-CB2-OB2
48	r	501	PEE	C42-C43-C44-C45
51	V	201	CDL	C15-C16-C17-C18
51	r	504	CDL	C71-C72-C73-C74
48	C	302	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	C57-C58-C59-C60
48	W	201	PEE	C1-C2-C3-O3
51	V	201	CDL	CB3-CB4-CB6-OB8
51	k	101	CDL	C76-C77-C78-C79
51	r	504	CDL	C72-C73-C74-C75
48	l	704	PEE	C32-C33-C34-C35
51	k	101	CDL	C75-C76-C77-C78
51	a	201	CDL	C71-C72-C73-C74
51	l	702	CDL	C17-C18-C19-C20
51	o	201	CDL	C32-C31-CA7-OA8
48	l	704	PEE	C24-C25-C26-C27
51	V	201	CDL	C52-C53-C54-C55
51	a	201	CDL	C44-C45-C46-C47
48	r	501	PEE	C39-C40-C41-C42
51	V	201	CDL	CA7-C31-C32-C33
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
48	B	303	PEE	C44-C45-C46-C47
48	l	703	PEE	C13-C14-C15-C16
49	r	503	PLX	C11-C12-C13-C14
51	o	201	CDL	C57-C58-C59-C60
51	I	201	CDL	CA6-CA4-OA6-CA5
51	V	201	CDL	CA6-CA4-OA6-CA5
51	i	401	CDL	CA6-CA4-OA6-CA5
49	r	502	PLX	C30-C31-C32-C33
51	l	702	CDL	C15-C16-C17-C18
51	o	201	CDL	C77-C78-C79-C80
46	A	502	FMN	C5'-O5'-P-O1P
50	G	201	8Q1	C28-O27-P24-O3
48	U	101	PEE	C12-C13-C14-C15
49	r	503	PLX	C14-C15-C16-C17
50	G	201	8Q1	C11-C12-C13-C14
50	X	201	8Q1	C7-C8-C9-C10
51	l	701	CDL	C75-C76-C77-C78
51	o	201	CDL	C64-C65-C66-C67
48	l	704	PEE	O3P-C1-C2-O2
49	j	202	PLX	O4-C3-C4-O6
49	C	303	PLX	C32-C33-C34-C35
49	r	503	PLX	C26-C27-C28-C29
51	l	701	CDL	C37-C38-C39-C40
51	l	702	CDL	C39-C40-C41-C42
48	l	704	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	O6-C4-C5-O8
51	k	101	CDL	OA6-CA4-CA6-OA8
48	U	101	PEE	C32-C33-C34-C35
49	r	502	PLX	C34-C35-C36-C37
51	i	401	CDL	C82-C83-C84-C85
51	k	101	CDL	C84-C85-C86-C87
49	r	503	PLX	C12-C13-C14-C15
48	l	703	PEE	O5-C30-O3-C3
49	j	202	PLX	C29-C30-C31-C32
51	r	504	CDL	C73-C74-C75-C76
53	J	402	UQ	C3-C2-O2-CM2
48	C	302	PEE	C42-C43-C44-C45
51	k	101	CDL	C52-C53-C54-C55
52	J	401	NDP	PN-O3-PA-O1A
49	g	201	PLX	C16-C17-C18-C19
51	l	702	CDL	C11-C12-C13-C14
49	j	202	PLX	C34-C35-C36-C37
51	a	201	CDL	C84-C85-C86-C87
49	g	201	PLX	C36-C37-C38-C39
51	l	701	CDL	C51-C52-C53-C54
49	j	202	PLX	C12-C13-C14-C15
50	X	201	8Q1	C12-C13-C14-C15
51	a	201	CDL	C76-C77-C78-C79
48	l	703	PEE	C18-C19-C20-C21
48	r	501	PEE	C38-C39-C40-C41
48	l	703	PEE	C14-C15-C16-C17
49	r	502	PLX	C14-C15-C16-C17
51	k	101	CDL	C14-C15-C16-C17
51	r	504	CDL	C62-C63-C64-C65
48	C	302	PEE	O3P-C1-C2-C3
49	C	303	PLX	O4-C3-C4-C5
49	J	403	PLX	O4-C3-C4-C5
51	i	401	CDL	OB5-CB3-CB4-CB6
51	k	101	CDL	OA5-CA3-CA4-CA6
51	o	201	CDL	OB5-CB3-CB4-CB6
48	r	501	PEE	O4P-C4-C5-N
48	l	704	PEE	C42-C43-C44-C45
48	l	704	PEE	C13-C14-C15-C16
49	a	202	PLX	C11-C10-C9-C8
51	a	201	CDL	C71-CB7-OB8-CB6
51	k	101	CDL	C31-CA7-OA8-CA6
48	l	703	PEE	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
48	l	705	PEE	C11-C12-C13-C14
51	V	201	CDL	C33-C34-C35-C36
51	o	201	CDL	C84-C85-C86-C87
51	m	201	CDL	C52-C53-C54-C55
49	J	403	PLX	C12-C13-C14-C15
48	C	302	PEE	C1-C2-C3-O3
48	l	703	PEE	C1-C2-C3-O3
48	l	705	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
51	i	401	CDL	CB3-CB4-CB6-OB8
51	o	201	CDL	CA3-CA4-CA6-OA8
48	r	501	PEE	C17-C18-C19-C20
49	J	403	PLX	C16-C17-C18-C19
49	a	202	PLX	C15-C16-C17-C18
51	k	101	CDL	C80-C81-C82-C83
48	C	302	PEE	C31-C32-C33-C34
51	i	401	CDL	C76-C77-C78-C79
51	m	201	CDL	C33-C34-C35-C36
51	m	201	CDL	C51-C52-C53-C54
48	U	101	PEE	C44-C45-C46-C47
49	a	202	PLX	C5-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
51	l	702	CDL	CB2-OB2-PB2-OB5
51	r	504	CDL	CB2-OB2-PB2-OB5
48	r	501	PEE	O3P-C1-C2-O2
49	C	303	PLX	O4-C3-C4-O6
49	J	403	PLX	C10-C11-C12-C13
51	V	201	CDL	C64-C65-C66-C67
49	j	202	PLX	C20-C21-C22-C23
51	l	702	CDL	C16-C17-C18-C19
51	k	101	CDL	C12-C13-C14-C15
51	m	201	CDL	C72-C73-C74-C75
48	B	303	PEE	O2-C2-C3-O3
48	C	302	PEE	O2-C2-C3-O3
51	k	101	CDL	OB6-CB4-CB6-OB8
51	l	702	CDL	OB6-CB4-CB6-OB8
48	j	201	PEE	C24-C25-C26-C27
49	C	303	PLX	C11-C12-C13-C14
51	o	201	CDL	C34-C35-C36-C37
51	m	201	CDL	CB2-C1-CA2-OA2
50	G	201	8Q1	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C11-C10-C9-C8
51	V	201	CDL	C14-C15-C16-C17
51	l	702	CDL	C79-C80-C81-C82
51	I	201	CDL	C1-CA2-OA2-PA1
51	r	504	CDL	C1-CB2-OB2-PB2
48	l	703	PEE	C34-C35-C36-C37
49	a	202	PLX	C27-C28-C29-C30
51	k	101	CDL	C18-C19-C20-C21
51	I	201	CDL	CA7-C31-C32-C33
51	V	201	CDL	C17-C18-C19-C20
51	l	701	CDL	C51-CB5-OB6-CB4
51	o	201	CDL	C79-C80-C81-C82
51	r	504	CDL	C37-C38-C39-C40
56	Q	501	970	C18-C19-O28-C29
48	j	201	PEE	C34-C35-C36-C37
49	a	202	PLX	C11-C12-C13-C14
49	J	403	PLX	O8-C24-C25-C26
49	a	202	PLX	O8-C24-C25-C26
49	j	202	PLX	O6-C6-C7-C8
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	O8-C24-C25-C26
51	a	201	CDL	C43-C44-C45-C46
51	r	504	CDL	C78-C79-C80-C81
48	l	703	PEE	O3P-C1-C2-C3
48	l	704	PEE	O3P-C1-C2-C3
51	V	201	CDL	OA5-CA3-CA4-CA6
51	m	201	CDL	OA5-CA3-CA4-CA6
51	m	201	CDL	O1-C1-CB2-OB2
49	C	303	PLX	C11-C10-C9-C8
51	a	201	CDL	C82-C83-C84-C85
48	U	101	PEE	C34-C35-C36-C37
51	V	201	CDL	C55-C56-C57-C58
51	a	201	CDL	C20-C21-C22-C23
51	i	401	CDL	C71-C72-C73-C74
51	m	201	CDL	C54-C55-C56-C57
51	m	201	CDL	C35-C36-C37-C38
51	r	504	CDL	C15-C16-C17-C18
51	l	701	CDL	C11-CA5-OA6-CA4
58	w	401	ADP	PA-O3A-PB-O1B
49	r	503	PLX	C33-C34-C35-C36
51	l	701	CDL	C78-C79-C80-C81
51	u	201	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	C37-C38-C39-C40
49	g	201	PLX	C3-C4-C5-O8
51	k	101	CDL	CB3-CB4-CB6-OB8
48	r	501	PEE	C14-C15-C16-C17
48	B	303	PEE	O3P-C1-C2-O2
48	C	302	PEE	O3P-C1-C2-O2
51	i	401	CDL	OB5-CB3-CB4-OB6
51	m	201	CDL	OA5-CA3-CA4-OA6
51	o	201	CDL	OA5-CA3-CA4-OA6
51	r	504	CDL	OB5-CB3-CB4-OB6
51	r	504	CDL	C39-C40-C41-C42
48	U	101	PEE	C38-C39-C40-C41
48	U	101	PEE	C11-C12-C13-C14
51	a	201	CDL	OB9-CB7-OB8-CB6
48	W	201	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
50	X	201	8Q1	C13-C14-C15-C16
47	A	503	NAI	C5B-O5B-PA-O3
52	J	401	NDP	C5D-O5D-PN-O3
48	B	303	PEE	C39-C40-C41-C42
53	J	402	UQ	C20-C19-C21-C22
51	k	101	CDL	OA9-CA7-OA8-CA6
51	l	701	CDL	OA7-CA5-OA6-CA4
51	l	701	CDL	OB7-CB5-OB6-CB4
51	V	201	CDL	C44-C45-C46-C47
51	r	504	CDL	C22-C23-C24-C25
51	r	504	CDL	C56-C57-C58-C59
48	r	501	PEE	C41-C42-C43-C44
51	a	201	CDL	C83-C84-C85-C86
48	C	302	PEE	C31-C30-O3-C3
51	a	201	CDL	C14-C15-C16-C17
51	a	201	CDL	C51-C52-C53-C54
48	l	703	PEE	C1-O3P-P-O4P
51	V	201	CDL	CB3-OB5-PB2-OB2
49	g	201	PLX	C20-C21-C22-C23
49	r	502	PLX	C4-C3-O4-P1
51	l	701	CDL	CA4-CA3-OA5-PA1
51	o	201	CDL	C1-CB2-OB2-PB2
48	B	303	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C4-O4P-P-O2P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C4-O4P-P-O2P
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C3-O4-P1-O3
51	I	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CA2-OA2-PA1-OA4
51	a	201	CDL	CA3-OA5-PA1-OA3
51	a	201	CDL	CA3-OA5-PA1-OA4
51	a	201	CDL	CB2-OB2-PB2-OB4
51	i	401	CDL	CB3-OB5-PB2-OB4
51	k	101	CDL	CA2-OA2-PA1-OA3
51	k	101	CDL	CB2-OB2-PB2-OB4
51	l	701	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CA2-OA2-PA1-OA4
51	u	201	CDL	CA2-OA2-PA1-OA4
51	u	201	CDL	CA3-OA5-PA1-OA3
53	s	401	UQ	C6-C7-C8-C9
58	w	401	ADP	C5'-O5'-PA-O1A
48	B	303	PEE	O3P-C1-C2-C3
49	j	202	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
51	o	201	CDL	OA5-CA3-CA4-CA6
51	r	504	CDL	OB5-CB3-CB4-CB6
51	i	401	CDL	C59-C60-C61-C62
46	A	502	FMN	C1'-C2'-C3'-O3'
48	l	705	PEE	C5-C4-O4P-P
48	r	501	PEE	C5-C4-O4P-P
49	J	403	PLX	C25-C24-O8-C5
56	Q	501	970	C01-C02-C04-C05
56	Q	501	970	C01-C02-C04-O08
51	m	201	CDL	CB7-C71-C72-C73
51	l	702	CDL	CA7-C31-C32-C33
51	u	201	CDL	C73-C74-C75-C76
51	V	201	CDL	C57-C58-C59-C60
49	J	403	PLX	O4-C3-C4-O6
49	r	503	PLX	O4-C3-C4-O6
48	r	501	PEE	C12-C13-C14-C15
51	V	201	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C54-C55-C56-C57
49	r	502	PLX	N1-C1-C2-O1
50	X	201	8Q1	O27-C28-C29-C32
51	l	702	CDL	CB3-CB4-CB6-OB8
49	r	502	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
51	r	504	CDL	OB6-CB4-CB6-OB8
51	m	201	CDL	C37-C38-C39-C40
48	C	302	PEE	O5-C30-O3-C3
48	j	201	PEE	C21-C22-C23-C24
51	i	401	CDL	C12-C13-C14-C15
51	u	201	CDL	C1-CB2-OB2-PB2
51	o	201	CDL	C55-C56-C57-C58
49	g	201	PLX	O8-C24-C25-C26
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	C30-C31-C32-C33
51	k	101	CDL	C16-C17-C18-C19
51	r	504	CDL	C34-C35-C36-C37
49	g	201	PLX	C33-C34-C35-C36
51	o	201	CDL	C16-C17-C18-C19
49	a	202	PLX	C28-C29-C30-C31
53	J	402	UQ	C4-C3-O3-CM3
49	j	202	PLX	C9-C10-C11-C12
51	r	504	CDL	C79-C80-C81-C82
48	U	101	PEE	C43-C44-C45-C46
51	l	701	CDL	C36-C37-C38-C39
49	r	503	PLX	C18-C19-C20-C21
51	k	101	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C19-C20-C21-C22
51	k	101	CDL	C53-C54-C55-C56
51	l	701	CDL	C84-C85-C86-C87
48	l	705	PEE	C2-C1-O3P-P
51	V	201	CDL	OA5-CA3-CA4-OA6
48	r	501	PEE	C37-C38-C39-C40
47	A	503	NAI	O4D-C1D-N1N-C2N
51	a	201	CDL	C53-C54-C55-C56
48	l	703	PEE	O2-C2-C3-O3
48	l	705	PEE	O2-C2-C3-O3
51	a	201	CDL	OA6-CA4-CA6-OA8
51	m	201	CDL	OB6-CB4-CB6-OB8
48	U	101	PEE	C1-O3P-P-O4P
48	U	101	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
48	l	705	PEE	C4-O4P-P-O3P
49	C	303	PLX	C2-O1-P1-O4
51	I	201	CDL	CB2-OB2-PB2-OB5
51	l	701	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CA2-OA2-PA1-OA5
51	m	201	CDL	CA3-OA5-PA1-OA2
51	m	201	CDL	CB3-OB5-PB2-OB2
51	u	201	CDL	CB2-OB2-PB2-OB5
47	A	503	NAI	C2D-C1D-N1N-C2N
51	V	201	CDL	C38-C39-C40-C41
51	a	201	CDL	C40-C41-C42-C43
49	J	403	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
51	I	201	CDL	CA3-CA4-CA6-OA8
51	i	401	CDL	C36-C37-C38-C39
49	C	303	PLX	C14-C15-C16-C17
52	J	401	NDP	PN-O3-PA-O2A
51	l	701	CDL	C58-C59-C60-C61
48	l	704	PEE	C2-C1-O3P-P
48	U	101	PEE	C20-C21-C22-C23
51	r	504	CDL	C54-C55-C56-C57
51	a	201	CDL	CA7-C31-C32-C33
48	U	101	PEE	C16-C17-C18-C19
48	r	501	PEE	C36-C37-C38-C39
49	C	303	PLX	C27-C28-C29-C30
49	j	202	PLX	C28-C29-C30-C31
48	C	302	PEE	C15-C16-C17-C18
49	J	403	PLX	C18-C19-C20-C21
51	l	701	CDL	C24-C25-C26-C27
49	r	502	PLX	C31-C32-C33-C34
49	r	503	PLX	C24-C25-C26-C27
52	J	401	NDP	O4D-C1D-N1N-C6N
51	l	701	CDL	C33-C34-C35-C36
51	o	201	CDL	C32-C31-CA7-OA9
51	k	101	CDL	OB9-CB7-OB8-CB6
51	l	701	CDL	C82-C83-C84-C85
50	X	201	8Q1	C10-C11-C12-C13
48	j	201	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
51	a	201	CDL	C33-C34-C35-C36
51	l	702	CDL	C38-C39-C40-C41
51	o	201	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	C33-C34-C35-C36
49	r	503	PLX	C31-C32-C33-C34
49	a	202	PLX	C25-C26-C27-C28
51	k	101	CDL	C32-C33-C34-C35
48	C	302	PEE	C41-C42-C43-C44
48	B	303	PEE	C1-C2-C3-O3
51	V	201	CDL	CB2-C1-CA2-OA2
51	k	101	CDL	CA3-CA4-CA6-OA8
51	m	201	CDL	CB3-CB4-CB6-OB8
51	r	504	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	C38-C39-C40-C41
51	V	201	CDL	O1-C1-CA2-OA2
51	m	201	CDL	C14-C15-C16-C17
48	U	101	PEE	C1-C2-O2-C10
48	l	703	PEE	C21-C22-C23-C24
48	U	101	PEE	C36-C37-C38-C39
51	r	504	CDL	CA2-OA2-PA1-OA5
49	C	303	PLX	C17-C18-C19-C20
51	I	201	CDL	OA5-CA3-CA4-OA6
51	l	701	CDL	OA5-CA3-CA4-OA6
49	a	202	PLX	C24-C25-C26-C27
51	r	504	CDL	C12-C13-C14-C15
51	I	201	CDL	OA5-CA3-CA4-CA6
48	j	201	PEE	C32-C33-C34-C35
51	k	101	CDL	C71-CB7-OB8-CB6
51	r	504	CDL	C42-C43-C44-C45
49	r	503	PLX	C2-C1-N1-C1B
51	l	701	CDL	C74-C75-C76-C77
51	l	701	CDL	C31-C32-C33-C34
51	r	504	CDL	C60-C61-C62-C63
49	g	201	PLX	O6-C4-C5-O8
48	U	101	PEE	C33-C34-C35-C36
49	g	201	PLX	C35-C36-C37-C38
49	j	202	PLX	C15-C16-C17-C18
51	u	201	CDL	C55-C56-C57-C58
48	B	303	PEE	C42-C43-C44-C45
48	W	201	PEE	C23-C24-C25-C26
48	U	101	PEE	C40-C41-C42-C43
48	l	705	PEE	C38-C39-C40-C41
49	a	202	PLX	C6-C7-C8-C9
49	r	503	PLX	C19-C20-C21-C22
49	r	503	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C17-C18-C19-C20
51	a	201	CDL	C56-C57-C58-C59
51	m	201	CDL	C75-C76-C77-C78
48	B	303	PEE	C2-C1-O3P-P
51	I	201	CDL	O1-C1-CB2-OB2
51	r	504	CDL	C76-C77-C78-C79
48	B	303	PEE	C11-C12-C13-C14
48	W	201	PEE	C16-C17-C18-C19
48	l	704	PEE	C1-C2-C3-O3
48	j	201	PEE	C18-C19-C20-C21
49	g	201	PLX	O4-C3-C4-O6
51	m	201	CDL	C78-C79-C80-C81
51	l	702	CDL	C40-C41-C42-C43
49	a	202	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
48	l	704	PEE	C11-C12-C13-C14
48	r	501	PEE	O3P-C1-C2-C3
46	A	502	FMN	O2'-C2'-C3'-C4'
51	I	201	CDL	OA6-CA4-CA6-OA8
51	V	201	CDL	OA6-CA4-CA6-OA8
51	a	201	CDL	OB6-CB4-CB6-OB8
51	l	701	CDL	C20-C21-C22-C23
51	o	201	CDL	C78-C79-C80-C81
51	l	702	CDL	C31-CA7-OA8-CA6
48	C	302	PEE	C18-C19-C20-C21
50	X	201	8Q1	O33-C32-C34-N36
52	J	401	NDP	C2B-O2B-P2B-O1X
48	U	101	PEE	O2-C10-C11-C12
51	I	201	CDL	C52-C51-CB5-OB6
51	l	702	CDL	C53-C54-C55-C56
50	X	201	8Q1	O27-C28-C29-C31
47	A	503	NAI	C2D-C1D-N1N-C6N
49	r	503	PLX	C2-C1-N1-C1C
49	r	503	PLX	C2-C1-N1-C1A
51	i	401	CDL	C39-C40-C41-C42
51	l	701	CDL	C80-C81-C82-C83
51	o	201	CDL	C40-C41-C42-C43
51	l	702	CDL	OA9-CA7-OA8-CA6
48	r	501	PEE	O2-C10-C11-C12
48	l	704	PEE	C36-C37-C38-C39
48	l	704	PEE	C38-C39-C40-C41
49	r	503	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C71-C72-C73-C74
51	u	201	CDL	C57-C58-C59-C60
51	V	201	CDL	C32-C31-CA7-OA8
51	o	201	CDL	C21-C22-C23-C24
53	J	402	UQ	C13-C14-C16-C17
51	i	401	CDL	CA3-CA4-CA6-OA8
51	o	201	CDL	C15-C16-C17-C18
48	W	201	PEE	C33-C34-C35-C36
51	a	201	CDL	C64-C65-C66-C67
51	m	201	CDL	C36-C37-C38-C39
58	w	401	ADP	PA-O3A-PB-O2B
58	w	401	ADP	PA-O3A-PB-O3B
53	s	401	UQ	C12-C13-C14-C16
51	l	702	CDL	C12-C11-CA5-OA6
49	j	202	PLX	O6-C4-C5-O8
51	i	401	CDL	OA6-CA4-CA6-OA8
49	r	503	PLX	C6-C7-C8-C9
48	B	303	PEE	C16-C17-C18-C19
49	a	202	PLX	C14-C15-C16-C17
51	o	201	CDL	C81-C82-C83-C84
51	a	201	CDL	C32-C31-CA7-OA8
49	C	303	PLX	O7-C6-C7-C8
52	J	401	NDP	C2B-O2B-P2B-O3X
51	m	201	CDL	C12-C11-CA5-OA6
51	m	201	CDL	C74-C75-C76-C77
51	l	702	CDL	C13-C14-C15-C16
48	B	303	PEE	C18-C19-C20-C21
48	l	703	PEE	C22-C23-C24-C25
51	i	401	CDL	C18-C19-C20-C21
53	J	402	UQ	C2-C3-O3-CM3
52	J	401	NDP	O4B-C4B-C5B-O5B
51	I	201	CDL	C72-C71-CB7-OB8
51	V	201	CDL	C41-C42-C43-C44
51	i	401	CDL	C51-C52-C53-C54
51	i	401	CDL	C53-C54-C55-C56
51	l	702	CDL	C78-C79-C80-C81
48	l	704	PEE	C18-C19-C20-C21
48	r	501	PEE	C31-C32-C33-C34
51	k	101	CDL	C32-C31-CA7-OA8
49	g	201	PLX	O6-C6-C7-C8
51	I	201	CDL	C52-C51-CB5-OB7
48	l	703	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C13-C14-C15-C16
48	j	201	PEE	C1-C2-C3-O3
49	j	202	PLX	C3-C4-C5-O8
51	V	201	CDL	CA3-CA4-CA6-OA8
48	l	704	PEE	C40-C41-C42-C43
49	g	201	PLX	C15-C16-C17-C18
49	g	201	PLX	C11-C12-C13-C14
50	X	201	8Q1	C11-C12-C13-C14
48	r	501	PEE	O4-C10-C11-C12
51	i	401	CDL	C52-C51-CB5-OB6
49	a	202	PLX	C4-C3-O4-P1
49	a	202	PLX	C17-C18-C19-C20
48	U	101	PEE	O4-C10-C11-C12
51	I	201	CDL	C72-C71-CB7-OB9
48	W	201	PEE	C18-C19-C20-C21
48	B	303	PEE	C4-O4P-P-O1P
48	U	101	PEE	C1-O3P-P-O1P
48	l	705	PEE	C4-O4P-P-O1P
49	a	202	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C2-O1-P1-O3
51	k	101	CDL	CB3-OB5-PB2-OB4
51	l	701	CDL	CB2-OB2-PB2-OB3
51	m	201	CDL	CB3-OB5-PB2-OB3
51	o	201	CDL	CB2-OB2-PB2-OB4
51	u	201	CDL	CB2-OB2-PB2-OB3
51	u	201	CDL	CB3-OB5-PB2-OB4
51	r	504	CDL	C72-C71-CB7-OB8
50	X	201	8Q1	C6-C7-C8-C9
51	l	701	CDL	C72-C73-C74-C75
48	l	703	PEE	C19-C20-C21-C22
50	X	201	8Q1	C9-C10-C11-C12
48	B	303	PEE	C12-C13-C14-C15
51	a	201	CDL	C12-C11-CA5-OA6
51	m	201	CDL	C12-C11-CA5-OA7
51	a	201	CDL	C58-C59-C60-C61
47	A	503	NAI	O4D-C1D-N1N-C6N
49	j	202	PLX	C25-C24-O8-C5
51	a	201	CDL	C21-C22-C23-C24
48	j	201	PEE	O3-C30-C31-C32
51	k	101	CDL	C21-C22-C23-C24
51	r	504	CDL	C19-C20-C21-C22

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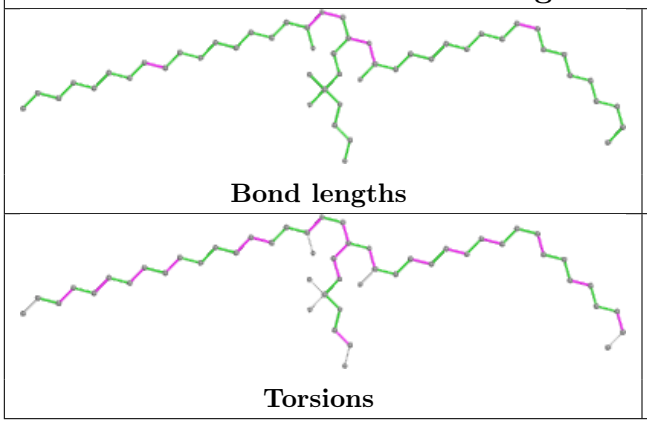
Mol	Chain	Res	Type	Atoms
48	U	101	PEE	O3-C30-C31-C32
51	l	702	CDL	CA2-C1-CB2-OB2
51	a	201	CDL	C32-C31-CA7-OA9
48	U	101	PEE	O3P-C1-C2-O2
53	s	401	UQ	C13-C14-C16-C17
51	k	101	CDL	C32-C31-CA7-OA9
48	B	303	PEE	C20-C21-C22-C23
51	a	201	CDL	C31-C32-C33-C34
51	k	101	CDL	C12-C11-CA5-OA6
56	Q	501	970	C19-C20-O26-C27
48	C	302	PEE	C36-C37-C38-C39

There are no ring outliers.

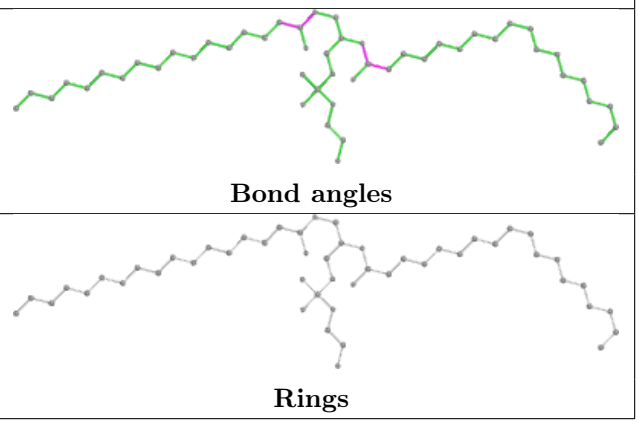
No monomer is involved in short contacts.

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 PEE l 704



Bond lengths

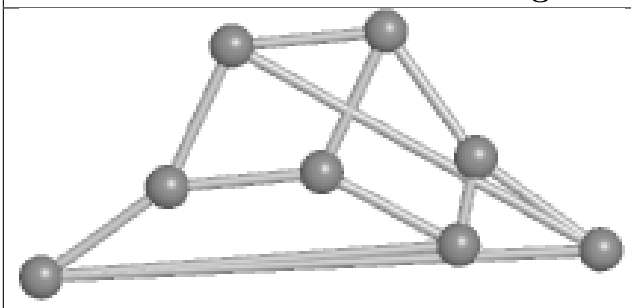


Bond angles

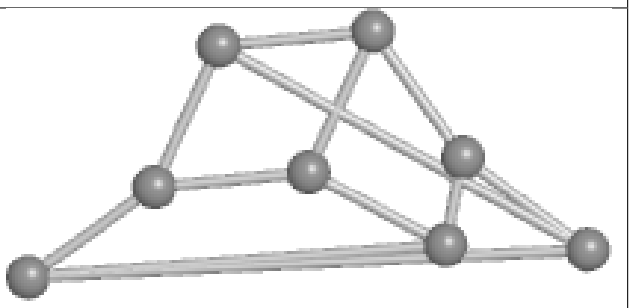
Torsions

Rings

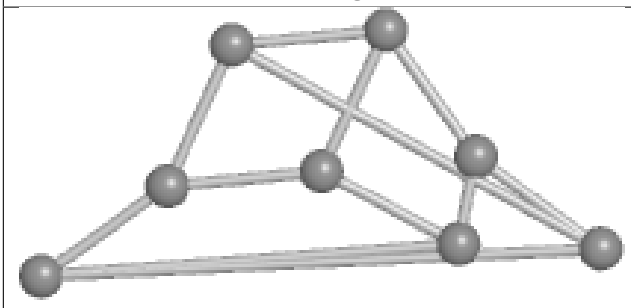
Ligand SF4 B 302



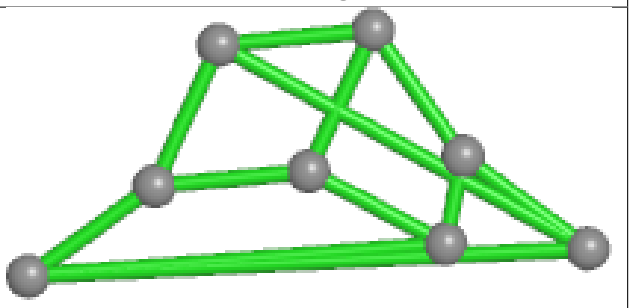
Bond lengths



Bond angles

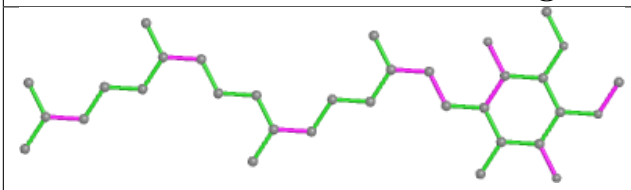


Torsions

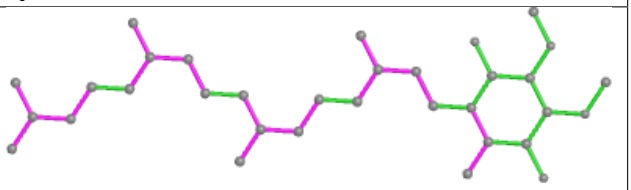


Rings

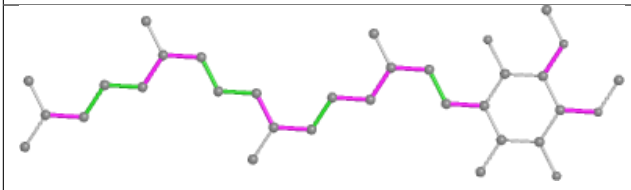
Ligand UQ J 402



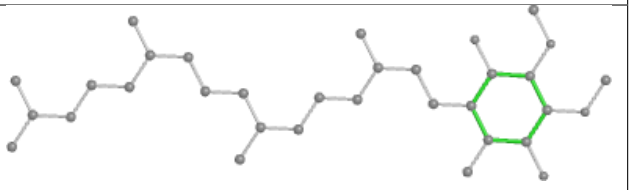
Bond lengths



Bond angles

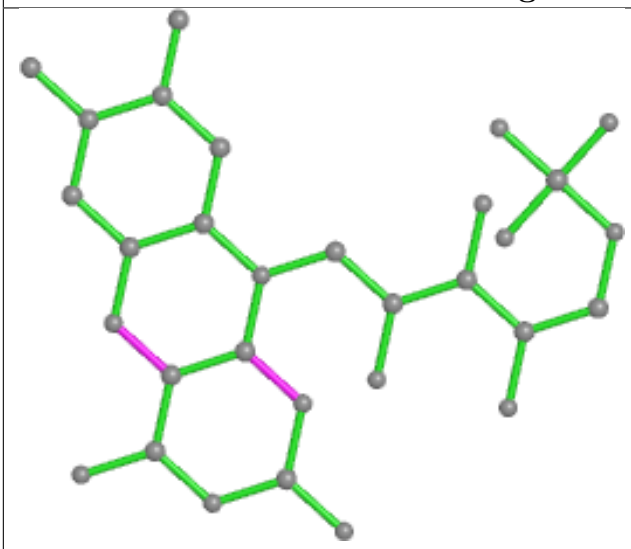


Torsions

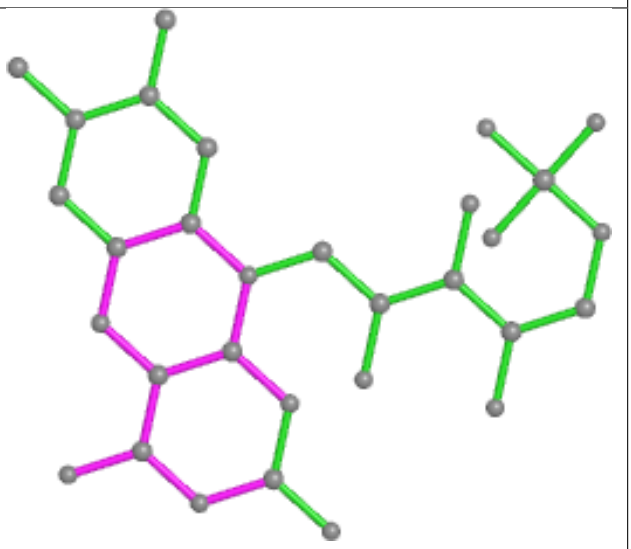


Rings

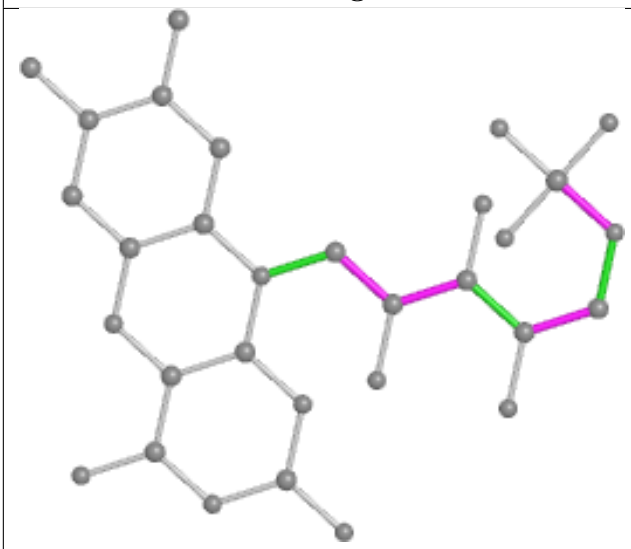
Ligand FMN A 502



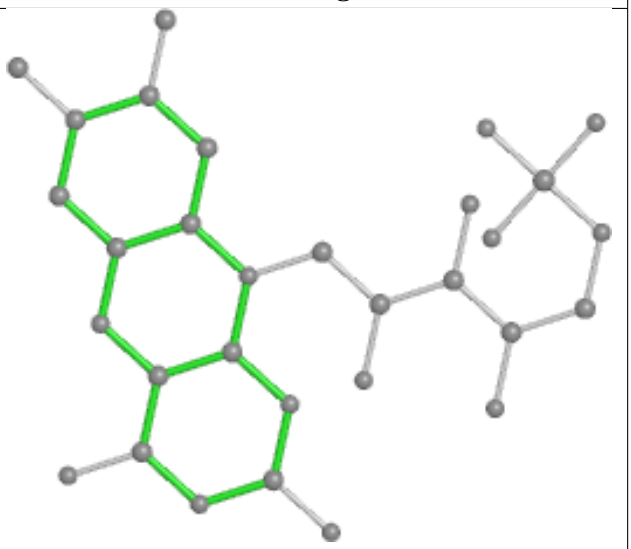
Bond lengths



Bond angles

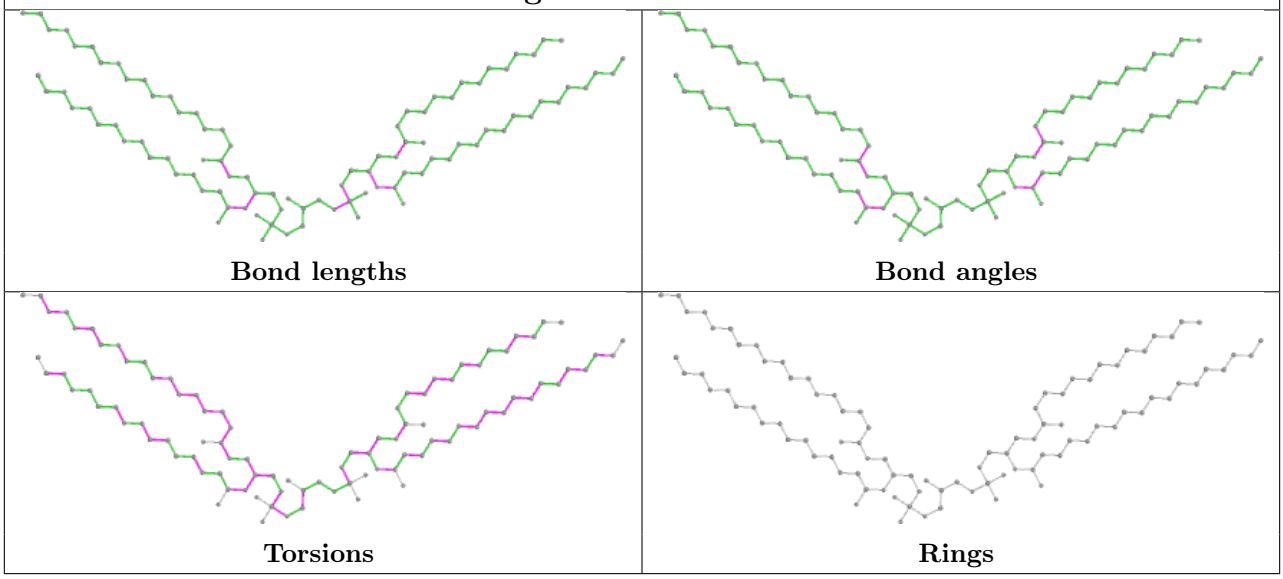


Torsions

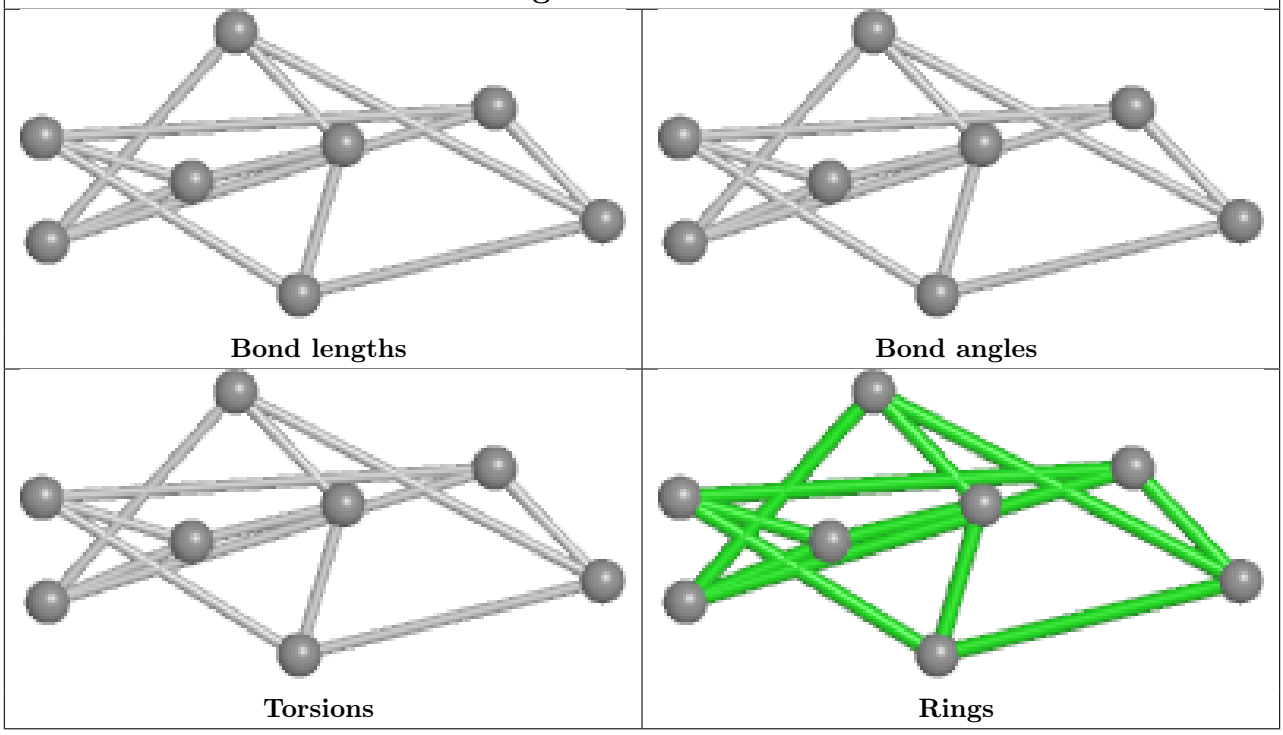


Rings

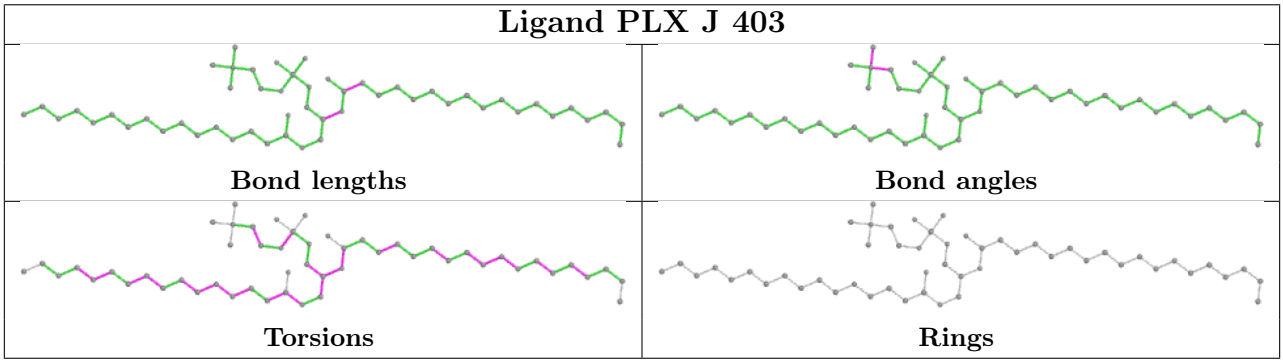
Ligand CDL V 201



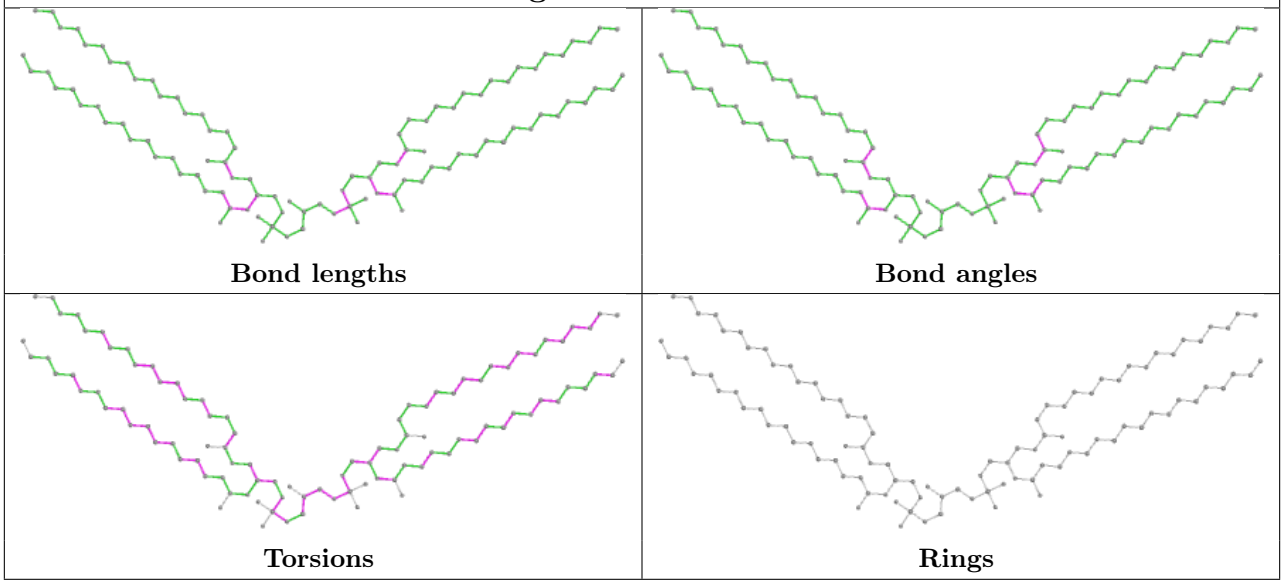
Ligand SF4 B 301



Ligand PLX J 403



Ligand CDL o 201



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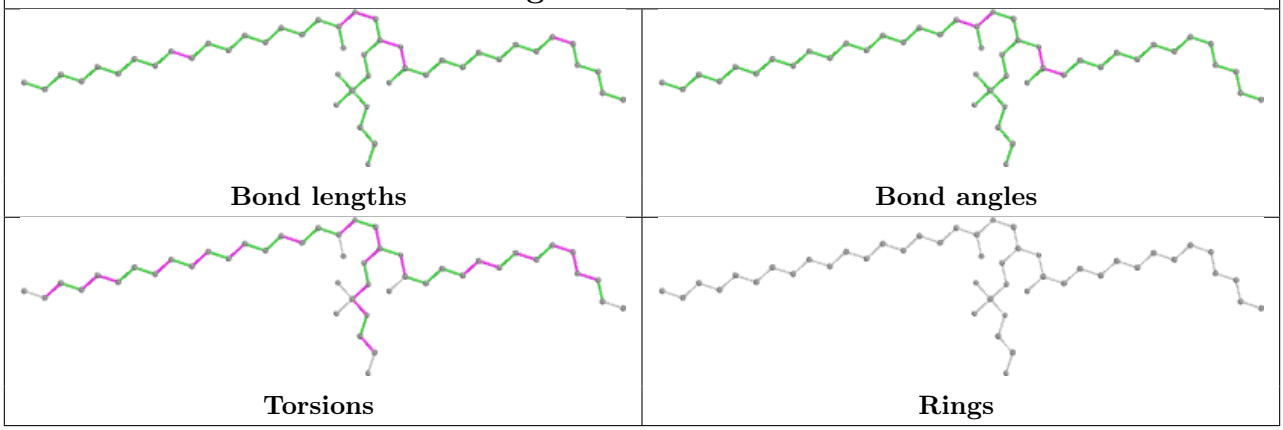
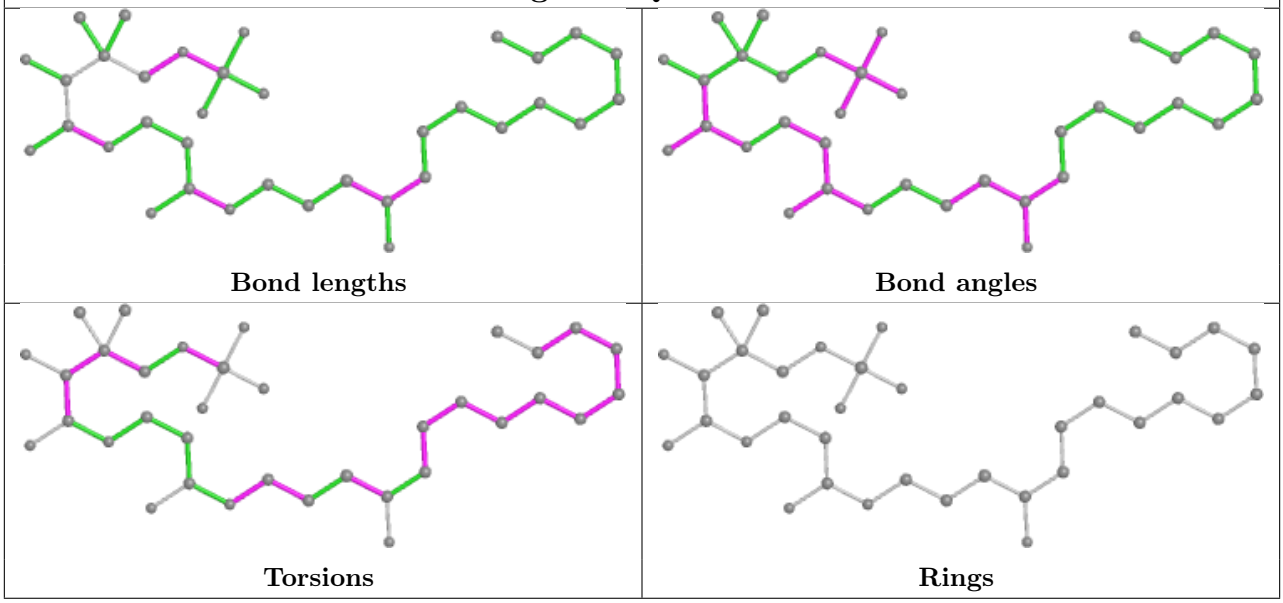


Ligand 8Q1 X 201



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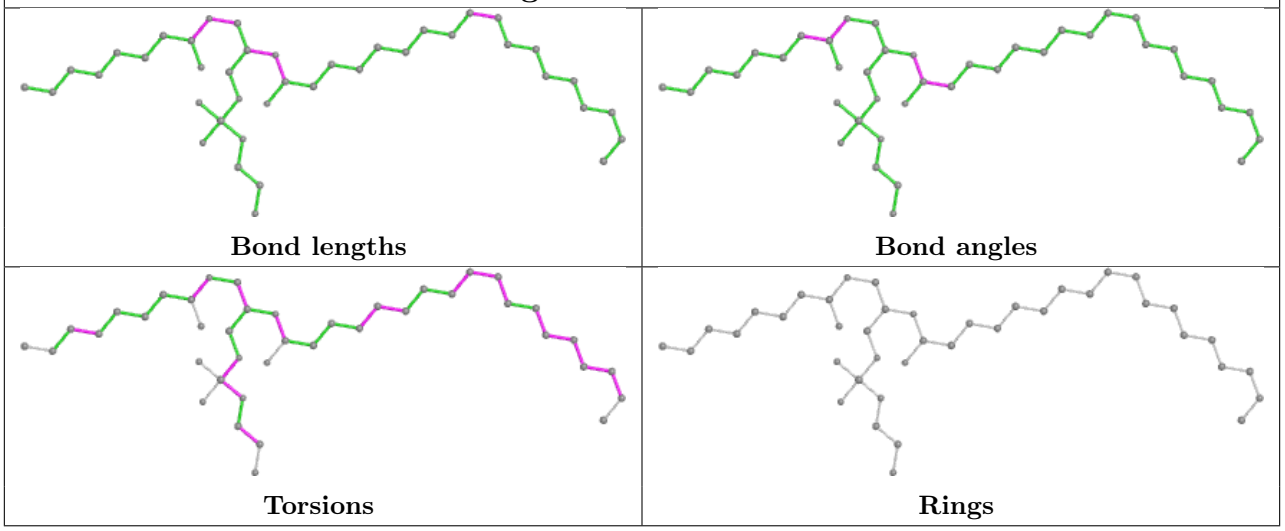

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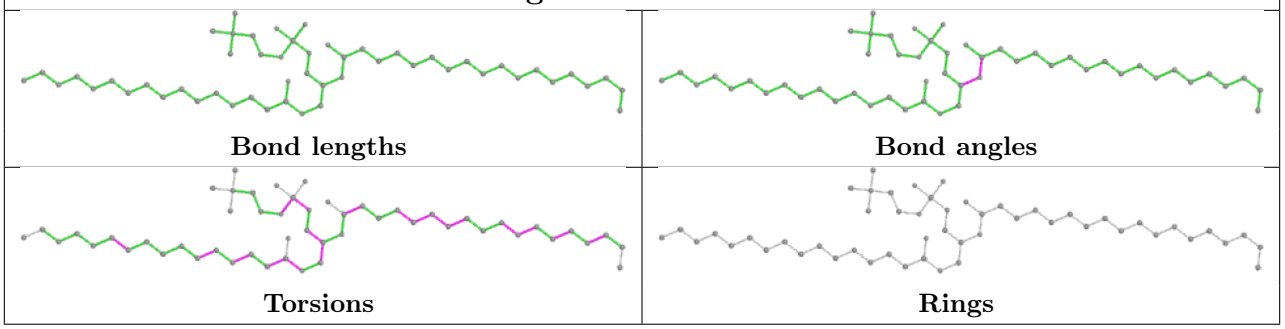
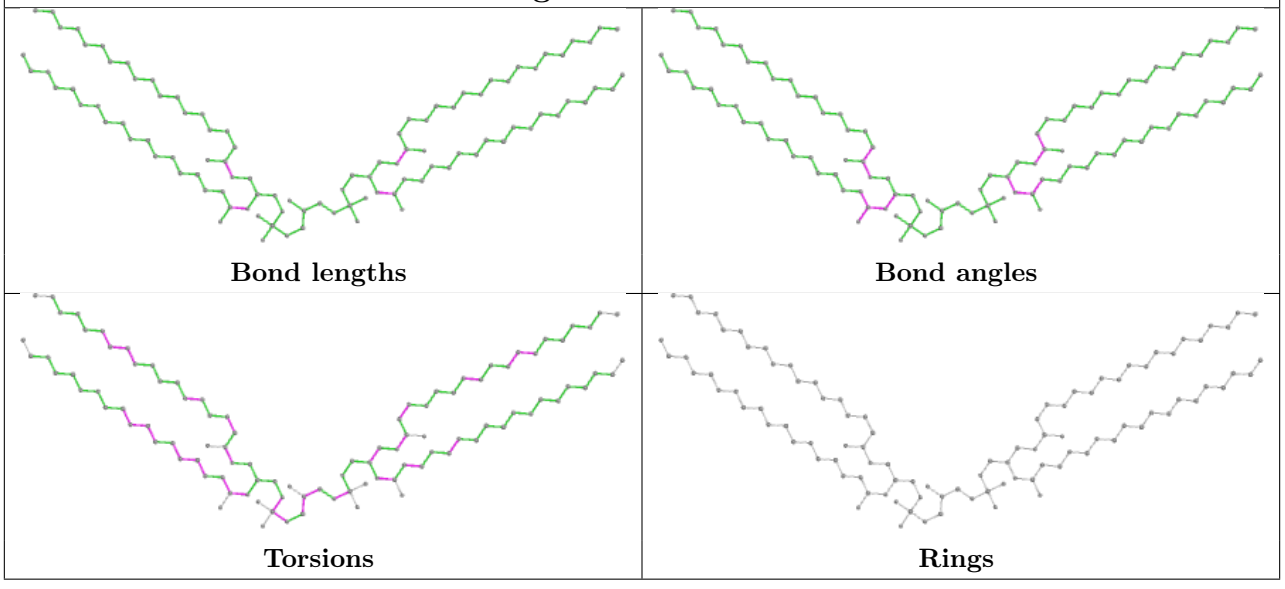
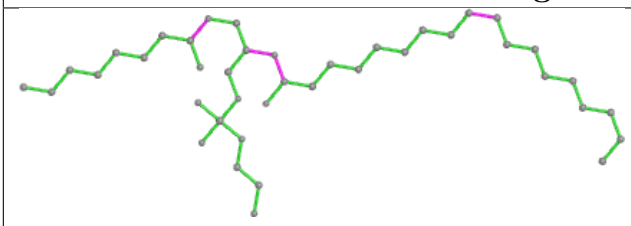


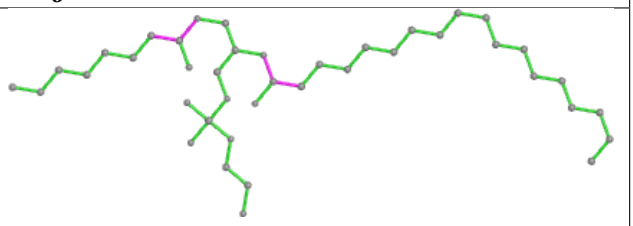
Ligand CDL l 702



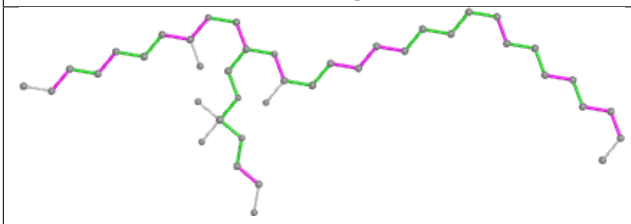
Ligand PEE j 201



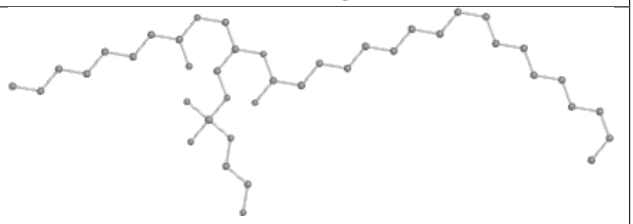
Bond lengths



Bond angles

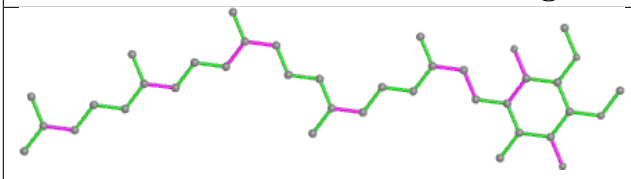


Torsions

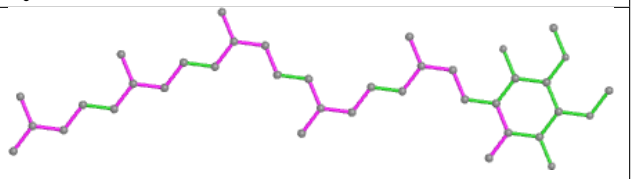


Rings

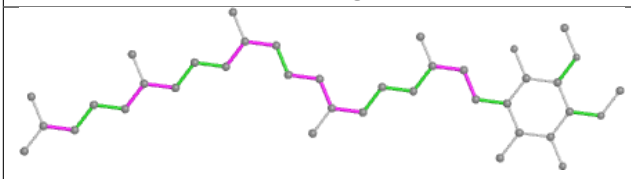
Ligand UQ s 401



Bond lengths



Bond angles



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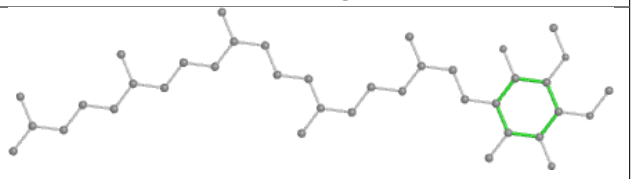
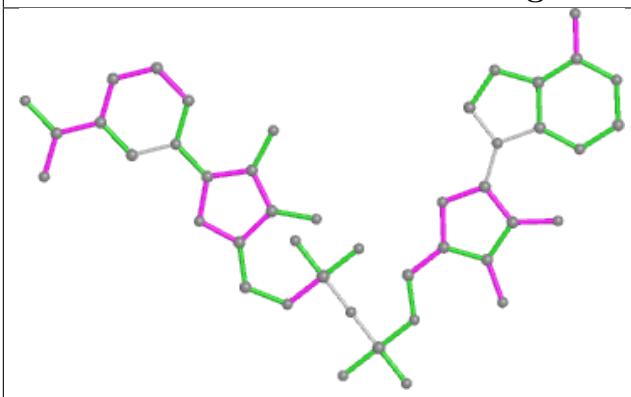
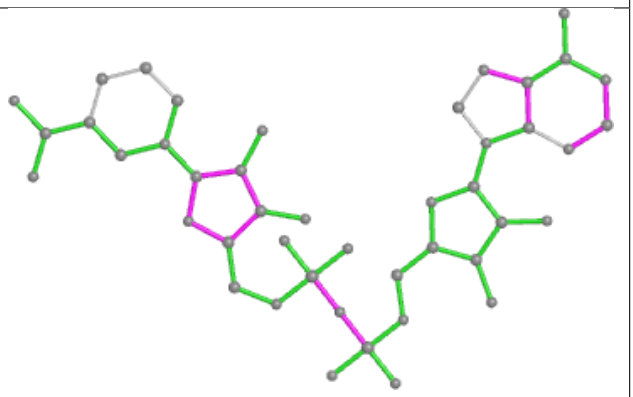


Rings

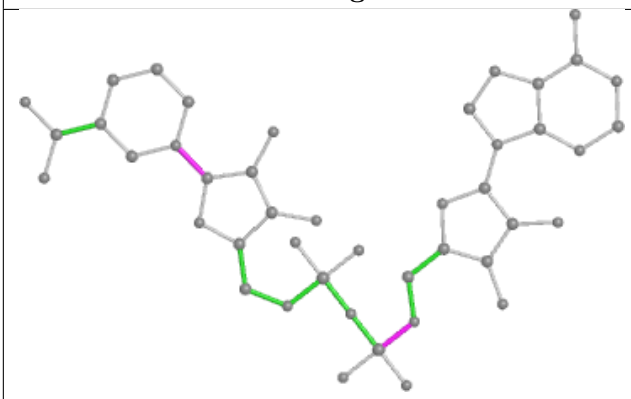
Ligand NAI A 503



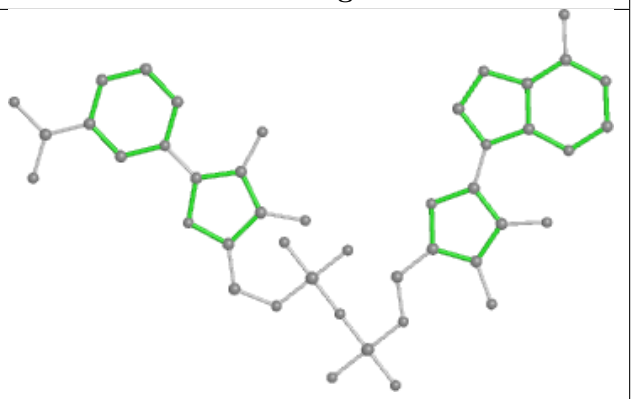
Bond lengths



Bond angles

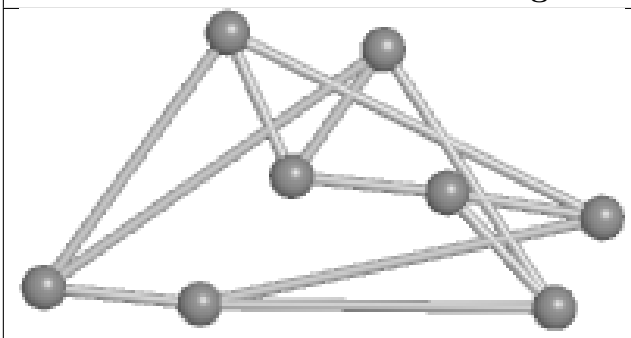


Torsions

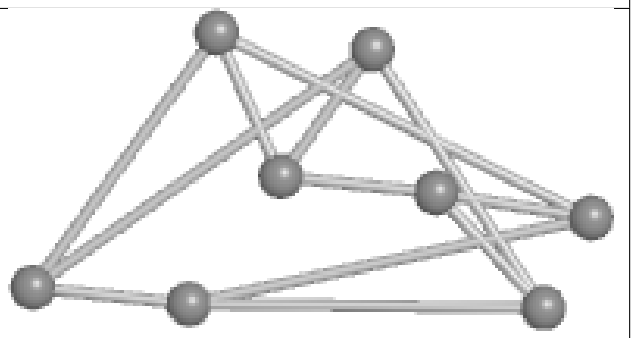


Rings

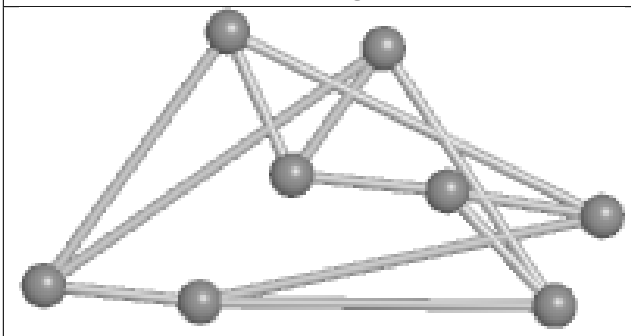
Ligand SF4 A 501



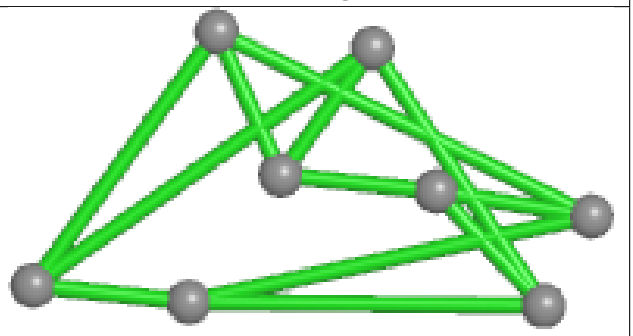
Bond lengths



Bond angles

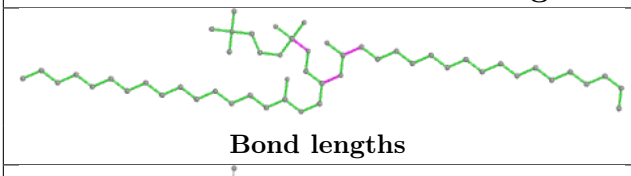


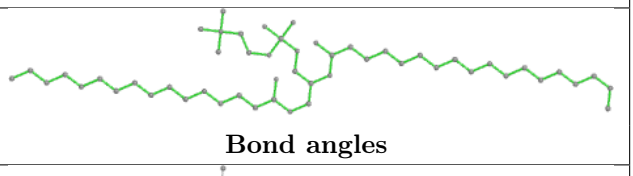
Torsions

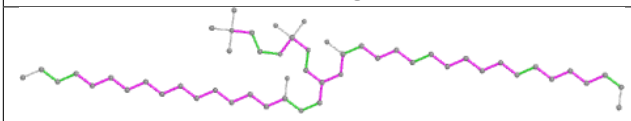


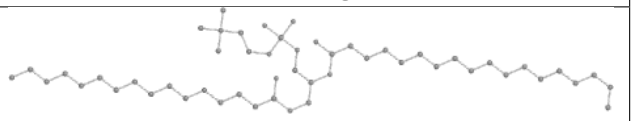
Rings

Ligand PLX r 503

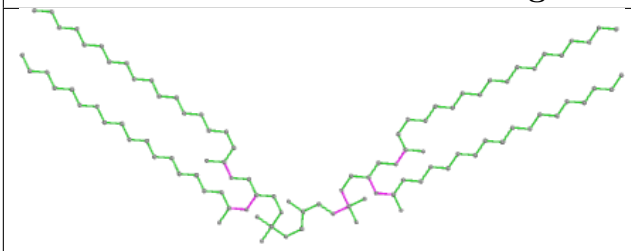

Bond lengths


Bond angles


Torsions


Rings

Ligand CDL a 201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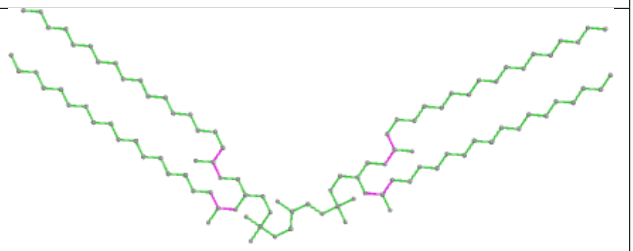
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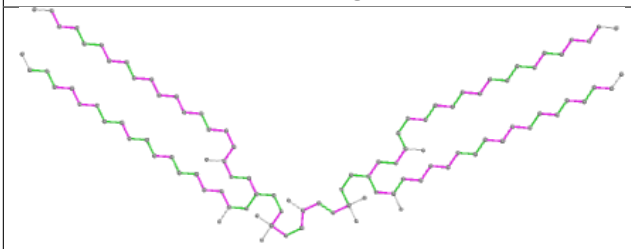
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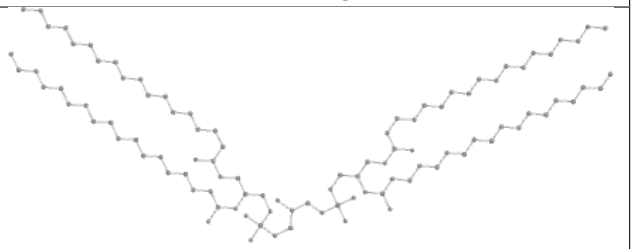
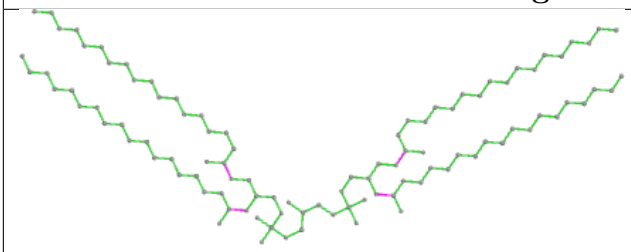

Rings

Ligand CDL i 401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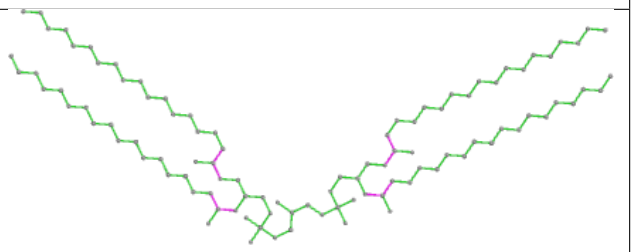
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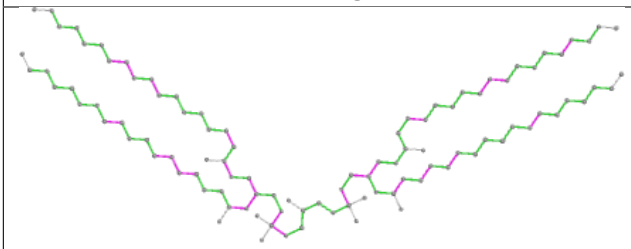
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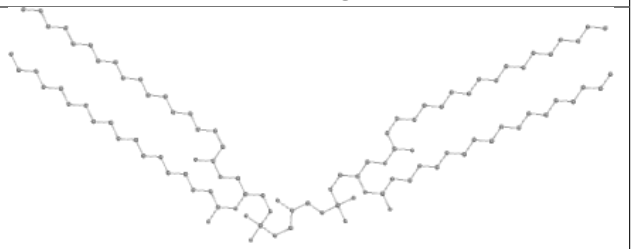
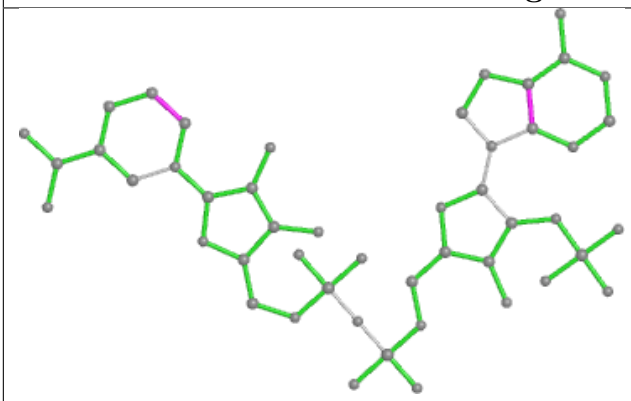

Rings

Ligand NDP J 401



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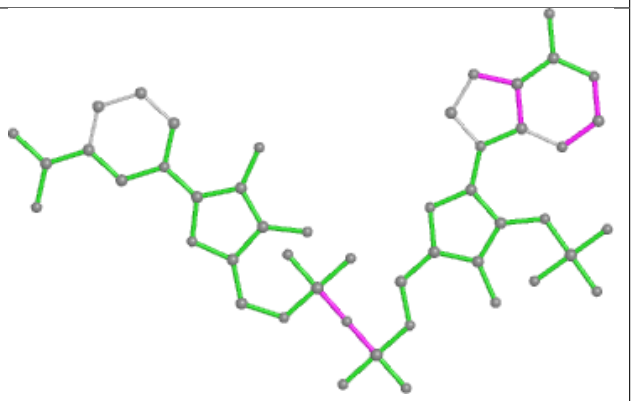

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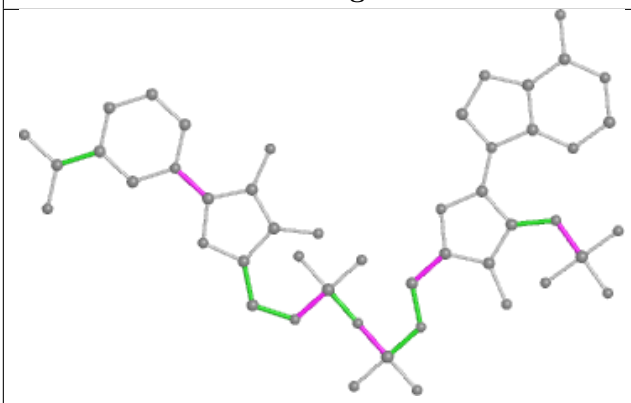

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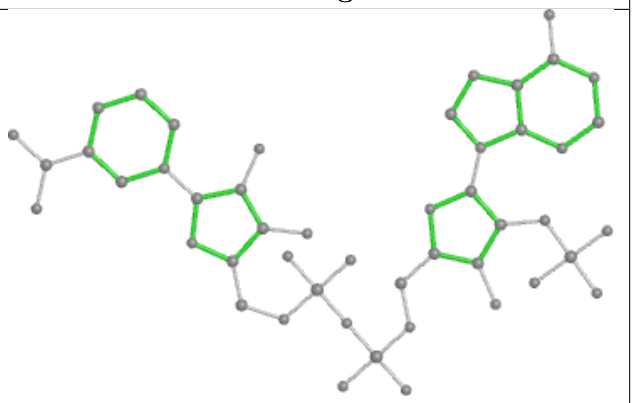
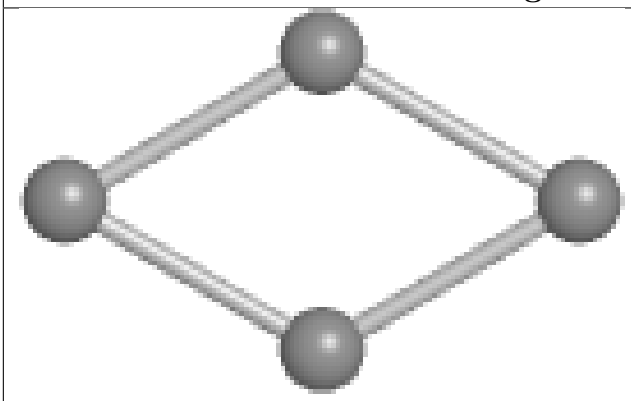


Rings

Ligand FES M 803



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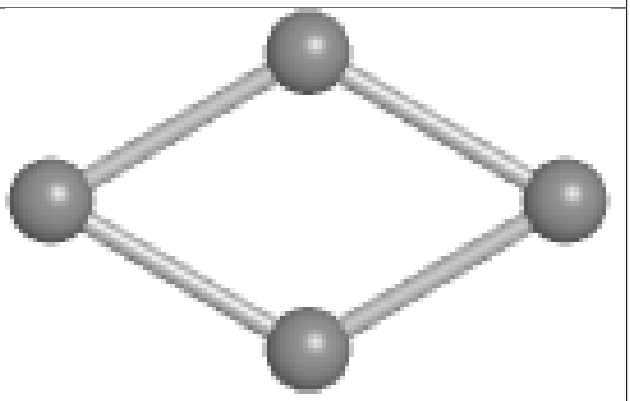

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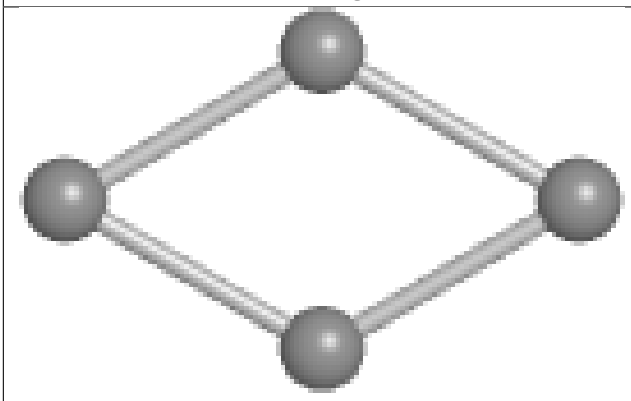

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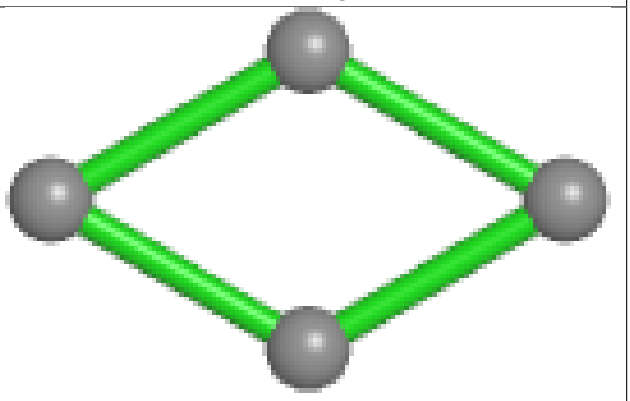
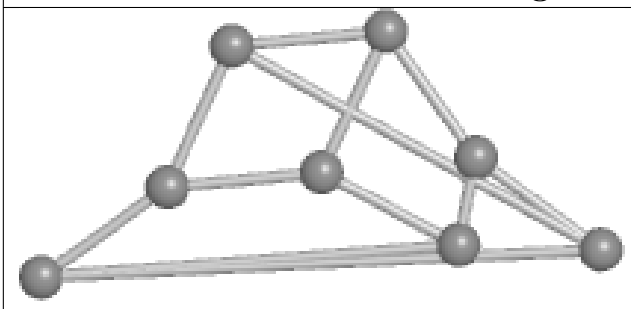


Rings

Ligand SF4 C 301



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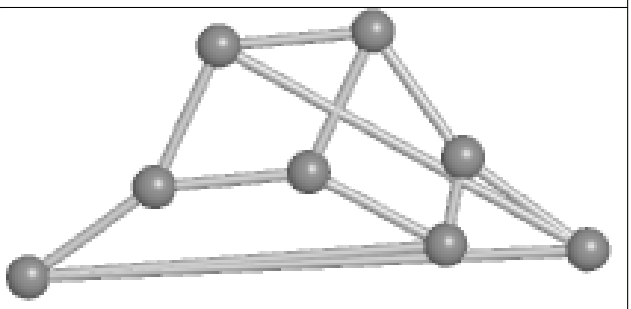

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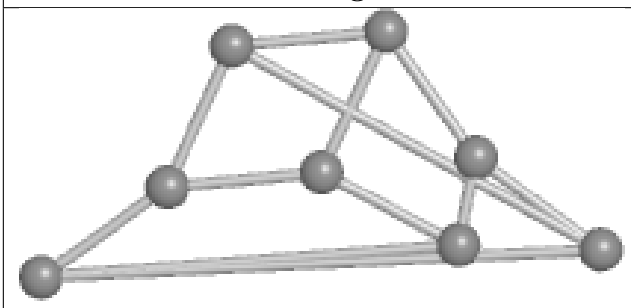

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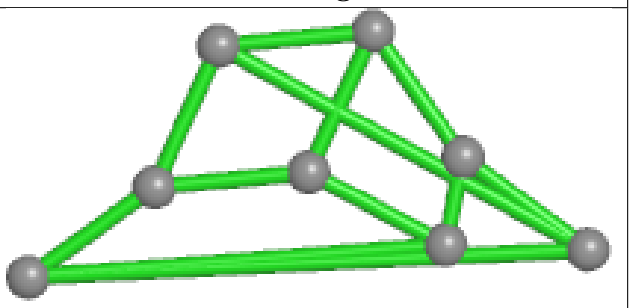
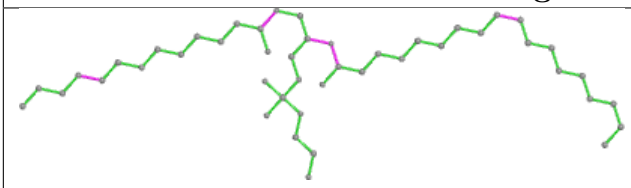


Rings

Ligand PEE l 705



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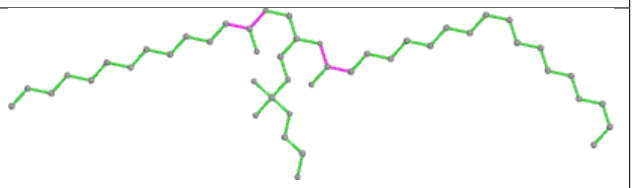

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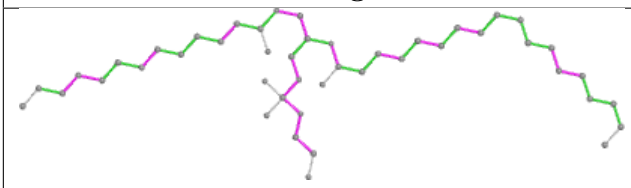

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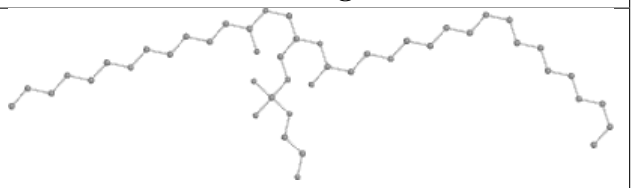
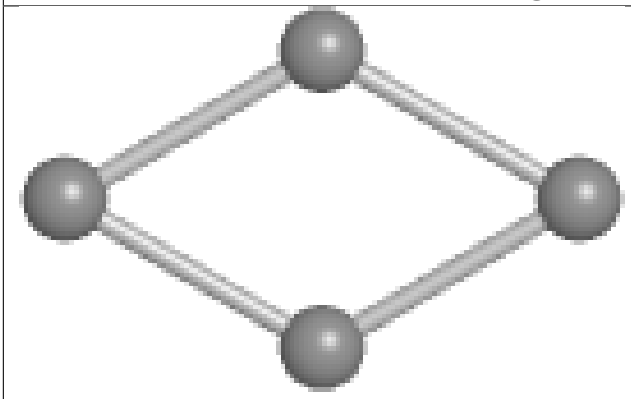


Rings

Ligand FES O 301



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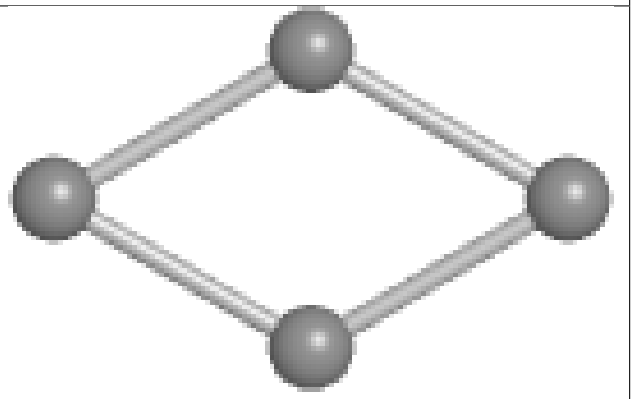

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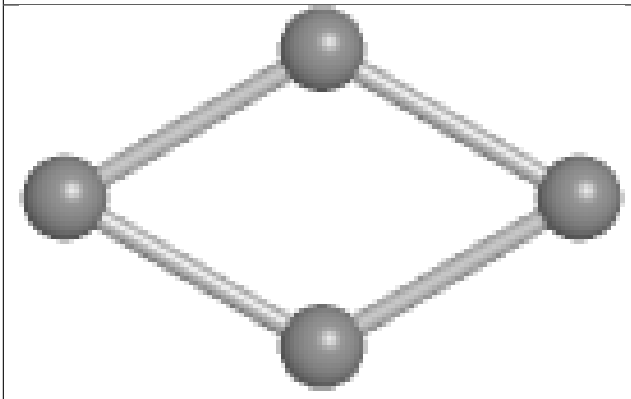

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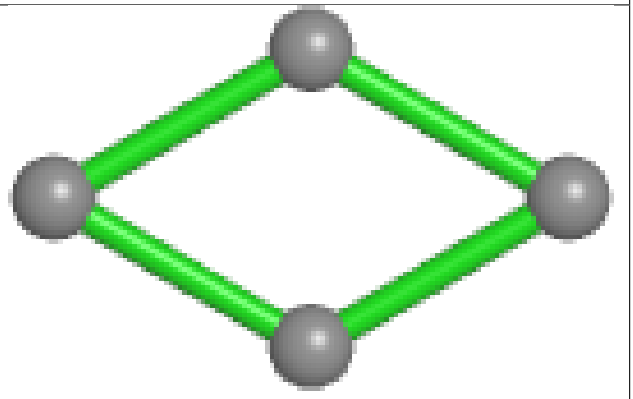
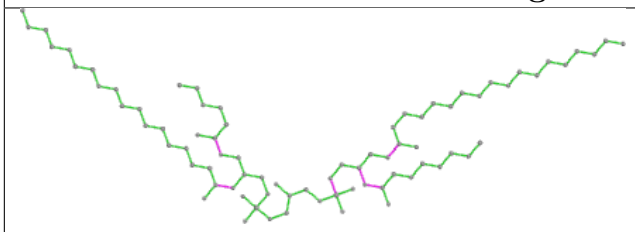


Rings

Ligand CDL k 101



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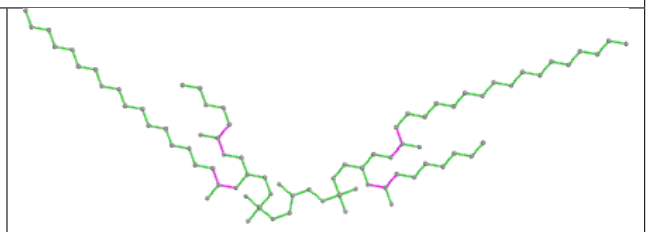

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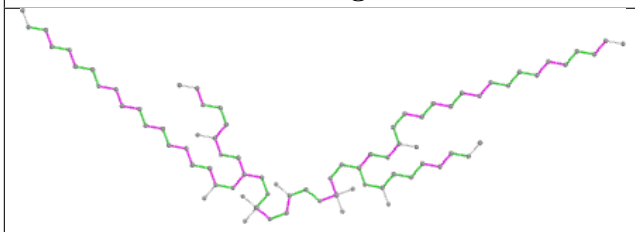

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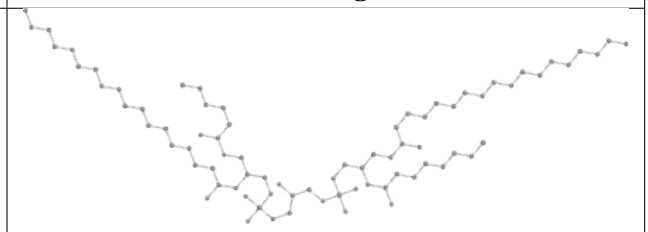
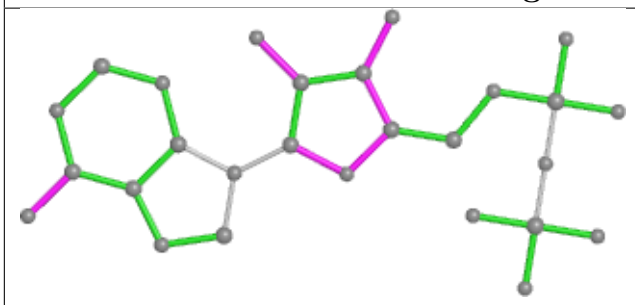


Rings

Ligand ADP w 401



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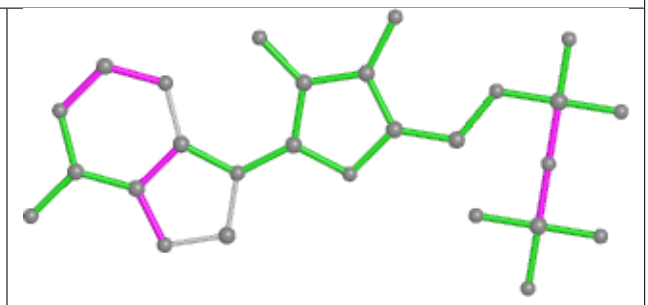
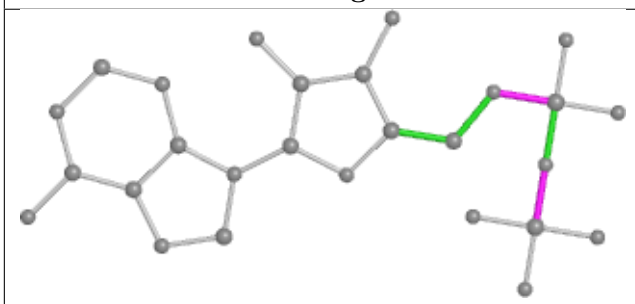


Bond angles



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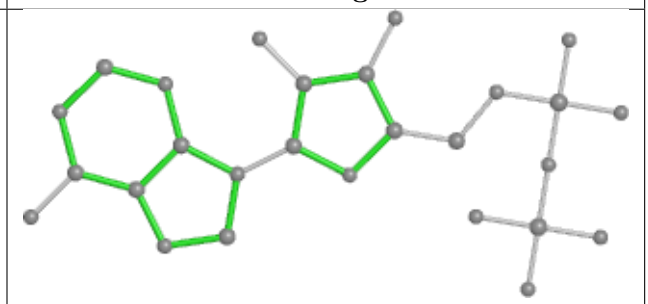

Rings

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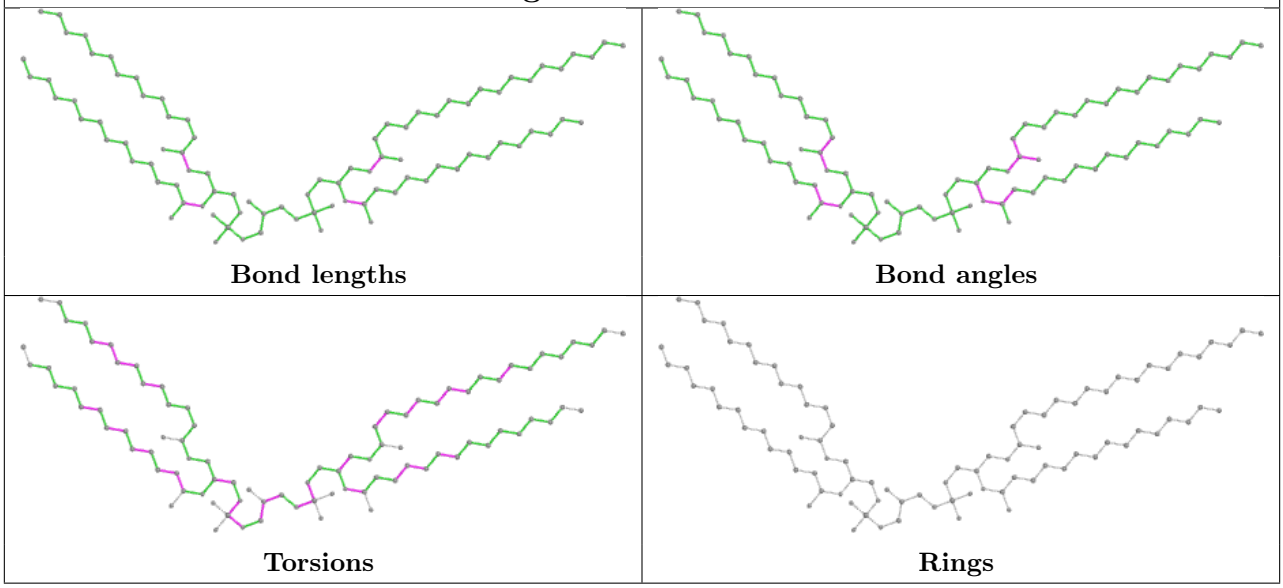
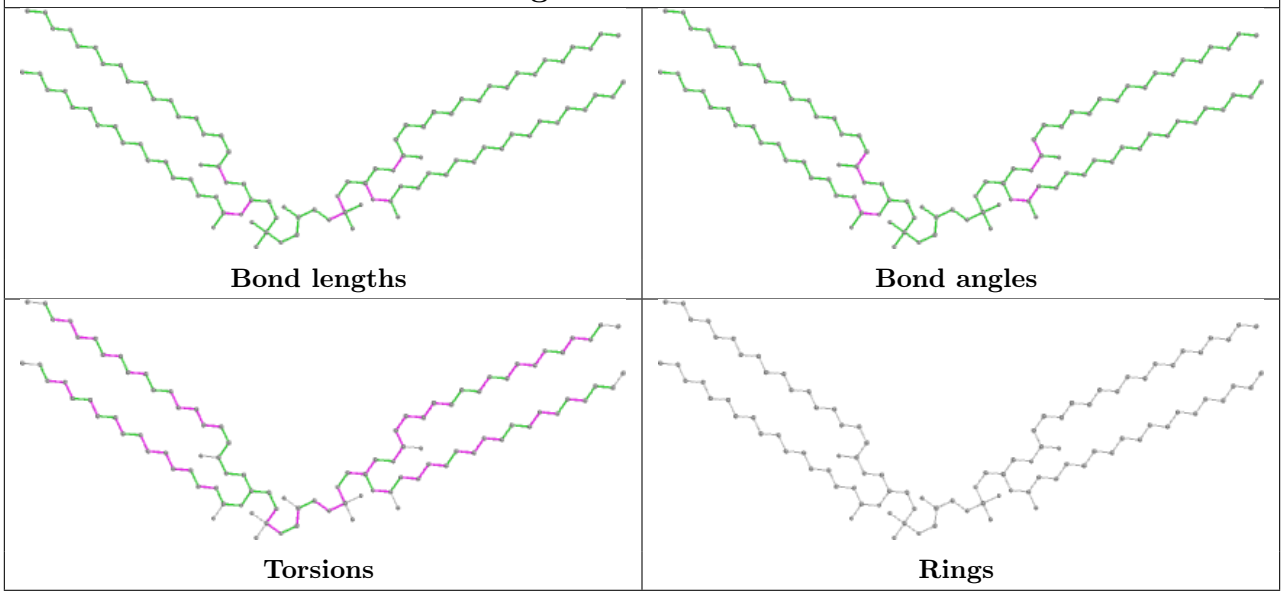
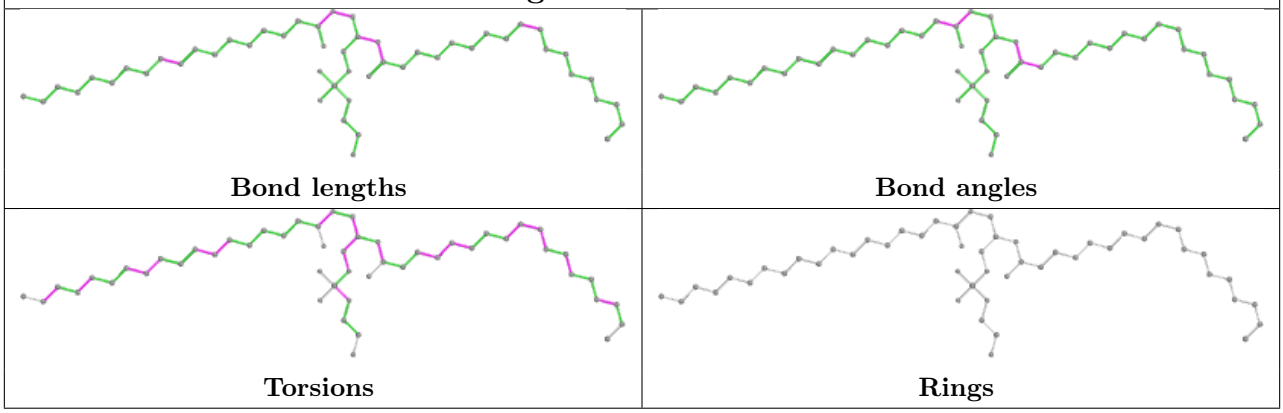


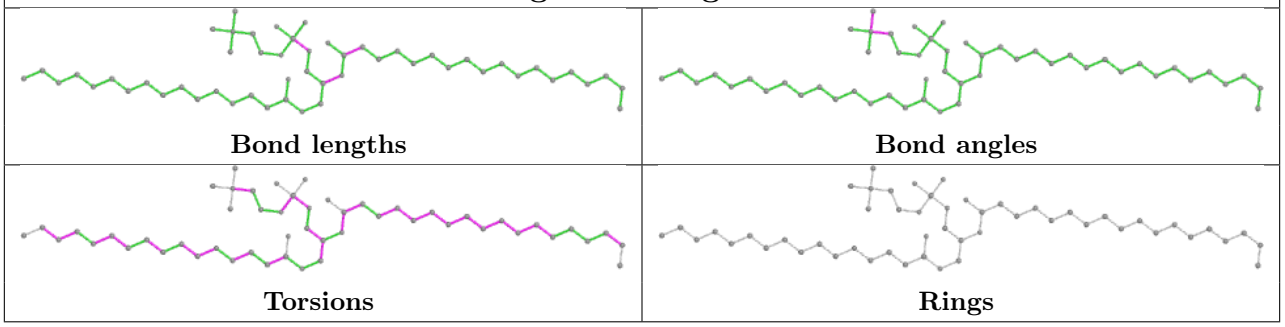
Ligand CDL r 504



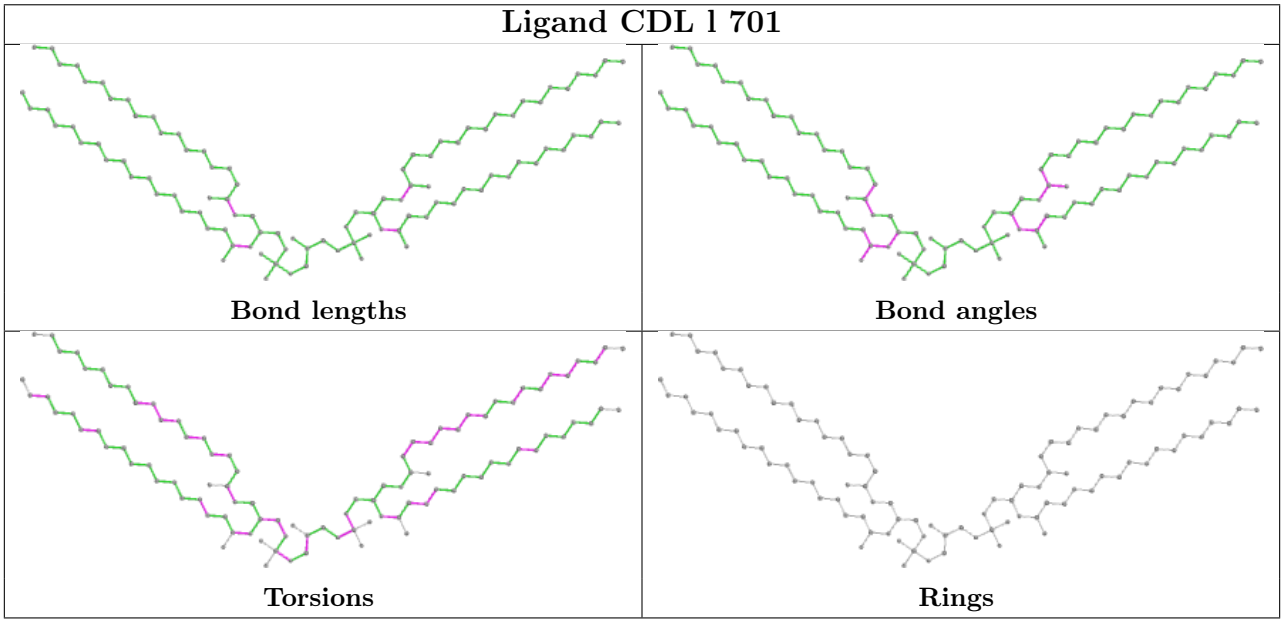
Ligand PEE B 303



Ligand PLX g 201



Ligand CDL l 701



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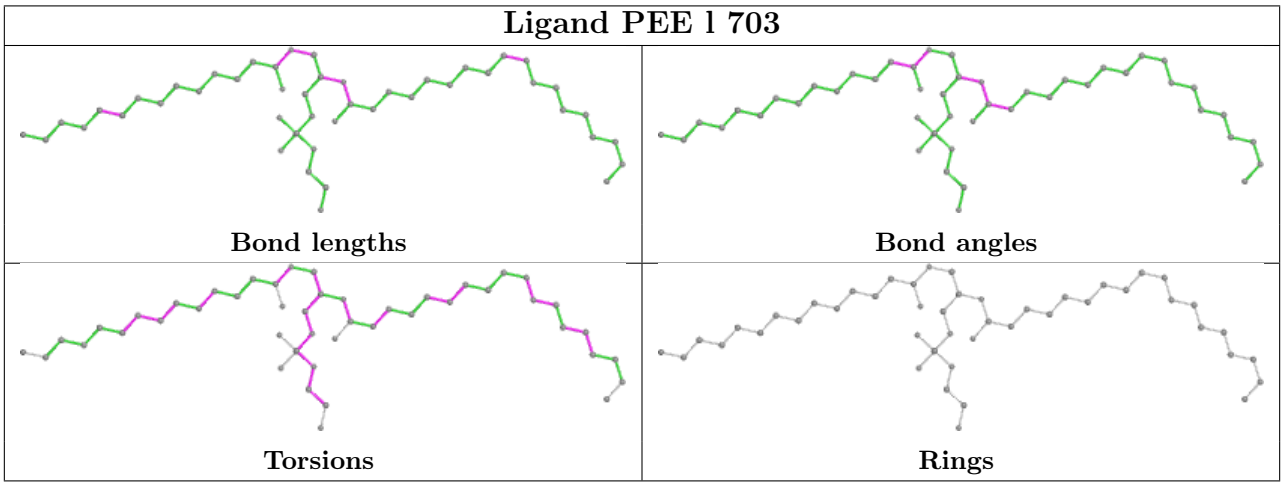

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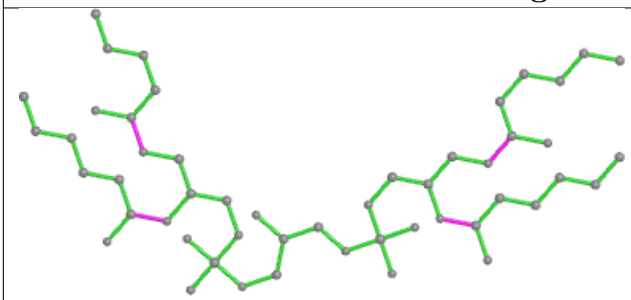
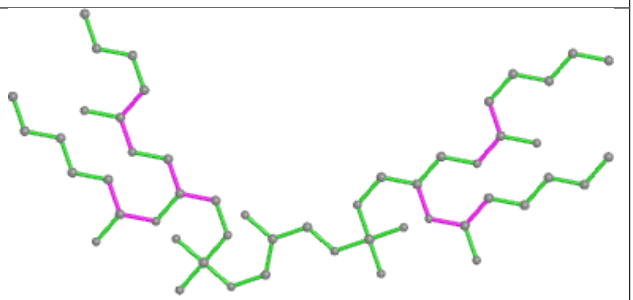
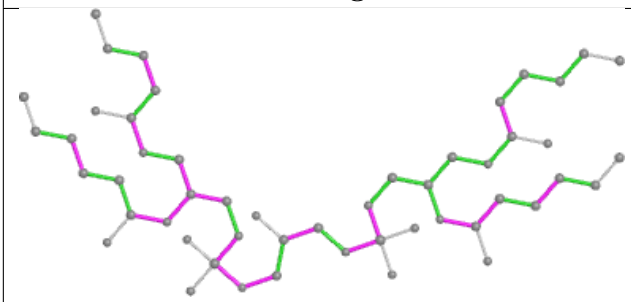


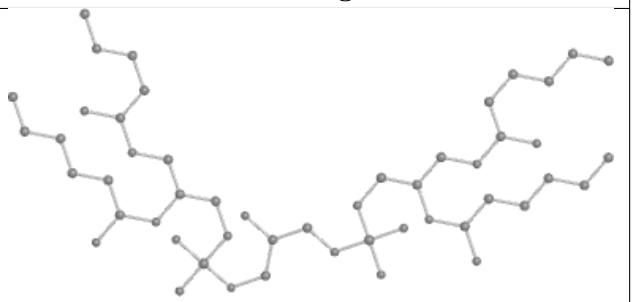
Bond lengths



Bond angles

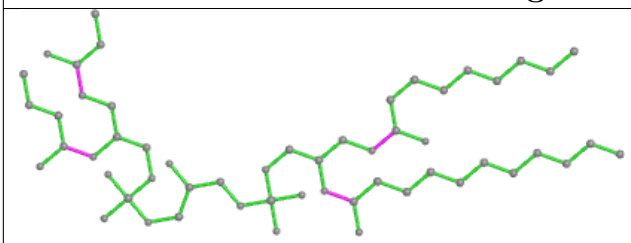


Torsions



Rings

Ligand CDL u 201



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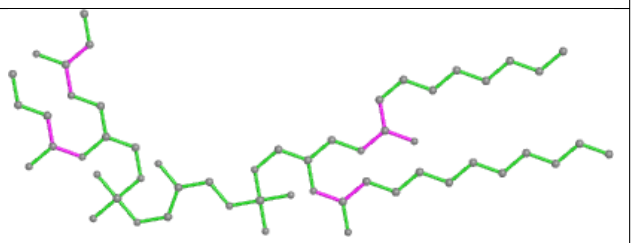
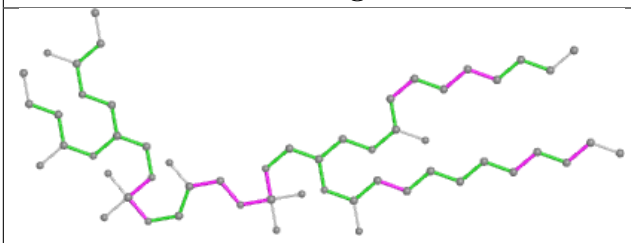


Bond angles



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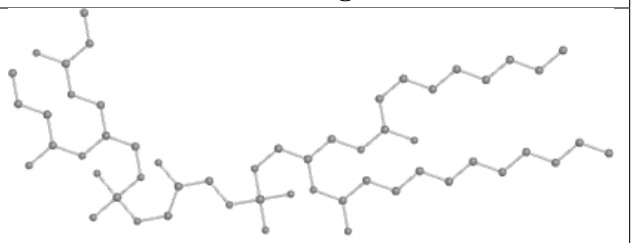
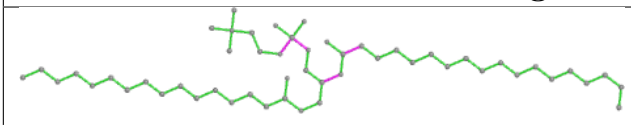


Rings

Ligand PLX a 202



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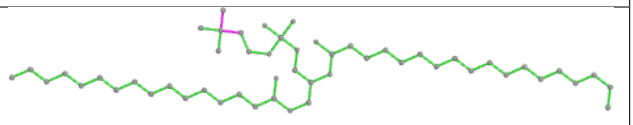
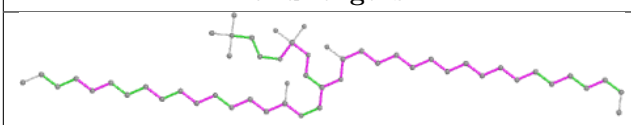


Bond angles



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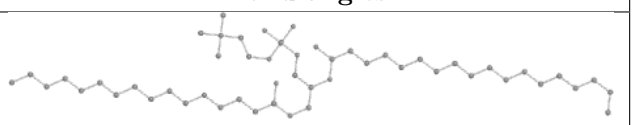
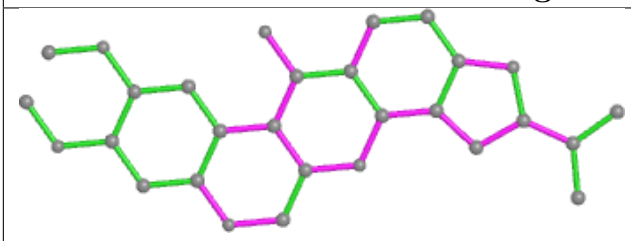
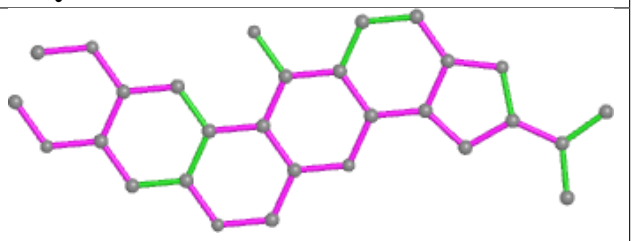


Rings

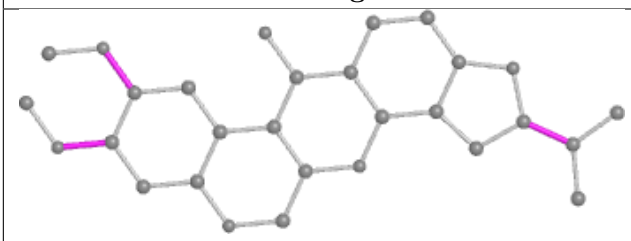
Ligand 970 Q 501



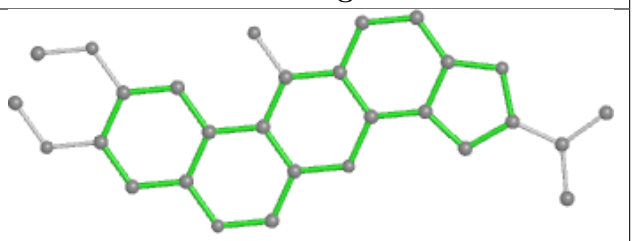
Bond lengths



Bond angles

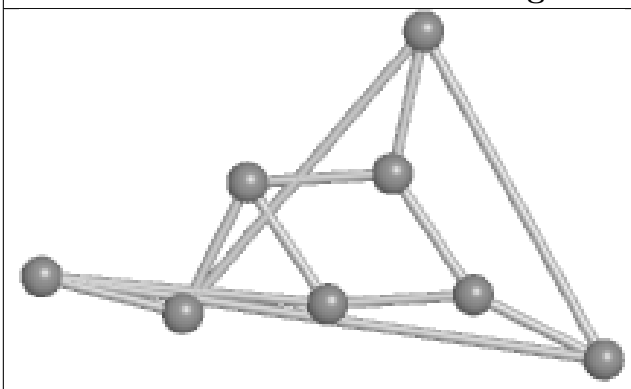


Torsions

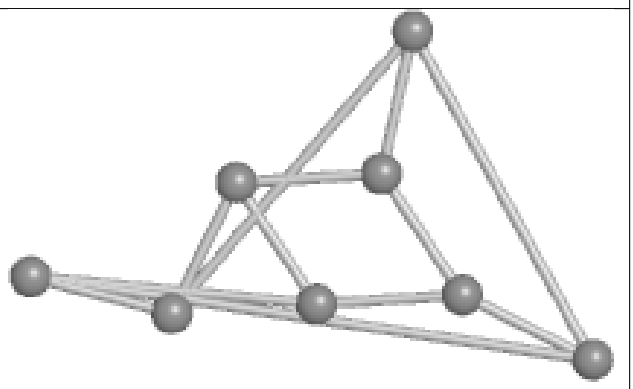


Rings

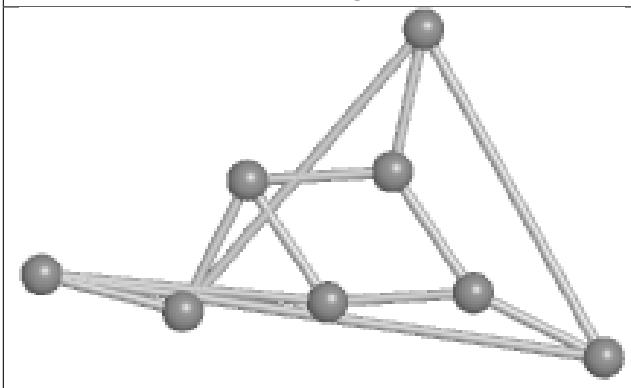
Ligand SF4 M 802



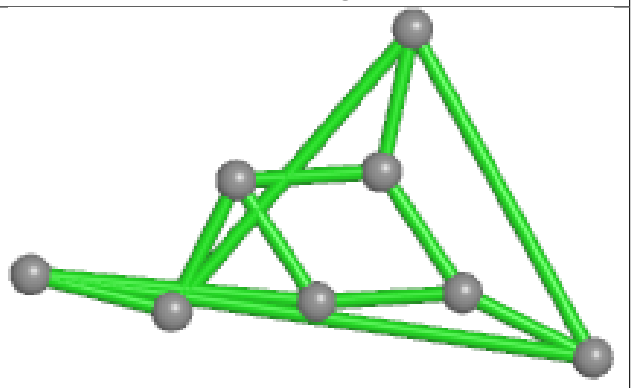
Bond lengths



Bond angles

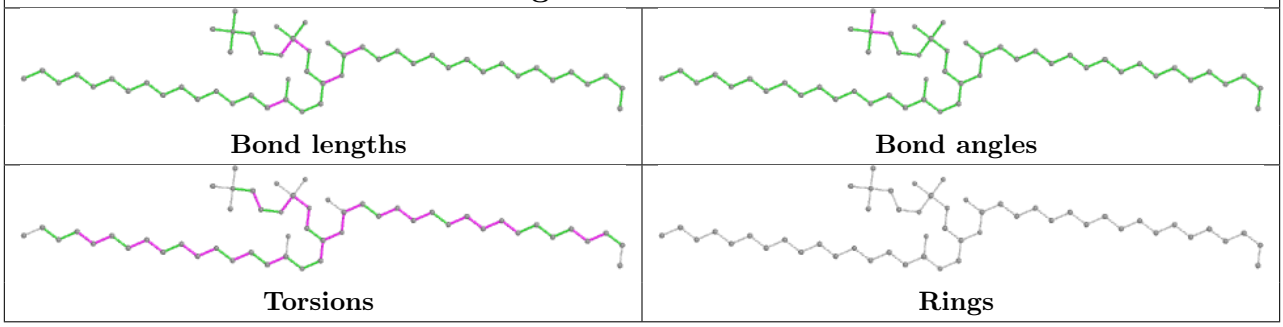


Torsions

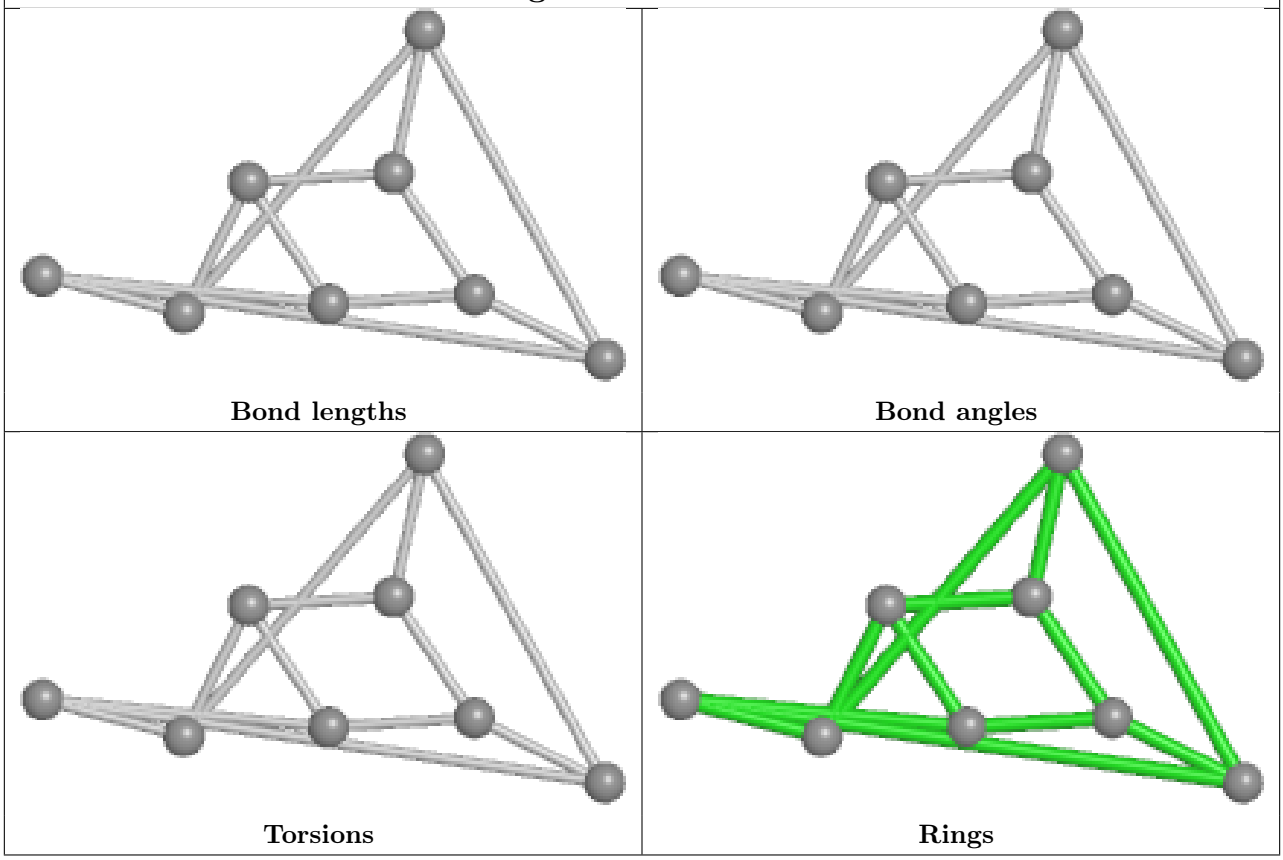


Rings

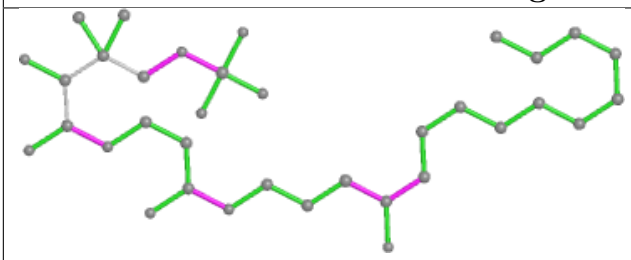
Ligand PLX r 502

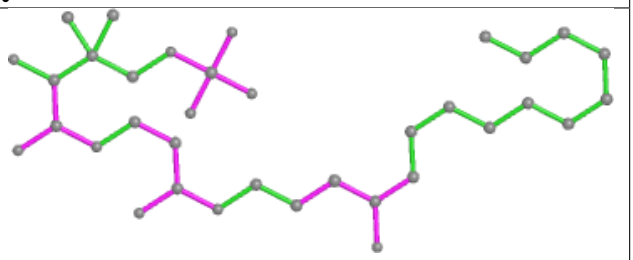


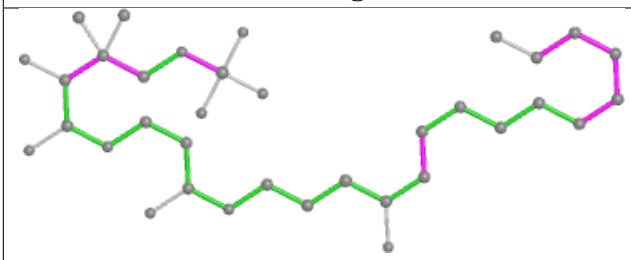
Ligand SF4 M 801

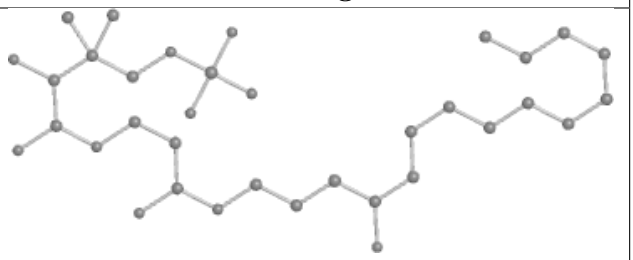


Ligand 8Q1 G 201

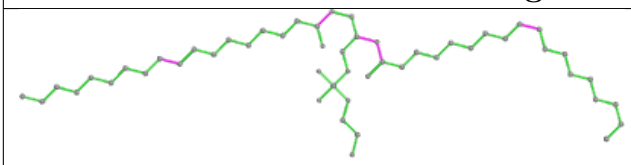

Bond lengths

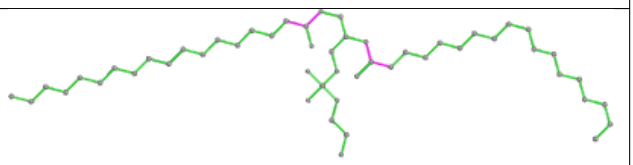

Bond angles

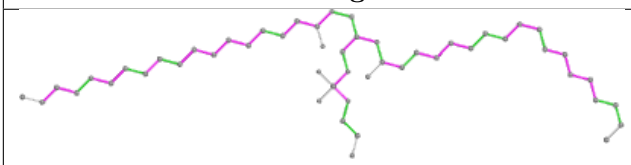

Torsions

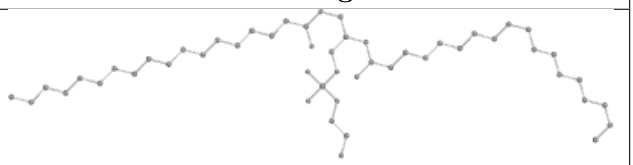

Rings

Ligand PEE U 101

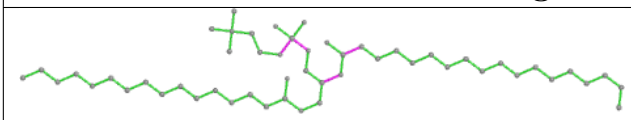

Bond lengths

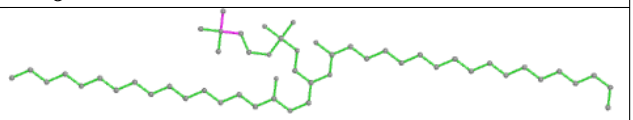

Bond angles

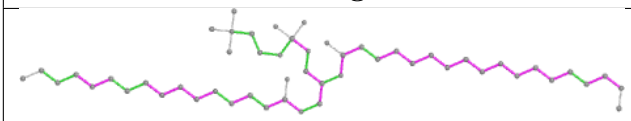

Torsions

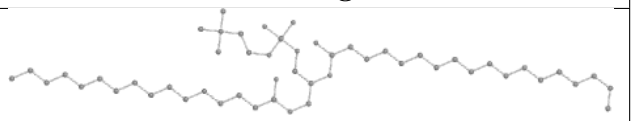

Rings

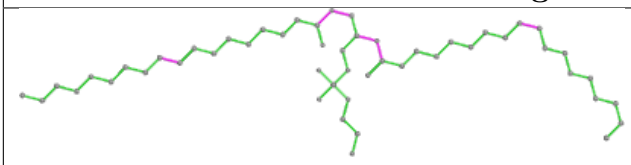
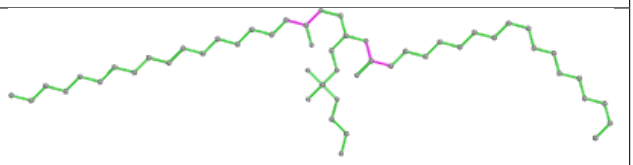
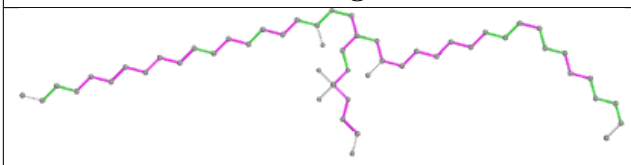
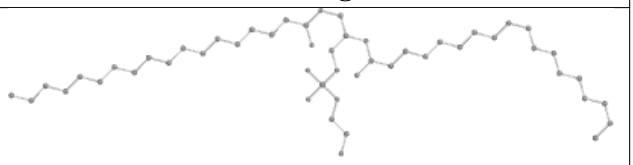
Ligand PLX j 202


Bond lengths


Bond angles


Torsions


Rings

Ligand PEE r 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

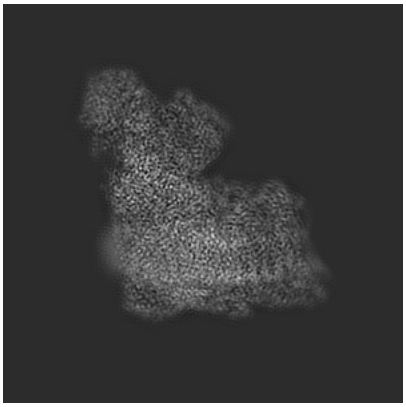
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31651. These allow visual inspection of the internal detail of the map and identification of artifacts.

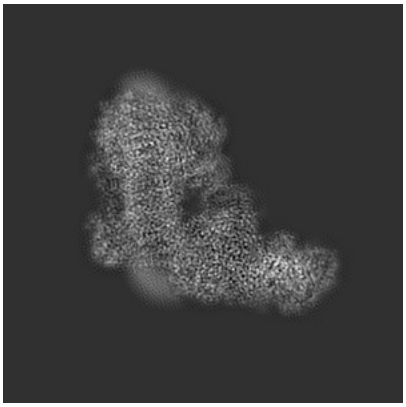
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

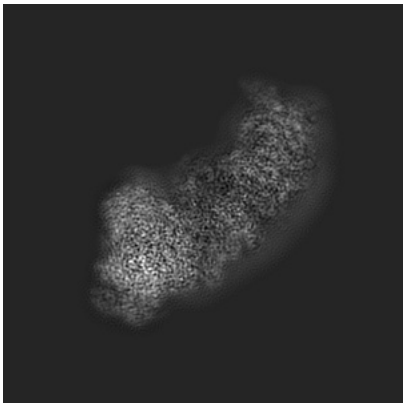
6.1.1 Primary map



X



Y

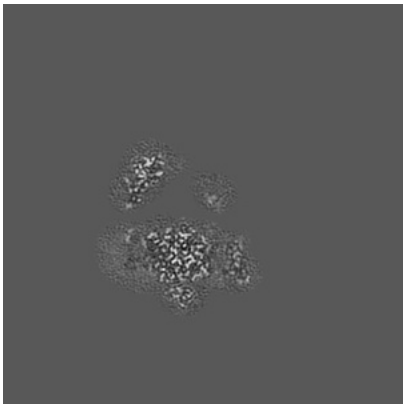


Z

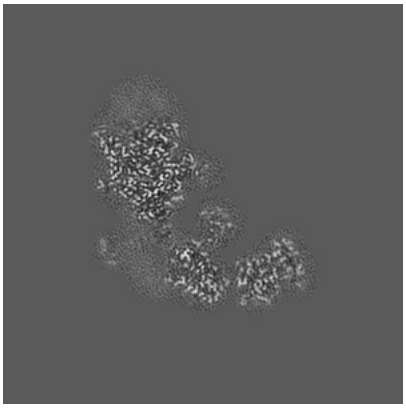
The images above show the map projected in three orthogonal directions.

6.2 Central slices

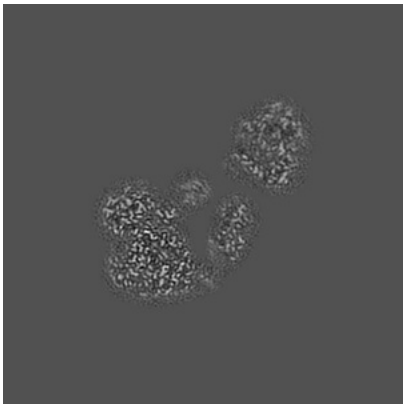
6.2.1 Primary map



X Index: 155



Y Index: 155



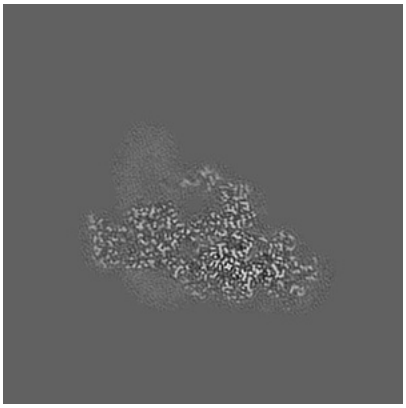
Z Index: 155

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

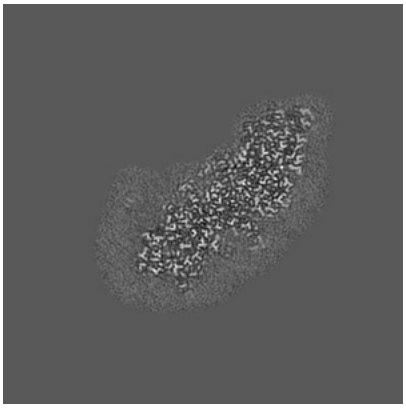
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 109



Y Index: 112

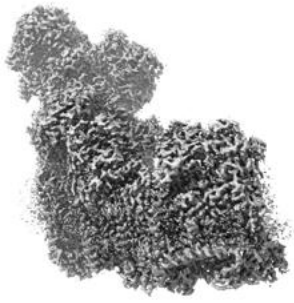


Z Index: 124

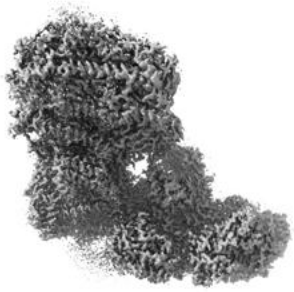
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

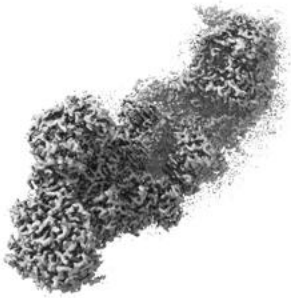
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0271. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

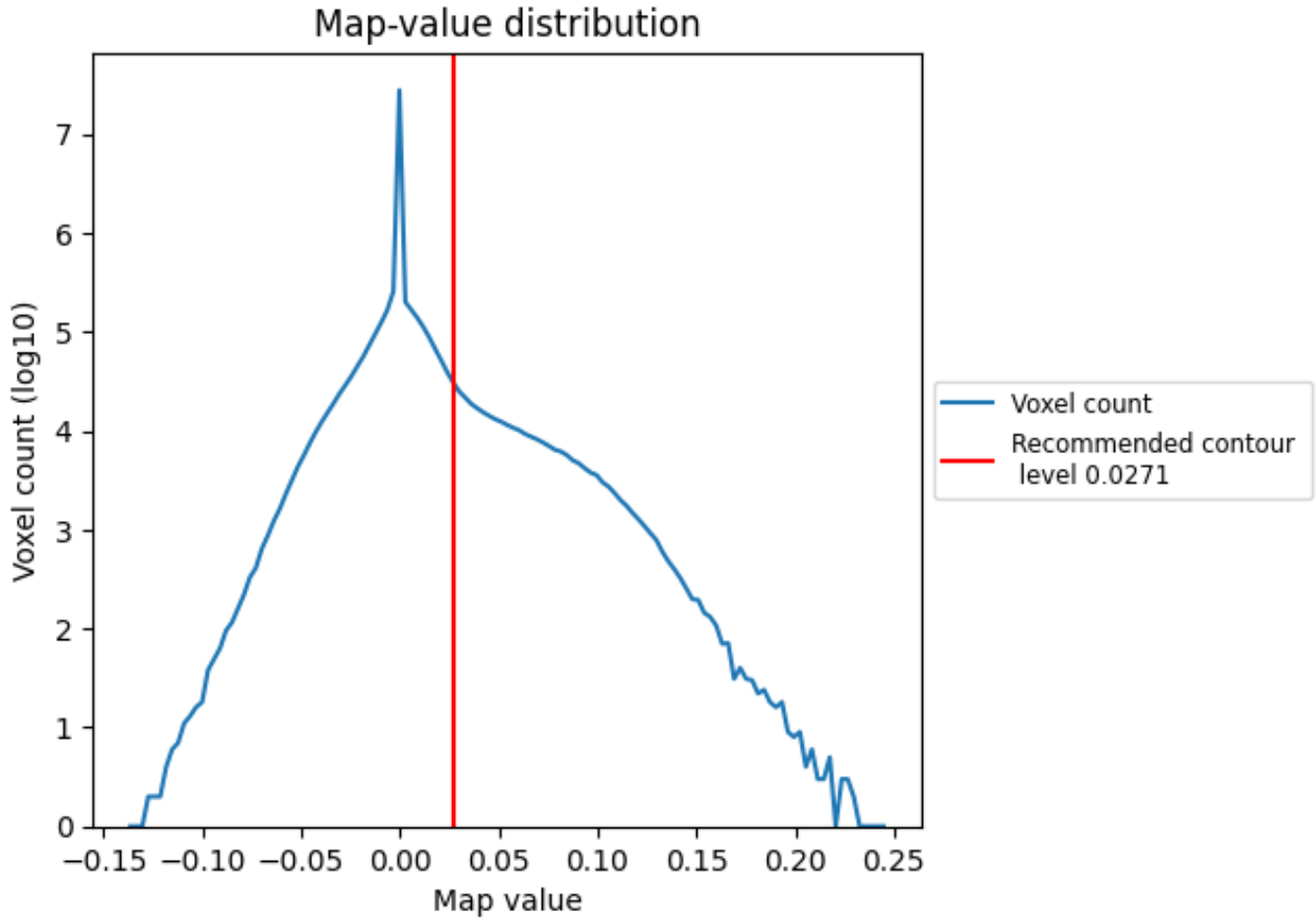
6.5 Mask visualisation (i)

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

7 Map analysis

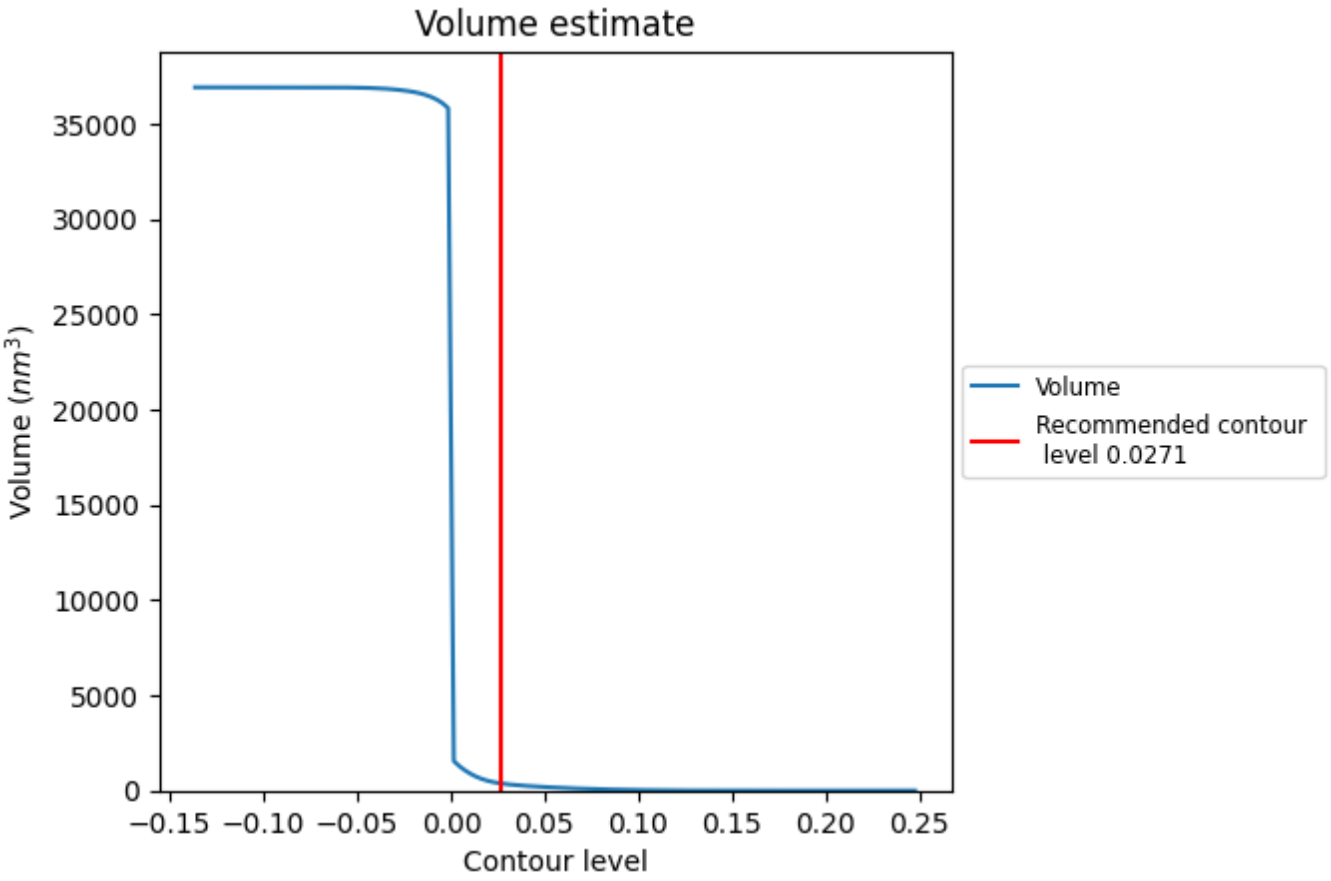
This section contains the results of statistical analysis of the map.

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.

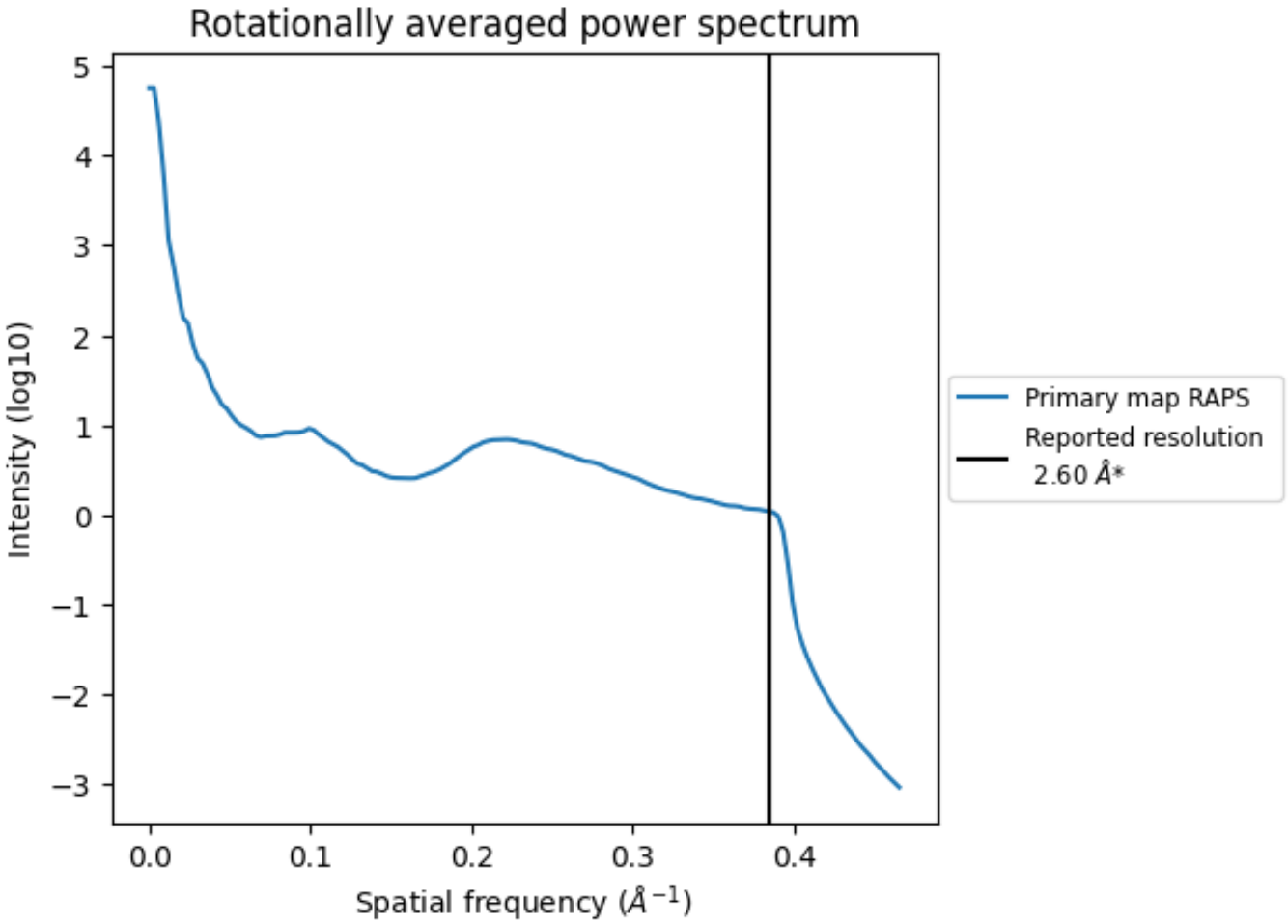
7.2 Volume estimate



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 0.385 $Å^{-1}$

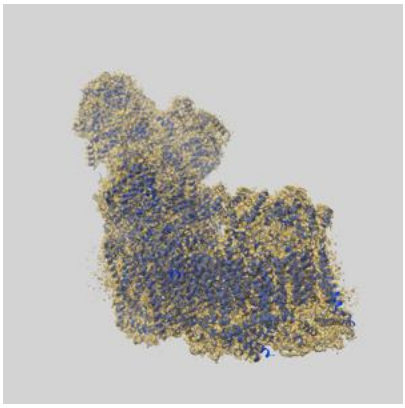
8 Fourier-Shell correlation

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

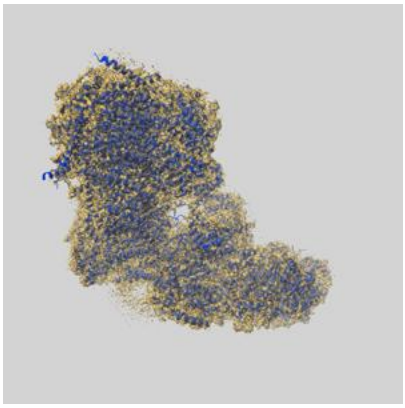
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31651 and PDB model 7V33. Per-residue inclusion information can be found in section 3 on page 22.

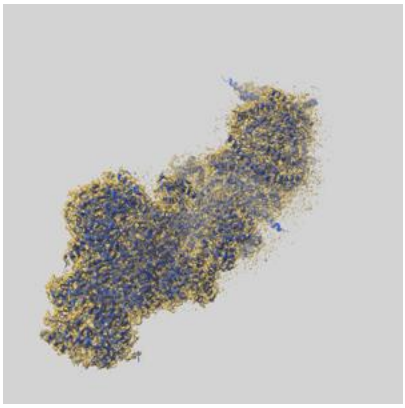
9.1 Map-model overlay



X



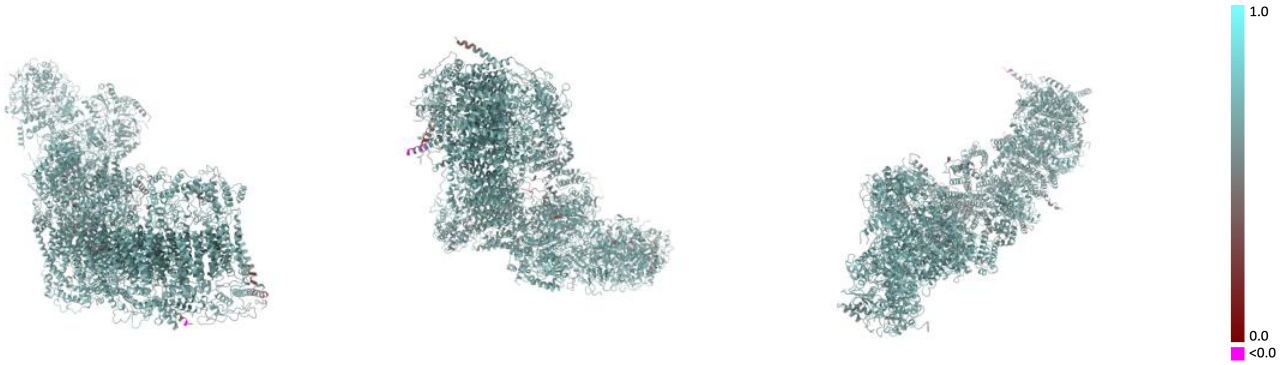
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0271 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.

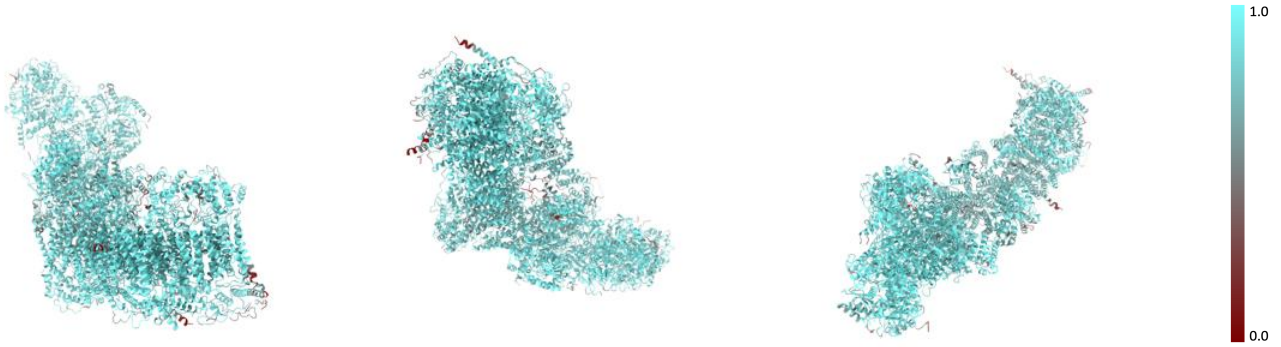
9.2 Q-score mapped to coordinate model (i)



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.

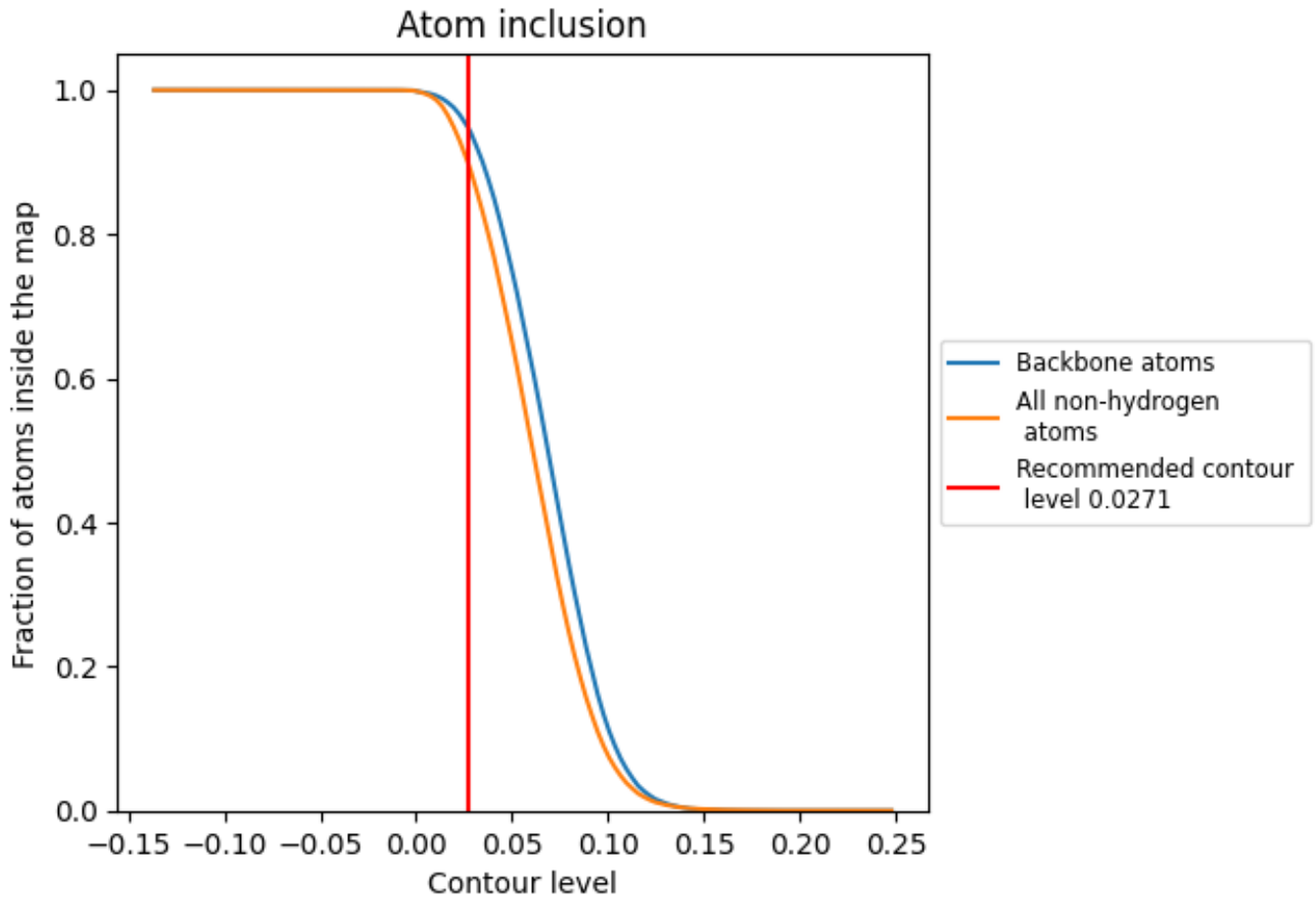
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0271).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.0271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8986	0.6490
A	0.9057	0.6390
B	0.9646	0.6870
C	0.9602	0.6870
E	0.9076	0.6600
F	0.8286	0.5970
G	0.6925	0.5290
H	0.9173	0.6420
I	0.8042	0.6240
J	0.9202	0.6570
K	0.8225	0.6020
L	0.9215	0.6720
M	0.9308	0.6570
N	0.8841	0.6480
O	0.8673	0.6220
P	0.9681	0.6890
Q	0.9610	0.6850
S	0.9583	0.6650
T	0.8892	0.6610
U	0.8721	0.6430
V	0.8586	0.6340
W	0.8973	0.6460
X	0.8083	0.6030
Y	0.7733	0.5930
Z	0.7360	0.5720
a	0.8992	0.6580
b	0.8262	0.6170
c	0.8600	0.6320
d	0.8481	0.6230
e	0.8487	0.6280
f	0.7507	0.5920
g	0.9133	0.6550
h	0.8913	0.6410
i	0.9447	0.6770
j	0.8978	0.6650

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	0.9402	0.6740
l	0.9105	0.6560
m	0.8497	0.6310
n	0.7500	0.5980
o	0.8255	0.6290
p	0.8734	0.6350
r	0.9530	0.6750
s	0.9613	0.6780
u	0.9036	0.6500
v	0.7463	0.5730
w	0.8638	0.6270