



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2023 – 10:35 AM JST

PDB ID : 7W00  
EMDB ID : EMD-32232  
Title : Deactive state CI from Q10 dataset, Subclass 1  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-11-17  
Resolution : 3.50 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:

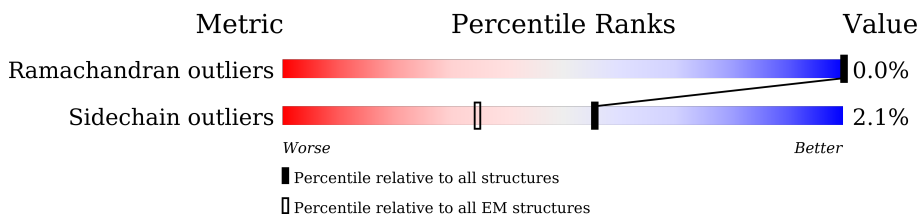
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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




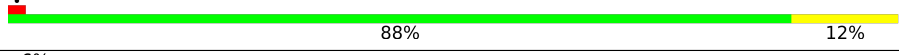
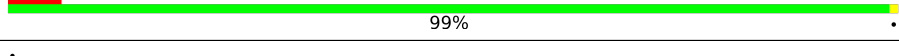
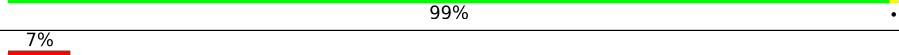
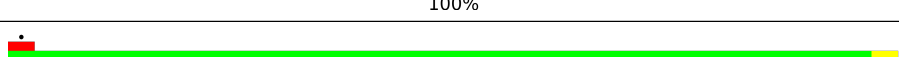
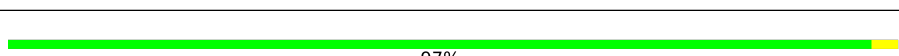
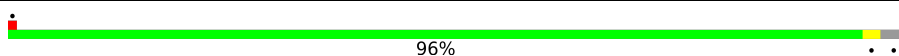
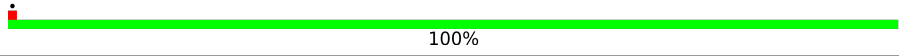
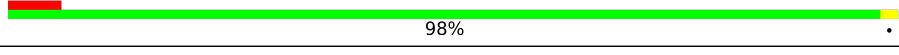
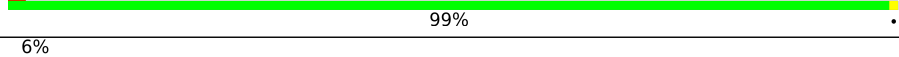
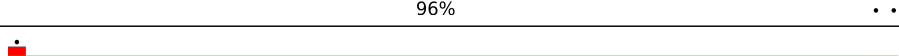
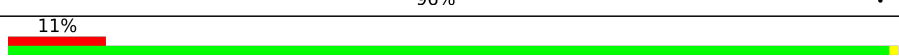
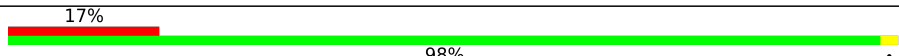
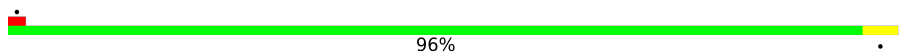

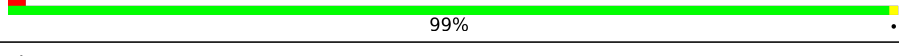
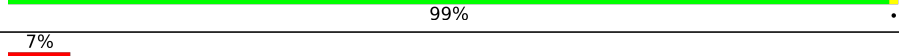
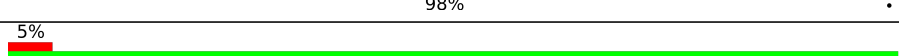
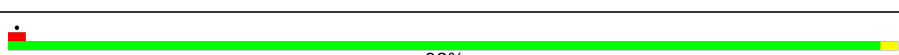
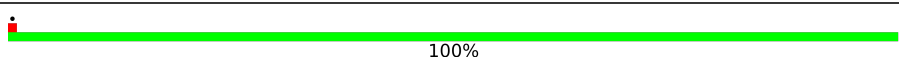
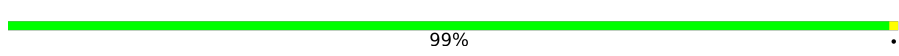




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	431	99% .
2	B	176	99% .
3	C	156	96% .
4	E	115	6% 97% .
5	F	86	6% 98% .
6	G	88	19% 99% .
6	X	88	6% 98% .
7	H	112	97% .
8	I	112	5% 84% . 13%

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Mol	Chain	Length	Quality of chain
9	J	341	 85% 13%
10	K	42	 88% 12%
11	L	125	 99% 6%
12	M	690	 99%
13	N	144	 100% 7%
14	O	217	 97%
15	P	208	 97%
16	Q	430	 96%
17	S	70	 100%
18	T	96	 98% 6%
19	U	83	 99%
20	V	140	 96% 6%
21	W	142	 96%
22	Y	70	 99% 11%
23	Z	84	 98% 17%
24	a	140	 96%
25	b	126	 79% 18% 8%
26	c	156	 99%
27	d	175	 99%
28	e	107	 98% 7%
29	f	42	 100% 5%
30	g	121	 98%
31	h	105	 100%
32	i	347	 99%
33	j	113	 84% 12% 6%

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Mol	Chain	Length	Quality of chain
34	k	98	 98%
35	l	603	 98%
36	m	175	 5% 71% 26%
37	n	56	 14% 98%
38	o	128	 96%
39	p	178	 98%
40	r	459	 99%
41	s	318	 94% 5%
42	u	171	 97%
43	v	124	 9% 95% 5%
44	w	320	 99%

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 66775 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3315	2094	591	610	20	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	967	617	179	166	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	687	432	128	125	2	0	0

- 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
			678	438	102	133	5		
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2348	1508	420	412	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5293	3319	923	1012	39		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1661	1060	279	312	10	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	419	3377	2162	578	613	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	567	364	104	94	5	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			875	571	158	145	1		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	156	1299	843	211	237	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	107	890	568	145	173	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	42	344	227	58	59	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	99	797	544	117	131	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4783	3172	741	819	51	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3630	2412	572	608	38	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	303	2390	1605	369	395	21	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2581	1645	437	489	10	0	0

- 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).



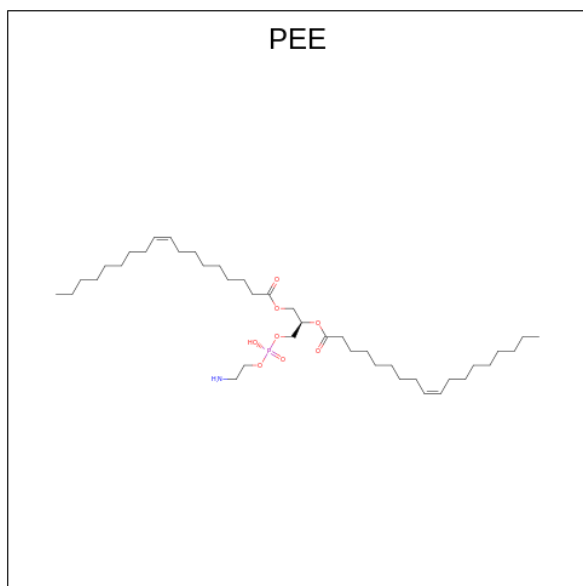
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



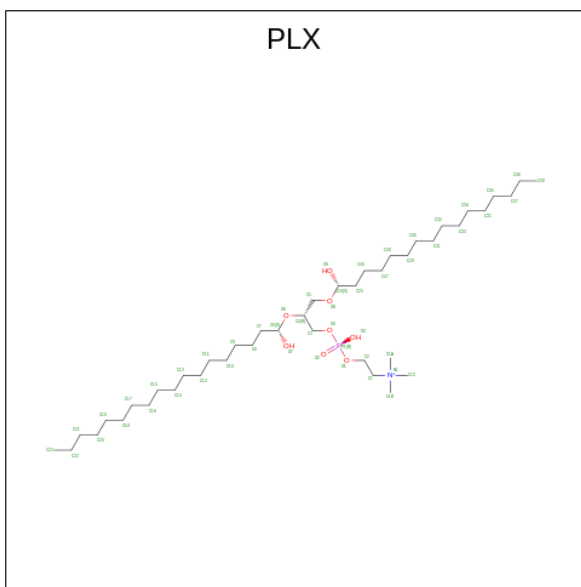
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	B	1	51	41	1	8	1	0
47	C	1	47	37	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	W	1	Total 41	C 31	N 1	O 8	P 1	0
47	b	1	Total 46	C 36	N 1	O 8	P 1	0
47	i	1	Total 47	C 37	N 1	O 8	P 1	0
47	j	1	Total 51	C 41	N 1	O 8	P 1	0
47	l	1	Total 40	C 30	N 1	O 8	P 1	0
47	l	1	Total 46	C 36	N 1	O 8	P 1	0
47	r	1	Total 51	C 41	N 1	O 8	P 1	0

- 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).



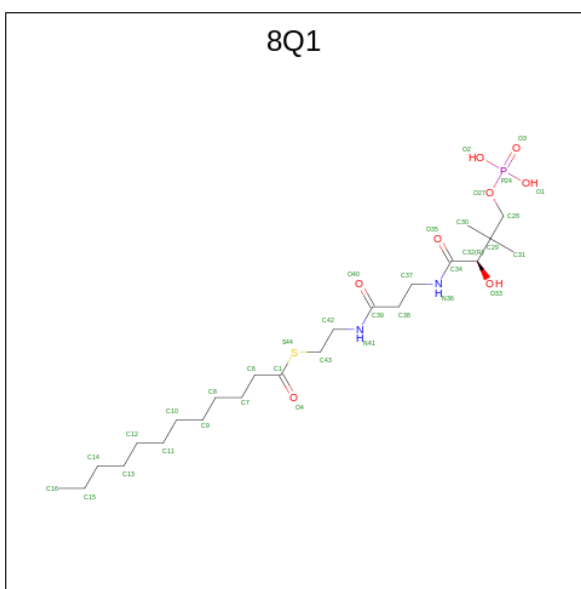
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	C	1	Total 52	C 42	N 1	O 8	P 1	0
48	a	1	Total 52	C 42	N 1	O 8	P 1	0
48	g	1	Total 52	C 42	N 1	O 8	P 1	0

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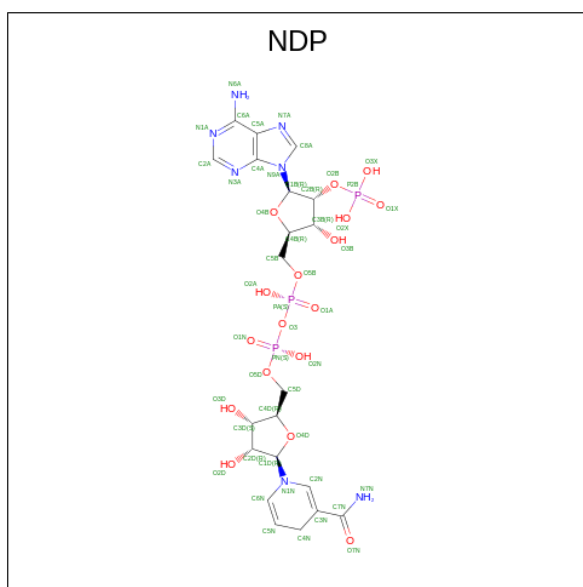
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)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).



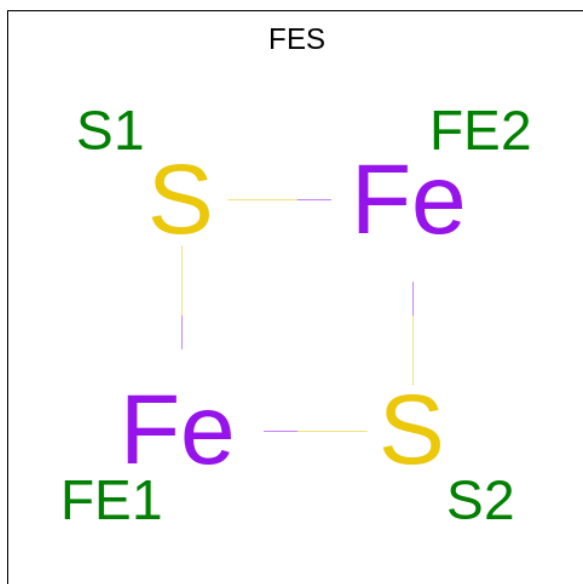
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<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).



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

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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



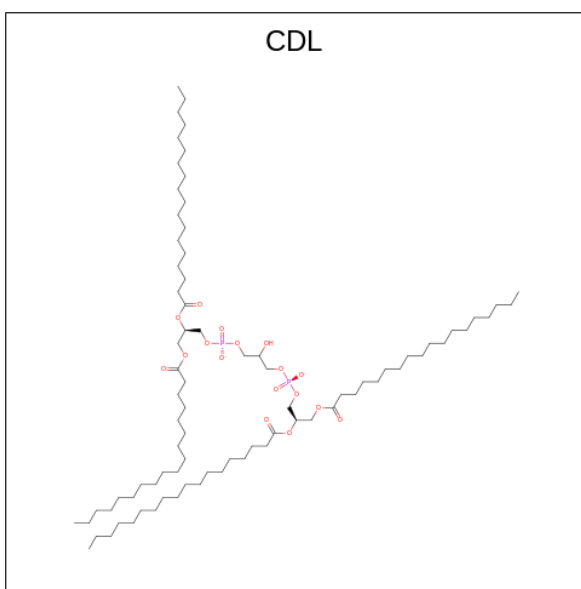
- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



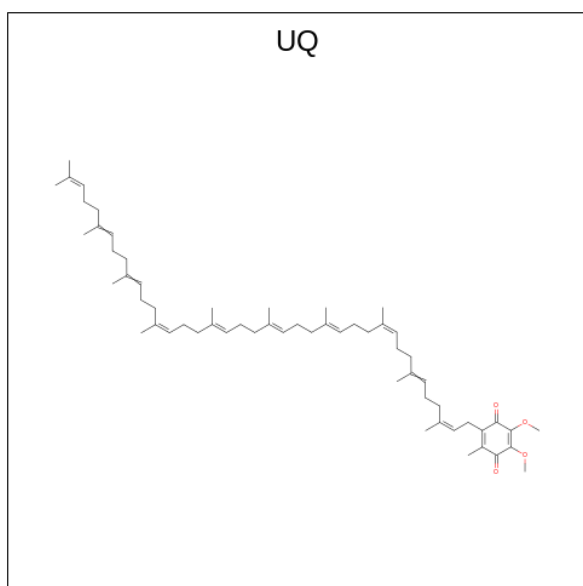
Mol	Chain	Residues	Atoms	AltConf
54	V	1	Total C O P 94 75 17 2	0
54	a	1	Total C O P 91 72 17 2	0
54	i	1	Total C O P 66 47 17 2	0
54	l	1	Total C O P 99 80 17 2	0
54	l	1	Total C O P 100 81 17 2	0

*Continued on next page...*

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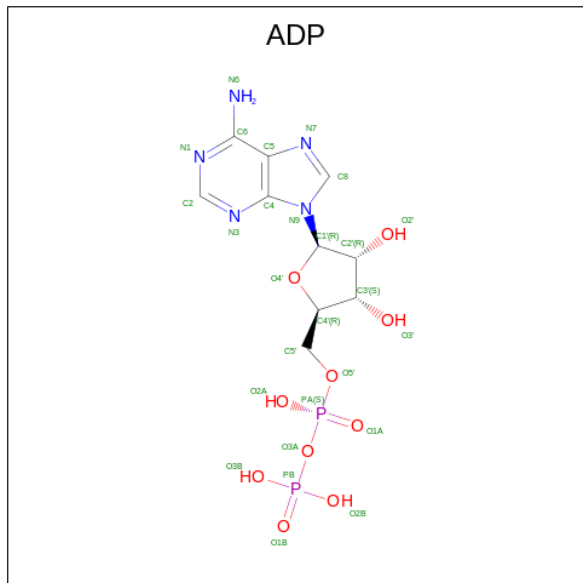
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
54	o	1	68	49	17	2	0
54	r	1	95	76	17	2	0
54	u	1	78	59	17	2	0

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

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

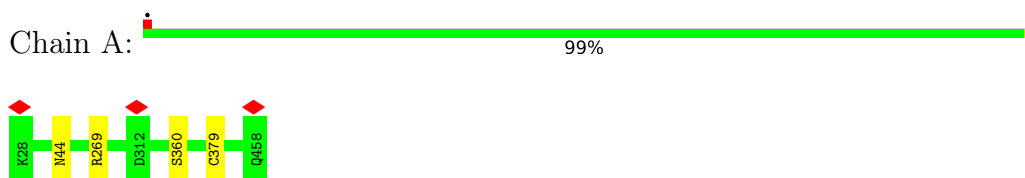


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	w	1	27	10	5	10	2	0

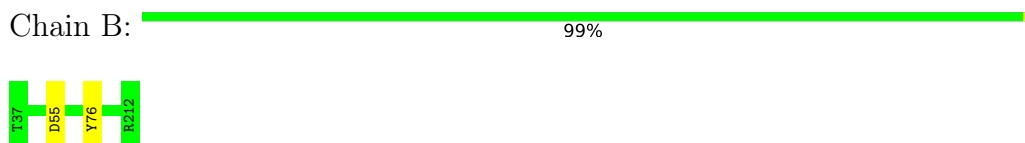
### 3 Residue-property plots [i](#)

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.

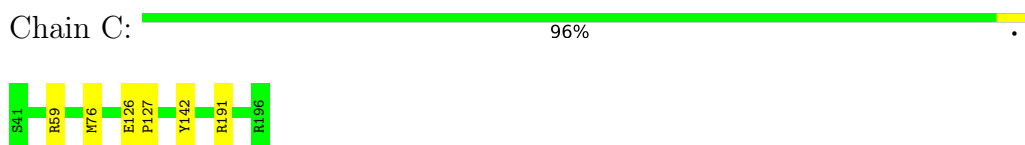
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



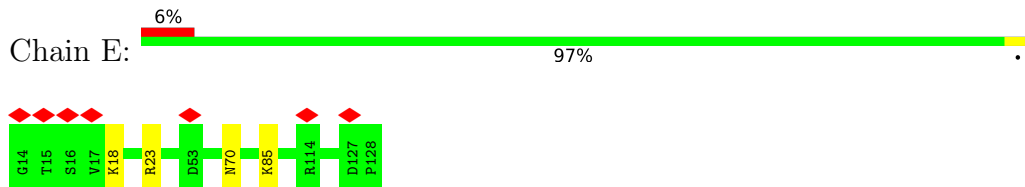
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



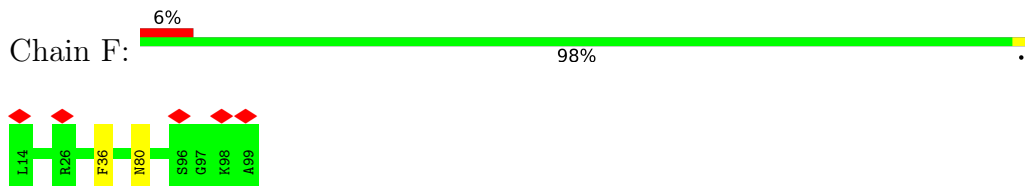
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



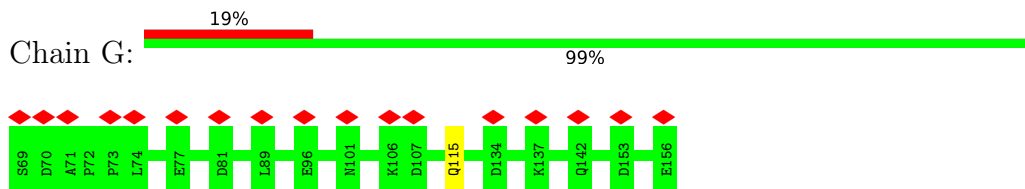
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



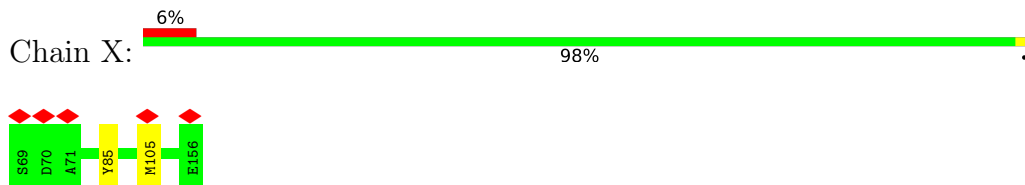
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



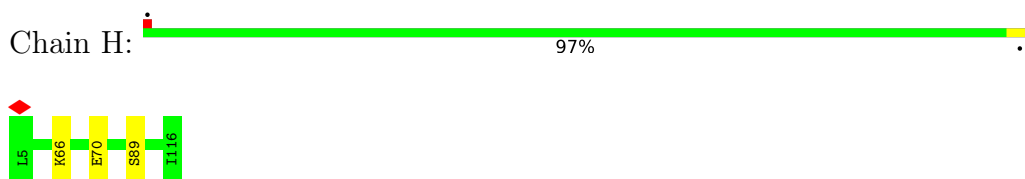
- Molecule 6: Acyl carrier protein



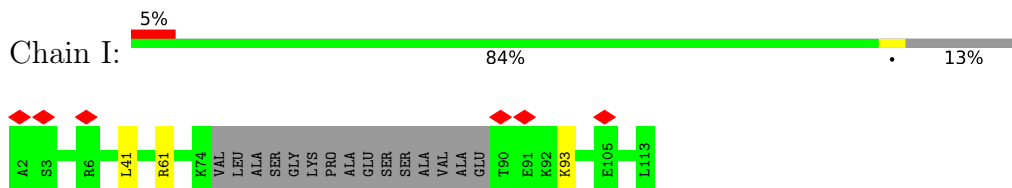
- Molecule 6: Acyl carrier protein



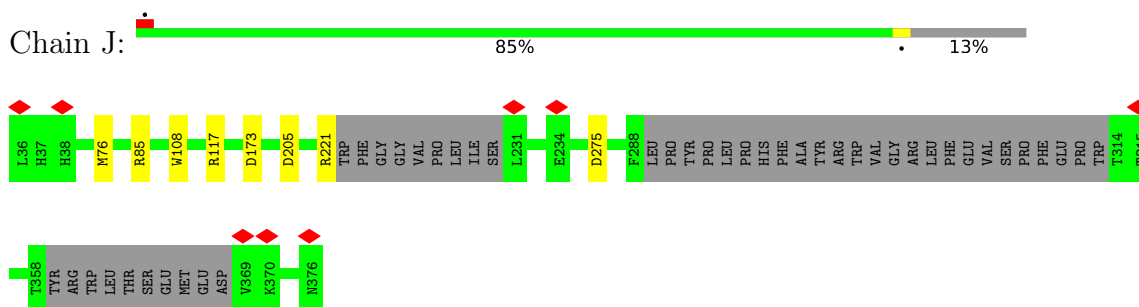
- Molecule 7: Complex I subunit B13



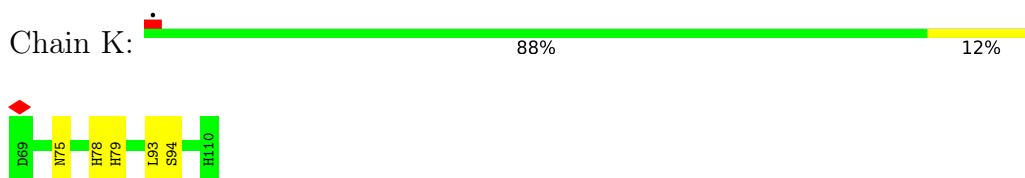
- Molecule 8: Complex I-B14.5a



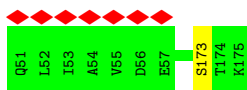
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



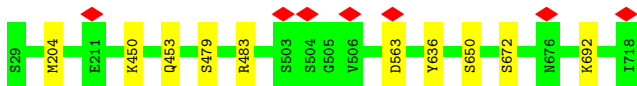
- Molecule 10: Complex I-9kD



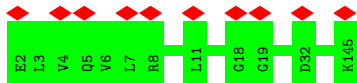
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



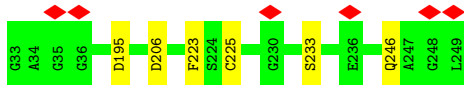
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



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



- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD

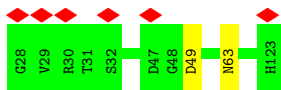


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

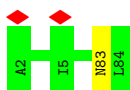




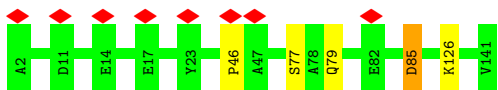
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



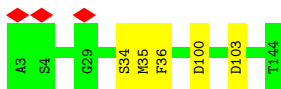
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



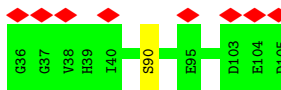
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



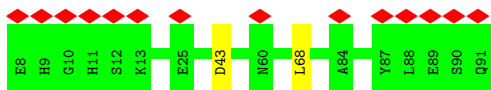
- Molecule 21: Complex I-B16.6



- Molecule 22: Complex I-AGGG



- Molecule 23: Complex I-B12




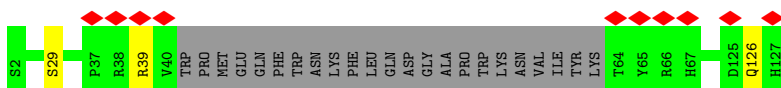
- Molecule 24: Complex I-SGDH

Chain a:  96%



- Molecule 25: Complex I-B17

Chain b:  8% 79% 18%



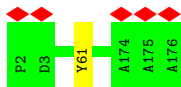
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  99%



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

Chain d:  99%



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

Chain e:  7% 98%



- Molecule 29: Complex I-KFYI

Chain f:  5% 100%



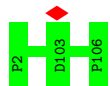
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  98%





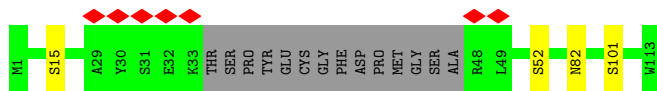
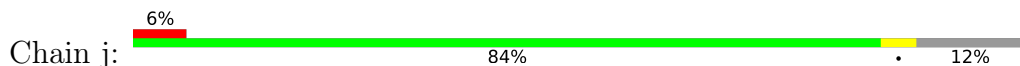
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



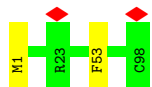
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



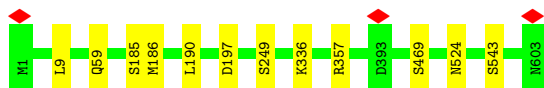
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



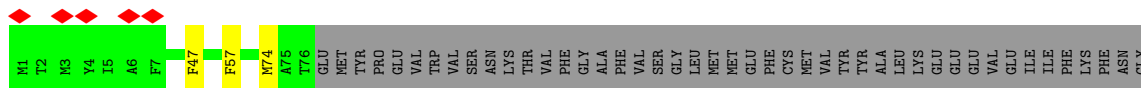
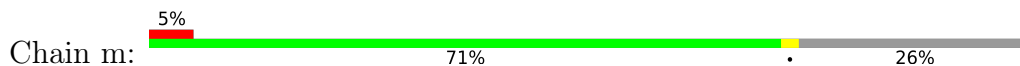
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

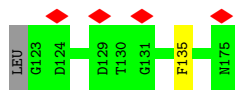


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

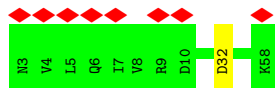


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6





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



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



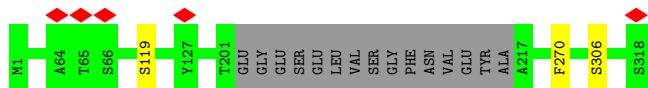
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



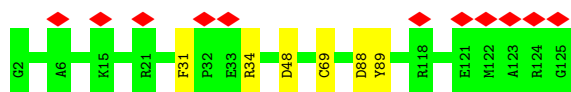
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



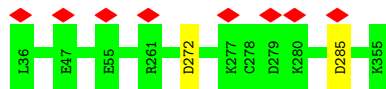
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88543	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	0.256	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0204	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.25	0/3390	0.49	0/4580
2	B	0.26	0/1443	0.51	0/1952
3	C	0.26	0/1279	0.61	1/1730 (0.1%)
4	E	0.26	0/991	0.55	0/1335
5	F	0.26	0/698	0.59	0/940
6	G	0.26	0/689	0.52	0/935
6	X	0.25	0/711	0.42	0/963
7	H	0.24	0/929	0.44	0/1258
8	I	0.25	0/798	0.53	0/1079
9	J	0.25	0/2400	0.49	0/3241
10	K	0.24	0/365	0.57	1/493 (0.2%)
11	L	0.25	0/1039	0.51	0/1403
12	M	0.25	0/5381	0.50	0/7291
13	N	0.25	0/1245	0.49	0/1694
14	O	0.25	0/1701	0.46	0/2316
15	P	0.26	0/1789	0.50	0/2436
16	Q	0.26	0/3451	0.48	0/4672
17	S	0.25	0/582	0.48	0/783
18	T	0.25	0/755	0.51	0/1018
19	U	0.25	0/664	0.43	0/912
20	V	0.26	0/1042	0.48	1/1411 (0.1%)
21	W	0.25	0/1198	0.49	0/1617
22	Y	0.25	0/623	0.45	0/853
23	Z	0.26	0/695	0.54	1/939 (0.1%)
24	a	0.27	0/1199	0.48	0/1623
25	b	0.26	0/902	0.53	0/1227
26	c	0.27	0/1355	0.48	0/1857
27	d	0.26	0/1494	0.51	0/2015
28	e	0.25	0/916	0.49	0/1246
29	f	0.24	0/353	0.41	0/477
30	g	0.26	0/1031	0.49	1/1394 (0.1%)
31	h	0.25	0/889	0.48	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.25	0/2773	0.45	0/3768
33	j	0.26	0/816	0.48	0/1113
34	k	0.26	0/759	0.44	0/1029
35	l	0.26	0/4912	0.45	0/6680
36	m	0.27	0/973	0.48	0/1320
37	n	0.24	0/491	0.50	0/663
38	o	0.27	0/1092	0.53	1/1481 (0.1%)
39	p	0.27	0/1590	0.53	0/2155
40	r	0.25	0/3722	0.44	0/5077
41	s	0.26	0/2460	0.46	0/3364
42	u	0.25	0/1436	0.49	1/1938 (0.1%)
43	v	0.28	0/1052	0.58	0/1411
44	w	0.26	0/2641	0.47	0/3577
All	All	0.26	0/66714	0.49	7/90456 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	126	GLU	C-N-CD	-12.02	94.16	120.60
10	K	93	LEU	CA-CB-CG	5.95	128.99	115.30
23	Z	43	ASP	CB-CG-OD1	5.53	123.28	118.30
20	V	85	ASP	CB-CG-OD1	5.46	123.22	118.30
38	o	84	PRO	CA-N-CD	-5.39	103.95	111.50
42	u	134	ASP	CB-CG-OD1	5.19	122.97	118.30
30	g	47	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	417 (97%)	12 (3%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	5 (3%)	1 (1%)	25	64
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	280 (97%)	9 (3%)	0	100	100
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	669 (97%)	19 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	399 (97%)	13 (3%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	61
21	W	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
24	a	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
25	b	99/126 (79%)	97 (98%)	2 (2%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
33	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
36	m	125/175 (71%)	113 (90%)	12 (10%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	168 (96%)	7 (4%)	1 (1%)	25	64
40	r	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
41	s	299/318 (94%)	289 (97%)	10 (3%)	0	100	100
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%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8308 (97%)	7721 (96%)	305 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	127	PRO
39	p	175	ARG
20	V	46	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/345 (100%)	340 (99%)	4 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	86
3	C	132/132 (100%)	128 (97%)	4 (3%)	41	71
4	E	106/107 (99%)	102 (96%)	4 (4%)	33	65
5	F	75/76 (99%)	73 (97%)	2 (3%)	44	73
6	G	72/81 (89%)	71 (99%)	1 (1%)	67	85
6	X	78/81 (96%)	76 (97%)	2 (3%)	46	74
7	H	99/99 (100%)	96 (97%)	3 (3%)	41	71
8	I	87/97 (90%)	84 (97%)	3 (3%)	37	68
9	J	252/295 (85%)	244 (97%)	8 (3%)	39	69
10	K	41/41 (100%)	37 (90%)	4 (10%)	8	33
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	90
12	M	579/580 (100%)	569 (98%)	10 (2%)	60	82
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	180/183 (98%)	174 (97%)	6 (3%)	38	68
15	P	190/190 (100%)	183 (96%)	7 (4%)	34	65
16	Q	361/370 (98%)	355 (98%)	6 (2%)	60	82
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	77 (98%)	2 (2%)	47	75
19	U	69/69 (100%)	68 (99%)	1 (1%)	67	85
20	V	101/101 (100%)	97 (96%)	4 (4%)	31	64
21	W	122/123 (99%)	117 (96%)	5 (4%)	30	63
22	Y	62/63 (98%)	61 (98%)	1 (2%)	62	83
23	Z	65/65 (100%)	64 (98%)	1 (2%)	65	84
24	a	122/122 (100%)	117 (96%)	5 (4%)	30	63
25	b	97/119 (82%)	94 (97%)	3 (3%)	40	70
26	c	137/141 (97%)	136 (99%)	1 (1%)	84	93
27	d	155/155 (100%)	154 (99%)	1 (1%)	86	94
28	e	99/99 (100%)	97 (98%)	2 (2%)	55	79
29	f	36/38 (95%)	36 (100%)	0	100	100
30	g	108/108 (100%)	106 (98%)	2 (2%)	57	80
31	h	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	311/311 (100%)	307 (99%)	4 (1%)	69	86
33	j	87/99 (88%)	83 (95%)	4 (5%)	27	61
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	76
35	l	536/537 (100%)	524 (98%)	12 (2%)	52	78
36	m	99/141 (70%)	95 (96%)	4 (4%)	31	64
37	n	53/53 (100%)	52 (98%)	1 (2%)	57	80
38	o	113/113 (100%)	109 (96%)	4 (4%)	36	67
39	p	159/159 (100%)	156 (98%)	3 (2%)	57	80
40	r	409/410 (100%)	405 (99%)	4 (1%)	76	88
41	s	262/275 (95%)	259 (99%)	3 (1%)	73	88
42	u	153/153 (100%)	148 (97%)	5 (3%)	38	68
43	v	104/111 (94%)	98 (94%)	6 (6%)	20	53
44	w	281/283 (99%)	279 (99%)	2 (1%)	84	93
All	All	7045/7234 (97%)	6896 (98%)	149 (2%)	56	79

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	269	ARG
1	A	360	SER
1	A	379	CYS
2	B	55	ASP
2	B	76	TYR
3	C	59	ARG
3	C	76	MET
3	C	142	TYR
3	C	191	ARG
4	E	18	LYS
4	E	23	ARG
4	E	70	ASN
4	E	85	LYS
5	F	36	PHE
5	F	80	ASN
6	G	115	GLN
7	H	66	LYS
7	H	70	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	H	89	SER
8	I	41	LEU
8	I	61	ARG
8	I	93	LYS
9	J	76	MET
9	J	85	ARG
9	J	108	TRP
9	J	117	ARG
9	J	173	ASP
9	J	205	ASP
9	J	221	ARG
9	J	275	ASP
10	K	75	ASN
10	K	78	HIS
10	K	79	HIS
10	K	94	SER
11	L	173	SER
12	M	204	MET
12	M	450	LYS
12	M	453	GLN
12	M	479	SER
12	M	483	ARG
12	M	563	ASP
12	M	636	TYR
12	M	650	SER
12	M	672	SER
12	M	692	LYS
14	O	195	ASP
14	O	206	ASP
14	O	223	PHE
14	O	225	CYS
14	O	233	SER
14	O	246	GLN
15	P	52	ASP
15	P	82	ASN
15	P	110	SER
15	P	134	SER
15	P	161	LYS
15	P	231	ARG
15	P	236	ASN
16	Q	83	ASN
16	Q	144	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	Q	222	MET
16	Q	359	ASP
16	Q	364	SER
16	Q	439	SER
18	T	49	ASP
18	T	63	ASN
19	U	83	ASN
20	V	77	SER
20	V	79	GLN
20	V	85	ASP
20	V	126	LYS
21	W	34	SER
21	W	35	MET
21	W	36	PHE
21	W	100	ASP
21	W	103	ASP
6	X	85	TYR
6	X	105	MET
22	Y	90	SER
23	Z	68	LEU
24	a	60	SER
24	a	76	LEU
24	a	77	LEU
24	a	84	ILE
24	a	87	THR
25	b	29	SER
25	b	39	ARG
25	b	126	GLN
26	c	110	ASP
27	d	61	TYR
28	e	77	ASP
28	e	86	ASN
30	g	27	LYS
30	g	115	LEU
32	i	100	MET
32	i	146	SER
32	i	300	SER
32	i	313	MET
33	j	15	SER
33	j	52	SER
33	j	82	ASN
33	j	101	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	k	1	MET
34	k	53	PHE
35	l	9	LEU
35	l	59	GLN
35	l	185	SER
35	l	186	MET
35	l	190	LEU
35	l	197	ASP
35	l	249	SER
35	l	336	LYS
35	l	357	ARG
35	l	469	SER
35	l	524	ASN
35	l	543	SER
36	m	47	PHE
36	m	57	PHE
36	m	74	MET
36	m	135	PHE
37	n	32	ASP
38	o	24	ASP
38	o	26	SER
38	o	41	SER
38	o	87	SER
39	p	105	ASP
39	p	132	SER
39	p	176	GLU
40	r	57	PHE
40	r	248	THR
40	r	256	TYR
40	r	339	SER
41	s	119	SER
41	s	270	PHE
41	s	306	SER
42	u	48	TRP
42	u	66	CYS
42	u	99	HIS
42	u	134	ASP
42	u	157	ASP
43	v	31	PHE
43	v	34	ARG
43	v	48	ASP
43	v	69	CYS

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Mol	Chain	Res	Type
43	v	88	ASP
43	v	89	TYR
44	w	272	ASP
44	w	285	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
4	E	70	ASN
4	E	95	ASN
8	I	13	ASN
12	M	260	ASN
12	M	569	GLN
12	M	604	GLN
14	O	69	ASN
18	T	63	ASN
35	l	541	ASN
40	r	169	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	2MR	Q	118	16	10,12,13	1.93	1 (10%)	5,13,15	6.10	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.54	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	12.51	130.95	119.48
16	Q	118	2MR	CD-NE-CZ	4.47	131.79	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.92	130.32	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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
54	CDL	a	201	-	90,90,99	1.14	8 (8%)	96,102,111	0.92	4 (4%)
48	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
54	CDL	l	702	-	98,98,99	1.09	8 (8%)	104,110,111	0.89	4 (3%)
48	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
49	8Q1	G	201	6	31,34,34	1.71	6 (19%)	40,43,43	1.54	6 (15%)
54	CDL	u	201	-	77,77,99	1.21	8 (10%)	83,89,111	0.96	4 (4%)
47	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.96	2 (4%)
47	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	0.98	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
54	CDL	V	201	-	93,93,99	1.12	8 (8%)	99,105,111	0.86	4 (4%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
47	PEE	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.99	2 (4%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
55	UQ	s	401	-	28,28,63	3.28	8 (28%)	34,37,79	2.76	11 (32%)
48	PLX	g	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
51	FES	O	301	14	0,4,4	-	-	-	-	-
47	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
47	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
47	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.05	2 (4%)
54	CDL	l	703	-	99,99,99	1.10	9 (9%)	105,111,111	0.84	4 (3%)
47	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
49	8Q1	X	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.57	6 (15%)
48	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
54	CDL	r	504	-	94,94,99	1.11	9 (9%)	100,106,111	0.87	4 (4%)
54	CDL	o	201	-	67,67,99	1.26	8 (11%)	73,79,111	1.02	4 (5%)
51	FES	M	803	12	0,4,4	-	-	-	-	-
45	SF4	B	302	2	0,12,12	-	-	-	-	-
54	CDL	i	401	-	65,65,99	1.28	9 (13%)	71,77,111	1.01	4 (5%)
47	PEE	l	704	-	45,45,50	1.23	6 (13%)	48,50,55	0.99	2 (4%)
50	NDP	J	401	-	45,52,52	4.58	20 (44%)	53,80,80	1.93	7 (13%)
45	SF4	C	301	16,3	0,12,12	-	-	-	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.20	8 (16%)
56	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.44	4 (13%)
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
48	PLX	C	303	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)

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
54	CDL	a	201	-	-	47/101/101/110	-
48	PLX	a	202	-	-	22/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
54	CDL	l	702	-	-	56/109/109/110	-
48	PLX	j	202	-	-	27/55/55/55	-
49	8Q1	G	201	6	-	12/41/41/41	-
54	CDL	u	201	-	-	36/88/88/110	-
47	PEE	C	302	-	-	19/50/50/54	-
47	PEE	i	402	-	-	20/50/50/54	-
54	CDL	V	201	-	-	57/104/104/110	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PLX	r	502	-	-	24/55/55/55	-
47	PEE	W	201	-	-	19/44/44/54	-
45	SF4	M	802	12	-	-	0/6/5/5
55	UQ	s	401	-	-	10/21/45/87	0/1/1/1
48	PLX	g	201	-	-	25/55/55/55	-
51	FES	O	301	14	-	-	0/1/1/1
47	PEE	b	201	-	-	31/49/49/54	-
47	PEE	j	201	-	-	30/54/54/54	-
47	PEE	l	701	-	-	32/43/43/54	-
54	CDL	l	703	-	-	58/110/110/110	-
47	PEE	r	501	-	-	30/54/54/54	-
49	8Q1	X	201	6	-	16/41/41/41	-
48	PLX	r	503	-	-	36/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
54	CDL	r	504	-	-	58/105/105/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CDL	o	201	-	-	45/78/78/110	-
51	FES	M	803	12	-	-	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
54	CDL	i	401	-	-	37/76/76/110	-
47	PEE	l	704	-	-	22/49/49/54	-
50	NDP	J	401	-	-	6/30/77/77	0/4/5/5
45	SF4	C	301	16,3	-	-	0/6/5/5
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
56	ADP	w	401	-	-	4/12/32/32	0/3/3/3
47	PEE	B	303	-	-	23/54/54/54	-
48	PLX	C	303	-	-	26/55/55/55	-

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-13.06	1.23	1.52
50	J	401	NDP	C6N-C5N	12.36	1.55	1.33
50	J	401	NDP	O4D-C4D	10.71	1.68	1.45
50	J	401	NDP	C3D-C4D	-9.83	1.27	1.53
55	s	401	UQ	C13-C14	9.31	1.55	1.33
55	s	401	UQ	C8-C9	9.00	1.54	1.33
56	w	401	ADP	C3'-C4'	-8.83	1.30	1.53
50	J	401	NDP	O4B-C1B	8.64	1.53	1.41
55	s	401	UQ	C18-C19	8.21	1.56	1.32
50	J	401	NDP	O4B-C4B	-7.82	1.27	1.45
56	w	401	ADP	O4'-C4'	7.69	1.62	1.45
50	J	401	NDP	C2N-C3N	7.43	1.55	1.34
56	w	401	ADP	O4'-C1'	-6.96	1.31	1.41
50	J	401	NDP	P2B-O2B	5.79	1.70	1.59
49	G	201	8Q1	C34-N36	5.49	1.45	1.33
49	X	201	8Q1	C39-N41	5.43	1.45	1.33
49	X	201	8Q1	C34-N36	5.39	1.45	1.33
49	G	201	8Q1	C39-N41	5.37	1.45	1.33
50	J	401	NDP	C3B-C4B	5.32	1.66	1.53
50	J	401	NDP	O4D-C1D	-4.91	1.30	1.42
50	J	401	NDP	C6N-N1N	4.82	1.49	1.37
50	J	401	NDP	C7N-N7N	4.23	1.44	1.33
50	J	401	NDP	O2D-C2D	-4.16	1.33	1.43
50	J	401	NDP	C6A-N6A	4.12	1.49	1.34
56	w	401	ADP	C6-N6	3.86	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	502	FMN	C4A-N5	3.77	1.38	1.30
47	W	201	PEE	C18-C19	3.75	1.53	1.31
47	l	701	PEE	C18-C19	3.74	1.53	1.31
47	B	303	PEE	C18-C19	3.74	1.53	1.31
47	C	302	PEE	C18-C19	3.74	1.53	1.31
47	l	704	PEE	C18-C19	3.73	1.53	1.31
47	b	201	PEE	C18-C19	3.73	1.53	1.31
47	r	501	PEE	C18-C19	3.72	1.53	1.31
47	j	201	PEE	C18-C19	3.72	1.53	1.31
47	i	402	PEE	C18-C19	3.72	1.53	1.31
47	C	302	PEE	C39-C38	3.67	1.53	1.31
47	j	201	PEE	C39-C38	3.65	1.52	1.31
47	i	402	PEE	C39-C38	3.65	1.52	1.31
47	l	704	PEE	C39-C38	3.65	1.52	1.31
47	b	201	PEE	C39-C38	3.65	1.52	1.31
47	l	701	PEE	C39-C38	3.65	1.52	1.31
47	r	501	PEE	C39-C38	3.64	1.52	1.31
47	B	303	PEE	C39-C38	3.64	1.52	1.31
54	V	201	CDL	OA8-CA7	3.50	1.43	1.33
54	o	201	CDL	OA8-CA7	3.48	1.43	1.33
54	u	201	CDL	OA8-CA7	3.48	1.43	1.33
54	a	201	CDL	OA8-CA7	3.46	1.43	1.33
54	l	703	CDL	OA8-CA7	3.46	1.43	1.33
54	l	702	CDL	OA8-CA7	3.45	1.43	1.33
54	r	504	CDL	OA8-CA7	3.45	1.43	1.33
54	i	401	CDL	OA8-CA7	3.43	1.43	1.33
56	w	401	ADP	O2'-C2'	-3.32	1.35	1.43
54	V	201	CDL	OA6-CA5	3.14	1.43	1.34
56	w	401	ADP	O3'-C3'	3.11	1.50	1.43
50	J	401	NDP	O3D-C3D	3.10	1.50	1.43
54	l	702	CDL	OB6-CB5	3.06	1.42	1.34
54	r	504	CDL	OB6-CB5	3.06	1.42	1.34
54	i	401	CDL	OB6-CB5	3.05	1.42	1.34
54	a	201	CDL	OB6-CB5	3.04	1.42	1.34
54	V	201	CDL	OB8-CB7	3.04	1.42	1.33
54	i	401	CDL	OA6-CA5	3.04	1.42	1.34
54	a	201	CDL	OA6-CA5	3.03	1.42	1.34
54	a	201	CDL	OB8-CB7	3.03	1.42	1.33
54	l	703	CDL	OB6-CB5	3.03	1.42	1.34
54	u	201	CDL	OB8-CB7	3.02	1.42	1.33
50	J	401	NDP	C7N-C3N	3.01	1.55	1.48
54	o	201	CDL	OB8-CB7	3.01	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	r	504	CDL	OB8-CB7	3.01	1.42	1.33
54	l	702	CDL	OB8-CB7	3.00	1.42	1.33
54	l	703	CDL	OB8-CB7	3.00	1.42	1.33
54	o	201	CDL	OA6-CA5	3.00	1.42	1.34
54	V	201	CDL	OB6-CB5	2.99	1.42	1.34
54	u	201	CDL	OB6-CB5	2.99	1.42	1.34
54	i	401	CDL	OB8-CB7	2.99	1.42	1.33
54	o	201	CDL	OB6-CB5	2.97	1.42	1.34
54	l	703	CDL	OA6-CA5	2.96	1.42	1.34
54	r	504	CDL	OA6-CA5	2.95	1.42	1.34
54	u	201	CDL	OA6-CA5	2.95	1.42	1.34
54	l	702	CDL	OA6-CA5	2.91	1.42	1.34
48	r	503	PLX	O6-C4	-2.76	1.40	1.44
55	s	401	UQ	C6-C1	2.76	1.54	1.46
48	a	202	PLX	O6-C4	-2.72	1.41	1.44
48	g	201	PLX	O6-C4	-2.67	1.41	1.44
48	C	303	PLX	O6-C4	-2.66	1.41	1.44
47	b	201	PEE	O3-C30	2.55	1.40	1.33
48	j	202	PLX	O6-C4	-2.53	1.41	1.44
47	r	501	PEE	O3-C30	2.51	1.40	1.33
47	C	302	PEE	O3-C30	2.50	1.40	1.33
47	B	303	PEE	O3-C30	2.49	1.40	1.33
47	l	701	PEE	O3-C30	2.48	1.40	1.33
47	i	402	PEE	O3-C30	2.47	1.40	1.33
47	C	302	PEE	O2-C2	-2.45	1.40	1.46
46	A	502	FMN	C10-N1	2.45	1.38	1.33
47	j	201	PEE	O3-C30	2.44	1.40	1.33
47	l	704	PEE	O2-C2	-2.44	1.40	1.46
47	l	704	PEE	O3-C30	2.43	1.40	1.33
54	u	201	CDL	OA6-CA4	-2.43	1.40	1.46
47	r	501	PEE	O2-C2	-2.43	1.40	1.46
49	X	201	8Q1	C1-S44	2.42	1.82	1.76
54	r	504	CDL	OA6-CA4	-2.42	1.40	1.46
50	J	401	NDP	O2B-C2B	2.41	1.52	1.44
49	G	201	8Q1	C1-S44	2.41	1.82	1.76
47	l	701	PEE	O2-C2	-2.40	1.40	1.46
49	G	201	8Q1	C6-C1	2.39	1.53	1.50
47	W	201	PEE	O3-C30	2.39	1.40	1.33
48	r	502	PLX	C7-C6	2.38	1.55	1.50
54	l	702	CDL	OA6-CA4	-2.38	1.40	1.46
54	o	201	CDL	OA6-CA4	-2.38	1.40	1.46
48	j	202	PLX	C7-C6	2.38	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	i	402	PEE	O2-C2	-2.37	1.40	1.46
50	J	401	NDP	C2D-C3D	2.37	1.59	1.53
48	g	201	PLX	C7-C6	2.37	1.55	1.50
47	b	201	PEE	O2-C2	-2.36	1.40	1.46
47	W	201	PEE	O2-C10	2.35	1.40	1.34
54	l	703	CDL	OA6-CA4	-2.35	1.40	1.46
54	i	401	CDL	OA6-CA4	-2.34	1.40	1.46
47	B	303	PEE	O2-C10	2.33	1.40	1.34
54	a	201	CDL	OA6-CA4	-2.32	1.40	1.46
47	j	201	PEE	O2-C2	-2.32	1.40	1.46
47	l	701	PEE	O2-C10	2.32	1.40	1.34
48	C	303	PLX	C7-C6	2.32	1.55	1.50
47	l	704	PEE	O2-C10	2.31	1.40	1.34
48	r	503	PLX	C7-C6	2.31	1.55	1.50
47	W	201	PEE	O2-C2	-2.31	1.40	1.46
47	j	201	PEE	O2-C10	2.31	1.40	1.34
47	B	303	PEE	O2-C2	-2.30	1.40	1.46
49	X	201	8Q1	C6-C1	2.30	1.53	1.50
47	r	501	PEE	O2-C10	2.29	1.40	1.34
48	a	202	PLX	C7-C6	2.28	1.55	1.50
47	C	302	PEE	O2-C10	2.28	1.40	1.34
47	b	201	PEE	O2-C10	2.28	1.40	1.34
47	i	402	PEE	O2-C10	2.27	1.40	1.34
54	u	201	CDL	PB2-OB2	2.26	1.68	1.59
48	r	502	PLX	O6-C4	-2.25	1.41	1.44
54	l	703	CDL	PB2-OB2	2.24	1.68	1.59
54	o	201	CDL	PB2-OB2	2.24	1.68	1.59
54	a	201	CDL	PB2-OB2	2.23	1.68	1.59
55	s	401	UQ	C7-C8	2.23	1.53	1.50
49	G	201	8Q1	O35-C34	-2.23	1.19	1.23
54	V	201	CDL	PB2-OB2	2.22	1.68	1.59
54	l	702	CDL	PB2-OB5	2.21	1.68	1.59
54	u	201	CDL	PB2-OB5	2.21	1.68	1.59
54	l	703	CDL	OB6-CB4	-2.21	1.41	1.46
54	r	504	CDL	PB2-OB2	2.21	1.68	1.59
54	V	201	CDL	OB6-CB4	-2.21	1.41	1.46
54	r	504	CDL	PB2-OB5	2.21	1.68	1.59
54	l	702	CDL	PB2-OB2	2.20	1.68	1.59
54	i	401	CDL	PB2-OB2	2.20	1.68	1.59
48	j	202	PLX	P1-O4	2.19	1.68	1.59
49	X	201	8Q1	O35-C34	-2.18	1.19	1.23
54	i	401	CDL	PB2-OB5	2.18	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	X	201	8Q1	O40-C39	-2.18	1.18	1.23
54	o	201	CDL	PB2-OB5	2.18	1.68	1.59
49	G	201	8Q1	O40-C39	-2.18	1.18	1.23
54	i	401	CDL	OB6-CB4	-2.18	1.41	1.46
54	l	703	CDL	PB2-OB5	2.17	1.68	1.59
55	s	401	UQ	O4-C4	-2.17	1.18	1.23
54	V	201	CDL	PB2-OB5	2.16	1.68	1.59
54	a	201	CDL	PB2-OB5	2.16	1.68	1.59
54	u	201	CDL	OB6-CB4	-2.16	1.41	1.46
48	a	202	PLX	P1-O4	2.15	1.68	1.59
54	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
54	o	201	CDL	OB6-CB4	-2.15	1.41	1.46
50	J	401	NDP	PA-O5B	2.15	1.68	1.59
47	W	201	PEE	O3-C3	-2.14	1.40	1.45
48	g	201	PLX	P1-O4	2.13	1.67	1.59
48	C	303	PLX	P1-O4	2.13	1.67	1.59
54	V	201	CDL	OA6-CA4	-2.12	1.41	1.46
54	l	702	CDL	OB6-CB4	-2.11	1.41	1.46
50	J	401	NDP	O7N-C7N	-2.11	1.19	1.24
47	j	201	PEE	O3-C3	-2.11	1.40	1.45
48	r	502	PLX	P1-O4	2.11	1.67	1.59
47	l	704	PEE	O3-C3	-2.11	1.40	1.45
48	r	503	PLX	P1-O4	2.10	1.67	1.59
54	r	504	CDL	OB6-CB4	-2.09	1.41	1.46
55	s	401	UQ	O1-C1	-2.07	1.18	1.23
48	j	202	PLX	P1-O1	2.06	1.67	1.59
48	C	303	PLX	P1-O1	2.06	1.67	1.59
48	r	502	PLX	P1-O1	2.05	1.67	1.59
47	r	501	PEE	O3-C3	-2.05	1.40	1.45
48	r	503	PLX	P1-O1	2.04	1.67	1.59
47	B	303	PEE	O3-C3	-2.04	1.40	1.45
47	l	701	PEE	O3-C3	-2.04	1.40	1.45
54	l	703	CDL	C11-CA5	2.03	1.56	1.50
55	s	401	UQ	O3-CM3	-2.03	1.40	1.45
47	C	302	PEE	O3-C3	-2.03	1.40	1.45
54	r	504	CDL	C11-CA5	2.03	1.56	1.50
48	a	202	PLX	P1-O1	2.02	1.67	1.59
48	g	201	PLX	P1-O1	2.02	1.67	1.59
47	b	201	PEE	O3-C3	-2.00	1.40	1.45
47	i	402	PEE	O3-C3	-2.00	1.40	1.45
54	i	401	CDL	C11-CA5	2.00	1.56	1.50

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	s	401	UQ	C7-C8-C9	-9.42	111.10	126.79
50	J	401	NDP	C3N-C2N-N1N	-7.64	112.19	123.10
50	J	401	NDP	C1D-N1N-C2N	-7.08	109.33	121.11
49	X	201	8Q1	C6-C1-S44	6.16	120.62	113.46
55	s	401	UQ	C12-C13-C14	-5.79	113.72	127.66
49	G	201	8Q1	C6-C1-S44	5.72	120.12	113.46
50	J	401	NDP	C1D-N1N-C6N	-5.27	109.48	120.83
56	w	401	ADP	N3-C2-N1	-4.46	121.71	128.68
55	s	401	UQ	C17-C18-C19	-4.23	113.28	127.75
47	B	303	PEE	O2-C10-C11	4.18	120.51	111.50
54	a	201	CDL	OB6-CB5-C51	4.15	120.45	111.50
55	s	401	UQ	C10-C9-C8	-4.15	113.04	123.68
54	o	201	CDL	OB6-CB5-C51	4.13	120.41	111.50
54	u	201	CDL	OB6-CB5-C51	4.13	120.41	111.50
50	J	401	NDP	N3A-C2A-N1A	-4.12	122.24	128.68
54	l	702	CDL	OB6-CB5-C51	4.11	120.36	111.50
54	a	201	CDL	OA6-CA5-C11	4.11	120.35	111.50
55	s	401	UQ	C11-C9-C8	-4.10	112.83	121.12
55	s	401	UQ	C15-C14-C13	-4.08	113.22	123.68
47	l	701	PEE	O2-C10-C11	4.06	120.24	111.50
54	i	401	CDL	OA6-CA5-C11	4.05	120.22	111.50
47	W	201	PEE	O2-C10-C11	4.03	120.18	111.50
54	l	702	CDL	OA6-CA5-C11	4.02	120.17	111.50
55	s	401	UQ	C16-C14-C13	-3.99	113.03	121.12
54	l	703	CDL	OA6-CA5-C11	3.98	120.09	111.50
54	r	504	CDL	OB6-CB5-C51	3.98	120.07	111.50
47	r	501	PEE	O2-C10-C11	3.95	120.01	111.50
47	j	201	PEE	O2-C10-C11	3.94	119.98	111.50
54	i	401	CDL	OB6-CB5-C51	3.92	119.95	111.50
54	o	201	CDL	OA6-CA5-C11	3.90	119.91	111.50
47	b	201	PEE	O2-C10-C11	3.90	119.90	111.50
47	i	402	PEE	O2-C10-C11	3.89	119.89	111.50
47	l	704	PEE	O2-C10-C11	3.89	119.88	111.50
54	u	201	CDL	OA6-CA5-C11	3.87	119.85	111.50
54	V	201	CDL	OA6-CA5-C11	3.87	119.83	111.50
54	l	703	CDL	OB6-CB5-C51	3.81	119.71	111.50
54	r	504	CDL	OA6-CA5-C11	3.79	119.68	111.50
47	C	302	PEE	O2-C10-C11	3.79	119.67	111.50
54	V	201	CDL	OB6-CB5-C51	3.72	119.52	111.50
49	X	201	8Q1	O4-C1-C6	-3.53	119.82	123.99
49	G	201	8Q1	O4-C1-C6	-3.34	120.04	123.99
55	s	401	UQ	C21-C19-C18	-3.22	113.33	122.65
55	s	401	UQ	C20-C19-C18	-3.18	113.45	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C4-N3-C2	-3.11	119.89	125.64
49	G	201	8Q1	C37-C38-C39	3.03	117.40	112.36
55	s	401	UQ	CM5-C5-C6	-2.84	119.76	124.40
47	B	303	PEE	O3-C30-C31	2.82	120.77	111.91
49	X	201	8Q1	C37-C38-C39	2.79	117.00	112.36
54	V	201	CDL	OB8-CB7-C71	2.79	120.65	111.91
47	r	501	PEE	O3-C30-C31	2.72	120.46	111.91
56	w	401	ADP	O4'-C1'-C2'	-2.70	102.98	106.93
54	o	201	CDL	OB8-CB7-C71	2.66	120.26	111.91
47	b	201	PEE	O3-C30-C31	2.66	120.25	111.91
47	i	402	PEE	O3-C30-C31	2.63	120.16	111.91
55	s	401	UQ	C7-C6-C1	2.62	121.64	118.48
56	w	401	ADP	PA-O3A-PB	-2.62	123.82	132.83
47	l	704	PEE	O3-C30-C31	2.62	120.13	111.91
54	u	201	CDL	OB8-CB7-C71	2.62	120.13	111.91
46	A	502	FMN	C4A-C4-N3	2.61	119.83	113.19
47	C	302	PEE	O3-C30-C31	2.61	120.11	111.91
54	l	702	CDL	OA8-CA7-C31	2.61	120.08	111.91
47	j	201	PEE	O3-C30-C31	2.60	120.05	111.91
54	i	401	CDL	OA8-CA7-C31	2.59	120.05	111.91
50	J	401	NDP	PN-O3-PA	-2.59	123.94	132.83
47	l	701	PEE	O3-C30-C31	2.58	120.00	111.91
54	a	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
54	u	201	CDL	OA8-CA7-C31	2.58	119.99	111.91
54	i	401	CDL	OB8-CB7-C71	2.56	119.95	111.91
54	l	702	CDL	OB8-CB7-C71	2.56	119.95	111.91
54	V	201	CDL	OA8-CA7-C31	2.56	119.93	111.91
54	l	703	CDL	OB8-CB7-C71	2.55	119.91	111.91
54	o	201	CDL	OA8-CA7-C31	2.55	119.90	111.91
54	l	703	CDL	OA8-CA7-C31	2.55	119.90	111.91
54	r	504	CDL	OB8-CB7-C71	2.54	119.88	111.91
54	a	201	CDL	OA8-CA7-C31	2.52	119.81	111.91
54	r	504	CDL	OA8-CA7-C31	2.50	119.77	111.91
47	W	201	PEE	O3-C30-C31	2.50	119.74	111.91
46	A	502	FMN	C4A-C10-N10	2.48	120.10	116.48
46	A	502	FMN	O4-C4-C4A	-2.48	120.03	126.60
48	r	502	PLX	C1A-N1-C1	2.43	119.85	109.92
48	j	202	PLX	C1A-N1-C1	2.40	119.75	109.92
48	r	503	PLX	C1A-N1-C1	2.40	119.73	109.92
48	a	202	PLX	C1A-N1-C1	2.38	119.67	109.92
48	g	201	PLX	C1A-N1-C1	2.38	119.66	109.92
49	G	201	8Q1	C43-S44-C1	2.38	109.28	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G	201	8Q1	C38-C39-N41	2.36	120.39	116.42
49	X	201	8Q1	O4-C1-S44	-2.36	119.56	122.61
49	X	201	8Q1	C38-C39-N41	2.34	120.35	116.42
50	J	401	NDP	C4A-C5A-N7A	-2.30	107.00	109.40
48	C	303	PLX	C1A-N1-C1	2.26	119.16	109.92
46	A	502	FMN	C10-C4A-N5	-2.19	120.20	124.86
46	A	502	FMN	C4A-C10-N1	-2.17	119.70	124.73
49	G	201	8Q1	O4-C1-S44	-2.13	119.84	122.61
46	A	502	FMN	C9A-C5A-N5	-2.13	120.12	122.43
56	w	401	ADP	C4-C5-N7	-2.10	107.21	109.40
49	X	201	8Q1	C43-S44-C1	2.07	108.31	101.87
46	A	502	FMN	C5A-C9A-N10	2.03	120.06	117.95
50	J	401	NDP	C2D-C3D-C4D	2.03	106.58	102.64

There are no chirality outliers.

All (834) 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	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	B	303	PEE	C37-C38-C39-C40
47	C	302	PEE	C1-O3P-P-O2P
47	C	302	PEE	C1-O3P-P-O1P
47	C	302	PEE	C1-O3P-P-O4P
47	W	201	PEE	C4-O4P-P-O1P
47	b	201	PEE	C1-O3P-P-O1P
47	b	201	PEE	C37-C38-C39-C40
47	i	402	PEE	C11-C10-O2-C2
47	j	201	PEE	C17-C18-C19-C20
47	j	201	PEE	C1-O3P-P-O2P
47	j	201	PEE	C1-O3P-P-O1P
47	j	201	PEE	C1-O3P-P-O4P
47	j	201	PEE	C4-O4P-P-O2P
47	l	701	PEE	C18-C19-C20-C21
47	l	701	PEE	C17-C18-C19-C20
47	l	701	PEE	O2-C2-C3-O3
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-O1P

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Mol	Chain	Res	Type	Atoms
47	r	501	PEE	C1-O3P-P-O1P
47	r	501	PEE	C4-O4P-P-O3P
47	r	501	PEE	C4-O4P-P-O2P
47	r	501	PEE	C4-O4P-P-O1P
48	C	303	PLX	O7-C6-O6-C4
48	C	303	PLX	C3-O4-P1-O1
48	C	303	PLX	N1-C1-C2-O1
48	a	202	PLX	O4-C3-C4-O6
48	a	202	PLX	C3-O4-P1-O1
48	a	202	PLX	C3-O4-P1-O2
48	a	202	PLX	C3-O4-P1-O3
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	C3-O4-P1-O3
48	g	201	PLX	O9-C24-C25-C26
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-C25-C26
48	r	503	PLX	O7-C6-O6-C4
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C3-O4-P1-O3
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
49	G	201	8Q1	N36-C37-C38-C39
49	G	201	8Q1	N41-C42-C43-S44
49	G	201	8Q1	C42-C43-S44-C1
49	G	201	8Q1	C28-O27-P24-O3
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1

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Mol	Chain	Res	Type	Atoms
49	X	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	J	401	NDP	C2N-C3N-C7N-N7N
54	V	201	CDL	CB2-C1-CA2-OA2
54	V	201	CDL	CA2-C1-CB2-OB2
54	V	201	CDL	CA2-OA2-PA1-OA4
54	V	201	CDL	CB2-OB2-PB2-OB4
54	V	201	CDL	CB3-OB5-PB2-OB3
54	V	201	CDL	CB3-OB5-PB2-OB4
54	a	201	CDL	CB2-C1-CA2-OA2
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CB2-OB2-PB2-OB3
54	a	201	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	CB3-OB5-PB2-OB3
54	l	702	CDL	O1-C1-CB2-OB2
54	l	702	CDL	CA2-C1-CB2-OB2
54	l	702	CDL	CB2-OB2-PB2-OB4
54	l	702	CDL	CB3-OB5-PB2-OB3
54	l	703	CDL	O1-C1-CA2-OA2
54	l	703	CDL	CA2-C1-CB2-OB2
54	l	703	CDL	OA6-CA4-CA6-OA8
54	l	703	CDL	CB2-OB2-PB2-OB3
54	l	703	CDL	CB2-OB2-PB2-OB4
54	l	703	CDL	CB2-OB2-PB2-OB5
54	l	703	CDL	OB6-CB4-CB6-OB8
54	o	201	CDL	CB2-C1-CA2-OA2
54	o	201	CDL	CA2-OA2-PA1-OA5
54	o	201	CDL	CA3-OA5-PA1-OA3
54	o	201	CDL	OA6-CA4-CA6-OA8
54	o	201	CDL	CB2-OB2-PB2-OB3
54	o	201	CDL	CB3-OB5-PB2-OB2
54	o	201	CDL	CB3-OB5-PB2-OB3
54	o	201	CDL	CB3-OB5-PB2-OB4
54	o	201	CDL	OB6-CB4-CB6-OB8
54	r	504	CDL	CB2-C1-CA2-OA2
54	r	504	CDL	CA2-OA2-PA1-OA3
54	r	504	CDL	CA2-OA2-PA1-OA4
54	r	504	CDL	CA3-OA5-PA1-OA3
54	r	504	CDL	CA3-OA5-PA1-OA4
54	r	504	CDL	CB3-OB5-PB2-OB3
54	r	504	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
54	u	201	CDL	O1-C1-CA2-OA2
54	u	201	CDL	CB2-C1-CA2-OA2
54	u	201	CDL	CA2-C1-CB2-OB2
54	u	201	CDL	CA2-OA2-PA1-OA4
54	u	201	CDL	CB2-OB2-PB2-OB3
55	s	401	UQ	C7-C8-C9-C11
55	s	401	UQ	C12-C11-C9-C8
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
54	i	401	CDL	OA9-CA7-OA8-CA6
54	l	702	CDL	OA9-CA7-OA8-CA6
47	i	402	PEE	O4-C10-O2-C2
54	i	401	CDL	C31-CA7-OA8-CA6
47	b	201	PEE	C31-C30-O3-C3
54	l	702	CDL	C31-CA7-OA8-CA6
54	r	504	CDL	C71-CB7-OB8-CB6
54	l	703	CDL	C75-C76-C77-C78
47	b	201	PEE	O5-C30-O3-C3
47	l	704	PEE	O5-C30-O3-C3
54	u	201	CDL	C52-C53-C54-C55
54	u	201	CDL	C75-C76-C77-C78
54	V	201	CDL	O1-C1-CA2-OA2
54	a	201	CDL	O1-C1-CB2-OB2
54	l	702	CDL	O1-C1-CA2-OA2
54	l	703	CDL	O1-C1-CB2-OB2
54	o	201	CDL	O1-C1-CA2-OA2
47	B	303	PEE	C11-C10-O2-C2
47	j	201	PEE	C11-C10-O2-C2
47	l	704	PEE	C11-C10-O2-C2
54	V	201	CDL	C11-CA5-OA6-CA4
48	g	201	PLX	C10-C11-C12-C13
54	u	201	CDL	C71-C72-C73-C74
54	r	504	CDL	OB9-CB7-OB8-CB6
47	l	701	PEE	C11-C12-C13-C14
48	a	202	PLX	C33-C34-C35-C36
48	j	202	PLX	C28-C29-C30-C31
48	r	502	PLX	C9-C10-C11-C12
54	V	201	CDL	C11-C12-C13-C14
54	l	703	CDL	C59-C60-C61-C62
47	l	704	PEE	C33-C34-C35-C36
47	l	704	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	O4-C10-O2-C2
54	V	201	CDL	OA7-CA5-OA6-CA4
54	V	201	CDL	C59-C60-C61-C62
54	l	703	CDL	C11-C12-C13-C14
54	o	201	CDL	C72-C73-C74-C75
55	s	401	UQ	C9-C11-C12-C13
48	r	502	PLX	C30-C31-C32-C33
48	r	503	PLX	C12-C13-C14-C15
54	l	703	CDL	C35-C36-C37-C38
55	s	401	UQ	C17-C18-C19-C20
54	a	201	CDL	CA2-C1-CB2-OB2
54	o	201	CDL	CA2-C1-CB2-OB2
47	j	201	PEE	O4-C10-O2-C2
47	W	201	PEE	C31-C30-O3-C3
47	j	201	PEE	C31-C30-O3-C3
47	l	701	PEE	C31-C30-O3-C3
54	l	702	CDL	C71-CB7-OB8-CB6
54	l	703	CDL	C71-CB7-OB8-CB6
54	V	201	CDL	C62-C63-C64-C65
54	o	201	CDL	C32-C33-C34-C35
54	r	504	CDL	C74-C75-C76-C77
48	g	201	PLX	C12-C13-C14-C15
47	l	701	PEE	O3P-C1-C2-O2
47	l	704	PEE	O3P-C1-C2-O2
54	a	201	CDL	O1-C1-CA2-OA2
54	u	201	CDL	O1-C1-CB2-OB2
54	l	703	CDL	OB9-CB7-OB8-CB6
47	b	201	PEE	C11-C10-O2-C2
54	V	201	CDL	CB7-C71-C72-C73
54	i	401	CDL	CB7-C71-C72-C73
54	r	504	CDL	C76-C77-C78-C79
54	l	702	CDL	CB7-C71-C72-C73
54	o	201	CDL	CB7-C71-C72-C73
54	r	504	CDL	CB5-C51-C52-C53
54	u	201	CDL	CB5-C51-C52-C53
47	C	302	PEE	C37-C38-C39-C40
54	V	201	CDL	C32-C33-C34-C35
54	a	201	CDL	CA5-C11-C12-C13
54	l	703	CDL	CB7-C71-C72-C73
54	r	504	CDL	CA7-C31-C32-C33
54	u	201	CDL	CB7-C71-C72-C73
54	l	702	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C15-C16-C17-C18
47	l	704	PEE	O4-C10-O2-C2
47	l	704	PEE	C30-C31-C32-C33
54	l	702	CDL	C58-C59-C60-C61
54	l	702	CDL	OB9-CB7-OB8-CB6
54	r	504	CDL	CA5-C11-C12-C13
47	j	201	PEE	C34-C35-C36-C37
47	W	201	PEE	O5-C30-O3-C3
47	l	701	PEE	C30-C31-C32-C33
54	V	201	CDL	O1-C1-CB2-OB2
54	i	401	CDL	O1-C1-CA2-OA2
54	o	201	CDL	O1-C1-CB2-OB2
54	r	504	CDL	O1-C1-CA2-OA2
54	i	401	CDL	C71-CB7-OB8-CB6
47	j	201	PEE	O5-C30-O3-C3
47	B	303	PEE	C17-C18-C19-C20
47	l	701	PEE	O5-C30-O3-C3
48	r	502	PLX	C11-C12-C13-C14
54	l	703	CDL	C39-C40-C41-C42
47	j	201	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O3P
48	r	503	PLX	C3-O4-P1-O1
54	V	201	CDL	CA2-OA2-PA1-OA5
54	V	201	CDL	CA3-OA5-PA1-OA2
54	V	201	CDL	CB2-OB2-PB2-OB5
54	V	201	CDL	CB3-OB5-PB2-OB2
54	a	201	CDL	CB3-OB5-PB2-OB2
54	i	401	CDL	CB3-OB5-PB2-OB2
54	l	702	CDL	CA2-OA2-PA1-OA5
54	l	702	CDL	CB3-OB5-PB2-OB2
54	l	703	CDL	CB3-OB5-PB2-OB2
54	r	504	CDL	CA2-OA2-PA1-OA5
54	r	504	CDL	CA3-OA5-PA1-OA2
54	r	504	CDL	CB3-OB5-PB2-OB2
54	u	201	CDL	CA2-OA2-PA1-OA5
50	J	401	NDP	C2D-C1D-N1N-C6N
54	l	703	CDL	C54-C55-C56-C57
54	a	201	CDL	C71-CB7-OB8-CB6
47	i	402	PEE	C30-C31-C32-C33
54	i	401	CDL	CB2-C1-CA2-OA2
54	l	702	CDL	CB2-C1-CA2-OA2
54	l	703	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	O4-C10-O2-C2
54	V	201	CDL	C31-CA7-OA8-CA6
54	o	201	CDL	C71-CB7-OB8-CB6
48	j	202	PLX	O6-C6-C7-C8
48	C	303	PLX	C15-C16-C17-C18
47	B	303	PEE	C39-C40-C41-C42
47	j	201	PEE	C30-C31-C32-C33
47	r	501	PEE	C13-C14-C15-C16
54	l	702	CDL	C52-C53-C54-C55
54	r	504	CDL	C35-C36-C37-C38
54	r	504	CDL	C51-CB5-OB6-CB4
47	i	402	PEE	C21-C22-C23-C24
48	g	201	PLX	C27-C28-C29-C30
54	a	201	CDL	C21-C22-C23-C24
54	a	201	CDL	C33-C34-C35-C36
54	l	702	CDL	C59-C60-C61-C62
54	l	702	CDL	C75-C76-C77-C78
54	r	504	CDL	C12-C13-C14-C15
48	g	201	PLX	C11-C10-C9-C8
48	r	502	PLX	C27-C28-C29-C30
48	r	503	PLX	C10-C11-C12-C13
54	V	201	CDL	C52-C53-C54-C55
54	r	504	CDL	OB7-CB5-OB6-CB4
46	A	502	FMN	O2'-C2'-C3'-C4'
48	r	503	PLX	C25-C26-C27-C28
54	V	201	CDL	C74-C75-C76-C77
54	a	201	CDL	C37-C38-C39-C40
54	l	702	CDL	C35-C36-C37-C38
54	l	702	CDL	C39-C40-C41-C42
54	l	703	CDL	C37-C38-C39-C40
54	o	201	CDL	C75-C76-C77-C78
54	u	201	CDL	C55-C56-C57-C58
47	r	501	PEE	C41-C42-C43-C44
48	C	303	PLX	C25-C26-C27-C28
48	g	201	PLX	C9-C10-C11-C12
54	l	702	CDL	C42-C43-C44-C45
54	l	703	CDL	C73-C74-C75-C76
54	o	201	CDL	C83-C84-C85-C86
48	j	202	PLX	C25-C26-C27-C28
48	r	502	PLX	C15-C16-C17-C18
54	r	504	CDL	C59-C60-C61-C62
47	l	704	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C7-C8-C9-C10
48	a	202	PLX	C28-C29-C30-C31
54	a	201	CDL	C75-C76-C77-C78
54	u	201	CDL	C11-C12-C13-C14
54	u	201	CDL	C13-C14-C15-C16
54	u	201	CDL	C59-C60-C61-C62
54	o	201	CDL	OB9-CB7-OB8-CB6
48	a	202	PLX	C25-C26-C27-C28
48	j	202	PLX	C10-C11-C12-C13
48	r	502	PLX	C7-C8-C9-C10
54	i	401	CDL	C33-C34-C35-C36
54	r	504	CDL	C56-C57-C58-C59
47	b	201	PEE	C33-C34-C35-C36
48	C	303	PLX	C16-C17-C18-C19
48	a	202	PLX	C14-C15-C16-C17
48	g	201	PLX	C25-C26-C27-C28
48	r	502	PLX	C13-C14-C15-C16
48	r	502	PLX	C12-C13-C14-C15
48	r	503	PLX	C14-C15-C16-C17
54	i	401	CDL	C32-C33-C34-C35
54	l	702	CDL	C11-C12-C13-C14
54	l	702	CDL	C82-C83-C84-C85
54	l	703	CDL	C55-C56-C57-C58
54	r	504	CDL	C72-C73-C74-C75
54	u	201	CDL	C17-C18-C19-C20
54	o	201	CDL	C55-C56-C57-C58
54	o	201	CDL	C51-CB5-OB6-CB4
47	b	201	PEE	C32-C33-C34-C35
48	C	303	PLX	C14-C15-C16-C17
48	r	503	PLX	C26-C27-C28-C29
54	o	201	CDL	C71-C72-C73-C74
47	i	402	PEE	C35-C36-C37-C38
54	a	201	CDL	CA7-C31-C32-C33
54	i	401	CDL	CA7-C31-C32-C33
54	l	703	CDL	CB5-C51-C52-C53
48	a	202	PLX	C32-C33-C34-C35
54	a	201	CDL	C73-C74-C75-C76
54	i	401	CDL	C52-C53-C54-C55
54	l	702	CDL	C73-C74-C75-C76
54	o	201	CDL	C73-C74-C75-C76
54	r	504	CDL	C32-C33-C34-C35
54	r	504	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
48	C	303	PLX	C9-C10-C11-C12
54	i	401	CDL	C14-C15-C16-C17
54	l	702	CDL	C20-C21-C22-C23
54	l	702	CDL	C71-C72-C73-C74
54	o	201	CDL	C56-C57-C58-C59
47	b	201	PEE	C23-C24-C25-C26
54	l	702	CDL	C32-C33-C34-C35
54	o	201	CDL	C52-C53-C54-C55
54	r	504	CDL	C14-C15-C16-C17
54	u	201	CDL	C14-C15-C16-C17
48	a	202	PLX	C11-C12-C13-C14
48	g	201	PLX	C29-C30-C31-C32
48	r	503	PLX	C13-C14-C15-C16
48	r	503	PLX	C27-C28-C29-C30
48	C	303	PLX	C31-C32-C33-C34
54	o	201	CDL	C82-C83-C84-C85
54	u	201	CDL	C72-C73-C74-C75
47	b	201	PEE	C22-C23-C24-C25
47	b	201	PEE	C31-C32-C33-C34
54	l	703	CDL	C56-C57-C58-C59
54	a	201	CDL	OB9-CB7-OB8-CB6
54	i	401	CDL	OB9-CB7-OB8-CB6
48	j	202	PLX	C27-C28-C29-C30
54	l	702	CDL	C14-C15-C16-C17
54	l	702	CDL	C74-C75-C76-C77
54	r	504	CDL	C43-C44-C45-C46
54	u	201	CDL	C57-C58-C59-C60
54	o	201	CDL	OB7-CB5-OB6-CB4
47	r	501	PEE	C17-C18-C19-C20
54	a	201	CDL	C52-C53-C54-C55
54	r	504	CDL	C73-C74-C75-C76
48	r	502	PLX	C14-C15-C16-C17
48	r	502	PLX	C31-C32-C33-C34
47	r	501	PEE	C11-C10-O2-C2
54	V	201	CDL	C51-CB5-OB6-CB4
54	V	201	CDL	C14-C15-C16-C17
54	l	702	CDL	C76-C77-C78-C79
54	r	504	CDL	C17-C18-C19-C20
48	r	503	PLX	O9-C24-C25-C26
47	l	701	PEE	C32-C33-C34-C35
54	i	401	CDL	C11-C12-C13-C14
46	A	502	FMN	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
47	i	402	PEE	C19-C20-C21-C22
47	r	501	PEE	C39-C40-C41-C42
54	V	201	CDL	OA9-CA7-OA8-CA6
48	C	303	PLX	C26-C27-C28-C29
50	J	401	NDP	O4B-C4B-C5B-O5B
54	i	401	CDL	C37-C38-C39-C40
54	V	201	CDL	C71-CB7-OB8-CB6
48	g	201	PLX	C33-C34-C35-C36
48	r	503	PLX	C33-C34-C35-C36
47	r	501	PEE	O4-C10-O2-C2
54	V	201	CDL	OB7-CB5-OB6-CB4
55	s	401	UQ	C12-C13-C14-C16
47	j	201	PEE	C41-C42-C43-C44
48	j	202	PLX	C12-C13-C14-C15
54	l	702	CDL	C36-C37-C38-C39
47	r	501	PEE	C11-C12-C13-C14
54	l	702	CDL	C56-C57-C58-C59
48	r	503	PLX	C2-C1-N1-C1A
48	C	303	PLX	C27-C28-C29-C30
48	g	201	PLX	C13-C14-C15-C16
47	b	201	PEE	C13-C14-C15-C16
54	V	201	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	C16-C17-C18-C19
54	l	703	CDL	C74-C75-C76-C77
47	C	302	PEE	C19-C20-C21-C22
47	l	701	PEE	O4-C10-O2-C2
54	u	201	CDL	OA7-CA5-OA6-CA4
54	r	504	CDL	C41-C42-C43-C44
48	j	202	PLX	C7-C8-C9-C10
48	j	202	PLX	C26-C27-C28-C29
48	C	303	PLX	C11-C12-C13-C14
54	V	201	CDL	C55-C56-C57-C58
47	r	501	PEE	C14-C15-C16-C17
47	r	501	PEE	C40-C41-C42-C43
47	l	701	PEE	C11-C10-O2-C2
54	u	201	CDL	C11-CA5-OA6-CA4
48	C	303	PLX	O4-C3-C4-O6
48	r	503	PLX	C16-C17-C18-C19
54	V	201	CDL	C40-C41-C42-C43
54	i	401	CDL	C73-C74-C75-C76
54	i	401	CDL	C35-C36-C37-C38
54	i	401	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	OB6-CB4-CB6-OB8
47	r	501	PEE	C31-C32-C33-C34
48	r	503	PLX	C2-C1-N1-C1C
48	C	303	PLX	C30-C31-C32-C33
48	a	202	PLX	C19-C20-C21-C22
47	l	701	PEE	C35-C36-C37-C38
55	s	401	UQ	C17-C18-C19-C21
47	B	303	PEE	C12-C13-C14-C15
48	r	503	PLX	C29-C30-C31-C32
54	l	703	CDL	C57-C58-C59-C60
47	l	704	PEE	C37-C38-C39-C40
54	V	201	CDL	C33-C34-C35-C36
54	r	504	CDL	C36-C37-C38-C39
54	r	504	CDL	C75-C76-C77-C78
47	B	303	PEE	C21-C22-C23-C24
54	a	201	CDL	C17-C18-C19-C20
47	j	201	PEE	C36-C37-C38-C39
47	r	501	PEE	C36-C37-C38-C39
47	r	501	PEE	C1-O3P-P-O4P
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CB2-OB2-PB2-OB5
54	l	702	CDL	CB2-OB2-PB2-OB5
54	u	201	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	C76-C77-C78-C79
54	l	703	CDL	C72-C73-C74-C75
47	B	303	PEE	C31-C30-O3-C3
47	l	701	PEE	O3P-C1-C2-C3
48	C	303	PLX	O4-C3-C4-C5
48	a	202	PLX	O4-C3-C4-C5
54	i	401	CDL	OA5-CA3-CA4-CA6
54	i	401	CDL	OB5-CB3-CB4-CB6
55	s	401	UQ	C7-C8-C9-C10
48	r	503	PLX	C28-C29-C30-C31
54	l	703	CDL	C71-C72-C73-C74
48	j	202	PLX	C13-C14-C15-C16
54	r	504	CDL	C60-C61-C62-C63
48	C	303	PLX	C17-C18-C19-C20
48	a	202	PLX	C11-C10-C9-C8
48	j	202	PLX	C14-C15-C16-C17
54	l	703	CDL	C52-C53-C54-C55
47	C	302	PEE	C35-C36-C37-C38
47	b	201	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
47	j	201	PEE	C39-C40-C41-C42
47	j	201	PEE	C32-C33-C34-C35
47	W	201	PEE	C12-C13-C14-C15
47	b	201	PEE	C14-C15-C16-C17
48	g	201	PLX	C11-C12-C13-C14
54	a	201	CDL	C43-C44-C45-C46
54	l	703	CDL	C60-C61-C62-C63
47	W	201	PEE	C1-C2-C3-O3
47	b	201	PEE	C1-C2-C3-O3
47	i	402	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
54	l	703	CDL	CA3-CA4-CA6-OA8
54	o	201	CDL	CA3-CA4-CA6-OA8
54	o	201	CDL	CB3-CB4-CB6-OB8
47	l	701	PEE	C12-C13-C14-C15
48	C	303	PLX	C33-C34-C35-C36
54	l	703	CDL	C64-C65-C66-C67
48	C	303	PLX	C7-C8-C9-C10
48	r	503	PLX	C31-C32-C33-C34
54	r	504	CDL	C42-C43-C44-C45
47	r	501	PEE	C10-C11-C12-C13
48	r	503	PLX	O8-C24-C25-C26
48	g	201	PLX	C28-C29-C30-C31
47	W	201	PEE	C23-C24-C25-C26
48	a	202	PLX	C9-C10-C11-C12
47	B	303	PEE	C20-C21-C22-C23
47	B	303	PEE	C11-C12-C13-C14
54	u	201	CDL	C53-C54-C55-C56
50	J	401	NDP	C3B-C4B-C5B-O5B
47	B	303	PEE	C40-C41-C42-C43
47	r	501	PEE	C21-C22-C23-C24
49	G	201	8Q1	O27-C28-C29-C30
49	G	201	8Q1	O27-C28-C29-C31
54	l	703	CDL	CA7-C31-C32-C33
54	o	201	CDL	C84-C85-C86-C87
54	r	504	CDL	C52-C53-C54-C55
54	r	504	CDL	CB4-CB3-OB5-PB2
54	i	401	CDL	C31-C32-C33-C34
54	l	703	CDL	C41-C42-C43-C44
47	b	201	PEE	O3P-C1-C2-O2
54	a	201	CDL	OA5-CA3-CA4-OA6
54	o	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C2-C1-N1-C1B
54	l	703	CDL	C58-C59-C60-C61
54	r	504	CDL	OA6-CA4-CA6-OA8
54	r	504	CDL	OB6-CB4-CB6-OB8
47	C	302	PEE	C43-C44-C45-C46
47	B	303	PEE	O5-C30-O3-C3
54	V	201	CDL	C58-C59-C60-C61
54	a	201	CDL	C55-C56-C57-C58
54	r	504	CDL	C13-C14-C15-C16
54	o	201	CDL	C32-C31-CA7-OA8
47	l	704	PEE	C14-C15-C16-C17
48	j	202	PLX	C33-C34-C35-C36
54	o	201	CDL	C54-C55-C56-C57
54	a	201	CDL	C60-C61-C62-C63
47	j	201	PEE	C31-C32-C33-C34
54	V	201	CDL	C34-C35-C36-C37
47	b	201	PEE	C34-C35-C36-C37
48	r	503	PLX	C30-C31-C32-C33
47	i	402	PEE	C11-C12-C13-C14
48	r	502	PLX	C28-C29-C30-C31
47	l	704	PEE	O3P-C1-C2-C3
48	j	202	PLX	O4-C3-C4-C5
54	a	201	CDL	OA5-CA3-CA4-CA6
54	o	201	CDL	OB5-CB3-CB4-CB6
54	r	504	CDL	C37-C38-C39-C40
48	j	202	PLX	C34-C35-C36-C37
49	X	201	8Q1	C29-C32-C34-O35
47	i	402	PEE	C10-C11-C12-C13
54	a	201	CDL	C71-C72-C73-C74
54	V	201	CDL	CB5-C51-C52-C53
47	B	303	PEE	C34-C35-C36-C37
48	r	503	PLX	C15-C16-C17-C18
47	l	704	PEE	C31-C32-C33-C34
54	a	201	CDL	C38-C39-C40-C41
54	V	201	CDL	C31-C32-C33-C34
54	l	702	CDL	C40-C41-C42-C43
54	r	504	CDL	C31-C32-C33-C34
47	l	701	PEE	C1-C2-C3-O3
48	r	503	PLX	C3-C4-C5-O8
54	i	401	CDL	CA3-CA4-CA6-OA8
54	i	401	CDL	CB3-CB4-CB6-OB8
54	r	504	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
54	r	504	CDL	CB3-CB4-CB6-OB8
48	j	202	PLX	C11-C12-C13-C14
48	j	202	PLX	C9-C10-C11-C12
48	r	503	PLX	C18-C19-C20-C21
54	i	401	CDL	C75-C76-C77-C78
48	r	503	PLX	C9-C10-C11-C12
47	B	303	PEE	C31-C32-C33-C34
48	j	202	PLX	C3-O4-P1-O1
48	C	303	PLX	O9-C24-C25-C26
54	l	703	CDL	OA5-CA3-CA4-OA6
54	r	504	CDL	C11-C12-C13-C14
47	b	201	PEE	O2-C2-C3-O3
54	i	401	CDL	OA6-CA4-CA6-OA8
47	i	402	PEE	C24-C25-C26-C27
48	C	303	PLX	C13-C14-C15-C16
47	W	201	PEE	C13-C14-C15-C16
47	B	303	PEE	C13-C14-C15-C16
47	i	402	PEE	C2-C1-O3P-P
47	B	303	PEE	C15-C16-C17-C18
47	W	201	PEE	C22-C23-C24-C25
48	r	502	PLX	C10-C11-C12-C13
47	r	501	PEE	C38-C39-C40-C41
47	C	302	PEE	C42-C43-C44-C45
48	r	503	PLX	C7-C8-C9-C10
54	V	201	CDL	C72-C73-C74-C75
49	G	201	8Q1	O4-C1-S44-C43
48	C	303	PLX	C28-C29-C30-C31
54	l	702	CDL	C23-C24-C25-C26
54	V	201	CDL	C64-C65-C66-C67
54	r	504	CDL	C57-C58-C59-C60
54	l	702	CDL	C34-C35-C36-C37
48	g	201	PLX	O8-C24-C25-C26
54	a	201	CDL	C19-C20-C21-C22
47	b	201	PEE	O3P-C1-C2-C3
47	i	402	PEE	O3P-C1-C2-C3
48	g	201	PLX	O4-C3-C4-C5
54	a	201	CDL	OB5-CB3-CB4-CB6
54	l	703	CDL	OA5-CA3-CA4-CA6
47	C	302	PEE	C18-C19-C20-C21
47	l	704	PEE	C19-C20-C21-C22
54	a	201	CDL	C14-C15-C16-C17
54	l	702	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	C12-C13-C14-C15
54	u	201	CDL	C60-C61-C62-C63
49	X	201	8Q1	O33-C32-C34-N36
48	j	202	PLX	C31-C32-C33-C34
54	r	504	CDL	C55-C56-C57-C58
47	j	201	PEE	C20-C21-C22-C23
49	G	201	8Q1	C6-C1-S44-C43
54	V	201	CDL	CA6-CA4-OA6-CA5
47	W	201	PEE	C33-C34-C35-C36
48	g	201	PLX	C14-C15-C16-C17
48	r	502	PLX	C3-C4-C5-O8
54	V	201	CDL	CA3-CA4-CA6-OA8
54	l	703	CDL	CB3-CB4-CB6-OB8
54	u	201	CDL	CA3-CA4-CA6-OA8
47	r	501	PEE	O3P-C1-C2-O2
48	j	202	PLX	O4-C3-C4-O6
54	V	201	CDL	OB5-CB3-CB4-OB6
54	a	201	CDL	OB5-CB3-CB4-OB6
47	W	201	PEE	O3-C30-C31-C32
54	l	703	CDL	C40-C41-C42-C43
50	J	401	NDP	O4D-C1D-N1N-C6N
47	l	704	PEE	C23-C24-C25-C26
49	G	201	8Q1	C9-C10-C11-C12
47	r	501	PEE	O2-C2-C3-O3
54	u	201	CDL	OA6-CA4-CA6-OA8
54	r	504	CDL	C54-C55-C56-C57
54	a	201	CDL	CB7-C71-C72-C73
47	C	302	PEE	C40-C41-C42-C43
54	i	401	CDL	C15-C16-C17-C18
48	a	202	PLX	C26-C27-C28-C29
54	a	201	CDL	C54-C55-C56-C57
47	b	201	PEE	C10-C11-C12-C13
54	V	201	CDL	C57-C58-C59-C60
47	l	704	PEE	C4-O4P-P-O3P
54	a	201	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA2-OA2-PA1-OA5
54	l	703	CDL	CA2-OA2-PA1-OA5
54	o	201	CDL	CB2-OB2-PB2-OB5
54	u	201	CDL	CB3-OB5-PB2-OB2
47	j	201	PEE	C4-O4P-P-O1P
47	l	701	PEE	C4-O4P-P-O2P
47	r	501	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	C	303	PLX	C3-O4-P1-O3
48	g	201	PLX	C2-O1-P1-O3
48	r	502	PLX	C2-O1-P1-O3
54	V	201	CDL	CA2-OA2-PA1-OA3
54	V	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CB3-OB5-PB2-OB4
54	l	702	CDL	CA2-OA2-PA1-OA3
54	l	702	CDL	CB2-OB2-PB2-OB3
54	l	702	CDL	CB3-OB5-PB2-OB4
54	l	703	CDL	CB3-OB5-PB2-OB3
54	l	703	CDL	CB3-OB5-PB2-OB4
54	o	201	CDL	CA2-OA2-PA1-OA4
54	o	201	CDL	CB2-OB2-PB2-OB4
54	u	201	CDL	CB2-OB2-PB2-OB4
54	u	201	CDL	CB3-OB5-PB2-OB4
47	l	701	PEE	C10-C11-C12-C13
47	B	303	PEE	O3P-C1-C2-C3
47	C	302	PEE	O3P-C1-C2-C3
47	j	201	PEE	O3P-C1-C2-C3
54	V	201	CDL	C75-C76-C77-C78
47	l	701	PEE	C37-C38-C39-C40
48	g	201	PLX	C16-C17-C18-C19
54	a	201	CDL	C53-C54-C55-C56
48	a	202	PLX	C25-C24-O8-C5
48	g	201	PLX	C25-C24-O8-C5
48	j	202	PLX	C25-C24-O8-C5
48	r	503	PLX	C25-C24-O8-C5
54	o	201	CDL	C33-C34-C35-C36
54	l	703	CDL	C43-C44-C45-C46
47	b	201	PEE	C11-C12-C13-C14
47	B	303	PEE	O3P-C1-C2-O2
47	i	402	PEE	O3P-C1-C2-O2
47	j	201	PEE	O3P-C1-C2-O2
48	g	201	PLX	O4-C3-C4-O6
54	i	401	CDL	OA5-CA3-CA4-OA6
54	o	201	CDL	C74-C75-C76-C77
47	C	302	PEE	C16-C17-C18-C19
54	l	702	CDL	C61-C62-C63-C64
54	r	504	CDL	C64-C65-C66-C67
54	l	702	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
54	l	702	CDL	CA7-C31-C32-C33
54	i	401	CDL	C71-C72-C73-C74
54	l	702	CDL	C24-C25-C26-C27
50	J	401	NDP	C2N-C3N-C7N-O7N
48	j	202	PLX	O6-C4-C5-O8
48	r	503	PLX	O6-C4-C5-O8
54	u	201	CDL	C74-C75-C76-C77
54	l	703	CDL	C76-C77-C78-C79
48	g	201	PLX	C31-C32-C33-C34
48	C	303	PLX	C18-C19-C20-C21
54	V	201	CDL	C53-C54-C55-C56
48	a	202	PLX	C27-C28-C29-C30
54	V	201	CDL	C12-C13-C14-C15
54	V	201	CDL	C71-C72-C73-C74
47	j	201	PEE	C10-C11-C12-C13
54	a	201	CDL	C31-C32-C33-C34
47	r	501	PEE	O3P-C1-C2-C3
48	r	503	PLX	C35-C36-C37-C38
47	j	201	PEE	C18-C19-C20-C21
54	i	401	CDL	OB5-CB3-CB4-OB6
47	B	303	PEE	C23-C24-C25-C26
54	l	703	CDL	C14-C15-C16-C17
47	W	201	PEE	O2-C2-C3-O3
47	i	402	PEE	O2-C2-C3-O3
48	r	502	PLX	O6-C4-C5-O8
54	a	201	CDL	C15-C16-C17-C18
48	a	202	PLX	C2-O1-P1-O4
48	r	502	PLX	C2-O1-P1-O4
54	l	703	CDL	CA3-OA5-PA1-OA2
47	W	201	PEE	C32-C33-C34-C35
54	a	201	CDL	C12-C13-C14-C15
54	l	703	CDL	C15-C16-C17-C18
47	i	402	PEE	C14-C15-C16-C17
49	G	201	8Q1	C6-C7-C8-C9
47	l	701	PEE	C13-C14-C15-C16
54	V	201	CDL	CA4-CA3-OA5-PA1
47	B	303	PEE	C36-C37-C38-C39
47	W	201	PEE	C18-C19-C20-C21
47	b	201	PEE	C16-C17-C18-C19
47	j	201	PEE	C38-C39-C40-C41
47	W	201	PEE	C31-C32-C33-C34
54	i	401	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
54	l	703	CDL	C32-C33-C34-C35
48	g	201	PLX	C6-C7-C8-C9
47	r	501	PEE	C12-C13-C14-C15
47	b	201	PEE	C38-C39-C40-C41
47	W	201	PEE	O4-C10-O2-C2
47	l	701	PEE	C39-C40-C41-C42
47	r	501	PEE	C20-C21-C22-C23
48	r	502	PLX	O8-C24-C25-C26
47	l	704	PEE	C38-C39-C40-C41
47	i	402	PEE	C23-C24-C25-C26
47	j	201	PEE	C12-C13-C14-C15
49	X	201	8Q1	C9-C10-C11-C12
48	j	202	PLX	C3-C4-C5-O8
47	b	201	PEE	C18-C19-C20-C21
47	i	402	PEE	C31-C32-C33-C34
48	a	202	PLX	C10-C11-C12-C13
49	X	201	8Q1	C29-C32-C34-N36
47	W	201	PEE	C19-C20-C21-C22
47	l	704	PEE	C1-C2-O2-C10
54	l	703	CDL	C12-C13-C14-C15
54	a	201	CDL	C36-C37-C38-C39
54	r	504	CDL	C23-C24-C25-C26
54	r	504	CDL	C39-C40-C41-C42
48	C	303	PLX	C3-C4-O6-C6
48	r	503	PLX	C5-C4-O6-C6
54	V	201	CDL	OA5-CA3-CA4-OA6
54	r	504	CDL	C44-C45-C46-C47
54	V	201	CDL	OB5-CB3-CB4-CB6
54	r	504	CDL	C78-C79-C80-C81
54	l	702	CDL	C44-C45-C46-C47
54	r	504	CDL	C33-C34-C35-C36
54	o	201	CDL	C32-C31-CA7-OA9
54	a	201	CDL	C35-C36-C37-C38
47	j	201	PEE	C24-C25-C26-C27
54	V	201	CDL	C60-C61-C62-C63
47	W	201	PEE	C16-C17-C18-C19
54	l	702	CDL	C80-C81-C82-C83
55	s	401	UQ	C5-C6-C7-C8
54	l	702	CDL	C62-C63-C64-C65
47	C	302	PEE	C31-C30-O3-C3
47	C	302	PEE	O5-C30-O3-C3
47	i	402	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	C16-C17-C18-C19
47	C	302	PEE	O3P-C1-C2-O2
47	l	701	PEE	C31-C32-C33-C34
48	a	202	PLX	C6-C7-C8-C9
48	j	202	PLX	C24-C25-C26-C27
48	C	303	PLX	O6-C6-C7-C8
48	g	201	PLX	O6-C6-C7-C8
54	V	201	CDL	C39-C40-C41-C42
54	l	702	CDL	C16-C17-C18-C19
47	b	201	PEE	O4P-C4-C5-N
47	i	402	PEE	C18-C19-C20-C21
54	V	201	CDL	OB6-CB4-CB6-OB8
47	j	201	PEE	C22-C23-C24-C25
54	l	703	CDL	C62-C63-C64-C65
47	b	201	PEE	C12-C13-C14-C15
47	W	201	PEE	C11-C10-O2-C2
47	b	201	PEE	C36-C37-C38-C39
47	l	704	PEE	C36-C37-C38-C39
55	s	401	UQ	C15-C14-C16-C17
54	u	201	CDL	C72-C71-CB7-OB8
54	l	702	CDL	C33-C34-C35-C36
55	s	401	UQ	C1-C6-C7-C8
54	l	702	CDL	C17-C18-C19-C20
54	l	702	CDL	C12-C11-CA5-OA6
47	i	402	PEE	C36-C37-C38-C39
47	l	701	PEE	C16-C17-C18-C19
47	l	701	PEE	C38-C39-C40-C41
47	l	704	PEE	C22-C23-C24-C25
47	l	704	PEE	C3-C2-O2-C10
54	r	504	CDL	C22-C23-C24-C25
47	C	302	PEE	C44-C45-C46-C47
54	r	504	CDL	C19-C20-C21-C22
47	r	501	PEE	C18-C19-C20-C21
47	r	501	PEE	C16-C17-C18-C19
54	o	201	CDL	C80-C81-C82-C83
48	j	202	PLX	C7-C6-O6-C4
54	o	201	CDL	OA7-CA5-OA6-CA4
47	r	501	PEE	C37-C38-C39-C40
47	j	201	PEE	O2-C10-C11-C12
54	V	201	CDL	C35-C36-C37-C38
47	l	701	PEE	C33-C34-C35-C36
54	V	201	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
54	l	703	CDL	OB5-CB3-CB4-CB6
54	i	401	CDL	C74-C75-C76-C77
54	l	703	CDL	C44-C45-C46-C47
47	l	701	PEE	O3-C30-C31-C32
54	l	702	CDL	OB6-CB4-CB6-OB8
54	o	201	CDL	CA7-C31-C32-C33
47	C	302	PEE	C36-C37-C38-C39
54	l	702	CDL	C72-C71-CB7-OB8
54	i	401	CDL	C38-C39-C40-C41
48	a	202	PLX	O9-C24-C25-C26
47	B	303	PEE	C14-C15-C16-C17
47	j	201	PEE	C16-C17-C18-C19
48	C	303	PLX	C24-C25-C26-C27
56	w	401	ADP	PB-O3A-PA-O1A
54	l	703	CDL	C79-C80-C81-C82
54	u	201	CDL	C72-C71-CB7-OB9
54	u	201	CDL	C61-C62-C63-C64
47	B	303	PEE	C18-C19-C20-C21
48	r	502	PLX	C25-C26-C27-C28
54	V	201	CDL	C54-C55-C56-C57
54	a	201	CDL	CB5-C51-C52-C53
47	j	201	PEE	O4-C10-C11-C12
54	l	702	CDL	C12-C11-CA5-OA7
47	B	303	PEE	C24-C25-C26-C27
47	b	201	PEE	O3-C30-C31-C32
48	j	202	PLX	C3-O4-P1-O3
54	l	702	CDL	CA3-OA5-PA1-OA3
54	u	201	CDL	CA3-OA5-PA1-OA3
54	l	703	CDL	C12-C11-CA5-OA6
48	r	503	PLX	C11-C12-C13-C14
47	C	302	PEE	C13-C14-C15-C16
47	W	201	PEE	O5-C30-C31-C32
54	o	201	CDL	C11-CA5-OA6-CA4
54	r	504	CDL	C15-C16-C17-C18
47	b	201	PEE	C5-C4-O4P-P
48	r	502	PLX	C25-C24-O8-C5
54	l	702	CDL	C72-C71-CB7-OB9
47	l	704	PEE	C13-C14-C15-C16
54	o	201	CDL	C52-C51-CB5-OB6
54	a	201	CDL	C72-C71-CB7-OB8
54	l	703	CDL	C32-C31-CA7-OA8
54	u	201	CDL	CA5-C11-C12-C13

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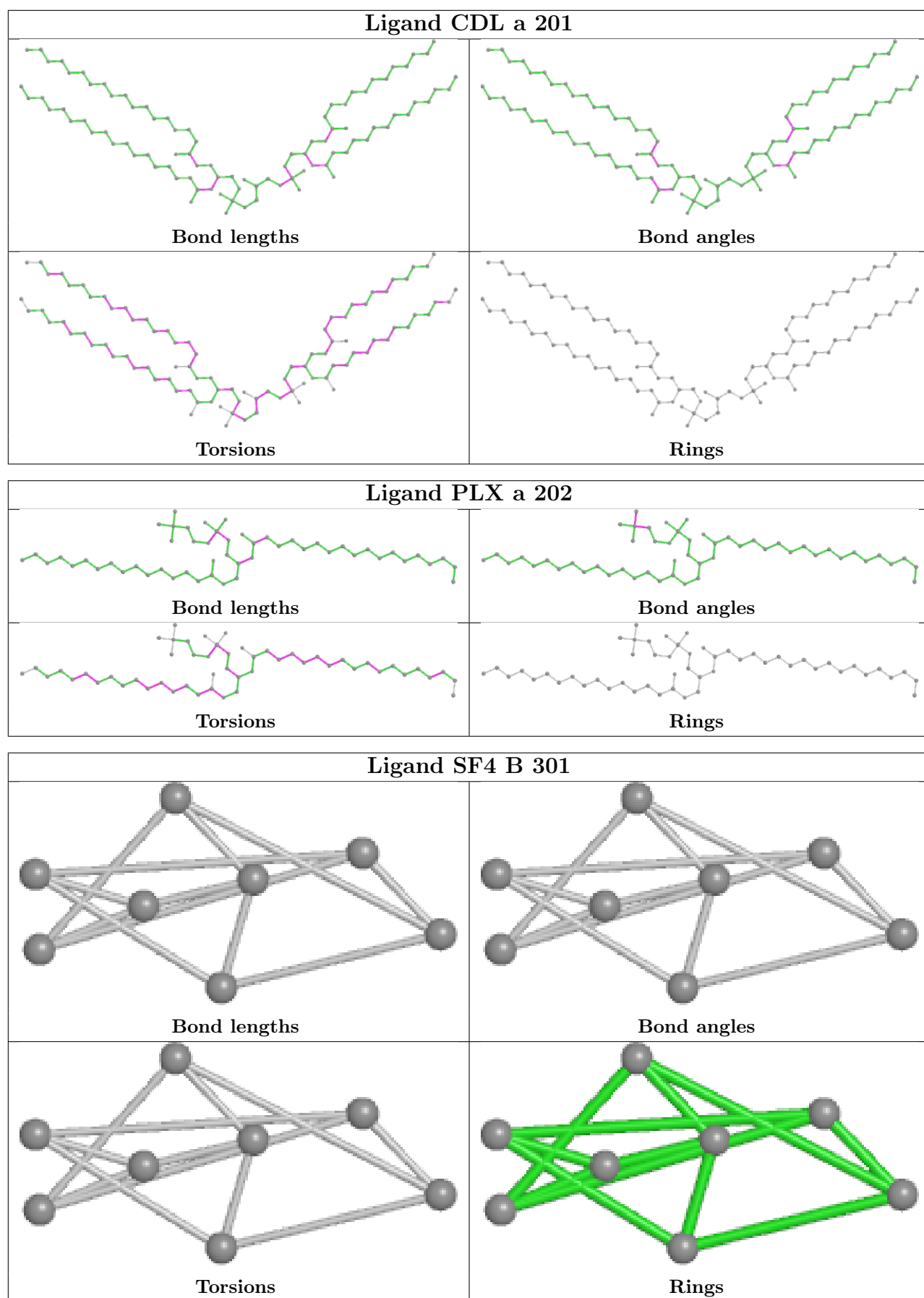
*Continued from previous page...*

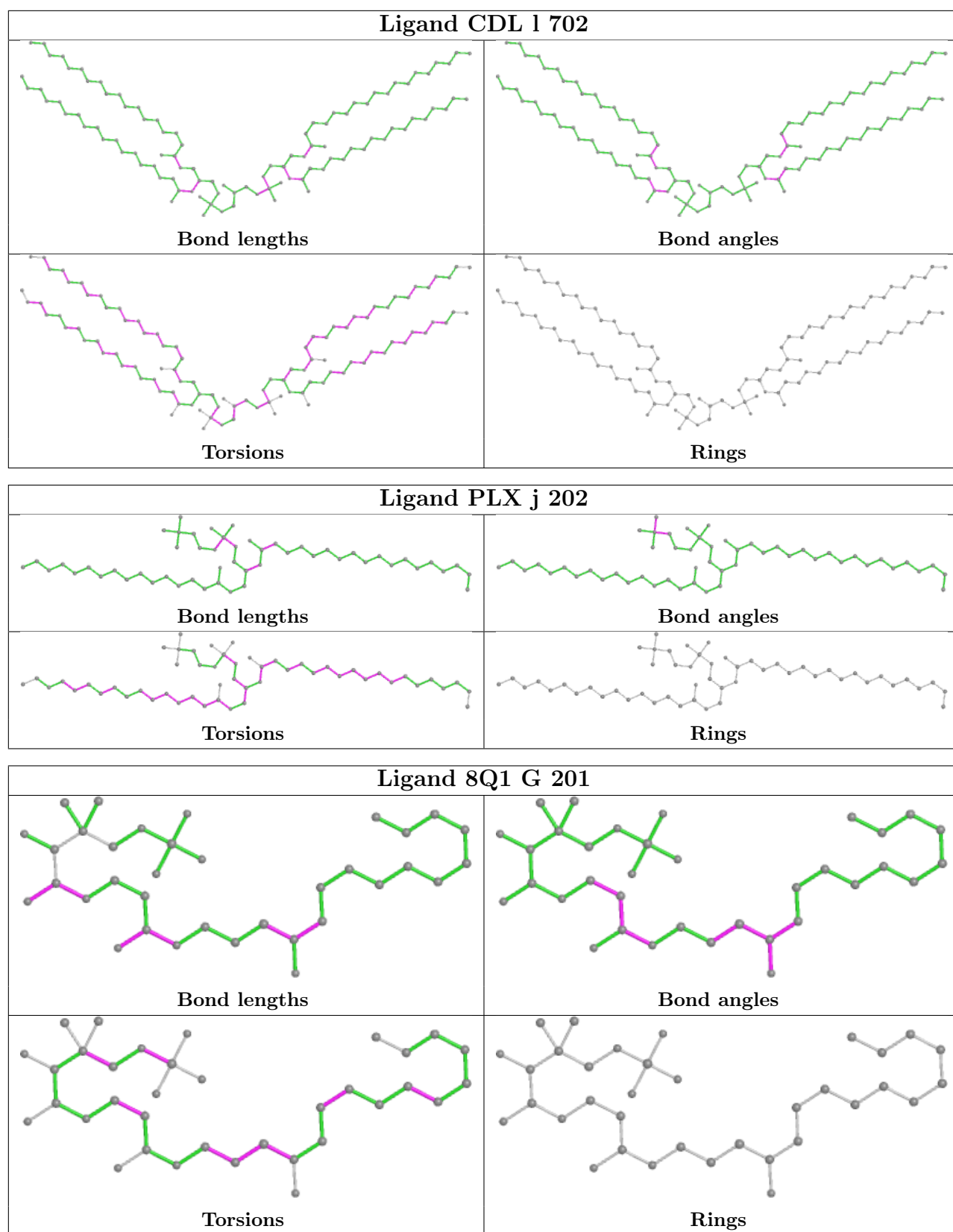
Mol	Chain	Res	Type	Atoms
54	l	703	CDL	OB5-CB3-CB4-OB6
54	a	201	CDL	C32-C31-CA7-OA8
47	l	701	PEE	O5-C30-C31-C32
54	l	703	CDL	C12-C11-CA5-OA7
47	b	201	PEE	C20-C21-C22-C23
47	b	201	PEE	O5-C30-C31-C32
47	l	701	PEE	C34-C35-C36-C37
48	r	503	PLX	C24-C25-C26-C27
54	V	201	CDL	C32-C31-CA7-OA8
54	l	703	CDL	C32-C31-CA7-OA9
47	r	501	PEE	C33-C34-C35-C36
47	C	302	PEE	O3-C30-C31-C32

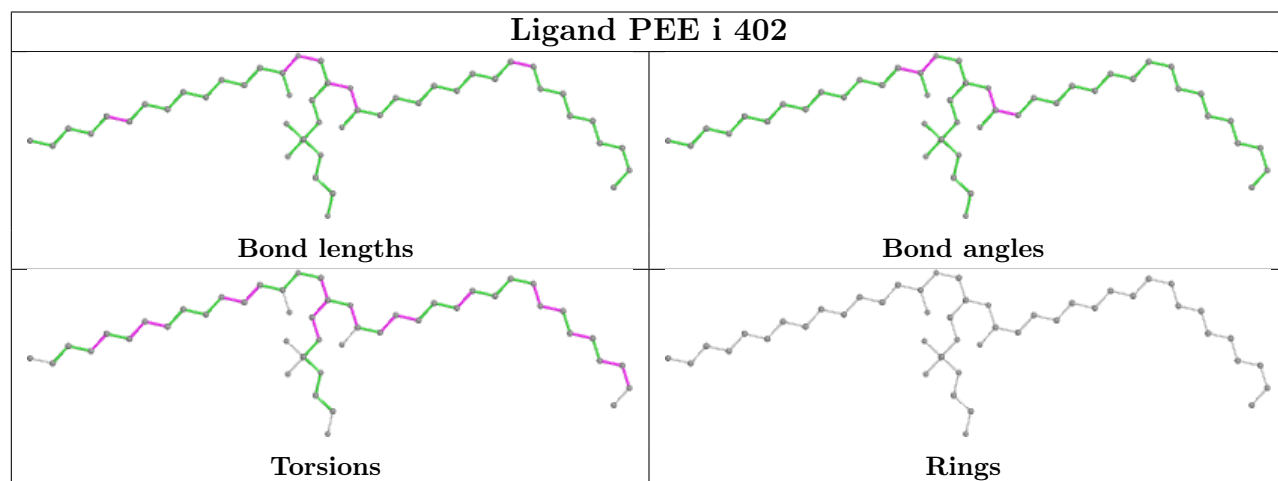
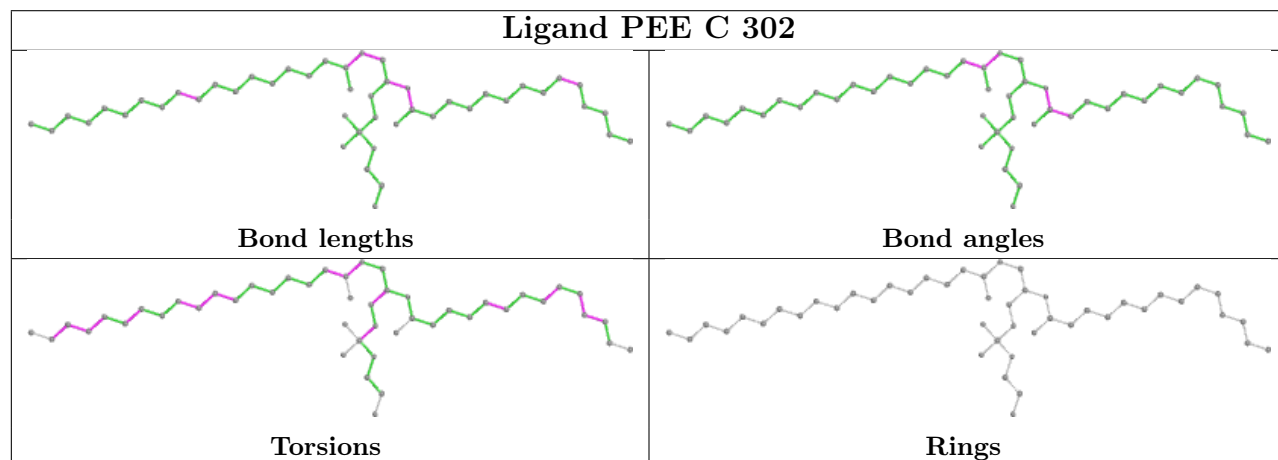
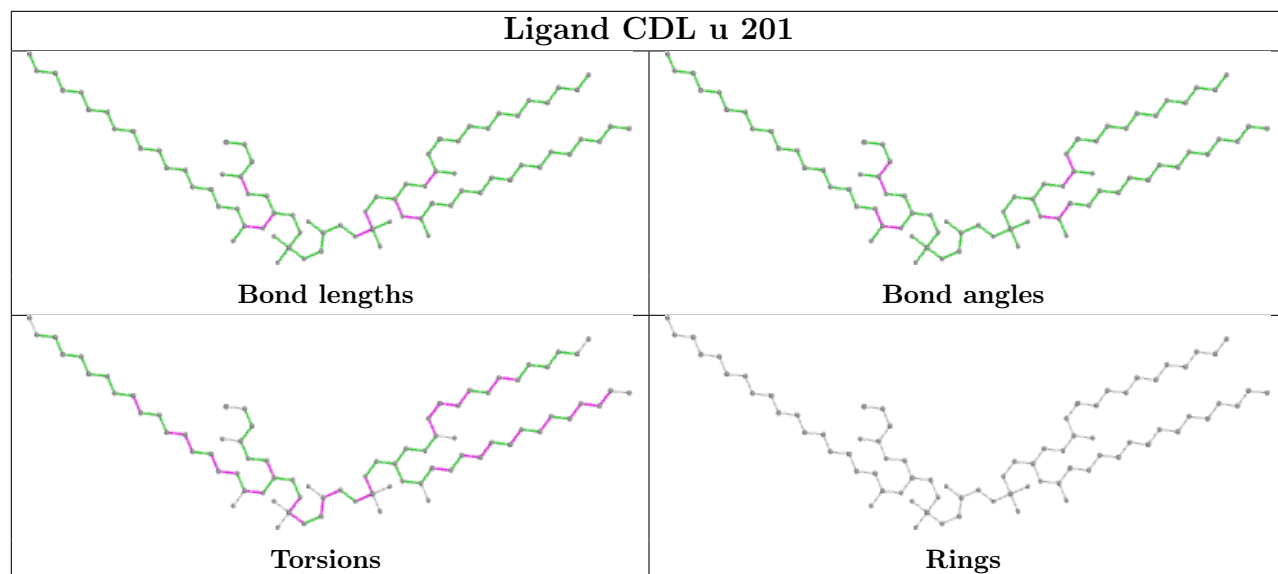
There are no ring outliers.

No monomer is involved in short contacts.

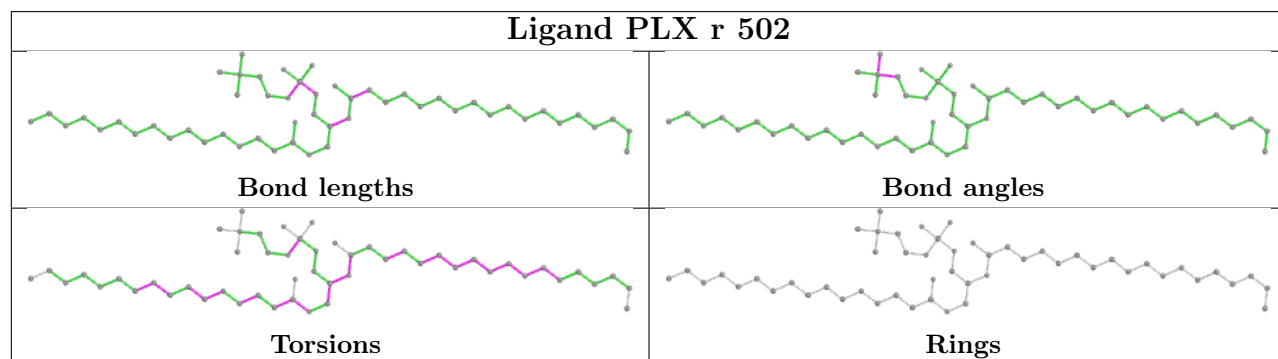
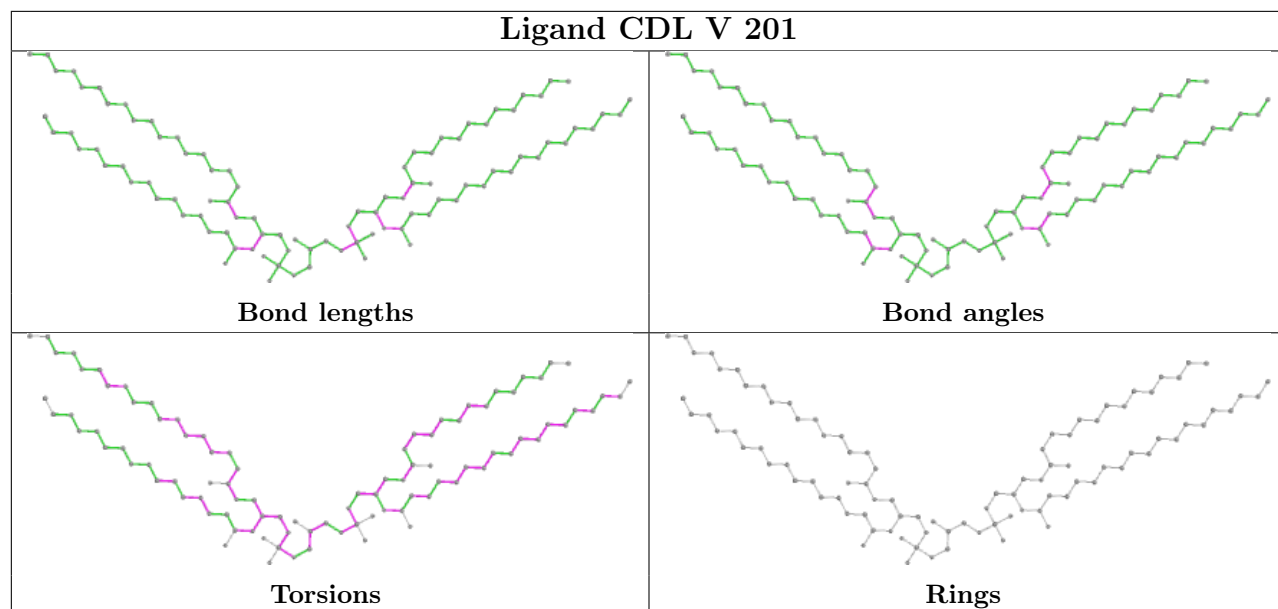
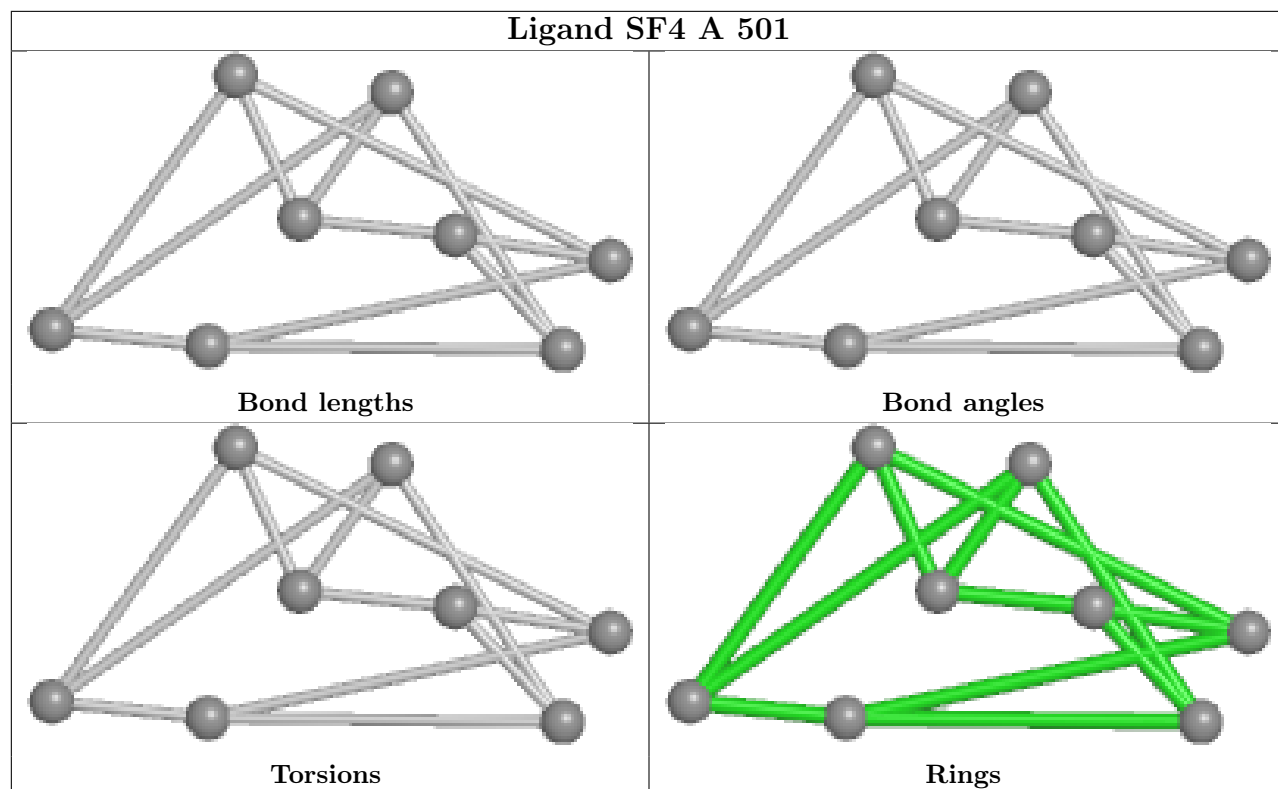
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

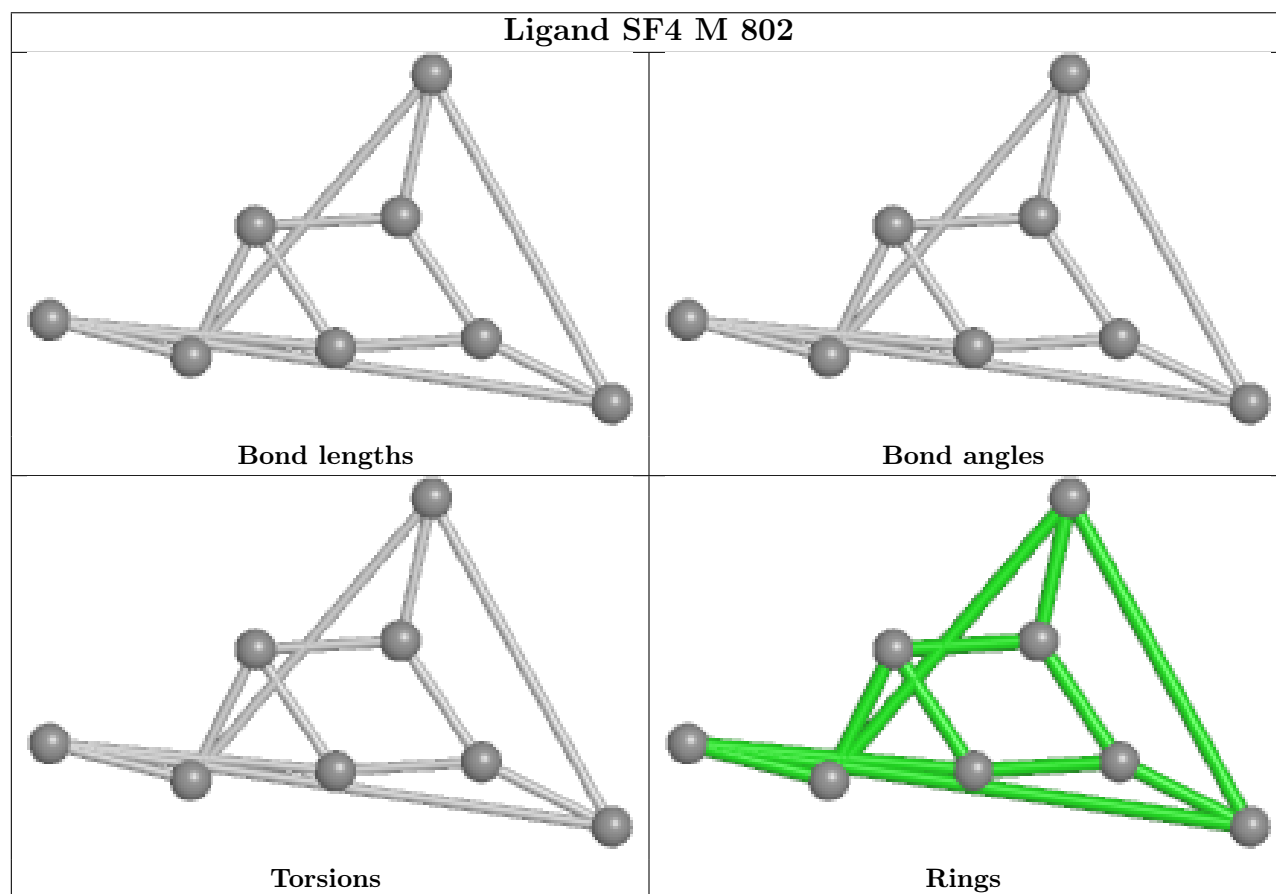
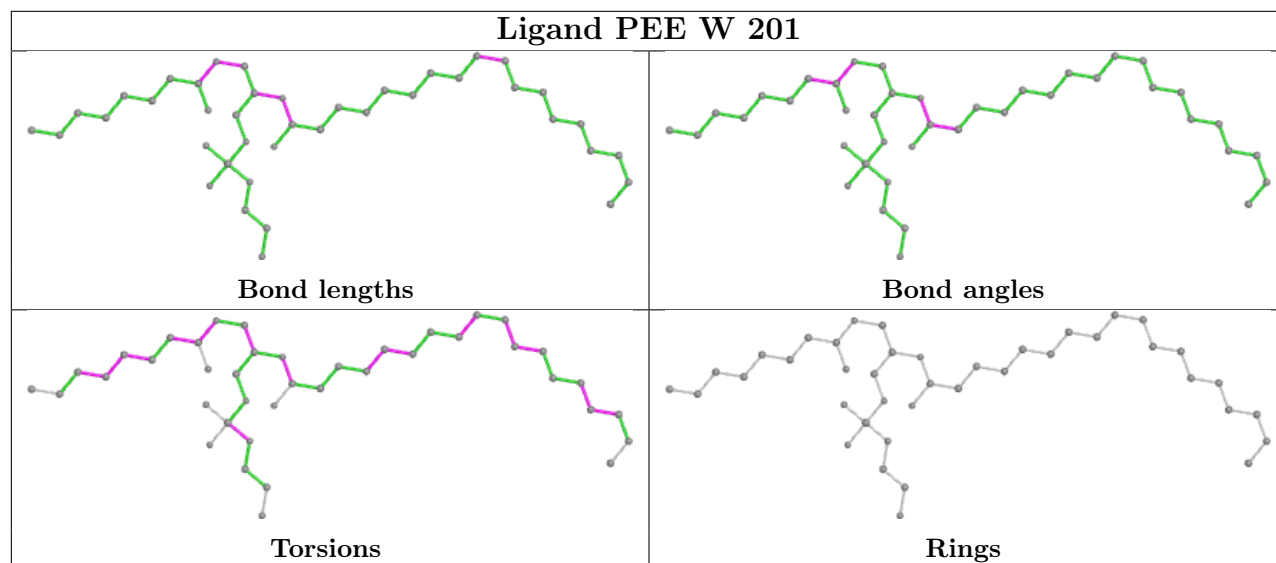


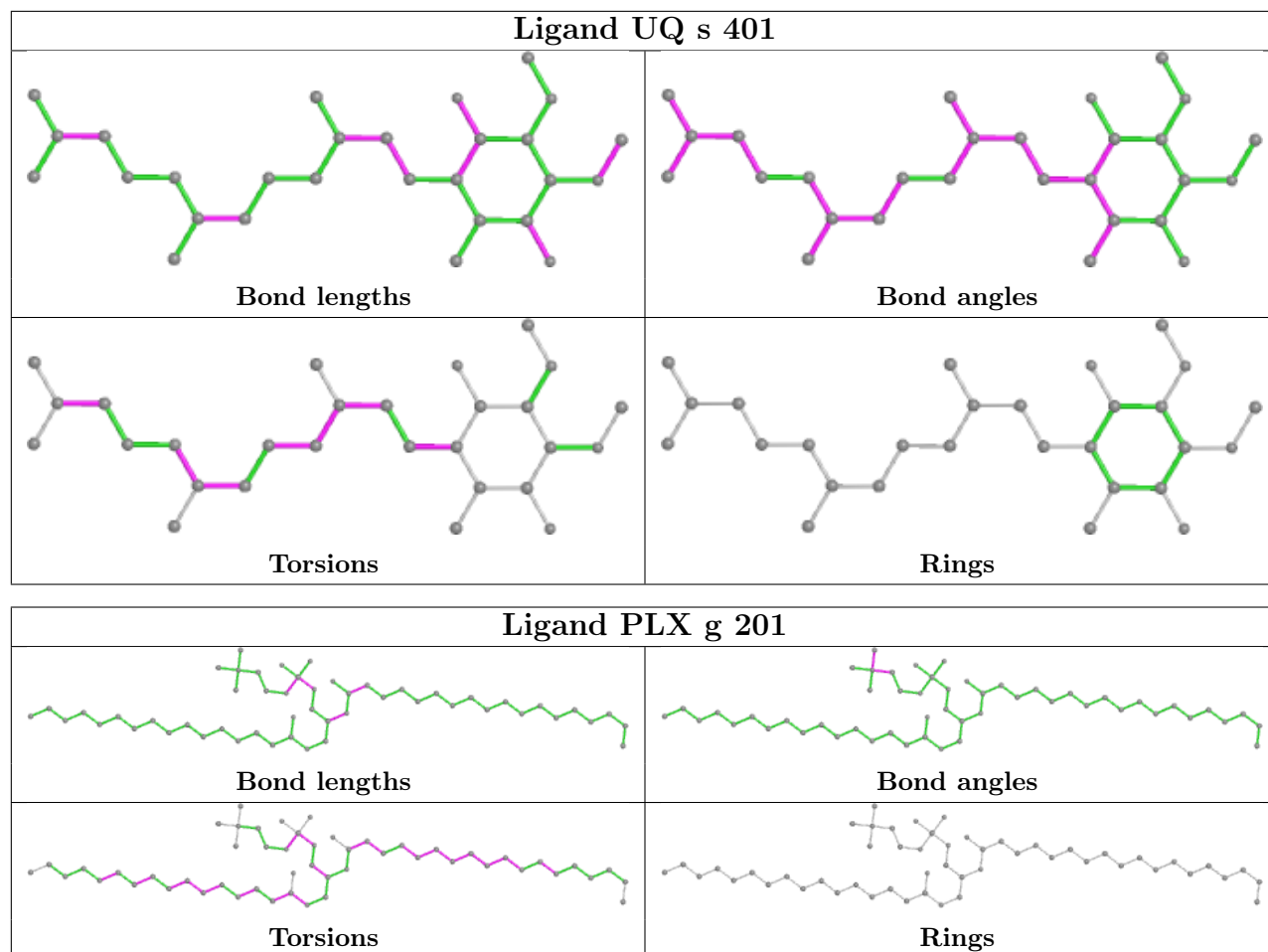


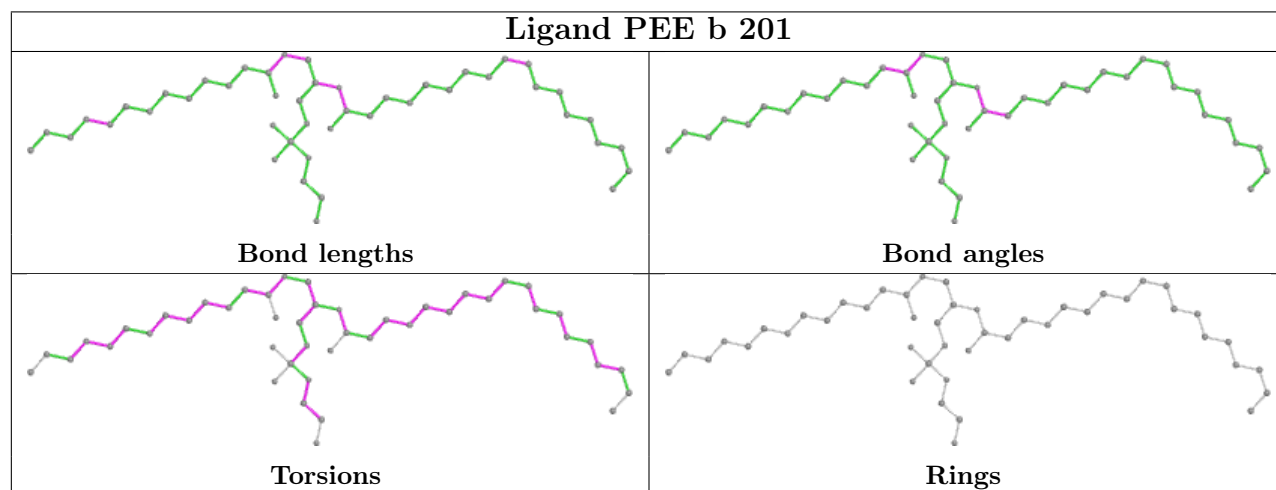
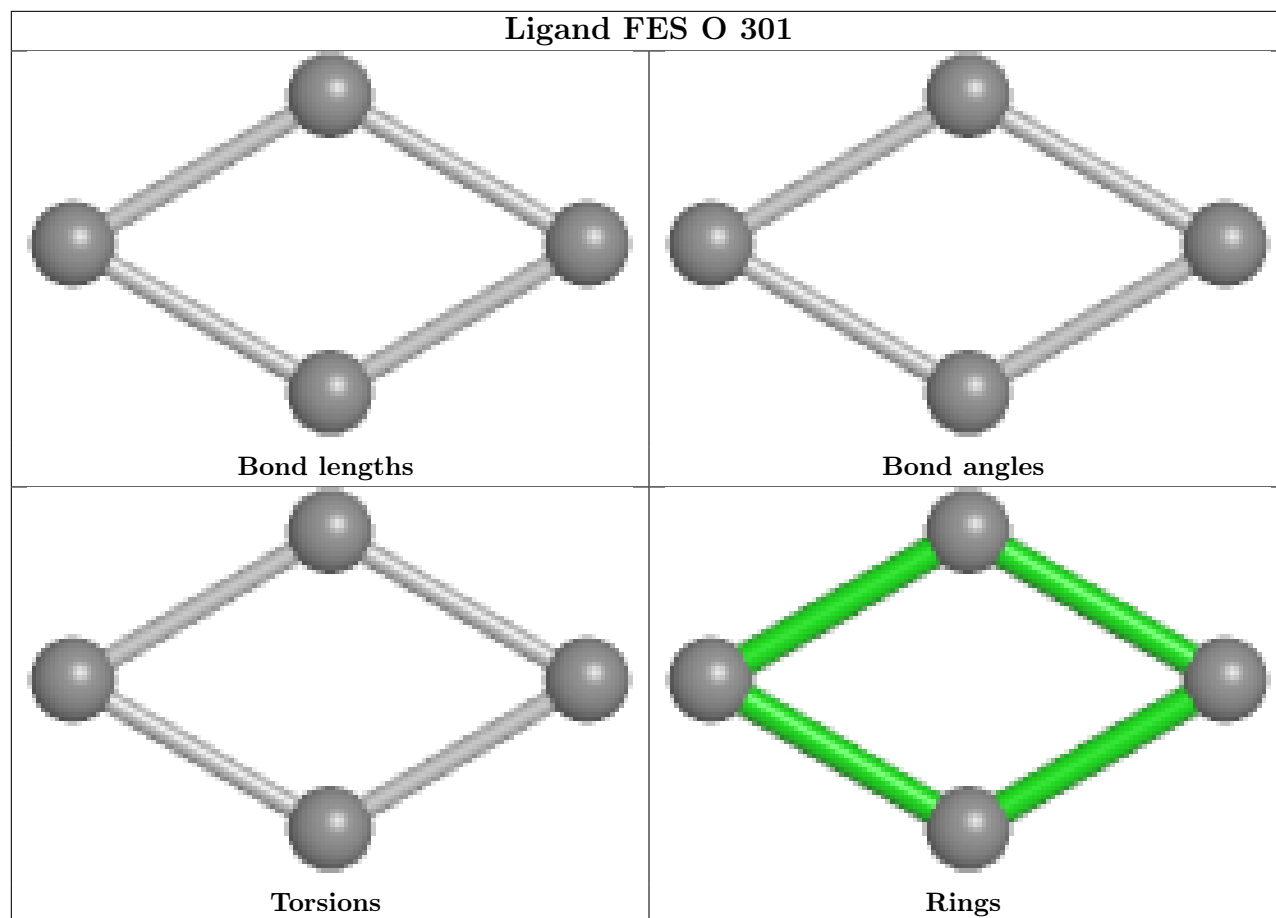


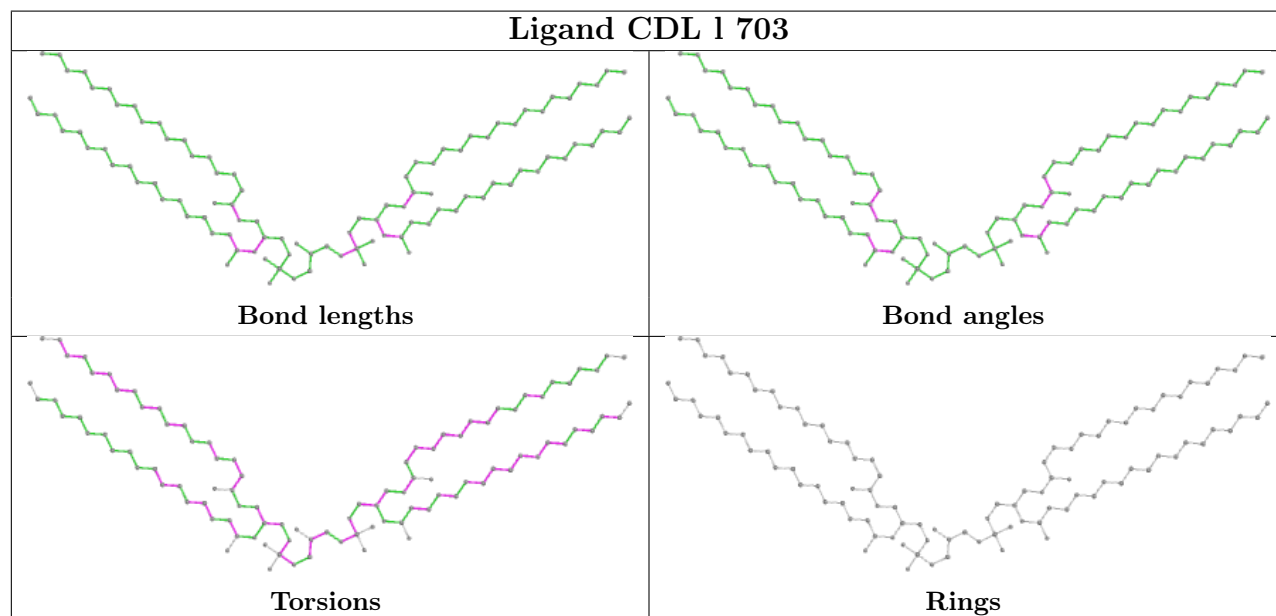
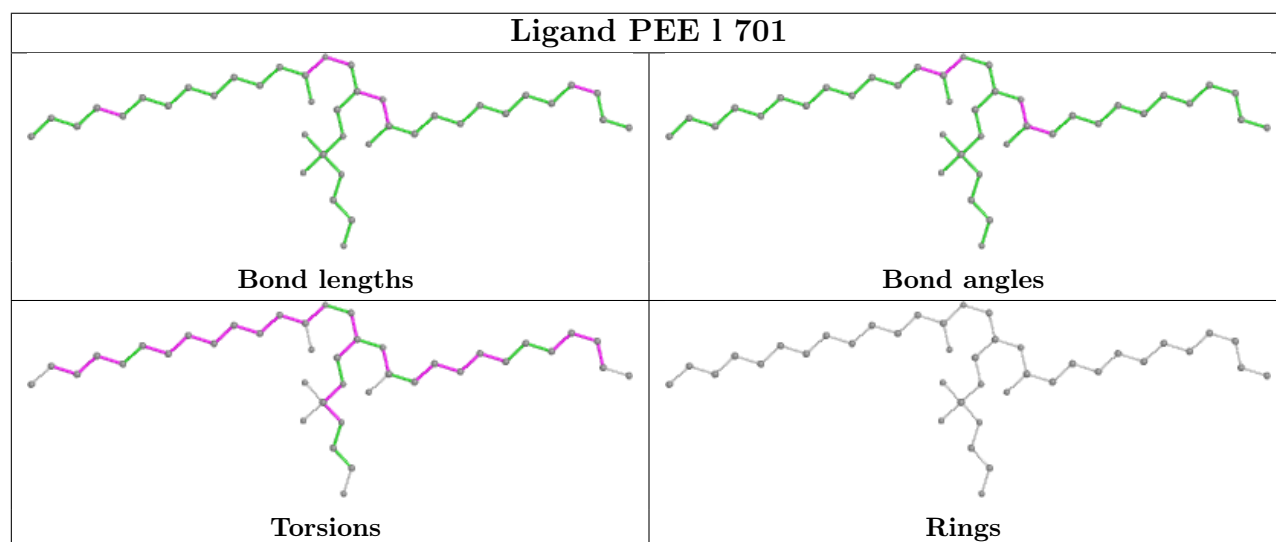
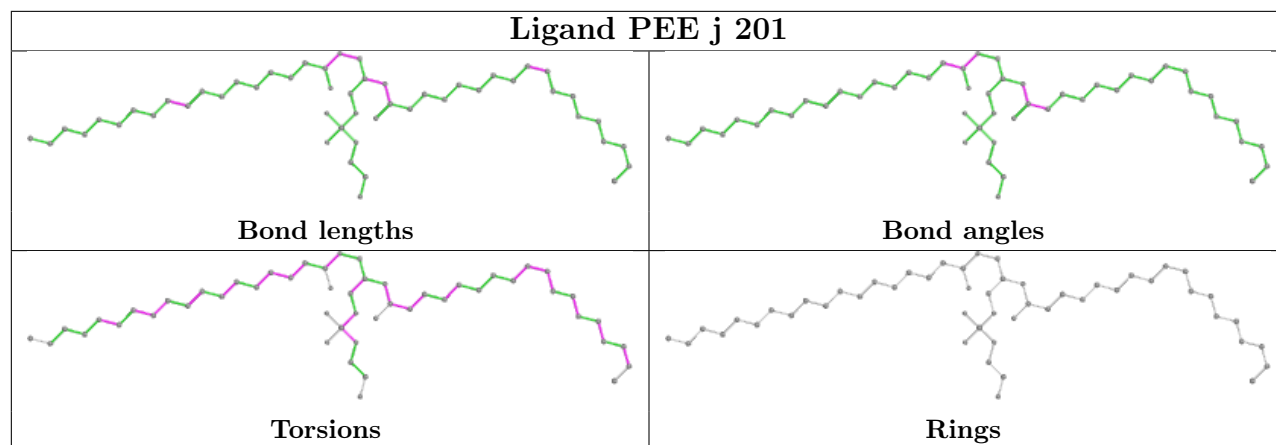


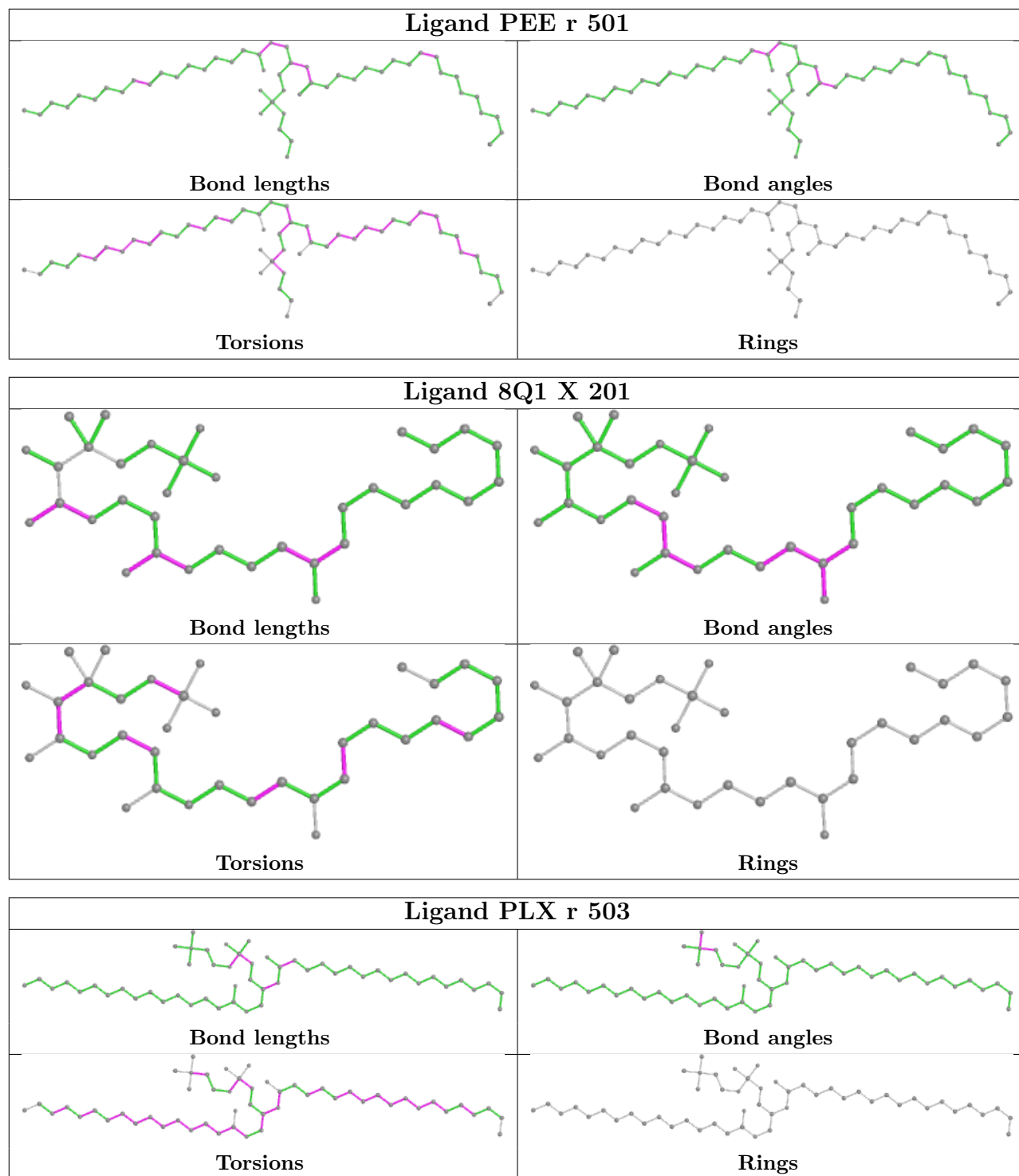


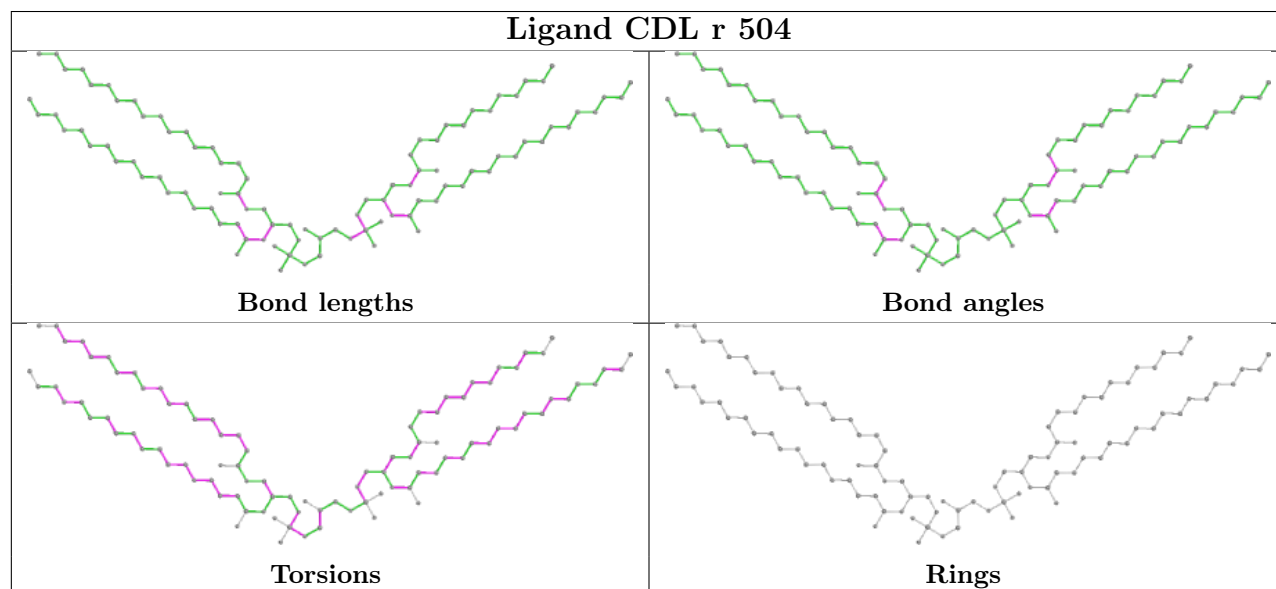
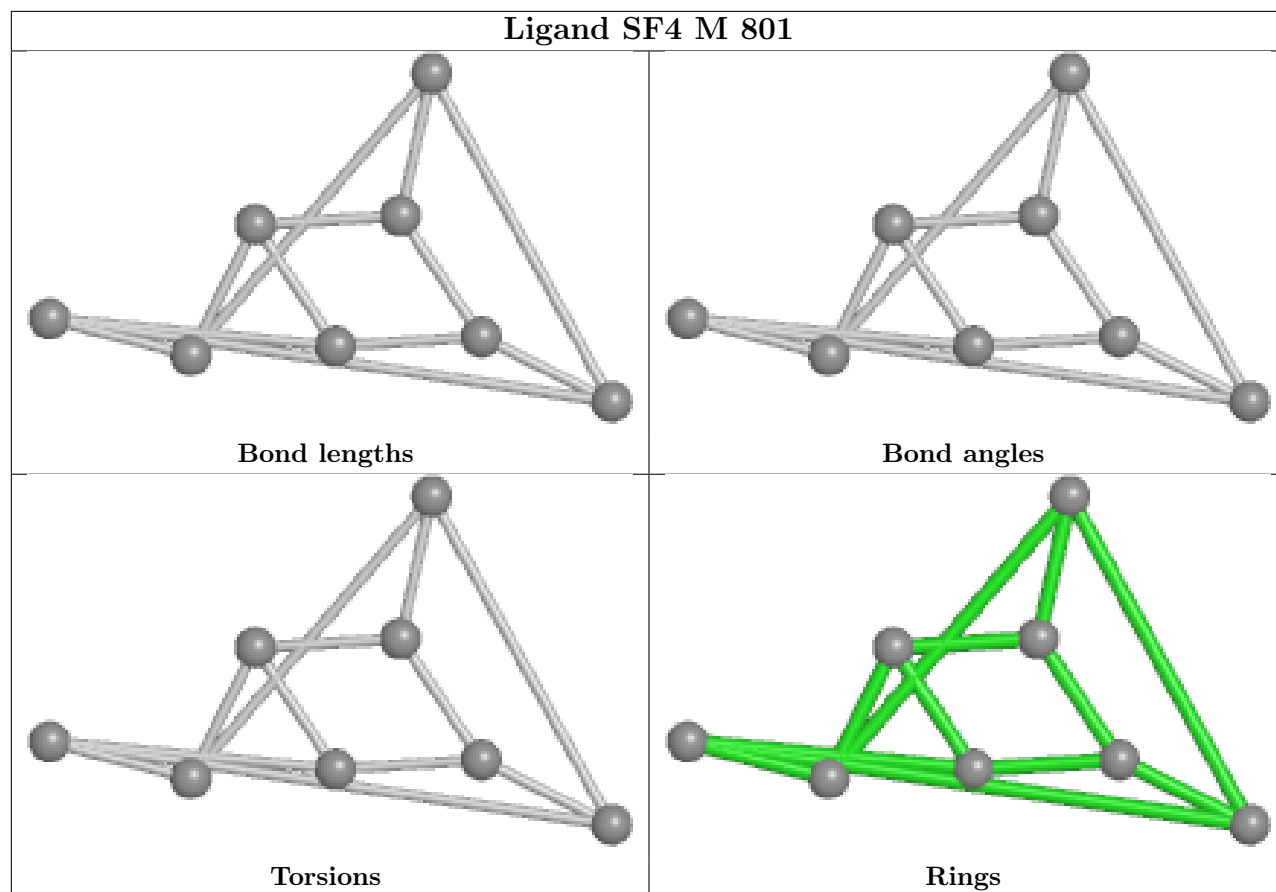


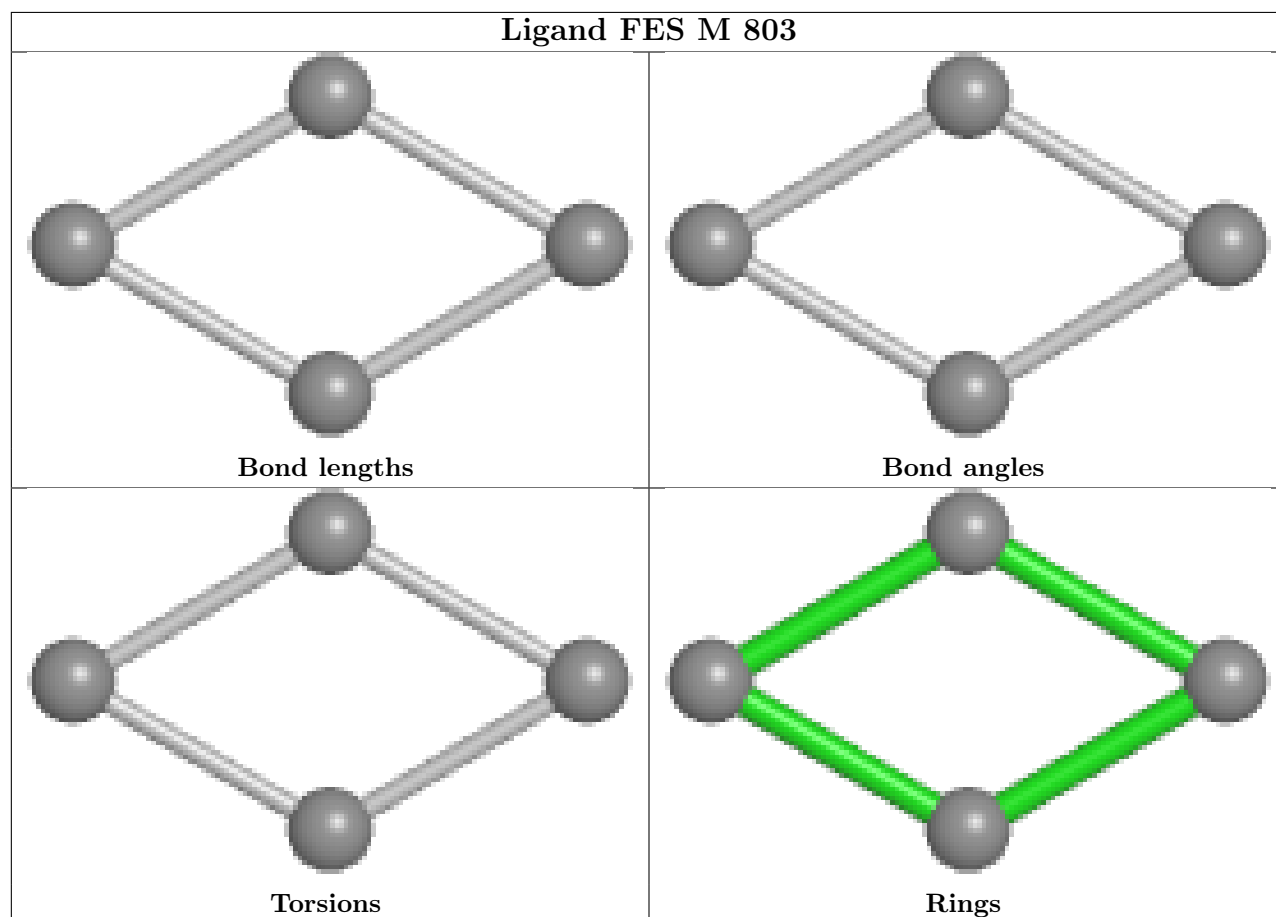
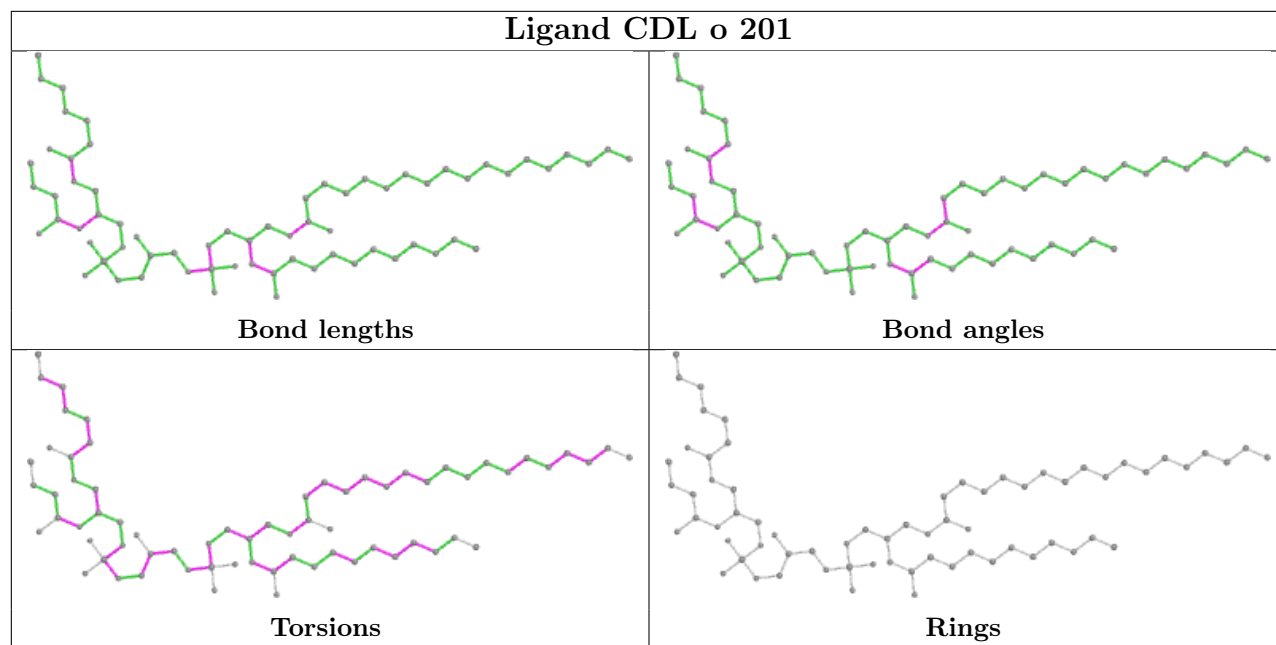




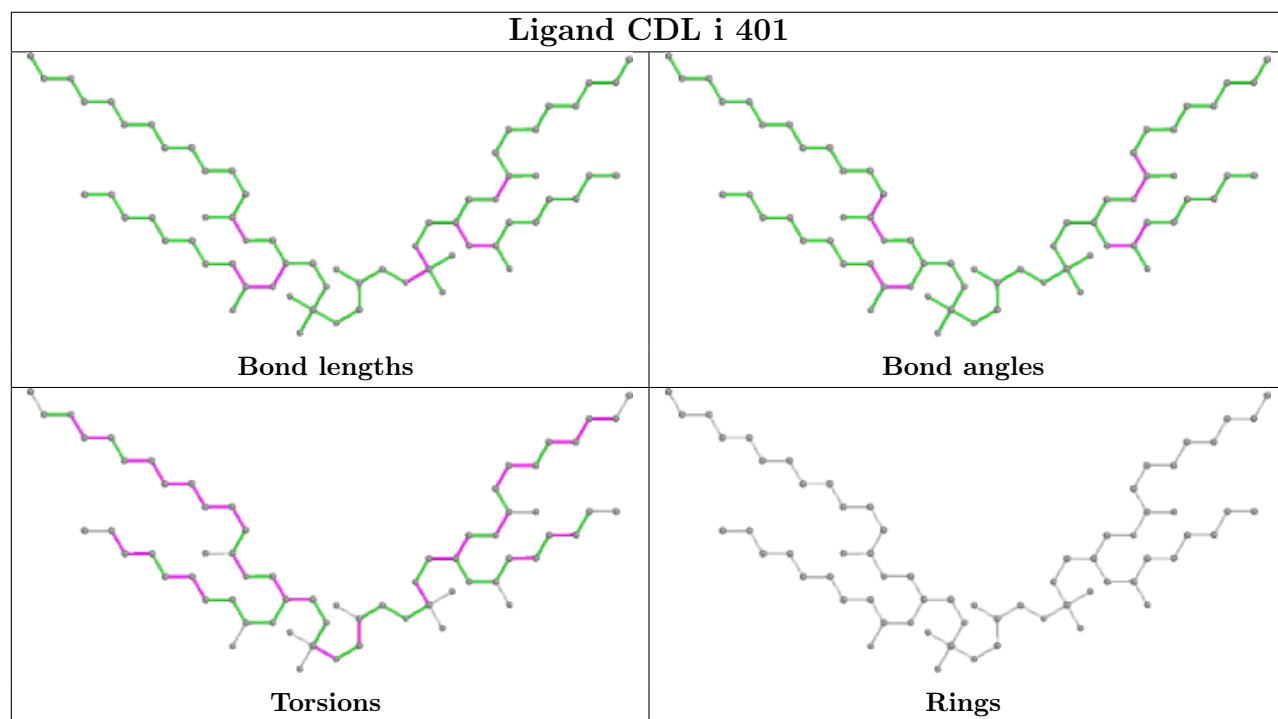
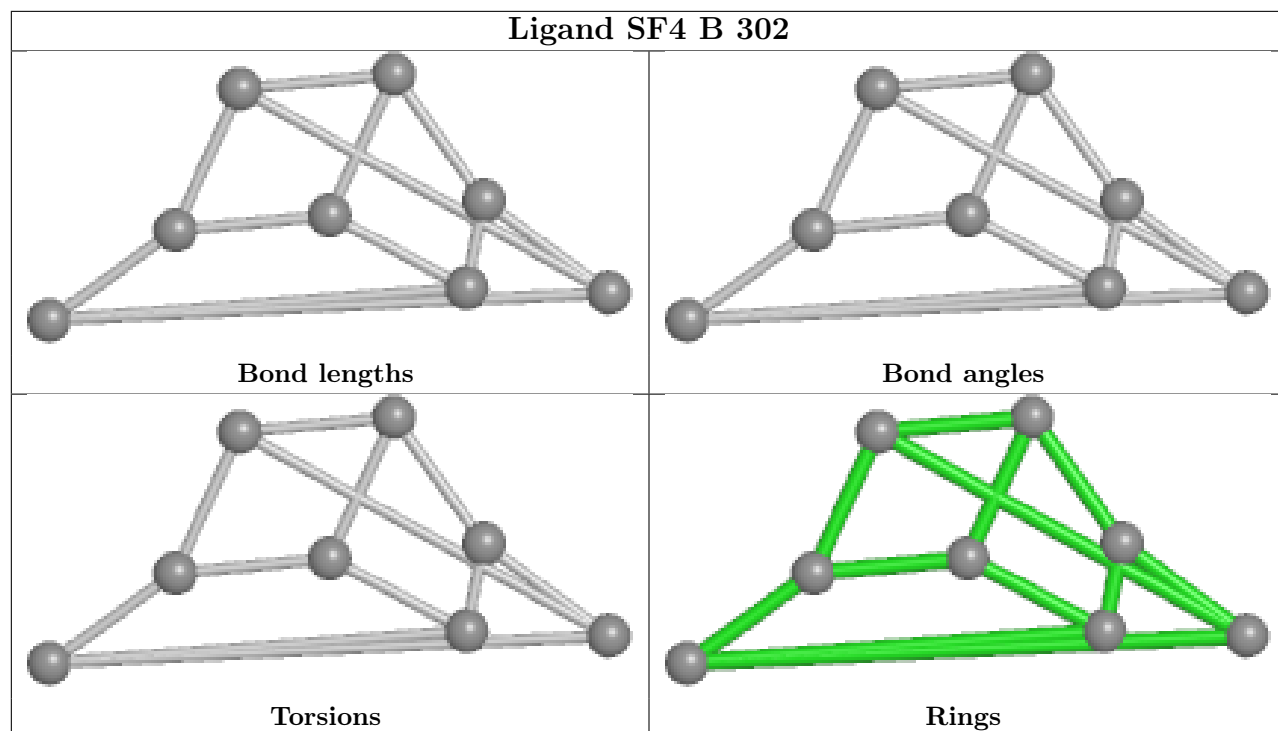


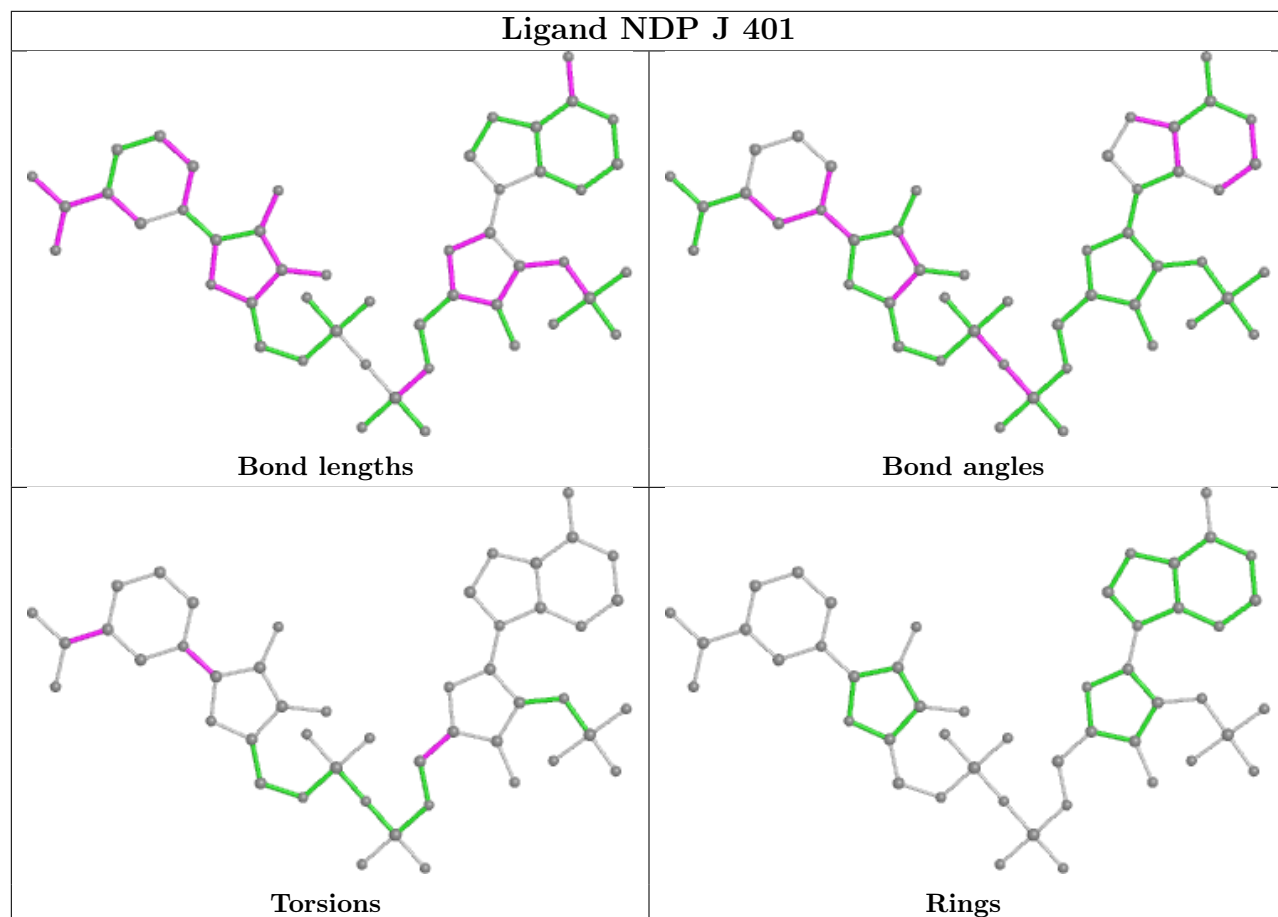
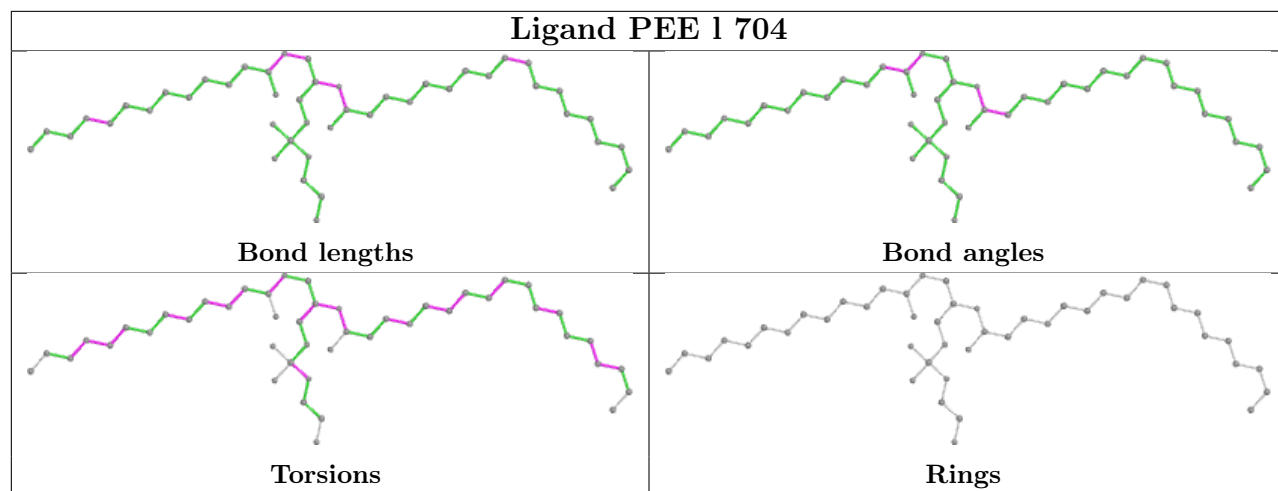


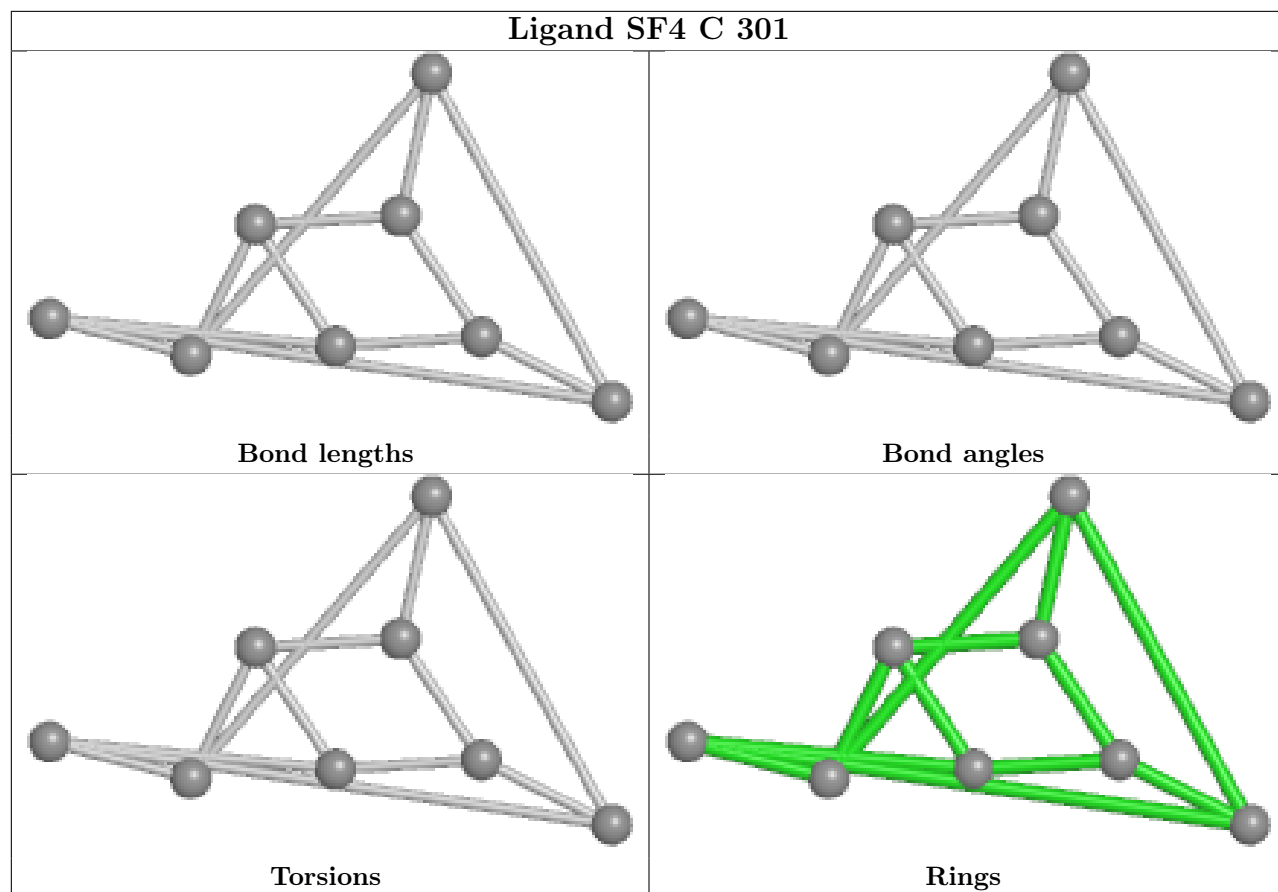


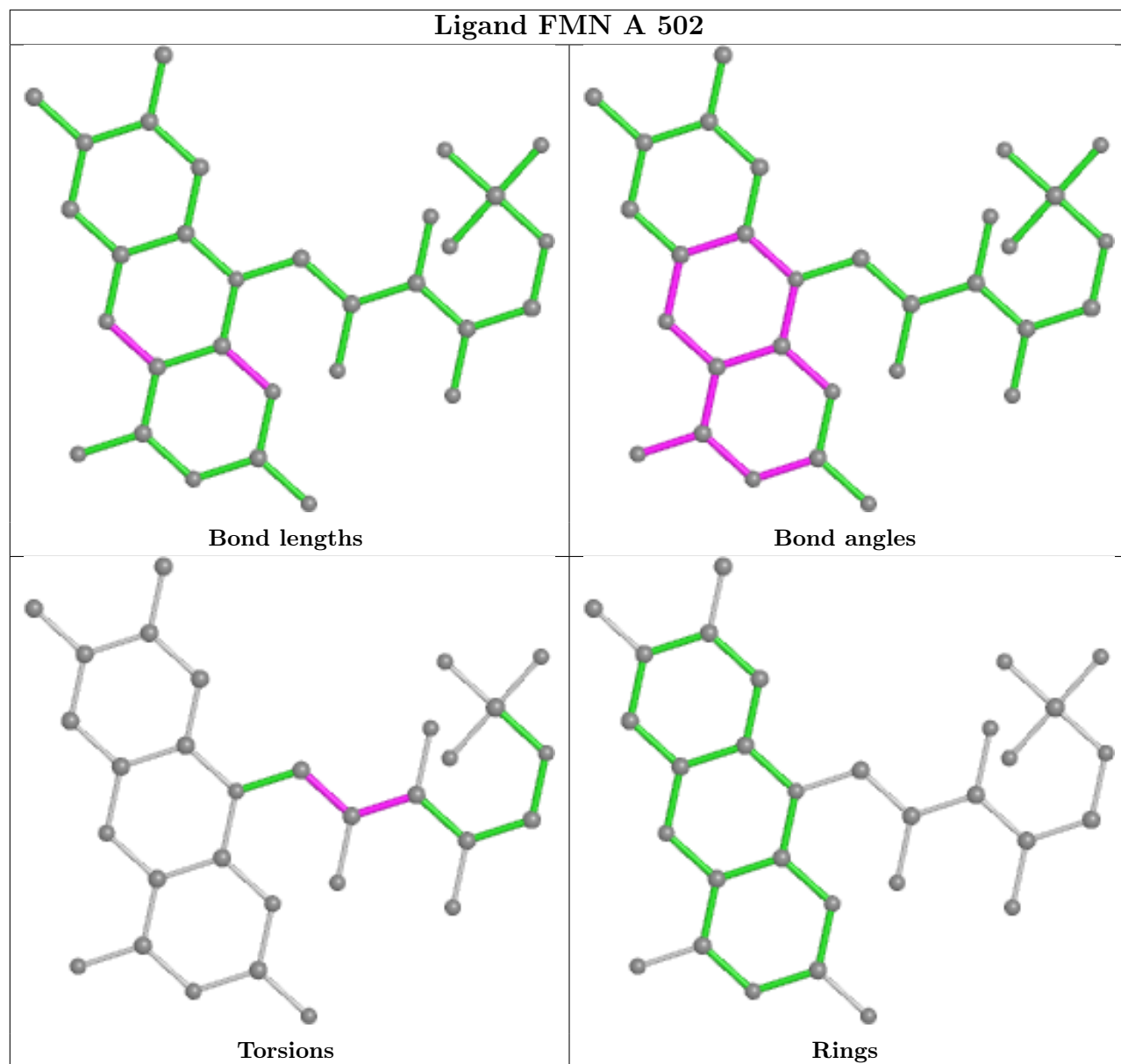


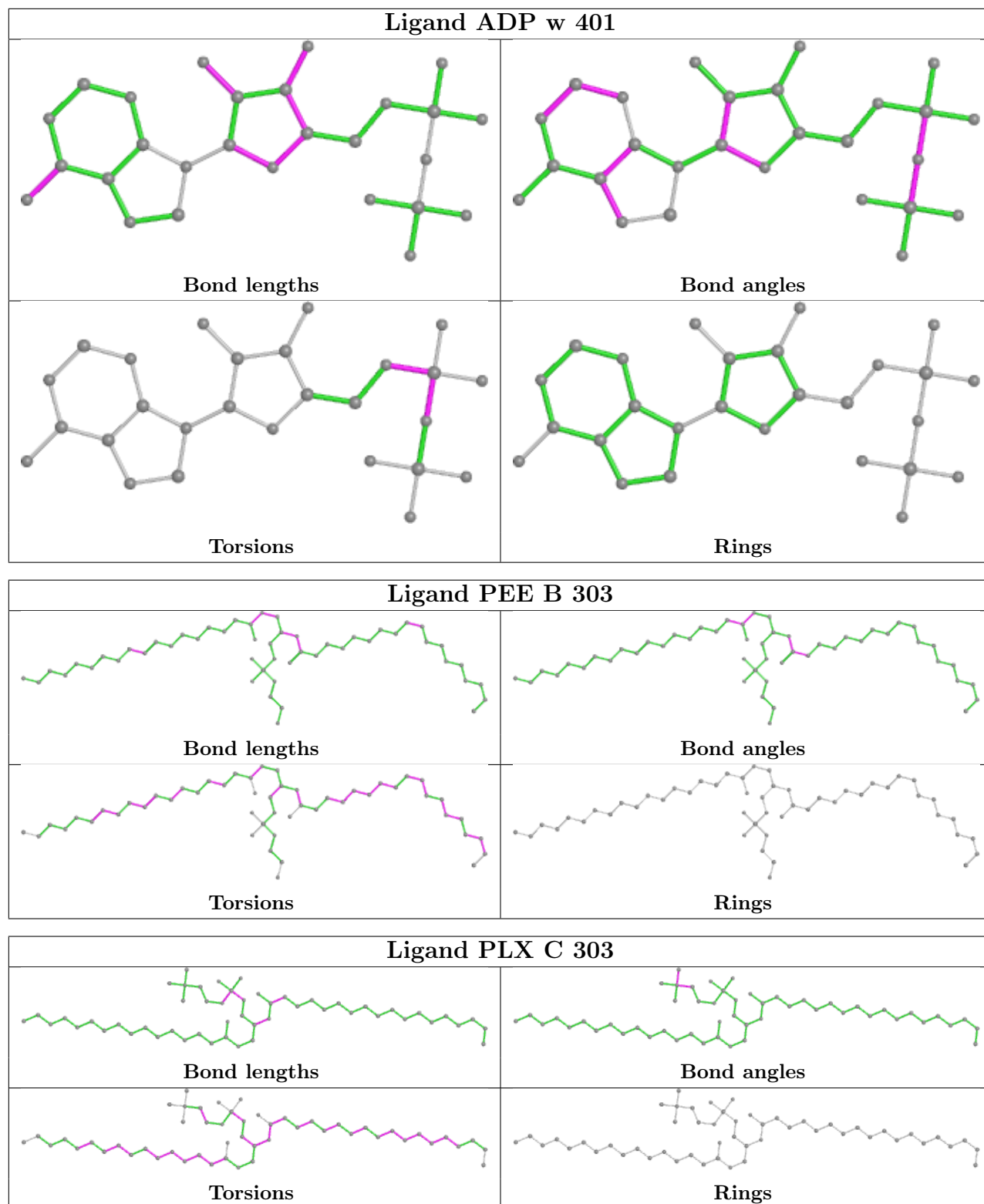












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

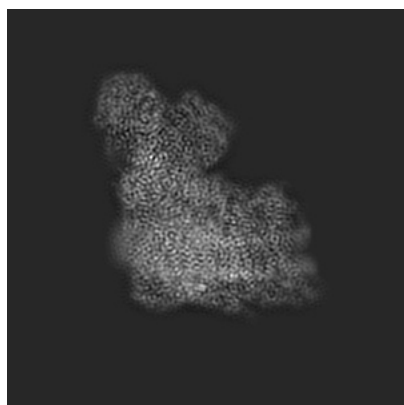
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32232. These allow visual inspection of the internal detail of the map and identification of artifacts.

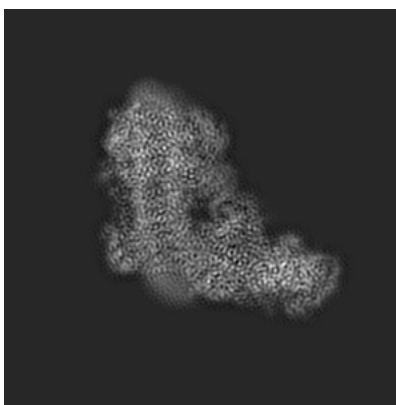
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

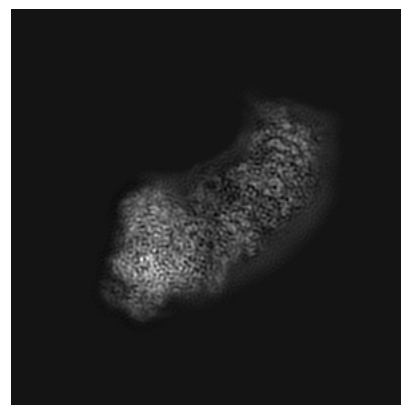
#### 6.1.1 Primary map



X



Y

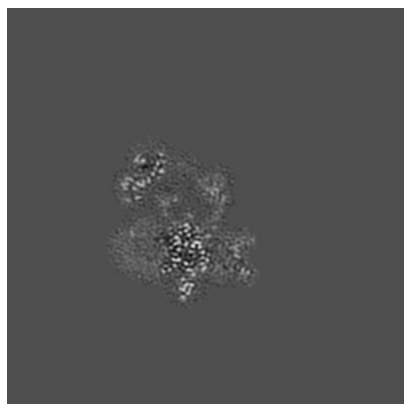


Z

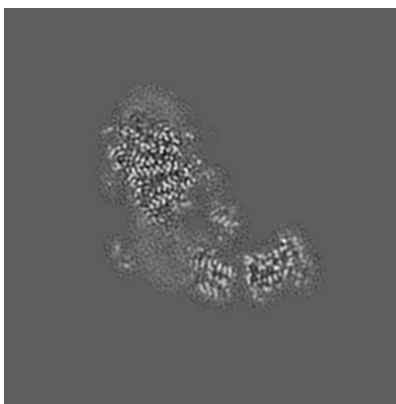
The images above show the map projected in three orthogonal directions.

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

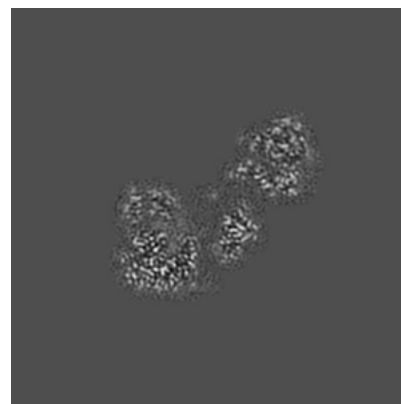
#### 6.2.1 Primary map



X Index: 165



Y Index: 165

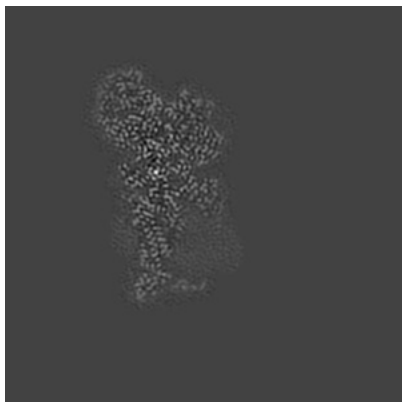


Z Index: 165

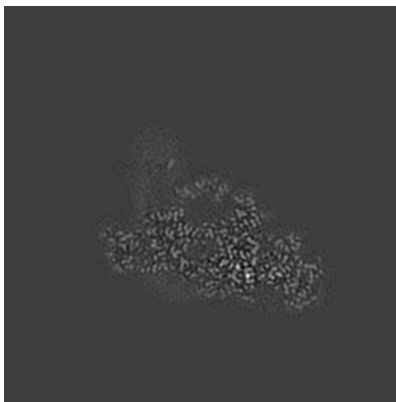
The images above show central slices of the map in three orthogonal directions.

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

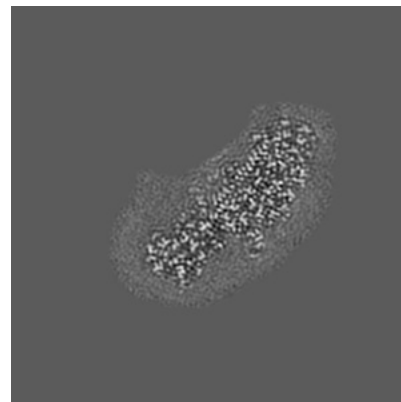
### 6.3.1 Primary map



X Index: 115



Y Index: 123

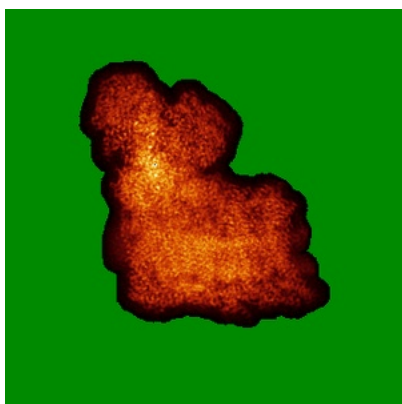


Z Index: 137

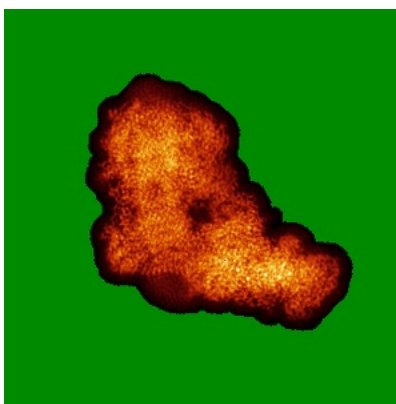
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

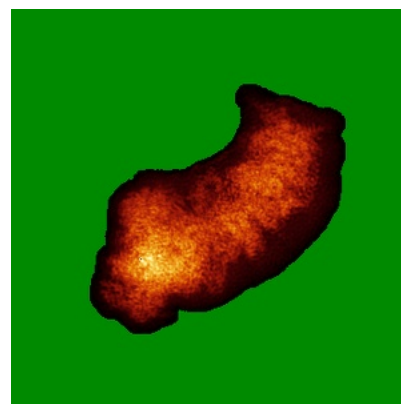
### 6.4.1 Primary map



X



Y



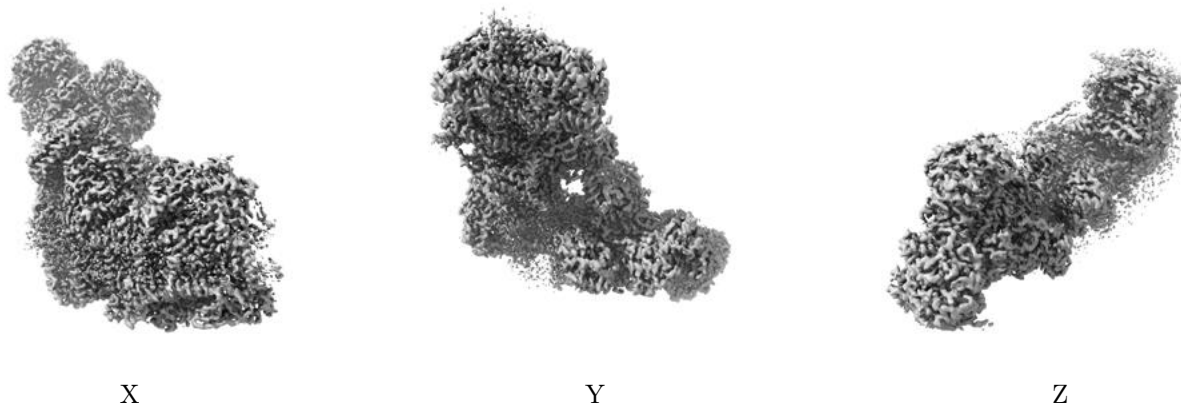
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

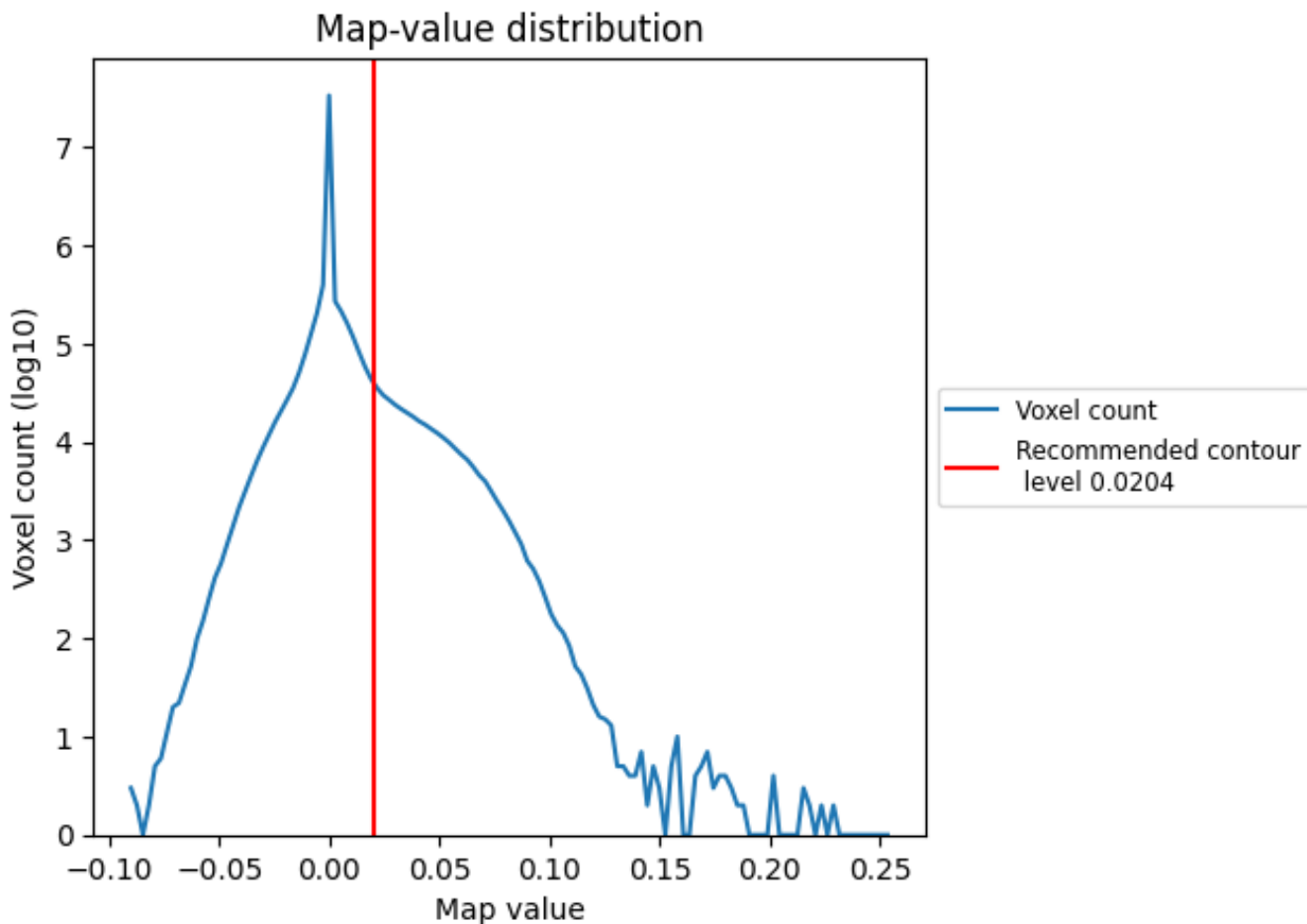
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

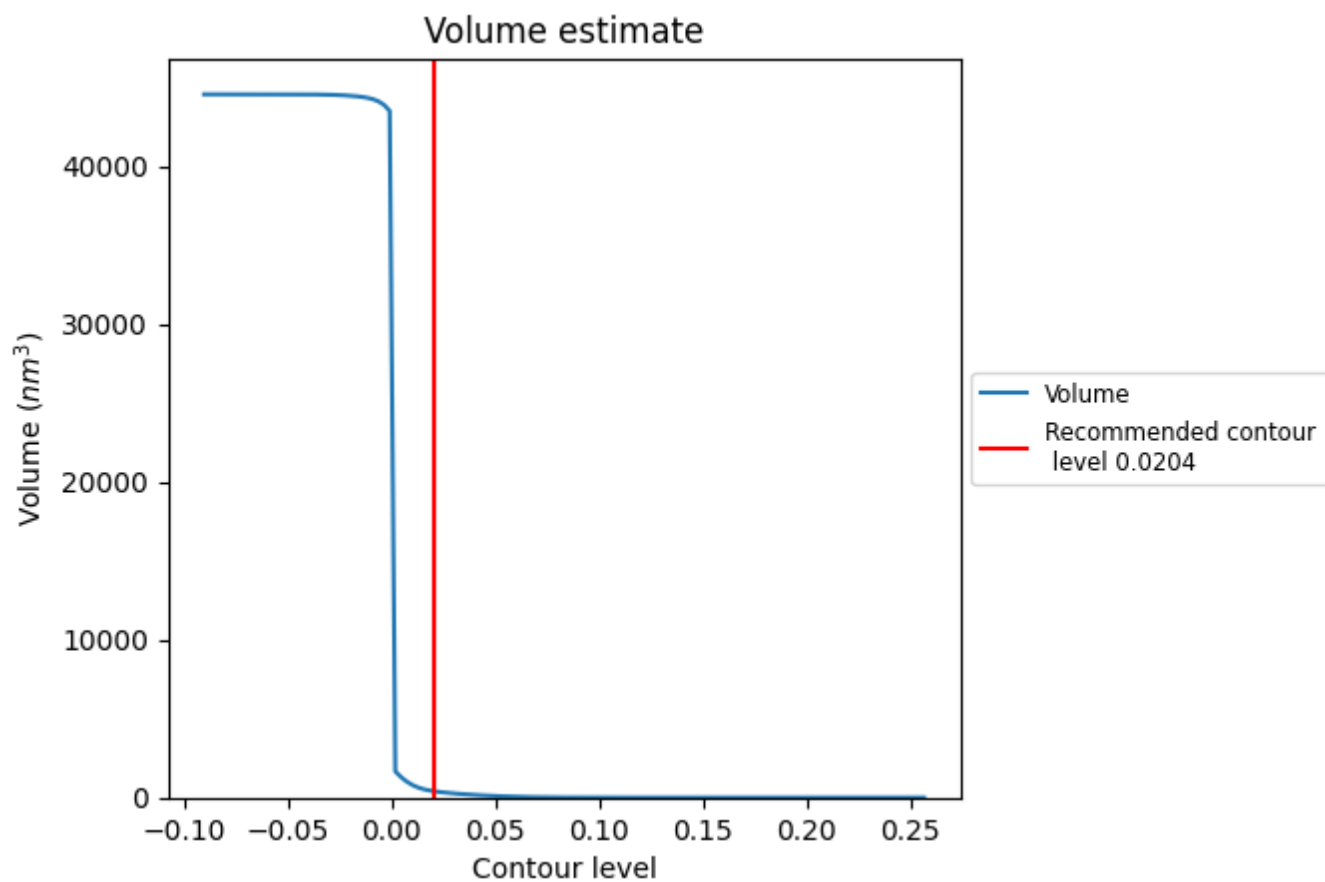
This section contains the results of statistical analysis of the map.

### 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.

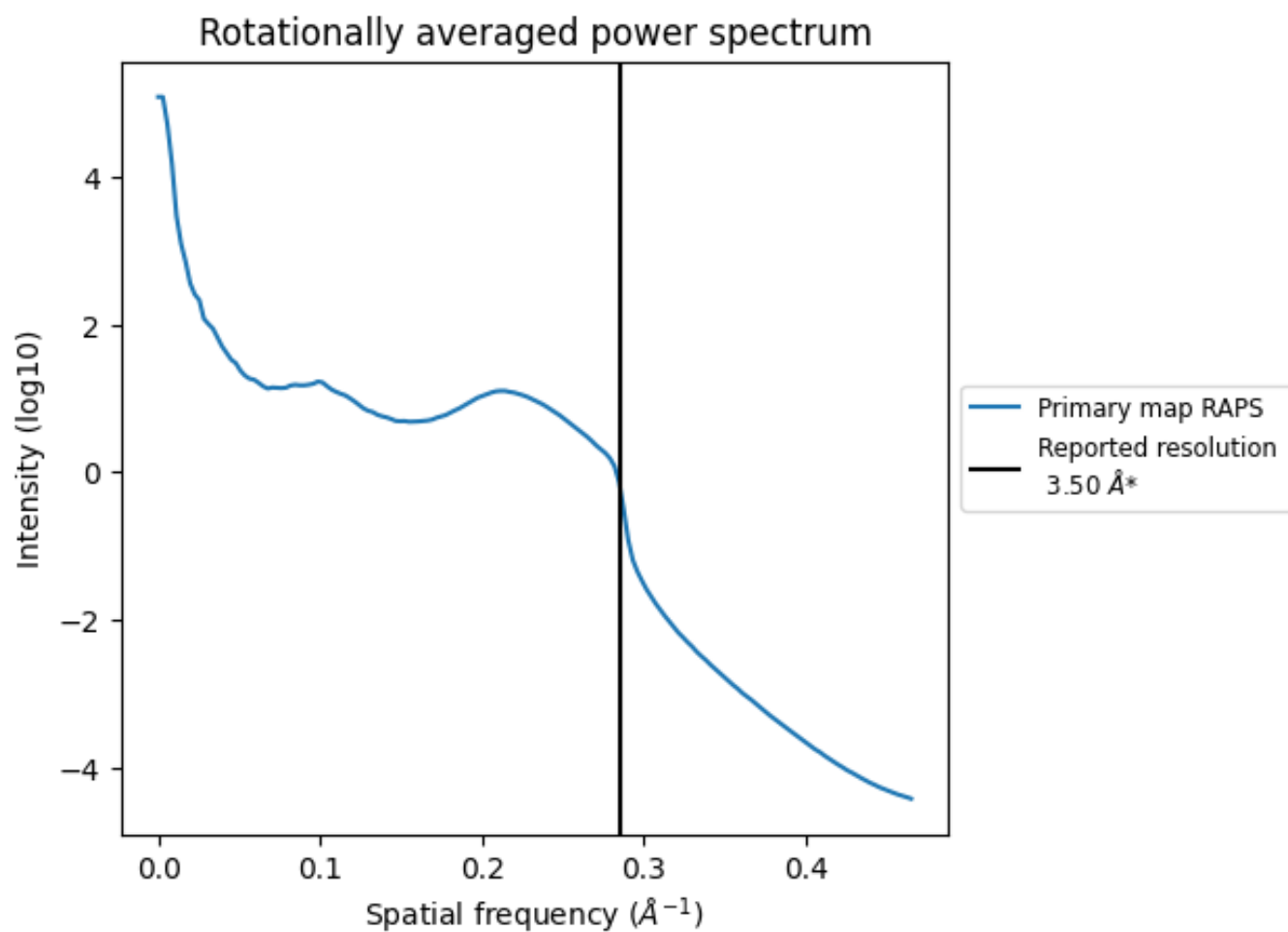
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404  $\text{nm}^3$ ; this corresponds to an approximate mass of 365 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.286 \text{\AA}^{-1}$

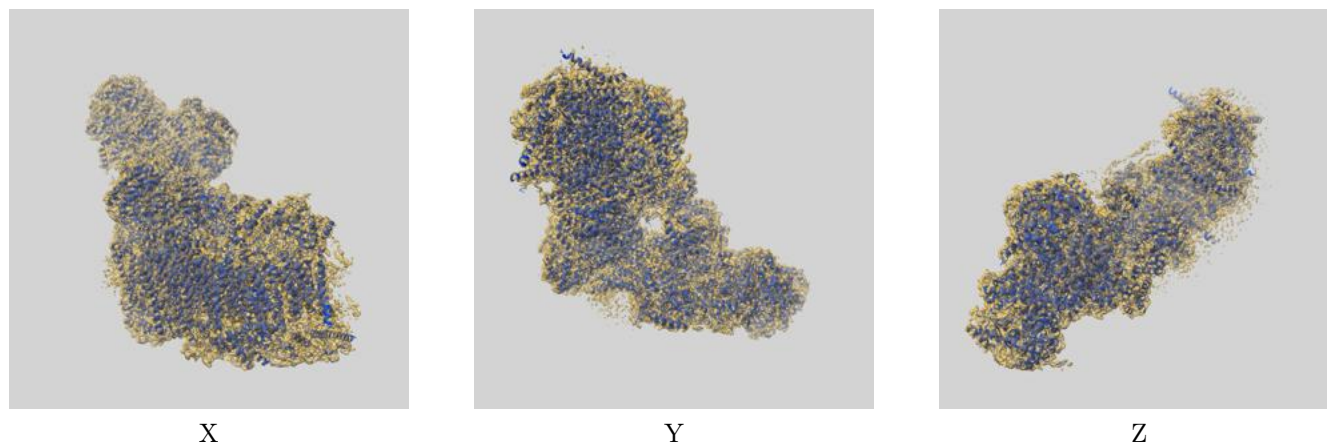
## 8 Fourier-Shell correlation

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

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

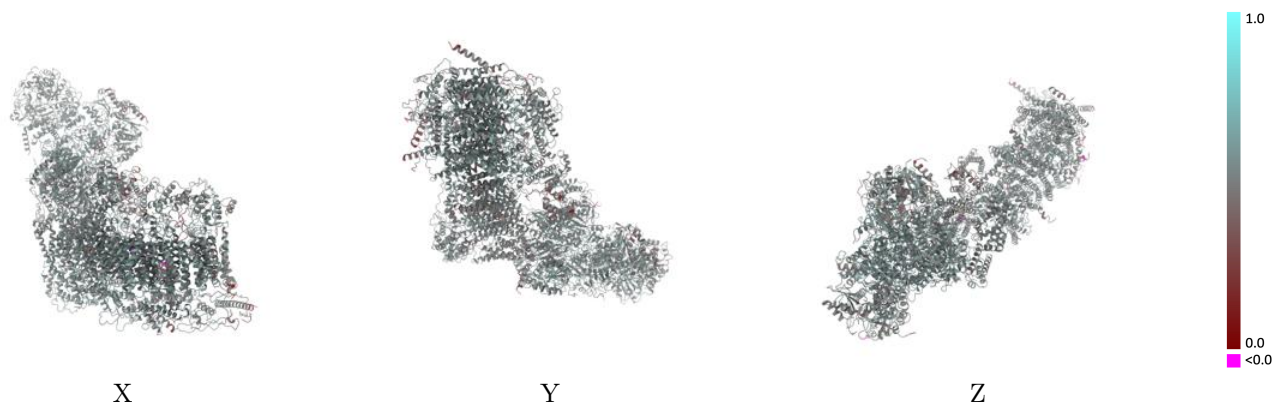
This section contains information regarding the fit between EMDB map EMD-32232 and PDB model 7W00. Per-residue inclusion information can be found in section 3 on page 20.

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



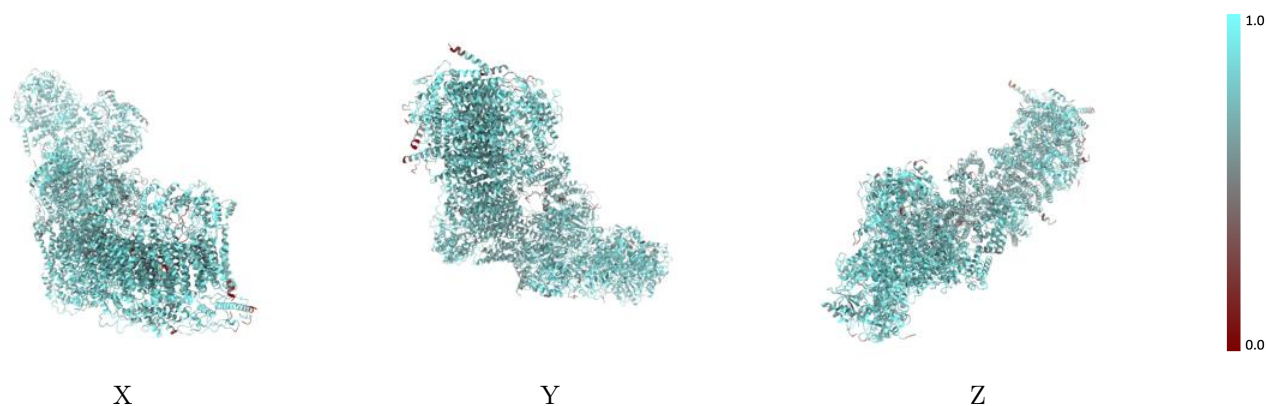
The images above show the 3D surface view of the map at the recommended contour level 0.0204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



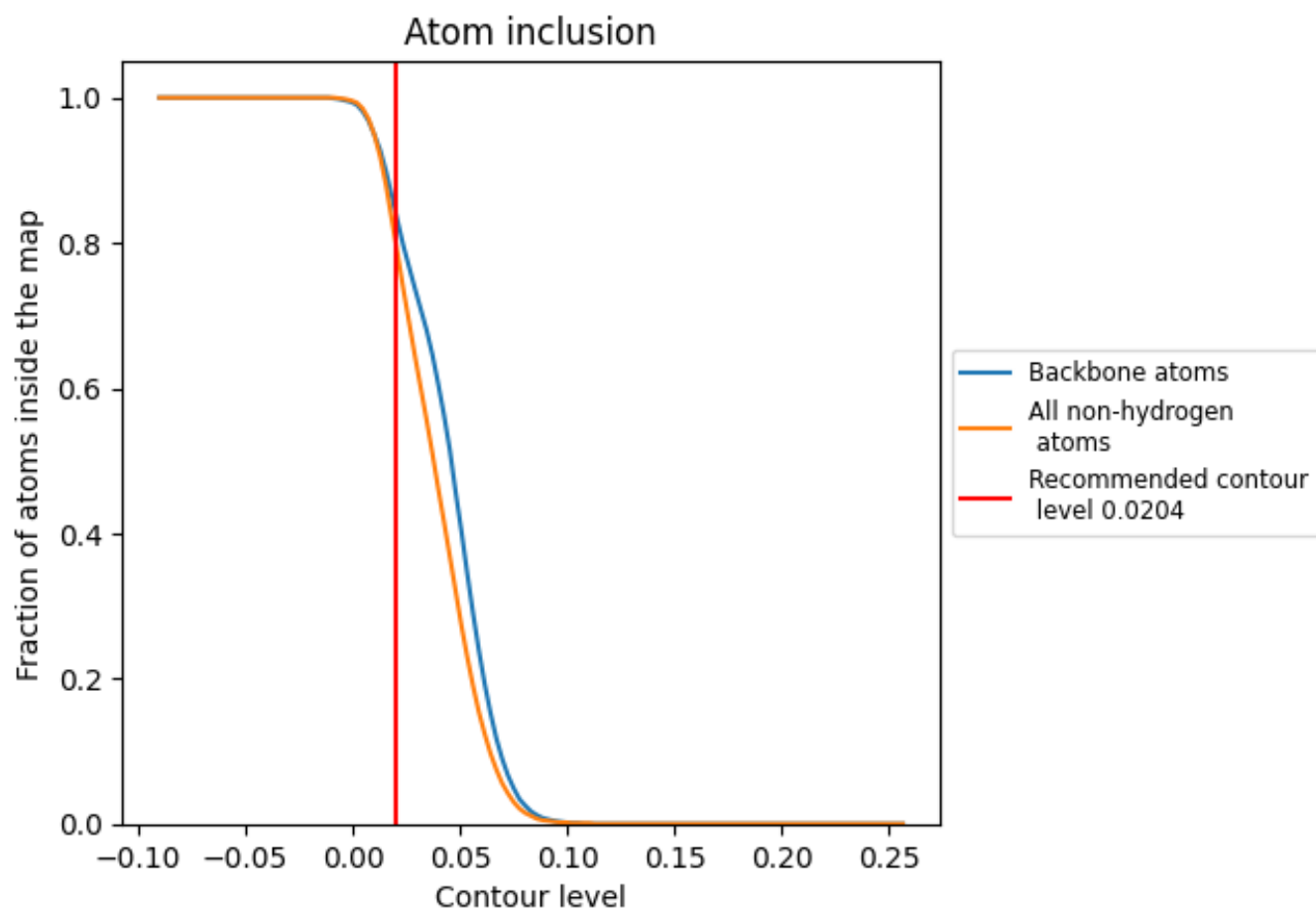
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0204).

## 9.4 Atom inclusion [i](#)









































































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 (0.0204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.5190
A	 0.8060	 0.5150
B	 0.8750	 0.5500
C	 0.8280	 0.5390
E	 0.7760	 0.5180
F	 0.7430	 0.4770
G	 0.6310	 0.4170
H	 0.7900	 0.5050
I	 0.7750	 0.5290
J	 0.7770	 0.5140
K	 0.7940	 0.5110
L	 0.7960	 0.5270
M	 0.8260	 0.5290
N	 0.7490	 0.5180
O	 0.7770	 0.5040
P	 0.8510	 0.5490
Q	 0.8380	 0.5420
S	 0.8480	 0.5290
T	 0.7940	 0.5360
U	 0.7920	 0.5120
V	 0.6590	 0.4780
W	 0.8130	 0.5260
X	 0.7430	 0.4880
Y	 0.7580	 0.4820
Z	 0.6670	 0.4490
a	 0.8070	 0.5390
b	 0.7190	 0.4870
c	 0.8040	 0.5260
d	 0.7820	 0.5060
e	 0.7500	 0.5020
f	 0.7530	 0.4940
g	 0.8220	 0.5300
h	 0.8010	 0.5270
i	 0.8300	 0.5360
j	 0.6940	 0.4960



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Chain	Atom inclusion	Q-score
k	 0.7560	 0.5150
l	 0.7960	 0.5260
m	 0.7490	 0.4970
n	 0.7000	 0.4940
o	 0.7610	 0.5180
p	 0.8070	 0.5170
r	 0.8140	 0.5360
s	 0.8130	 0.5220
u	 0.8200	 0.5260
v	 0.7540	 0.4850
w	 0.7840	 0.5110