



Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 02:01 PM JST

PDB ID : 7V2E
EMDB ID : EMD-31643
Title : Active state complex I from Q10-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-08
Resolution : 2.80 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:

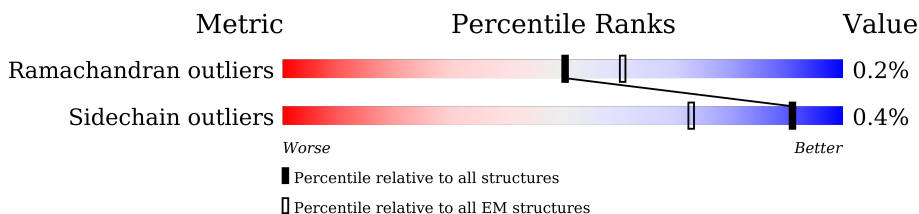
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.80 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.



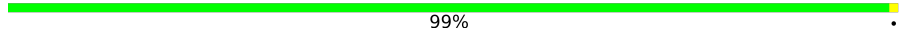

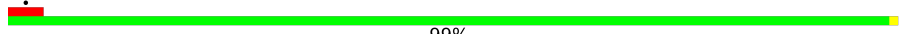
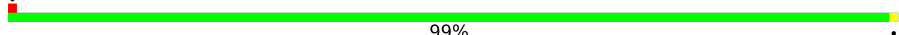
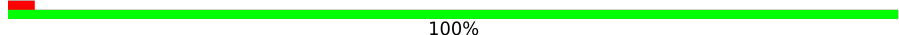
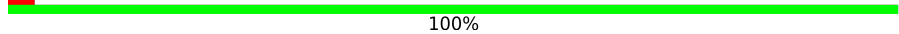
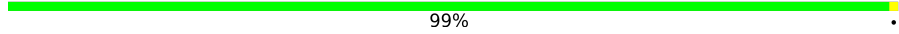
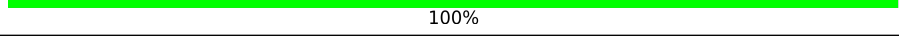
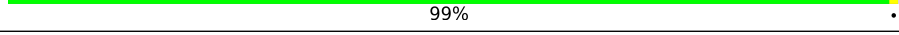
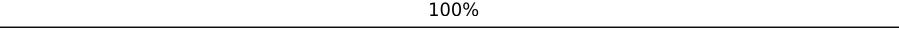
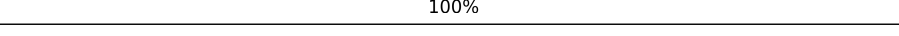
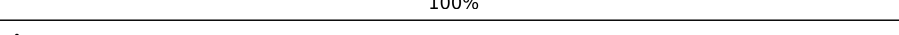
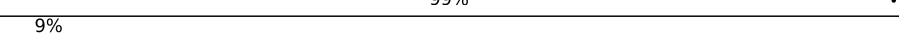
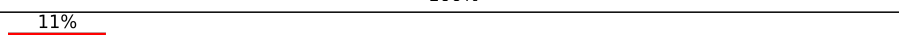





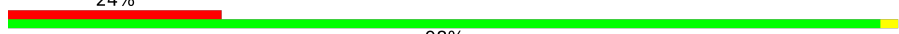
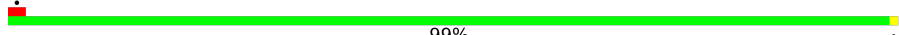
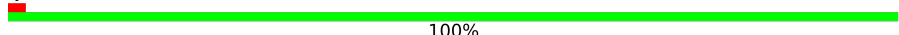
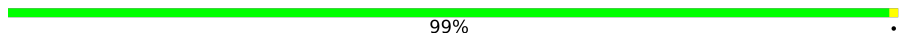
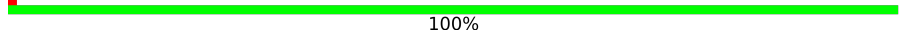

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	100%
2	B	176	99%
3	C	156	99%
4	E	115	98%
5	F	86	7% 99%
6	G	88	30% 99%
6	X	88	5% 100%
7	H	112	98%
8	I	112	5% 81% 5% 13%

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Mol	Chain	Length	Quality of chain
9	J	342	 99%
10	K	43	 5% 100%
11	L	125	 99%
12	M	690	 99%
13	N	144	 100%
14	O	217	 100%
15	P	208	 99%
16	Q	430	 100%
17	S	70	 99%
18	T	96	 100%
19	U	83	 100%
20	V	140	 100%
21	W	142	 99%
22	Y	67	 9% 100%
23	Z	80	 11% 100%
24	a	138	 100%
25	b	126	 5% 78% 22%
26	c	156	 100%
27	d	175	 5% 99%
28	e	104	 10% 100%
29	f	49	 24% 98%
30	g	121	 99%
31	h	105	 100%
32	i	347	 99%
33	j	115	 100%

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Mol	Chain	Length	Quality of chain
34	k	98	 98%
35	l	606	 99%
36	m	175	 99%
37	n	56	 100%
38	o	128	 100%
39	p	178	 99%
40	r	459	 100%
41	s	318	 99%
42	u	171	 98%
43	v	125	 99%
44	w	320	 99%

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68244 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	687	432	129	124	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0
6	X	88	704	454	104	141	5	0	0

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

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	342	2751	1783	481	478	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	43	366	228	68	69	1	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1671	1065	281	315	10	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	430	3459	2212	594	629	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	566	364	103	94	5	0	0

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

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

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

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

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

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	67	584	385	95	103	1	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	98	819	537	144	137	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	156	1315	853	213	241	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	175	1461	916	265	272	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	104	867	553	142	168	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	49	378	246	65	67	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2710	1782	420	462	46	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	115	914	615	134	158	7	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	606	4800	3182	744	823	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	175	1295	864	188	230	13	0	0

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

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

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	o	128	1062	691	182	189	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3631	2412	572	609	38	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	318	2508	1678	385	424	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	171	1398	887	250	251	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1059	658	202	189	10	0	0

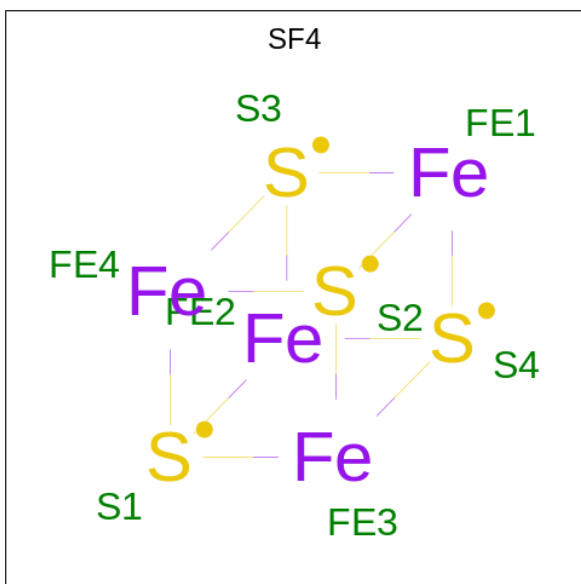
There is a discrepancy between the modelled and reference sequences:

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.

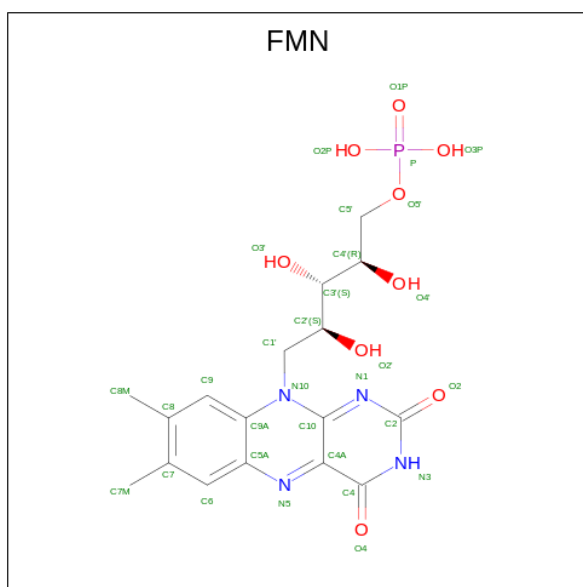
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2582	1643	438	491	10	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



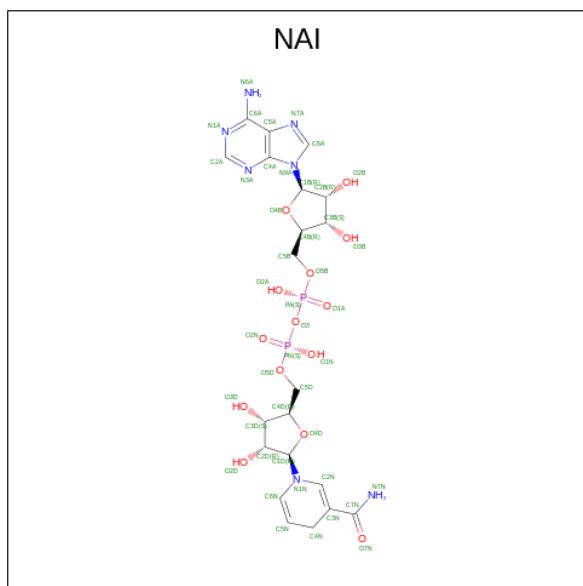
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



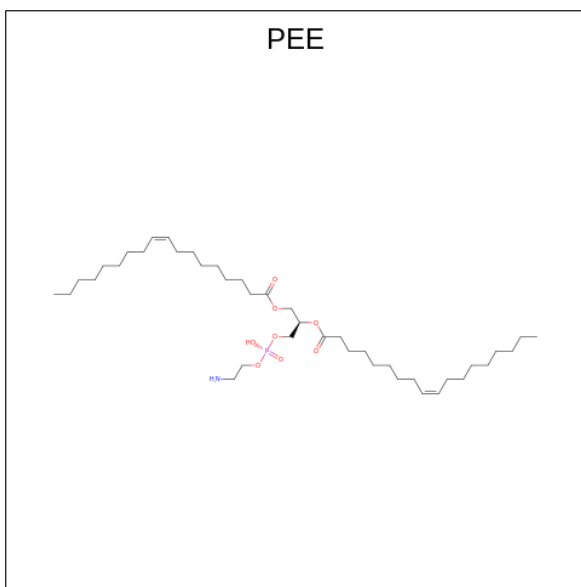
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- 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).



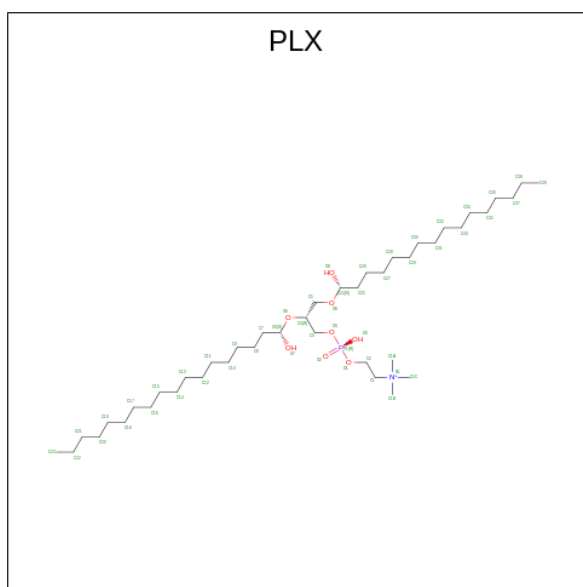
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- 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).



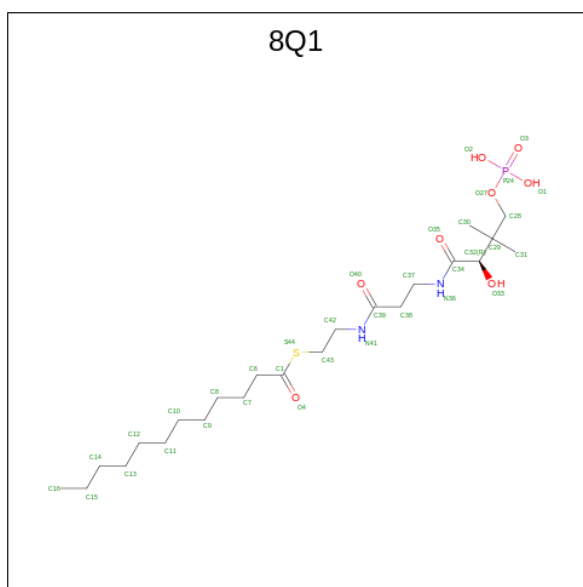
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	Total 51	41	1	8	1	0
48	C	1	Total 47	37	1	8	1	0
48	Q	1	Total 47	37	1	8	1	0
48	W	1	Total 41	31	1	8	1	0
48	b	1	Total 46	36	1	8	1	0
48	j	1	Total 92	72	2	16	2	0
48	j	1	Total 92	72	2	16	2	0
48	l	1	Total 91	71	2	16	2	0
48	l	1	Total 91	71	2	16	2	0
48	r	1	Total 51	41	1	8	1	0

- 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: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



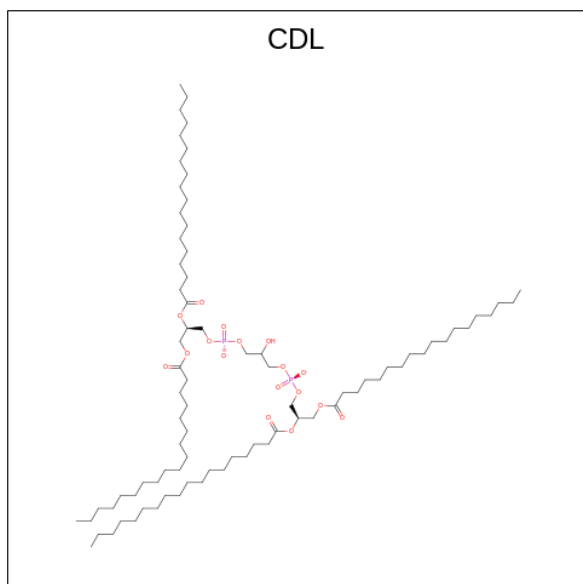
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	52	42	1	8	1	0
49	J	1	52	42	1	8	1	0
49	a	1	52	42	1	8	1	0
49	g	1	52	42	1	8	1	0
49	j	1	52	42	1	8	1	0
49	r	1	104	84	2	16	2	0
49	r	1	104	84	2	16	2	0

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



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

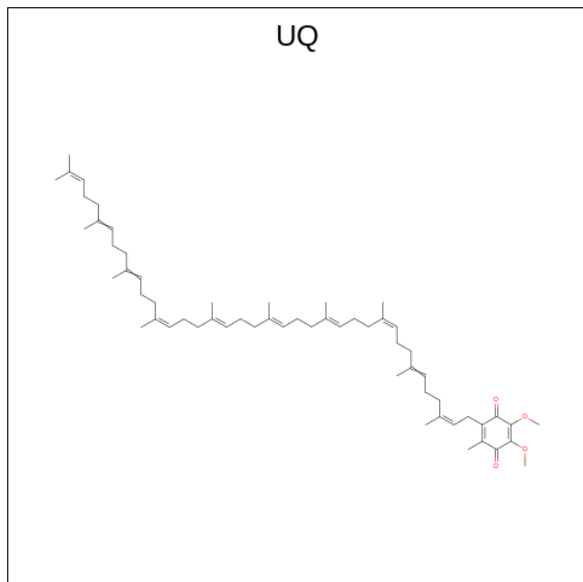
- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
51	I	1	51	32	17	2	0

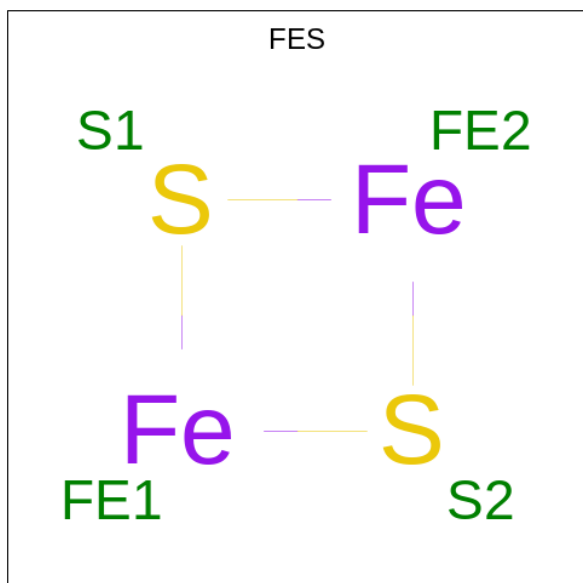
Continued on next page...

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

- 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	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

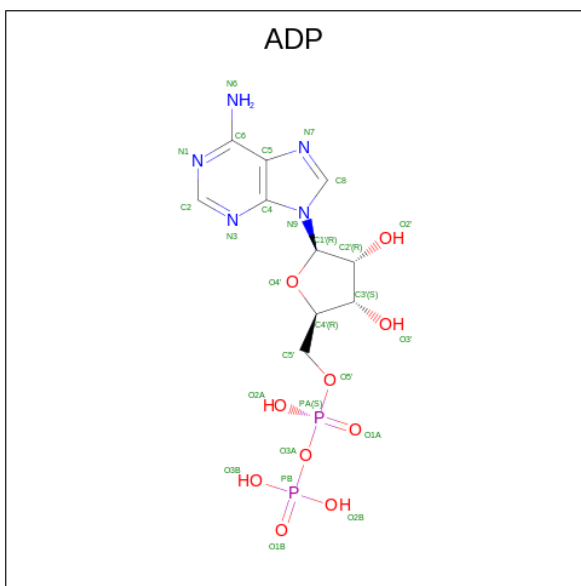
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

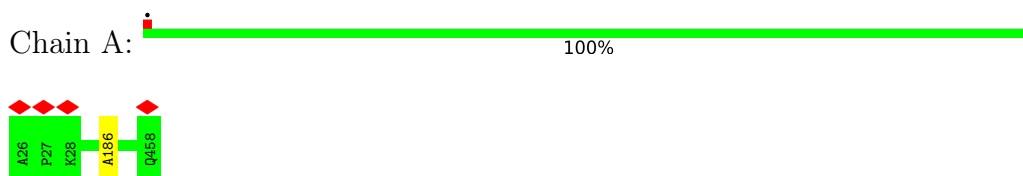


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

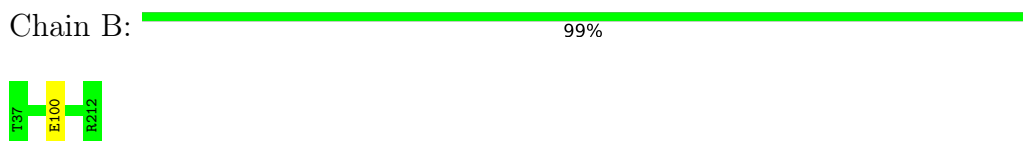
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

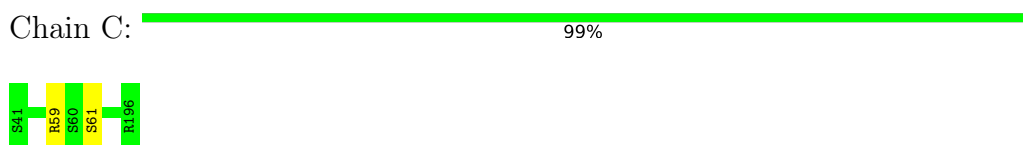
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



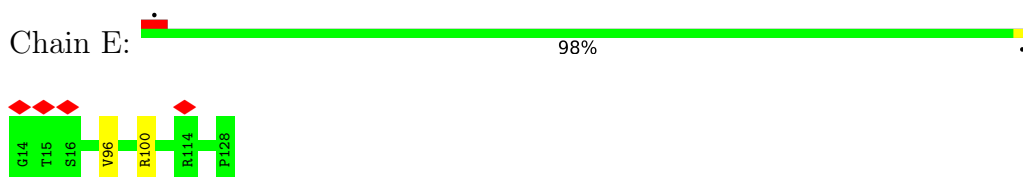
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



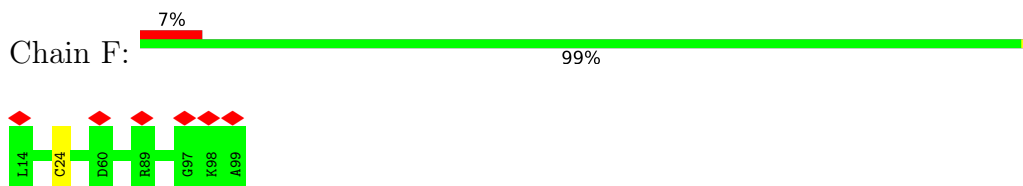
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



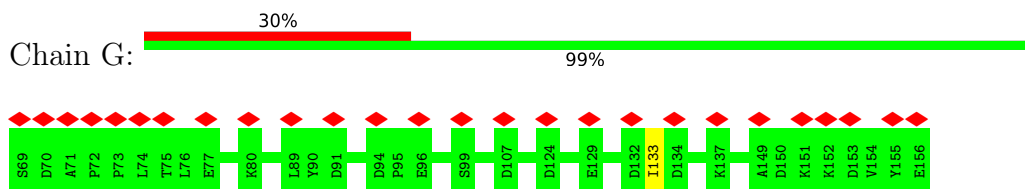
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



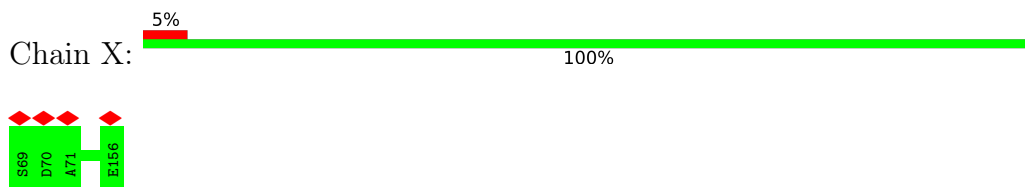
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



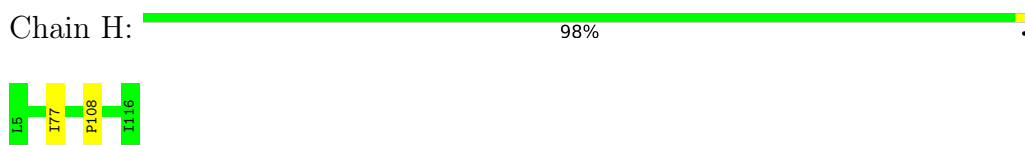
- Molecule 6: Acyl carrier protein, mitochondrial



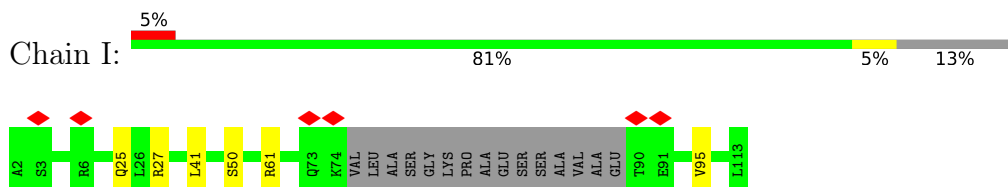
- Molecule 6: Acyl carrier protein, mitochondrial



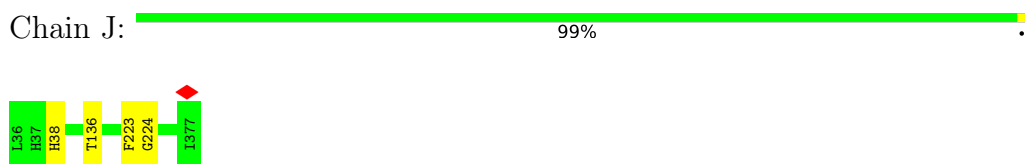
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



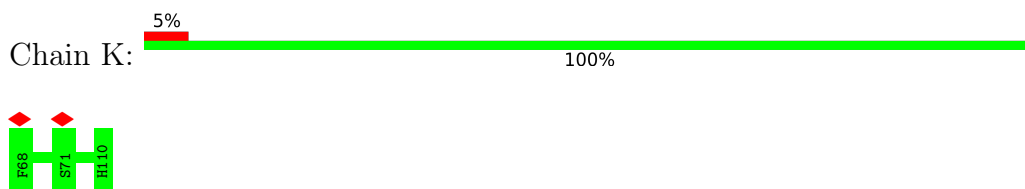
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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



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

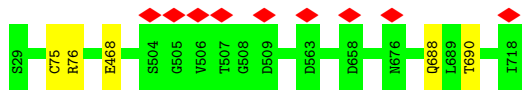


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





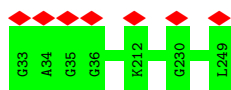
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



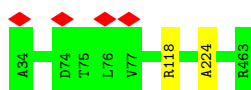
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



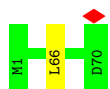
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



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



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



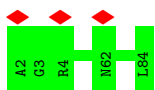
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  100%



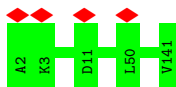
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  100%



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

Chain V:  100%



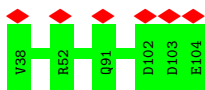
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  99%



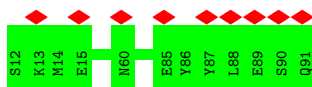
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  9% 100%



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

Chain Z:  11% 100%

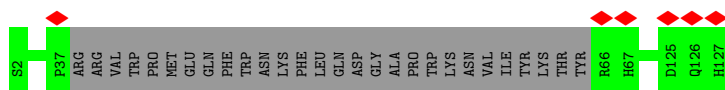
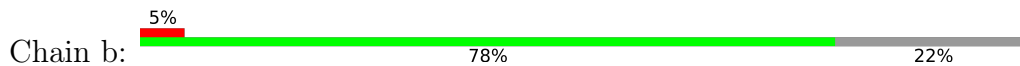


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  100%

There are no outlier residues recorded for this chain.

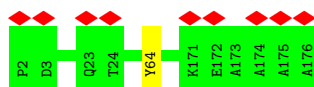
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



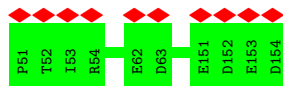
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



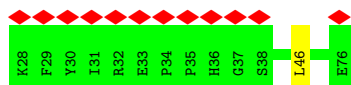
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



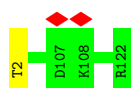
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

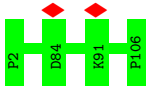


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



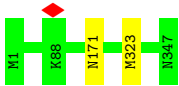
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  100%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  99%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  100%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  98%



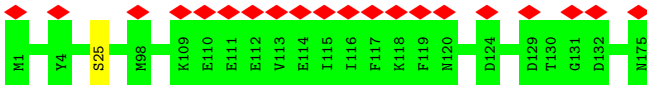
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  99%



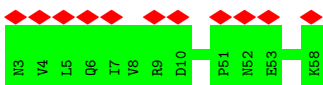
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  11%  99%



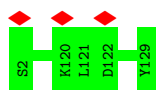
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  20%  100%



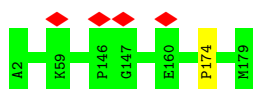
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  100%



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

Chain p:  99%



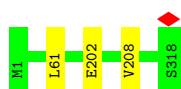
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  100%



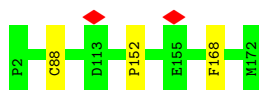
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  99%



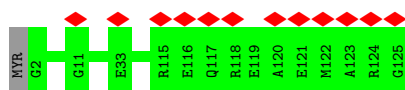
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  98%



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

Chain v:  10% 99%



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

Chain w:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152604	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 ($e^-/\text{\AA}^2$)	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	0.205	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0258	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: 8Q1, PLX, MG, 2MR, NDP, CDL, UQ, PEE, NAI, ZN, FES, SF4, ADP, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/3406	0.50	0/4603
2	B	0.32	0/1443	0.53	0/1952
3	C	0.32	0/1279	0.53	0/1730
4	E	0.27	0/995	0.49	0/1340
5	F	0.37	1/698 (0.1%)	0.60	0/940
6	G	0.26	0/705	0.52	0/956
6	X	0.27	0/716	0.46	0/968
7	H	0.25	0/929	0.46	0/1258
8	I	0.27	0/798	0.54	0/1079
9	J	0.29	0/2828	0.50	0/3834
10	K	0.27	0/377	0.51	0/509
11	L	0.28	0/1039	0.51	0/1403
12	M	0.28	0/5384	0.53	0/7295
13	N	0.28	0/1245	0.51	0/1694
14	O	0.27	0/1711	0.49	0/2328
15	P	0.31	0/1789	0.54	0/2436
16	Q	0.31	0/3538	0.52	0/4796
17	S	0.27	0/581	0.53	0/781
18	T	0.28	0/755	0.53	0/1018
19	U	0.27	0/664	0.43	0/912
20	V	0.26	0/1042	0.49	0/1411
21	W	0.29	0/1198	0.52	0/1617
22	Y	0.26	0/610	0.44	0/836
23	Z	0.26	0/660	0.46	0/892
24	a	0.29	0/1184	0.52	0/1603
25	b	0.27	0/844	0.50	0/1149
26	c	0.28	0/1371	0.48	0/1875
27	d	0.27	0/1494	0.52	0/2015
28	e	0.27	0/891	0.50	0/1210
29	f	0.27	0/386	0.55	1/523 (0.2%)
30	g	0.29	0/1031	0.48	0/1394
31	h	0.27	0/889	0.53	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.28	0/2773	0.49	0/3768
33	j	0.27	0/938	0.43	0/1281
34	k	0.30	0/759	0.58	0/1029
35	l	0.28	0/4929	0.46	0/6704
36	m	0.30	0/1328	0.50	0/1804
37	n	0.25	0/491	0.52	0/663
38	o	0.27	0/1092	0.50	0/1481
39	p	0.27	0/1590	0.50	0/2155
40	r	0.28	0/3723	0.50	0/5078
41	s	0.29	0/2581	0.49	0/3529
42	u	0.29	0/1436	0.54	1/1938 (0.1%)
43	v	0.26	0/1083	0.53	0/1448
44	w	0.27	0/2642	0.49	0/3580
All	All	0.28	1/67845 (0.0%)	0.50	2/92005 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	24	CYS	CB-SG	5.76	1.92	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
29	f	46	LEU	CA-CB-CG	6.05	129.22	115.30
42	u	88	CYS	CA-CB-SG	5.99	124.78	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ALA	Peptide

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%)	17 (4%)	0	100	100
2	B	174/176 (99%)	169 (97%)	4 (2%)	1 (1%)	25	56
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	107 (95%)	4 (4%)	2 (2%)	8	28
5	F	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
6	G	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	13	39
6	X	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
7	H	110/112 (98%)	104 (94%)	4 (4%)	2 (2%)	8	28
8	I	93/112 (83%)	84 (90%)	8 (9%)	1 (1%)	14	41
9	J	340/342 (99%)	321 (94%)	16 (5%)	3 (1%)	17	46
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	664 (96%)	24 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	202 (98%)	4 (2%)	0	100	100
16	Q	427/430 (99%)	413 (97%)	13 (3%)	1 (0%)	47	78
17	S	68/70 (97%)	64 (94%)	3 (4%)	1 (2%)	10	33
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	81 (100%)	0	0	100	100
20	V	138/140 (99%)	137 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
23	Z	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
24	a	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
28	e	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	581 (96%)	23 (4%)	0	100	100
36	m	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	25	56
37	n	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	25	56
40	r	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
41	s	316/318 (99%)	307 (97%)	8 (2%)	1 (0%)	41	72
42	u	169/171 (99%)	164 (97%)	3 (2%)	2 (1%)	13	39
43	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	301 (95%)	16 (5%)	1 (0%)	41	72
All	All	8174/8313 (98%)	7859 (96%)	297 (4%)	18 (0%)	50	78

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	100	GLU
7	H	108	PRO
16	Q	224	ALA
42	u	168	PHE
6	G	133	ILE

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Mol	Chain	Res	Type
17	S	66	LEU
4	E	100	ARG
44	w	227	MET
8	I	41	LEU
9	J	38	HIS
9	J	223	PHE
41	s	208	VAL
7	H	77	ILE
9	J	224	GLY
4	E	96	VAL
36	m	25	SER
39	p	174	PRO
42	u	152	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%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	130 (98%)	2 (2%)	65	89
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	79/81 (98%)	79 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	82 (94%)	5 (6%)	20	50
9	J	296/296 (100%)	295 (100%)	1 (0%)	92	98
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	94
12	M	580/580 (100%)	575 (99%)	5 (1%)	78	94
13	N	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	188 (99%)	2 (1%)	73	92
16	Q	370/370 (100%)	370 (100%)	0	100	100
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	121 (99%)	1 (1%)	81	94
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	154 (99%)	1 (1%)	86	96
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	94
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	309 (99%)	2 (1%)	86	96
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	81
35	l	537/540 (99%)	533 (99%)	4 (1%)	84	95
36	m	130/141 (92%)	130 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	408 (100%)	2 (0%)	88	96
41	s	275/275 (100%)	273 (99%)	2 (1%)	84	95
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	111/111 (100%)	111 (100%)	0	100	100
44	w	281/283 (99%)	280 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7166/7240 (99%)	7134 (100%)	32 (0%)	91 97

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	59	ARG
3	C	61	SER
8	I	25	GLN
8	I	27	ARG
8	I	50	SER
8	I	61	ARG
8	I	95	VAL
9	J	136	THR
11	L	86	ASN
12	M	75	CYS
12	M	76	ARG
12	M	468	GLU
12	M	688	GLN
12	M	690	THR
15	P	161	LYS
15	P	201	ASP
21	W	99	LYS
27	d	64	TYR
30	g	2	THR
32	i	171	ASN
32	i	323	MET
34	k	50	ASN
34	k	53	PHE
35	l	320	ASN
35	l	423	SER
35	l	425	ARG
35	l	541	ASN
40	r	255	ASN
40	r	256	TYR
41	s	61	LEU
41	s	202	GLU
44	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
7	H	50	GLN
8	I	29	GLN
9	J	138	ASN
10	K	78	HIS
11	L	88	GLN
12	M	260	ASN
12	M	334	GLN
12	M	336	ASN
12	M	514	ASN
12	M	604	GLN
14	O	69	ASN
14	O	131	HIS
17	S	31	ASN
18	T	43	GLN
27	d	107	GLN
31	h	45	HIS
32	i	273	ASN
35	l	534	HIS
38	o	79	ASN
40	r	255	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	2.00	2 (20%)	5,13,15	6.28	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	5.55	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.07	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.88	131.29	119.48
16	Q	118	2MR	CD-NE-CZ	4.59	132.00	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.86	130.20	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 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.97	2 (4%)
48	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.97	2 (3%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
50	8Q1	X	201	-	31,34,34	2.04	6 (19%)	40,43,43	1.73	11 (27%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PEE	l	701	-	39,39,50	1.30	6 (15%)	41,44,55	1.07	3 (7%)
51	CDL	l	702	-	98,98,99	1.09	8 (8%)	104,110,111	0.89	4 (3%)
49	PLX	r	502	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
51	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
54	FES	O	301	14	0,4,4	-	-	-	-	-
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.39	4 (13%)
48	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	1.03	2 (4%)
51	CDL	l	703	-	99,99,99	0.92	4 (4%)	105,111,111	1.02	5 (4%)
49	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.65	1 (1%)
48	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)
46	FMN	A	502	-	33,33,33	1.40	5 (15%)	48,50,50	1.29	7 (14%)
51	CDL	V	201	-	93,93,99	1.11	9 (9%)	99,105,111	0.87	4 (4%)
51	CDL	n	101	-	54,54,99	1.23	4 (7%)	60,66,111	1.24	5 (8%)
53	UQ	s	402	-	38,38,63	3.54	10 (26%)	46,49,79	2.83	16 (34%)
50	8Q1	G	201	-	31,34,34	2.04	6 (19%)	40,43,43	1.73	12 (30%)
49	PLX	a	202	-	51,51,51	1.15	3 (5%)	55,59,59	0.58	1 (1%)
52	NDP	J	401	-	45,52,52	2.22	4 (8%)	53,80,80	1.74	10 (18%)
49	PLX	J	403	-	51,51,51	1.14	3 (5%)	55,59,59	0.59	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
49	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
51	CDL	s	401	-	88,88,99	1.13	8 (9%)	94,100,111	0.94	4 (4%)
51	CDL	I	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.32	6 (10%)
48	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
54	FES	M	803	12	0,4,4	-	-	-	-	-
45	SF4	M	802	12	0,12,12	-	-	-	-	-
45	SF4	C	301	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
47	NAI	A	503	-	42,48,48	4.94	18 (42%)	47,73,73	1.30	7 (14%)
51	CDL	V	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
51	CDL	r	504	-	99,99,99	1.07	8 (8%)	105,111,111	0.89	4 (3%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
48	PEE	l	704	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
49	PLX	C	303	-	51,51,51	0.62	0	55,59,59	0.73	1 (1%)
53	UQ	J	402	-	33,33,63	3.44	10 (30%)	40,43,79	2.79	14 (35%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
51	CDL	k	101	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
48	PEE	j	202	-	40,40,50	1.15	5 (12%)	43,45,55	1.07	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	W	201	-	-	21/44/44/54	-
48	PEE	j	201	-	-	29/54/54/54	-
48	PEE	B	303	-	-	30/54/54/54	-
50	8Q1	X	201	-	-	22/41/41/41	-
51	CDL	l	702	-	-	60/109/109/110	-
48	PEE	l	701	-	-	24/43/43/54	-
45	SF4	A	501	1	-	-	0/6/5/5
49	PLX	r	502	-	-	35/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
51	CDL	a	201	-	-	55/110/110/110	-
54	FES	O	301	14	-	-	0/1/1/1
57	ADP	w	401	-	-	3/12/32/32	0/3/3/3
48	PEE	Q	501	-	-	21/50/50/54	-
51	CDL	l	703	-	-	71/110/110/110	-
49	PLX	g	201	-	-	32/55/55/55	-
48	PEE	C	302	-	-	23/50/50/54	-
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
51	CDL	V	201	-	-	60/104/104/110	-
51	CDL	n	101	-	-	24/65/65/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	UQ	s	402	-	-	13/33/57/87	0/1/1/1
50	8Q1	G	201	-	-	14/41/41/41	-
49	PLX	a	202	-	-	33/55/55/55	-
52	NDP	J	401	-	-	4/30/77/77	0/5/5/5
49	PLX	r	503	-	-	30/55/55/55	-
49	PLX	J	403	-	-	29/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
51	CDL	s	401	-	-	55/99/99/110	-
51	CDL	I	201	-	-	28/61/61/110	-
48	PEE	b	201	-	-	24/49/49/54	-
54	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	j	203	-	-	25/55/55/55	-
47	NAI	A	503	-	-	9/25/72/72	0/5/5/5
51	CDL	V	202	-	-	66/110/110/110	-
51	CDL	r	504	-	-	64/110/110/110	-
48	PEE	r	501	-	-	30/54/54/54	-
48	PEE	l	704	-	-	33/54/54/54	-
49	PLX	C	303	-	-	26/55/55/55	-
53	UQ	J	402	-	-	12/27/51/87	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
51	CDL	k	101	-	-	56/110/110/110	-
48	PEE	j	202	-	-	25/44/44/54	-

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.18	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.56	1.30	1.53
52	J	401	NDP	P2B-O2B	12.42	1.82	1.59
47	A	503	NAI	C3D-C4D	-10.34	1.26	1.53
53	s	402	UQ	C18-C19	9.60	1.56	1.33
53	J	402	UQ	C18-C19	9.56	1.55	1.33
53	s	402	UQ	C13-C14	9.29	1.55	1.33
53	J	402	UQ	C13-C14	9.13	1.54	1.33
53	s	402	UQ	C23-C24	9.09	1.54	1.33
53	J	402	UQ	C8-C9	9.05	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	w	401	ADP	C3'-C4'	-8.96	1.30	1.53
53	s	402	UQ	C8-C9	8.95	1.54	1.33
47	A	503	NAI	O4B-C4B	-8.24	1.26	1.45
53	J	402	UQ	C23-C24	7.86	1.55	1.32
53	s	402	UQ	C28-C29	7.70	1.54	1.32
57	w	401	ADP	O4'-C4'	7.69	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.68	1.28	1.53
50	X	201	8Q1	P24-O27	7.56	1.84	1.60
50	G	201	8Q1	P24-O27	7.34	1.83	1.60
57	w	401	ADP	O4'-C1'	-6.80	1.31	1.41
47	A	503	NAI	O4D-C4D	6.78	1.60	1.45
47	A	503	NAI	C2D-C3D	5.84	1.69	1.53
47	A	503	NAI	C7N-N7N	5.73	1.48	1.33
47	A	503	NAI	O4D-C1D	5.31	1.54	1.42
47	A	503	NAI	C4N-C3N	-5.06	1.40	1.49
46	A	502	FMN	C9A-C5A	4.69	1.49	1.41
47	A	503	NAI	O2B-C2B	4.52	1.53	1.43
51	I	201	CDL	OA8-CA7	4.27	1.45	1.33
51	l	703	CDL	OB8-CB7	4.25	1.45	1.33
51	n	101	CDL	OA8-CA7	4.24	1.45	1.33
51	I	201	CDL	OB8-CB7	4.23	1.45	1.33
51	l	703	CDL	OA8-CA7	4.23	1.45	1.33
51	n	101	CDL	OB8-CB7	4.20	1.45	1.33
51	n	101	CDL	OB6-CB5	4.14	1.46	1.34
51	l	703	CDL	OA6-CA5	4.13	1.45	1.34
51	I	201	CDL	OA6-CA5	4.10	1.45	1.34
51	n	101	CDL	OA6-CA5	4.09	1.45	1.34
51	I	201	CDL	OB6-CB5	4.06	1.45	1.34
51	l	703	CDL	OB6-CB5	4.05	1.45	1.34
47	A	503	NAI	C6N-C5N	3.96	1.40	1.33
50	X	201	8Q1	C1-S44	3.87	1.85	1.76
57	w	401	ADP	C6-N6	3.84	1.48	1.34
50	G	201	8Q1	C1-S44	3.82	1.85	1.76
48	l	704	PEE	C18-C19	3.76	1.53	1.31
48	j	202	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.74	1.53	1.31
48	C	302	PEE	C18-C19	3.73	1.53	1.31
48	b	201	PEE	C18-C19	3.73	1.53	1.31
48	l	701	PEE	C18-C19	3.71	1.53	1.31
48	B	303	PEE	C18-C19	3.71	1.53	1.31
48	W	201	PEE	C18-C19	3.69	1.53	1.31
48	j	201	PEE	C18-C19	3.68	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	501	PEE	C18-C19	3.67	1.53	1.31
48	l	701	PEE	C39-C38	3.65	1.52	1.31
48	l	704	PEE	C39-C38	3.65	1.52	1.31
48	b	201	PEE	C39-C38	3.65	1.52	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
52	J	401	NDP	PN-O5D	3.64	1.74	1.59
48	C	302	PEE	C39-C38	3.62	1.52	1.31
48	j	201	PEE	C39-C38	3.62	1.52	1.31
48	B	303	PEE	C39-C38	3.62	1.52	1.31
48	Q	501	PEE	C39-C38	3.61	1.52	1.31
51	l	702	CDL	OA8-CA7	3.59	1.43	1.33
50	G	201	8Q1	C34-N36	3.55	1.41	1.33
47	A	503	NAI	C6A-N6A	3.50	1.46	1.34
51	s	401	CDL	OA8-CA7	3.48	1.43	1.33
47	A	503	NAI	C7N-C3N	3.47	1.56	1.48
50	X	201	8Q1	C34-N36	3.46	1.41	1.33
51	a	201	CDL	OA8-CA7	3.44	1.43	1.33
51	V	202	CDL	OA8-CA7	3.41	1.43	1.33
51	V	201	CDL	OA8-CA7	3.39	1.43	1.33
51	k	101	CDL	OA8-CA7	3.39	1.43	1.33
50	G	201	8Q1	O27-C28	-3.36	1.33	1.43
50	X	201	8Q1	O27-C28	-3.35	1.33	1.43
51	r	504	CDL	OA8-CA7	3.35	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.32	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.29	1.40	1.48
50	G	201	8Q1	C6-C1	3.26	1.54	1.50
57	w	401	ADP	O3'-C3'	3.20	1.50	1.43
51	V	201	CDL	OA6-CA5	3.17	1.43	1.34
51	k	101	CDL	OA6-CA5	3.12	1.43	1.34
46	A	502	FMN	C8-C7	3.11	1.48	1.40
51	a	201	CDL	OB6-CB5	3.08	1.43	1.34
52	J	401	NDP	O2B-C2B	-3.07	1.32	1.44
51	l	702	CDL	OB8-CB7	3.05	1.42	1.33
51	s	401	CDL	OA6-CA5	3.01	1.42	1.34
50	X	201	8Q1	C39-N41	3.00	1.40	1.33
51	V	202	CDL	OB6-CB5	3.00	1.42	1.34
51	k	101	CDL	OB6-CB5	2.98	1.42	1.34
51	s	401	CDL	OB6-CB5	2.97	1.42	1.34
51	k	101	CDL	OB8-CB7	2.96	1.42	1.33
51	r	504	CDL	OB6-CB5	2.96	1.42	1.34
51	l	702	CDL	OB6-CB5	2.96	1.42	1.34
51	V	202	CDL	OB8-CB7	2.95	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	a	201	CDL	OB8-CB7	2.94	1.41	1.33
51	r	504	CDL	OB8-CB7	2.93	1.41	1.33
51	V	202	CDL	OA6-CA5	2.93	1.42	1.34
51	a	201	CDL	OA6-CA5	2.92	1.42	1.34
51	V	201	CDL	OB8-CB7	2.88	1.41	1.33
51	r	504	CDL	OA6-CA5	2.88	1.42	1.34
49	g	201	PLX	O6-C4	-2.88	1.40	1.44
49	a	202	PLX	O6-C4	-2.87	1.40	1.44
51	V	201	CDL	OB6-CB5	2.84	1.42	1.34
51	l	702	CDL	OA6-CA5	2.83	1.42	1.34
51	s	401	CDL	OB8-CB7	2.81	1.41	1.33
50	G	201	8Q1	C39-N41	2.79	1.39	1.33
46	A	502	FMN	C4-N3	-2.73	1.33	1.38
53	s	402	UQ	C6-C1	2.73	1.54	1.46
49	j	203	PLX	O6-C4	-2.68	1.41	1.44
49	r	502	PLX	O6-C4	-2.65	1.41	1.44
53	J	402	UQ	C6-C1	2.60	1.53	1.46
48	B	303	PEE	O2-C2	-2.60	1.40	1.46
50	X	201	8Q1	C6-C1	2.56	1.53	1.50
48	C	302	PEE	O2-C2	-2.56	1.40	1.46
51	l	702	CDL	OA6-CA4	-2.55	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.55	1.37	1.43
49	r	503	PLX	O6-C4	-2.55	1.41	1.44
48	j	202	PEE	O2-C2	-2.53	1.40	1.46
51	r	504	CDL	OA6-CA4	-2.52	1.40	1.46
48	j	201	PEE	O2-C2	-2.51	1.40	1.46
48	W	201	PEE	O2-C2	-2.48	1.40	1.46
53	J	402	UQ	C7-C8	2.48	1.54	1.50
53	s	402	UQ	C7-C8	2.48	1.54	1.50
51	a	201	CDL	OA6-CA4	-2.46	1.40	1.46
48	l	704	PEE	O2-C2	-2.45	1.40	1.46
48	j	202	PEE	O3-C30	2.44	1.40	1.33
49	j	203	PLX	C7-C6	2.44	1.55	1.50
48	r	501	PEE	O2-C2	-2.43	1.40	1.46
48	Q	501	PEE	O2-C2	-2.43	1.40	1.46
48	B	303	PEE	O3-C30	2.43	1.40	1.33
48	C	302	PEE	O3-C30	2.43	1.40	1.33
48	b	201	PEE	O3-C30	2.42	1.40	1.33
48	l	701	PEE	O3-C30	2.41	1.40	1.33
49	J	403	PLX	C7-C6	2.41	1.55	1.50
48	r	501	PEE	O3-C30	2.40	1.40	1.33
51	V	202	CDL	OA6-CA4	-2.38	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	704	PEE	O3-C30	2.38	1.40	1.33
48	W	201	PEE	O2-C10	2.37	1.41	1.34
51	s	401	CDL	OA6-CA4	-2.37	1.40	1.46
49	r	502	PLX	C7-C6	2.37	1.55	1.50
48	l	701	PEE	O2-C2	-2.35	1.40	1.46
48	Q	501	PEE	O3-C30	2.35	1.40	1.33
48	b	201	PEE	O2-C2	-2.35	1.40	1.46
47	A	503	NAI	PN-O5D	2.32	1.68	1.59
51	V	201	CDL	OB6-CB4	-2.32	1.40	1.46
48	j	201	PEE	O3-C30	2.32	1.40	1.33
48	W	201	PEE	O3-C30	2.32	1.40	1.33
46	A	502	FMN	C4A-N5	2.31	1.35	1.30
49	a	202	PLX	C7-C6	2.30	1.55	1.50
49	r	503	PLX	C7-C6	2.29	1.55	1.50
51	k	101	CDL	OB6-CB4	-2.27	1.40	1.46
48	b	201	PEE	O2-C10	2.26	1.40	1.34
49	g	201	PLX	C7-C6	2.26	1.55	1.50
47	A	503	NAI	C5B-C4B	2.25	1.58	1.51
48	W	201	PEE	O3-C3	-2.25	1.40	1.45
48	l	701	PEE	O2-C10	2.24	1.40	1.34
48	r	501	PEE	O3-C3	-2.23	1.40	1.45
51	V	202	CDL	PB2-OB2	2.22	1.68	1.59
48	Q	501	PEE	O3-C3	-2.21	1.40	1.45
53	J	402	UQ	O4-C4	-2.20	1.18	1.23
51	V	201	CDL	PB2-OB2	2.20	1.68	1.59
48	j	202	PEE	O2-C10	2.19	1.40	1.34
51	V	202	CDL	OB6-CB4	-2.19	1.41	1.46
48	C	302	PEE	O2-C10	2.19	1.40	1.34
48	Q	501	PEE	O2-C10	2.19	1.40	1.34
48	B	303	PEE	O3-C3	-2.19	1.40	1.45
51	l	702	CDL	OB6-CB4	-2.19	1.41	1.46
48	j	201	PEE	O3-C3	-2.19	1.40	1.45
51	s	401	CDL	PB2-OB2	2.19	1.68	1.59
51	k	101	CDL	OA6-CA4	-2.18	1.41	1.46
48	l	704	PEE	O2-C10	2.18	1.40	1.34
53	s	402	UQ	O4-C4	-2.18	1.18	1.23
51	s	401	CDL	OB6-CB4	-2.18	1.41	1.46
48	r	501	PEE	O2-C10	2.18	1.40	1.34
51	l	702	CDL	PB2-OB5	2.18	1.68	1.59
51	V	202	CDL	PB2-OB5	2.17	1.68	1.59
51	r	504	CDL	PB2-OB2	2.16	1.68	1.59
51	a	201	CDL	PB2-OB5	2.16	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	101	CDL	PB2-OB5	2.16	1.68	1.59
48	j	201	PEE	O2-C10	2.15	1.40	1.34
51	k	101	CDL	PB2-OB2	2.15	1.68	1.59
51	r	504	CDL	PB2-OB5	2.15	1.68	1.59
49	J	403	PLX	O6-C4	-2.15	1.41	1.44
51	V	201	CDL	C11-CA5	2.14	1.57	1.50
48	B	303	PEE	O2-C10	2.14	1.40	1.34
48	b	201	PEE	O3-C3	-2.14	1.40	1.45
51	a	201	CDL	PB2-OB2	2.14	1.68	1.59
46	A	502	FMN	C5A-N5	-2.13	1.35	1.39
51	l	702	CDL	PB2-OB2	2.13	1.67	1.59
49	a	202	PLX	P1-O4	2.13	1.67	1.59
51	r	504	CDL	OB6-CB4	-2.13	1.41	1.46
52	J	401	NDP	O5D-C5D	-2.13	1.36	1.44
51	V	201	CDL	PB2-OB5	2.10	1.67	1.59
48	C	302	PEE	O3-C3	-2.10	1.40	1.45
49	J	403	PLX	P1-O4	2.10	1.67	1.59
51	a	201	CDL	OB6-CB4	-2.10	1.41	1.46
49	r	502	PLX	P1-O4	2.09	1.67	1.59
49	j	203	PLX	P1-O4	2.08	1.67	1.59
48	j	202	PEE	O3-C3	-2.07	1.40	1.45
49	r	503	PLX	P1-O4	2.06	1.67	1.59
53	J	402	UQ	O1-C1	-2.06	1.18	1.23
48	l	701	PEE	O3-C3	-2.06	1.40	1.45
53	s	402	UQ	C21-C19	2.05	1.55	1.51
51	s	401	CDL	PB2-OB5	2.04	1.67	1.59
53	J	402	UQ	O3-CM3	-2.03	1.40	1.45
53	J	402	UQ	C21-C19	2.03	1.55	1.51
53	s	402	UQ	O1-C1	-2.02	1.19	1.23
49	j	203	PLX	P1-O1	2.01	1.67	1.59
51	V	201	CDL	OA6-CA4	-2.01	1.41	1.46
49	g	201	PLX	P1-O4	2.01	1.67	1.59
49	r	503	PLX	P1-O1	2.01	1.67	1.59
49	r	502	PLX	P1-O1	2.01	1.67	1.59
48	l	704	PEE	O3-C3	-2.00	1.40	1.45

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C7-C8-C9	-7.91	113.62	126.79
53	s	402	UQ	C7-C8-C9	-7.83	113.75	126.79
52	J	401	NDP	PN-O3-PA	-7.11	108.43	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C12-C13-C14	-6.28	112.53	127.66
53	J	402	UQ	C17-C18-C19	-6.24	112.64	127.66
53	s	402	UQ	C22-C23-C24	-5.94	113.35	127.66
53	s	402	UQ	C12-C13-C14	-5.76	113.80	127.66
53	s	402	UQ	C17-C18-C19	-5.71	113.92	127.66
50	G	201	8Q1	C6-C1-S44	4.72	118.95	113.46
50	X	201	8Q1	C6-C1-S44	4.61	118.83	113.46
57	w	401	ADP	N3-C2-N1	-4.48	121.67	128.68
53	J	402	UQ	C22-C23-C24	-4.46	112.50	127.75
53	s	402	UQ	C10-C9-C8	-4.46	112.24	123.68
47	A	503	NAI	N3A-C2A-N1A	-4.44	121.74	128.68
48	r	501	PEE	O2-C10-C11	4.40	120.99	111.50
53	J	402	UQ	C15-C14-C13	-4.38	112.44	123.68
48	j	202	PEE	O2-C10-C11	4.31	120.79	111.50
53	s	402	UQ	C21-C19-C18	-4.26	112.49	121.12
53	s	402	UQ	C25-C24-C23	-4.26	112.75	123.68
53	s	402	UQ	C27-C28-C29	-4.23	113.31	127.75
53	J	402	UQ	C10-C9-C8	-4.21	112.87	123.68
51	V	201	CDL	OA6-CA5-C11	4.21	120.57	111.50
51	s	401	CDL	OB6-CB5-C51	4.16	120.47	111.50
53	s	402	UQ	C16-C14-C13	-4.15	112.71	121.12
53	s	402	UQ	C11-C9-C8	-4.15	112.71	121.12
51	s	401	CDL	OA6-CA5-C11	4.12	120.39	111.50
53	J	402	UQ	C16-C14-C13	-4.10	112.82	121.12
53	J	402	UQ	C20-C19-C18	-4.09	113.18	123.68
51	l	702	CDL	OB6-CB5-C51	4.06	120.25	111.50
51	l	703	CDL	OB6-CB5-C51	4.04	120.22	111.50
48	l	704	PEE	O2-C10-C11	4.04	120.22	111.50
51	k	101	CDL	OB6-CB5-C51	4.04	120.21	111.50
51	I	201	CDL	OA6-CA5-C11	4.04	120.20	111.50
51	l	703	CDL	OA6-CA5-C11	4.03	120.18	111.50
53	J	402	UQ	C11-C9-C8	-4.02	112.97	121.12
51	V	202	CDL	OB6-CB5-C51	4.02	120.17	111.50
51	I	201	CDL	OB6-CB5-C51	4.01	120.14	111.50
48	l	701	PEE	O2-C10-C11	4.01	120.14	111.50
48	b	201	PEE	O2-C10-C11	3.99	120.09	111.50
48	C	302	PEE	O2-C10-C11	3.98	120.09	111.50
51	n	101	CDL	OB6-CB5-C51	3.97	120.06	111.50
51	r	504	CDL	OB6-CB5-C51	3.97	120.05	111.50
51	a	201	CDL	OA6-CA5-C11	3.96	120.04	111.50
51	a	201	CDL	OB6-CB5-C51	3.96	120.04	111.50
53	s	402	UQ	C20-C19-C18	-3.94	113.58	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	r	504	CDL	OA6-CA5-C11	3.91	119.93	111.50
53	s	402	UQ	C26-C24-C23	-3.91	113.20	121.12
53	s	402	UQ	C15-C14-C13	-3.91	113.65	123.68
48	j	201	PEE	O2-C10-C11	3.91	119.92	111.50
51	l	702	CDL	OA6-CA5-C11	3.91	119.92	111.50
51	V	202	CDL	OA6-CA5-C11	3.85	119.81	111.50
51	n	101	CDL	OA6-CA5-C11	3.80	119.69	111.50
51	V	201	CDL	OB6-CB5-C51	3.79	119.67	111.50
48	Q	501	PEE	O2-C10-C11	3.77	119.63	111.50
48	B	303	PEE	O2-C10-C11	3.75	119.58	111.50
50	G	201	8Q1	C43-S44-C1	3.73	113.50	101.87
48	W	201	PEE	O2-C10-C11	3.73	119.55	111.50
50	X	201	8Q1	O35-C34-N36	-3.66	115.13	122.99
50	X	201	8Q1	C43-S44-C1	3.62	113.13	101.87
53	J	402	UQ	C21-C19-C18	-3.61	113.81	121.12
51	k	101	CDL	OA6-CA5-C11	3.57	119.20	111.50
53	s	402	UQ	C30-C29-C28	-3.41	112.81	122.65
52	J	401	NDP	O2B-P2B-O1X	-3.31	96.62	109.39
53	J	402	UQ	C26-C24-C23	-3.28	113.17	122.65
53	s	402	UQ	C31-C29-C28	-3.26	113.23	122.65
53	J	402	UQ	C25-C24-C23	-3.17	113.50	122.65
50	G	201	8Q1	O35-C34-N36	-3.15	116.22	122.99
51	n	101	CDL	OA8-CA7-C31	3.11	119.53	111.38
51	n	101	CDL	OB8-CB7-C71	3.07	121.55	111.91
47	A	503	NAI	C4D-O4D-C1D	-3.06	102.71	109.47
48	Q	501	PEE	O3-C30-C31	3.03	121.41	111.91
52	J	401	NDP	PA-O5B-C5B	-3.02	103.95	121.68
50	X	201	8Q1	O2-P24-O27	-2.94	98.90	106.73
50	X	201	8Q1	C32-C34-N36	2.93	122.41	116.58
47	A	503	NAI	C3D-C2D-C1D	2.92	106.97	101.43
48	B	303	PEE	O3-C30-C31	2.88	120.96	111.91
51	l	702	CDL	OA8-CA7-C31	2.87	120.90	111.91
48	l	704	PEE	O3-C30-C31	2.86	120.89	111.91
50	G	201	8Q1	O2-P24-O27	-2.81	99.25	106.73
51	l	703	CDL	OB8-CB7-C71	2.81	120.72	111.91
52	J	401	NDP	PN-O5D-C5D	-2.80	105.23	121.68
46	A	502	FMN	C4A-C10-N1	-2.77	118.29	124.73
51	k	101	CDL	OB8-CB7-C71	2.77	120.60	111.91
51	I	201	CDL	OA8-CA7-C31	2.74	120.51	111.91
51	a	201	CDL	OB8-CB7-C71	2.72	120.45	111.91
51	V	202	CDL	OB8-CB7-C71	2.71	120.41	111.91
51	r	504	CDL	OB8-CB7-C71	2.71	120.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	l	703	CDL	OA8-CA7-C31	2.71	120.40	111.91
51	V	202	CDL	OA8-CA7-C31	2.68	120.31	111.91
51	I	201	CDL	OB8-CB7-C71	2.68	120.31	111.91
51	l	702	CDL	OB8-CB7-C71	2.67	120.28	111.91
50	X	201	8Q1	O40-C39-N41	-2.66	117.99	123.01
51	V	201	CDL	OB8-CB7-C71	2.64	120.20	111.91
51	s	401	CDL	OA8-CA7-C31	2.63	120.16	111.91
50	G	201	8Q1	O40-C39-N41	-2.63	118.05	123.01
57	w	401	ADP	PA-O3A-PB	-2.63	123.81	132.83
48	r	501	PEE	O3-C30-C31	2.62	120.14	111.91
50	G	201	8Q1	C37-C38-C39	2.62	116.72	112.36
49	g	201	PLX	C1A-N1-C1	2.62	120.63	109.92
48	j	202	PEE	O3-C30-C31	2.61	120.11	111.91
51	k	101	CDL	OA8-CA7-C31	2.61	120.11	111.91
47	A	503	NAI	C2D-C3D-C4D	2.59	107.68	102.64
52	J	401	NDP	O4B-C4B-C3B	2.59	110.24	105.11
48	b	201	PEE	O3-C30-C31	2.57	119.97	111.91
51	I	201	CDL	CB4-OB6-CB5	-2.57	111.48	117.79
51	a	201	CDL	OA8-CA7-C31	2.56	119.95	111.91
48	W	201	PEE	O3-C30-C31	2.56	119.93	111.91
51	s	401	CDL	OB8-CB7-C71	2.55	119.91	111.91
52	J	401	NDP	O3X-P2B-O2X	2.55	117.37	107.64
51	r	504	CDL	OA8-CA7-C31	2.54	119.89	111.91
48	C	302	PEE	O3-C30-C31	2.54	119.89	111.91
50	G	201	8Q1	C32-C34-N36	2.52	121.60	116.58
53	J	402	UQ	CM5-C5-C6	-2.51	120.30	124.40
51	I	201	CDL	CA6-CA4-CA3	-2.48	105.92	111.79
48	j	201	PEE	O3-C30-C31	2.47	119.65	111.91
52	J	401	NDP	C2A-N1A-C6A	-2.46	114.54	118.75
47	A	503	NAI	C4A-C5A-N7A	-2.46	106.83	109.40
49	j	203	PLX	C1A-N1-C1	2.46	119.97	109.92
46	A	502	FMN	C4-C4A-N5	2.45	121.72	118.23
49	r	503	PLX	C1A-N1-C1	2.45	119.93	109.92
48	l	701	PEE	O3-C30-C31	2.44	119.57	111.91
50	X	201	8Q1	O4-C1-C6	-2.44	121.10	123.99
50	G	201	8Q1	O4-C1-S44	-2.43	119.46	122.61
48	j	202	PEE	C2-O2-C10	-2.39	111.90	117.79
51	l	703	CDL	CB4-OB6-CB5	-2.39	111.90	117.79
49	r	502	PLX	C1A-N1-C1	2.39	119.68	109.92
52	J	401	NDP	O5D-PN-O1N	-2.38	99.76	109.07
50	G	201	8Q1	O1-P24-O2	2.38	116.74	107.64
49	a	202	PLX	C1A-N1-C1	2.35	119.52	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G	201	8Q1	C38-C39-N41	2.35	120.37	116.42
50	X	201	8Q1	O1-P24-O2	2.34	116.60	107.64
50	X	201	8Q1	C38-C39-N41	2.33	120.35	116.42
49	J	403	PLX	C1A-N1-C1	2.32	119.41	109.92
52	J	401	NDP	O2N-PN-O1N	2.32	123.69	112.24
46	A	502	FMN	O2-C2-N1	-2.30	118.02	121.83
51	V	201	CDL	OA8-CA7-C31	2.28	119.06	111.91
47	A	503	NAI	C3B-C2B-C1B	2.25	104.36	100.98
53	s	402	UQ	CM5-C5-C6	-2.24	120.75	124.40
46	A	502	FMN	O4-C4-C4A	-2.23	120.69	126.60
57	w	401	ADP	C4-C5-N7	-2.19	107.11	109.40
46	A	502	FMN	C10-N1-C2	2.17	121.25	116.90
51	n	101	CDL	OB8-CB7-OB9	-2.17	118.11	123.59
52	J	401	NDP	C5B-C4B-C3B	-2.17	107.06	115.18
50	G	201	8Q1	O27-P24-O3	-2.13	100.50	106.47
46	A	502	FMN	C4A-C4-N3	2.11	118.55	113.19
46	A	502	FMN	C4-N3-C2	-2.11	121.75	125.64
50	X	201	8Q1	C37-C38-C39	2.10	115.86	112.36
53	J	402	UQ	C10-C9-C11	-2.07	111.80	115.27
48	l	701	PEE	C2-O2-C10	-2.06	112.71	117.79
57	w	401	ADP	O4'-C1'-C2'	-2.06	103.92	106.93
49	C	303	PLX	C6-O6-C4	-2.04	111.12	115.20
50	G	201	8Q1	O4-C1-C6	-2.04	121.58	123.99
50	X	201	8Q1	O27-P24-O3	-2.02	100.80	106.47
47	A	503	NAI	PN-O3-PA	-2.02	125.89	132.83

There are no chirality outliers.

All (1094) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C2'-C1'-N10-C10
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	A	503	NAI	C5B-O5B-PA-O3
48	B	303	PEE	O4P-C4-C5-N
48	C	302	PEE	C11-C10-O2-C2
48	C	302	PEE	O4P-C4-C5-N
48	Q	501	PEE	C11-C10-O2-C2
48	Q	501	PEE	O4-C10-O2-C2
48	Q	501	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	Q	501	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C4-O4P-P-O1P
48	W	201	PEE	O4P-C4-C5-N
48	b	201	PEE	C37-C38-C39-C40
48	j	201	PEE	C19-C20-C21-C22
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O1P
48	l	701	PEE	C11-C10-O2-C2
48	l	701	PEE	C2-C1-O3P-P
48	l	701	PEE	C4-O4P-P-O1P
48	l	701	PEE	C39-C40-C41-C42
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	C4-O4P-P-O3P
48	l	704	PEE	C4-O4P-P-O2P
48	l	704	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	C1-C2-O1-P1
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	O9-C24-O8-C5
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C5-C4-O6-C6
49	a	202	PLX	C3-O4-P1-O2
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-C25-C26
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O6-C4-C5-O8
49	g	201	PLX	O9-C24-C25-C26
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	O9-C24-O8-C5
49	j	203	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	C25-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C2-O1-P1-O2
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	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	C28-O27-P24-O3
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	O27-C28-C29-C30
50	X	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	C29-C32-C34-N36
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C42-C43-S44-C1
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	CA6-CA4-OA6-CA5
51	I	201	CDL	CB2-OB2-PB2-OB4
51	I	201	CDL	CB3-OB5-PB2-OB4
51	V	201	CDL	CA2-C1-CB2-OB2
51	V	201	CDL	CA2-OA2-PA1-OA3
51	V	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CA2-OA2-PA1-OA5
51	V	201	CDL	C11-CA5-OA6-CA4
51	V	201	CDL	CB2-OB2-PB2-OB3
51	V	201	CDL	CB3-OB5-PB2-OB3
51	V	201	CDL	CB3-OB5-PB2-OB4
51	V	202	CDL	CB2-C1-CA2-OA2
51	V	202	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	CA3-OA5-PA1-OA3
51	V	202	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CA2-C1-CB2-OB2
51	a	201	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CB3-OB5-PB2-OB4
51	k	101	CDL	CA2-OA2-PA1-OA3
51	k	101	CDL	CA3-OA5-PA1-OA2
51	k	101	CDL	OA5-CA3-CA4-OA6
51	k	101	CDL	OB5-CB3-CB4-OB6
51	l	702	CDL	CA2-C1-CB2-OB2
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	CA3-OA5-PA1-OA3
51	l	702	CDL	OA9-CA7-OA8-CA6
51	l	702	CDL	C31-CA7-OA8-CA6
51	l	702	CDL	CB2-OB2-PB2-OB3
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	703	CDL	CA2-OA2-PA1-OA4
51	l	703	CDL	CA3-OA5-PA1-OA2
51	l	703	CDL	CA3-OA5-PA1-OA3
51	l	703	CDL	CA3-OA5-PA1-OA4
51	l	703	CDL	CB3-OB5-PB2-OB4
51	n	101	CDL	CA2-OA2-PA1-OA3
51	n	101	CDL	CA2-OA2-PA1-OA4
51	n	101	CDL	CA2-OA2-PA1-OA5
51	n	101	CDL	CA3-OA5-PA1-OA3
51	n	101	CDL	CB3-OB5-PB2-OB2
51	n	101	CDL	CB3-OB5-PB2-OB3
51	n	101	CDL	CB3-OB5-PB2-OB4
51	r	504	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CB3-OB5-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB4
51	s	401	CDL	CA2-C1-CB2-OB2
51	s	401	CDL	CA2-OA2-PA1-OA3
51	s	401	CDL	CA2-OA2-PA1-OA4
53	J	402	UQ	C7-C8-C9-C10
53	J	402	UQ	C12-C11-C9-C10
53	J	402	UQ	C17-C18-C19-C20
53	s	402	UQ	C7-C8-C9-C10
53	s	402	UQ	C7-C8-C9-C11
53	s	402	UQ	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
57	w	401	ADP	C5'-O5'-PA-O3A
51	s	401	CDL	OA9-CA7-OA8-CA6
51	l	703	CDL	CA4-CA6-OA8-CA7
51	s	401	CDL	C31-CA7-OA8-CA6
48	Q	501	PEE	O5-C30-O3-C3
48	C	302	PEE	O4-C10-O2-C2
48	l	701	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
51	I	201	CDL	OA7-CA5-OA6-CA4
51	V	201	CDL	OA7-CA5-OA6-CA4
48	Q	501	PEE	C31-C30-O3-C3
51	I	201	CDL	C11-CA5-OA6-CA4
53	J	402	UQ	C18-C19-C21-C22
48	j	202	PEE	C31-C30-O3-C3
48	j	201	PEE	C17-C18-C19-C20
53	J	402	UQ	C7-C8-C9-C11
53	J	402	UQ	C12-C13-C14-C16
53	s	402	UQ	C17-C18-C19-C21
53	s	402	UQ	C22-C23-C24-C26
48	j	202	PEE	O5-C30-O3-C3
49	g	201	PLX	C9-C10-C11-C12
51	I	201	CDL	O1-C1-CA2-OA2
51	I	201	CDL	O1-C1-CB2-OB2
51	V	201	CDL	O1-C1-CA2-OA2
51	V	202	CDL	O1-C1-CA2-OA2
51	a	201	CDL	O1-C1-CA2-OA2
51	k	101	CDL	O1-C1-CB2-OB2
51	l	703	CDL	O1-C1-CA2-OA2
51	s	401	CDL	O1-C1-CA2-OA2
49	g	201	PLX	C7-C8-C9-C10
48	j	202	PEE	C11-C10-O2-C2
51	V	202	CDL	C51-CB5-OB6-CB4
51	a	201	CDL	C51-CB5-OB6-CB4
51	r	504	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C30-C31-C32-C33
48	W	201	PEE	C22-C23-C24-C25
51	V	202	CDL	C32-C33-C34-C35
51	r	504	CDL	C60-C61-C62-C63
51	s	401	CDL	C37-C38-C39-C40
51	a	201	CDL	C36-C37-C38-C39
51	k	101	CDL	C73-C74-C75-C76
52	J	401	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	OB7-CB5-OB6-CB4
51	r	504	CDL	C74-C75-C76-C77
51	V	201	CDL	C62-C63-C64-C65
53	J	402	UQ	C22-C23-C24-C26
53	J	402	UQ	C13-C14-C16-C17
51	l	703	CDL	C35-C36-C37-C38
53	J	402	UQ	C19-C21-C22-C23
51	l	702	CDL	C55-C56-C57-C58
48	l	701	PEE	C31-C30-O3-C3
51	l	703	CDL	C71-CB7-OB8-CB6
49	g	201	PLX	C17-C18-C19-C20
49	r	502	PLX	C7-C8-C9-C10
53	s	402	UQ	C27-C28-C29-C31
48	B	303	PEE	C22-C23-C24-C25
48	b	201	PEE	C10-C11-C12-C13
51	a	201	CDL	CB2-C1-CA2-OA2
51	r	504	CDL	OB7-CB5-OB6-CB4
48	l	701	PEE	O5-C30-O3-C3
51	l	703	CDL	OB9-CB7-OB8-CB6
48	C	302	PEE	C41-C42-C43-C44
48	W	201	PEE	C11-C12-C13-C14
51	V	201	CDL	C59-C60-C61-C62
49	g	201	PLX	C2-C1-N1-C1A
48	j	201	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
51	I	201	CDL	C31-CA7-OA8-CA6
51	V	201	CDL	C71-CB7-OB8-CB6
51	l	702	CDL	C71-CB7-OB8-CB6
51	s	401	CDL	C71-CB7-OB8-CB6
49	j	203	PLX	C13-C14-C15-C16
50	X	201	8Q1	C10-C11-C12-C13
48	j	201	PEE	C32-C33-C34-C35
51	k	101	CDL	C40-C41-C42-C43
51	V	202	CDL	O1-C1-CB2-OB2
51	l	702	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CB2-OB2
51	l	702	CDL	CB5-C51-C52-C53
48	Q	501	PEE	C11-C12-C13-C14
51	l	702	CDL	C58-C59-C60-C61
48	l	701	PEE	C11-C12-C13-C14
49	J	403	PLX	C11-C10-C9-C8
51	k	101	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	C17-C18-C19-C20
49	r	502	PLX	C9-C10-C11-C12
46	A	502	FMN	O2'-C2'-C3'-O3'
53	s	402	UQ	C22-C23-C24-C25
48	r	501	PEE	C10-C11-C12-C13
51	a	201	CDL	CB5-C51-C52-C53
51	l	702	CDL	CB7-C71-C72-C73
51	n	101	CDL	CB7-C71-C72-C73
52	J	401	NDP	C3D-C4D-C5D-O5D
51	V	201	CDL	C34-C35-C36-C37
51	r	504	CDL	C23-C24-C25-C26
48	j	202	PEE	O4-C10-O2-C2
51	a	201	CDL	OB7-CB5-OB6-CB4
49	g	201	PLX	C2-C1-N1-C1B
51	l	702	CDL	CA7-C31-C32-C33
51	k	101	CDL	C11-CA5-OA6-CA4
51	k	101	CDL	C36-C37-C38-C39
48	l	704	PEE	O5-C30-O3-C3
51	l	702	CDL	OB9-CB7-OB8-CB6
51	s	401	CDL	OB9-CB7-OB8-CB6
48	j	201	PEE	O5-C30-O3-C3
51	I	201	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	OB9-CB7-OB8-CB6
53	s	402	UQ	C14-C16-C17-C18
51	l	703	CDL	CB5-C51-C52-C53
51	V	201	CDL	O1-C1-CB2-OB2
51	a	201	CDL	O1-C1-CB2-OB2
51	k	101	CDL	C16-C17-C18-C19
48	l	704	PEE	C37-C38-C39-C40
50	X	201	8Q1	C6-C7-C8-C9
48	B	303	PEE	C11-C10-O2-C2
48	b	201	PEE	C11-C10-O2-C2
48	Q	501	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	l	701	PEE	C1-O3P-P-O4P
49	C	303	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O4
51	I	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
51	I	201	CDL	CA3-OA5-PA1-OA2
51	I	201	CDL	CB2-OB2-PB2-OB5
51	I	201	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	CB2-OB2-PB2-OB5
51	V	201	CDL	CB3-OB5-PB2-OB2
51	V	202	CDL	CA2-OA2-PA1-OA5
51	V	202	CDL	CB2-OB2-PB2-OB5
51	V	202	CDL	CB3-OB5-PB2-OB2
51	a	201	CDL	CB3-OB5-PB2-OB2
51	k	101	CDL	CB3-OB5-PB2-OB2
51	l	703	CDL	CA2-OA2-PA1-OA5
51	r	504	CDL	CB2-OB2-PB2-OB5
51	s	401	CDL	CA2-OA2-PA1-OA5
51	s	401	CDL	C33-C34-C35-C36
51	k	101	CDL	C60-C61-C62-C63
51	k	101	CDL	C58-C59-C60-C61
51	V	201	CDL	CB2-C1-CA2-OA2
51	s	401	CDL	CB2-C1-CA2-OA2
48	B	303	PEE	O4-C10-O2-C2
48	b	201	PEE	O4-C10-O2-C2
51	k	101	CDL	OA7-CA5-OA6-CA4
53	J	402	UQ	C20-C19-C21-C22
51	s	401	CDL	C31-C32-C33-C34
48	W	201	PEE	C31-C30-O3-C3
48	b	201	PEE	C31-C30-O3-C3
49	r	502	PLX	O6-C6-C7-C8
49	g	201	PLX	C28-C29-C30-C31
50	G	201	8Q1	C10-C11-C12-C13
48	r	501	PEE	C11-C10-O2-C2
51	I	201	CDL	C51-CB5-OB6-CB4
51	l	703	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	C31-C32-C33-C34
48	C	302	PEE	C13-C14-C15-C16
49	C	303	PLX	C14-C15-C16-C17
49	C	303	PLX	C11-C12-C13-C14
49	C	303	PLX	C10-C11-C12-C13
49	a	202	PLX	C14-C15-C16-C17
49	a	202	PLX	C25-C26-C27-C28
49	j	203	PLX	C16-C17-C18-C19
51	V	201	CDL	C55-C56-C57-C58
51	V	202	CDL	C13-C14-C15-C16
51	V	202	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
51	k	101	CDL	C55-C56-C57-C58
51	l	702	CDL	C56-C57-C58-C59
51	l	702	CDL	C71-C72-C73-C74
51	l	702	CDL	C74-C75-C76-C77
51	l	703	CDL	C34-C35-C36-C37
51	s	401	CDL	C17-C18-C19-C20
51	s	401	CDL	C52-C53-C54-C55
50	X	201	8Q1	O27-C28-C29-C31
51	l	703	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C13-C14-C15-C16
48	B	303	PEE	C12-C13-C14-C15
48	W	201	PEE	C13-C14-C15-C16
48	b	201	PEE	C31-C32-C33-C34
48	r	501	PEE	C11-C12-C13-C14
49	J	403	PLX	C14-C15-C16-C17
49	J	403	PLX	C7-C8-C9-C10
49	g	201	PLX	C13-C14-C15-C16
49	j	203	PLX	C14-C15-C16-C17
49	r	502	PLX	C34-C35-C36-C37
51	V	202	CDL	C37-C38-C39-C40
51	l	702	CDL	C36-C37-C38-C39
51	l	702	CDL	C62-C63-C64-C65
51	l	702	CDL	C75-C76-C77-C78
51	r	504	CDL	C31-C32-C33-C34
48	r	501	PEE	O4-C10-O2-C2
51	l	703	CDL	OB7-CB5-OB6-CB4
51	n	101	CDL	CB5-C51-C52-C53
46	A	502	FMN	O2'-C2'-C3'-C4'
49	J	403	PLX	C13-C14-C15-C16
49	a	202	PLX	C13-C14-C15-C16
49	g	201	PLX	C32-C33-C34-C35
49	j	203	PLX	C31-C32-C33-C34
51	V	201	CDL	C52-C53-C54-C55
51	s	401	CDL	C73-C74-C75-C76
51	a	201	CDL	OB9-CB7-OB8-CB6
48	W	201	PEE	C17-C18-C19-C20
48	B	303	PEE	C42-C43-C44-C45
48	W	201	PEE	C12-C13-C14-C15
49	J	403	PLX	C25-C26-C27-C28
49	a	202	PLX	C35-C36-C37-C38
49	j	203	PLX	C34-C35-C36-C37
49	r	502	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C60-C61-C62-C63
51	l	702	CDL	C51-C52-C53-C54
51	r	504	CDL	C75-C76-C77-C78
51	V	201	CDL	C35-C36-C37-C38
51	s	401	CDL	C11-C12-C13-C14
48	l	701	PEE	C10-C11-C12-C13
48	l	704	PEE	C31-C32-C33-C34
48	r	501	PEE	C13-C14-C15-C16
49	r	503	PLX	C25-C26-C27-C28
51	V	202	CDL	C56-C57-C58-C59
51	k	101	CDL	C21-C22-C23-C24
51	l	702	CDL	C19-C20-C21-C22
51	s	401	CDL	C75-C76-C77-C78
48	l	704	PEE	C21-C22-C23-C24
49	j	203	PLX	C7-C8-C9-C10
49	r	503	PLX	C12-C13-C14-C15
51	V	202	CDL	C55-C56-C57-C58
51	a	201	CDL	C35-C36-C37-C38
51	a	201	CDL	C37-C38-C39-C40
51	l	703	CDL	C71-C72-C73-C74
53	s	402	UQ	C23-C24-C26-C27
51	r	504	CDL	CA7-C31-C32-C33
48	j	201	PEE	C42-C43-C44-C45
48	l	704	PEE	C34-C35-C36-C37
49	J	403	PLX	C27-C28-C29-C30
49	g	201	PLX	C30-C31-C32-C33
51	V	201	CDL	C37-C38-C39-C40
51	V	202	CDL	C54-C55-C56-C57
51	k	101	CDL	C71-C72-C73-C74
51	l	702	CDL	C52-C53-C54-C55
51	l	703	CDL	C54-C55-C56-C57
51	r	504	CDL	C71-C72-C73-C74
51	s	401	CDL	C51-C52-C53-C54
49	j	203	PLX	C29-C30-C31-C32
49	r	503	PLX	C35-C36-C37-C38
51	V	202	CDL	C33-C34-C35-C36
51	a	201	CDL	C60-C61-C62-C63
51	l	703	CDL	C58-C59-C60-C61
51	l	703	CDL	C59-C60-C61-C62
51	I	201	CDL	OB7-CB5-OB6-CB4
48	C	302	PEE	C42-C43-C44-C45
49	C	303	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C10-C11-C12-C13
51	V	201	CDL	C58-C59-C60-C61
51	r	504	CDL	C62-C63-C64-C65
51	s	401	CDL	CB5-C51-C52-C53
48	B	303	PEE	C23-C24-C25-C26
48	b	201	PEE	C33-C34-C35-C36
48	l	701	PEE	C32-C33-C34-C35
48	r	501	PEE	C40-C41-C42-C43
49	C	303	PLX	C11-C10-C9-C8
49	J	403	PLX	C9-C10-C11-C12
49	j	203	PLX	C33-C34-C35-C36
51	V	201	CDL	C71-C72-C73-C74
51	V	202	CDL	C34-C35-C36-C37
51	V	202	CDL	C52-C53-C54-C55
51	a	201	CDL	C52-C53-C54-C55
51	k	101	CDL	C75-C76-C77-C78
51	s	401	CDL	C55-C56-C57-C58
51	s	401	CDL	C71-C72-C73-C74
49	g	201	PLX	C2-C1-N1-C1C
49	J	403	PLX	O4-C3-C4-C5
48	C	302	PEE	C43-C44-C45-C46
51	V	201	CDL	C12-C13-C14-C15
51	a	201	CDL	C73-C74-C75-C76
51	l	702	CDL	C73-C74-C75-C76
51	s	401	CDL	C54-C55-C56-C57
49	J	403	PLX	C33-C34-C35-C36
51	l	703	CDL	C33-C34-C35-C36
51	r	504	CDL	C57-C58-C59-C60
51	V	201	CDL	CA5-C11-C12-C13
49	r	503	PLX	C13-C14-C15-C16
51	a	201	CDL	C32-C33-C34-C35
51	r	504	CDL	C32-C33-C34-C35
51	r	504	CDL	C83-C84-C85-C86
51	s	401	CDL	C59-C60-C61-C62
51	l	703	CDL	C51-C52-C53-C54
49	r	503	PLX	C31-C32-C33-C34
51	k	101	CDL	C59-C60-C61-C62
51	l	703	CDL	C21-C22-C23-C24
48	j	201	PEE	C22-C23-C24-C25
49	g	201	PLX	C33-C34-C35-C36
51	l	702	CDL	C59-C60-C61-C62
51	l	703	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C13-C14-C15-C16
49	g	201	PLX	C10-C11-C12-C13
51	l	703	CDL	C72-C73-C74-C75
51	V	202	CDL	C71-CB7-OB8-CB6
49	a	202	PLX	C16-C17-C18-C19
51	l	702	CDL	C13-C14-C15-C16
49	r	502	PLX	C33-C34-C35-C36
51	a	201	CDL	C22-C23-C24-C25
51	r	504	CDL	C43-C44-C45-C46
51	s	401	CDL	C35-C36-C37-C38
48	l	701	PEE	C35-C36-C37-C38
48	W	201	PEE	O5-C30-O3-C3
48	b	201	PEE	O5-C30-O3-C3
48	W	201	PEE	C10-C11-C12-C13
51	V	201	CDL	C75-C76-C77-C78
51	k	101	CDL	C20-C21-C22-C23
51	r	504	CDL	C63-C64-C65-C66
51	s	401	CDL	C36-C37-C38-C39
51	s	401	CDL	CB7-C71-C72-C73
48	Q	501	PEE	C21-C22-C23-C24
49	g	201	PLX	C18-C19-C20-C21
51	a	201	CDL	C74-C75-C76-C77
51	l	703	CDL	C74-C75-C76-C77
51	l	703	CDL	OA9-CA7-OA8-CA6
49	J	403	PLX	C29-C30-C31-C32
49	a	202	PLX	C10-C11-C12-C13
51	V	201	CDL	C72-C73-C74-C75
51	V	202	CDL	C75-C76-C77-C78
49	C	303	PLX	C19-C20-C21-C22
49	r	502	PLX	C31-C32-C33-C34
49	r	503	PLX	C15-C16-C17-C18
51	k	101	CDL	C14-C15-C16-C17
51	l	703	CDL	C17-C18-C19-C20
48	j	201	PEE	C40-C41-C42-C43
49	J	403	PLX	C31-C32-C33-C34
51	V	202	CDL	C76-C77-C78-C79
51	r	504	CDL	C41-C42-C43-C44
49	r	502	PLX	C11-C10-C9-C8
51	a	201	CDL	C62-C63-C64-C65
51	l	703	CDL	C38-C39-C40-C41
53	s	402	UQ	C27-C28-C29-C30
50	X	201	8Q1	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	OB9-CB7-OB8-CB6
48	W	201	PEE	C24-C25-C26-C27
48	j	202	PEE	C11-C12-C13-C14
48	B	303	PEE	C35-C36-C37-C38
48	Q	501	PEE	C19-C20-C21-C22
48	j	202	PEE	C19-C20-C21-C22
48	j	201	PEE	O4-C10-O2-C2
49	r	503	PLX	C30-C31-C32-C33
51	l	702	CDL	C32-C33-C34-C35
49	j	203	PLX	C9-C10-C11-C12
49	r	503	PLX	C28-C29-C30-C31
51	n	101	CDL	C73-C74-C75-C76
48	l	704	PEE	C30-C31-C32-C33
49	a	202	PLX	C9-C10-C11-C12
51	k	101	CDL	C52-C53-C54-C55
51	k	101	CDL	C56-C57-C58-C59
51	k	101	CDL	C79-C80-C81-C82
51	l	702	CDL	C12-C13-C14-C15
49	r	502	PLX	C14-C15-C16-C17
51	V	202	CDL	C42-C43-C44-C45
51	k	101	CDL	C41-C42-C43-C44
51	l	702	CDL	C37-C38-C39-C40
51	r	504	CDL	C59-C60-C61-C62
48	j	201	PEE	C11-C10-O2-C2
51	V	201	CDL	C51-CB5-OB6-CB4
51	l	702	CDL	C11-CA5-OA6-CA4
51	s	401	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	C41-C42-C43-C44
48	l	704	PEE	C32-C33-C34-C35
49	j	203	PLX	C12-C13-C14-C15
49	r	503	PLX	C16-C17-C18-C19
51	r	504	CDL	C54-C55-C56-C57
51	l	702	CDL	OA7-CA5-OA6-CA4
51	V	202	CDL	OA6-CA4-CA6-OA8
51	l	702	CDL	OA6-CA4-CA6-OA8
51	s	401	CDL	OB6-CB4-CB6-OB8
51	a	201	CDL	C76-C77-C78-C79
49	r	502	PLX	C28-C29-C30-C31
51	V	201	CDL	C32-C33-C34-C35
51	V	202	CDL	C62-C63-C64-C65
48	Q	501	PEE	C35-C36-C37-C38
51	a	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
48	Q	501	PEE	C23-C24-C25-C26
48	l	704	PEE	C13-C14-C15-C16
47	A	503	NAI	C3D-C4D-C5D-O5D
48	b	201	PEE	C13-C14-C15-C16
49	r	502	PLX	C30-C31-C32-C33
48	B	303	PEE	C11-C12-C13-C14
49	a	202	PLX	C30-C31-C32-C33
51	s	401	CDL	C14-C15-C16-C17
49	C	303	PLX	C35-C36-C37-C38
51	a	201	CDL	C75-C76-C77-C78
48	r	501	PEE	C38-C39-C40-C41
48	l	701	PEE	C4-O4P-P-O3P
49	r	502	PLX	C2-O1-P1-O4
51	V	202	CDL	CA3-OA5-PA1-OA2
48	l	704	PEE	C44-C45-C46-C47
49	j	203	PLX	C27-C28-C29-C30
49	r	502	PLX	C19-C20-C21-C22
49	r	502	PLX	C11-C12-C13-C14
48	l	701	PEE	C31-C32-C33-C34
49	r	503	PLX	C7-C8-C9-C10
51	a	201	CDL	C18-C19-C20-C21
48	B	303	PEE	C31-C30-O3-C3
51	k	101	CDL	OA5-CA3-CA4-CA6
51	k	101	CDL	OB5-CB3-CB4-CB6
51	s	401	CDL	OA5-CA3-CA4-CA6
48	b	201	PEE	C22-C23-C24-C25
49	a	202	PLX	C33-C34-C35-C36
48	j	202	PEE	C10-C11-C12-C13
51	l	703	CDL	C19-C20-C21-C22
51	r	504	CDL	C84-C85-C86-C87
48	j	202	PEE	C23-C24-C25-C26
48	j	202	PEE	C22-C23-C24-C25
51	l	702	CDL	C17-C18-C19-C20
48	W	201	PEE	C19-C20-C21-C22
48	j	202	PEE	C15-C16-C17-C18
51	l	703	CDL	CB7-C71-C72-C73
49	g	201	PLX	C25-C26-C27-C28
51	V	202	CDL	C73-C74-C75-C76
51	k	101	CDL	C15-C16-C17-C18
51	l	702	CDL	C42-C43-C44-C45
48	B	303	PEE	C21-C22-C23-C24
48	B	303	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	C14-C15-C16-C17
51	r	504	CDL	C17-C18-C19-C20
51	V	202	CDL	C11-CA5-OA6-CA4
48	b	201	PEE	C1-C2-C3-O3
49	J	403	PLX	C28-C29-C30-C31
49	r	503	PLX	C3-C4-C5-O8
51	l	703	CDL	C22-C23-C24-C25
49	C	303	PLX	C4-C5-O8-C24
49	J	403	PLX	C36-C37-C38-C39
51	a	201	CDL	C84-C85-C86-C87
51	l	703	CDL	C24-C25-C26-C27
51	a	201	CDL	C39-C40-C41-C42
51	k	101	CDL	C32-C33-C34-C35
51	l	703	CDL	C64-C65-C66-C67
49	C	303	PLX	O6-C6-C7-C8
50	X	201	8Q1	O33-C32-C34-O35
53	J	402	UQ	C9-C11-C12-C13
48	j	201	PEE	C14-C15-C16-C17
51	n	101	CDL	C52-C53-C54-C55
48	l	704	PEE	C39-C40-C41-C42
48	r	501	PEE	C33-C34-C35-C36
49	r	503	PLX	C14-C15-C16-C17
51	l	703	CDL	C63-C64-C65-C66
51	a	201	CDL	C11-CA5-OA6-CA4
51	s	401	CDL	C11-CA5-OA6-CA4
51	V	202	CDL	C84-C85-C86-C87
51	n	101	CDL	C72-C73-C74-C75
48	C	302	PEE	C11-C12-C13-C14
51	r	504	CDL	C64-C65-C66-C67
51	k	101	CDL	CA6-CA4-OA6-CA5
51	V	201	CDL	OB7-CB5-OB6-CB4
49	j	203	PLX	C26-C27-C28-C29
50	X	201	8Q1	C13-C14-C15-C16
49	j	203	PLX	C25-C26-C27-C28
51	V	201	CDL	C64-C65-C66-C67
48	j	201	PEE	C38-C39-C40-C41
51	l	702	CDL	C80-C81-C82-C83
48	l	701	PEE	C17-C18-C19-C20
48	j	202	PEE	C14-C15-C16-C17
49	a	202	PLX	C28-C29-C30-C31
48	j	201	PEE	C44-C45-C46-C47
51	s	401	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C74-C75-C76-C77
51	l	703	CDL	C43-C44-C45-C46
51	l	703	CDL	C44-C45-C46-C47
51	l	703	CDL	C84-C85-C86-C87
48	l	701	PEE	O2-C2-C3-O3
51	k	101	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C32-C33-C34-C35
48	l	704	PEE	C33-C34-C35-C36
51	V	202	CDL	C35-C36-C37-C38
48	B	303	PEE	O5-C30-O3-C3
50	G	201	8Q1	C30-C29-C32-O33
48	l	701	PEE	C33-C34-C35-C36
48	Q	501	PEE	C34-C35-C36-C37
49	g	201	PLX	C27-C28-C29-C30
51	k	101	CDL	C71-CB7-OB8-CB6
51	k	101	CDL	CA2-C1-CB2-OB2
51	a	201	CDL	C54-C55-C56-C57
48	W	201	PEE	C21-C22-C23-C24
49	C	303	PLX	C33-C34-C35-C36
48	r	501	PEE	C17-C18-C19-C20
49	j	203	PLX	C11-C12-C13-C14
51	V	202	CDL	C17-C18-C19-C20
51	V	202	CDL	C82-C83-C84-C85
51	a	201	CDL	OA5-CA3-CA4-CA6
51	a	201	CDL	OB5-CB3-CB4-CB6
49	r	503	PLX	C27-C28-C29-C30
51	l	703	CDL	C20-C21-C22-C23
51	r	504	CDL	C15-C16-C17-C18
48	l	704	PEE	C10-C11-C12-C13
51	k	101	CDL	C74-C75-C76-C77
51	l	702	CDL	C15-C16-C17-C18
51	s	401	CDL	C40-C41-C42-C43
49	g	201	PLX	C12-C13-C14-C15
51	r	504	CDL	C35-C36-C37-C38
48	r	501	PEE	C31-C30-O3-C3
48	Q	501	PEE	C10-C11-C12-C13
51	r	504	CDL	CA5-C11-C12-C13
49	C	303	PLX	C7-C8-C9-C10
49	a	202	PLX	C19-C20-C21-C22
51	a	201	CDL	C71-C72-C73-C74
51	k	101	CDL	C37-C38-C39-C40
51	k	101	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C16-C17-C18-C19
49	r	502	PLX	C12-C13-C14-C15
50	X	201	8Q1	C9-C10-C11-C12
48	j	202	PEE	C1-C2-C3-O3
48	l	701	PEE	C1-C2-C3-O3
49	J	403	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
51	V	202	CDL	CA3-CA4-CA6-OA8
51	k	101	CDL	CB3-CB4-CB6-OB8
51	l	702	CDL	CA3-CA4-CA6-OA8
51	n	101	CDL	CA3-CA4-CA6-OA8
51	s	401	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	C34-C35-C36-C37
49	r	502	PLX	C13-C14-C15-C16
51	l	703	CDL	C15-C16-C17-C18
49	r	503	PLX	C32-C33-C34-C35
51	a	201	CDL	C20-C21-C22-C23
51	l	703	CDL	C39-C40-C41-C42
49	J	403	PLX	C3-C4-O6-C6
49	a	202	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O1
49	r	503	PLX	C5-C4-O6-C6
49	J	403	PLX	O9-C24-C25-C26
48	r	501	PEE	C21-C22-C23-C24
50	G	201	8Q1	C11-C12-C13-C14
48	b	201	PEE	O3P-C1-C2-O2
49	J	403	PLX	O4-C3-C4-O6
49	r	502	PLX	O4-C3-C4-O6
51	V	202	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	OB5-CB3-CB4-OB6
48	j	201	PEE	C34-C35-C36-C37
48	r	501	PEE	C42-C43-C44-C45
49	r	502	PLX	C18-C19-C20-C21
51	V	202	CDL	C39-C40-C41-C42
51	k	101	CDL	OB9-CB7-OB8-CB6
49	j	203	PLX	C36-C37-C38-C39
51	s	401	CDL	C34-C35-C36-C37
51	V	202	CDL	C12-C13-C14-C15
49	r	502	PLX	O6-C4-C5-O8
51	V	201	CDL	OB6-CB4-CB6-OB8
51	V	202	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
51	n	101	CDL	OA6-CA4-CA6-OA8
51	r	504	CDL	OA6-CA4-CA6-OA8
48	B	303	PEE	C36-C37-C38-C39
51	k	101	CDL	C33-C34-C35-C36
51	V	202	CDL	C21-C22-C23-C24
51	r	504	CDL	C19-C20-C21-C22
51	I	201	CDL	CA2-C1-CB2-OB2
51	l	703	CDL	CB2-C1-CA2-OA2
48	C	302	PEE	C12-C13-C14-C15
49	r	502	PLX	C10-C11-C12-C13
51	r	504	CDL	C13-C14-C15-C16
51	V	202	CDL	OA7-CA5-OA6-CA4
51	a	201	CDL	OA7-CA5-OA6-CA4
51	s	401	CDL	OA7-CA5-OA6-CA4
51	V	201	CDL	C43-C44-C45-C46
49	J	403	PLX	C10-C11-C12-C13
49	a	202	PLX	C7-C8-C9-C10
51	V	201	CDL	C44-C45-C46-C47
51	r	504	CDL	C53-C54-C55-C56
48	W	201	PEE	C34-C35-C36-C37
51	k	101	CDL	C77-C78-C79-C80
48	l	701	PEE	C18-C19-C20-C21
51	a	201	CDL	C11-C12-C13-C14
51	k	101	CDL	C84-C85-C86-C87
49	j	203	PLX	O6-C6-C7-C8
48	B	303	PEE	O3P-C1-C2-C3
51	V	201	CDL	OB5-CB3-CB4-CB6
51	l	702	CDL	OA5-CA3-CA4-CA6
51	l	703	CDL	C75-C76-C77-C78
51	r	504	CDL	C77-C78-C79-C80
51	n	101	CDL	C51-C52-C53-C54
48	j	201	PEE	C21-C22-C23-C24
48	j	201	PEE	C13-C14-C15-C16
48	r	501	PEE	C36-C37-C38-C39
51	V	202	CDL	C83-C84-C85-C86
48	l	704	PEE	C3-C2-O2-C10
51	V	201	CDL	CA6-CA4-OA6-CA5
51	V	202	CDL	C11-C12-C13-C14
48	C	302	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	g	201	PLX	C3-C4-C5-O8
51	k	101	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C11-C10-C9-C8
51	k	101	CDL	C51-C52-C53-C54
48	j	201	PEE	O3P-C1-C2-O2
48	l	701	PEE	O3P-C1-C2-O2
49	r	503	PLX	O4-C3-C4-O6
51	V	201	CDL	OB5-CB3-CB4-OB6
51	a	201	CDL	OA5-CA3-CA4-OA6
51	a	201	CDL	OB5-CB3-CB4-OB6
51	r	504	CDL	C72-C71-CB7-OB8
51	k	101	CDL	C64-C65-C66-C67
51	V	202	CDL	C64-C65-C66-C67
49	r	502	PLX	C6-C7-C8-C9
48	j	201	PEE	C36-C37-C38-C39
51	l	702	CDL	CB2-C1-CA2-OA2
51	l	703	CDL	C41-C42-C43-C44
48	r	501	PEE	O5-C30-O3-C3
51	s	401	CDL	C16-C17-C18-C19
51	r	504	CDL	C36-C37-C38-C39
48	b	201	PEE	O2-C2-C3-O3
48	j	202	PEE	O2-C2-C3-O3
51	r	504	CDL	C56-C57-C58-C59
51	l	703	CDL	C37-C38-C39-C40
47	A	503	NAI	C5D-O5D-PN-O3
51	k	101	CDL	C62-C63-C64-C65
48	C	302	PEE	C15-C16-C17-C18
49	C	303	PLX	C15-C16-C17-C18
51	a	201	CDL	C31-C32-C33-C34
48	B	303	PEE	C38-C39-C40-C41
49	J	403	PLX	C24-C25-C26-C27
48	r	501	PEE	C34-C35-C36-C37
50	G	201	8Q1	C7-C8-C9-C10
51	V	202	CDL	C32-C31-CA7-OA8
48	j	202	PEE	C24-C25-C26-C27
51	l	703	CDL	CA7-C31-C32-C33
51	l	703	CDL	C76-C77-C78-C79
51	k	101	CDL	C11-C12-C13-C14
48	j	201	PEE	C15-C16-C17-C18
49	J	403	PLX	C2-O1-P1-O4
51	a	201	CDL	CB2-OB2-PB2-OB5
51	n	101	CDL	CA3-OA5-PA1-OA2
51	n	101	CDL	CB2-OB2-PB2-OB5
52	J	401	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	CA7-C31-C32-C33
48	r	501	PEE	C32-C33-C34-C35
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O2A
48	Q	501	PEE	C4-O4P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	l	701	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C4-O4P-P-O2P
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C2-O1-P1-O3
49	g	201	PLX	C2-O1-P1-O3
49	j	203	PLX	C2-O1-P1-O3
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C2-O1-P1-O3
51	I	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CA2-OA2-PA1-OA4
51	V	202	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB3-OB5-PB2-OB3
51	V	202	CDL	CB3-OB5-PB2-OB4
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CB2-OB2-PB2-OB4
51	k	101	CDL	CA3-OA5-PA1-OA4
51	k	101	CDL	CB2-OB2-PB2-OB4
51	k	101	CDL	CB3-OB5-PB2-OB4
51	l	702	CDL	CB3-OB5-PB2-OB4
51	r	504	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CB2-OB2-PB2-OB4
53	s	402	UQ	C6-C7-C8-C9
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
49	J	403	PLX	C16-C17-C18-C19
48	b	201	PEE	O3P-C1-C2-C3
48	l	701	PEE	O3P-C1-C2-C3
49	r	502	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
51	V	201	CDL	OA5-CA3-CA4-CA6
51	V	202	CDL	OA5-CA3-CA4-CA6
51	V	201	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C11-C12-C13-C14
51	a	201	CDL	C14-C15-C16-C17
51	s	401	CDL	C18-C19-C20-C21
48	j	202	PEE	C12-C13-C14-C15
48	B	303	PEE	C5-C4-O4P-P
48	r	501	PEE	C5-C4-O4P-P
49	a	202	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
51	k	101	CDL	CB5-C51-C52-C53
51	r	504	CDL	CB5-C51-C52-C53
48	l	704	PEE	C22-C23-C24-C25
51	r	504	CDL	C71-CB7-OB8-CB6
51	I	201	CDL	CB2-C1-CA2-OA2
48	b	201	PEE	C34-C35-C36-C37
51	V	202	CDL	CB7-C71-C72-C73
51	a	201	CDL	C38-C39-C40-C41
51	r	504	CDL	C12-C13-C14-C15
46	A	502	FMN	O4'-C4'-C5'-O5'
51	n	101	CDL	C54-C55-C56-C57
48	l	704	PEE	C40-C41-C42-C43
51	V	201	CDL	C74-C75-C76-C77
51	l	702	CDL	C54-C55-C56-C57
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	C11-C12-C13-C14
49	a	202	PLX	C3-C4-C5-O8
51	l	703	CDL	C62-C63-C64-C65
51	r	504	CDL	CA3-CA4-CA6-OA8
48	C	302	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
49	r	502	PLX	C16-C17-C18-C19
49	C	303	PLX	C16-C17-C18-C19
49	r	502	PLX	C4-C5-O8-C24
51	a	201	CDL	C57-C58-C59-C60
51	V	201	CDL	CA4-CA3-OA5-PA1
51	k	101	CDL	C1-CB2-OB2-PB2
51	r	504	CDL	C1-CB2-OB2-PB2
50	X	201	8Q1	C12-C13-C14-C15
48	l	704	PEE	C43-C44-C45-C46
49	g	201	PLX	O6-C6-C7-C8
49	j	203	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C39-C40-C41-C42
48	b	201	PEE	C14-C15-C16-C17
48	b	201	PEE	C30-C31-C32-C33
49	j	203	PLX	C30-C31-C32-C33
51	a	201	CDL	C64-C65-C66-C67
51	l	703	CDL	C11-C12-C13-C14
51	n	101	CDL	O1-C1-CB2-OB2
51	r	504	CDL	O1-C1-CA2-OA2
51	r	504	CDL	O1-C1-CB2-OB2
51	V	201	CDL	C73-C74-C75-C76
51	s	401	CDL	C77-C78-C79-C80
49	r	502	PLX	C35-C36-C37-C38
51	r	504	CDL	C44-C45-C46-C47
48	l	704	PEE	C14-C15-C16-C17
49	r	503	PLX	C11-C12-C13-C14
51	l	702	CDL	C12-C11-CA5-OA6
48	B	303	PEE	C44-C45-C46-C47
51	a	201	CDL	C12-C13-C14-C15
48	j	202	PEE	C33-C34-C35-C36
49	a	202	PLX	C18-C19-C20-C21
51	l	702	CDL	C24-C25-C26-C27
51	l	703	CDL	C32-C33-C34-C35
48	B	303	PEE	O3P-C1-C2-O2
51	V	201	CDL	OA5-CA3-CA4-OA6
51	s	401	CDL	C83-C84-C85-C86
48	l	704	PEE	C41-C42-C43-C44
48	b	201	PEE	C16-C17-C18-C19
48	C	302	PEE	C20-C21-C22-C23
49	J	403	PLX	O6-C4-C5-O8
51	l	703	CDL	C77-C78-C79-C80
48	b	201	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
51	l	703	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CA3-OA5-PA1-OA2
51	s	401	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	C38-C39-C40-C41
51	V	202	CDL	C19-C20-C21-C22
51	V	202	CDL	CB3-CB4-CB6-OB8
51	r	504	CDL	C39-C40-C41-C42
49	j	203	PLX	C18-C19-C20-C21
51	V	202	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
51	l	703	CDL	C18-C19-C20-C21
48	C	302	PEE	C35-C36-C37-C38
47	A	503	NAI	O4D-C1D-N1N-C2N
51	l	703	CDL	C13-C14-C15-C16
51	V	202	CDL	C36-C37-C38-C39
51	n	101	CDL	C75-C76-C77-C78
51	V	201	CDL	CB4-CB3-OB5-PB2
51	k	101	CDL	C1-CA2-OA2-PA1
48	C	302	PEE	C44-C45-C46-C47
48	B	303	PEE	C18-C19-C20-C21
48	Q	501	PEE	C16-C17-C18-C19
48	b	201	PEE	C18-C19-C20-C21
53	J	402	UQ	C11-C12-C13-C14
51	r	504	CDL	C52-C53-C54-C55
47	A	503	NAI	C2D-C1D-N1N-C2N
48	r	501	PEE	C18-C19-C20-C21
48	Q	501	PEE	C24-C25-C26-C27
52	J	401	NDP	O4B-C4B-C5B-O5B
49	C	303	PLX	O4-C3-C4-O6
51	l	703	CDL	OA5-CA3-CA4-OA6
51	n	101	CDL	OA5-CA3-CA4-OA6
49	a	202	PLX	C27-C28-C29-C30
51	I	201	CDL	C51-C52-C53-C54
51	n	101	CDL	O1-C1-CA2-OA2
51	a	201	CDL	C56-C57-C58-C59
48	l	704	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
49	g	201	PLX	O8-C24-C25-C26
51	l	703	CDL	OA6-CA4-CA6-OA8
51	l	703	CDL	C78-C79-C80-C81
51	l	702	CDL	CB4-CB3-OB5-PB2
48	C	302	PEE	C16-C17-C18-C19
51	l	702	CDL	C82-C83-C84-C85
48	C	302	PEE	C32-C33-C34-C35
48	j	202	PEE	C13-C14-C15-C16
48	j	201	PEE	C23-C24-C25-C26
48	Q	501	PEE	C22-C23-C24-C25
51	l	703	CDL	CB6-CB4-OB6-CB5
51	a	201	CDL	C21-C22-C23-C24
51	s	401	CDL	C38-C39-C40-C41
48	j	202	PEE	C16-C17-C18-C19
48	r	501	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
51	k	101	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CA3-OA5-PA1-OA2
51	r	504	CDL	C61-C62-C63-C64
48	W	201	PEE	C20-C21-C22-C23
51	V	202	CDL	C63-C64-C65-C66
48	l	704	PEE	O3P-C1-C2-O2
51	n	101	CDL	OB5-CB3-CB4-OB6
51	l	703	CDL	C42-C43-C44-C45
48	j	201	PEE	O3P-C1-C2-C3
51	l	703	CDL	OA5-CA3-CA4-CA6
51	V	201	CDL	C40-C41-C42-C43
51	r	504	CDL	C42-C43-C44-C45
51	V	201	CDL	C36-C37-C38-C39
51	V	201	CDL	C80-C81-C82-C83
49	C	303	PLX	C34-C35-C36-C37
48	j	201	PEE	C2-C3-O3-C30
51	a	201	CDL	C44-C45-C46-C47
48	B	303	PEE	C37-C38-C39-C40
48	j	202	PEE	C17-C18-C19-C20
48	r	501	PEE	C37-C38-C39-C40
51	s	401	CDL	C15-C16-C17-C18
51	l	703	CDL	C61-C62-C63-C64
51	l	702	CDL	C23-C24-C25-C26
49	J	403	PLX	C30-C31-C32-C33
51	s	401	CDL	C19-C20-C21-C22
49	C	303	PLX	C3-C4-C5-O8
51	s	401	CDL	C57-C58-C59-C60
47	A	503	NAI	O4D-C4D-C5D-O5D
51	s	401	CDL	C72-C71-CB7-OB8
48	l	704	PEE	C24-C25-C26-C27
48	l	704	PEE	C19-C20-C21-C22
48	B	303	PEE	C16-C17-C18-C19
48	Q	501	PEE	C36-C37-C38-C39
48	W	201	PEE	C16-C17-C18-C19
48	l	701	PEE	C38-C39-C40-C41
48	l	704	PEE	C36-C37-C38-C39
48	r	501	PEE	C16-C17-C18-C19
51	V	202	CDL	OB5-CB3-CB4-OB6
49	a	202	PLX	C24-C25-C26-C27
49	g	201	PLX	C6-C7-C8-C9
51	l	703	CDL	C12-C11-CA5-OA6
49	g	201	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
51	l	702	CDL	OB5-CB3-CB4-CB6
51	V	202	CDL	C61-C62-C63-C64
48	Q	501	PEE	C38-C39-C40-C41
51	k	101	CDL	C52-C51-CB5-OB6
48	r	501	PEE	C24-C25-C26-C27
51	l	703	CDL	OB6-CB4-CB6-OB8
49	r	503	PLX	C24-C25-C26-C27
51	I	201	CDL	C72-C71-CB7-OB8
51	V	201	CDL	C53-C54-C55-C56
49	a	202	PLX	C36-C37-C38-C39
48	b	201	PEE	C2-C3-O3-C30
48	j	202	PEE	C2-C3-O3-C30
48	W	201	PEE	C4-O4P-P-O3P
51	V	201	CDL	C51-C52-C53-C54
51	l	703	CDL	O1-C1-CB2-OB2
51	V	202	CDL	C52-C51-CB5-OB6
49	g	201	PLX	C20-C21-C22-C23
51	V	201	CDL	C12-C11-CA5-OA6
51	s	401	CDL	C12-C11-CA5-OA6
51	l	702	CDL	C77-C78-C79-C80
48	C	302	PEE	C18-C19-C20-C21
48	l	701	PEE	C16-C17-C18-C19
48	C	302	PEE	C39-C40-C41-C42
51	n	101	CDL	C71-C72-C73-C74
48	l	704	PEE	C1-C2-C3-O3
49	j	203	PLX	C7-C6-O6-C4
50	X	201	8Q1	C28-O27-P24-O3
51	I	201	CDL	OA5-CA3-CA4-OA6
51	a	201	CDL	C32-C31-CA7-OA8
49	g	201	PLX	C14-C15-C16-C17
48	r	501	PEE	C14-C15-C16-C17
48	b	201	PEE	C38-C39-C40-C41
48	l	704	PEE	C16-C17-C18-C19
51	r	504	CDL	OA7-CA5-OA6-CA4
51	I	201	CDL	C52-C51-CB5-OB6
51	l	702	CDL	C72-C71-CB7-OB8
51	r	504	CDL	C51-C52-C53-C54
53	s	402	UQ	C12-C13-C14-C16
48	j	202	PEE	C20-C21-C22-C23
51	V	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
51	l	703	CDL	C52-C51-CB5-OB6
49	a	202	PLX	C34-C35-C36-C37
48	j	202	PEE	C18-C19-C20-C21
51	a	201	CDL	C12-C11-CA5-OA6
51	r	504	CDL	C12-C11-CA5-OA6
51	r	504	CDL	C52-C51-CB5-OB6
51	s	401	CDL	C84-C85-C86-C87
51	s	401	CDL	CA7-C31-C32-C33
49	a	202	PLX	C29-C30-C31-C32
51	V	201	CDL	C14-C15-C16-C17
51	l	702	CDL	C60-C61-C62-C63
51	s	401	CDL	C74-C75-C76-C77
51	s	401	CDL	C56-C57-C58-C59
49	a	202	PLX	C12-C13-C14-C15
48	Q	501	PEE	C18-C19-C20-C21
51	a	201	CDL	C32-C31-CA7-OA9
51	k	101	CDL	C52-C51-CB5-OB7
51	s	401	CDL	C12-C11-CA5-OA7
49	r	503	PLX	C19-C20-C21-C22
50	G	201	8Q1	C12-C13-C14-C15
51	I	201	CDL	C52-C51-CB5-OB7
51	I	201	CDL	C72-C71-CB7-OB9
51	V	201	CDL	CB3-CB4-CB6-OB8
51	l	703	CDL	CB3-CB4-CB6-OB8
51	l	702	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	C22-C23-C24-C25
48	l	704	PEE	C42-C43-C44-C45
49	j	203	PLX	C10-C11-C12-C13
51	r	504	CDL	C58-C59-C60-C61
51	V	201	CDL	C12-C11-CA5-OA7
51	V	202	CDL	C52-C51-CB5-OB7
51	l	702	CDL	C72-C71-CB7-OB9
51	r	504	CDL	C12-C11-CA5-OA7
48	b	201	PEE	C24-C25-C26-C27
48	b	201	PEE	C1-O3P-P-O1P
49	C	303	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O2
51	I	201	CDL	CA3-OA5-PA1-OA3
51	l	703	CDL	CB3-OB5-PB2-OB3
51	r	504	CDL	CA2-OA2-PA1-OA4
51	s	401	CDL	CB3-OB5-PB2-OB3
51	V	201	CDL	CA7-C31-C32-C33

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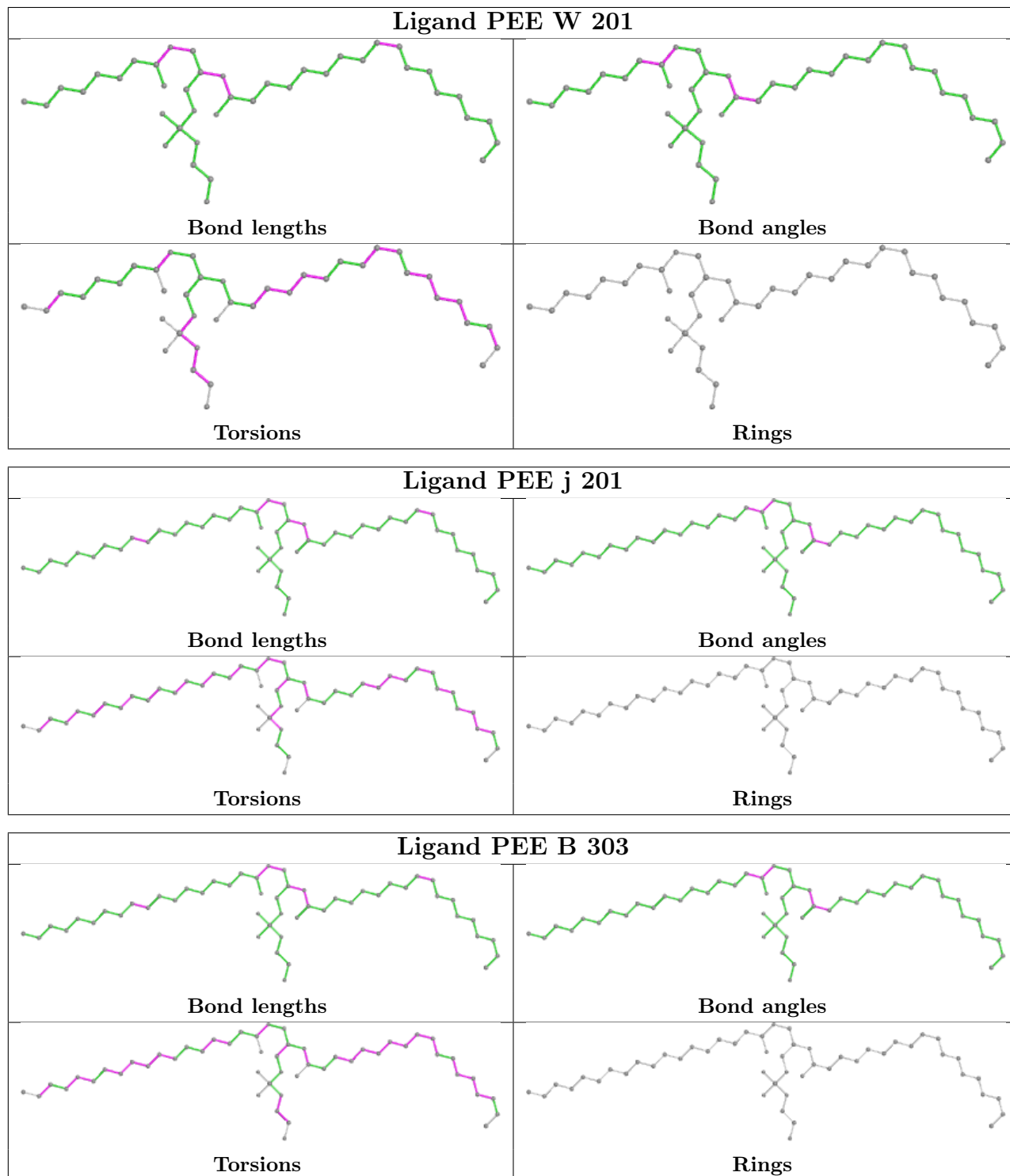
Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C31-C32-C33-C34
48	C	302	PEE	O5-C30-O3-C3
51	a	201	CDL	C24-C25-C26-C27
51	a	201	CDL	C12-C11-CA5-OA7
51	r	504	CDL	C52-C51-CB5-OB7
51	r	504	CDL	C37-C38-C39-C40
50	G	201	8Q1	O27-C28-C29-C30
49	a	202	PLX	C15-C16-C17-C18
48	C	302	PEE	C31-C30-O3-C3
51	l	703	CDL	C72-C71-CB7-OB8
51	l	703	CDL	C52-C51-CB5-OB7
51	I	201	CDL	C11-C12-C13-C14
48	l	704	PEE	C11-C12-C13-C14
48	W	201	PEE	C5-C4-O4P-P
49	J	403	PLX	C1-C2-O1-P1
51	l	703	CDL	CB3-CB4-OB6-CB5
49	r	503	PLX	C18-C19-C20-C21
47	A	503	NAI	C2D-C1D-N1N-C6N
51	r	504	CDL	C11-CA5-OA6-CA4
48	C	302	PEE	O3-C30-C31-C32
51	l	703	CDL	C32-C31-CA7-OA8
49	r	503	PLX	C29-C30-C31-C32
51	s	401	CDL	C13-C14-C15-C16
51	r	504	CDL	CB4-CB3-OB5-PB2
53	s	402	UQ	C13-C14-C16-C17
51	V	202	CDL	C77-C78-C79-C80
49	g	201	PLX	C11-C12-C13-C14
48	B	303	PEE	C15-C16-C17-C18
51	l	702	CDL	C16-C17-C18-C19
49	r	503	PLX	C26-C27-C28-C29
48	B	303	PEE	C20-C21-C22-C23
51	V	201	CDL	C52-C51-CB5-OB6

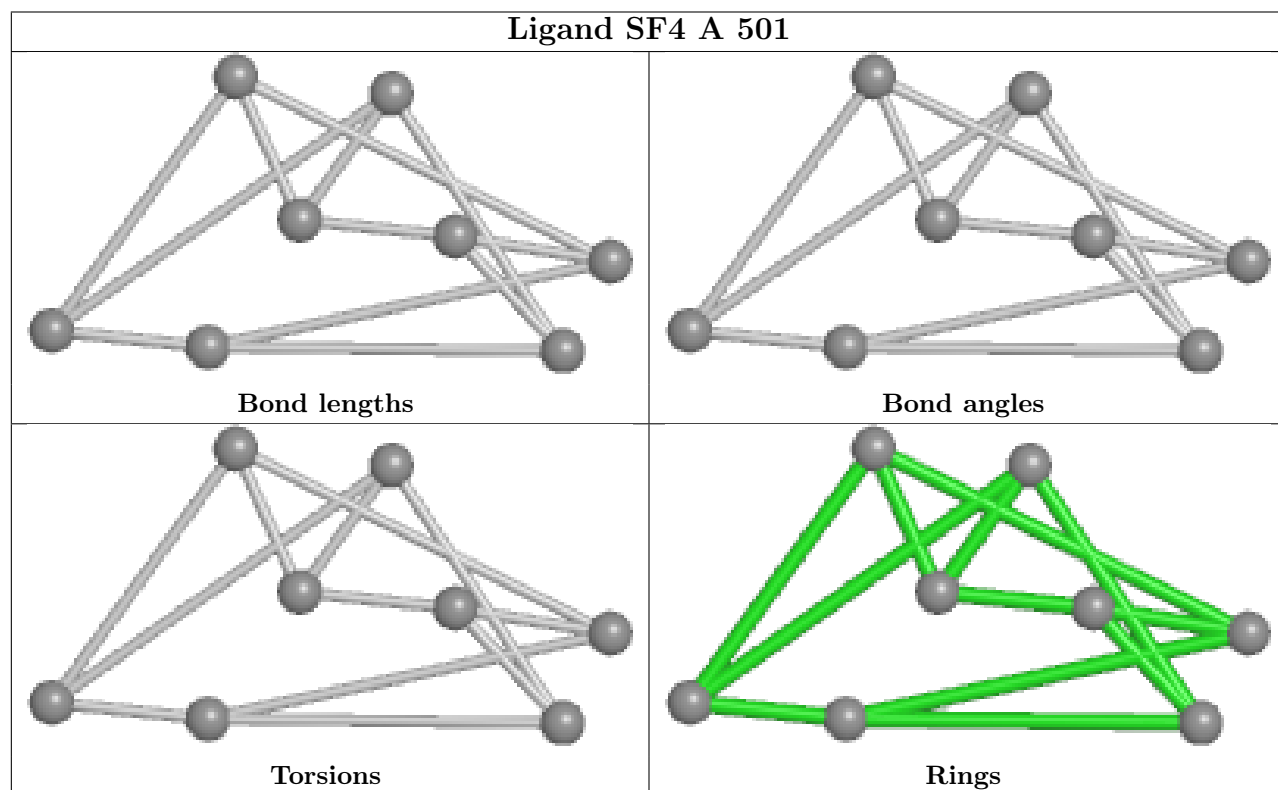
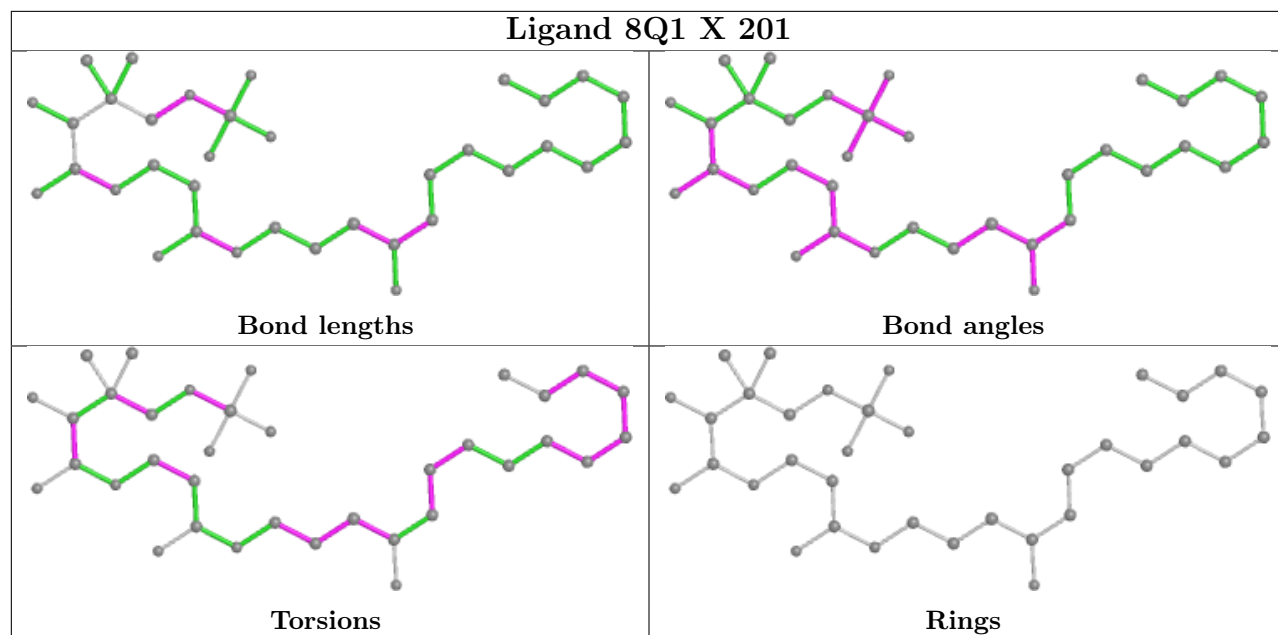
There are no ring outliers.

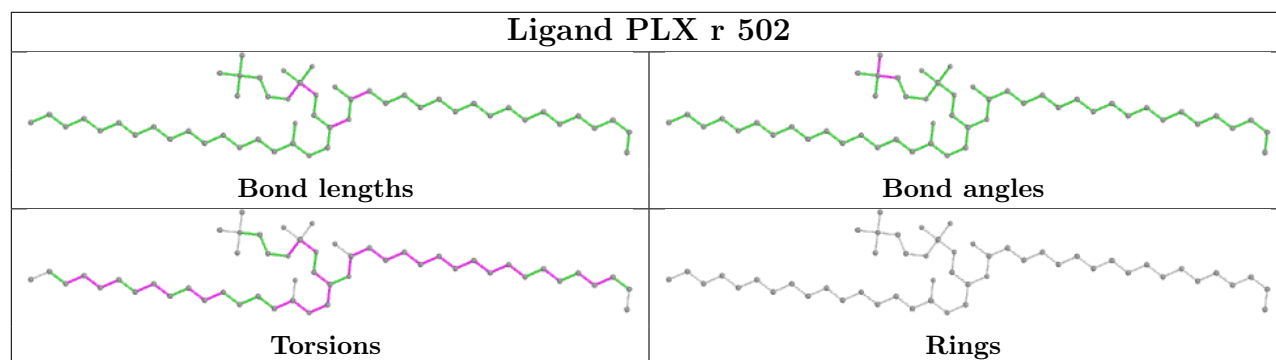
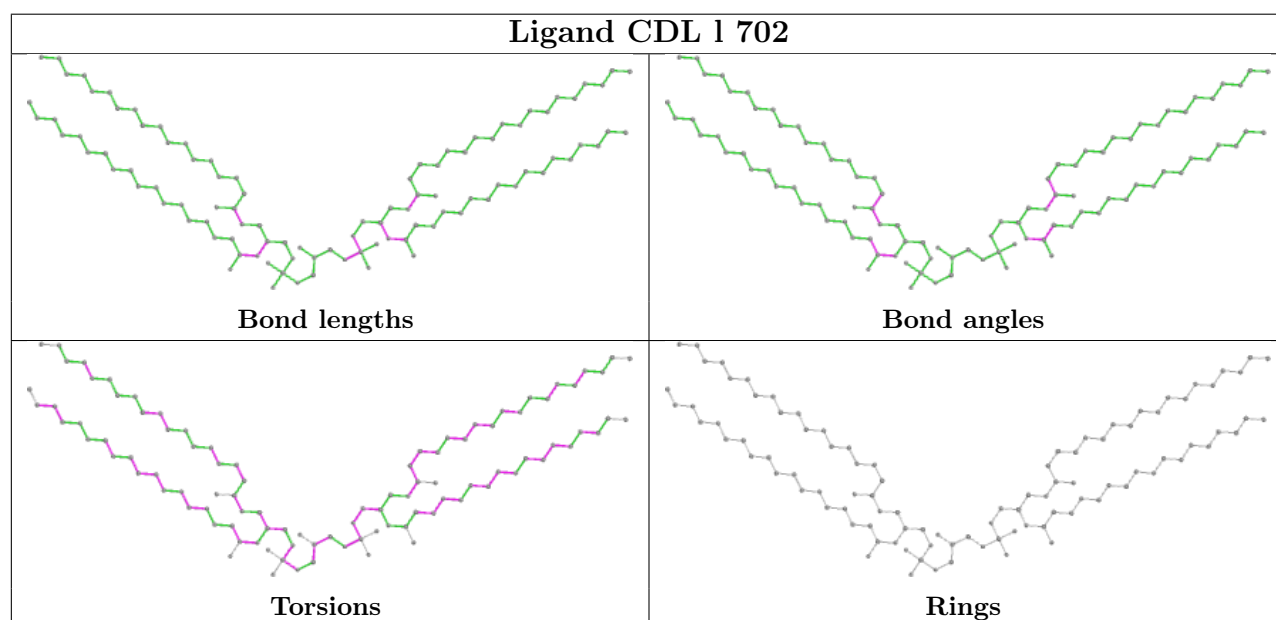
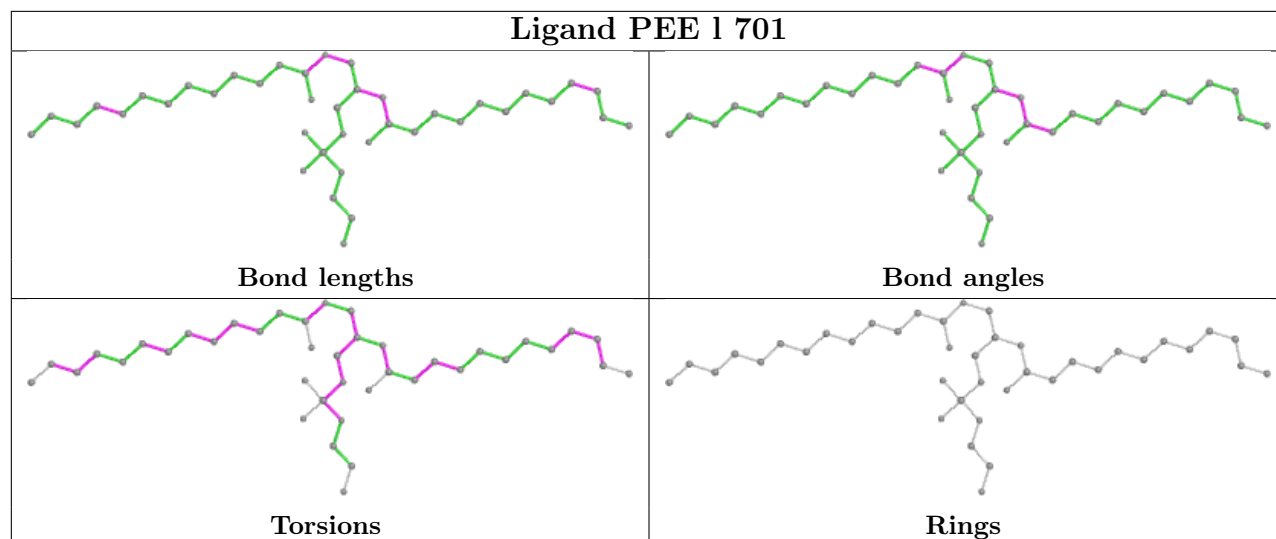
No monomer is involved in short contacts.

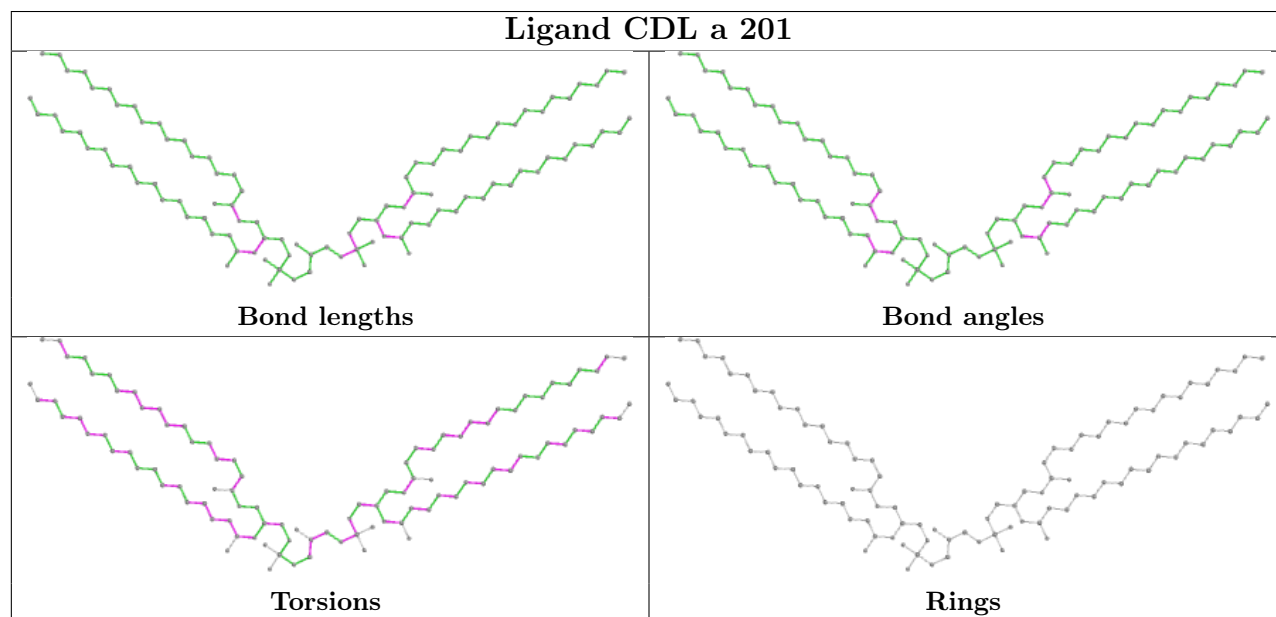
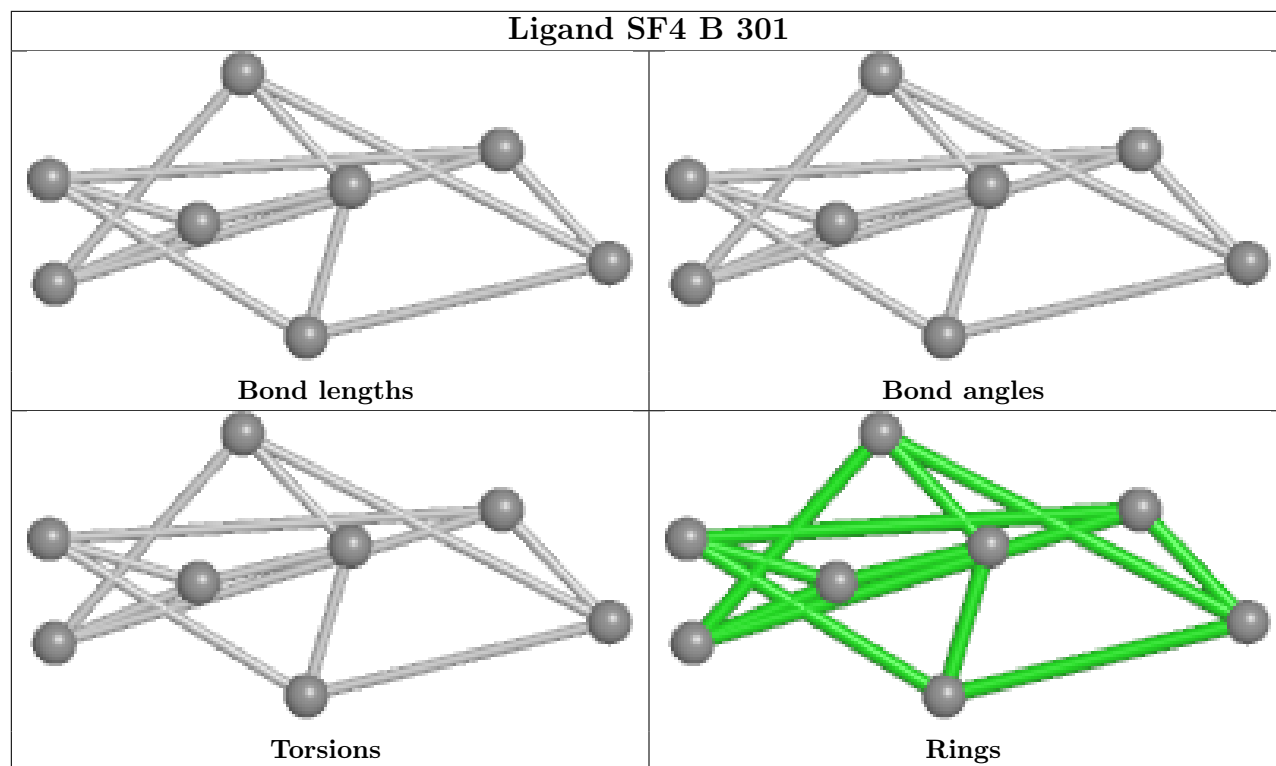
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

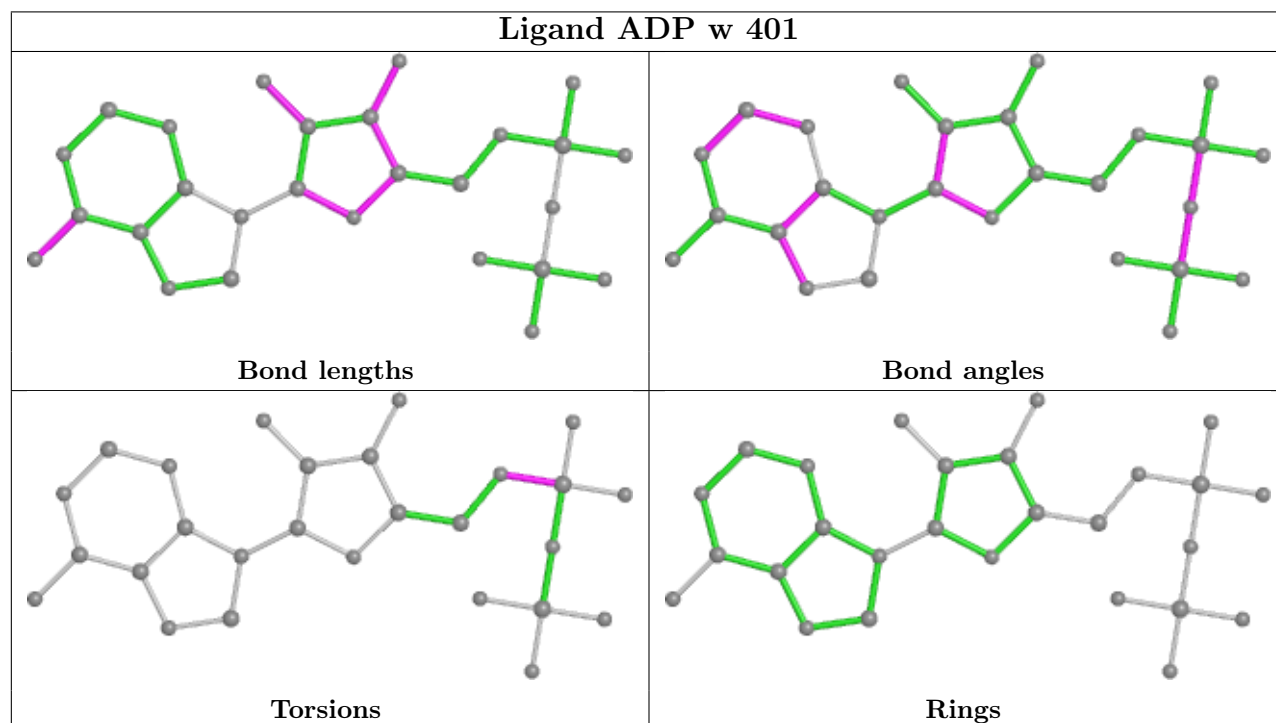
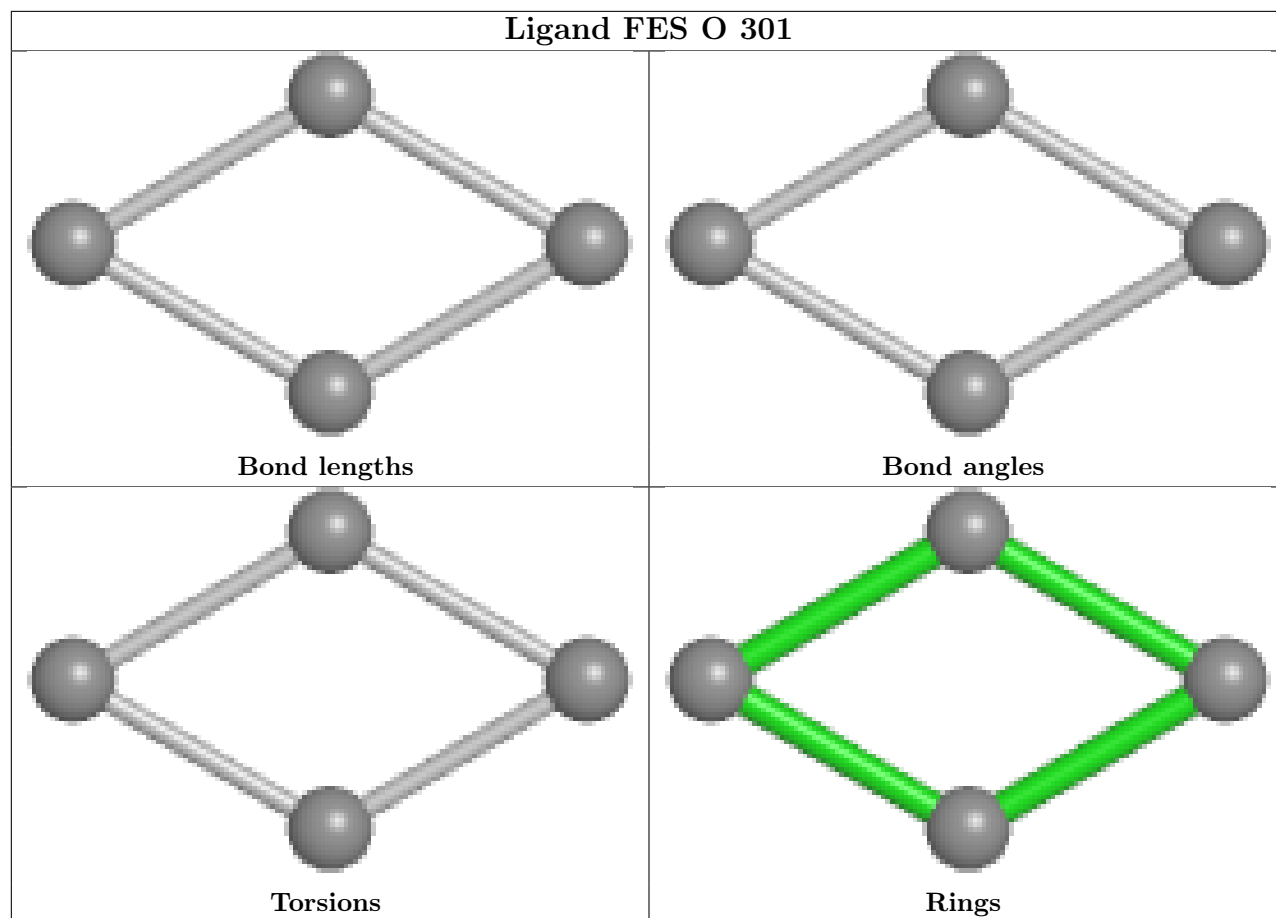
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

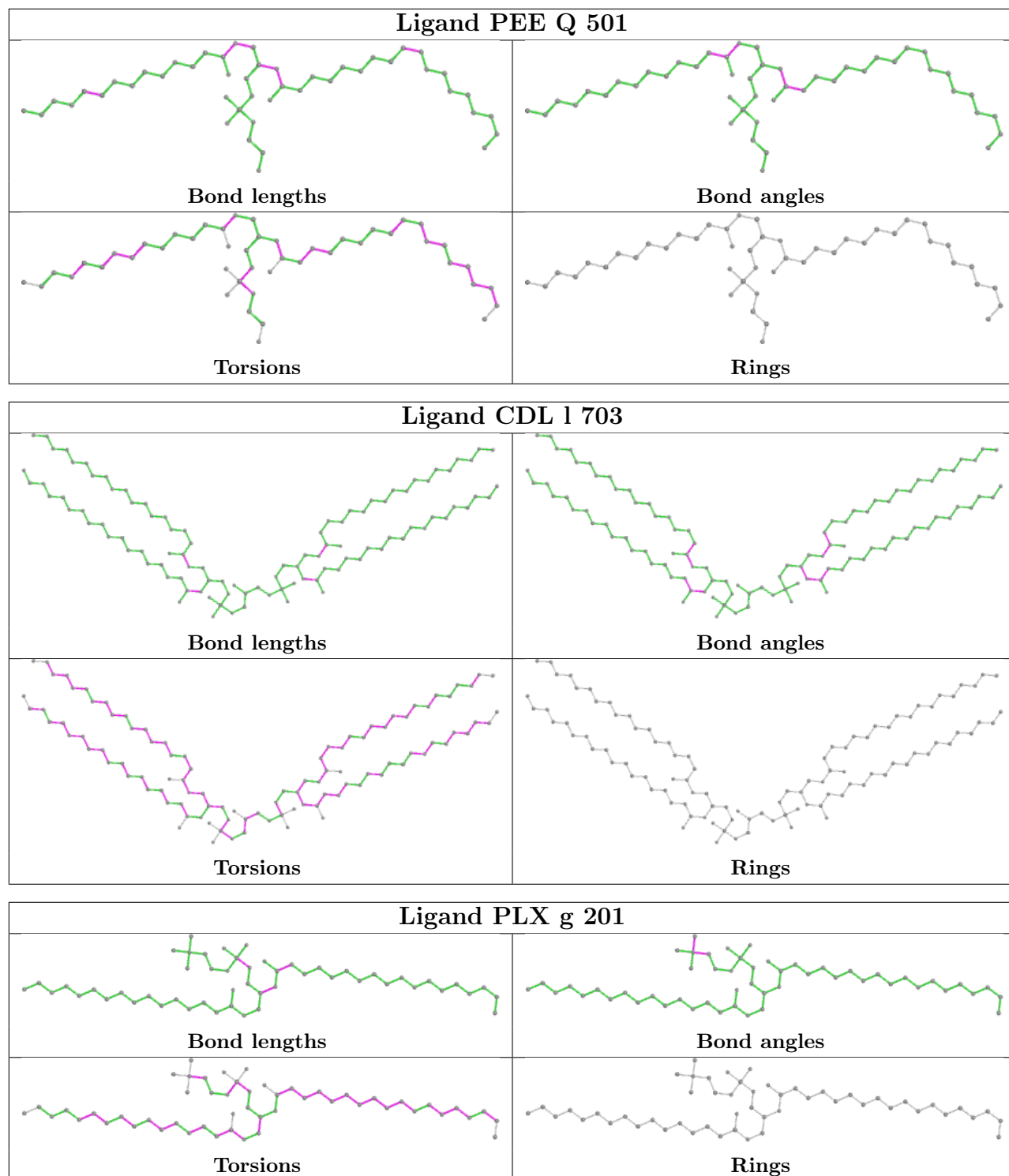


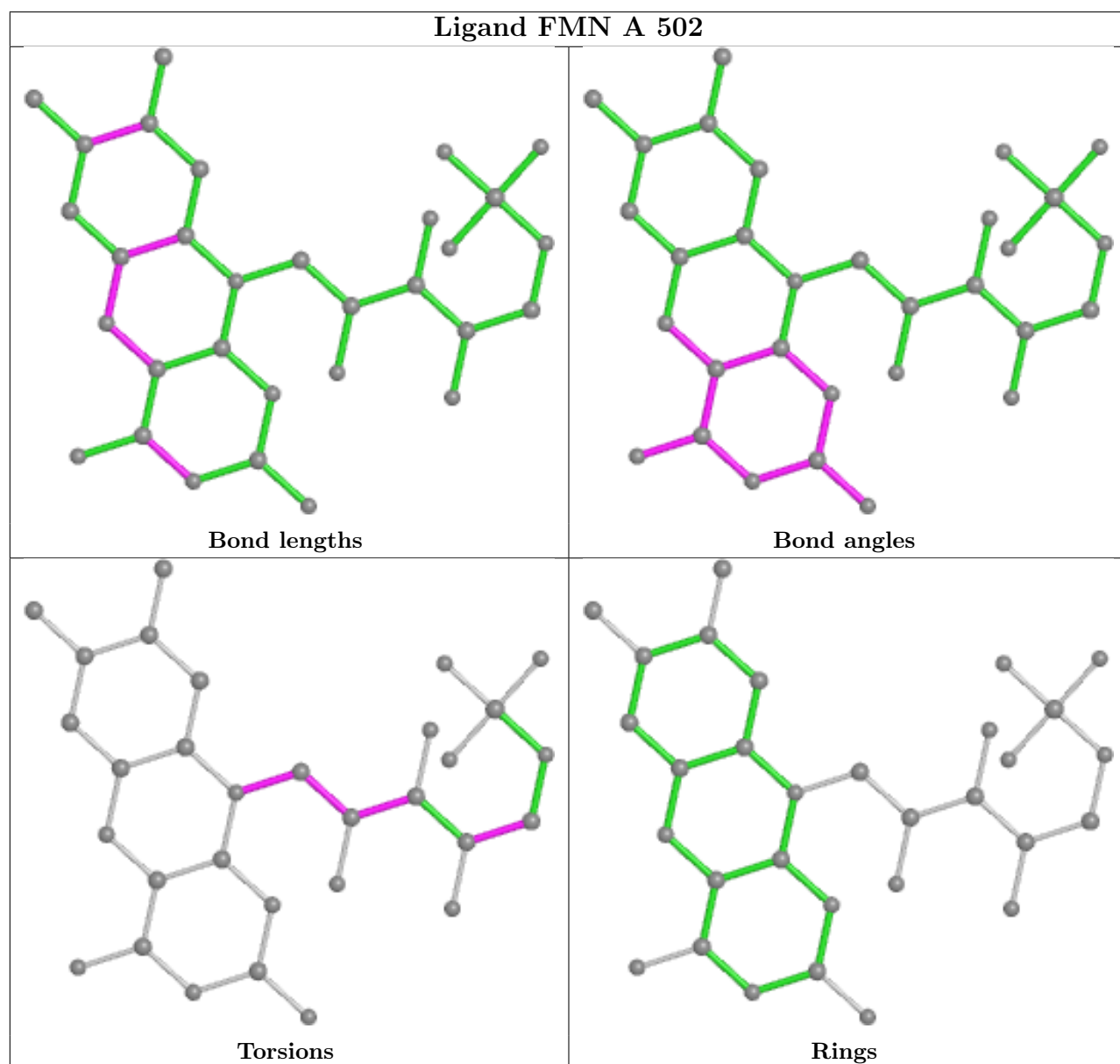
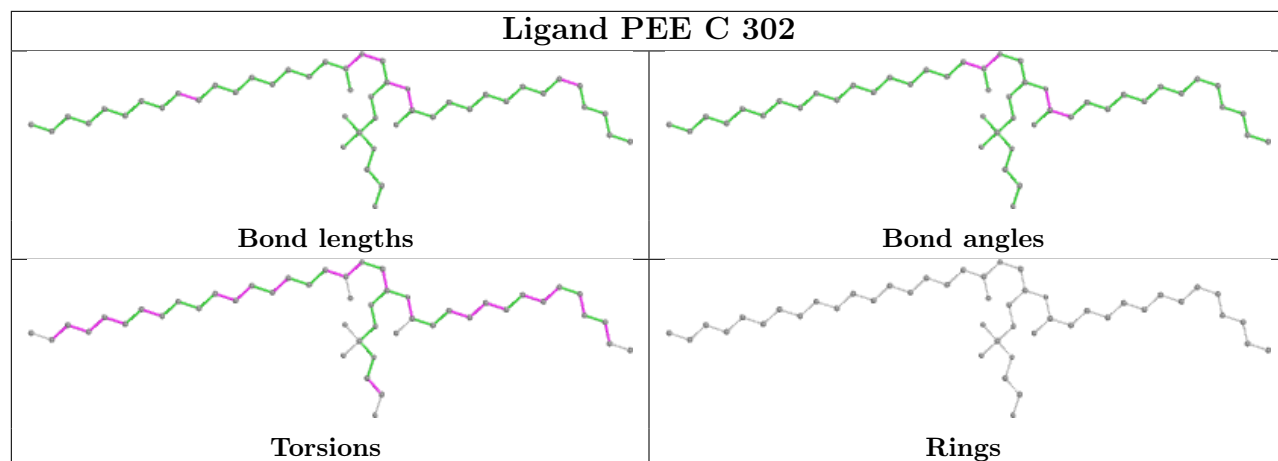


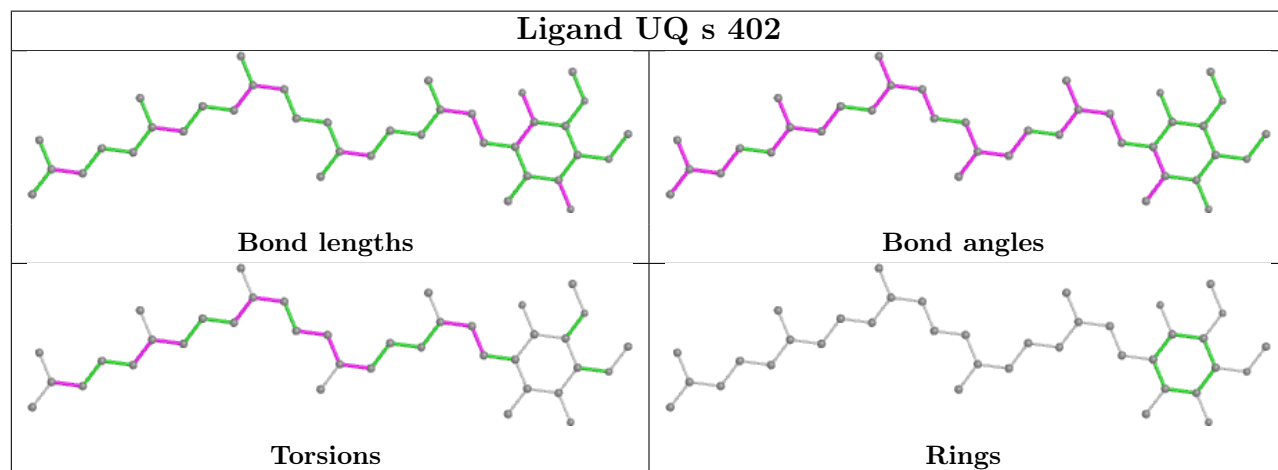
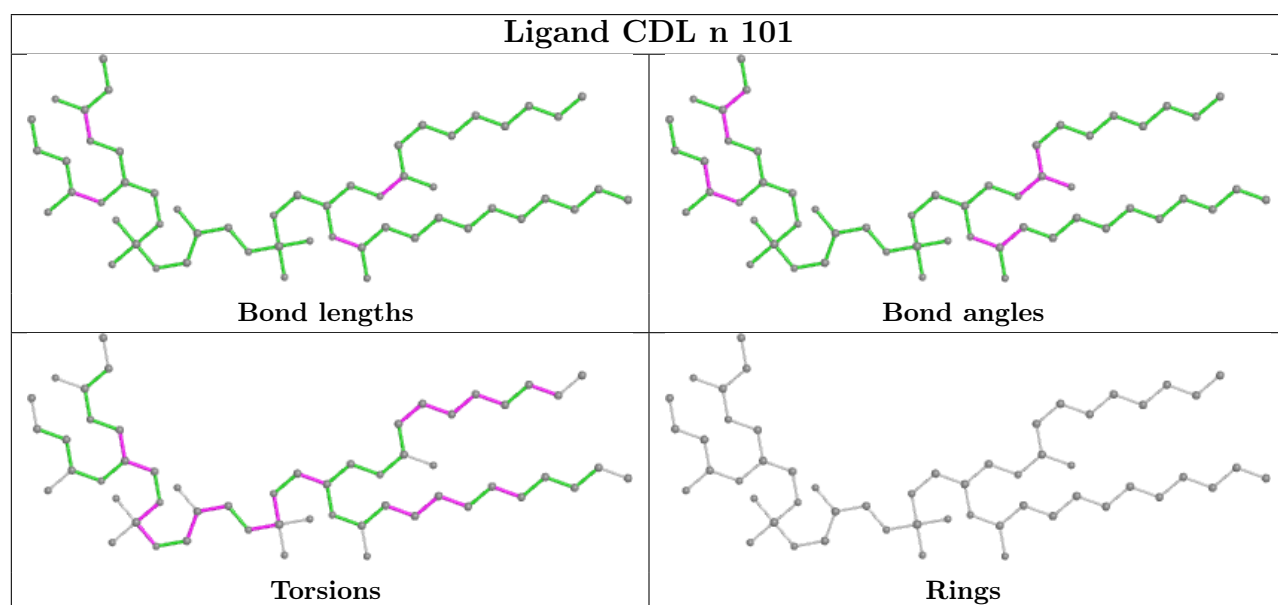
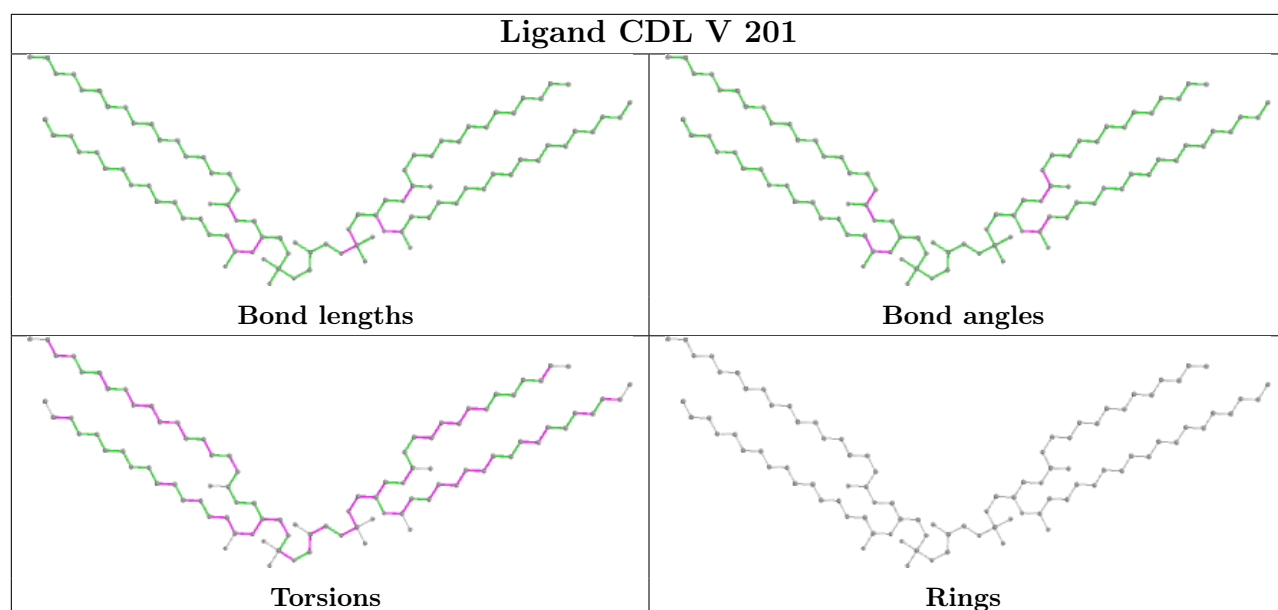


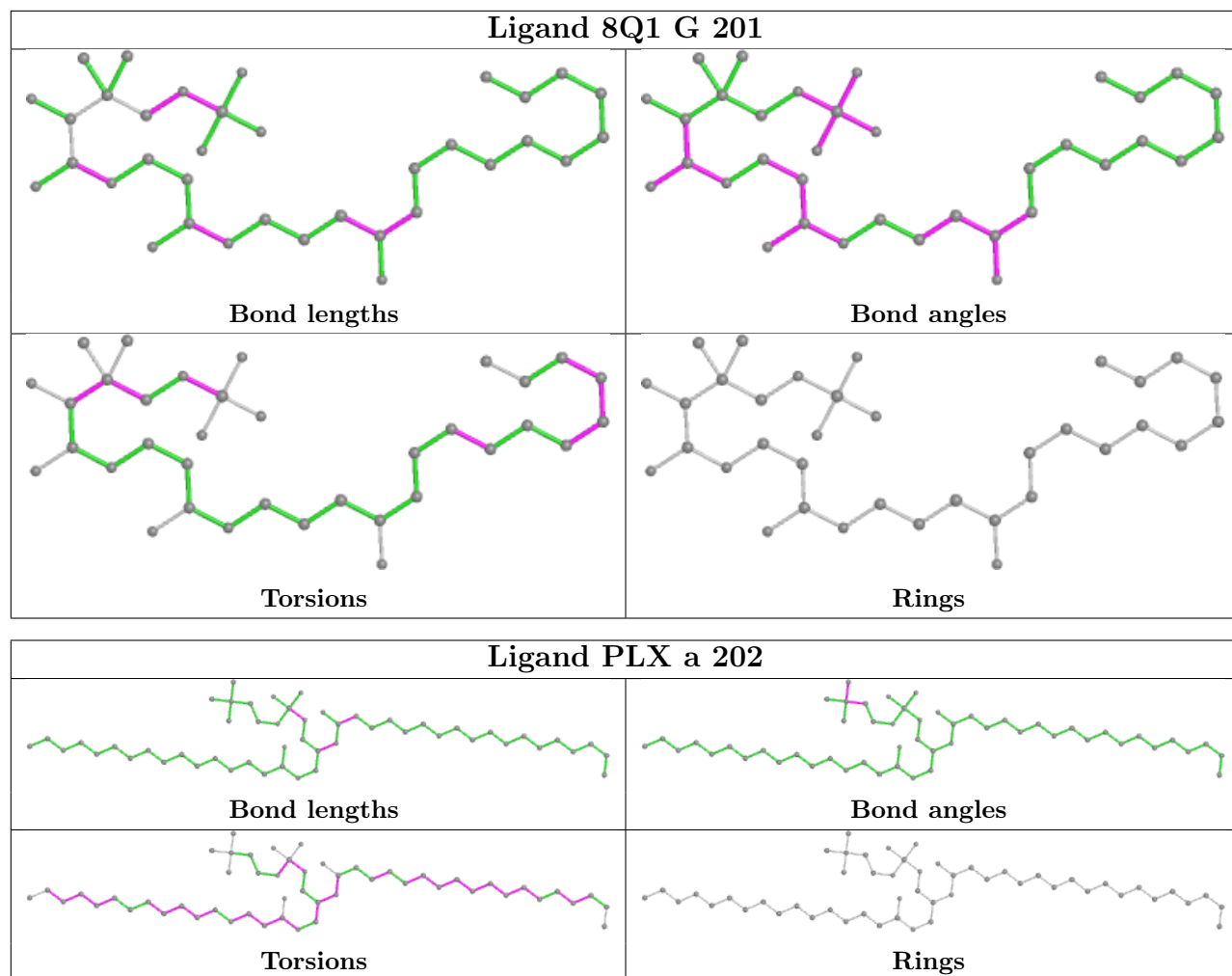


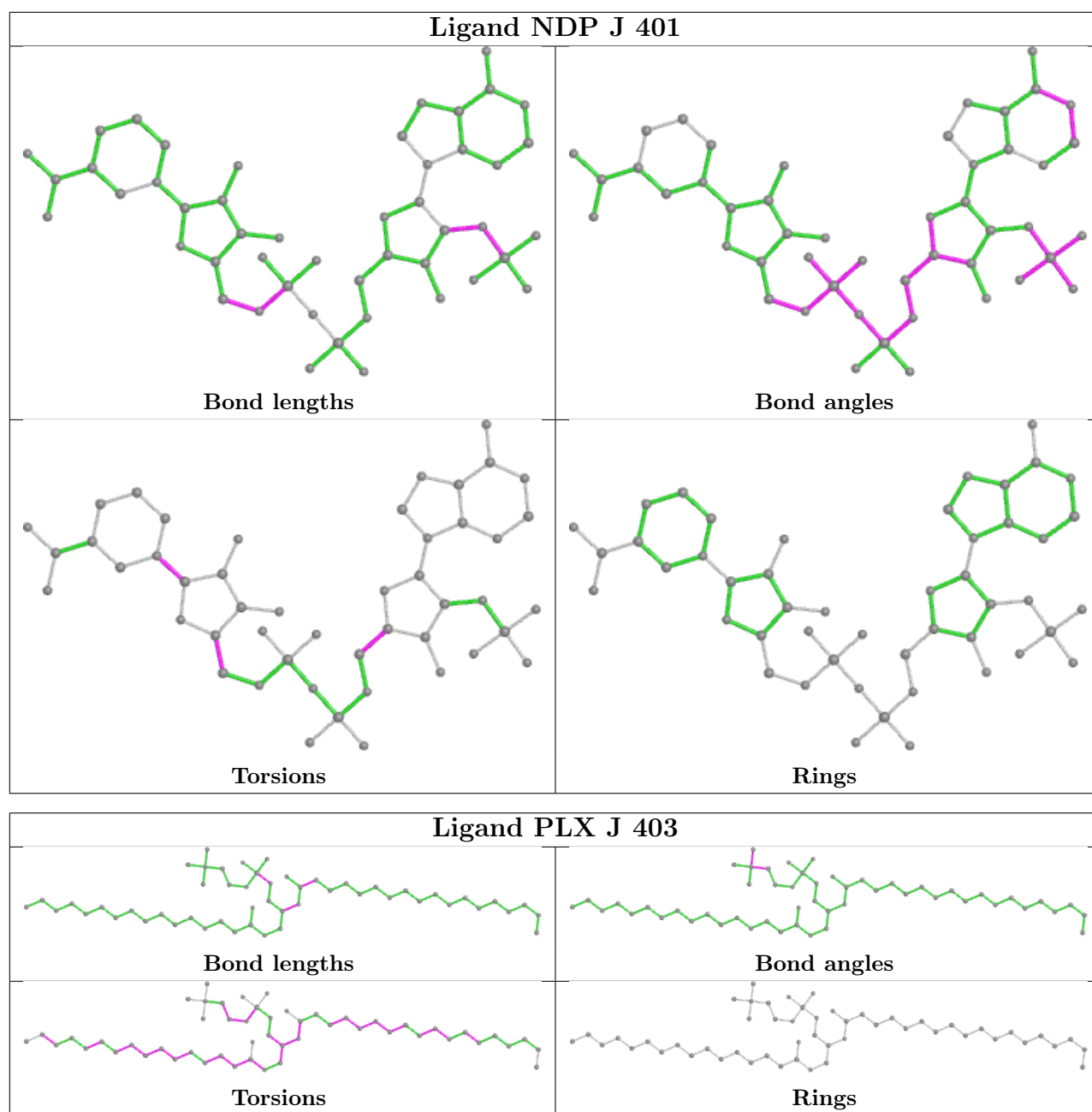


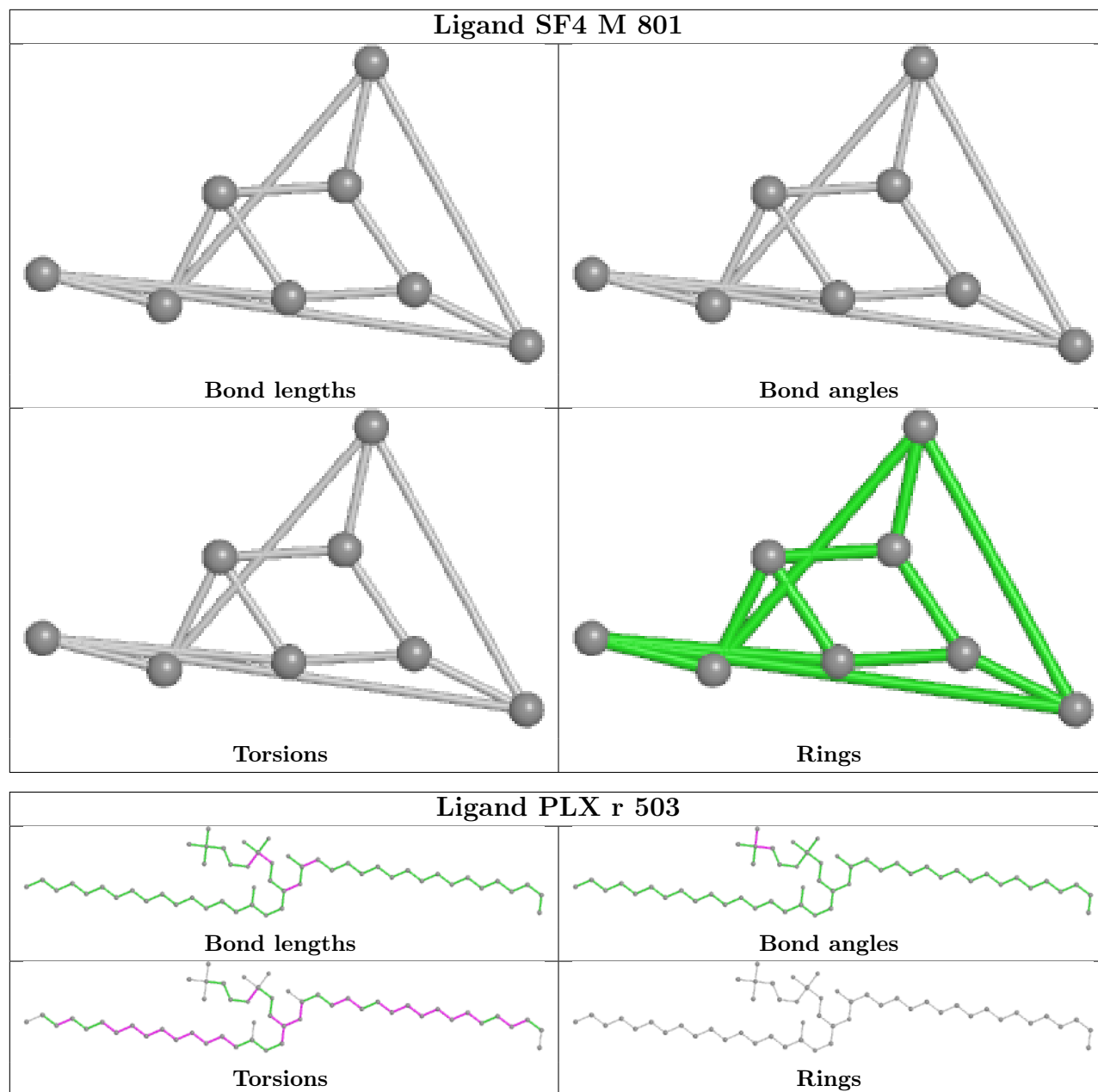


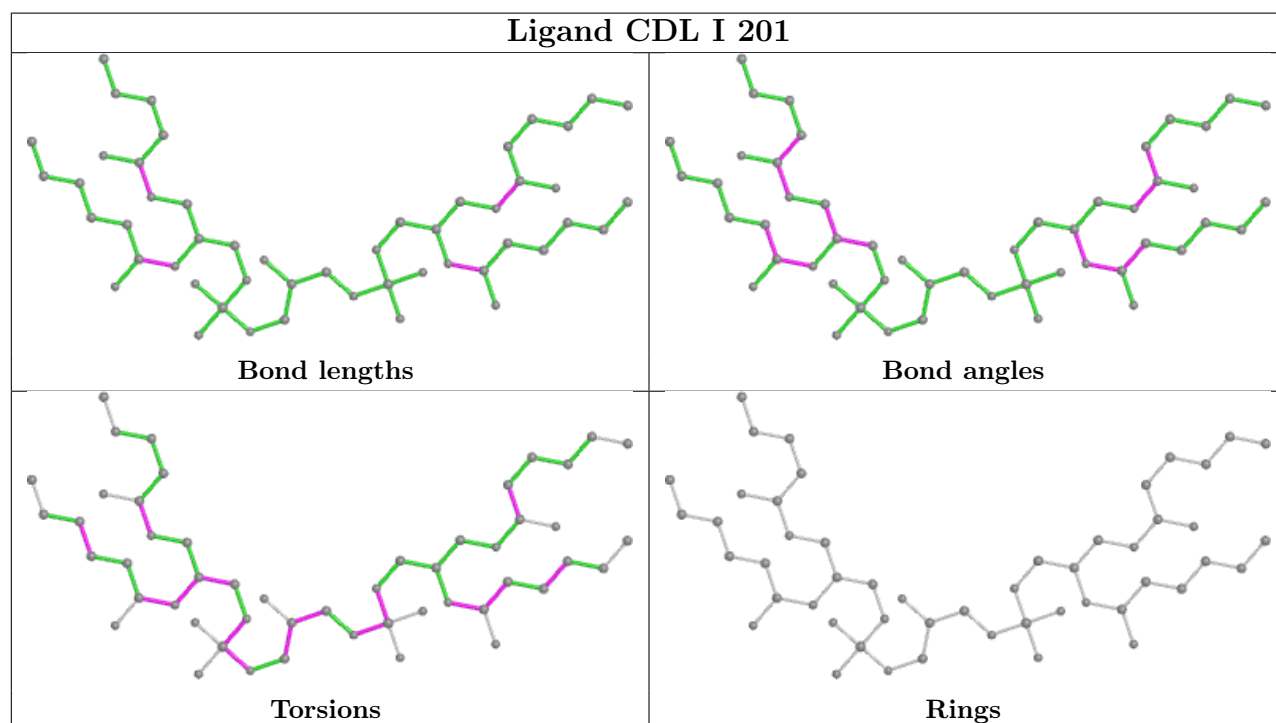
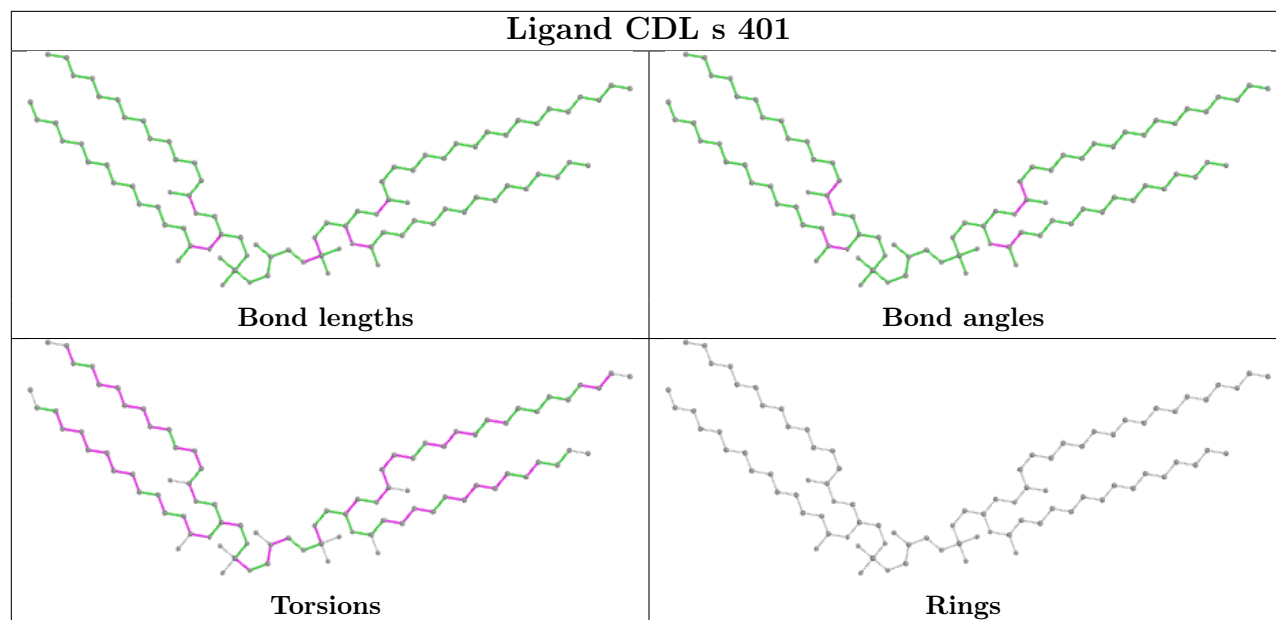


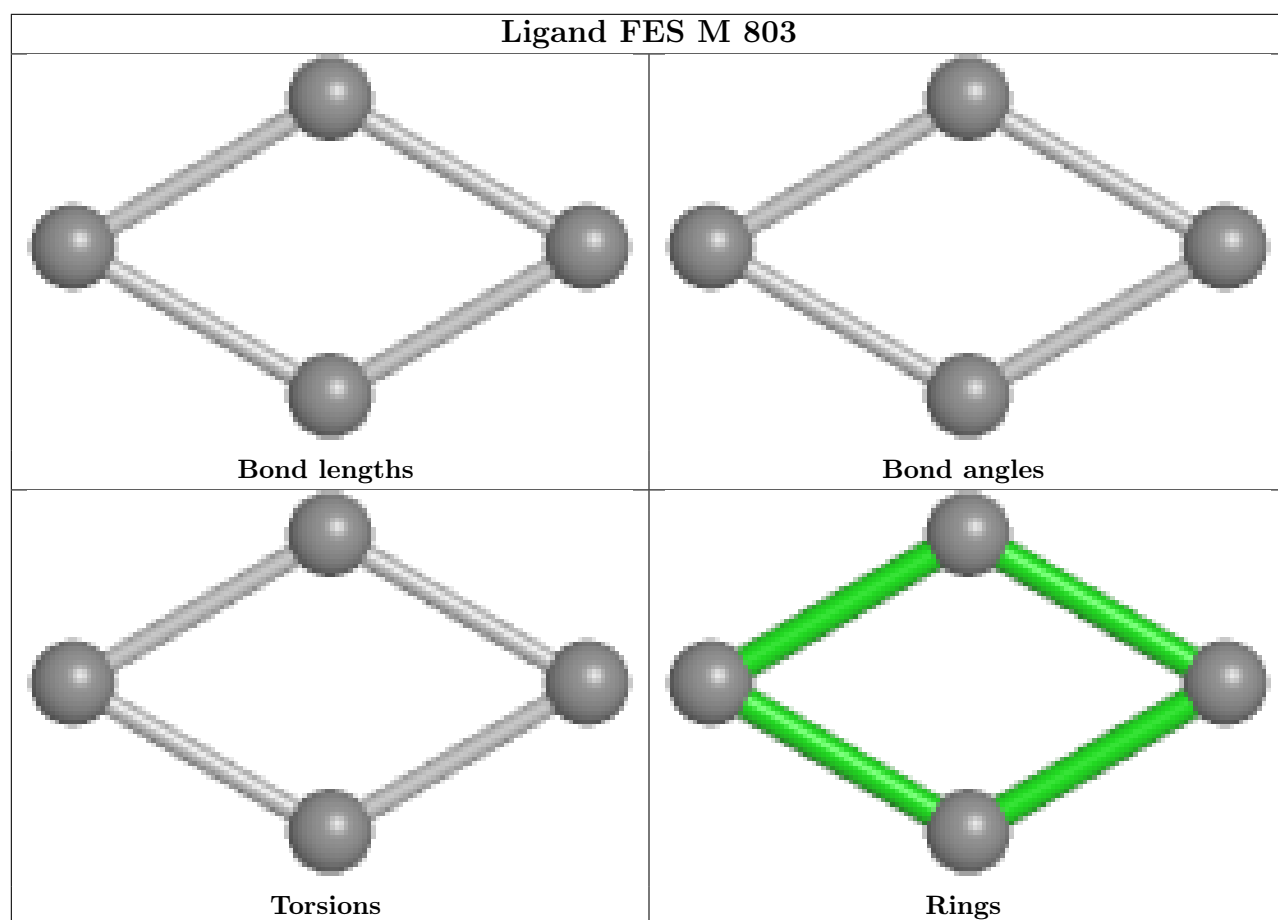
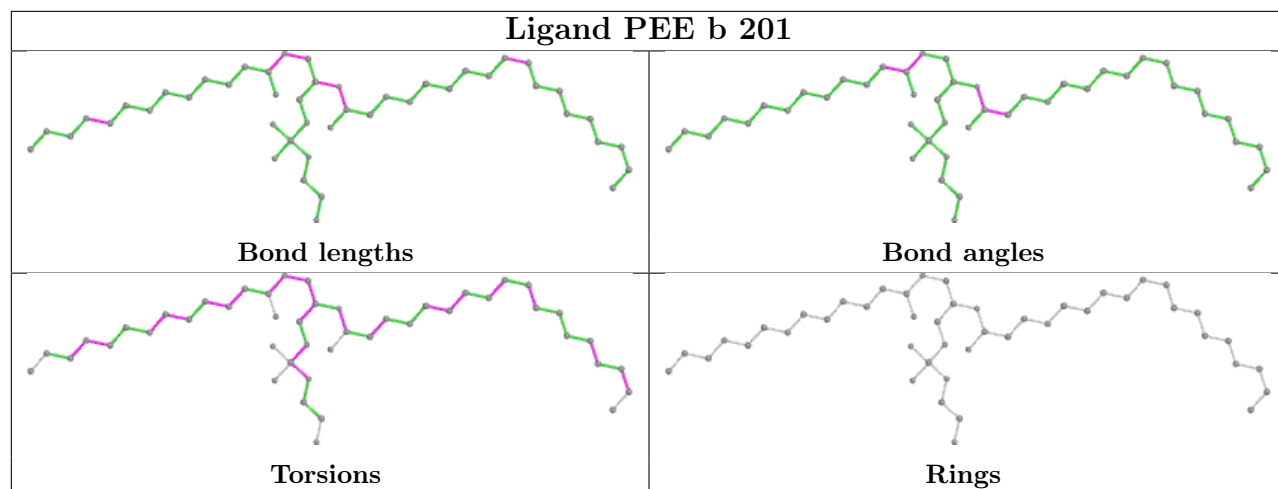


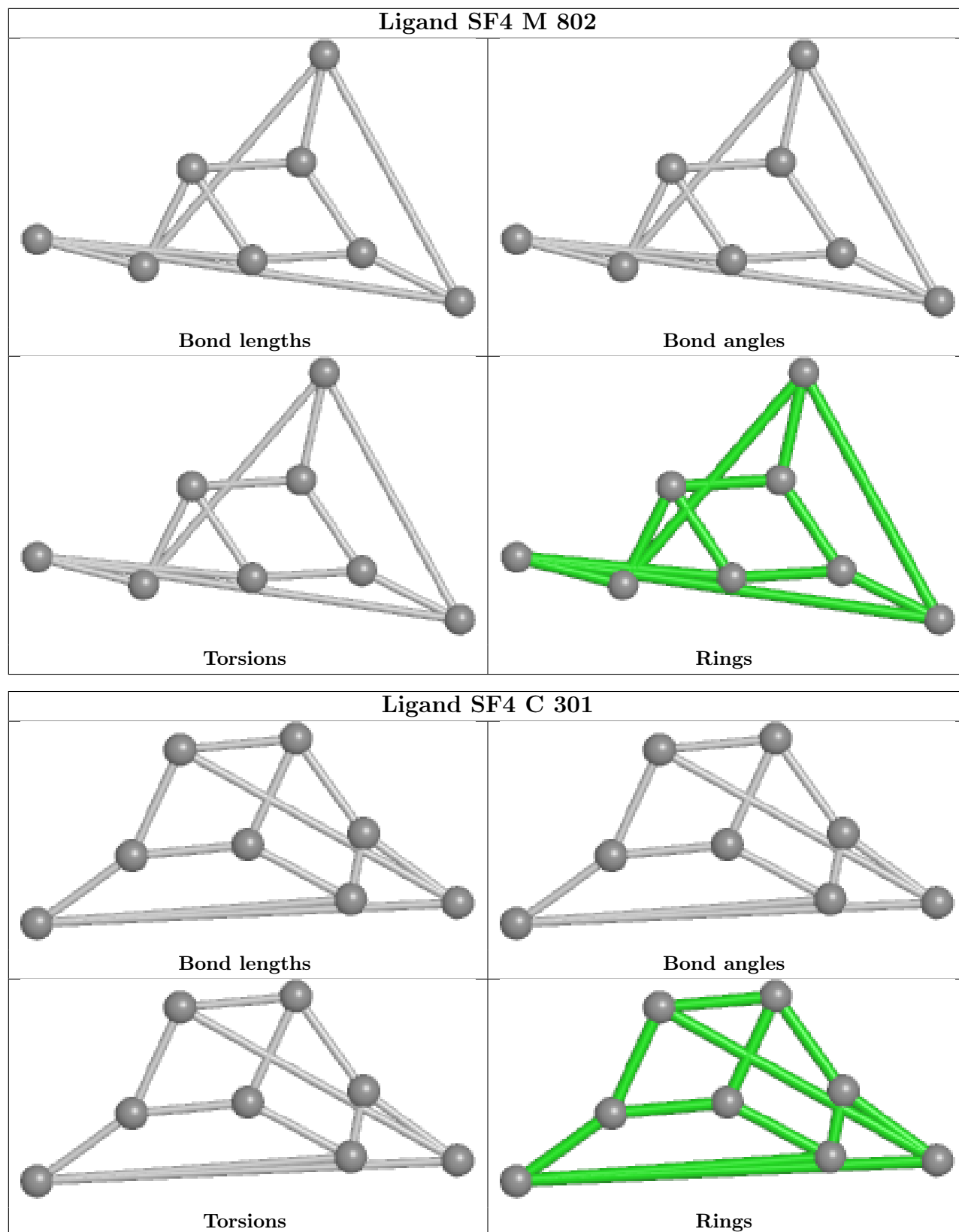


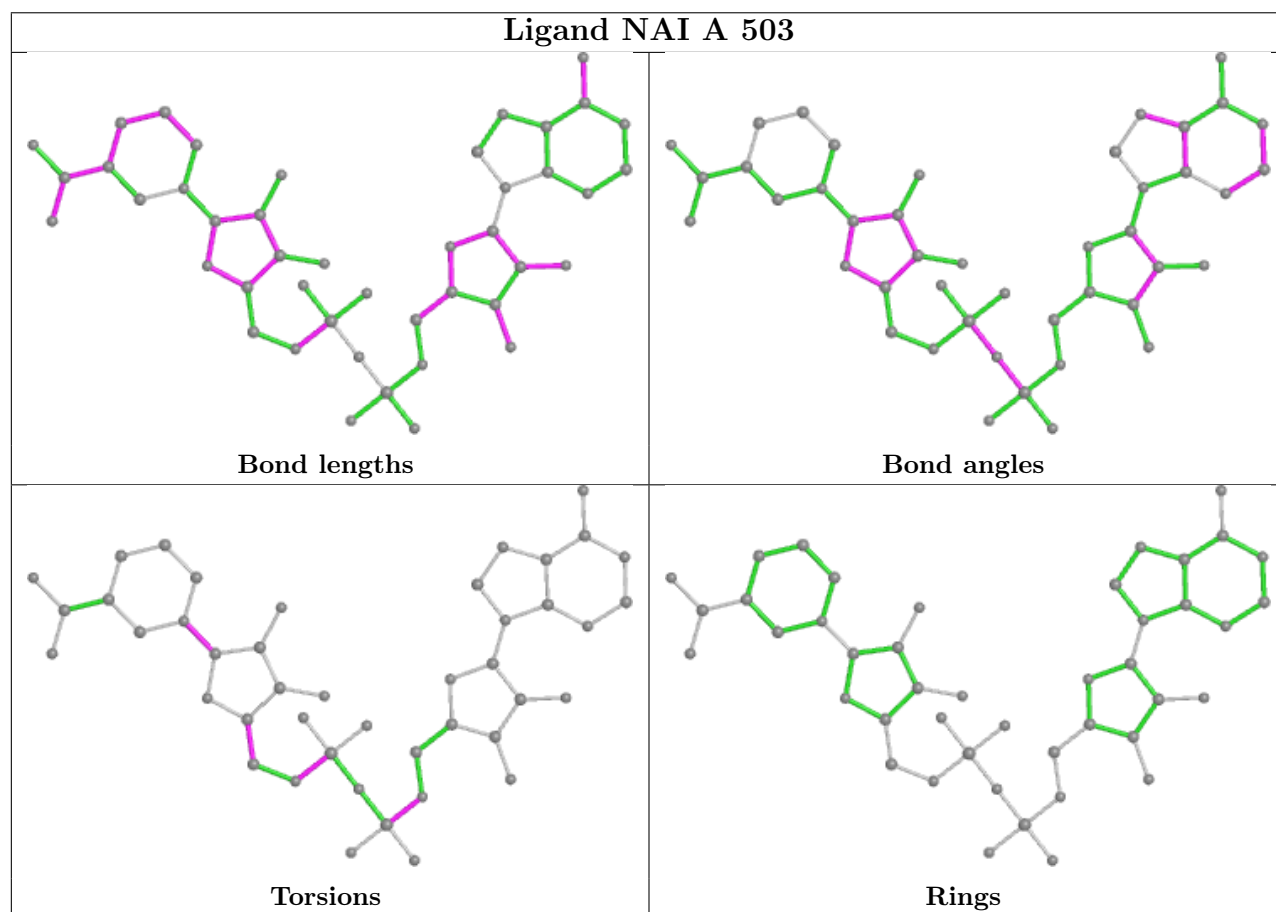
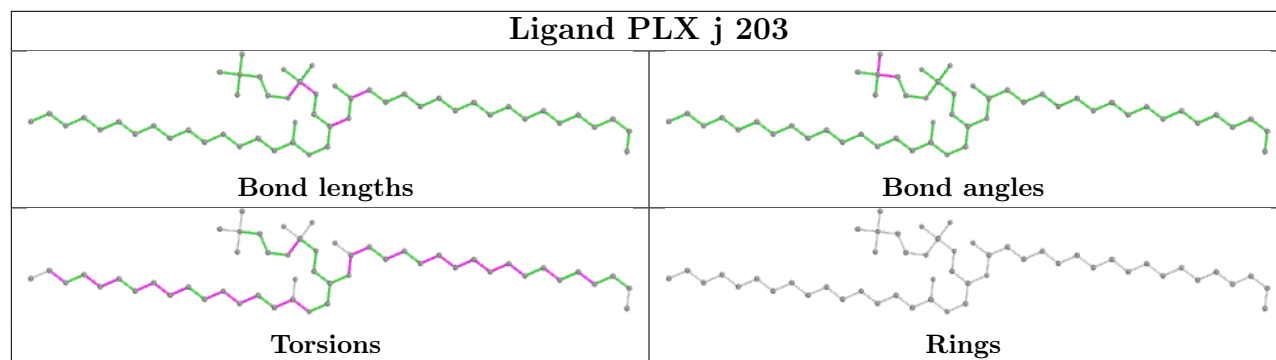


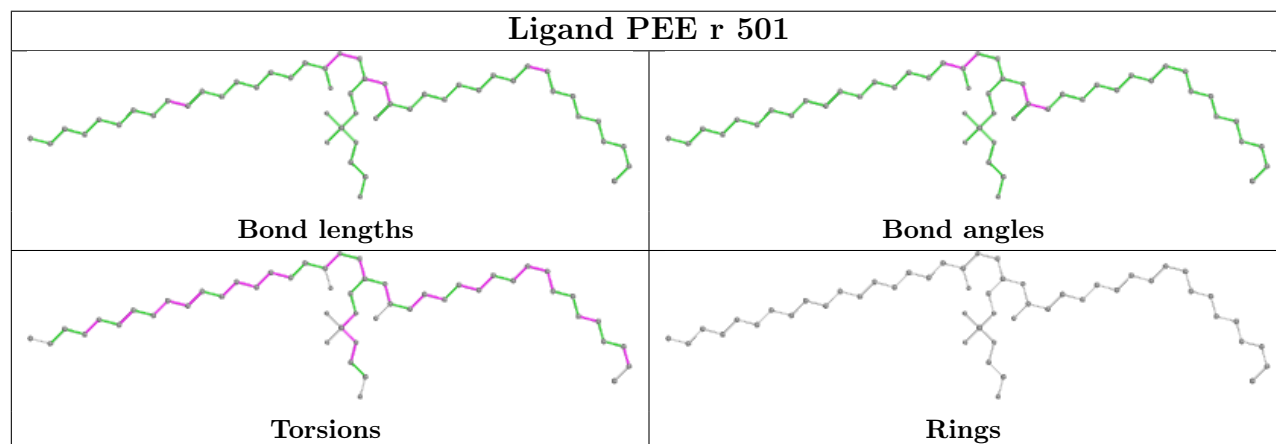
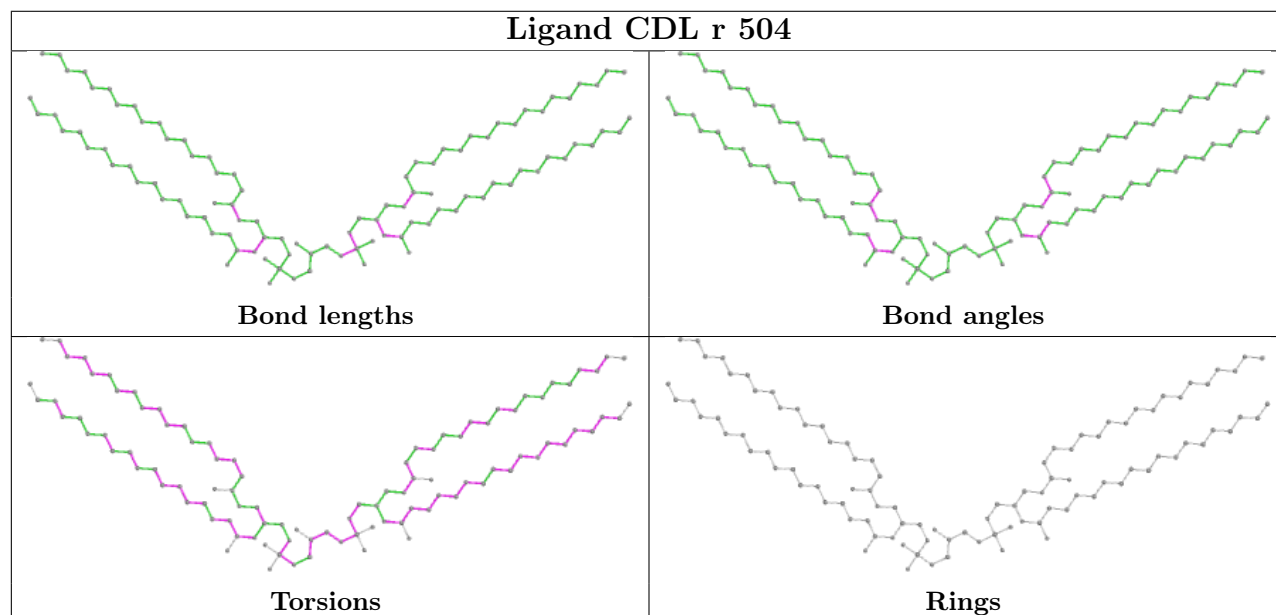
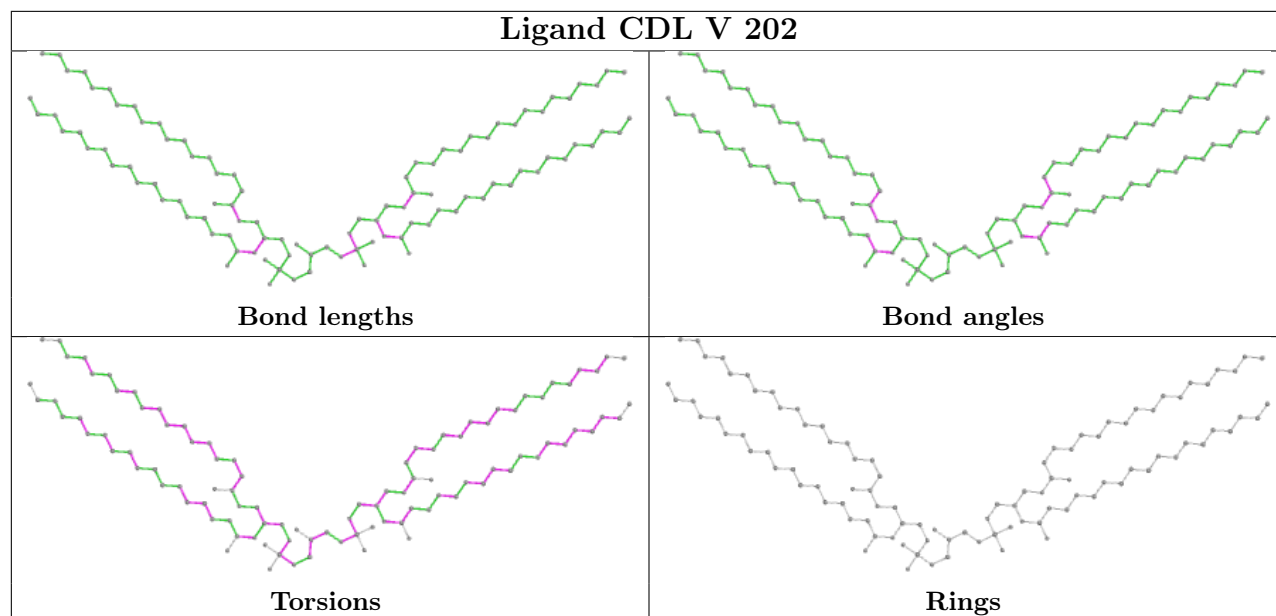


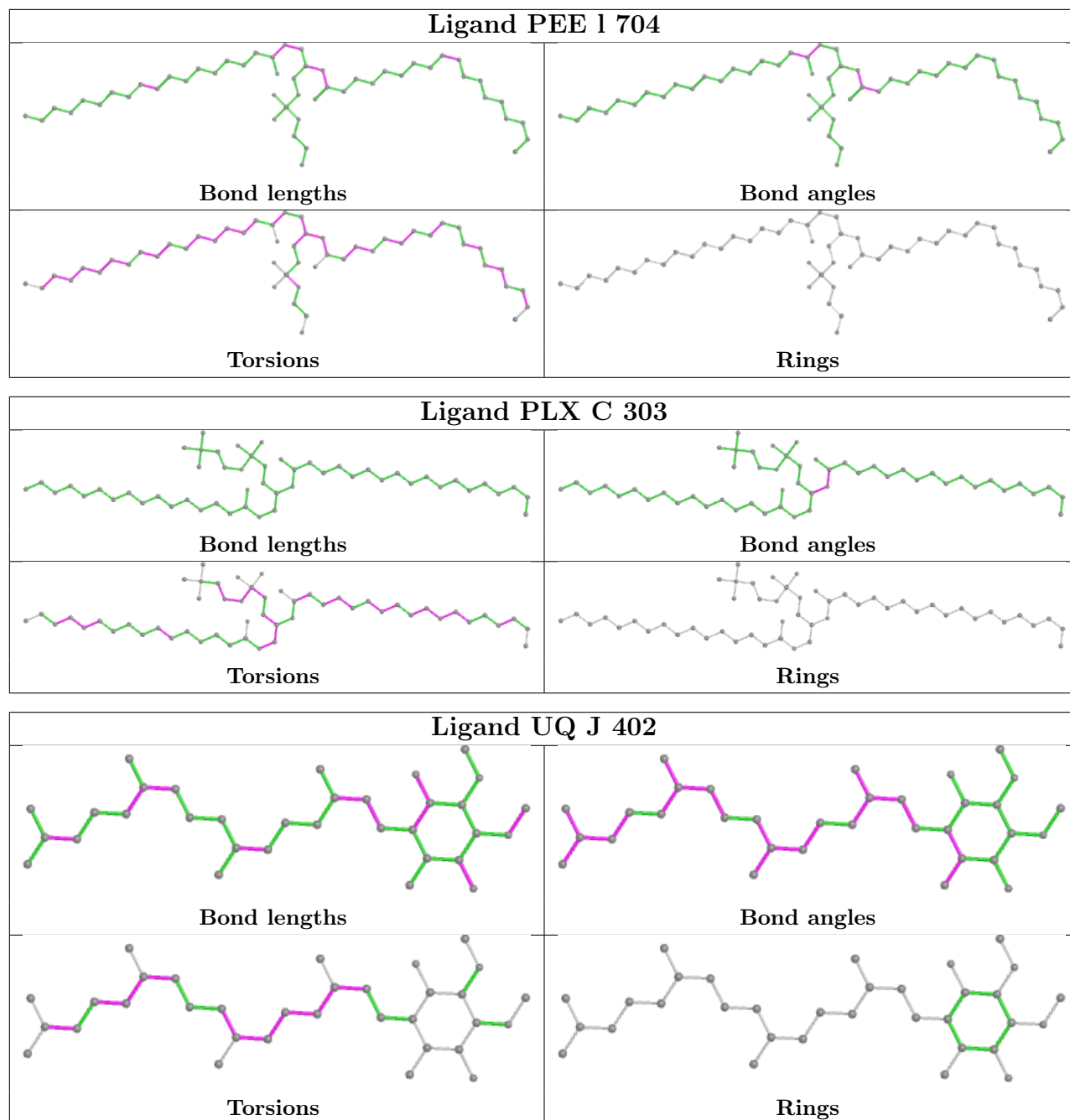


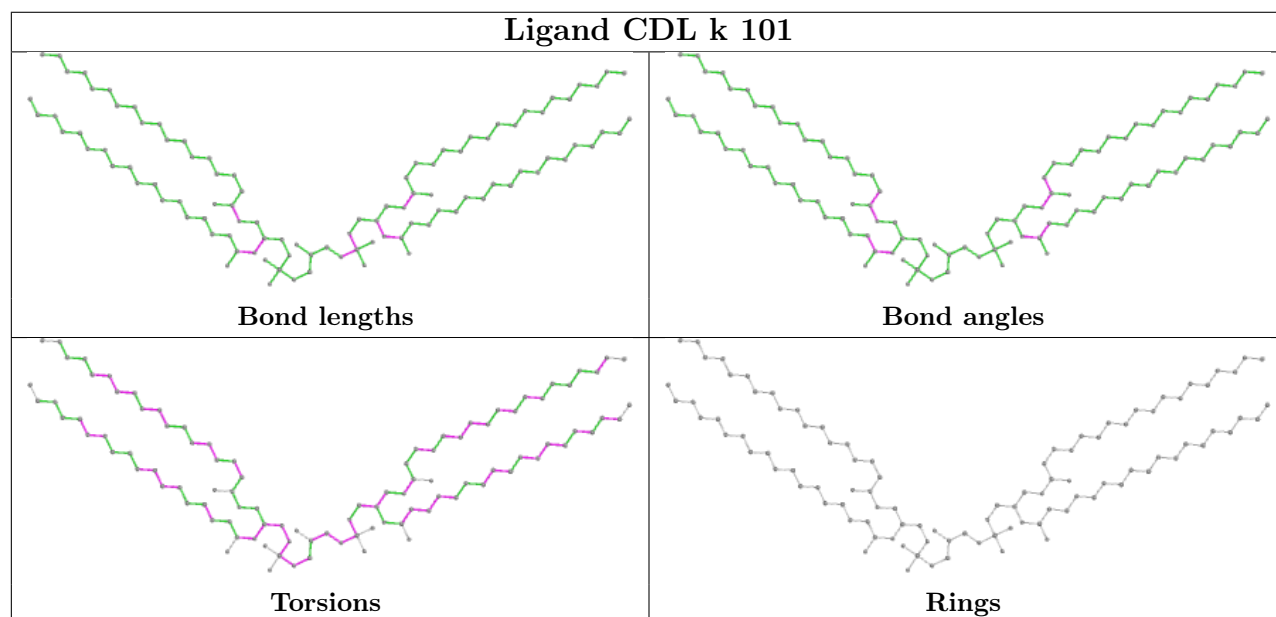
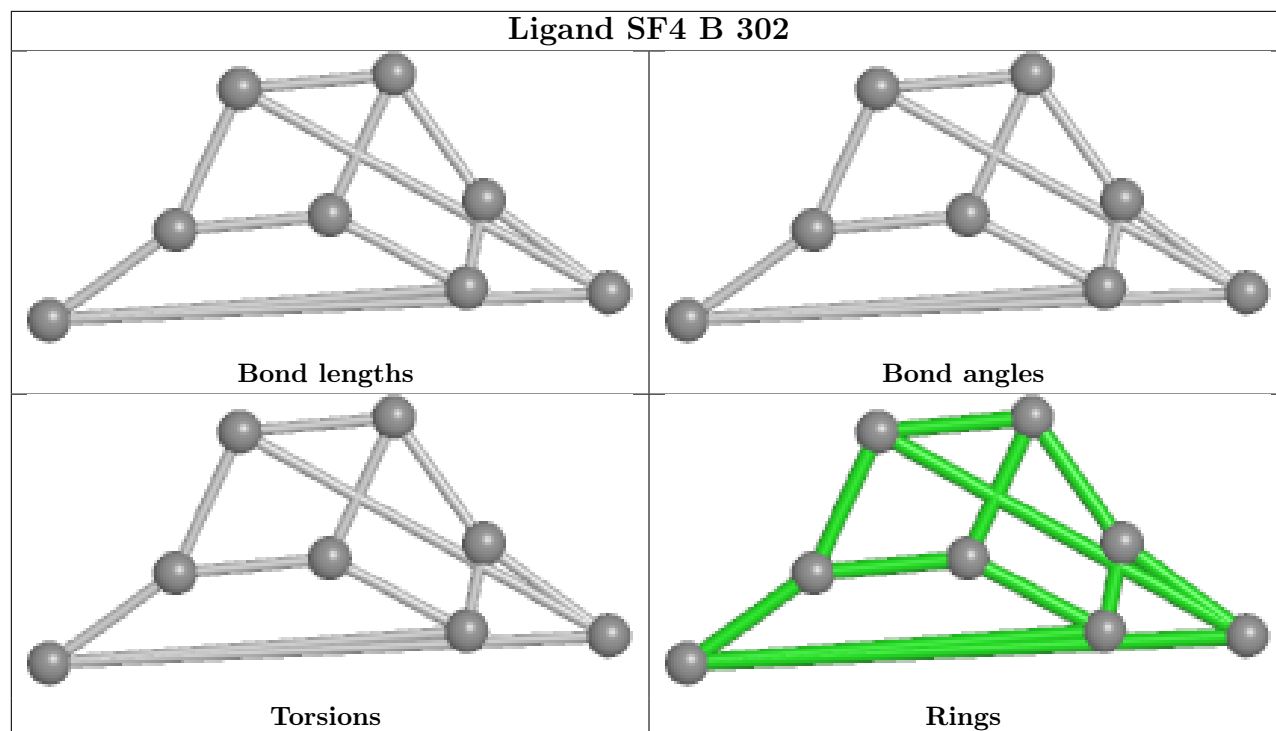


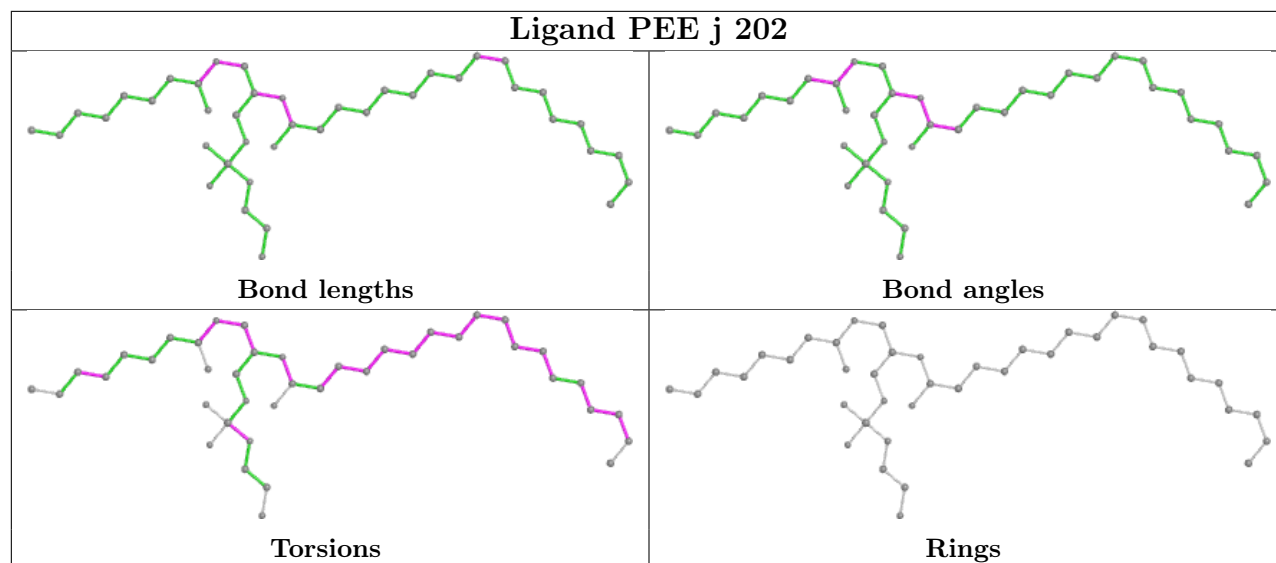












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

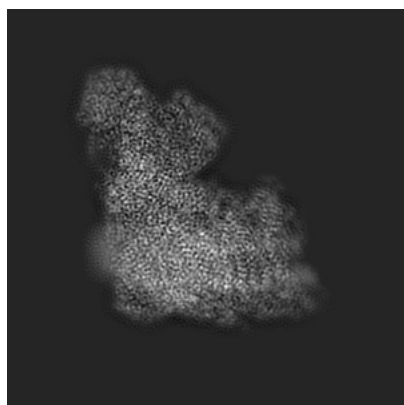
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31643. These allow visual inspection of the internal detail of the map and identification of artifacts.

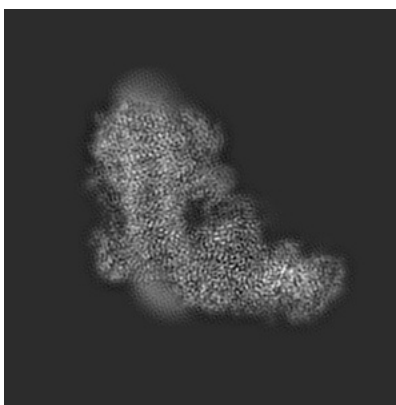
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

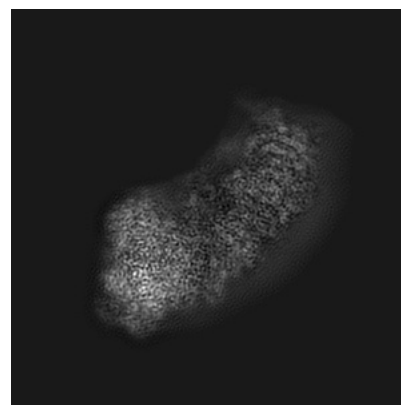
6.1.1 Primary map



X



Y

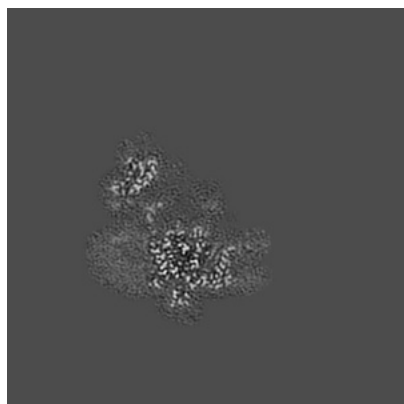


Z

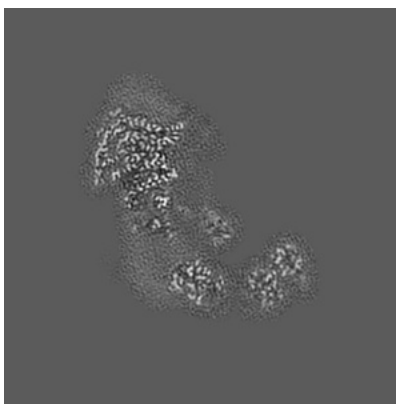
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

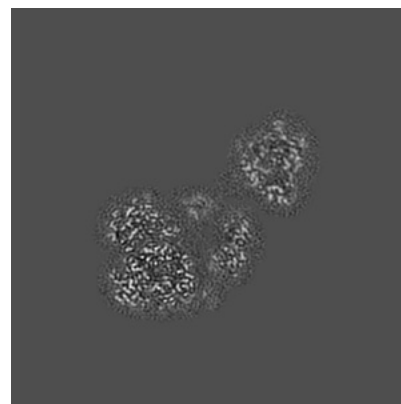
6.2.1 Primary map



X Index: 155



Y Index: 155

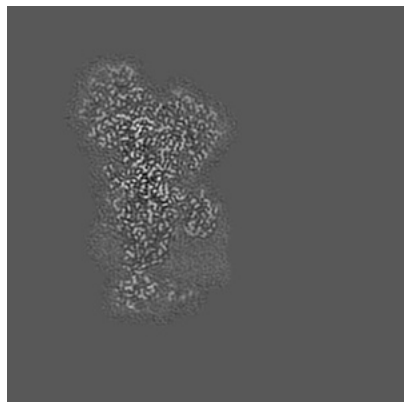


Z Index: 155

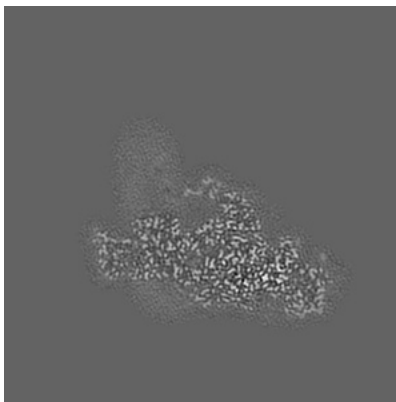
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

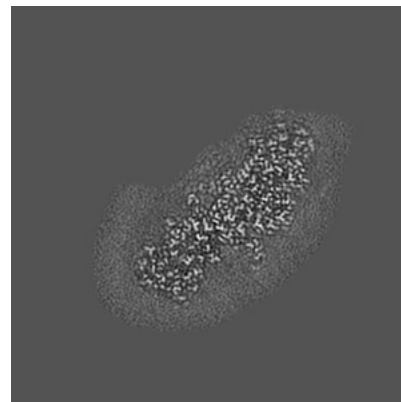
6.3.1 Primary map



X Index: 105



Y Index: 102

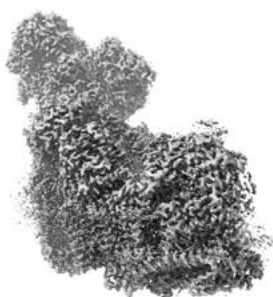


Z Index: 122

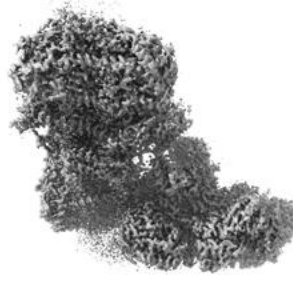
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

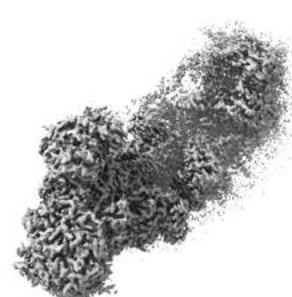
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0258. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

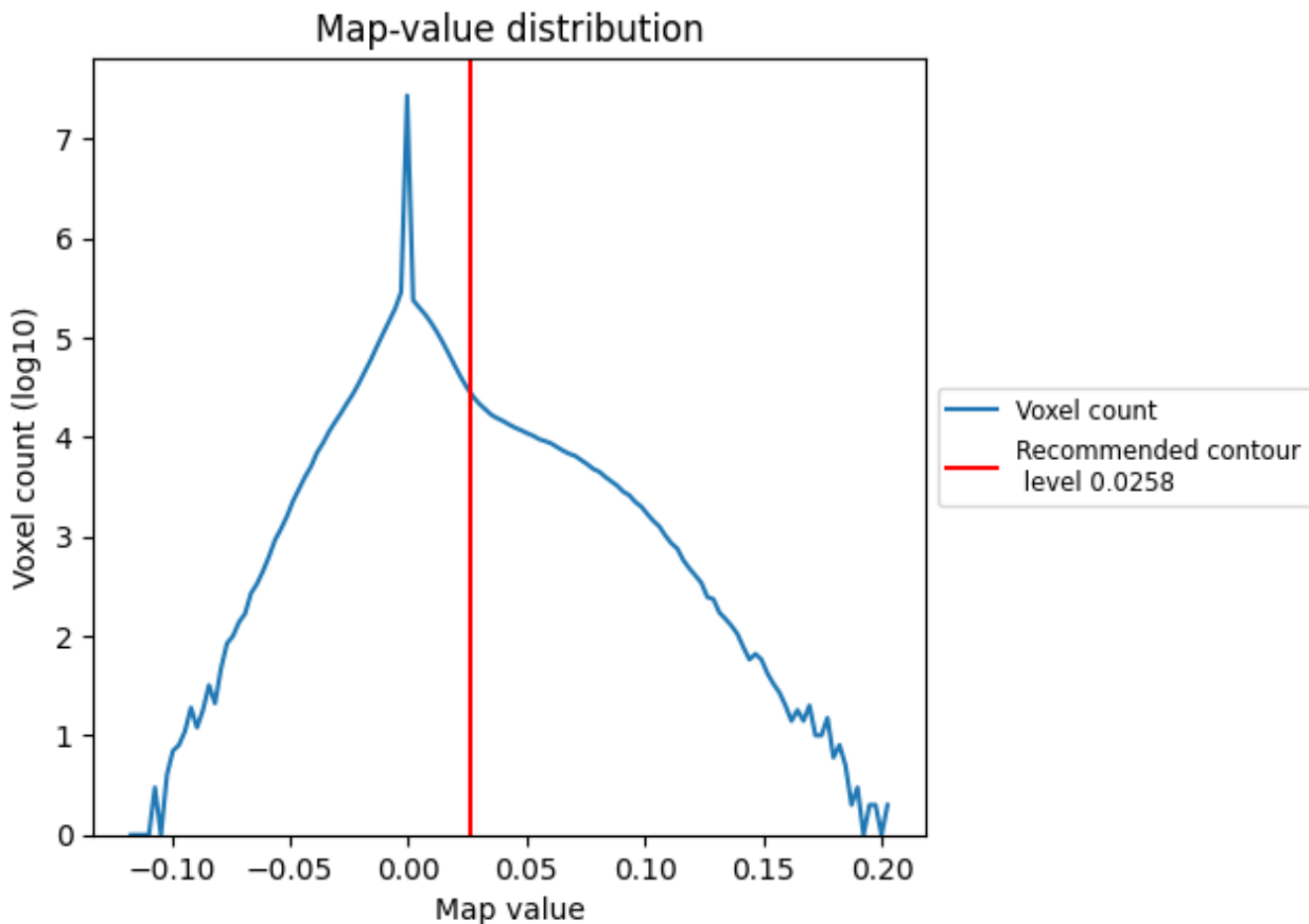
6.5 Mask visualisation

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

7 Map analysis [i](#)

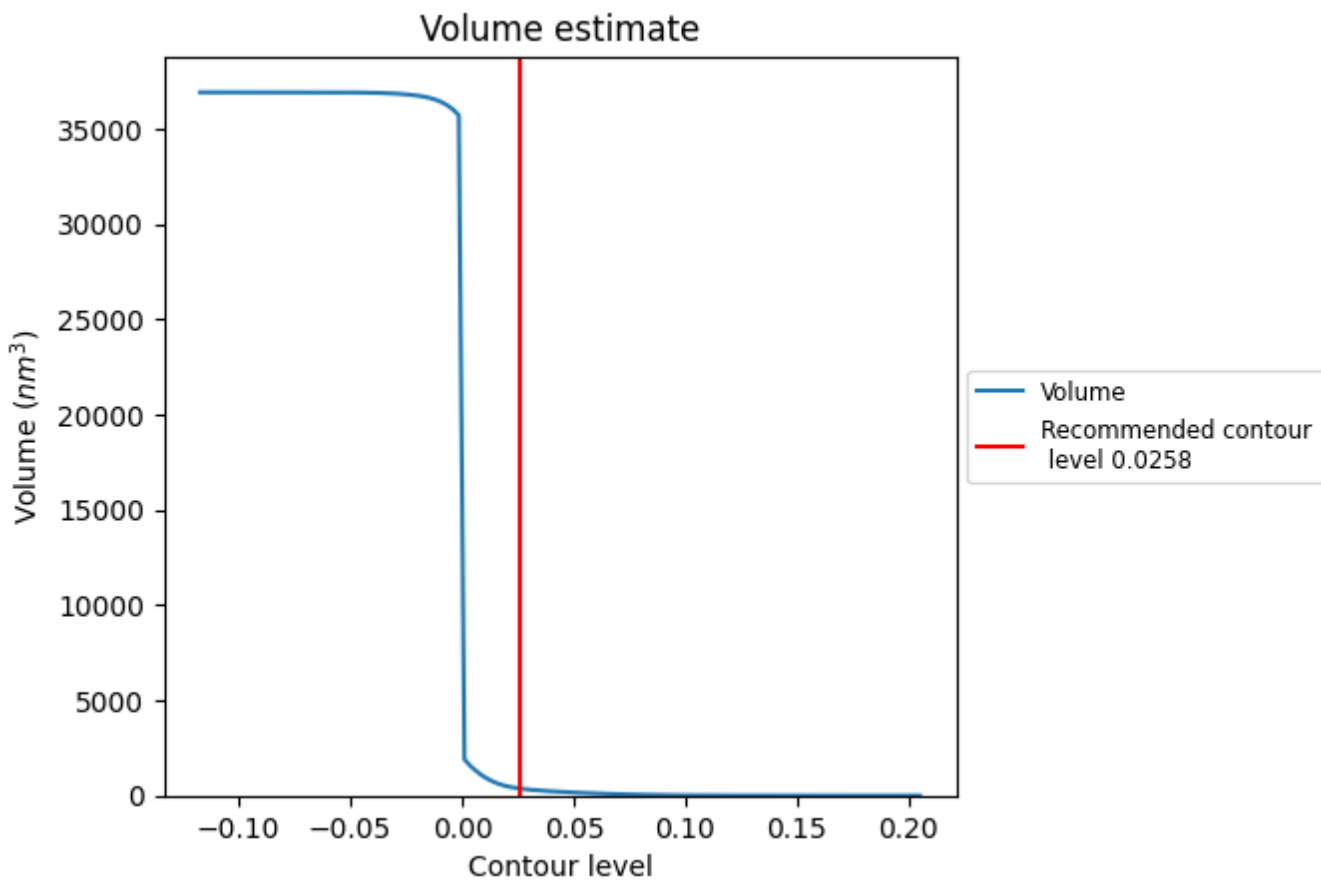
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

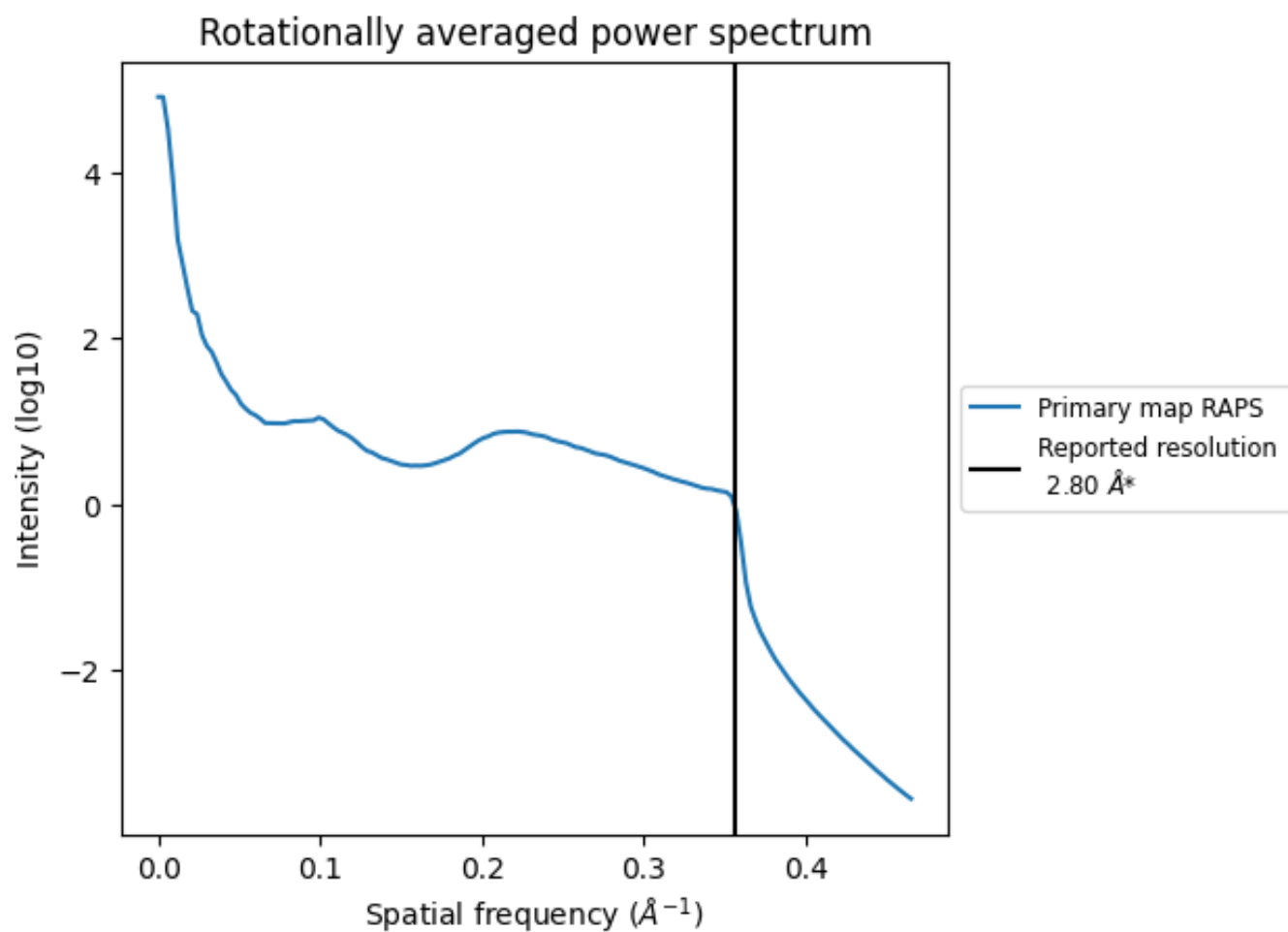
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 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 0.357\AA^{-1}

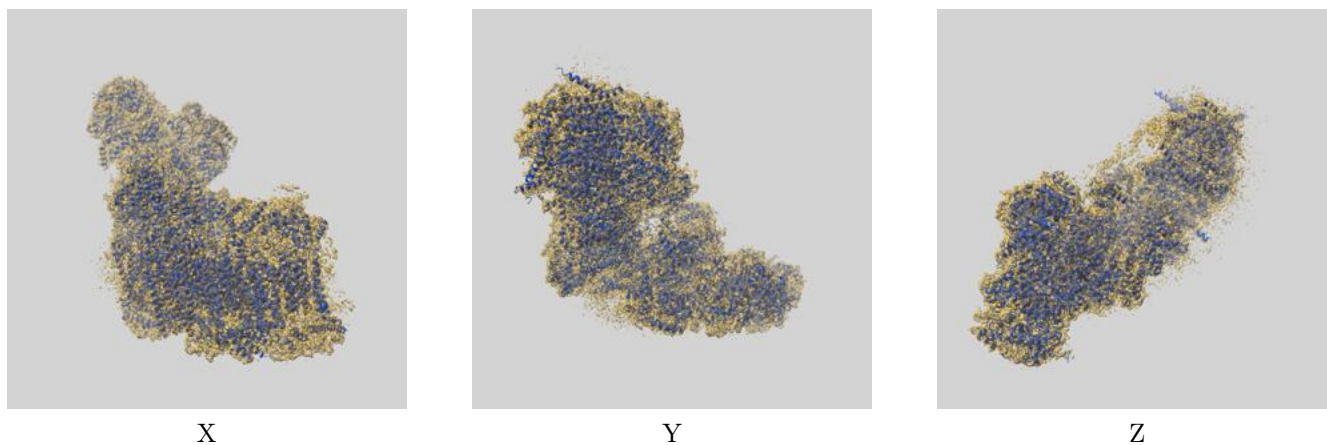
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

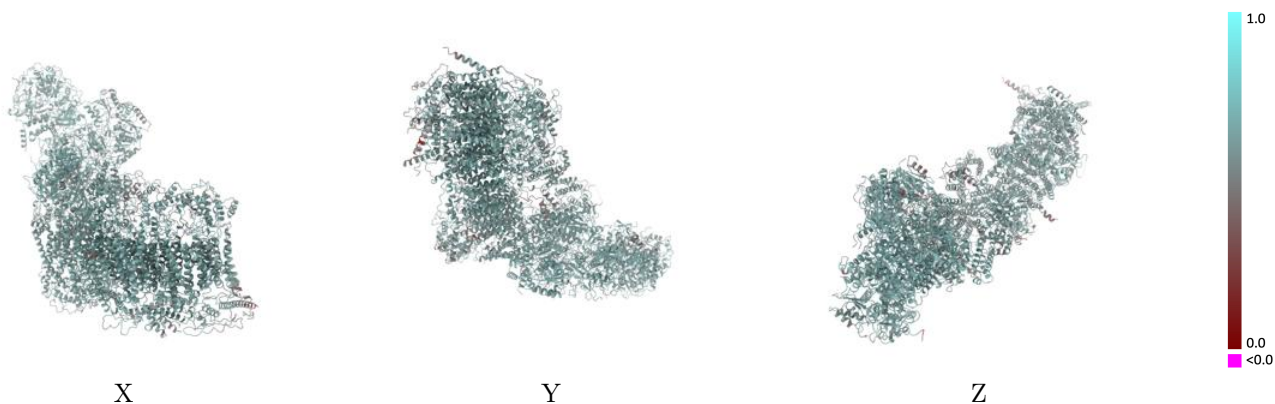
This section contains information regarding the fit between EMDB map EMD-31643 and PDB model 7V2E. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



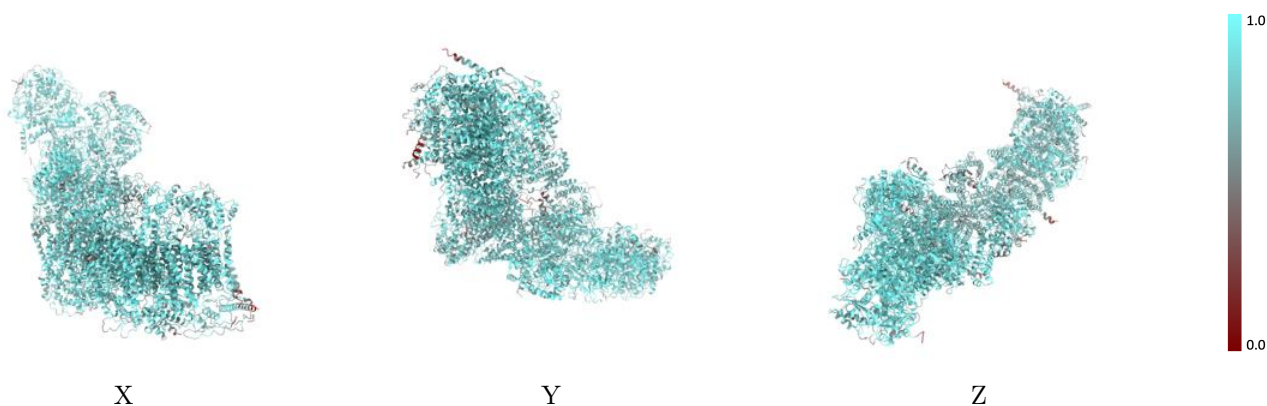
The images above show the 3D surface view of the map at the recommended contour level 0.0258 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



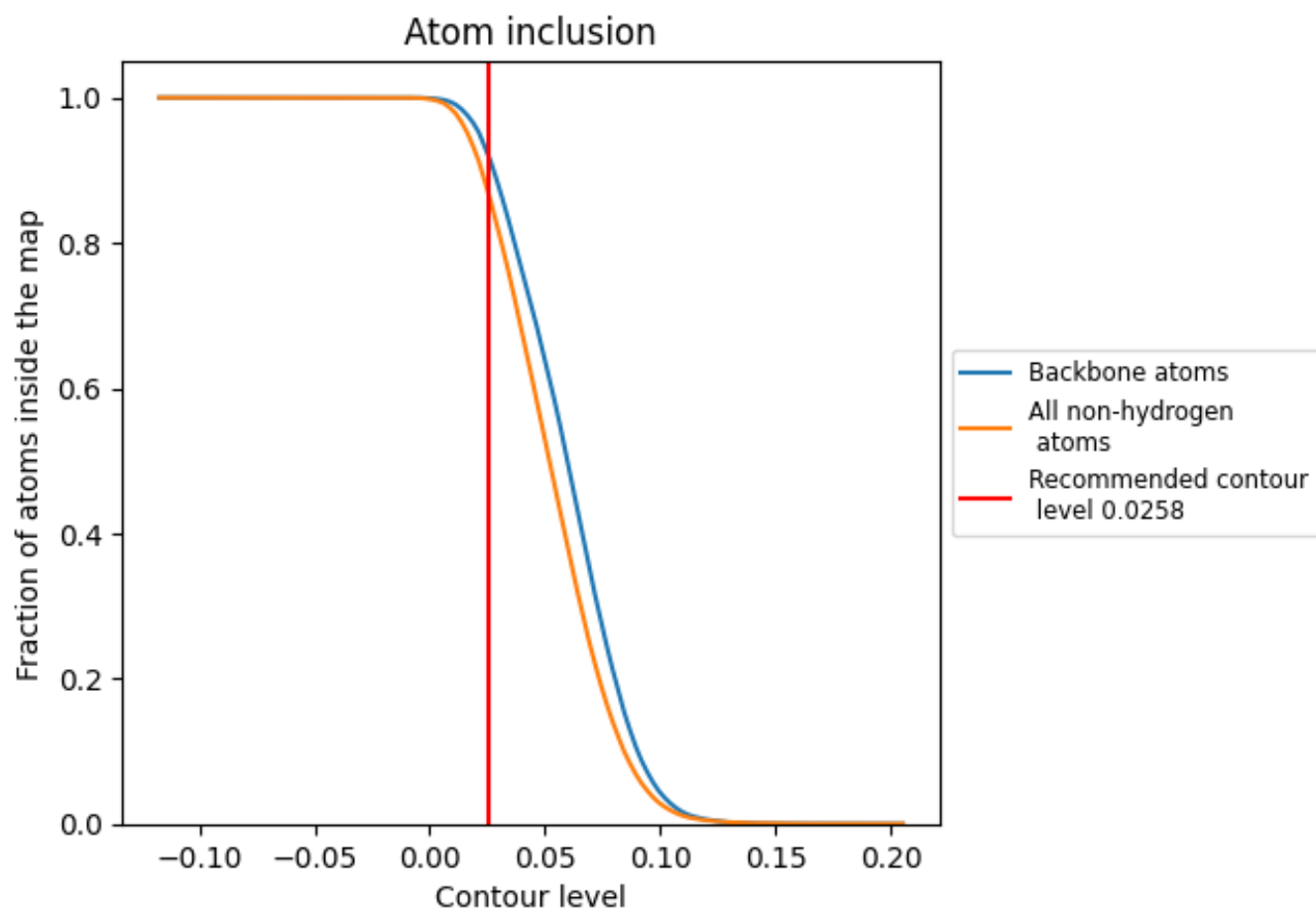
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0258).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.0258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8639	 0.6090
A	 0.8823	 0.6090
B	 0.9500	 0.6500
C	 0.9342	 0.6500
E	 0.8715	 0.6170
F	 0.7769	 0.5480
G	 0.5720	 0.4790
H	 0.8849	 0.6060
I	 0.8166	 0.6040
J	 0.8918	 0.6160
K	 0.8535	 0.6030
L	 0.8974	 0.6350
M	 0.9103	 0.6230
N	 0.8575	 0.6160
O	 0.8376	 0.5910
P	 0.9568	 0.6510
Q	 0.9381	 0.6460
S	 0.9112	 0.6230
T	 0.8947	 0.6220
U	 0.8347	 0.5960
V	 0.7347	 0.5850
W	 0.8618	 0.6040
X	 0.7640	 0.5640
Y	 0.7346	 0.5480
Z	 0.6976	 0.5320
a	 0.8551	 0.6140
b	 0.7774	 0.5700
c	 0.8421	 0.5980
d	 0.8021	 0.5840
e	 0.8038	 0.5870
f	 0.6703	 0.5300
g	 0.8678	 0.6160
h	 0.8475	 0.5850
i	 0.9389	 0.6340
j	 0.8561	 0.6260



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Chain	Atom inclusion	Q-score
k	 0.8551	 0.6140
l	 0.8604	 0.6160
m	 0.8069	 0.5810
n	 0.7052	 0.5550
o	 0.8455	 0.6010
p	 0.8402	 0.5920
r	 0.9020	 0.6280
s	 0.9095	 0.6290
u	 0.8397	 0.5900
v	 0.7098	 0.5310
w	 0.8503	 0.5960