



## Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 05:41 PM JST

PDB ID : 7VZW  
EMDB ID : EMD-32231  
Title : Active state CI from Q10 dataset, Subclass 2  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-11-16  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

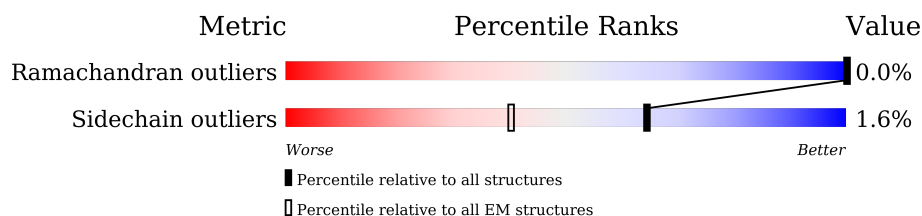
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



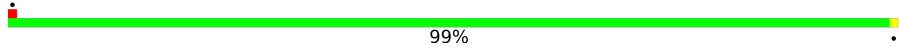

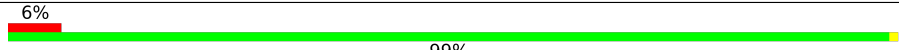
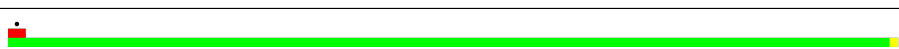
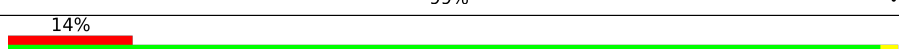
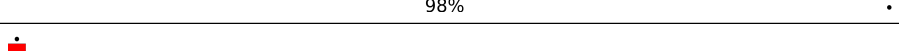
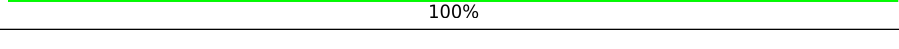
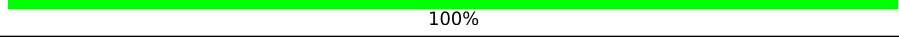
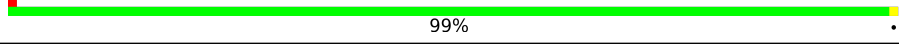

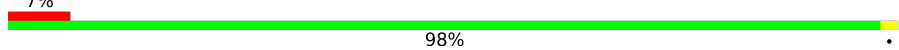

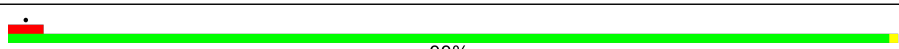

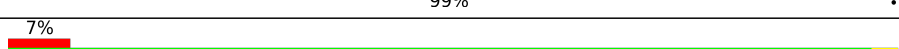
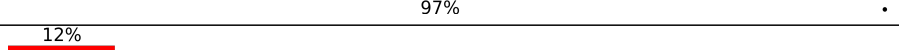
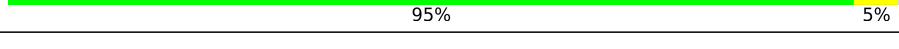
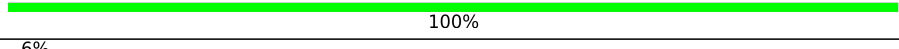

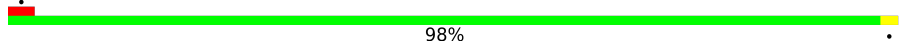
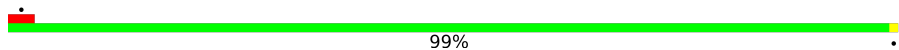
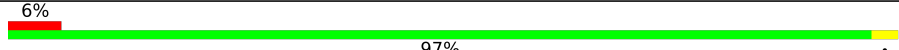

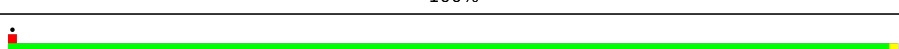
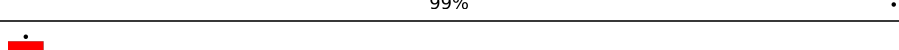
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	

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

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Mol	Chain	Length	Quality of chain
34	k	98	 98% .
35	l	606	 98% .
36	m	175	 8% 97% .
37	n	56	 16% 96% .
38	o	128	 98% .
39	p	178	 98% .
40	r	459	 99% .
41	s	318	 98% .
42	u	171	 99% .
43	v	124	 7% 97% .
44	w	320	 99% .

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 68165 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3326	2101	593	612	20		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			687	432	129	124	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			694	447	103	139	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1735	1123	298	312	2		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1161	749	197	206	9		

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2706	1779	419	462	46		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1291	861	188	229	13		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1526	978	279	261	8		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

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

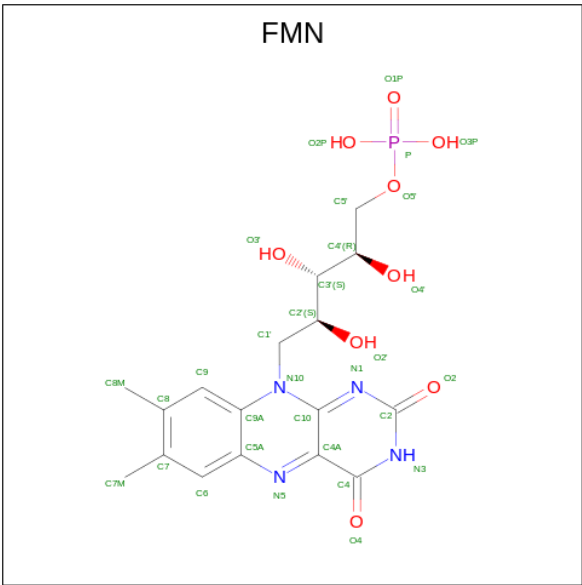
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2579	1643	438	488	10		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

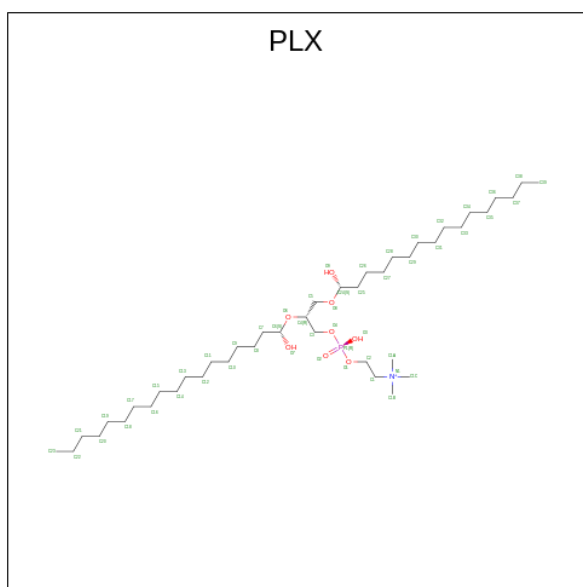
- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
47	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	l	1	Total	C	N	O	P	0
			137	107	3	24	3	
47	l	1	Total	C	N	O	P	0
			137	107	3	24	3	
47	l	1	Total	C	N	O	P	0
			137	107	3	24	3	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	s	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



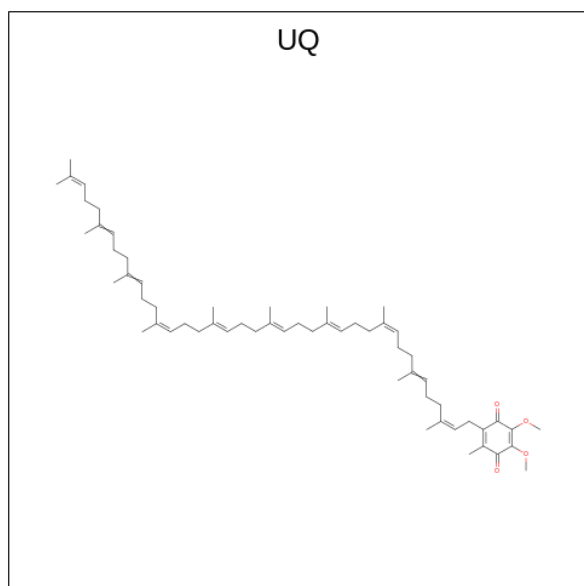
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	N	1	Total	C	N	O	P	0
			52	42	1	8	1	

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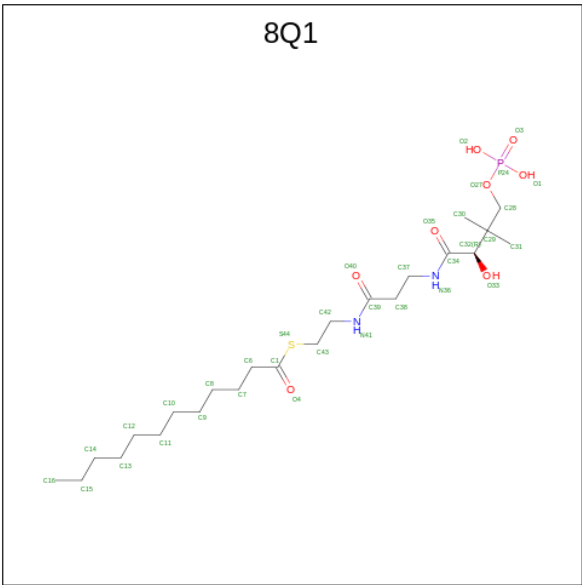
Mol	Chain	Residues	Atoms					AltConf
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			104	84	2	16	2	
48	j	1	Total	C	N	O	P	0
			104	84	2	16	2	
48	n	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



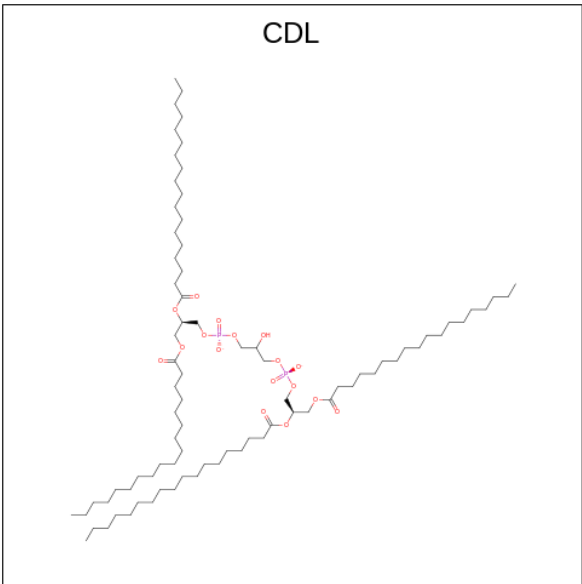
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			63	59	4	
49	J	1	Total	C	O	0
			33	29	4	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



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

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



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

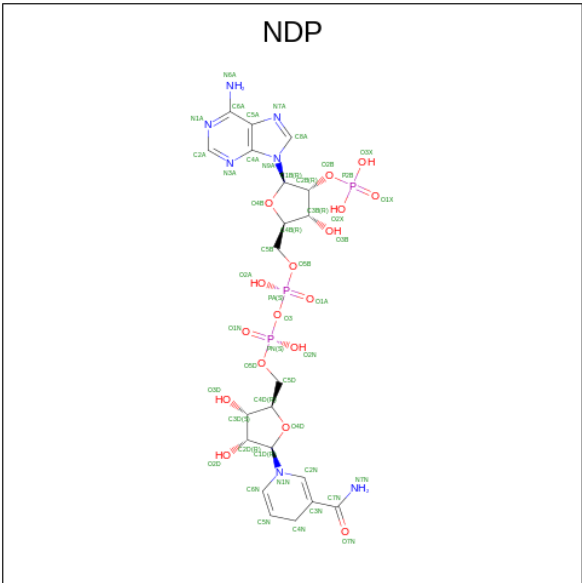
Continued on next page...



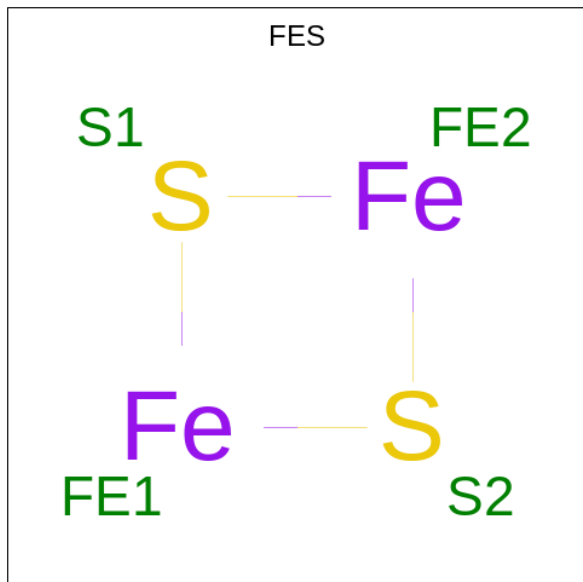
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			194	156	34	4	
51	V	1	Total	C	O	P	0
			194	156	34	4	
51	a	1	Total	C	O	P	0
			100	81	17	2	
51	l	1	Total	C	O	P	0
			199	161	34	4	
51	l	1	Total	C	O	P	0
			199	161	34	4	
51	m	1	Total	C	O	P	0
			100	81	17	2	
51	n	1	Total	C	O	P	0
			55	36	17	2	
51	r	1	Total	C	O	P	0
			100	81	17	2	
51	s	1	Total	C	O	P	0
			89	70	17	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

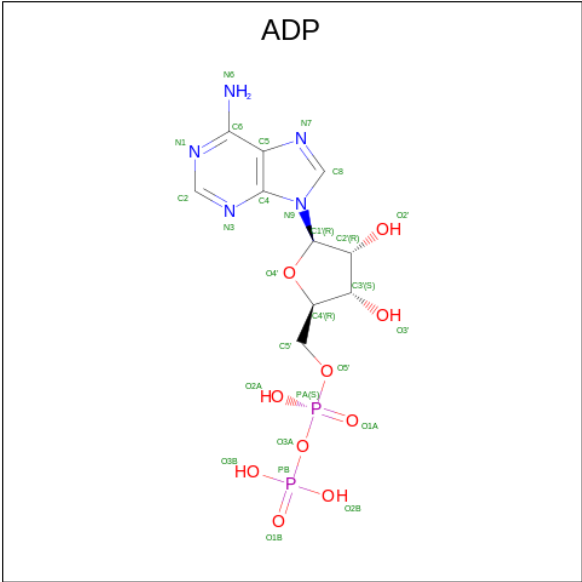
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

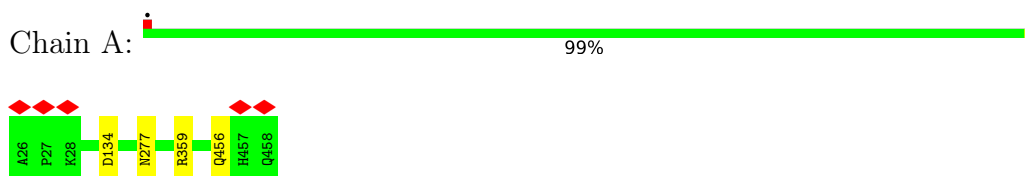


Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

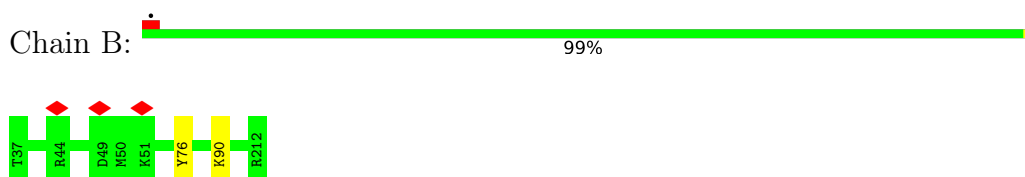
### 3 Residue-property plots [i](#)

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

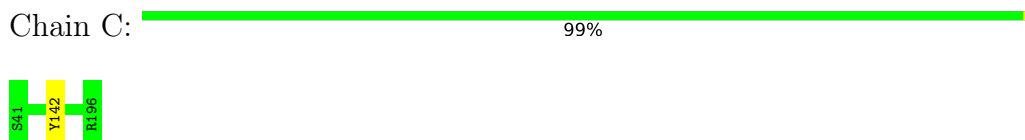
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



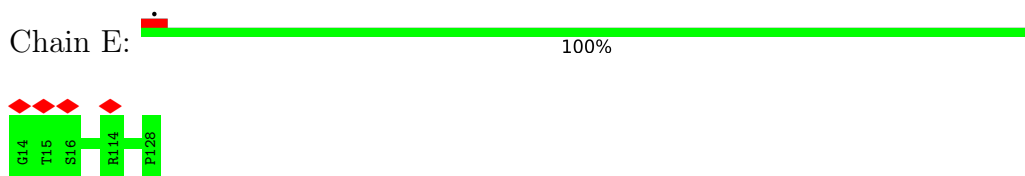
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



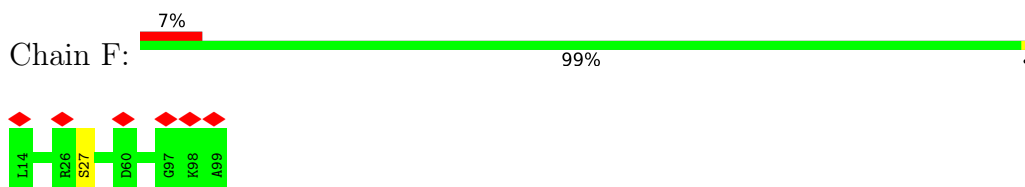
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



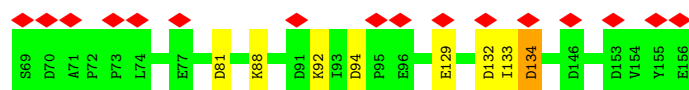
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



- Molecule 6: Acyl carrier protein



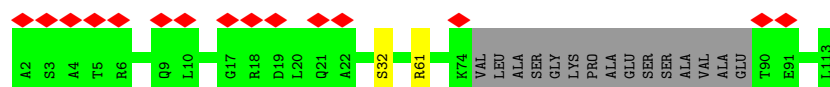
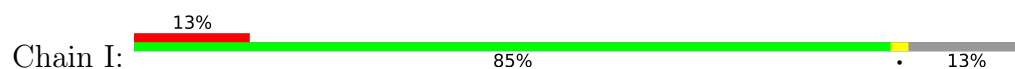
- Molecule 6: Acyl carrier protein



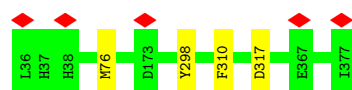
- Molecule 7: Complex I subunit B13



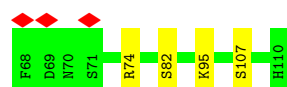
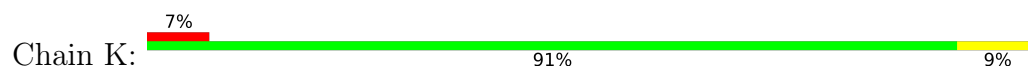
- Molecule 8: Complex I-B14.5a



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



- Molecule 10: Complex I-9kD



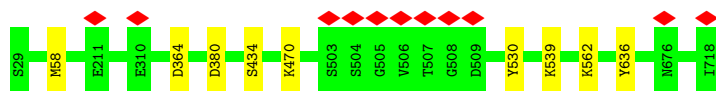
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





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

Chain M: 99%



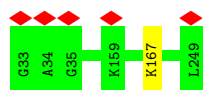
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N: 14% 98%



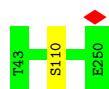
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O: 100%



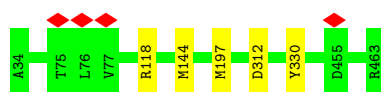
- Molecule 15: Complex I-30kD

Chain P: 100%



- Molecule 16: Complex I-49kD

Chain Q: 99%

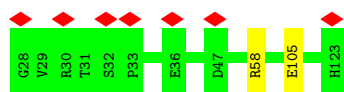


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

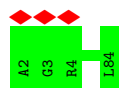
Chain S: 100%



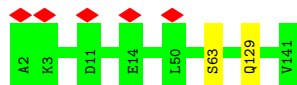
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



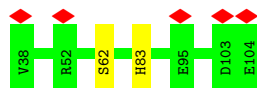
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



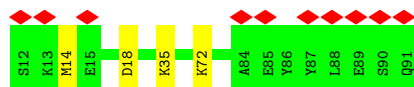
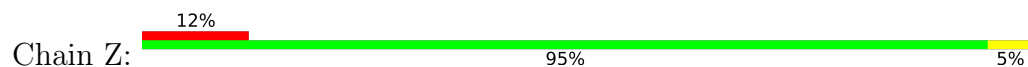
- Molecule 21: Complex I-B16.6



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



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

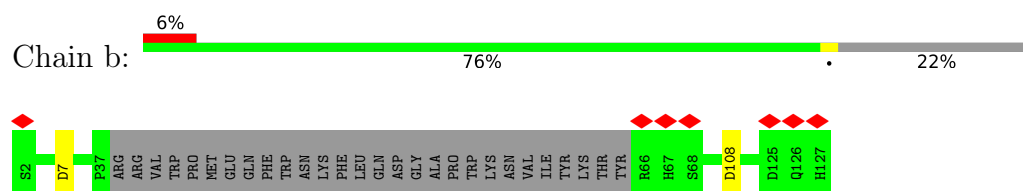


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

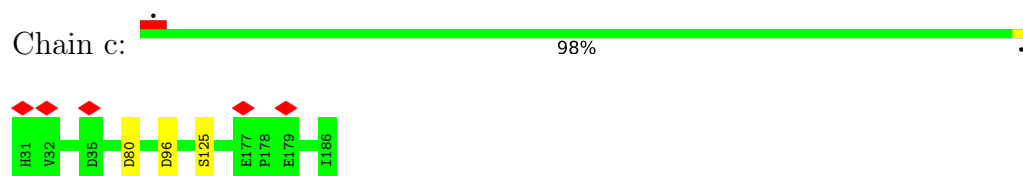


There are no outlier residues recorded for this chain.

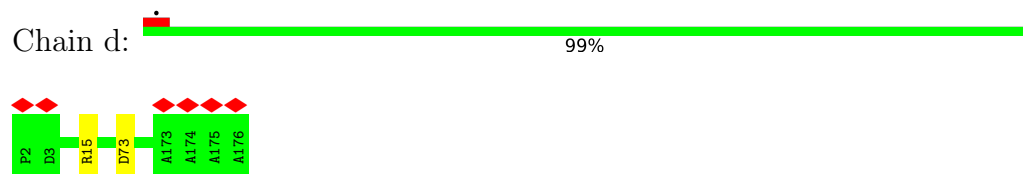
- Molecule 25: Complex I-B17



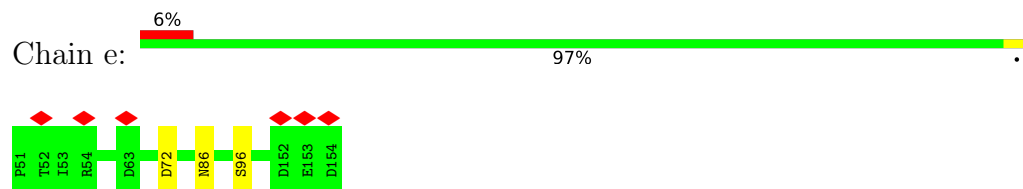
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



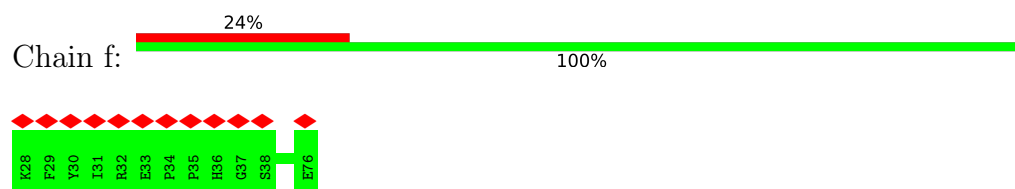
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



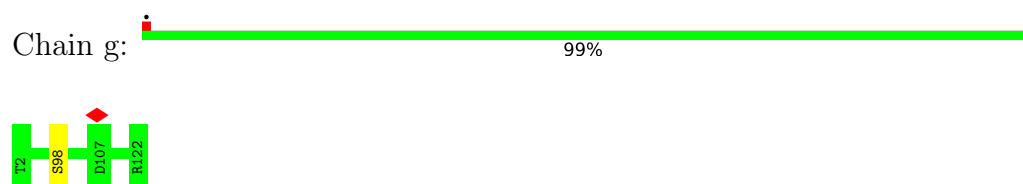
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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



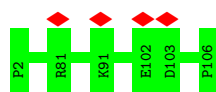
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

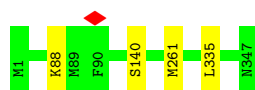


Chain h:  100%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  99%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  98%



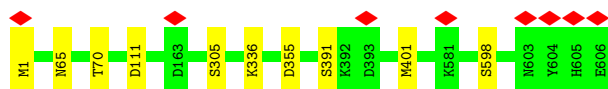
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  98%



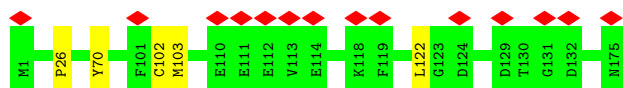
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  98%



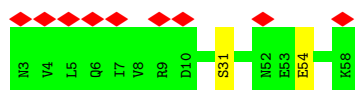
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  8% 97%



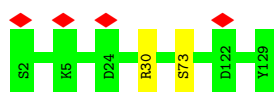
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  16% 96%



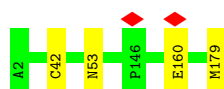
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  98%



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

Chain p:  98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  99%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  98%



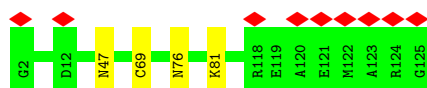
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  99%



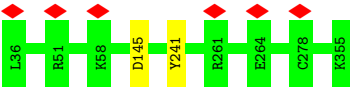
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  7% 97%



- 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	128783	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	0.217	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0219	Depositor
Map size ( $\text{\AA}$ )	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0742, 1.0742, 1.0742	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.27	0/3402	0.49	0/4598
2	B	0.30	0/1443	0.51	0/1952
3	C	0.29	0/1279	0.50	0/1730
4	E	0.27	0/995	0.50	0/1340
5	F	0.26	0/698	0.54	0/940
6	G	0.27	0/702	0.55	1/952 (0.1%)
6	X	0.27	0/705	0.45	0/954
7	H	0.25	0/929	0.43	0/1258
8	I	0.26	0/798	0.52	0/1079
9	J	0.27	0/2828	0.47	0/3834
10	K	0.26	0/377	0.51	0/509
11	L	0.26	0/1039	0.49	0/1403
12	M	0.26	0/5384	0.49	0/7295
13	N	0.26	0/1245	0.51	0/1694
14	O	0.27	0/1711	0.47	0/2328
15	P	0.29	0/1786	0.50	0/2432
16	Q	0.29	0/3538	0.49	0/4796
17	S	0.26	0/581	0.48	0/781
18	T	0.27	0/755	0.52	0/1018
19	U	0.26	0/664	0.44	0/912
20	V	0.26	0/1042	0.46	0/1411
21	W	0.28	0/1192	0.49	0/1610
22	Y	0.26	0/610	0.46	0/836
23	Z	0.28	0/660	0.48	0/892
24	a	0.29	0/1184	0.49	0/1603
25	b	0.27	0/844	0.50	0/1149
26	c	0.28	0/1371	0.45	0/1875
27	d	0.26	0/1494	0.51	0/2015
28	e	0.26	0/891	0.47	0/1210
29	f	0.25	0/386	0.41	0/523
30	g	0.28	0/1031	0.49	0/1394
31	h	0.27	0/889	0.52	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.27	0/2769	0.43	0/3764
33	j	0.26	0/938	0.43	0/1281
34	k	0.27	0/759	0.43	0/1029
35	l	0.27	0/4947	0.45	0/6728
36	m	0.29	0/1323	0.46	0/1797
37	n	0.25	0/491	0.50	0/663
38	o	0.28	0/1092	0.51	0/1481
39	p	0.26	0/1582	0.48	0/2145
40	r	0.27	0/3723	0.45	0/5078
41	s	0.28	0/2581	0.45	0/3529
42	u	0.27	0/1436	0.49	0/1938
43	v	0.27	0/1052	0.52	0/1411
44	w	0.27	0/2639	0.47	0/3575
All	All	0.27	0/67785	0.48	1/91932 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	134	ASP	CB-CG-OD2	5.74	123.46	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	417 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	49
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	101 (92%)	8 (7%)	1 (1%)	17	56
8	I	93/112 (83%)	78 (84%)	15 (16%)	0	100	100
9	J	340/342 (99%)	327 (96%)	13 (4%)	0	100	100
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	660 (96%)	28 (4%)	0	100	100
13	N	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	415 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	91 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	96 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	330 (96%)	15 (4%)	0	100	100
33	j	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
34	k	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
35	l	604/606 (100%)	571 (94%)	33 (6%)	0	100	100
36	m	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	25	64
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
41	s	316/318 (99%)	303 (96%)	12 (4%)	1 (0%)	41	74
42	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
43	v	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8174/8312 (98%)	7859 (96%)	311 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
36	m	26	PRO
7	H	77	ILE
41	s	208	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/346 (100%)	341 (99%)	4 (1%)	71	88
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	87
3	C	132/132 (100%)	131 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	74 (99%)	1 (1%)	69	87
6	G	75/81 (93%)	68 (91%)	7 (9%)	9	33
6	X	76/81 (94%)	73 (96%)	3 (4%)	32	67
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	85 (98%)	2 (2%)	50	78
9	J	296/296 (100%)	292 (99%)	4 (1%)	67	86
10	K	42/42 (100%)	38 (90%)	4 (10%)	8	32
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	91
12	M	580/580 (100%)	571 (98%)	9 (2%)	62	84
13	N	130/130 (100%)	127 (98%)	3 (2%)	50	78
14	O	183/183 (100%)	182 (100%)	1 (0%)	88	95
15	P	189/190 (100%)	188 (100%)	1 (0%)	88	95
16	Q	370/370 (100%)	366 (99%)	4 (1%)	73	88
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	77 (98%)	2 (2%)	47	77
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	99 (98%)	2 (2%)	55	80
21	W	121/123 (98%)	120 (99%)	1 (1%)	81	93
22	Y	62/62 (100%)	60 (97%)	2 (3%)	39	71
23	Z	62/62 (100%)	58 (94%)	4 (6%)	17	51
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	88 (98%)	2 (2%)	52	79
26	c	141/141 (100%)	138 (98%)	3 (2%)	53	79
27	d	155/155 (100%)	153 (99%)	2 (1%)	69	87
28	e	96/96 (100%)	93 (97%)	3 (3%)	40	72
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	91
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	306 (99%)	4 (1%)	69	87
33	j	100/100 (100%)	98 (98%)	2 (2%)	55	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	77
35	l	540/540 (100%)	530 (98%)	10 (2%)	57	81
36	m	130/141 (92%)	126 (97%)	4 (3%)	40	72
37	n	53/53 (100%)	51 (96%)	2 (4%)	33	67
38	o	113/113 (100%)	111 (98%)	2 (2%)	59	82
39	p	157/159 (99%)	153 (98%)	4 (2%)	47	77
40	r	410/410 (100%)	407 (99%)	3 (1%)	84	94
41	s	275/275 (100%)	270 (98%)	5 (2%)	59	82
42	u	153/153 (100%)	152 (99%)	1 (1%)	84	94
43	v	104/111 (94%)	100 (96%)	4 (4%)	33	67
44	w	280/283 (99%)	278 (99%)	2 (1%)	84	94
All	All	7151/7240 (99%)	7037 (98%)	114 (2%)	64	84

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	277	ASN
1	A	359	ARG
1	A	456	GLN
2	B	76	TYR
2	B	90	LYS
3	C	142	TYR
5	F	27	SER
6	G	81	ASP
6	G	88	LYS
6	G	92	LYS
6	G	94	ASP
6	G	129	GLU
6	G	132	ASP
6	G	134	ASP
8	I	32	SER
8	I	61	ARG
9	J	76	MET
9	J	298	TYR
9	J	310	PHE
9	J	317	ASP
10	K	74	ARG

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Mol	Chain	Res	Type
10	K	82	SER
10	K	95	LYS
10	K	107	SER
11	L	154	LYS
12	M	58	MET
12	M	364	ASP
12	M	380	ASP
12	M	434	SER
12	M	470	LYS
12	M	530	TYR
12	M	539	LYS
12	M	562	LYS
12	M	636	TYR
13	N	15	SER
13	N	107	LYS
13	N	118	SER
14	O	167	LYS
15	P	110	SER
16	Q	144	MET
16	Q	197	MET
16	Q	312	ASP
16	Q	330	TYR
18	T	58	ARG
18	T	105	GLU
20	V	63	SER
20	V	129	GLN
21	W	88	ARG
6	X	98	LEU
6	X	105	MET
6	X	129	GLU
22	Y	62	SER
22	Y	83	HIS
23	Z	14	MET
23	Z	18	ASP
23	Z	35	LYS
23	Z	72	LYS
25	b	7	ASP
25	b	108	ASP
26	c	80	ASP
26	c	96	ASP
26	c	125	SER
27	d	15	ARG

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Mol	Chain	Res	Type
27	d	73	ASP
28	e	72	ASP
28	e	86	ASN
28	e	96	SER
30	g	98	SER
32	i	88	LYS
32	i	140	SER
32	i	261	MET
32	i	335	LEU
33	j	44	MET
33	j	101	SER
34	k	53	PHE
34	k	82	SER
35	l	1	MET
35	l	65	ASN
35	l	70	THR
35	l	111	ASP
35	l	305	SER
35	l	336	LYS
35	l	355	ASP
35	l	391	SER
35	l	401	MET
35	l	598	SER
36	m	70	TYR
36	m	102	CYS
36	m	103	MET
36	m	122	LEU
37	n	31	SER
37	n	54	GLU
38	o	30	ARG
38	o	73	SER
39	p	42	CYS
39	p	53	ASN
39	p	160	GLU
39	p	179	MET
40	r	168	GLN
40	r	253	LEU
40	r	401	MET
41	s	156	MET
41	s	174	MET
41	s	202	GLU
41	s	204	GLU

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Mol	Chain	Res	Type
41	s	289	LEU
42	u	48	TRP
43	v	47	ASN
43	v	69	CYS
43	v	76	ASN
43	v	81	LYS
44	w	145	ASP
44	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
12	M	652	ASN
14	O	69	ASN
27	d	149	HIS
35	l	541	ASN
40	r	251	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	2MR	Q	118	16	10,12,13	1.96	1 (10%)	5,13,15	5.95	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (1) bond length outliers are listed below:

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

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.22	130.68	119.48
16	Q	118	2MR	CD-NE-CZ	4.00	130.90	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.17	130.86	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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	$\# Z  > 2$
49	UQ	C	304	-	63,63,63	3.63	16 (25%)	76,79,79	3.18	32 (42%)
49	UQ	J	402	-	33,33,63	3.45	9 (27%)	40,43,79	2.78	13 (32%)
47	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	1.00	2 (4%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
47	PEE	s	401	-	40,40,50	1.15	5 (12%)	43,45,55	1.02	2 (4%)
51	CDL	s	402	-	88,88,99	1.13	8 (9%)	94,100,111	0.92	4 (4%)
52	NDP	J	401	-	45,52,52	4.56	20 (44%)	53,80,80	1.92	6 (11%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.23	8 (16%)
47	PEE	Q	501	-	46,46,50	1.19	6 (13%)	49,51,55	1.03	2 (4%)
48	PLX	n	101	-	51,51,51	1.14	4 (7%)	55,59,59	0.59	1 (1%)
48	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.64	1 (1%)
48	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
50	8Q1	G	201	-	31,34,34	1.68	6 (19%)	40,43,43	1.60	6 (15%)
50	8Q1	X	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.51	6 (15%)
51	CDL	l	703	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)
53	FES	O	301	14	0,4,4	-	-	-	-	-
51	CDL	I	201	-	50,50,99	1.40	8 (16%)	56,62,111	1.13	4 (7%)
56	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.45	5 (17%)
51	CDL	r	503	-	99,99,99	1.07	8 (8%)	105,111,111	0.88	4 (3%)
47	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.04	2 (4%)
48	PLX	j	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.62	1 (1%)
53	FES	M	803	12	0,4,4	-	-	-	-	-
47	PEE	U	101	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
51	CDL	l	702	-	98,98,99	1.09	8 (8%)	104,110,111	0.90	4 (3%)
51	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.87	4 (4%)
48	PLX	C	303	-	51,51,51	1.13	3 (5%)	55,59,59	0.61	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
45	SF4	A	501	1	0,12,12	-	-	-	-	-
47	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
51	CDL	n	102	-	54,54,99	1.36	8 (14%)	60,66,111	1.11	4 (6%)
47	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.58	1 (1%)
51	CDL	V	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	CDL	a	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
47	PEE	l	705	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
47	PEE	l	704	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
48	PLX	N	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
51	CDL	m	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	UQ	C	304	-	-	25/63/87/87	0/1/1/1
49	UQ	J	402	-	-	15/27/51/87	0/1/1/1
47	PEE	C	302	-	-	29/50/50/54	-
45	SF4	M	802	12	-	-	0/6/5/5
47	PEE	s	401	-	-	19/44/44/54	-
51	CDL	s	402	-	-	52/99/99/110	-
52	NDP	J	401	-	-	11/30/77/77	0/4/5/5
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
47	PEE	Q	501	-	-	24/50/50/54	-
48	PLX	n	101	-	-	26/55/55/55	-
48	PLX	g	201	-	-	29/55/55/55	-
48	PLX	j	202	-	-	25/55/55/55	-
50	8Q1	G	201	-	-	11/41/41/41	-
50	8Q1	X	201	6	-	16/41/41/41	-
51	CDL	l	703	-	-	58/110/110/110	-
53	FES	O	301	14	-	-	0/1/1/1
51	CDL	I	201	-	-	30/61/61/110	-
56	ADP	w	401	-	-	4/12/32/32	0/3/3/3
51	CDL	r	503	-	-	55/110/110/110	-
47	PEE	l	701	-	-	26/43/43/54	-
48	PLX	j	201	-	-	32/55/55/55	-
53	FES	M	803	12	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	U	101	-	-	21/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
51	CDL	l	702	-	-	56/109/109/110	-
51	CDL	V	201	-	-	50/104/104/110	-
48	PLX	C	303	-	-	26/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
47	PEE	r	501	-	-	27/54/54/54	-
51	CDL	n	102	-	-	25/65/65/110	-
47	PEE	W	201	-	-	25/44/44/54	-
48	PLX	r	502	-	-	30/55/55/55	-
51	CDL	V	202	-	-	54/110/110/110	-
51	CDL	a	201	-	-	58/110/110/110	-
47	PEE	l	705	-	-	28/49/49/54	-
47	PEE	l	704	-	-	29/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
48	PLX	N	201	-	-	25/55/55/55	-
47	PEE	B	303	-	-	21/54/54/54	-
51	CDL	m	201	-	-	64/110/110/110	-

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-13.08	1.23	1.52
52	J	401	NDP	C6N-C5N	12.43	1.55	1.33
52	J	401	NDP	O4D-C4D	10.56	1.68	1.45
52	J	401	NDP	C3D-C4D	-9.99	1.27	1.53
49	J	402	UQ	C18-C19	9.58	1.56	1.33
49	C	304	UQ	C18-C19	9.58	1.56	1.33
49	C	304	UQ	C13-C14	9.32	1.55	1.33
49	J	402	UQ	C13-C14	9.18	1.55	1.33
49	C	304	UQ	C23-C24	9.05	1.54	1.33
49	J	402	UQ	C8-C9	9.02	1.54	1.33
49	C	304	UQ	C8-C9	8.95	1.54	1.33
56	w	401	ADP	C3'-C4'	-8.95	1.30	1.53
49	C	304	UQ	C28-C29	8.85	1.54	1.33
49	C	304	UQ	C33-C34	8.53	1.53	1.33
52	J	401	NDP	O4B-C1B	8.46	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	304	UQ	C38-C39	8.25	1.52	1.33
49	C	304	UQ	C43-C44	8.24	1.52	1.33
52	J	401	NDP	O4B-C4B	-7.92	1.27	1.45
49	C	304	UQ	C48-C49	7.85	1.51	1.33
49	J	402	UQ	C23-C24	7.82	1.54	1.32
56	w	401	ADP	O4'-C4'	7.57	1.61	1.45
49	C	304	UQ	C53-C54	7.38	1.53	1.32
52	J	401	NDP	C2N-C3N	7.24	1.55	1.34
56	w	401	ADP	O4'-C1'	-6.97	1.31	1.41
50	X	201	8Q1	C34-N36	5.49	1.45	1.33
52	J	401	NDP	P2B-O2B	5.42	1.69	1.59
50	G	201	8Q1	C34-N36	5.35	1.45	1.33
50	G	201	8Q1	C39-N41	5.28	1.45	1.33
50	X	201	8Q1	C39-N41	5.27	1.45	1.33
52	J	401	NDP	C3B-C4B	5.19	1.66	1.53
52	J	401	NDP	O4D-C1D	-4.97	1.30	1.42
52	J	401	NDP	C6N-N1N	4.82	1.49	1.37
52	J	401	NDP	O2D-C2D	-4.29	1.32	1.43
52	J	401	NDP	C7N-N7N	4.19	1.44	1.33
52	J	401	NDP	C6A-N6A	4.07	1.48	1.34
56	w	401	ADP	C6-N6	3.83	1.48	1.34
47	l	701	PEE	C18-C19	3.75	1.53	1.31
47	s	401	PEE	C18-C19	3.74	1.53	1.31
46	A	502	FMN	C4A-N5	3.73	1.38	1.30
47	B	303	PEE	C18-C19	3.73	1.53	1.31
47	l	704	PEE	C18-C19	3.73	1.53	1.31
47	C	302	PEE	C18-C19	3.73	1.53	1.31
47	W	201	PEE	C18-C19	3.72	1.53	1.31
47	r	501	PEE	C18-C19	3.72	1.53	1.31
47	l	705	PEE	C18-C19	3.72	1.53	1.31
47	U	101	PEE	C18-C19	3.72	1.53	1.31
47	Q	501	PEE	C18-C19	3.69	1.53	1.31
47	l	701	PEE	C39-C38	3.66	1.53	1.31
47	U	101	PEE	C39-C38	3.66	1.53	1.31
47	B	303	PEE	C39-C38	3.65	1.52	1.31
47	r	501	PEE	C39-C38	3.65	1.52	1.31
47	C	302	PEE	C39-C38	3.64	1.52	1.31
47	l	705	PEE	C39-C38	3.64	1.52	1.31
47	l	704	PEE	C39-C38	3.62	1.52	1.31
47	Q	501	PEE	C39-C38	3.62	1.52	1.31
51	V	201	CDL	OA8-CA7	3.49	1.43	1.33
51	V	202	CDL	OA8-CA7	3.46	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	s	402	CDL	OA8-CA7	3.45	1.43	1.33
51	n	102	CDL	OA8-CA7	3.44	1.43	1.33
51	I	201	CDL	OA8-CA7	3.43	1.43	1.33
51	l	702	CDL	OA8-CA7	3.42	1.43	1.33
51	r	503	CDL	OA8-CA7	3.42	1.43	1.33
51	l	703	CDL	OA8-CA7	3.40	1.43	1.33
56	w	401	ADP	O2'-C2'	-3.39	1.35	1.43
51	m	201	CDL	OA8-CA7	3.37	1.43	1.33
51	a	201	CDL	OA8-CA7	3.37	1.43	1.33
51	V	201	CDL	OA6-CA5	3.09	1.43	1.34
51	m	201	CDL	OA6-CA5	3.05	1.42	1.34
56	w	401	ADP	O3'-C3'	3.05	1.50	1.43
51	I	201	CDL	OB6-CB5	3.03	1.42	1.34
52	J	401	NDP	O3D-C3D	3.03	1.50	1.43
51	a	201	CDL	OB6-CB5	3.01	1.42	1.34
51	r	503	CDL	OB6-CB5	3.00	1.42	1.34
51	l	702	CDL	OB6-CB5	3.00	1.42	1.34
51	V	202	CDL	OB6-CB5	3.00	1.42	1.34
51	m	201	CDL	OB8-CB7	3.00	1.42	1.33
51	m	201	CDL	OB6-CB5	3.00	1.42	1.34
51	n	102	CDL	OB8-CB7	2.99	1.42	1.33
51	s	402	CDL	OB6-CB5	2.99	1.42	1.34
51	a	201	CDL	OB8-CB7	2.98	1.42	1.33
51	V	201	CDL	OB6-CB5	2.97	1.42	1.34
51	I	201	CDL	OB8-CB7	2.97	1.42	1.33
51	s	402	CDL	OA6-CA5	2.97	1.42	1.34
51	I	201	CDL	OA6-CA5	2.96	1.42	1.34
51	l	703	CDL	OB6-CB5	2.96	1.42	1.34
51	l	702	CDL	OB8-CB7	2.96	1.42	1.33
51	n	102	CDL	OA6-CA5	2.95	1.42	1.34
51	r	503	CDL	OB8-CB7	2.94	1.41	1.33
51	V	201	CDL	OB8-CB7	2.94	1.41	1.33
51	l	703	CDL	OB8-CB7	2.93	1.41	1.33
52	J	401	NDP	C7N-C3N	2.93	1.55	1.48
51	V	202	CDL	OA6-CA5	2.93	1.42	1.34
51	n	102	CDL	OB6-CB5	2.92	1.42	1.34
51	l	703	CDL	OA6-CA5	2.90	1.42	1.34
51	a	201	CDL	OA6-CA5	2.89	1.42	1.34
51	V	202	CDL	OB8-CB7	2.89	1.41	1.33
51	l	702	CDL	OA6-CA5	2.88	1.42	1.34
51	s	402	CDL	OB8-CB7	2.87	1.41	1.33
51	r	503	CDL	OA6-CA5	2.81	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	303	PLX	O6-C4	-2.79	1.40	1.44
48	n	101	PLX	O6-C4	-2.79	1.40	1.44
48	g	201	PLX	O6-C4	-2.79	1.40	1.44
49	J	402	UQ	C6-C1	2.70	1.54	1.46
48	N	201	PLX	O6-C4	-2.67	1.41	1.44
49	C	304	UQ	C6-C1	2.64	1.54	1.46
48	r	502	PLX	O6-C4	-2.63	1.41	1.44
48	j	202	PLX	O6-C4	-2.59	1.41	1.44
48	j	201	PLX	O6-C4	-2.52	1.41	1.44
51	l	703	CDL	OA6-CA4	-2.50	1.40	1.46
47	W	201	PEE	O2-C2	-2.50	1.40	1.46
51	l	702	CDL	OA6-CA4	-2.48	1.40	1.46
47	l	701	PEE	O3-C30	2.48	1.40	1.33
47	C	302	PEE	O2-C2	-2.48	1.40	1.46
51	r	503	CDL	OA6-CA4	-2.48	1.40	1.46
47	B	303	PEE	O3-C30	2.47	1.40	1.33
47	l	704	PEE	O2-C2	-2.47	1.40	1.46
47	r	501	PEE	O2-C2	-2.46	1.40	1.46
48	j	202	PLX	C7-C6	2.46	1.56	1.50
51	n	102	CDL	OA6-CA4	-2.45	1.40	1.46
47	s	401	PEE	O3-C30	2.45	1.40	1.33
47	r	501	PEE	O3-C30	2.45	1.40	1.33
49	J	402	UQ	C7-C8	2.44	1.54	1.50
47	Q	501	PEE	O2-C2	-2.44	1.40	1.46
47	l	701	PEE	O2-C2	-2.44	1.40	1.46
47	B	303	PEE	O2-C2	-2.43	1.40	1.46
47	U	101	PEE	O3-C30	2.43	1.40	1.33
47	l	705	PEE	O2-C2	-2.43	1.40	1.46
47	C	302	PEE	O3-C30	2.43	1.40	1.33
51	a	201	CDL	OA6-CA4	-2.43	1.40	1.46
47	l	705	PEE	O3-C30	2.43	1.40	1.33
47	s	401	PEE	O2-C2	-2.41	1.40	1.46
51	V	202	CDL	OA6-CA4	-2.40	1.40	1.46
49	C	304	UQ	C7-C8	2.40	1.54	1.50
47	l	704	PEE	O3-C30	2.40	1.40	1.33
47	Q	501	PEE	O3-C30	2.40	1.40	1.33
51	s	402	CDL	OA6-CA4	-2.38	1.40	1.46
51	I	201	CDL	OA6-CA4	-2.38	1.40	1.46
47	U	101	PEE	O2-C2	-2.38	1.40	1.46
47	W	201	PEE	O3-C30	2.35	1.40	1.33
50	X	201	8Q1	O40-C39	-2.35	1.18	1.23
50	X	201	8Q1	C1-S44	2.35	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	G	201	8Q1	C1-S44	2.33	1.81	1.76
52	J	401	NDP	O2B-C2B	2.33	1.52	1.44
48	r	502	PLX	C7-C6	2.33	1.55	1.50
50	G	201	8Q1	O40-C39	-2.32	1.18	1.23
48	j	201	PLX	C7-C6	2.32	1.55	1.50
46	A	502	FMN	C10-N1	2.32	1.37	1.33
48	g	201	PLX	C7-C6	2.31	1.55	1.50
51	n	102	CDL	PB2-OB2	2.30	1.68	1.59
50	G	201	8Q1	O35-C34	-2.30	1.18	1.23
51	n	102	CDL	OB6-CB4	-2.29	1.40	1.46
48	N	201	PLX	C7-C6	2.28	1.55	1.50
47	l	704	PEE	O2-C10	2.28	1.40	1.34
48	n	101	PLX	C7-C6	2.27	1.55	1.50
47	r	501	PEE	O2-C10	2.26	1.40	1.34
47	l	704	PEE	O3-C3	-2.25	1.40	1.45
50	X	201	8Q1	O35-C34	-2.25	1.18	1.23
47	B	303	PEE	O2-C10	2.25	1.40	1.34
51	V	201	CDL	OB6-CB4	-2.25	1.41	1.46
47	l	701	PEE	O2-C10	2.25	1.40	1.34
47	l	705	PEE	O2-C10	2.25	1.40	1.34
51	s	402	CDL	OB6-CB4	-2.24	1.41	1.46
51	V	201	CDL	PB2-OB2	2.24	1.68	1.59
47	U	101	PEE	O2-C10	2.24	1.40	1.34
51	l	703	CDL	OB6-CB4	-2.23	1.41	1.46
51	m	201	CDL	OB6-CB4	-2.23	1.41	1.46
48	C	303	PLX	C7-C6	2.23	1.55	1.50
52	J	401	NDP	C2D-C3D	2.23	1.59	1.53
47	s	401	PEE	O2-C10	2.22	1.40	1.34
51	V	202	CDL	PB2-OB2	2.21	1.68	1.59
51	V	202	CDL	OB6-CB4	-2.21	1.41	1.46
51	I	201	CDL	PB2-OB2	2.20	1.68	1.59
47	C	302	PEE	O2-C10	2.20	1.40	1.34
51	a	201	CDL	PB2-OB2	2.19	1.68	1.59
47	W	201	PEE	O3-C3	-2.19	1.40	1.45
49	C	304	UQ	O4-C4	-2.18	1.18	1.23
51	r	503	CDL	OB6-CB4	-2.18	1.41	1.46
51	V	202	CDL	PB2-OB5	2.18	1.68	1.59
49	J	402	UQ	O4-C4	-2.18	1.18	1.23
51	I	201	CDL	PB2-OB5	2.18	1.68	1.59
47	W	201	PEE	O2-C10	2.18	1.40	1.34
51	a	201	CDL	OB6-CB4	-2.17	1.41	1.46
51	l	703	CDL	PB2-OB2	2.17	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	I	201	CDL	OB6-CB4	-2.17	1.41	1.46
51	m	201	CDL	PB2-OB2	2.17	1.68	1.59
51	r	503	CDL	PB2-OB2	2.17	1.68	1.59
51	l	702	CDL	PB2-OB2	2.17	1.68	1.59
51	m	201	CDL	OA6-CA4	-2.17	1.41	1.46
47	Q	501	PEE	O2-C10	2.17	1.40	1.34
51	V	201	CDL	PB2-OB5	2.16	1.68	1.59
47	Q	501	PEE	O3-C3	-2.16	1.40	1.45
51	l	702	CDL	PB2-OB5	2.16	1.68	1.59
52	J	401	NDP	O7N-C7N	-2.16	1.19	1.24
51	m	201	CDL	PB2-OB5	2.16	1.68	1.59
51	a	201	CDL	PB2-OB5	2.15	1.68	1.59
48	N	201	PLX	P1-O4	2.15	1.68	1.59
47	U	101	PEE	O3-C3	-2.14	1.40	1.45
51	s	402	CDL	PB2-OB2	2.14	1.68	1.59
51	l	702	CDL	OB6-CB4	-2.14	1.41	1.46
51	n	102	CDL	PB2-OB5	2.13	1.67	1.59
47	s	401	PEE	O3-C3	-2.13	1.40	1.45
48	j	202	PLX	P1-O4	2.13	1.67	1.59
48	g	201	PLX	P1-O4	2.12	1.67	1.59
51	r	503	CDL	PB2-OB5	2.11	1.67	1.59
47	l	705	PEE	O3-C3	-2.11	1.40	1.45
51	l	703	CDL	PB2-OB5	2.10	1.67	1.59
48	n	101	PLX	P1-O4	2.10	1.67	1.59
47	C	302	PEE	O3-C3	-2.10	1.40	1.45
48	C	303	PLX	P1-O4	2.08	1.67	1.59
51	V	201	CDL	OA6-CA4	-2.07	1.41	1.46
48	r	502	PLX	P1-O4	2.07	1.67	1.59
49	C	304	UQ	O2-CM2	-2.06	1.40	1.45
48	j	202	PLX	P1-O1	2.06	1.67	1.59
47	l	701	PEE	O3-C3	-2.06	1.40	1.45
48	N	201	PLX	P1-O1	2.05	1.67	1.59
47	B	303	PEE	O3-C3	-2.05	1.40	1.45
47	r	501	PEE	O3-C3	-2.04	1.40	1.45
52	J	401	NDP	PA-O5B	2.04	1.67	1.59
48	j	201	PLX	P1-O4	2.04	1.67	1.59
50	X	201	8Q1	C6-C1	2.04	1.52	1.50
48	r	502	PLX	P1-O1	2.04	1.67	1.59
51	s	402	CDL	PB2-OB5	2.03	1.67	1.59
49	J	402	UQ	O1-C1	-2.03	1.19	1.23
48	n	101	PLX	P1-O1	2.03	1.67	1.59
50	G	201	8Q1	C6-C1	2.03	1.52	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	J	402	UQ	C21-C19	2.02	1.55	1.51
49	C	304	UQ	O3-CM3	-2.00	1.40	1.45
49	C	304	UQ	O1-C1	-2.00	1.19	1.23

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	J	402	UQ	C7-C8-C9	-8.02	113.44	126.79
52	J	401	NDP	C3N-C2N-N1N	-8.00	111.67	123.10
49	C	304	UQ	C7-C8-C9	-7.85	113.72	126.79
52	J	401	NDP	C1D-N1N-C2N	-6.62	110.10	121.11
49	C	304	UQ	C42-C43-C44	-6.57	111.84	127.66
49	J	402	UQ	C12-C13-C14	-6.28	112.53	127.66
49	C	304	UQ	C47-C48-C49	-6.28	112.54	127.66
50	G	201	8Q1	C6-C1-S44	6.11	120.57	113.46
49	C	304	UQ	C37-C38-C39	-6.08	113.02	127.66
49	C	304	UQ	C22-C23-C24	-5.94	113.36	127.66
49	C	304	UQ	C27-C28-C29	-5.93	113.38	127.66
49	J	402	UQ	C17-C18-C19	-5.87	113.52	127.66
49	C	304	UQ	C12-C13-C14	-5.79	113.72	127.66
49	C	304	UQ	C17-C18-C19	-5.78	113.74	127.66
49	C	304	UQ	C32-C33-C34	-5.74	113.85	127.66
50	X	201	8Q1	C6-C1-S44	5.37	119.71	113.46
52	J	401	NDP	C1D-N1N-C6N	-5.06	109.94	120.83
49	C	304	UQ	C30-C29-C28	-4.73	111.54	123.68
49	C	304	UQ	C45-C44-C43	-4.55	111.99	123.68
56	w	401	ADP	N3-C2-N1	-4.49	121.66	128.68
49	C	304	UQ	C31-C29-C28	-4.48	112.06	121.12
49	C	304	UQ	C20-C19-C18	-4.37	112.46	123.68
49	C	304	UQ	C41-C39-C38	-4.37	112.28	121.12
49	J	402	UQ	C22-C23-C24	-4.35	112.89	127.75
49	J	402	UQ	C21-C19-C18	-4.33	112.35	121.12
49	C	304	UQ	C51-C49-C48	-4.30	112.41	121.12
49	C	304	UQ	C50-C49-C48	-4.28	112.70	123.68
49	J	402	UQ	C11-C9-C8	-4.26	112.49	121.12
49	C	304	UQ	C10-C9-C8	-4.25	112.78	123.68
49	C	304	UQ	C40-C39-C38	-4.22	112.85	123.68
49	J	402	UQ	C10-C9-C8	-4.22	112.85	123.68
49	C	304	UQ	C36-C34-C33	-4.20	112.62	121.12
49	C	304	UQ	C21-C19-C18	-4.18	112.66	121.12
47	s	401	PEE	O2-C10-C11	4.16	120.47	111.50
49	C	304	UQ	C52-C53-C54	-4.14	113.60	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	l	702	CDL	OB6-CB5-C51	4.13	120.41	111.50
49	C	304	UQ	C25-C24-C23	-4.13	113.07	123.68
49	J	402	UQ	C15-C14-C13	-4.11	113.14	123.68
51	m	201	CDL	OB6-CB5-C51	4.10	120.34	111.50
49	J	402	UQ	C20-C19-C18	-4.09	113.19	123.68
49	C	304	UQ	C46-C44-C43	-4.08	112.87	121.12
51	I	201	CDL	OB6-CB5-C51	4.07	120.27	111.50
52	J	401	NDP	N3A-C2A-N1A	-4.07	122.32	128.68
47	B	303	PEE	O2-C10-C11	4.04	120.21	111.50
47	C	302	PEE	O2-C10-C11	4.02	120.16	111.50
47	U	101	PEE	O2-C10-C11	4.01	120.15	111.50
51	s	402	CDL	OA6-CA5-C11	4.00	120.12	111.50
51	V	201	CDL	OA6-CA5-C11	3.99	120.11	111.50
47	r	501	PEE	O2-C10-C11	3.99	120.11	111.50
47	W	201	PEE	O2-C10-C11	3.99	120.10	111.50
51	l	702	CDL	OA6-CA5-C11	3.98	120.09	111.50
51	s	402	CDL	OB6-CB5-C51	3.98	120.08	111.50
47	Q	501	PEE	O2-C10-C11	3.98	120.07	111.50
51	a	201	CDL	OB6-CB5-C51	3.96	120.04	111.50
49	J	402	UQ	C16-C14-C13	-3.96	113.10	121.12
51	I	201	CDL	OA6-CA5-C11	3.96	120.04	111.50
51	a	201	CDL	OA6-CA5-C11	3.96	120.03	111.50
51	V	202	CDL	OB6-CB5-C51	3.95	120.02	111.50
51	r	503	CDL	OA6-CA5-C11	3.95	120.01	111.50
47	l	705	PEE	O2-C10-C11	3.95	120.01	111.50
51	V	202	CDL	OA6-CA5-C11	3.93	119.98	111.50
49	C	304	UQ	C11-C9-C8	-3.92	113.19	121.12
49	C	304	UQ	C35-C34-C33	-3.91	113.64	123.68
47	l	701	PEE	O2-C10-C11	3.91	119.92	111.50
51	n	102	CDL	OB6-CB5-C51	3.91	119.92	111.50
51	n	102	CDL	OA6-CA5-C11	3.90	119.91	111.50
47	l	704	PEE	O2-C10-C11	3.89	119.88	111.50
51	V	201	CDL	OB6-CB5-C51	3.86	119.82	111.50
51	r	503	CDL	OB6-CB5-C51	3.83	119.75	111.50
49	C	304	UQ	C26-C24-C23	-3.82	113.38	121.12
49	C	304	UQ	C15-C14-C13	-3.81	113.91	123.68
49	C	304	UQ	C16-C14-C13	-3.80	113.43	121.12
51	l	703	CDL	OA6-CA5-C11	3.74	119.57	111.50
50	G	201	8Q1	O4-C1-C6	-3.73	119.58	123.99
51	l	703	CDL	OB6-CB5-C51	3.72	119.52	111.50
51	m	201	CDL	OA6-CA5-C11	3.66	119.40	111.50
49	C	304	UQ	C55-C54-C53	-3.46	112.64	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	J	402	UQ	C26-C24-C23	-3.42	112.77	122.65
50	X	201	8Q1	O4-C1-C6	-3.42	119.95	123.99
49	J	402	UQ	C25-C24-C23	-3.38	112.88	122.65
51	n	102	CDL	OA8-CA7-C31	3.27	119.95	111.38
46	A	502	FMN	C4-N3-C2	-3.20	119.73	125.64
50	G	201	8Q1	C37-C38-C39	3.08	117.49	112.36
49	C	304	UQ	C56-C54-C53	-3.07	113.77	122.65
52	J	401	NDP	PN-O3-PA	-2.85	123.03	132.83
49	C	304	UQ	CM5-C5-C6	-2.84	119.76	124.40
51	m	201	CDL	OB8-CB7-C71	2.82	120.76	111.91
51	r	503	CDL	OB8-CB7-C71	2.77	120.59	111.91
47	B	303	PEE	O3-C30-C31	2.76	120.56	111.91
51	l	702	CDL	OA8-CA7-C31	2.75	120.55	111.91
47	r	501	PEE	O3-C30-C31	2.73	120.48	111.91
47	Q	501	PEE	O3-C30-C31	2.72	120.45	111.91
51	a	201	CDL	OB8-CB7-C71	2.71	120.41	111.91
51	l	703	CDL	OB8-CB7-C71	2.68	120.32	111.91
46	A	502	FMN	C4A-C4-N3	2.67	119.97	113.19
51	V	202	CDL	OB8-CB7-C71	2.66	120.26	111.91
47	l	701	PEE	O3-C30-C31	2.65	120.22	111.91
51	V	201	CDL	OB8-CB7-C71	2.65	120.21	111.91
47	s	401	PEE	O3-C30-C31	2.63	120.16	111.91
50	X	201	8Q1	C38-C39-N41	2.63	120.84	116.42
51	s	402	CDL	OA8-CA7-C31	2.62	120.14	111.91
51	l	702	CDL	OB8-CB7-C71	2.62	120.13	111.91
51	I	201	CDL	OA8-CA7-C31	2.62	120.12	111.91
51	m	201	CDL	OA8-CA7-C31	2.62	120.12	111.91
51	I	201	CDL	OB8-CB7-C71	2.61	120.08	111.91
56	w	401	ADP	PA-O3A-PB	-2.60	123.90	132.83
47	l	704	PEE	O3-C30-C31	2.60	120.06	111.91
47	U	101	PEE	O3-C30-C31	2.60	120.06	111.91
47	l	705	PEE	O3-C30-C31	2.59	120.04	111.91
47	W	201	PEE	O3-C30-C31	2.58	120.00	111.91
47	C	302	PEE	O3-C30-C31	2.57	119.98	111.91
51	V	202	CDL	OA8-CA7-C31	2.56	119.95	111.91
51	a	201	CDL	OA8-CA7-C31	2.56	119.94	111.91
51	r	503	CDL	OA8-CA7-C31	2.56	119.94	111.91
51	s	402	CDL	OB8-CB7-C71	2.54	119.89	111.91
51	n	102	CDL	OB8-CB7-C71	2.54	119.88	111.91
50	X	201	8Q1	C37-C38-C39	2.53	116.58	112.36
46	A	502	FMN	C4A-C10-N10	2.53	120.18	116.48
49	J	402	UQ	CM5-C5-C6	-2.53	120.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	401	ADP	O4'-C1'-C2'	-2.53	103.24	106.93
51	l	703	CDL	OA8-CA7-C31	2.50	119.77	111.91
48	g	201	PLX	C1A-N1-C1	2.50	120.13	109.92
46	A	502	FMN	O4-C4-C4A	-2.49	119.99	126.60
51	V	201	CDL	OA8-CA7-C31	2.48	119.69	111.91
48	j	202	PLX	C1A-N1-C1	2.41	119.77	109.92
48	r	502	PLX	C1A-N1-C1	2.40	119.74	109.92
48	N	201	PLX	C1A-N1-C1	2.38	119.64	109.92
48	n	101	PLX	C1A-N1-C1	2.32	119.43	109.92
52	J	401	NDP	C4A-C5A-N7A	-2.30	107.00	109.40
50	G	201	8Q1	C38-C39-N41	2.29	120.28	116.42
46	A	502	FMN	C4A-C10-N1	-2.27	119.46	124.73
48	j	201	PLX	C1A-N1-C1	2.25	119.10	109.92
48	C	303	PLX	C1A-N1-C1	2.24	119.07	109.92
46	A	502	FMN	C10-C4A-N5	-2.23	120.11	124.86
50	X	201	8Q1	C42-N41-C39	-2.21	118.73	122.84
50	G	201	8Q1	O4-C1-S44	-2.13	119.84	122.61
56	w	401	ADP	C4-C5-N7	-2.13	107.18	109.40
50	X	201	8Q1	C43-S44-C1	2.12	108.47	101.87
49	C	304	UQ	C20-C19-C21	-2.11	111.73	115.27
50	G	201	8Q1	C43-S44-C1	2.08	108.35	101.87
46	A	502	FMN	C5A-C9A-N10	2.06	120.08	117.95
46	A	502	FMN	C9A-C5A-N5	-2.03	120.22	122.43
56	w	401	ADP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (1031) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C5'-O5'-P-O1P
46	A	502	FMN	C5'-O5'-P-O2P
47	B	303	PEE	C11-C10-O2-C2
47	C	302	PEE	C11-C10-O2-C2
47	C	302	PEE	C1-O3P-P-O2P
47	C	302	PEE	C1-O3P-P-O1P
47	Q	501	PEE	C11-C10-O2-C2
47	U	101	PEE	C17-C18-C19-C20
47	U	101	PEE	C1-O3P-P-O2P
47	U	101	PEE	C1-O3P-P-O1P
47	W	201	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	C4-O4P-P-O1P
47	l	701	PEE	C11-C10-O2-C2
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O2P
47	l	704	PEE	O3P-C1-C2-O2
47	l	705	PEE	C37-C38-C39-C40
47	r	501	PEE	C1-O3P-P-O1P
47	s	401	PEE	C4-O4P-P-O2P
48	C	303	PLX	N1-C1-C2-O1
48	C	303	PLX	C25-C24-O8-C5
48	N	201	PLX	O7-C6-O6-C4
48	N	201	PLX	C2-O1-P1-O2
48	N	201	PLX	C2-O1-P1-O3
48	N	201	PLX	O9-C24-O8-C5
48	j	201	PLX	O7-C6-O6-C4
48	j	201	PLX	O9-C24-C25-C26
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	C25-C24-O8-C5
48	r	502	PLX	C3-O4-P1-O2
49	C	304	UQ	C12-C13-C14-C16
49	C	304	UQ	C16-C17-C18-C19
49	C	304	UQ	C17-C18-C19-C20
49	C	304	UQ	C17-C18-C19-C21
49	C	304	UQ	C22-C23-C24-C26
49	C	304	UQ	C27-C28-C29-C31
49	C	304	UQ	C37-C38-C39-C40
49	C	304	UQ	C42-C43-C44-C45
49	C	304	UQ	C42-C43-C44-C46
49	C	304	UQ	C47-C48-C49-C51
49	J	402	UQ	C7-C8-C9-C10
49	J	402	UQ	C9-C11-C12-C13
49	J	402	UQ	C12-C13-C14-C15
49	J	402	UQ	C12-C13-C14-C16
49	J	402	UQ	C14-C16-C17-C18
49	J	402	UQ	C17-C18-C19-C21
49	J	402	UQ	C19-C21-C22-C23
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-O33

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C42-C43-S44-C1
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	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
51	I	201	CDL	CB2-C1-CA2-OA2
51	I	201	CDL	O1-C1-CB2-OB2
51	I	201	CDL	CA2-OA2-PA1-OA5
51	I	201	CDL	CA3-OA5-PA1-OA3
51	I	201	CDL	CB2-OB2-PB2-OB3
51	I	201	CDL	CB2-OB2-PB2-OB4
51	I	201	CDL	CB2-OB2-PB2-OB5
51	I	201	CDL	CB3-OB5-PB2-OB3
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	CA3-OA5-PA1-OA3
51	V	202	CDL	CB2-OB2-PB2-OB3
51	V	202	CDL	C51-CB5-OB6-CB4
51	a	201	CDL	O1-C1-CA2-OA2
51	a	201	CDL	CA2-OA2-PA1-OA3
51	a	201	CDL	OB7-CB5-OB6-CB4
51	l	702	CDL	O1-C1-CA2-OA2
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	CB3-OB5-PB2-OB3
51	l	703	CDL	CA3-OA5-PA1-OA4
51	l	703	CDL	CB2-OB2-PB2-OB3
51	l	703	CDL	CB2-OB2-PB2-OB4
51	m	201	CDL	CB2-C1-CA2-OA2
51	m	201	CDL	CA2-OA2-PA1-OA3
51	m	201	CDL	CA2-OA2-PA1-OA4
51	m	201	CDL	CA2-OA2-PA1-OA5
51	m	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	CB3-OB5-PB2-OB2
51	m	201	CDL	CB3-OB5-PB2-OB3
51	m	201	CDL	CB3-OB5-PB2-OB4
51	n	102	CDL	O1-C1-CB2-OB2
51	n	102	CDL	CA2-C1-CB2-OB2
51	n	102	CDL	CA2-OA2-PA1-OA5
51	r	503	CDL	CA2-OA2-PA1-OA3
51	r	503	CDL	CA3-OA5-PA1-OA2
51	r	503	CDL	CA3-OA5-PA1-OA3
51	r	503	CDL	CB2-OB2-PB2-OB3
51	r	503	CDL	CB2-OB2-PB2-OB4
51	r	503	CDL	CB2-OB2-PB2-OB5
51	r	503	CDL	CB3-OB5-PB2-OB3
51	r	503	CDL	CB3-OB5-PB2-OB4
51	r	503	CDL	C51-CB5-OB6-CB4
51	s	402	CDL	CB2-C1-CA2-OA2
51	s	402	CDL	CA2-OA2-PA1-OA3
51	s	402	CDL	CA2-OA2-PA1-OA4
51	s	402	CDL	OB6-CB4-CB6-OB8
52	J	401	NDP	C2B-O2B-P2B-O3X
52	J	401	NDP	O4D-C1D-N1N-C6N
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
51	s	402	CDL	OA9-CA7-OA8-CA6
51	l	702	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	O4-C10-O2-C2
47	C	302	PEE	O4-C10-O2-C2
47	Q	501	PEE	O4-C10-O2-C2
47	l	701	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
51	V	201	CDL	OA7-CA5-OA6-CA4
51	V	202	CDL	OB7-CB5-OB6-CB4
51	r	503	CDL	OB7-CB5-OB6-CB4
51	s	402	CDL	C31-CA7-OA8-CA6
47	l	704	PEE	C11-C10-O2-C2
51	a	201	CDL	C51-CB5-OB6-CB4
49	J	402	UQ	C22-C23-C24-C26
47	l	704	PEE	O5-C30-O3-C3
49	J	402	UQ	C15-C14-C16-C17
51	V	201	CDL	C71-CB7-OB8-CB6
51	l	702	CDL	C31-CA7-OA8-CA6
47	B	303	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
47	W	201	PEE	C17-C18-C19-C20
49	C	304	UQ	C7-C8-C9-C10
49	C	304	UQ	C27-C28-C29-C30
51	s	402	CDL	OB7-CB5-OB6-CB4
49	J	402	UQ	C7-C8-C9-C11
47	Q	501	PEE	O5-C30-O3-C3
51	I	201	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CB2-OB2
51	l	703	CDL	O1-C1-CA2-OA2
51	l	703	CDL	O1-C1-CB2-OB2
51	r	503	CDL	O1-C1-CA2-OA2
51	s	402	CDL	O1-C1-CA2-OA2
51	s	402	CDL	O1-C1-CB2-OB2
47	l	704	PEE	C31-C30-O3-C3
47	U	101	PEE	C11-C10-O2-C2
47	l	705	PEE	C11-C10-O2-C2
51	m	201	CDL	C11-CA5-OA6-CA4
51	s	402	CDL	C51-CB5-OB6-CB4
51	V	201	CDL	C59-C60-C61-C62
51	V	202	CDL	C11-C12-C13-C14
48	g	201	PLX	C9-C10-C11-C12
51	V	201	CDL	C32-C33-C34-C35
51	V	202	CDL	C32-C33-C34-C35
51	m	201	CDL	C73-C74-C75-C76
51	n	102	CDL	C74-C75-C76-C77
51	r	503	CDL	C74-C75-C76-C77
51	s	402	CDL	C37-C38-C39-C40
48	C	303	PLX	C9-C10-C11-C12
48	g	201	PLX	C7-C8-C9-C10
52	J	401	NDP	O4B-C4B-C5B-O5B
47	Q	501	PEE	C31-C30-O3-C3
47	U	101	PEE	O4-C10-O2-C2
51	n	102	CDL	C1-CB2-OB2-PB2
49	C	304	UQ	C52-C53-C54-C55
49	J	402	UQ	C12-C11-C9-C10
49	C	304	UQ	C43-C44-C46-C47
49	C	304	UQ	C48-C49-C51-C52
49	J	402	UQ	C18-C19-C21-C22
51	l	702	CDL	C55-C56-C57-C58
51	V	201	CDL	OB9-CB7-OB8-CB6
48	C	303	PLX	C33-C34-C35-C36
48	j	202	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C62-C63-C64-C65
49	C	304	UQ	C47-C48-C49-C50
51	I	201	CDL	CA2-C1-CB2-OB2
51	a	201	CDL	CB2-C1-CA2-OA2
51	l	702	CDL	CA2-C1-CB2-OB2
51	l	703	CDL	CB2-C1-CA2-OA2
51	r	503	CDL	CB2-C1-CA2-OA2
51	s	402	CDL	CA2-C1-CB2-OB2
47	l	705	PEE	O4-C10-O2-C2
51	m	201	CDL	OA7-CA5-OA6-CA4
51	l	702	CDL	C34-C35-C36-C37
51	l	703	CDL	C35-C36-C37-C38
48	g	201	PLX	C2-C1-N1-C1A
47	U	101	PEE	C31-C30-O3-C3
47	W	201	PEE	C31-C30-O3-C3
47	l	701	PEE	C31-C30-O3-C3
51	l	702	CDL	C58-C59-C60-C61
48	N	201	PLX	C31-C32-C33-C34
51	I	201	CDL	OA5-CA3-CA4-OA6
51	m	201	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	C16-C17-C18-C19
51	l	702	CDL	C32-C33-C34-C35
51	V	202	CDL	CB7-C71-C72-C73
48	g	201	PLX	O6-C4-C5-O8
51	s	402	CDL	C14-C15-C16-C17
51	a	201	CDL	CA5-C11-C12-C13
51	l	702	CDL	CA7-C31-C32-C33
51	l	702	CDL	CB7-C71-C72-C73
47	U	101	PEE	O5-C30-O3-C3
47	U	101	PEE	C30-C31-C32-C33
51	l	702	CDL	CB5-C51-C52-C53
51	r	503	CDL	CA5-C11-C12-C13
47	l	701	PEE	C17-C18-C19-C20
51	l	703	CDL	C17-C18-C19-C20
47	l	701	PEE	O5-C30-O3-C3
51	a	201	CDL	CA7-C31-C32-C33
51	s	402	CDL	CA7-C31-C32-C33
52	J	401	NDP	C3B-C4B-C5B-O5B
51	l	703	CDL	C71-CB7-OB8-CB6
49	C	304	UQ	C32-C33-C34-C36
51	m	201	CDL	C36-C37-C38-C39
48	g	201	PLX	C2-C1-N1-C1B

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Mol	Chain	Res	Type	Atoms
51	I	201	CDL	CB7-C71-C72-C73
51	l	703	CDL	CB7-C71-C72-C73
51	s	402	CDL	CB7-C71-C72-C73
49	C	304	UQ	C34-C36-C37-C38
47	W	201	PEE	O5-C30-O3-C3
47	l	701	PEE	C10-C11-C12-C13
47	l	704	PEE	C37-C38-C39-C40
51	l	703	CDL	C51-C52-C53-C54
51	I	201	CDL	C11-C12-C13-C14
51	r	503	CDL	C60-C61-C62-C63
47	C	302	PEE	C1-O3P-P-O4P
47	U	101	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O3P
47	l	705	PEE	C1-O3P-P-O4P
48	g	201	PLX	C2-O1-P1-O4
48	j	201	PLX	C3-O4-P1-O1
48	r	502	PLX	C3-O4-P1-O1
51	V	201	CDL	CB2-OB2-PB2-OB5
51	V	201	CDL	CB3-OB5-PB2-OB2
51	V	202	CDL	CB3-OB5-PB2-OB2
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CB3-OB5-PB2-OB2
51	l	703	CDL	CA2-OA2-PA1-OA5
51	l	703	CDL	CA3-OA5-PA1-OA2
51	l	703	CDL	CB2-OB2-PB2-OB5
51	m	201	CDL	CA3-OA5-PA1-OA2
51	r	503	CDL	CA2-OA2-PA1-OA5
51	r	503	CDL	CB3-OB5-PB2-OB2
51	s	402	CDL	CA2-OA2-PA1-OA5
51	s	402	CDL	CA3-OA5-PA1-OA2
51	s	402	CDL	CB3-OB5-PB2-OB2
51	l	702	CDL	C71-CB7-OB8-CB6
51	l	703	CDL	OB9-CB7-OB8-CB6
47	r	501	PEE	C10-C11-C12-C13
51	l	703	CDL	CA2-C1-CB2-OB2
49	C	304	UQ	C25-C24-C26-C27
51	s	402	CDL	C31-C32-C33-C34
47	l	705	PEE	C31-C30-O3-C3
51	V	202	CDL	C71-CB7-OB8-CB6
51	V	202	CDL	C72-C73-C74-C75
51	s	402	CDL	C33-C34-C35-C36
48	j	201	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
48	n	101	PLX	O8-C24-C25-C26
47	r	501	PEE	C13-C14-C15-C16
51	a	201	CDL	C17-C18-C19-C20
51	l	703	CDL	C55-C56-C57-C58
47	W	201	PEE	C11-C10-O2-C2
51	V	201	CDL	C51-CB5-OB6-CB4
47	r	501	PEE	C40-C41-C42-C43
47	s	401	PEE	C23-C24-C25-C26
48	C	303	PLX	C25-C26-C27-C28
48	N	201	PLX	C14-C15-C16-C17
48	g	201	PLX	C27-C28-C29-C30
48	j	201	PLX	C7-C8-C9-C10
48	j	201	PLX	C30-C31-C32-C33
48	j	201	PLX	C31-C32-C33-C34
48	j	202	PLX	C31-C32-C33-C34
48	r	502	PLX	C13-C14-C15-C16
51	V	201	CDL	C11-C12-C13-C14
51	V	201	CDL	C37-C38-C39-C40
51	V	202	CDL	C14-C15-C16-C17
51	l	702	CDL	C14-C15-C16-C17
51	r	503	CDL	C57-C58-C59-C60
51	s	402	CDL	C75-C76-C77-C78
51	V	201	CDL	C31-CA7-OA8-CA6
48	N	201	PLX	C29-C30-C31-C32
48	g	201	PLX	C11-C12-C13-C14
48	j	201	PLX	C28-C29-C30-C31
51	a	201	CDL	C62-C63-C64-C65
51	l	702	CDL	C11-C12-C13-C14
51	l	702	CDL	C75-C76-C77-C78
51	r	503	CDL	C11-C12-C13-C14
47	W	201	PEE	O4-C10-O2-C2
51	V	201	CDL	OB7-CB5-OB6-CB4
47	W	201	PEE	C21-C22-C23-C24
47	l	705	PEE	C31-C32-C33-C34
51	V	201	CDL	C31-C32-C33-C34
51	V	202	CDL	C59-C60-C61-C62
51	a	201	CDL	C33-C34-C35-C36
51	m	201	CDL	C32-C33-C34-C35
51	r	503	CDL	C32-C33-C34-C35
51	m	201	CDL	CA4-CA3-OA5-PA1
47	U	101	PEE	C23-C24-C25-C26
47	s	401	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
48	g	201	PLX	C25-C26-C27-C28
48	n	101	PLX	C27-C28-C29-C30
48	r	502	PLX	C25-C26-C27-C28
51	V	201	CDL	C33-C34-C35-C36
51	V	201	CDL	C52-C53-C54-C55
51	V	201	CDL	C74-C75-C76-C77
51	V	202	CDL	C33-C34-C35-C36
51	a	201	CDL	C73-C74-C75-C76
51	a	201	CDL	C75-C76-C77-C78
51	l	702	CDL	C71-C72-C73-C74
51	m	201	CDL	C60-C61-C62-C63
51	r	503	CDL	C35-C36-C37-C38
51	m	201	CDL	O1-C1-CA2-OA2
48	C	303	PLX	C17-C18-C19-C20
48	j	202	PLX	C7-C8-C9-C10
48	C	303	PLX	O6-C4-C5-O8
51	a	201	CDL	C71-CB7-OB8-CB6
48	C	303	PLX	C27-C28-C29-C30
48	j	201	PLX	C9-C10-C11-C12
48	r	502	PLX	C10-C11-C12-C13
50	G	201	8Q1	C12-C13-C14-C15
51	l	702	CDL	C81-C82-C83-C84
51	V	202	CDL	OB9-CB7-OB8-CB6
47	l	705	PEE	C33-C34-C35-C36
48	j	202	PLX	C14-C15-C16-C17
51	m	201	CDL	C14-C15-C16-C17
51	I	201	CDL	CA7-C31-C32-C33
47	r	501	PEE	C31-C32-C33-C34
48	C	303	PLX	C14-C15-C16-C17
48	N	201	PLX	C27-C28-C29-C30
48	r	502	PLX	C27-C28-C29-C30
50	X	201	8Q1	C10-C11-C12-C13
51	V	202	CDL	C37-C38-C39-C40
51	V	202	CDL	C42-C43-C44-C45
51	a	201	CDL	C60-C61-C62-C63
51	l	702	CDL	C18-C19-C20-C21
51	l	703	CDL	C79-C80-C81-C82
51	s	402	CDL	C71-C72-C73-C74
48	g	201	PLX	C14-C15-C16-C17
48	j	202	PLX	C25-C26-C27-C28
48	n	101	PLX	C9-C10-C11-C12
50	X	201	8Q1	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	C75-C76-C77-C78
47	C	302	PEE	C42-C43-C44-C45
47	Q	501	PEE	C21-C22-C23-C24
47	l	705	PEE	C22-C23-C24-C25
48	n	101	PLX	C10-C11-C12-C13
51	V	202	CDL	C35-C36-C37-C38
51	V	202	CDL	C74-C75-C76-C77
51	l	703	CDL	C11-C12-C13-C14
51	m	201	CDL	C13-C14-C15-C16
51	m	201	CDL	C55-C56-C57-C58
47	r	501	PEE	C39-C40-C41-C42
51	V	202	CDL	CA7-C31-C32-C33
47	W	201	PEE	C12-C13-C14-C15
48	N	201	PLX	C33-C34-C35-C36
48	g	201	PLX	C28-C29-C30-C31
48	g	201	PLX	C32-C33-C34-C35
48	j	201	PLX	C11-C12-C13-C14
48	j	202	PLX	C9-C10-C11-C12
48	j	202	PLX	C28-C29-C30-C31
48	j	202	PLX	C33-C34-C35-C36
48	n	101	PLX	C13-C14-C15-C16
48	n	101	PLX	C31-C32-C33-C34
48	r	502	PLX	C30-C31-C32-C33
51	V	202	CDL	C52-C53-C54-C55
51	V	202	CDL	C75-C76-C77-C78
51	l	702	CDL	C52-C53-C54-C55
51	l	703	CDL	C14-C15-C16-C17
51	n	102	CDL	C55-C56-C57-C58
51	r	503	CDL	C62-C63-C64-C65
51	s	402	CDL	C17-C18-C19-C20
51	s	402	CDL	C52-C53-C54-C55
47	l	704	PEE	C31-C32-C33-C34
48	g	201	PLX	C13-C14-C15-C16
51	a	201	CDL	C37-C38-C39-C40
51	n	102	CDL	C52-C53-C54-C55
47	W	201	PEE	C13-C14-C15-C16
48	j	202	PLX	C12-C13-C14-C15
48	n	101	PLX	C14-C15-C16-C17
51	l	702	CDL	C74-C75-C76-C77
51	l	702	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	C14-C15-C16-C17
48	j	201	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	C34-C35-C36-C37
48	C	303	PLX	C11-C12-C13-C14
48	g	201	PLX	C12-C13-C14-C15
48	j	201	PLX	C13-C14-C15-C16
51	V	202	CDL	C73-C74-C75-C76
47	l	701	PEE	C11-C12-C13-C14
48	C	303	PLX	C7-C8-C9-C10
48	j	202	PLX	C16-C17-C18-C19
51	V	202	CDL	C82-C83-C84-C85
51	m	201	CDL	C59-C60-C61-C62
51	n	102	CDL	C71-C72-C73-C74
51	r	503	CDL	C71-C72-C73-C74
51	s	402	CDL	C73-C74-C75-C76
48	n	101	PLX	C3-C4-C5-O8
51	m	201	CDL	CB3-CB4-CB6-OB8
47	r	501	PEE	C17-C18-C19-C20
47	B	303	PEE	C31-C32-C33-C34
51	a	201	CDL	C52-C53-C54-C55
51	a	201	CDL	C71-C72-C73-C74
48	r	502	PLX	C11-C10-C9-C8
51	V	201	CDL	C58-C59-C60-C61
51	V	201	CDL	C71-C72-C73-C74
47	r	501	PEE	C11-C10-O2-C2
51	m	201	CDL	C79-C80-C81-C82
48	C	303	PLX	O7-C6-C7-C8
48	C	303	PLX	O9-C24-C25-C26
48	g	201	PLX	O9-C24-C25-C26
48	r	502	PLX	O9-C24-C25-C26
48	j	201	PLX	C25-C26-C27-C28
48	j	201	PLX	C32-C33-C34-C35
51	V	201	CDL	C55-C56-C57-C58
51	l	702	CDL	C56-C57-C58-C59
51	l	703	CDL	C37-C38-C39-C40
51	l	703	CDL	C71-C72-C73-C74
51	m	201	CDL	C71-C72-C73-C74
51	s	402	CDL	C82-C83-C84-C85
47	Q	501	PEE	C19-C20-C21-C22
47	W	201	PEE	C15-C16-C17-C18
47	l	705	PEE	O5-C30-O3-C3
51	r	503	CDL	C41-C42-C43-C44
51	V	202	CDL	O1-C1-CA2-OA2
48	j	202	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	C15-C16-C17-C18
51	a	201	CDL	C31-C32-C33-C34
51	l	703	CDL	C59-C60-C61-C62
51	r	503	CDL	C75-C76-C77-C78
51	s	402	CDL	CB5-C51-C52-C53
51	l	702	CDL	CB2-C1-CA2-OA2
47	r	501	PEE	C21-C22-C23-C24
51	r	503	CDL	C43-C44-C45-C46
47	r	501	PEE	O4-C10-O2-C2
47	l	704	PEE	C11-C12-C13-C14
48	j	201	PLX	C33-C34-C35-C36
51	m	201	CDL	C61-C62-C63-C64
51	r	503	CDL	C37-C38-C39-C40
51	V	201	CDL	OA9-CA7-OA8-CA6
51	a	201	CDL	OB9-CB7-OB8-CB6
51	V	202	CDL	C17-C18-C19-C20
51	r	503	CDL	C14-C15-C16-C17
51	r	503	CDL	C31-C32-C33-C34
48	g	201	PLX	C2-C1-N1-C1C
47	l	704	PEE	C43-C44-C45-C46
51	l	703	CDL	C32-C33-C34-C35
51	m	201	CDL	C37-C38-C39-C40
51	s	402	CDL	C71-CB7-OB8-CB6
48	n	101	PLX	C25-C26-C27-C28
51	V	201	CDL	C14-C15-C16-C17
51	l	702	CDL	C35-C36-C37-C38
51	l	702	CDL	C37-C38-C39-C40
51	r	503	CDL	C73-C74-C75-C76
51	V	201	CDL	C34-C35-C36-C37
51	s	402	CDL	C51-C52-C53-C54
51	l	702	CDL	C62-C63-C64-C65
51	m	201	CDL	C11-C12-C13-C14
47	s	401	PEE	C19-C20-C21-C22
47	s	401	PEE	O4-C10-O2-C2
47	B	303	PEE	C10-C11-C12-C13
51	V	202	CDL	CB5-C51-C52-C53
51	r	503	CDL	CA7-C31-C32-C33
48	N	201	PLX	C10-C11-C12-C13
48	n	101	PLX	C7-C8-C9-C10
51	a	201	CDL	C38-C39-C40-C41
48	g	201	PLX	C30-C31-C32-C33
51	V	202	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
48	g	201	PLX	C33-C34-C35-C36
51	l	702	CDL	C59-C60-C61-C62
47	r	501	PEE	C41-C42-C43-C44
48	j	201	PLX	C27-C28-C29-C30
48	j	202	PLX	C11-C12-C13-C14
48	j	202	PLX	C29-C30-C31-C32
51	s	402	CDL	C55-C56-C57-C58
47	s	401	PEE	C11-C10-O2-C2
51	l	702	CDL	C51-CB5-OB6-CB4
47	W	201	PEE	O3P-C1-C2-O2
51	V	201	CDL	OB5-CB3-CB4-OB6
49	J	402	UQ	C11-C12-C13-C14
51	l	703	CDL	C82-C83-C84-C85
47	r	501	PEE	C36-C37-C38-C39
47	r	501	PEE	C14-C15-C16-C17
47	l	704	PEE	C30-C31-C32-C33
48	n	101	PLX	O6-C4-C5-O8
51	V	202	CDL	OA6-CA4-CA6-OA8
51	l	703	CDL	OA6-CA4-CA6-OA8
51	m	201	CDL	OB6-CB4-CB6-OB8
51	l	703	CDL	C31-C32-C33-C34
48	C	303	PLX	C10-C11-C12-C13
48	N	201	PLX	C28-C29-C30-C31
48	r	502	PLX	C28-C29-C30-C31
51	V	202	CDL	C62-C63-C64-C65
51	s	402	CDL	C54-C55-C56-C57
47	B	303	PEE	C35-C36-C37-C38
47	l	701	PEE	C35-C36-C37-C38
49	C	304	UQ	C13-C14-C16-C17
51	s	402	CDL	C59-C60-C61-C62
51	s	402	CDL	OB9-CB7-OB8-CB6
48	N	201	PLX	C25-C26-C27-C28
51	a	201	CDL	C21-C22-C23-C24
51	m	201	CDL	C33-C34-C35-C36
51	n	102	CDL	C73-C74-C75-C76
51	l	703	CDL	C75-C76-C77-C78
51	s	402	CDL	C35-C36-C37-C38
51	a	201	CDL	C11-C12-C13-C14
51	m	201	CDL	C16-C17-C18-C19
47	B	303	PEE	C36-C37-C38-C39
47	s	401	PEE	C4-O4P-P-O3P
48	N	201	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
48	n	101	PLX	C3-O4-P1-O1
51	I	201	CDL	CB3-OB5-PB2-OB2
51	V	202	CDL	CA3-OA5-PA1-OA2
51	n	102	CDL	CB3-OB5-PB2-OB2
48	C	303	PLX	C18-C19-C20-C21
49	C	304	UQ	C52-C53-C54-C56
47	C	302	PEE	O3P-C1-C2-C3
47	Q	501	PEE	O3P-C1-C2-C3
47	l	704	PEE	O3P-C1-C2-C3
51	V	201	CDL	OB5-CB3-CB4-CB6
48	g	201	PLX	C10-C11-C12-C13
48	r	502	PLX	C11-C12-C13-C14
47	s	401	PEE	C31-C32-C33-C34
51	r	503	CDL	C83-C84-C85-C86
48	n	101	PLX	C29-C30-C31-C32
51	V	202	CDL	CB2-C1-CA2-OA2
51	m	201	CDL	C19-C20-C21-C22
51	l	703	CDL	CA7-C31-C32-C33
47	W	201	PEE	C24-C25-C26-C27
47	C	302	PEE	C1-C2-C3-O3
47	W	201	PEE	C1-C2-C3-O3
47	l	705	PEE	C1-C2-C3-O3
48	g	201	PLX	C3-C4-C5-O8
48	j	201	PLX	C3-C4-C5-O8
48	j	202	PLX	C3-C4-C5-O8
50	X	201	8Q1	C6-C7-C8-C9
51	I	201	CDL	CA3-CA4-CA6-OA8
51	l	703	CDL	C74-C75-C76-C77
51	m	201	CDL	C18-C19-C20-C21
51	m	201	CDL	C52-C53-C54-C55
51	n	102	CDL	C75-C76-C77-C78
51	l	703	CDL	C61-C62-C63-C64
47	W	201	PEE	C10-C11-C12-C13
47	l	701	PEE	C32-C33-C34-C35
48	N	201	PLX	C12-C13-C14-C15
51	V	202	CDL	C41-C42-C43-C44
51	l	703	CDL	C21-C22-C23-C24
50	X	201	8Q1	O33-C32-C34-O35
47	s	401	PEE	C22-C23-C24-C25
48	N	201	PLX	C7-C8-C9-C10
51	m	201	CDL	C17-C18-C19-C20
51	s	402	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C64-C65-C66-C67
47	B	303	PEE	C39-C40-C41-C42
47	l	704	PEE	C19-C20-C21-C22
47	B	303	PEE	C34-C35-C36-C37
48	r	502	PLX	C18-C19-C20-C21
51	I	201	CDL	C71-C72-C73-C74
51	l	703	CDL	C51-CB5-OB6-CB4
51	l	702	CDL	C63-C64-C65-C66
51	r	503	CDL	CB7-C71-C72-C73
48	r	502	PLX	C31-C32-C33-C34
51	r	503	CDL	C77-C78-C79-C80
51	a	201	CDL	C36-C37-C38-C39
51	m	201	CDL	CA6-CA4-OA6-CA5
47	B	303	PEE	C42-C43-C44-C45
51	r	503	CDL	C54-C55-C56-C57
51	V	201	CDL	C54-C55-C56-C57
51	m	201	CDL	C71-CB7-OB8-CB6
51	r	503	CDL	C71-CB7-OB8-CB6
47	l	705	PEE	O3P-C1-C2-O2
47	s	401	PEE	O3P-C1-C2-O2
51	V	201	CDL	C72-C73-C74-C75
51	r	503	CDL	C42-C43-C44-C45
51	r	503	CDL	C64-C65-C66-C67
47	U	101	PEE	C34-C35-C36-C37
51	r	503	CDL	CB5-C51-C52-C53
51	a	201	CDL	C32-C33-C34-C35
47	l	704	PEE	O2-C2-C3-O3
47	l	705	PEE	O2-C2-C3-O3
50	G	201	8Q1	C30-C29-C32-O33
47	r	501	PEE	C11-C12-C13-C14
51	s	402	CDL	C40-C41-C42-C43
47	U	101	PEE	C36-C37-C38-C39
47	s	401	PEE	C14-C15-C16-C17
47	C	302	PEE	C32-C33-C34-C35
48	C	303	PLX	C30-C31-C32-C33
51	V	202	CDL	C34-C35-C36-C37
47	l	705	PEE	C13-C14-C15-C16
47	Q	501	PEE	C34-C35-C36-C37
47	s	401	PEE	C11-C12-C13-C14
48	g	201	PLX	C11-C10-C9-C8
51	a	201	CDL	CA2-C1-CB2-OB2
51	l	702	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	C15-C16-C17-C18
47	Q	501	PEE	C32-C33-C34-C35
47	B	303	PEE	C12-C13-C14-C15
48	n	101	PLX	C26-C27-C28-C29
51	V	202	CDL	C84-C85-C86-C87
47	U	101	PEE	C38-C39-C40-C41
51	l	702	CDL	C36-C37-C38-C39
47	r	501	PEE	O3P-C1-C2-C3
51	I	201	CDL	OA5-CA3-CA4-CA6
51	l	703	CDL	OB5-CB3-CB4-CB6
51	m	201	CDL	OA5-CA3-CA4-CA6
51	r	503	CDL	C33-C34-C35-C36
51	V	202	CDL	C40-C41-C42-C43
51	l	703	CDL	C62-C63-C64-C65
51	r	503	CDL	C84-C85-C86-C87
51	m	201	CDL	C20-C21-C22-C23
48	n	101	PLX	C28-C29-C30-C31
51	m	201	CDL	C84-C85-C86-C87
47	l	701	PEE	C14-C15-C16-C17
51	r	503	CDL	C1-CB2-OB2-PB2
48	N	201	PLX	C16-C17-C18-C19
51	a	201	CDL	C35-C36-C37-C38
51	m	201	CDL	C35-C36-C37-C38
48	j	201	PLX	C34-C35-C36-C37
51	a	201	CDL	C22-C23-C24-C25
51	m	201	CDL	C41-C42-C43-C44
51	s	402	CDL	C34-C35-C36-C37
47	B	303	PEE	C31-C30-O3-C3
47	Q	501	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	C	303	PLX	C3-C4-C5-O8
51	l	703	CDL	CA3-CA4-CA6-OA8
51	n	102	CDL	CA3-CA4-CA6-OA8
51	l	703	CDL	C12-C13-C14-C15
51	V	201	CDL	C21-C22-C23-C24
48	j	201	PLX	C35-C36-C37-C38
47	r	501	PEE	C1-O3P-P-O4P
48	j	201	PLX	C3-C4-O6-C6
51	I	201	CDL	CA3-OA5-PA1-OA2
51	m	201	CDL	OB9-CB7-OB8-CB6
47	l	704	PEE	C21-C22-C23-C24
48	g	201	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
48	n	101	PLX	O7-C6-C7-C8
48	N	201	PLX	C13-C14-C15-C16
47	U	101	PEE	O3P-C1-C2-O2
48	N	201	PLX	O4-C3-C4-O6
48	n	101	PLX	O4-C3-C4-O6
51	l	702	CDL	OB5-CB3-CB4-OB6
51	m	201	CDL	OB5-CB3-CB4-OB6
47	B	303	PEE	C23-C24-C25-C26
48	n	101	PLX	C16-C17-C18-C19
51	a	201	CDL	C84-C85-C86-C87
51	l	702	CDL	C24-C25-C26-C27
51	s	402	CDL	C84-C85-C86-C87
51	r	503	CDL	OB9-CB7-OB8-CB6
48	n	101	PLX	C11-C12-C13-C14
51	a	201	CDL	C82-C83-C84-C85
51	l	703	CDL	C44-C45-C46-C47
48	r	502	PLX	O6-C4-C5-O8
51	I	201	CDL	OA6-CA4-CA6-OA8
51	n	102	CDL	OA6-CA4-CA6-OA8
51	m	201	CDL	C82-C83-C84-C85
51	V	202	CDL	C24-C25-C26-C27
51	I	201	CDL	C52-C53-C54-C55
51	l	703	CDL	OB7-CB5-OB6-CB4
49	C	304	UQ	C12-C11-C9-C8
51	l	703	CDL	C12-C11-CA5-OA6
51	m	201	CDL	C39-C40-C41-C42
51	V	201	CDL	C1-CB2-OB2-PB2
48	n	101	PLX	C30-C31-C32-C33
51	r	503	CDL	C59-C60-C61-C62
47	r	501	PEE	C20-C21-C22-C23
48	j	201	PLX	C10-C11-C12-C13
51	l	703	CDL	C64-C65-C66-C67
47	B	303	PEE	C38-C39-C40-C41
47	C	302	PEE	C43-C44-C45-C46
47	l	701	PEE	C18-C19-C20-C21
48	C	303	PLX	C36-C37-C38-C39
48	C	303	PLX	O8-C24-C25-C26
48	j	202	PLX	O6-C6-C7-C8
47	W	201	PEE	O3P-C1-C2-C3
47	l	705	PEE	O3P-C1-C2-C3
48	n	101	PLX	O4-C3-C4-C5
51	I	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
47	Q	501	PEE	C18-C19-C20-C21
47	r	501	PEE	C38-C39-C40-C41
47	r	501	PEE	C15-C16-C17-C18
47	Q	501	PEE	C24-C25-C26-C27
47	s	401	PEE	C12-C13-C14-C15
51	V	201	CDL	C75-C76-C77-C78
51	m	201	CDL	C64-C65-C66-C67
48	j	201	PLX	C11-C10-C9-C8
51	m	201	CDL	C43-C44-C45-C46
47	l	704	PEE	C32-C33-C34-C35
48	r	502	PLX	C3-C4-C5-O8
51	V	202	CDL	CA3-CA4-CA6-OA8
51	m	201	CDL	CA3-CA4-CA6-OA8
48	C	303	PLX	C35-C36-C37-C38
47	Q	501	PEE	O3P-C1-C2-O2
47	l	701	PEE	O3P-C1-C2-O2
48	r	502	PLX	O4-C3-C4-O6
51	I	201	CDL	OB5-CB3-CB4-OB6
51	V	201	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	C21-C22-C23-C24
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-C34
48	j	201	PLX	C12-C13-C14-C15
48	r	502	PLX	C7-C8-C9-C10
51	n	102	CDL	C54-C55-C56-C57
47	C	302	PEE	O2-C2-C3-O3
47	Q	501	PEE	O2-C2-C3-O3
51	V	201	CDL	OB6-CB4-CB6-OB8
51	I	201	CDL	C71-CB7-OB8-CB6
48	j	201	PLX	C26-C27-C28-C29
51	r	503	CDL	C51-C52-C53-C54
47	B	303	PEE	O5-C30-O3-C3
48	C	303	PLX	C13-C14-C15-C16
48	g	201	PLX	C31-C32-C33-C34
47	l	701	PEE	C13-C14-C15-C16
47	l	705	PEE	C23-C24-C25-C26
47	Q	501	PEE	C11-C12-C13-C14
47	Q	501	PEE	C10-C11-C12-C13
51	V	202	CDL	C71-C72-C73-C74
47	W	201	PEE	C1-O3P-P-O4P
47	l	704	PEE	C4-O4P-P-O3P
51	V	202	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	CB2-OB2-PB2-OB5
51	a	201	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	CA4-CA3-OA5-PA1
51	I	201	CDL	OB9-CB7-OB8-CB6
47	C	302	PEE	C4-O4P-P-O2P
47	Q	501	PEE	C4-O4P-P-O2P
47	W	201	PEE	C1-O3P-P-O1P
47	l	701	PEE	C4-O4P-P-O1P
47	l	705	PEE	C1-O3P-P-O2P
47	l	705	PEE	C1-O3P-P-O1P
47	r	501	PEE	C1-O3P-P-O2P
47	s	401	PEE	C4-O4P-P-O1P
48	g	201	PLX	C2-O1-P1-O3
48	j	201	PLX	C3-O4-P1-O3
48	j	201	PLX	C2-O1-P1-O3
48	n	101	PLX	C3-O4-P1-O3
48	r	502	PLX	C3-O4-P1-O3
51	I	201	CDL	CB3-OB5-PB2-OB4
51	V	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CB2-OB2-PB2-OB4
51	a	201	CDL	CB3-OB5-PB2-OB3
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB3-OB5-PB2-OB4
51	l	703	CDL	CA2-OA2-PA1-OA4
51	m	201	CDL	CA3-OA5-PA1-OA4
51	n	102	CDL	CA2-OA2-PA1-OA4
51	n	102	CDL	CB3-OB5-PB2-OB3
51	r	503	CDL	CA2-OA2-PA1-OA4
51	s	402	CDL	CA3-OA5-PA1-OA3
51	s	402	CDL	CA3-OA5-PA1-OA4
51	s	402	CDL	CB3-OB5-PB2-OB4
56	w	401	ADP	C5'-O5'-PA-O1A
51	n	102	CDL	C71-CB7-OB8-CB6
47	U	101	PEE	O3P-C1-C2-C3
47	l	701	PEE	O3P-C1-C2-C3
47	s	401	PEE	O3P-C1-C2-C3
48	N	201	PLX	O4-C3-C4-C5
48	r	502	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	OA5-CA3-CA4-CA6
51	a	201	CDL	OB5-CB3-CB4-CB6
51	I	201	CDL	C51-C52-C53-C54
48	r	502	PLX	C34-C35-C36-C37
48	g	201	PLX	C25-C24-O8-C5
48	j	201	PLX	C25-C24-O8-C5
51	l	702	CDL	C82-C83-C84-C85
47	U	101	PEE	C24-C25-C26-C27
48	r	502	PLX	C36-C37-C38-C39
51	r	503	CDL	C56-C57-C58-C59
47	C	302	PEE	O3P-C1-C2-O2
47	r	501	PEE	O3P-C1-C2-O2
50	X	201	8Q1	C28-C29-C32-C34
51	a	201	CDL	OA5-CA3-CA4-OA6
51	a	201	CDL	OB5-CB3-CB4-OB6
51	l	703	CDL	OA5-CA3-CA4-OA6
51	l	703	CDL	OB5-CB3-CB4-OB6
52	J	401	NDP	O4D-C4D-C5D-O5D
47	l	704	PEE	C34-C35-C36-C37
50	X	201	8Q1	C13-C14-C15-C16
51	m	201	CDL	C58-C59-C60-C61
47	s	401	PEE	C24-C25-C26-C27
51	m	201	CDL	C62-C63-C64-C65
51	l	703	CDL	C73-C74-C75-C76
51	n	102	CDL	OB9-CB7-OB8-CB6
51	a	201	CDL	O1-C1-CB2-OB2
52	J	401	NDP	C2D-C1D-N1N-C2N
47	l	704	PEE	C1-C2-C3-O3
48	j	201	PLX	N1-C1-C2-O1
51	s	402	CDL	CB3-CB4-CB6-OB8
47	r	501	PEE	O2-C2-C3-O3
48	j	201	PLX	O6-C4-C5-O8
48	j	202	PLX	O6-C4-C5-O8
51	V	202	CDL	C12-C13-C14-C15
51	a	201	CDL	C58-C59-C60-C61
51	r	503	CDL	C13-C14-C15-C16
47	l	705	PEE	C11-C12-C13-C14
48	j	202	PLX	C18-C19-C20-C21
48	r	502	PLX	O7-C6-C7-C8
51	a	201	CDL	C14-C15-C16-C17
51	s	402	CDL	C11-C12-C13-C14
48	N	201	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C35-C36-C37-C38
51	V	202	CDL	C58-C59-C60-C61
51	s	402	CDL	C12-C13-C14-C15
48	n	101	PLX	C12-C13-C14-C15
47	l	704	PEE	C1-C2-O2-C10
51	V	201	CDL	CA6-CA4-OA6-CA5
51	a	201	CDL	OA5-CA3-CA4-CA6
51	l	703	CDL	OA5-CA3-CA4-CA6
47	C	302	PEE	C12-C13-C14-C15
51	m	201	CDL	C42-C43-C44-C45
51	s	402	CDL	C72-C71-CB7-OB8
48	j	202	PLX	O4-C3-C4-O6
48	n	101	PLX	C15-C16-C17-C18
51	V	202	CDL	C32-C31-CA7-OA8
51	m	201	CDL	C74-C75-C76-C77
49	C	304	UQ	C39-C41-C42-C43
47	W	201	PEE	O2-C2-C3-O3
51	s	402	CDL	OA6-CA4-CA6-OA8
47	C	302	PEE	C13-C14-C15-C16
47	Q	501	PEE	C4-O4P-P-O3P
48	C	303	PLX	C3-O4-P1-O1
51	V	202	CDL	CA2-OA2-PA1-OA5
51	n	102	CDL	CB2-OB2-PB2-OB5
50	X	201	8Q1	C30-C29-C32-O33
48	C	303	PLX	C28-C29-C30-C31
51	l	703	CDL	C43-C44-C45-C46
47	l	705	PEE	C34-C35-C36-C37
51	V	202	CDL	C54-C55-C56-C57
47	l	705	PEE	C18-C19-C20-C21
51	V	202	CDL	C60-C61-C62-C63
51	l	702	CDL	C73-C74-C75-C76
48	r	502	PLX	C15-C16-C17-C18
51	m	201	CDL	C31-C32-C33-C34
47	B	303	PEE	C21-C22-C23-C24
47	B	303	PEE	C44-C45-C46-C47
47	U	101	PEE	C16-C17-C18-C19
47	l	705	PEE	C16-C17-C18-C19
47	C	302	PEE	C15-C16-C17-C18
47	l	704	PEE	C35-C36-C37-C38
47	r	501	PEE	C37-C38-C39-C40
51	V	201	CDL	CA7-C31-C32-C33
48	C	303	PLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
51	r	503	CDL	C15-C16-C17-C18
51	V	202	CDL	C31-C32-C33-C34
51	a	201	CDL	C74-C75-C76-C77
48	j	202	PLX	C24-C25-C26-C27
47	l	705	PEE	O4P-C4-C5-N
51	l	703	CDL	C15-C16-C17-C18
49	J	402	UQ	C21-C22-C23-C24
47	l	704	PEE	C23-C24-C25-C26
51	l	703	CDL	C33-C34-C35-C36
47	l	704	PEE	C42-C43-C44-C45
51	l	703	CDL	C41-C42-C43-C44
47	B	303	PEE	C13-C14-C15-C16
47	r	501	PEE	C33-C34-C35-C36
48	g	201	PLX	O6-C6-C7-C8
51	I	201	CDL	C31-C32-C33-C34
47	l	704	PEE	C40-C41-C42-C43
48	j	201	PLX	C16-C17-C18-C19
51	s	402	CDL	CA3-CA4-CA6-OA8
51	a	201	CDL	C44-C45-C46-C47
47	r	501	PEE	C12-C13-C14-C15
51	l	703	CDL	C39-C40-C41-C42
51	m	201	CDL	C77-C78-C79-C80
51	r	503	CDL	C52-C53-C54-C55
51	l	702	CDL	C41-C42-C43-C44
47	C	302	PEE	C4-O4P-P-O3P
51	l	702	CDL	C20-C21-C22-C23
51	l	703	CDL	C36-C37-C38-C39
51	l	702	CDL	C54-C55-C56-C57
51	n	102	CDL	OB5-CB3-CB4-OB6
47	l	704	PEE	C15-C16-C17-C18
48	j	201	PLX	C29-C30-C31-C32
48	C	303	PLX	C6-C7-C8-C9
51	r	503	CDL	OA6-CA4-CA6-OA8
48	g	201	PLX	C36-C37-C38-C39
52	J	401	NDP	O4D-C1D-N1N-C2N
51	n	102	CDL	CB7-C71-C72-C73
47	C	302	PEE	C33-C34-C35-C36
49	C	304	UQ	C40-C39-C41-C42
48	r	502	PLX	C16-C17-C18-C19
47	W	201	PEE	C16-C17-C18-C19
47	l	704	PEE	C13-C14-C15-C16
48	j	202	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C53-C54-C55-C56
51	l	702	CDL	C44-C45-C46-C47
51	V	201	CDL	C64-C65-C66-C67
51	V	202	CDL	C16-C17-C18-C19
51	r	503	CDL	C72-C71-CB7-OB8
47	C	302	PEE	C38-C39-C40-C41
51	s	402	CDL	C15-C16-C17-C18
48	g	201	PLX	C6-C7-C8-C9
51	l	702	CDL	C76-C77-C78-C79
47	l	704	PEE	C16-C17-C18-C19
47	s	401	PEE	C18-C19-C20-C21
48	N	201	PLX	O8-C24-C25-C26
51	l	702	CDL	OB5-CB3-CB4-CB6
51	m	201	CDL	OB5-CB3-CB4-CB6
47	W	201	PEE	O4P-C4-C5-N
47	C	302	PEE	C16-C17-C18-C19
47	U	101	PEE	C41-C42-C43-C44
47	l	704	PEE	C39-C40-C41-C42
48	N	201	PLX	O6-C4-C5-O8
47	B	303	PEE	C11-C12-C13-C14
52	J	401	NDP	C3D-C4D-C5D-O5D
47	B	303	PEE	C16-C17-C18-C19
47	C	302	PEE	C18-C19-C20-C21
47	l	701	PEE	C38-C39-C40-C41
47	s	401	PEE	C16-C17-C18-C19
46	A	502	FMN	C5'-O5'-P-O3P
48	r	502	PLX	C29-C30-C31-C32
51	a	201	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	C72-C71-CB7-OB8
47	C	302	PEE	C44-C45-C46-C47
47	Q	501	PEE	C15-C16-C17-C18
47	U	101	PEE	C19-C20-C21-C22
51	l	702	CDL	C60-C61-C62-C63
51	l	702	CDL	C51-C52-C53-C54
47	l	701	PEE	O3-C30-C31-C32
51	n	102	CDL	C72-C71-CB7-OB8
51	s	402	CDL	C12-C11-CA5-OA6
47	W	201	PEE	C18-C19-C20-C21
47	l	705	PEE	C38-C39-C40-C41
47	C	302	PEE	C20-C21-C22-C23
51	l	702	CDL	C22-C23-C24-C25
51	s	402	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	C3-C2-O2-C10
51	a	201	CDL	C16-C17-C18-C19
48	r	502	PLX	C33-C34-C35-C36
47	U	101	PEE	O2-C10-C11-C12
51	I	201	CDL	C72-C71-CB7-OB8
51	a	201	CDL	C64-C65-C66-C67
51	r	503	CDL	C39-C40-C41-C42
51	l	703	CDL	C72-C71-CB7-OB8
47	Q	501	PEE	C36-C37-C38-C39
47	l	705	PEE	C15-C16-C17-C18
48	N	201	PLX	C3-C4-C5-O8
48	j	202	PLX	C7-C6-O6-C4
47	C	302	PEE	O3-C30-C31-C32
51	V	202	CDL	C44-C45-C46-C47
51	a	201	CDL	C32-C31-CA7-OA8
50	X	201	8Q1	C31-C29-C32-C34
51	m	201	CDL	C53-C54-C55-C56
47	Q	501	PEE	C22-C23-C24-C25
47	C	302	PEE	O2-C10-C11-C12
47	l	705	PEE	O3-C30-C31-C32
47	l	701	PEE	O2-C2-C3-O3
51	a	201	CDL	C12-C13-C14-C15
52	J	401	NDP	C5B-O5B-PA-O3
47	Q	501	PEE	C23-C24-C25-C26
51	a	201	CDL	C51-C52-C53-C54
51	s	402	CDL	C74-C75-C76-C77
48	N	201	PLX	C26-C27-C28-C29
51	r	503	CDL	C21-C22-C23-C24
51	V	201	CDL	C40-C41-C42-C43
47	r	501	PEE	C16-C17-C18-C19
51	a	201	CDL	C41-C42-C43-C44
48	r	502	PLX	C19-C20-C21-C22
51	l	703	CDL	C56-C57-C58-C59
51	n	102	CDL	C72-C71-CB7-OB9
56	w	401	ADP	PB-O3A-PA-O2A
51	V	202	CDL	C39-C40-C41-C42
48	r	502	PLX	C26-C27-C28-C29
51	a	201	CDL	C43-C44-C45-C46
48	C	303	PLX	O6-C6-C7-C8
49	J	402	UQ	C17-C18-C19-C20
51	V	201	CDL	CB2-C1-CA2-OA2
47	Q	501	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
47	C	302	PEE	O5-C30-C31-C32
51	s	402	CDL	C12-C11-CA5-OA7
51	m	201	CDL	C54-C55-C56-C57
51	V	201	CDL	CB3-CB4-CB6-OB8
47	l	701	PEE	O2-C10-C11-C12
51	a	201	CDL	C12-C11-CA5-OA6
47	l	701	PEE	O5-C30-C31-C32
47	C	302	PEE	C34-C35-C36-C37
51	m	201	CDL	C44-C45-C46-C47
49	C	304	UQ	C15-C14-C16-C17
47	U	101	PEE	O4-C10-C11-C12
51	a	201	CDL	C13-C14-C15-C16
47	B	303	PEE	C18-C19-C20-C21
47	s	401	PEE	C1-O3P-P-O2P
48	g	201	PLX	C3-O4-P1-O2
48	j	201	PLX	C3-O4-P1-O2
48	j	202	PLX	C2-O1-P1-O3
48	n	101	PLX	C2-O1-P1-O3
51	V	202	CDL	CB3-OB5-PB2-OB4
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CB3-OB5-PB2-OB4
51	l	703	CDL	CA3-OA5-PA1-OA3
51	n	102	CDL	CB3-OB5-PB2-OB4
52	J	401	NDP	C5B-O5B-PA-O2A
52	J	401	NDP	C5D-O5D-PN-O1N
47	C	302	PEE	O4-C10-C11-C12
51	l	702	CDL	C72-C71-CB7-OB9
51	l	703	CDL	C12-C11-CA5-OA7
51	m	201	CDL	C12-C11-CA5-OA6
48	j	202	PLX	O4-C3-C4-C5
51	n	102	CDL	OB5-CB3-CB4-CB6
51	a	201	CDL	C32-C31-CA7-OA9
47	C	302	PEE	C35-C36-C37-C38
47	W	201	PEE	C34-C35-C36-C37
47	W	201	PEE	C5-C4-O4P-P
48	N	201	PLX	C1-C2-O1-P1
50	X	201	8Q1	C29-C32-C34-O35
51	I	201	CDL	C72-C71-CB7-OB9
51	l	703	CDL	C72-C71-CB7-OB9
51	a	201	CDL	C53-C54-C55-C56
47	l	705	PEE	O5-C30-C31-C32
51	r	503	CDL	C82-C83-C84-C85

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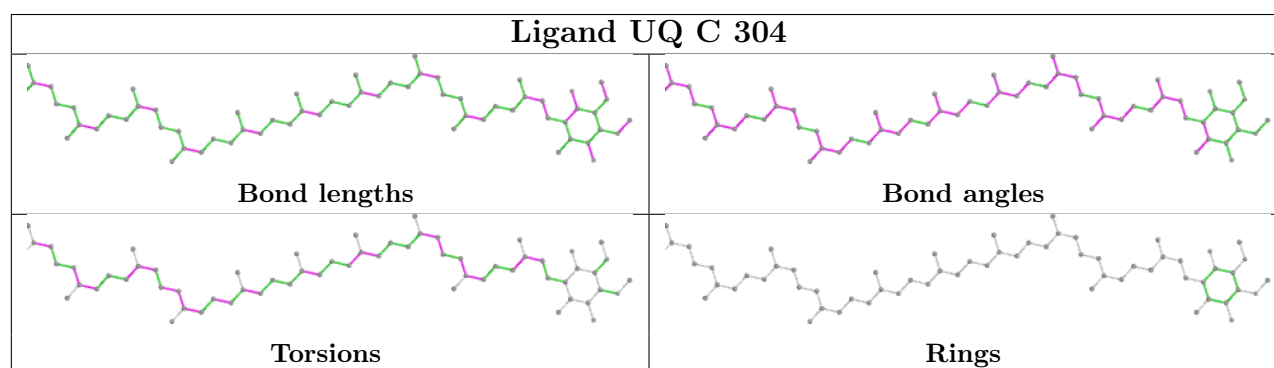
*Continued from previous page...*

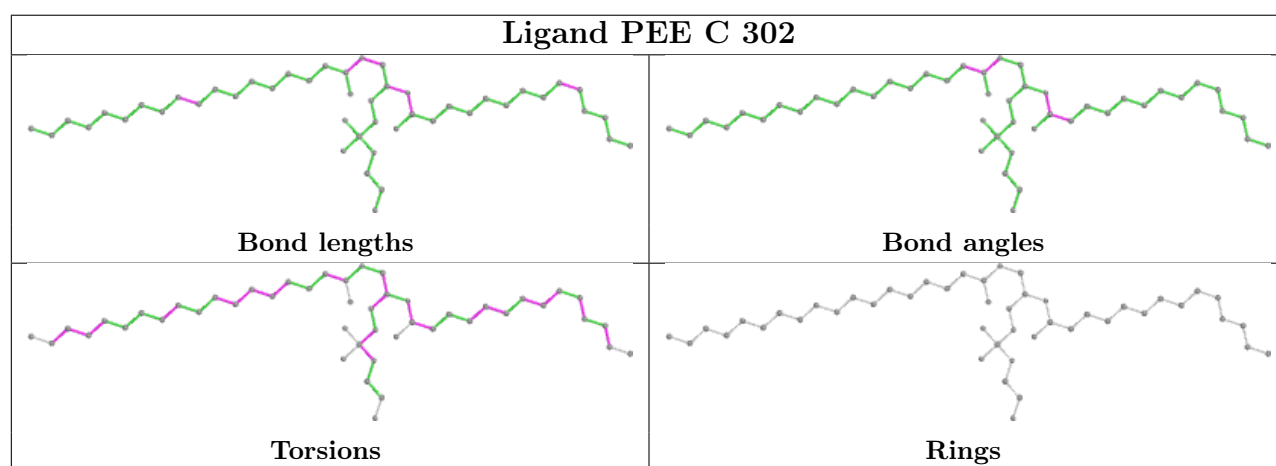
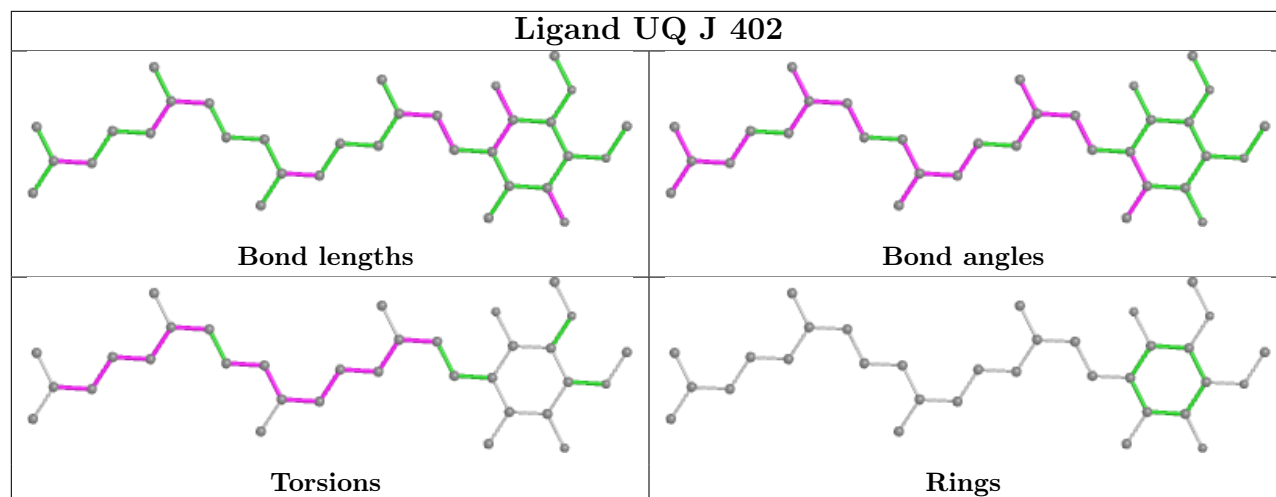
Mol	Chain	Res	Type	Atoms
51	a	201	CDL	C12-C11-CA5-OA7
51	l	703	CDL	OA7-CA5-OA6-CA4
47	Q	501	PEE	C2-C1-O3P-P
47	l	701	PEE	O4-C10-C11-C12
47	l	705	PEE	C14-C15-C16-C17
47	l	704	PEE	C14-C15-C16-C17
48	n	101	PLX	C6-C7-C8-C9
51	V	201	CDL	C57-C58-C59-C60
51	V	202	CDL	C55-C56-C57-C58
47	l	705	PEE	C30-C31-C32-C33

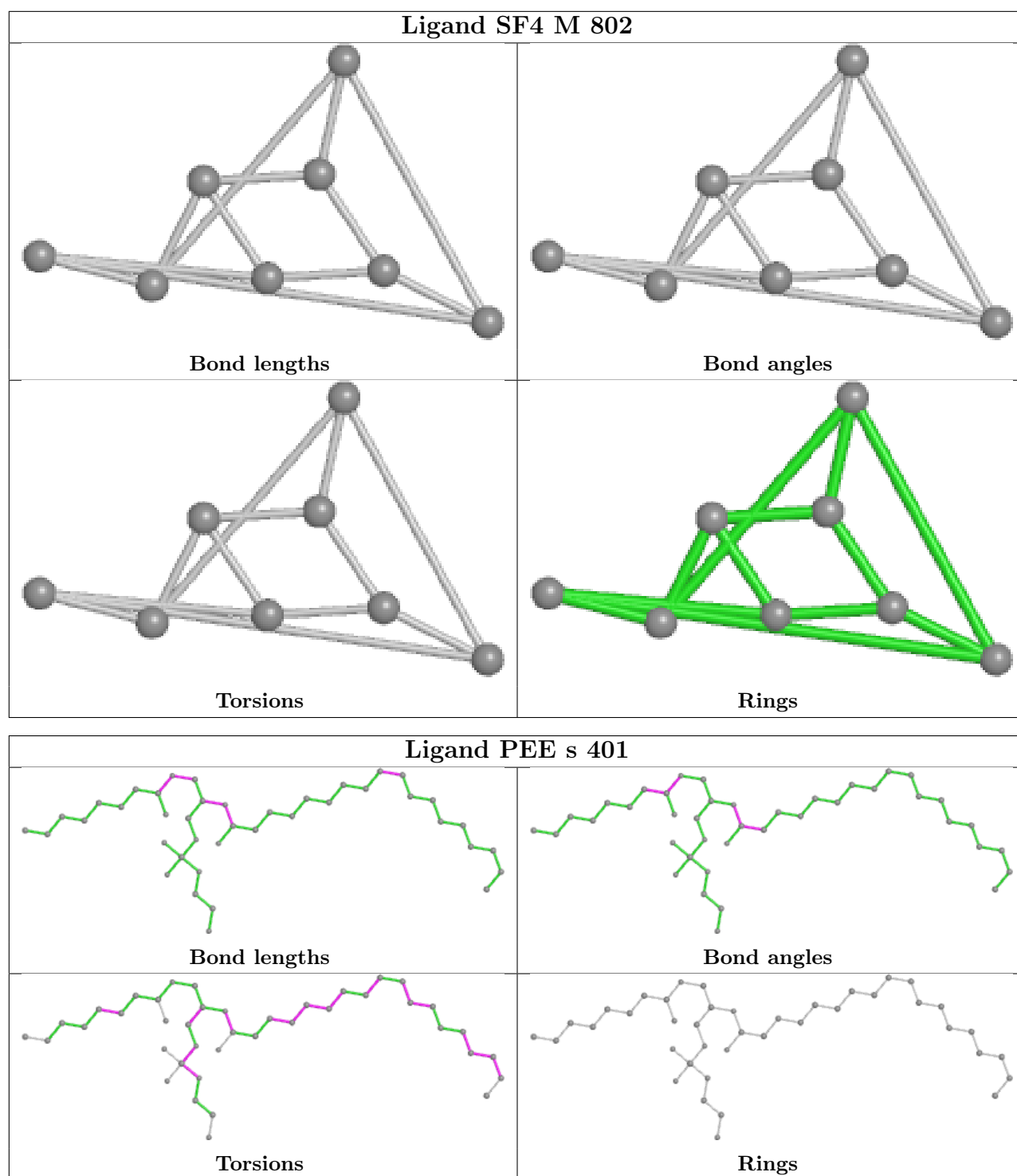
There are no ring outliers.

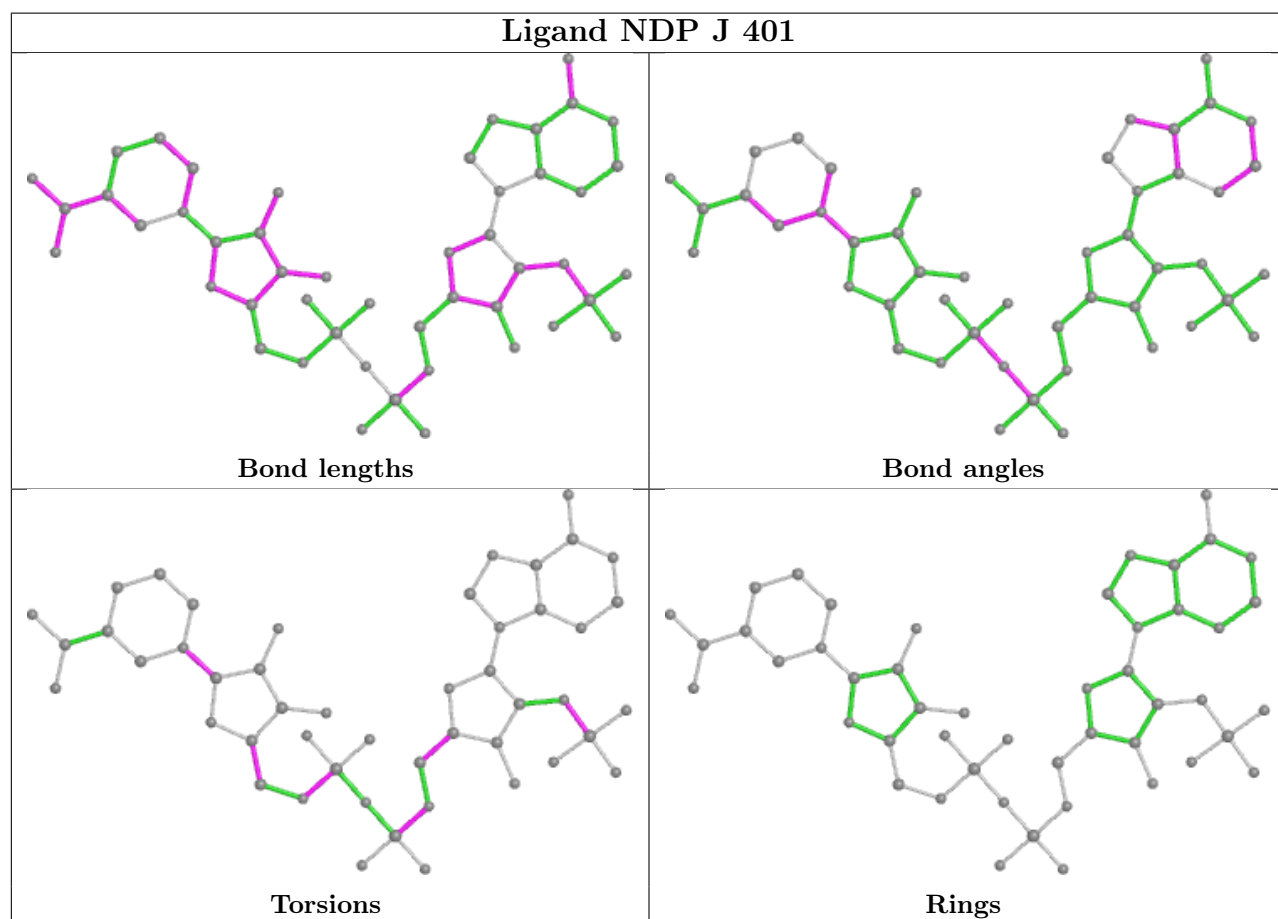
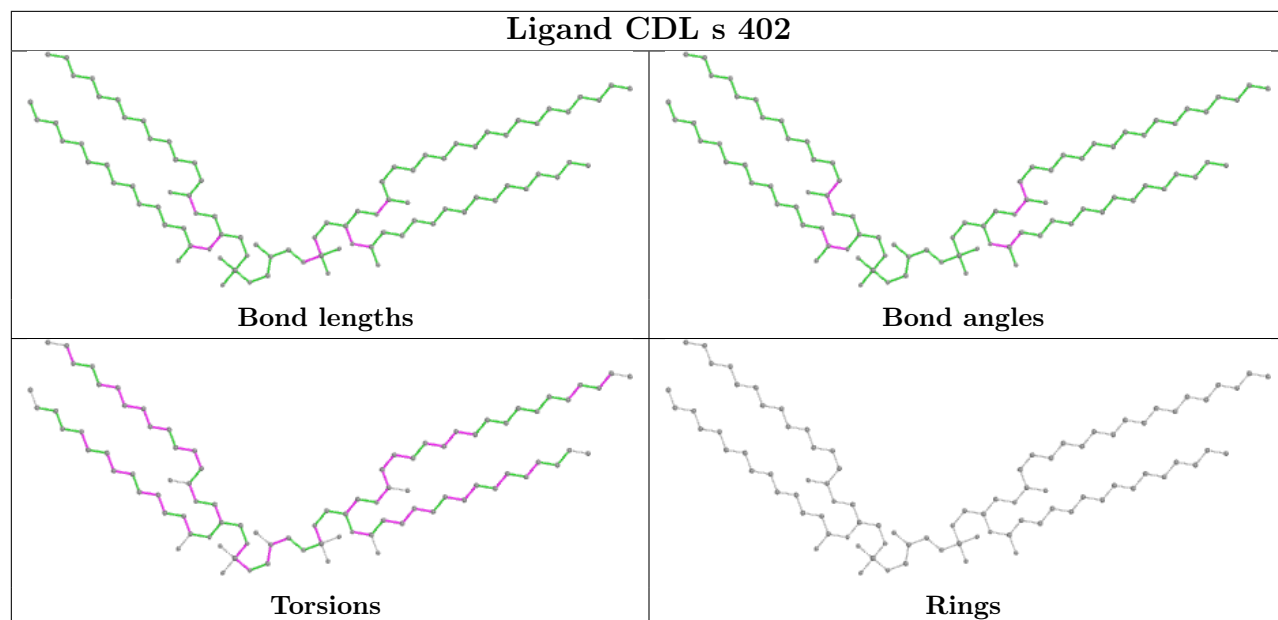
No monomer is involved in short contacts.

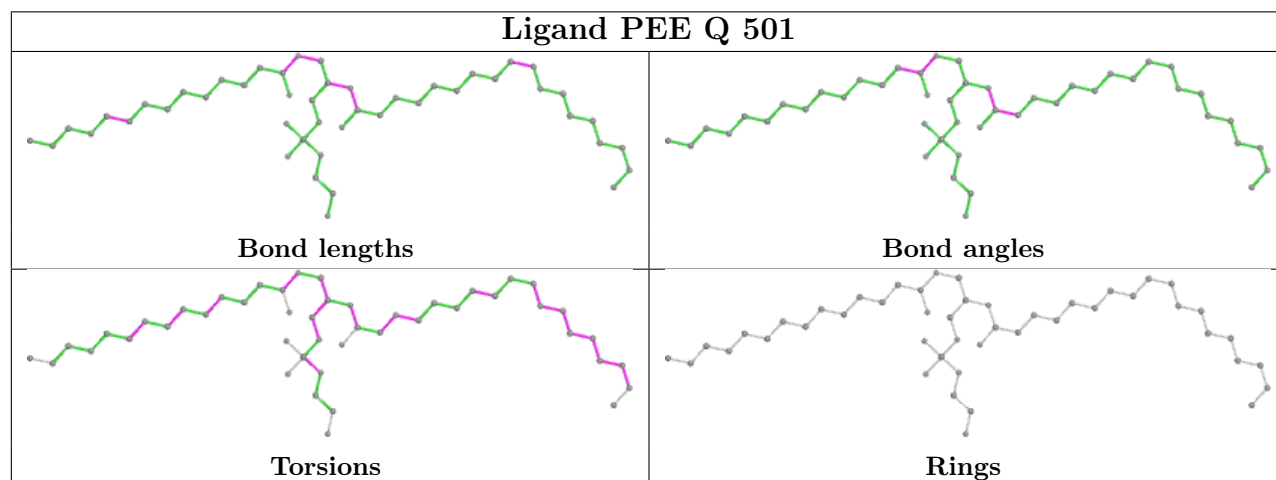
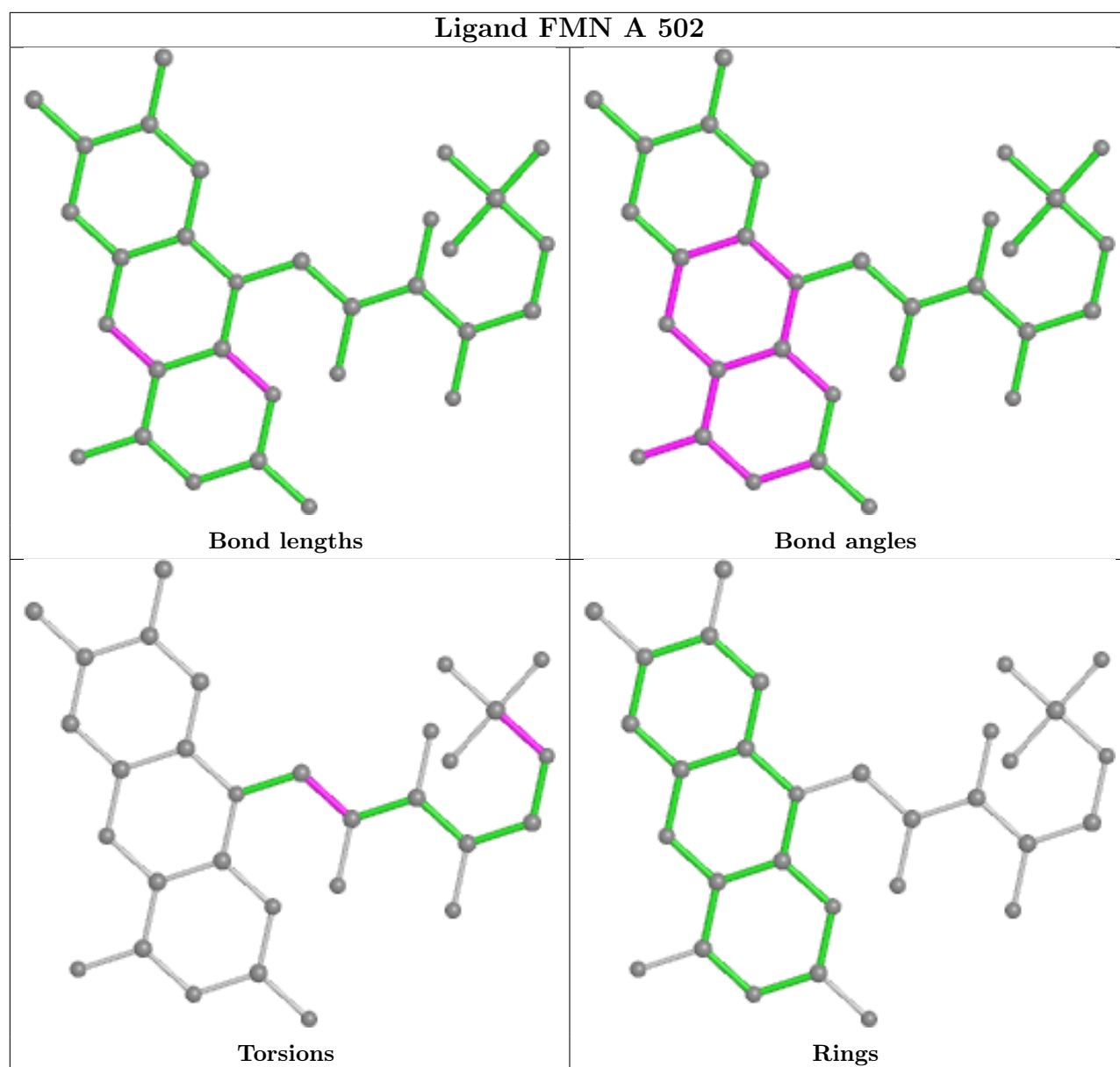
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

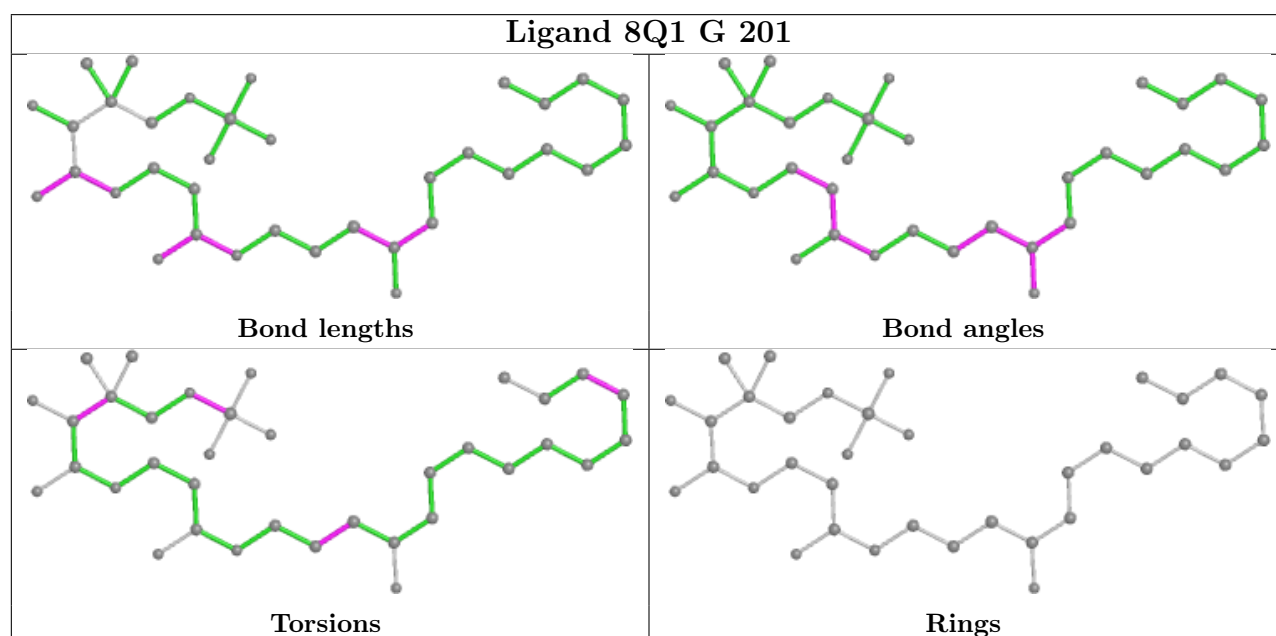
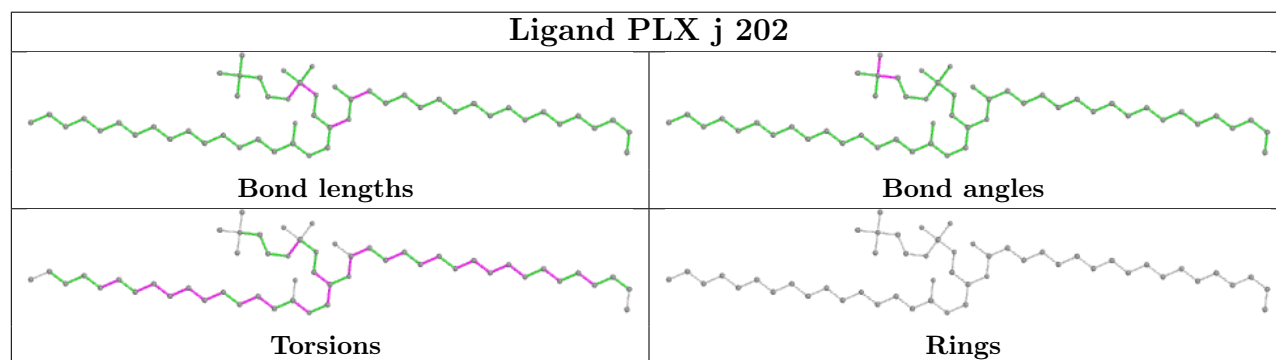
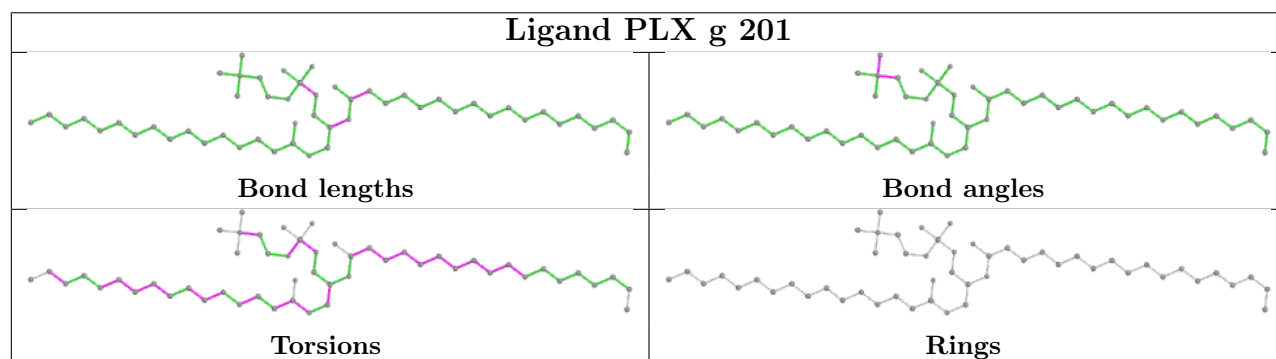
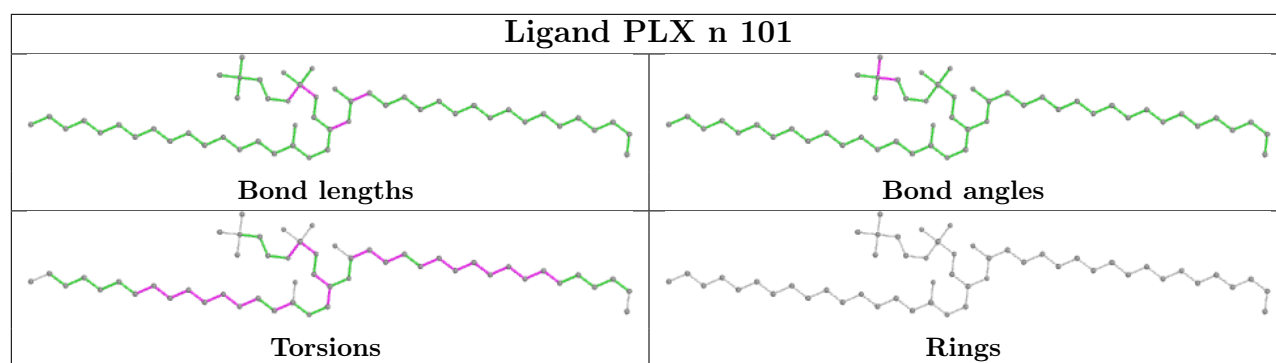




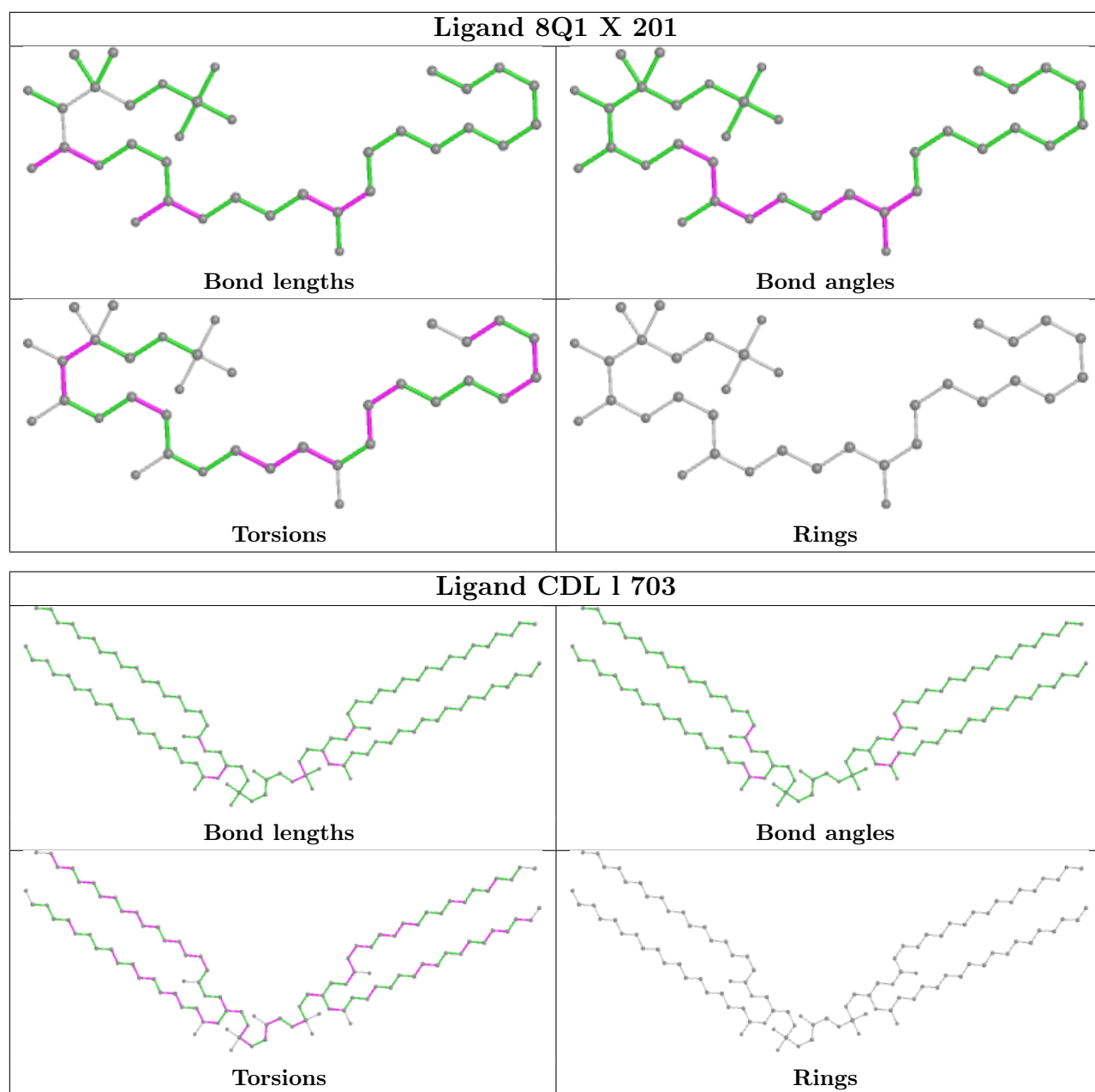


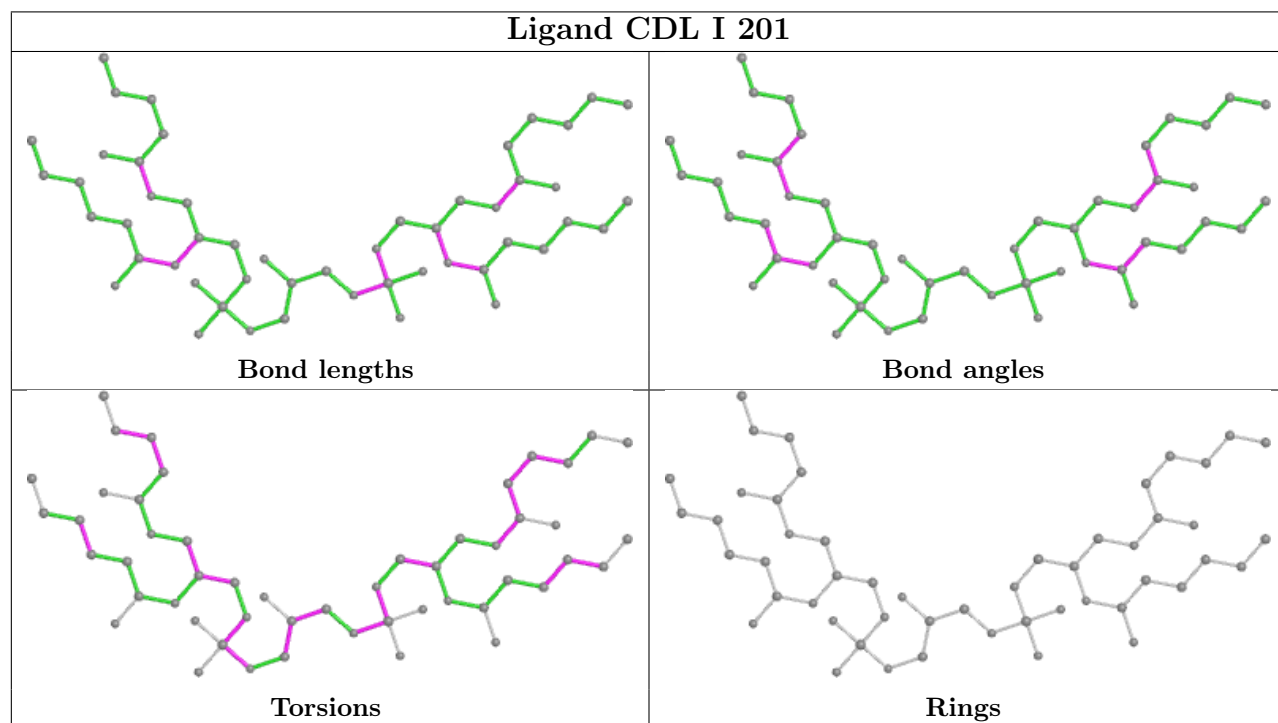
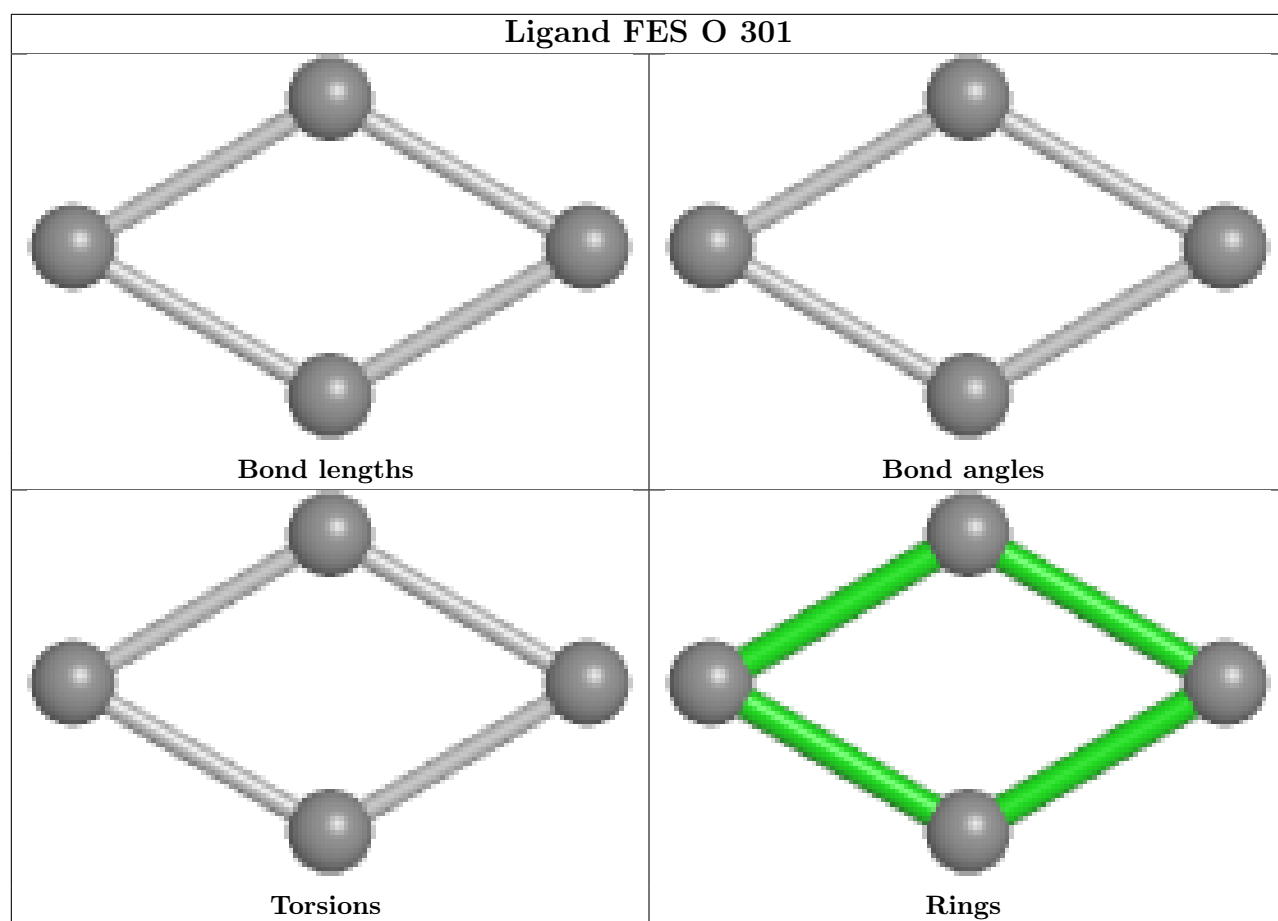


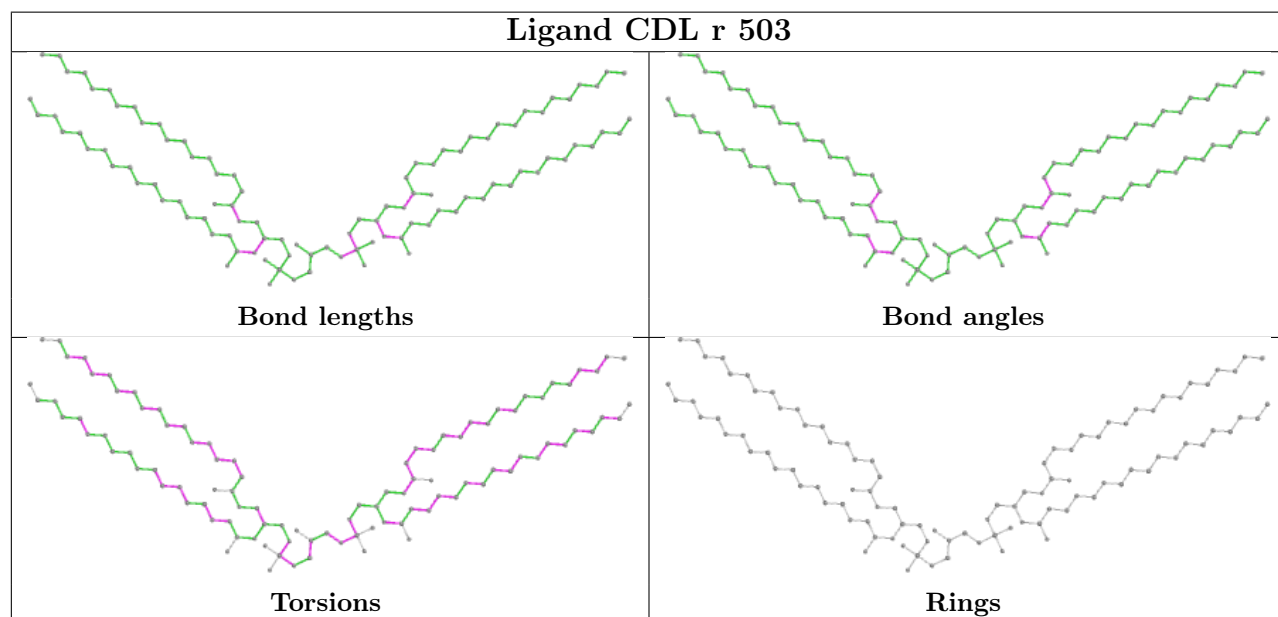
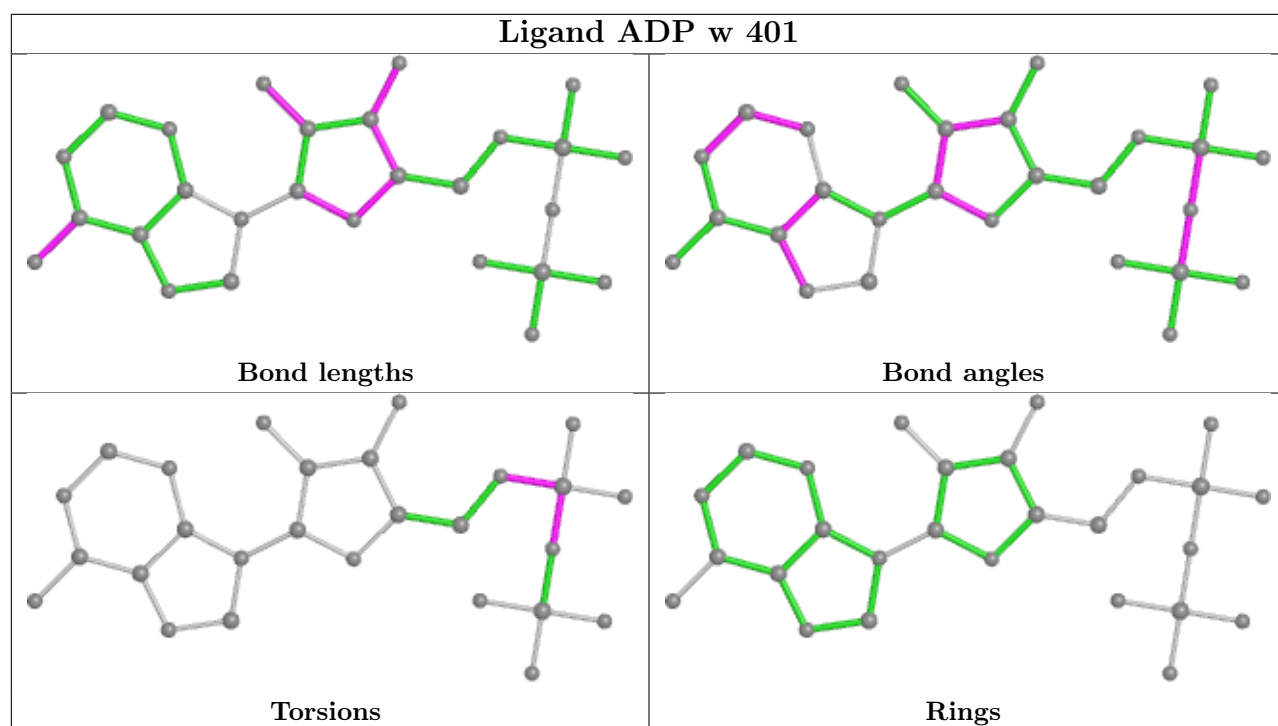


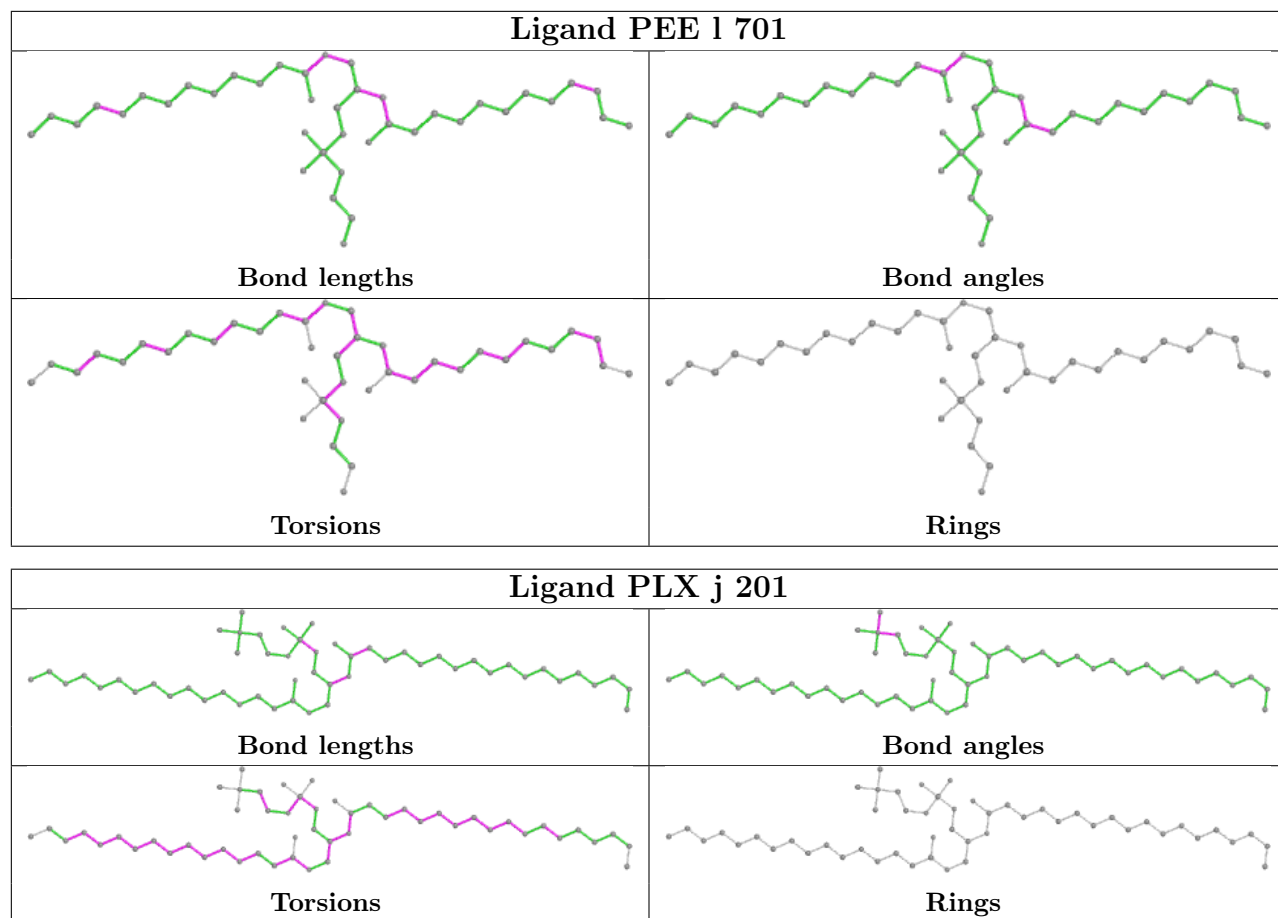


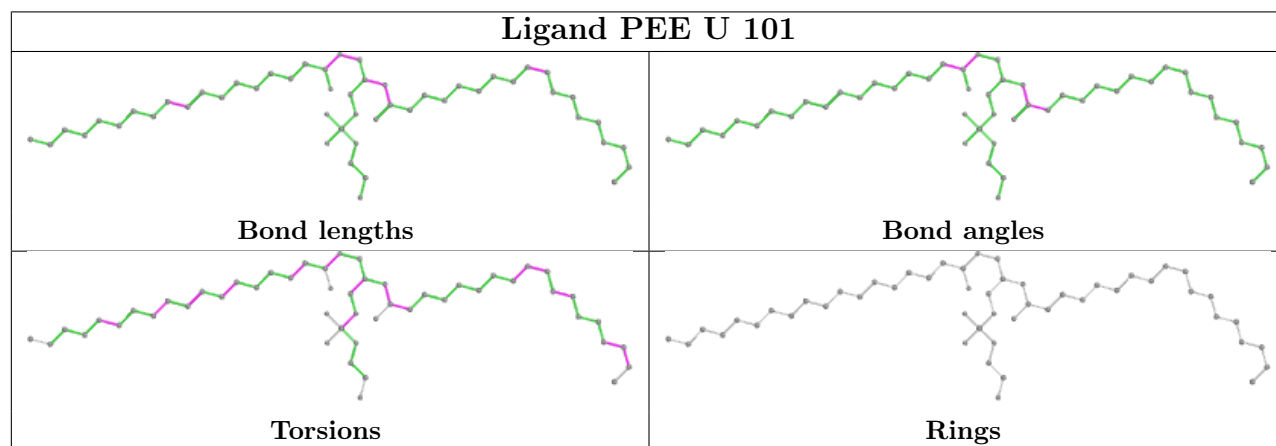
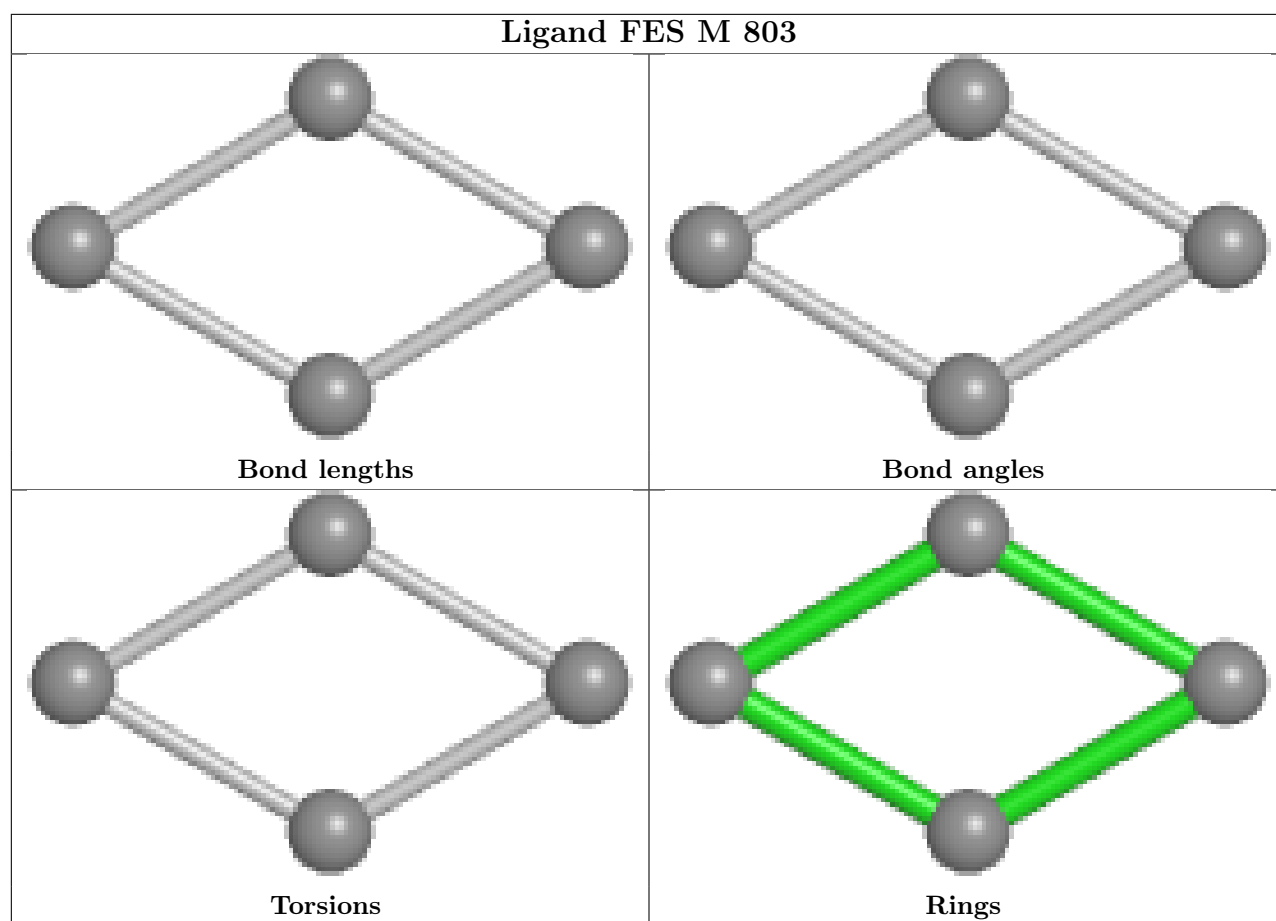


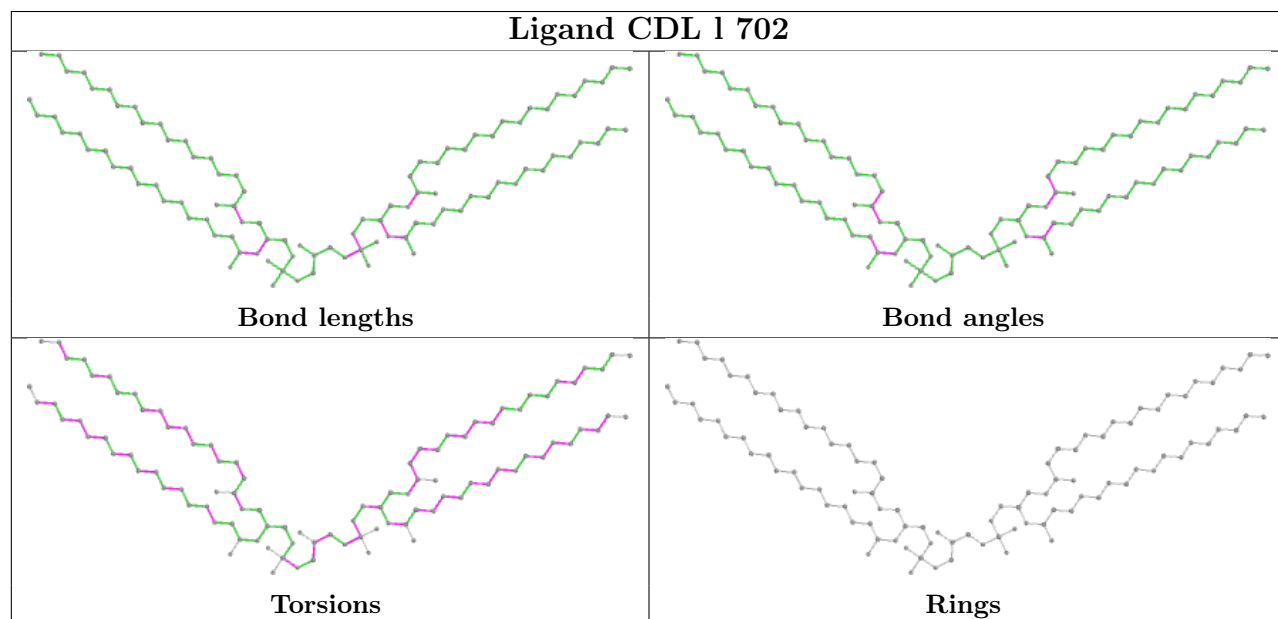
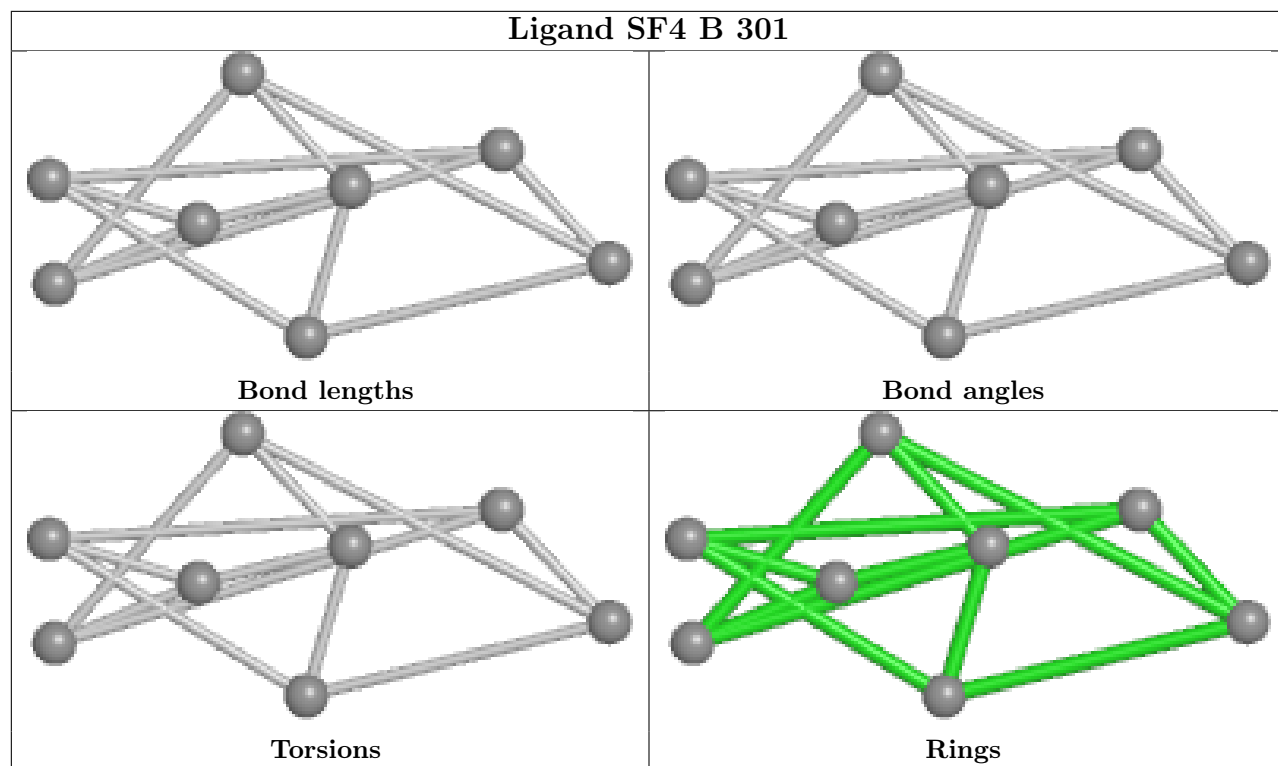


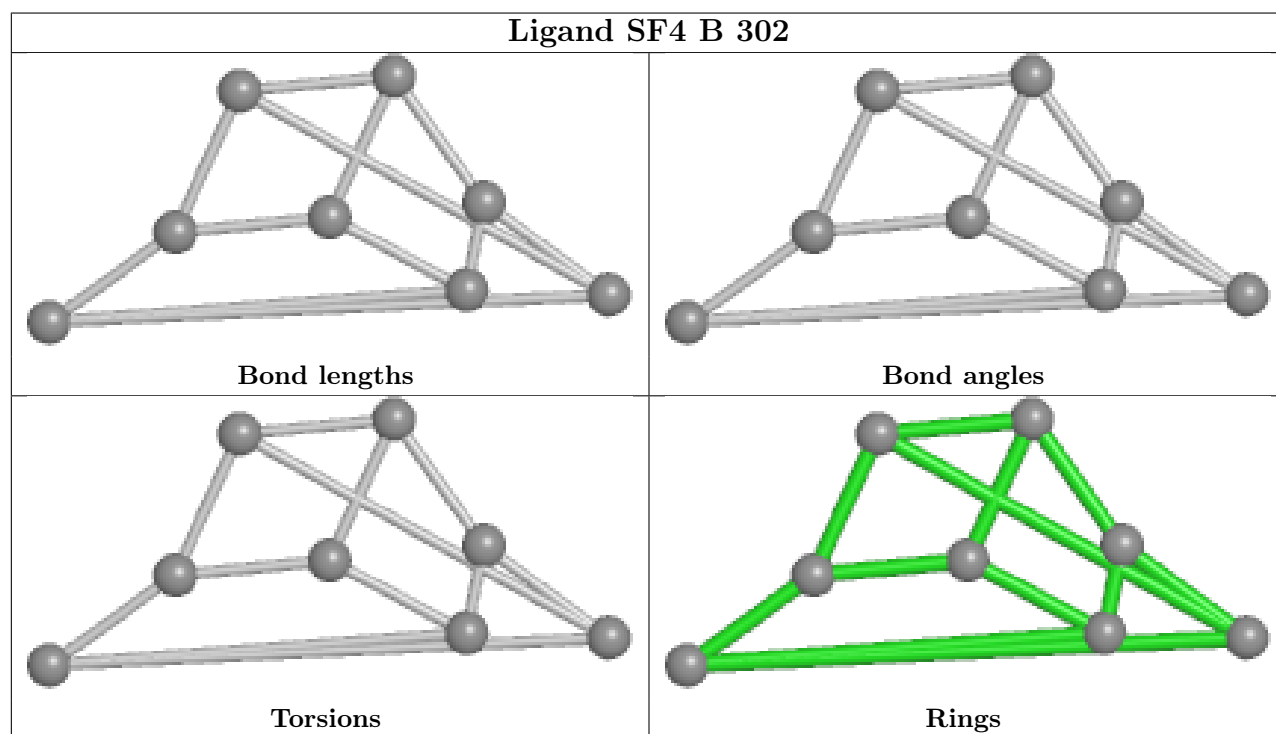
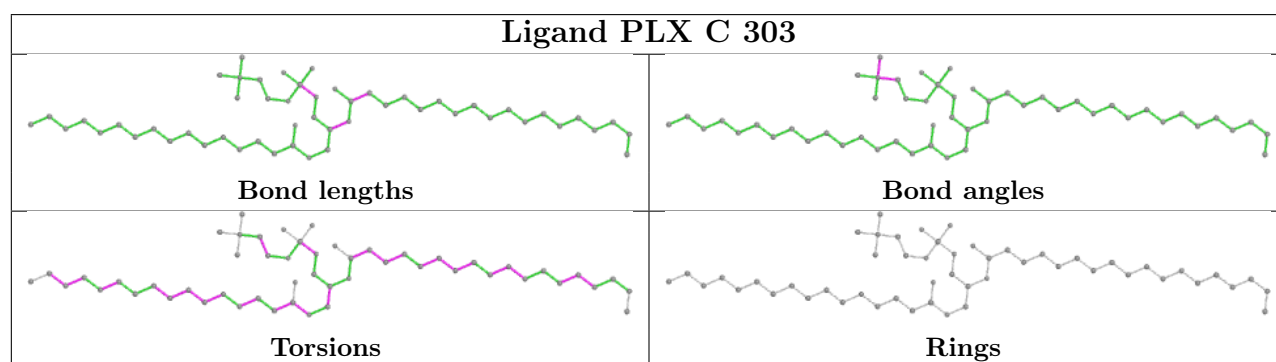
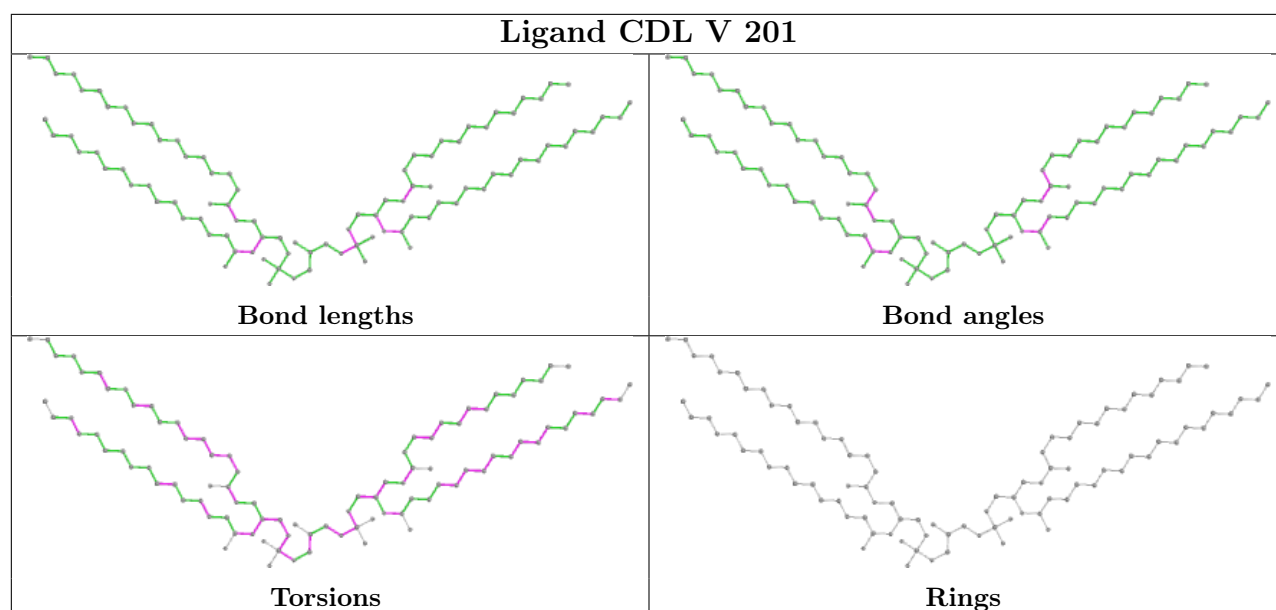


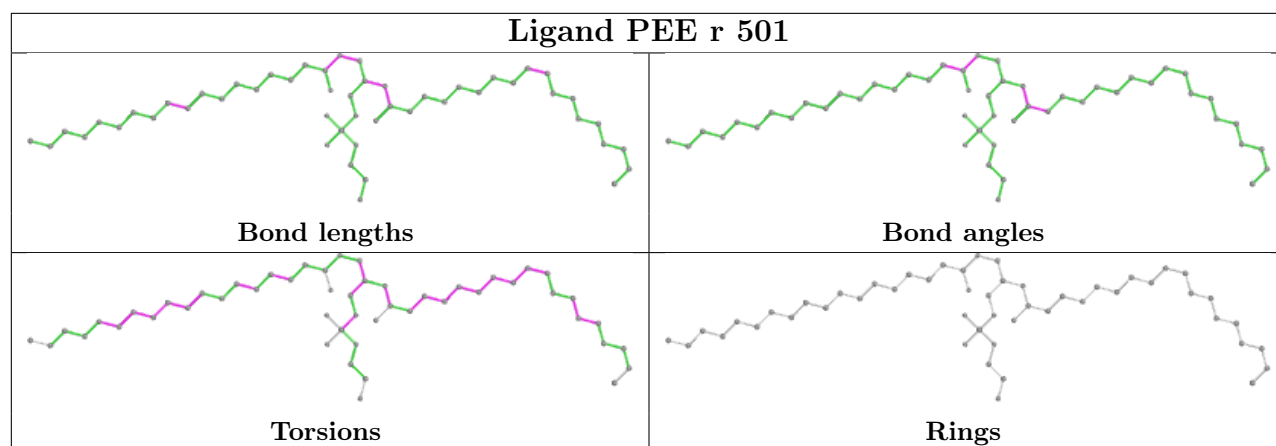
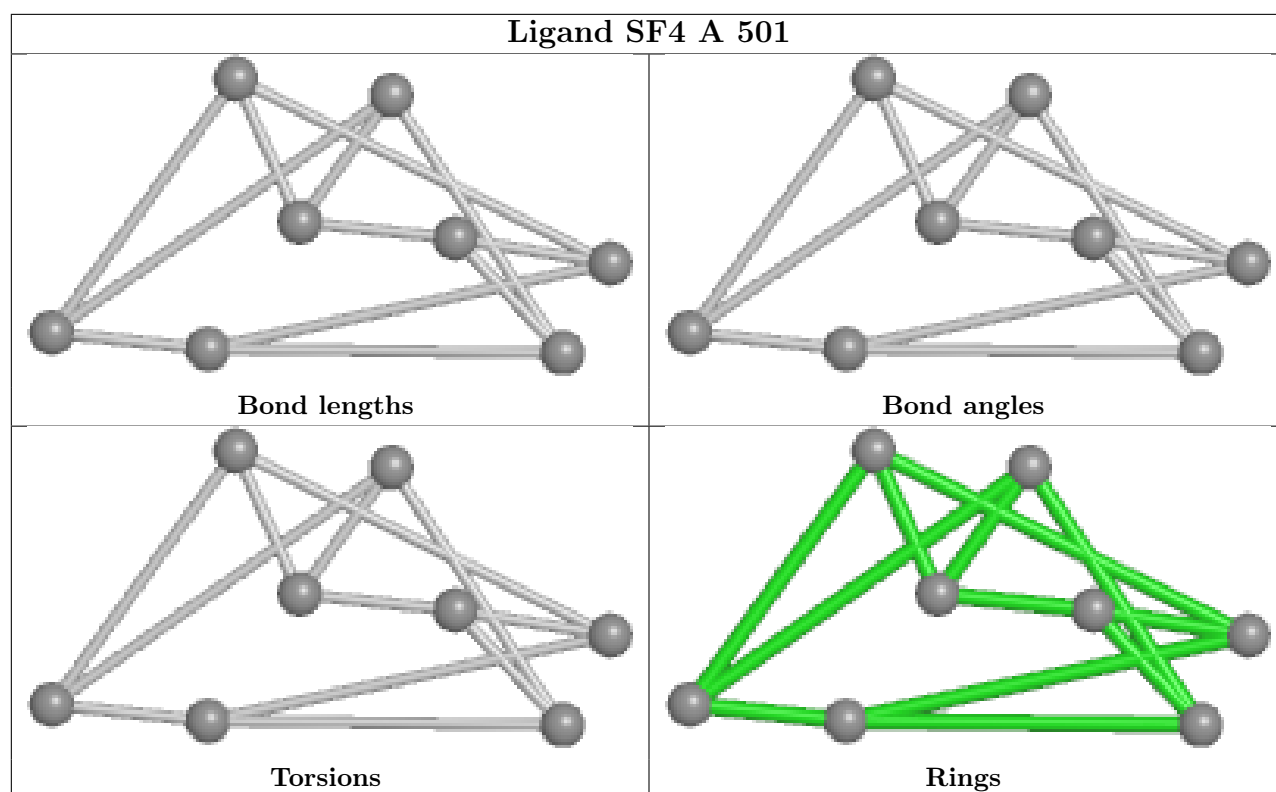




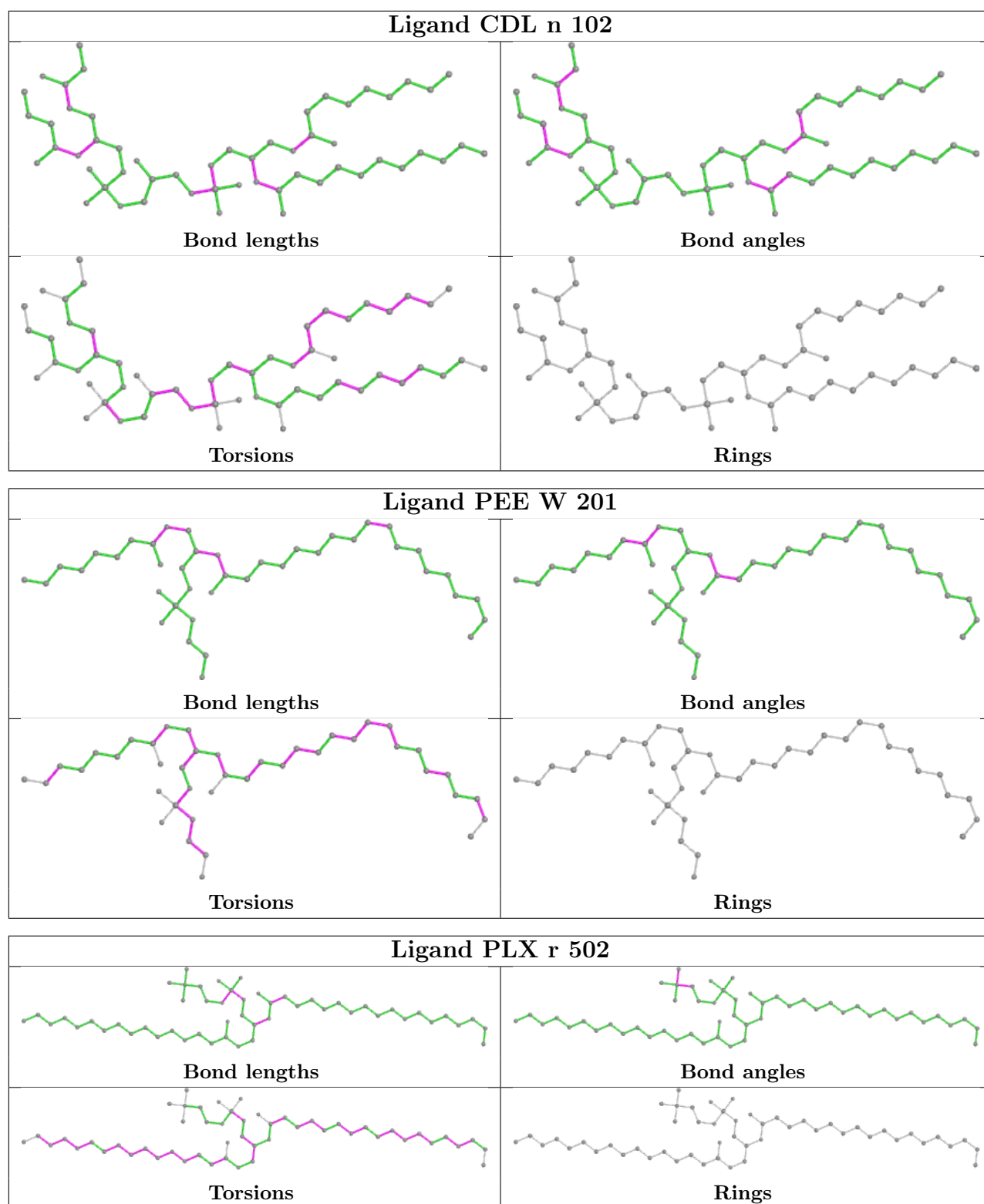


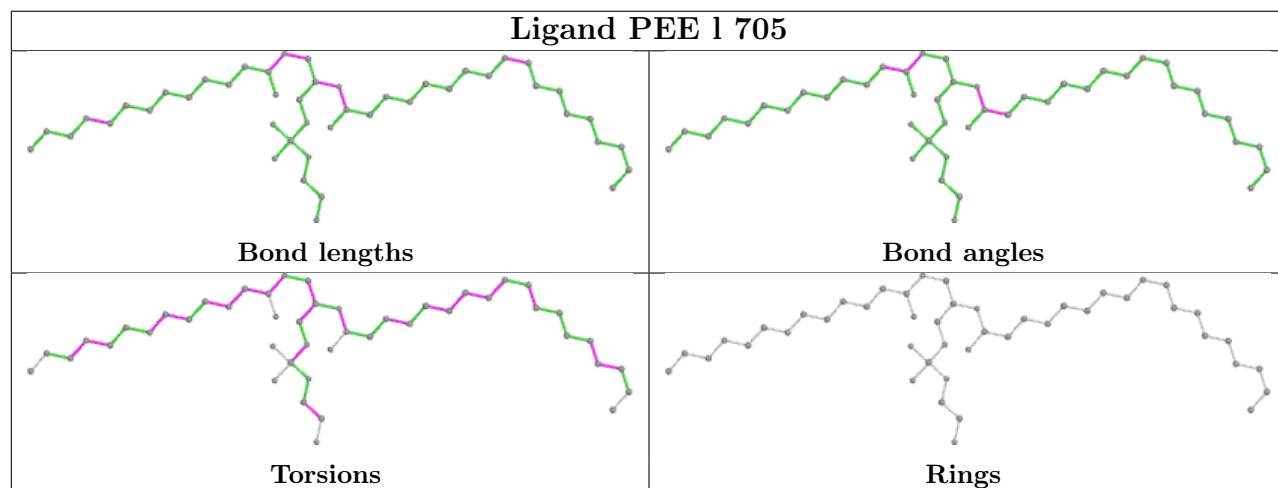
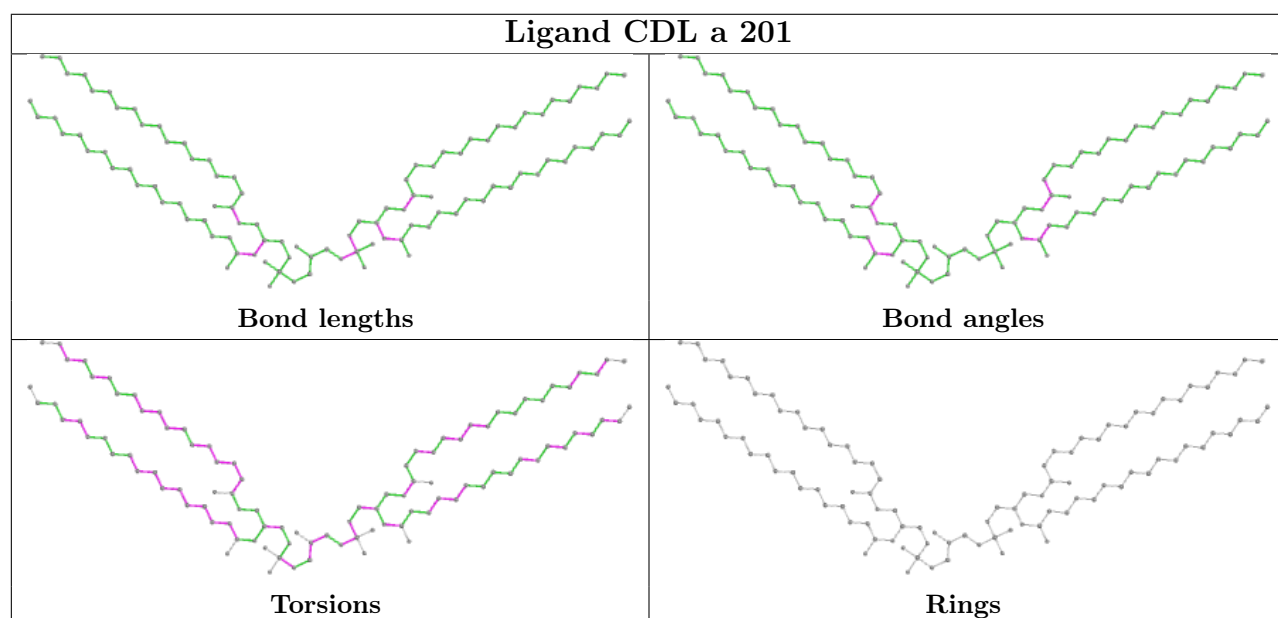
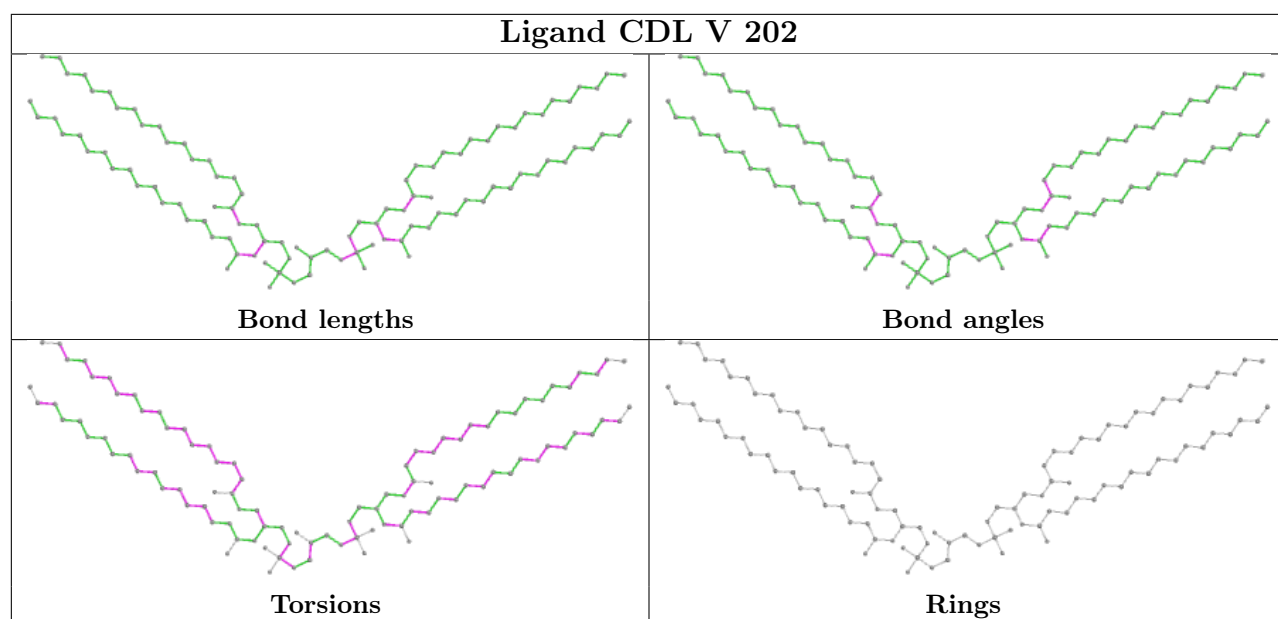


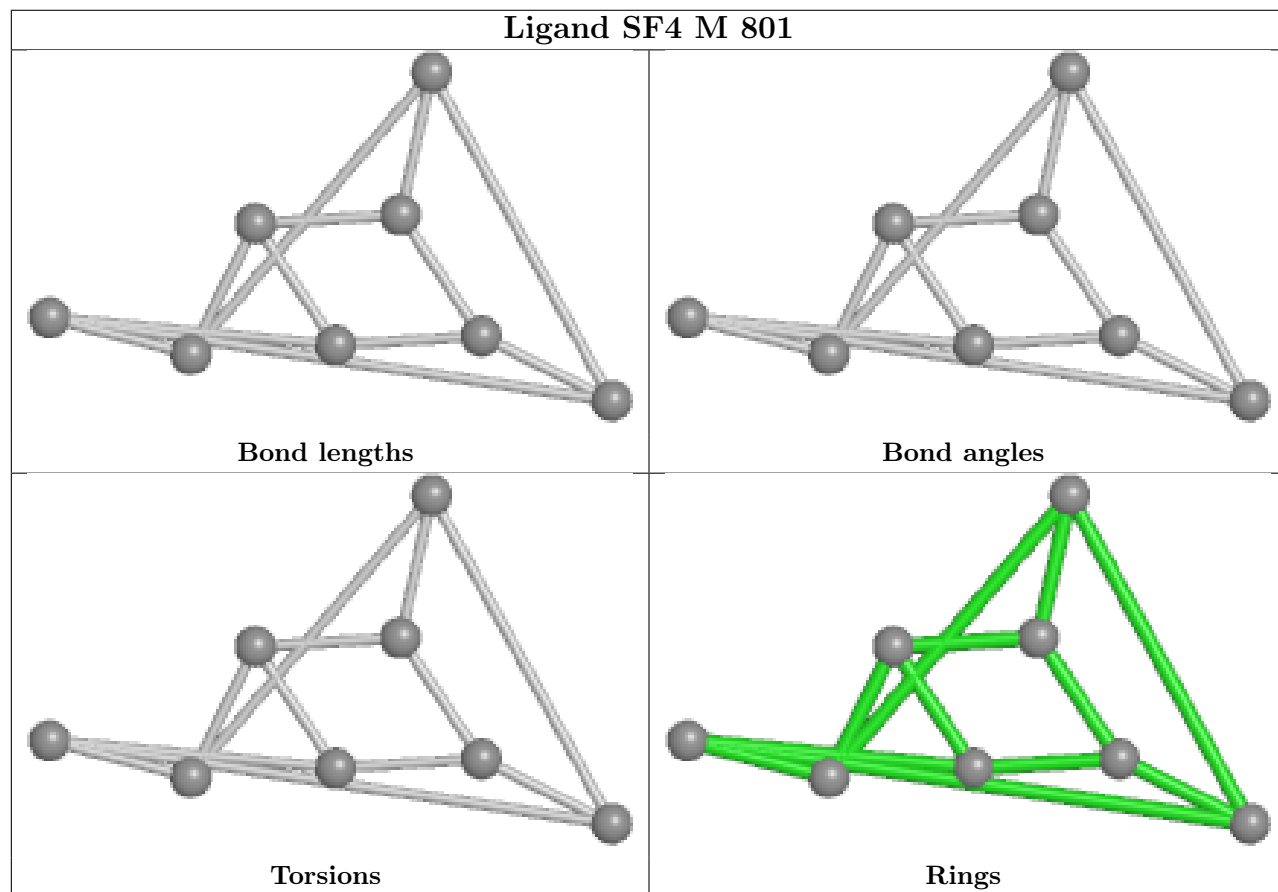
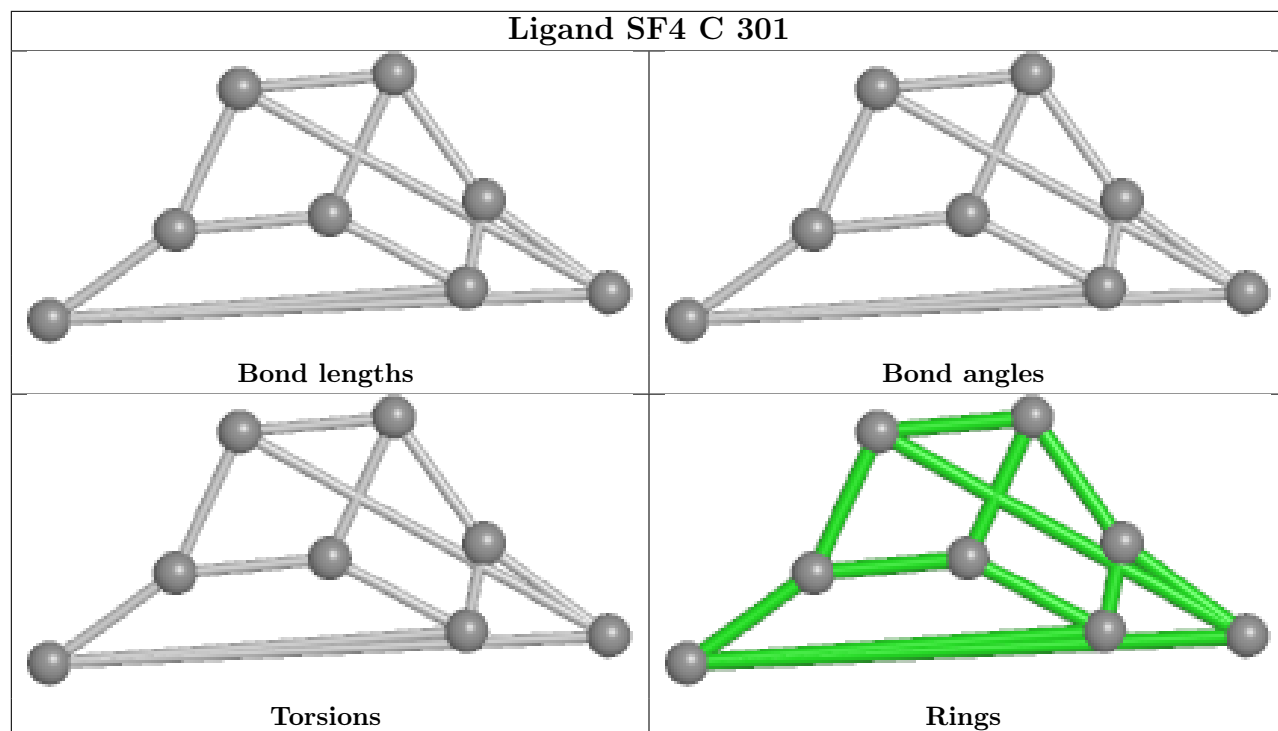


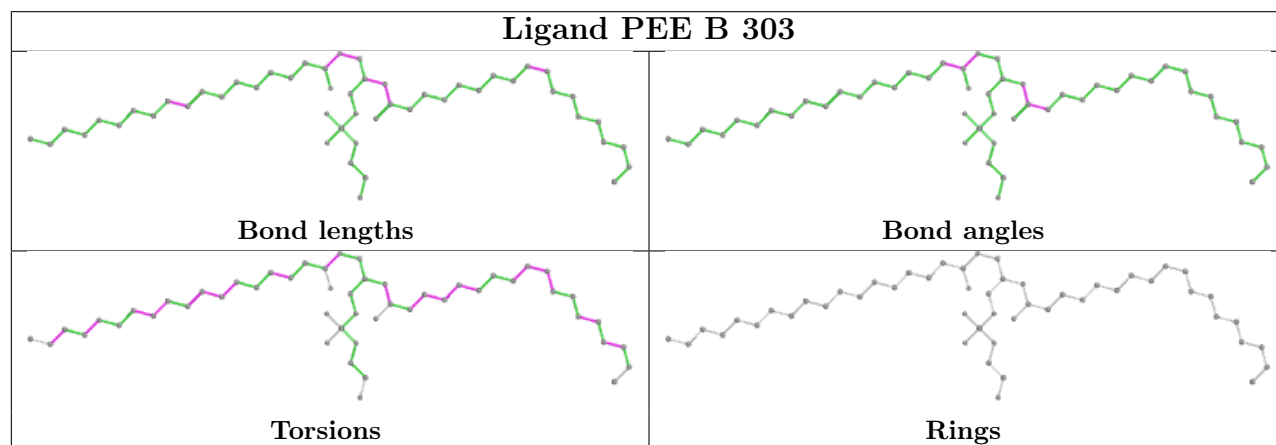
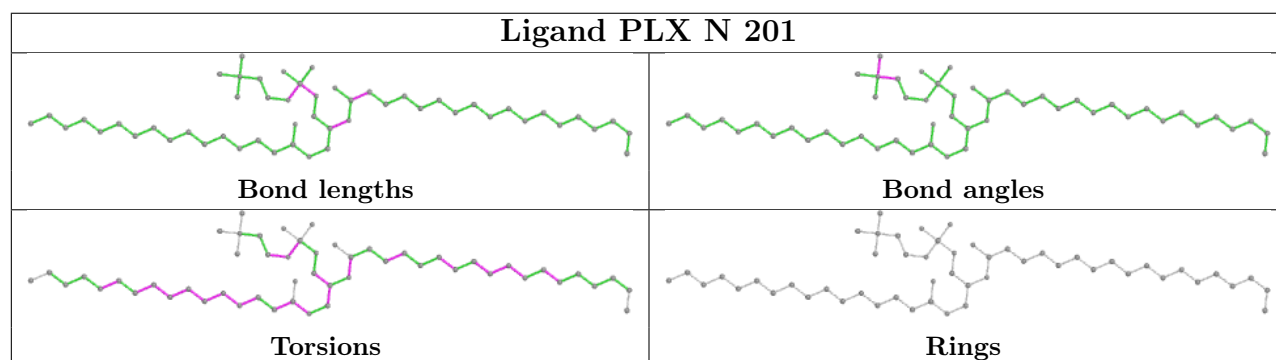
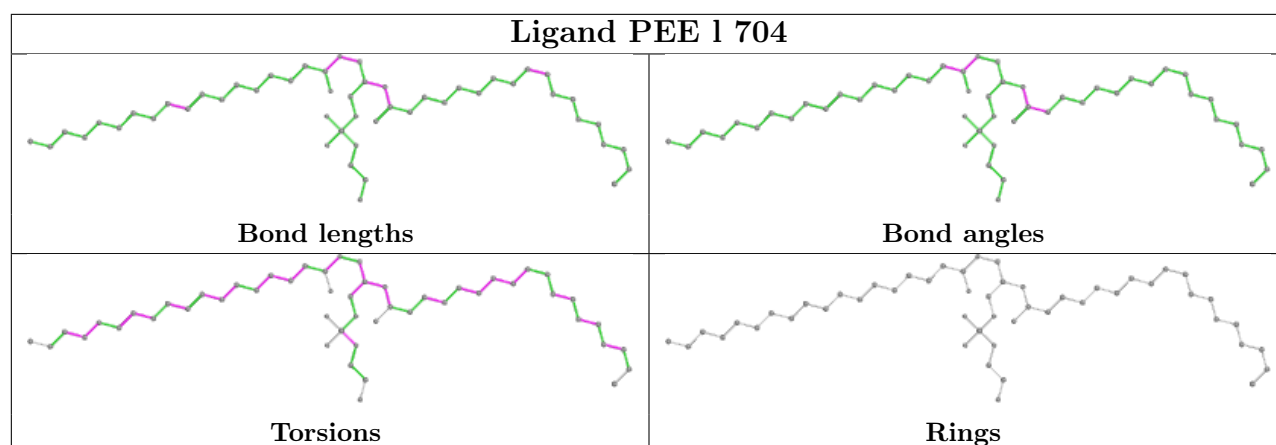


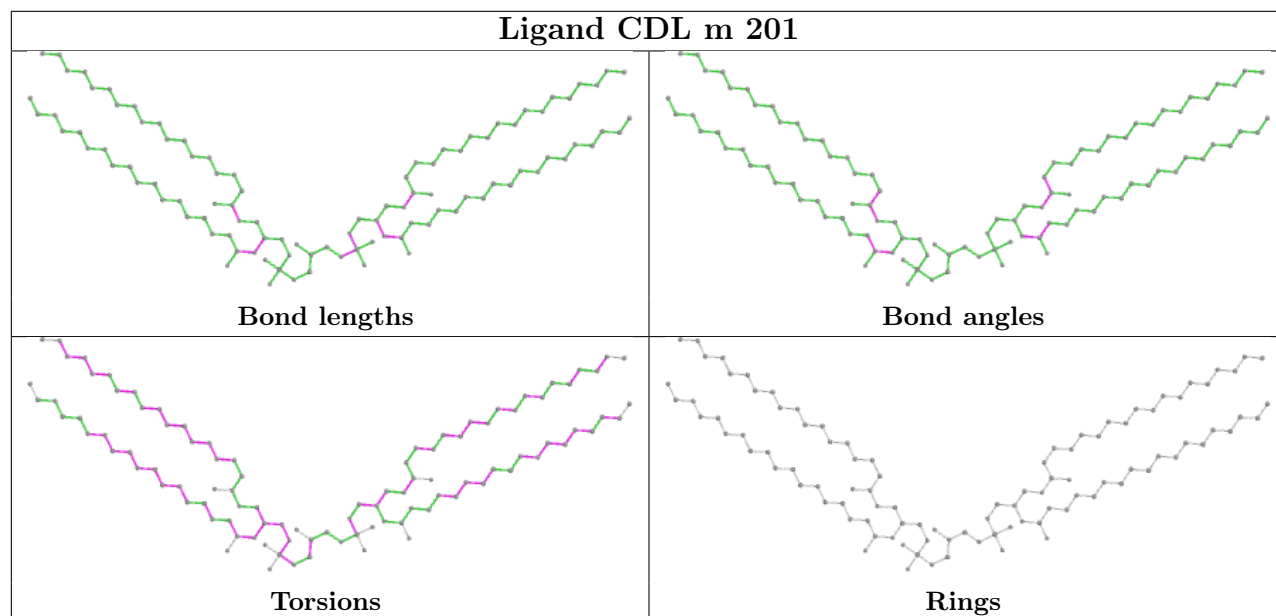












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

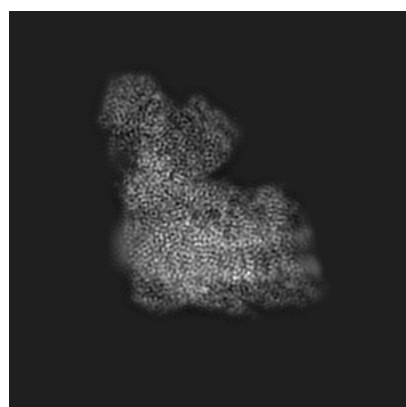
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32231. These allow visual inspection of the internal detail of the map and identification of artifacts.

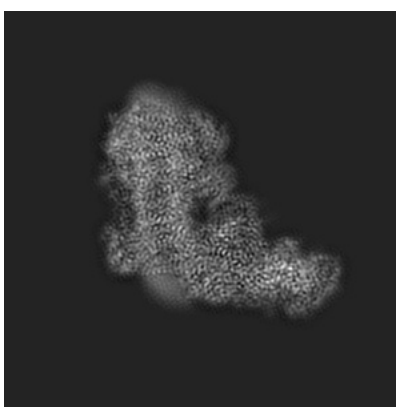
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

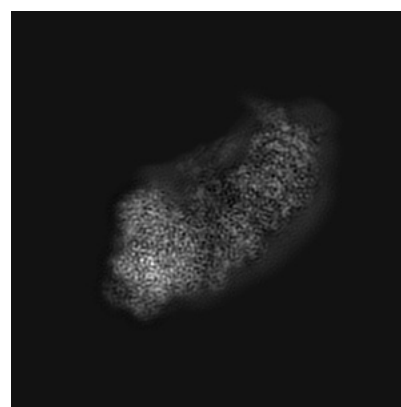
#### 6.1.1 Primary map



X



Y

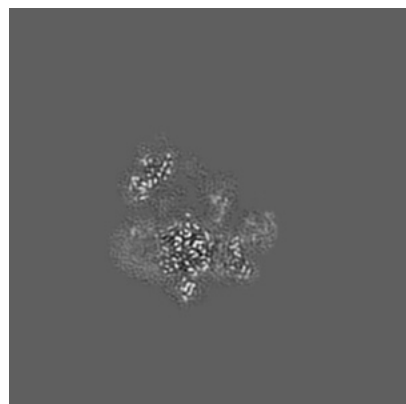


Z

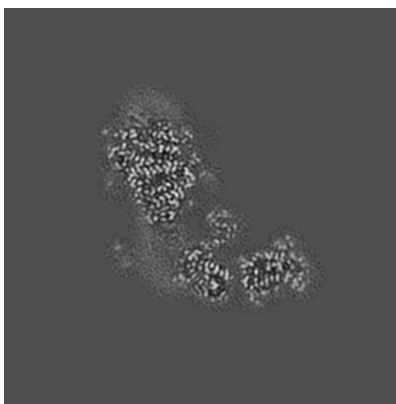
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

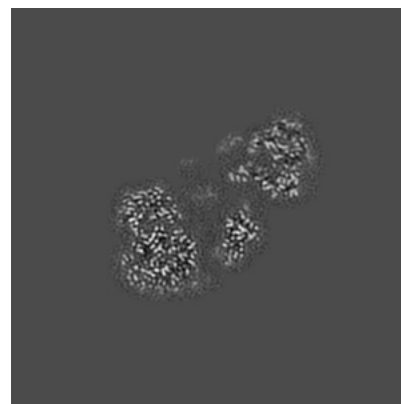
#### 6.2.1 Primary map



X Index: 165



Y Index: 165

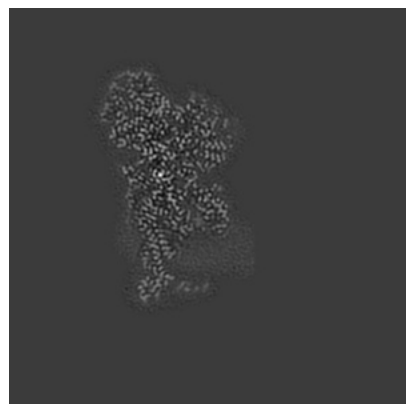


Z Index: 165

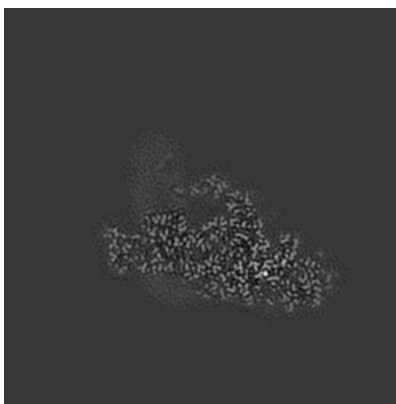
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

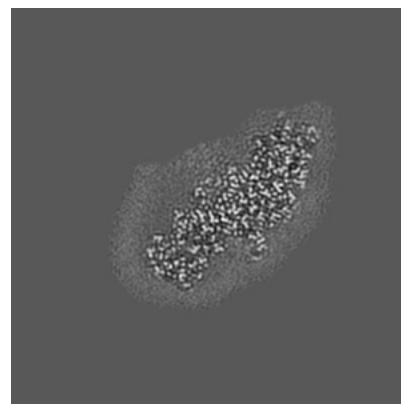
### 6.3.1 Primary map



X Index: 115



Y Index: 120



Z Index: 136

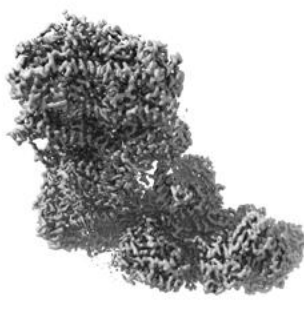
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.0219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

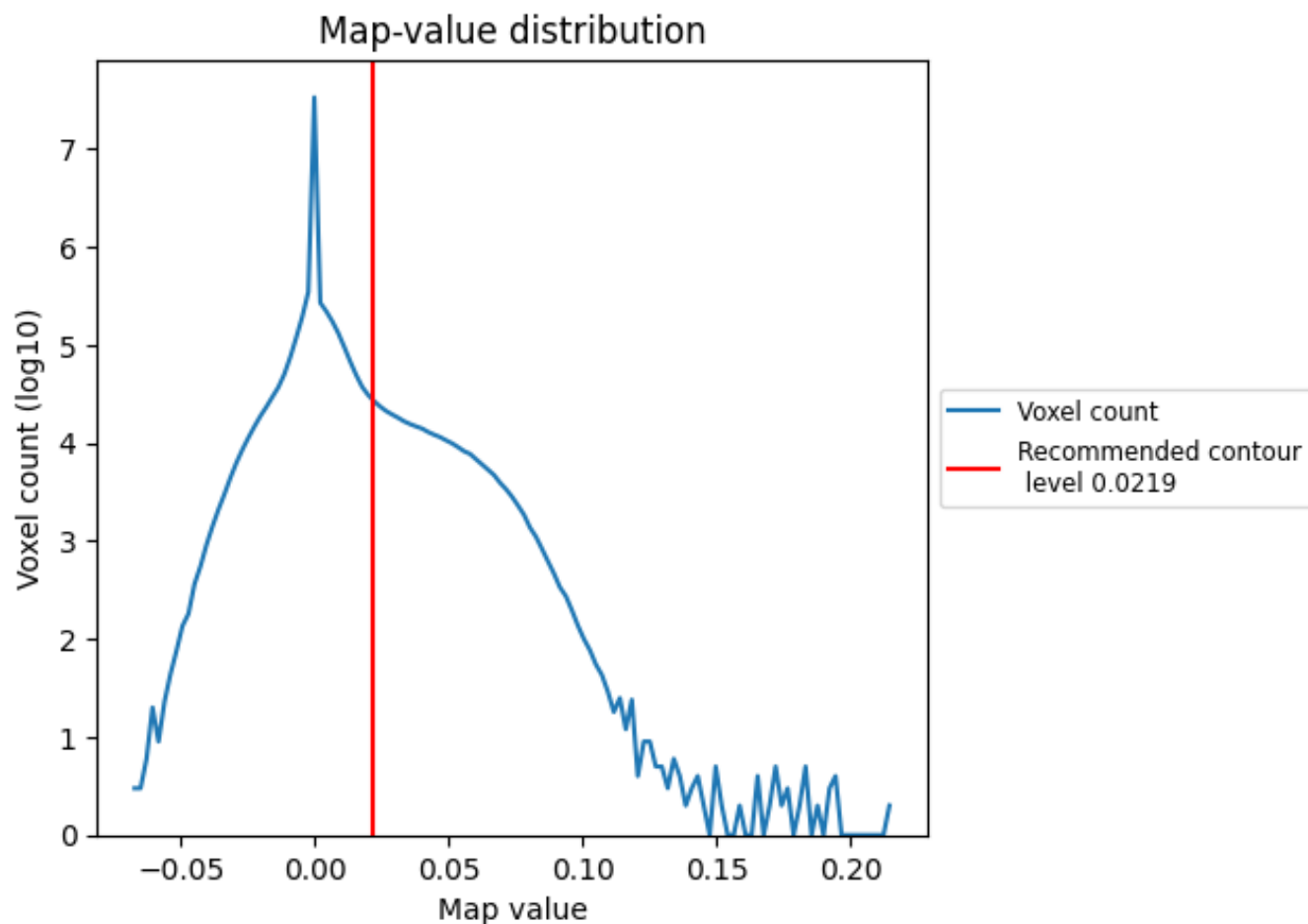
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

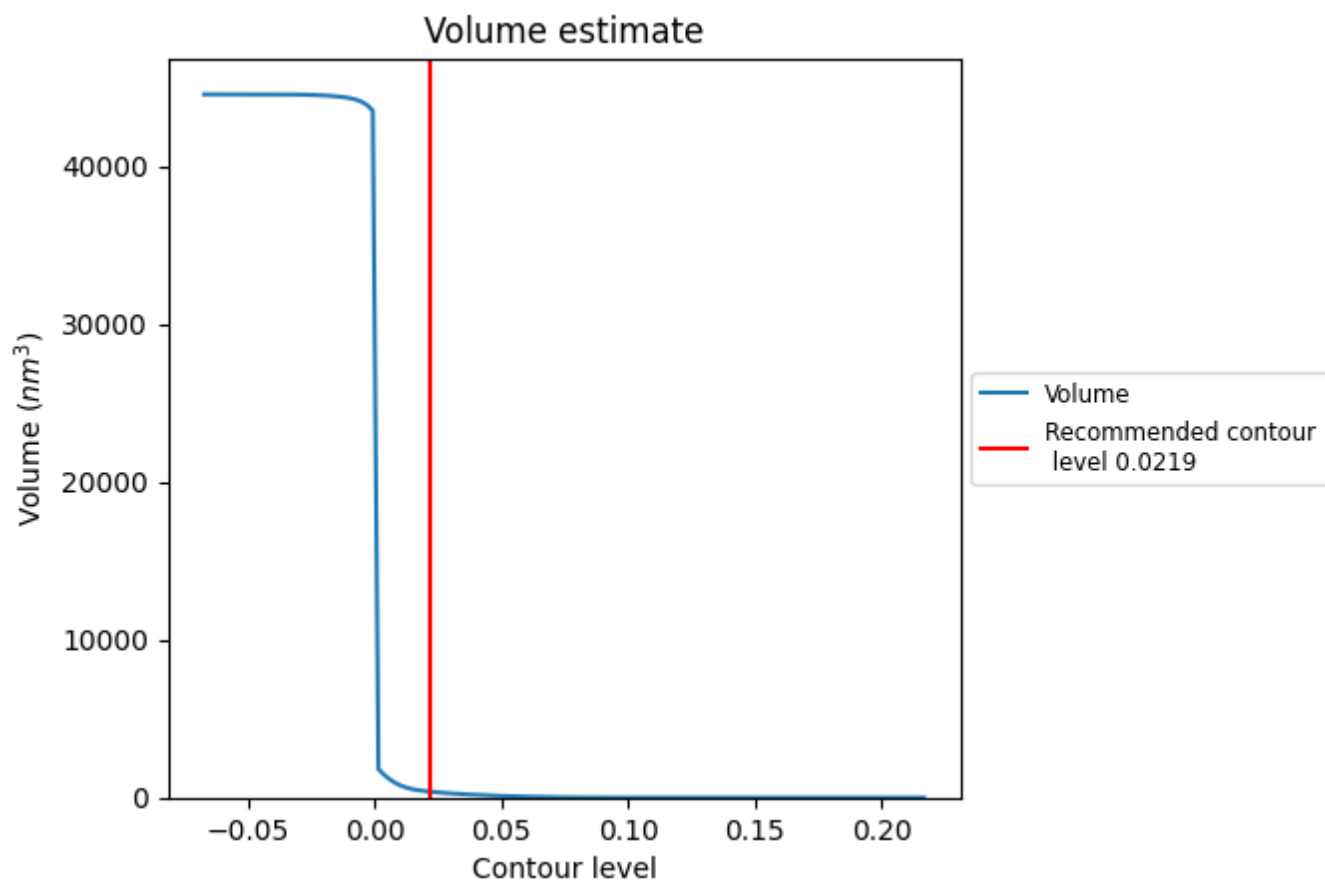
This section contains the results of statistical analysis of the map.

### 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.

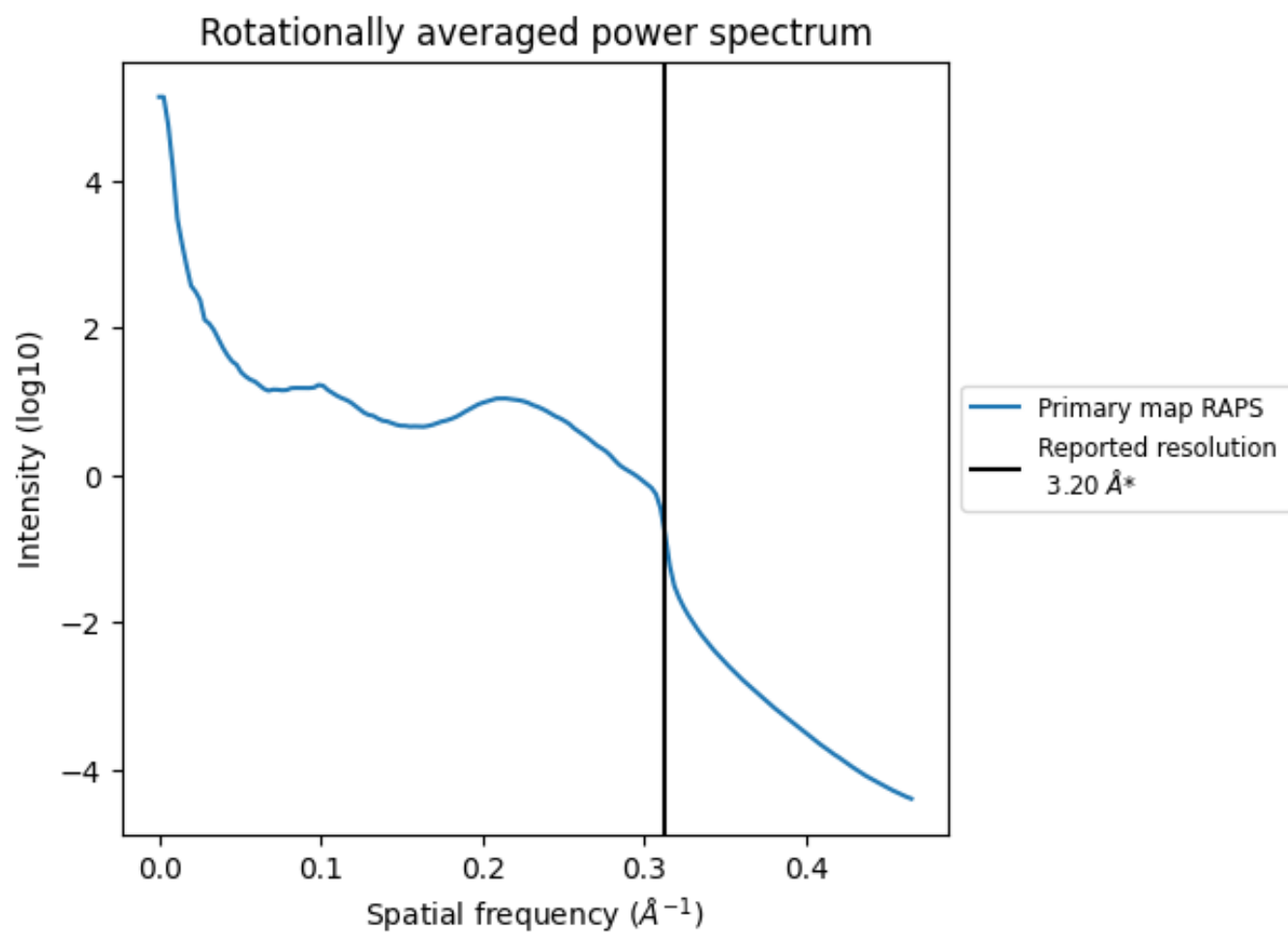
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 369  $\text{nm}^3$ ; this corresponds to an approximate mass of 333 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

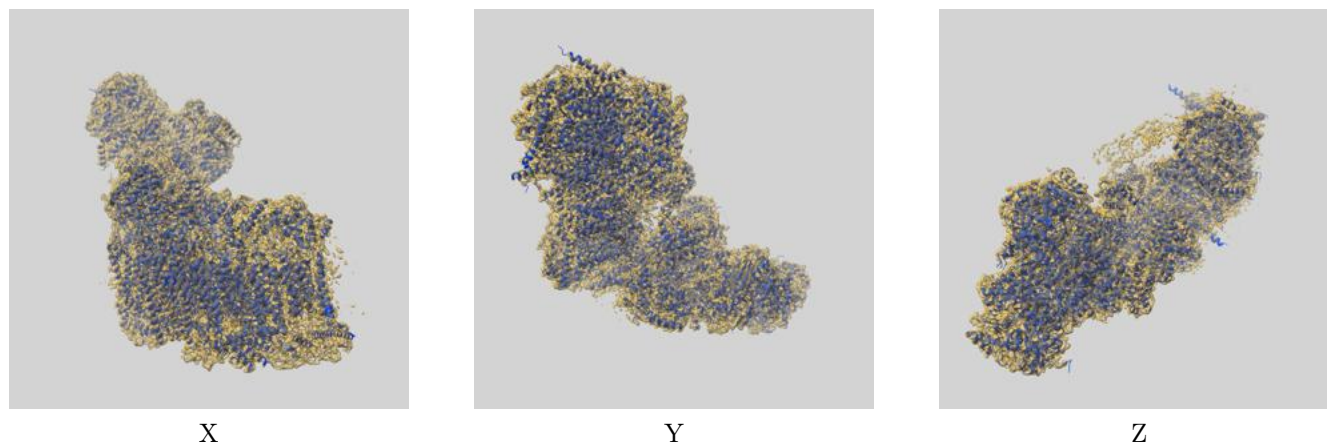
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

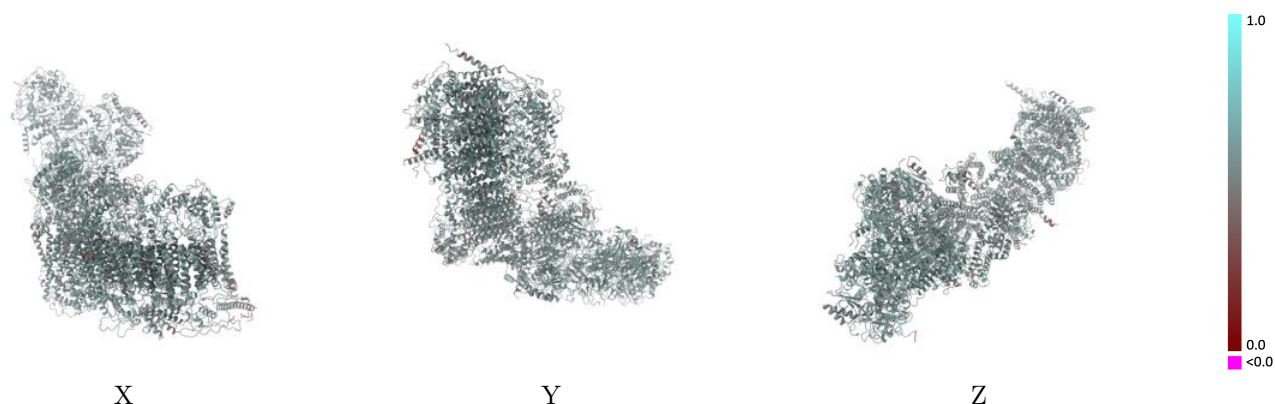
This section contains information regarding the fit between EMDB map EMD-32231 and PDB model 7VZW. Per-residue inclusion information can be found in section [3](#) on page [20](#).

### 9.1 Map-model overlay [i](#)



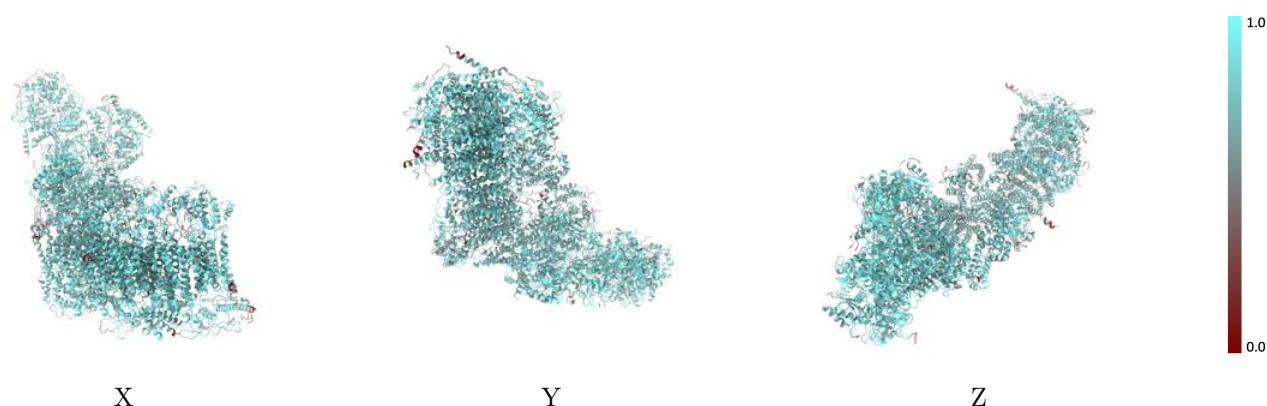
The images above show the 3D surface view of the map at the recommended contour level 0.0219 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



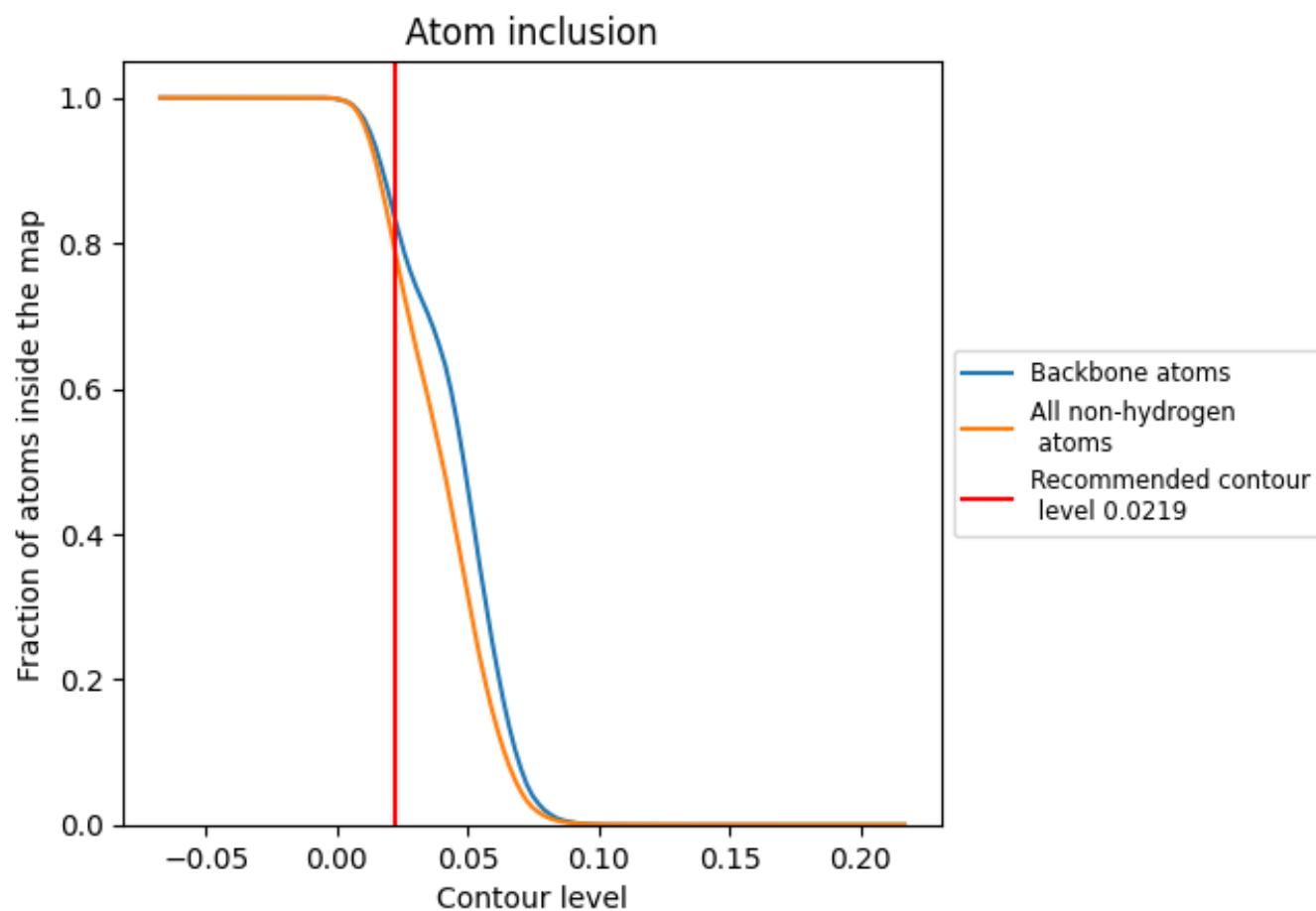
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0219).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.0219) and Q-score for the entire model and for each chain.























Chain	Atom inclusion	Q-score
All	 0.7925	 0.5560
A	 0.8092	 0.5550
B	 0.8757	 0.5770
C	 0.8204	 0.5770
E	 0.7941	 0.5580
F	 0.7470	 0.5250
G	 0.6064	 0.4690
H	 0.8000	 0.5550
I	 0.6691	 0.5400
J	 0.8226	 0.5670
K	 0.7662	 0.5480
L	 0.8018	 0.5690
M	 0.8319	 0.5670
N	 0.6993	 0.5500
O	 0.7988	 0.5510
P	 0.8655	 0.5840
Q	 0.8441	 0.5780
S	 0.8370	 0.5610
T	 0.7784	 0.5660
U	 0.7471	 0.5470
V	 0.6887	 0.5340
W	 0.7800	 0.5530
X	 0.7358	 0.5300
Y	 0.7381	 0.5210
Z	 0.6624	 0.5100
a	 0.8013	 0.5640
b	 0.7557	 0.5340
c	 0.7834	 0.5500
d	 0.7647	 0.5350
e	 0.7553	 0.5430
f	 0.6676	 0.5220
g	 0.8022	 0.5610
h	 0.7742	 0.5400
i	 0.8396	 0.5670
j	 0.7493	 0.5570



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Chain	Atom inclusion	Q-score
k	 0.8315	 0.5700
l	 0.7838	 0.5550
m	 0.7347	 0.5330
n	 0.6515	 0.5200
o	 0.7687	 0.5480
p	 0.8039	 0.5530
r	 0.8166	 0.5680
s	 0.8205	 0.5640
u	 0.8031	 0.5530
v	 0.7573	 0.5280
w	 0.7819	 0.5470