



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2023 – 12:09 PM JST

PDB ID : 7W4L  
EMDB ID : EMD-32307  
Title : Deactive state CI from Q1-NADH dataset, Subclass 3  
Authors : Gu, J.; Yang, M.  
Deposited on : 2021-11-28  
Resolution : 3.10 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:

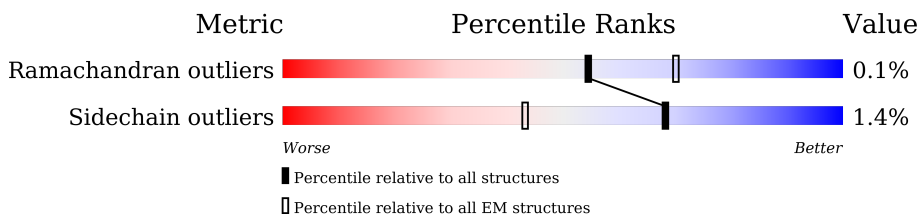
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal 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 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	

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Mol	Chain	Length	Quality of chain
9	J	342	16% 85% 13%
10	K	43	28% 95%
11	L	125	6% 98%
12	M	690	9% 100%
13	N	144	7% 99%
14	O	217	28% 98%
15	P	208	97%
16	Q	430	96%
17	S	70	100%
18	T	96	12% 97%
19	U	83	10% 99%
20	V	140	33% 98%
21	W	142	6% 100%
22	Y	70	21% 93% 7%
23	Z	84	24% 99%
24	a	140	99%
25	b	126	11% 79% 18%
26	c	156	8% 99%
27	d	175	9% 97%
28	e	107	12% 99%
29	f	49	12% 86% 14%
30	g	122	98%
31	h	105	8% 99%
32	i	347	99%
33	j	115	12% 85% 14%

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Mol	Chain	Length	Quality of chain
34	k	98	<p>7% 96%</p>
35	l	603	<p>99%</p>
36	m	175	<p>11% 71% 26%</p>
37	n	56	<p>18% 96%</p>
38	o	128	<p>5% 100%</p>
39	p	178	<p>99%</p>
40	r	459	<p>99%</p>
41	s	318	<p>5% 94% 5%</p>
42	u	171	<p>98%</p>
43	v	124	<p>15% 98%</p>
44	w	320	<p>12% 99%</p>

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66469 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	3300	2085	590	605	20	0	0

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			686	441	102	138	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2352	1510	420	414	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
			5295	3320	923	1013	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	1671	1065	281	315	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
			1014	648	171	189	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
			1173	755	203	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
			587	386	98	102	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
			867	567	152	147	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	1307	849	213	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	1457	914	265	270	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 NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	42	342	225	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	996	647	172	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	2707	1780	420	462	45	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	799	545	118	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	4781	3172	740	818	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	948	636	138	166	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	473	308	85	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	1058	689	182	187	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	1528	979	279	262	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	303	2394	1607	369	397	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	1386	881	250	245	10	0	0

- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1016	636	189	182	9	0	0

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

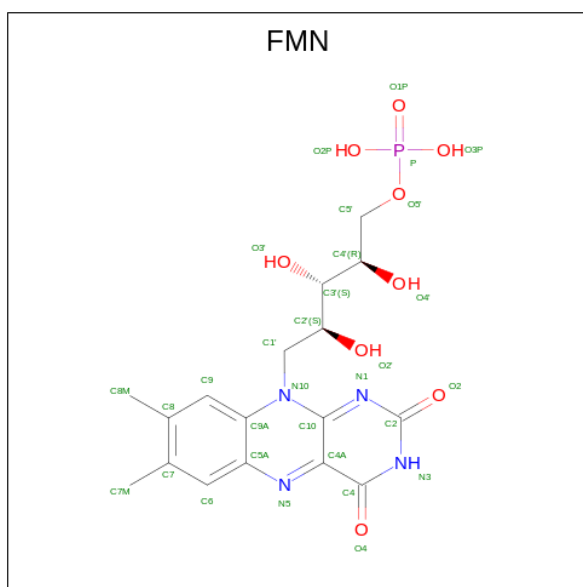
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2582	1643	438	491	10	0	0

- 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).



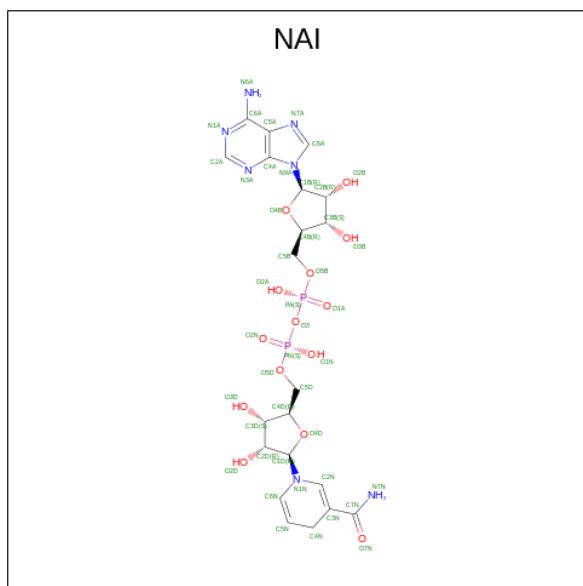
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	8	4	4	0
45	B	1	8	4	4	0
45	C	1	8	4	4	0
45	M	1	8	4	4	0
45	M	1	8	4	4	0

- 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).



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

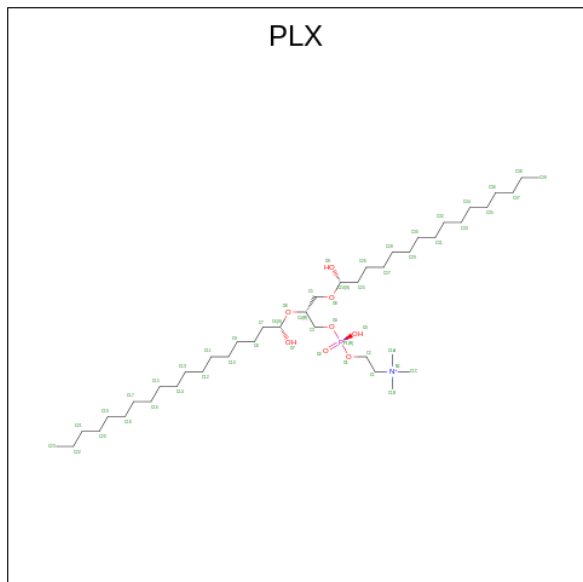
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

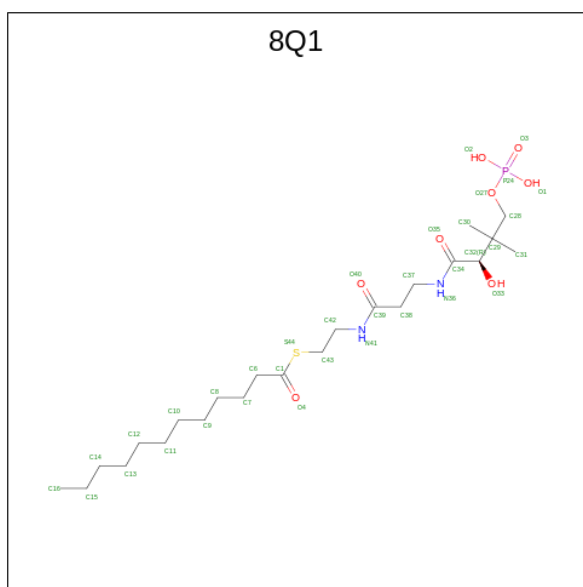
- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSA

NE-6,6,11-TRIOL (three-letter code: PLX) (formula:  $C_{42}H_{89}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



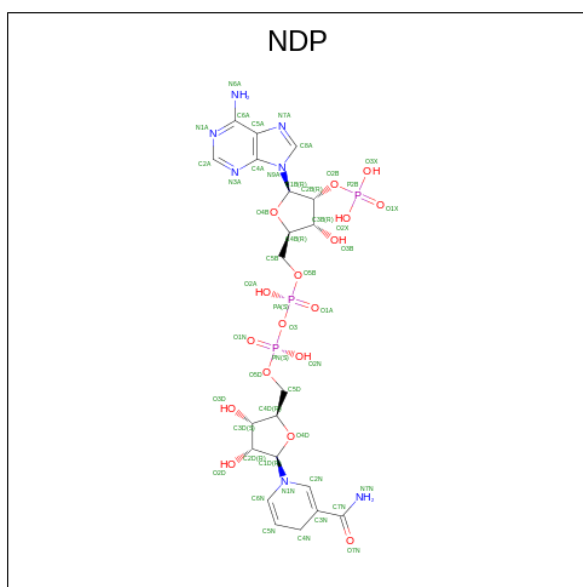
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	C	1	Total 52	C 42	N 1	O 8	P 1	0
48	a	1	Total 52	C 42	N 1	O 8	P 1	0
48	g	1	Total 52	C 42	N 1	O 8	P 1	0
48	j	1	Total 52	C 42	N 1	O 8	P 1	0
48	r	1	Total 52	C 42	N 1	O 8	P 1	0
48	r	1	Total 52	C 42	N 1	O 8	P 1	0

- 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:  $C_{23}H_{45}N_2O_8PS$ ).



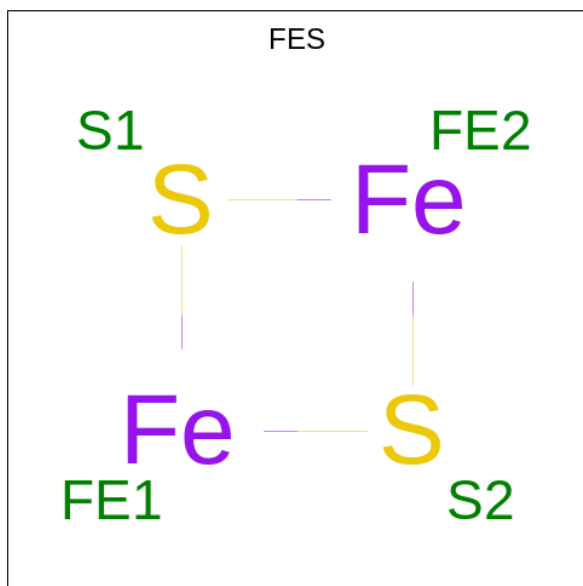
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



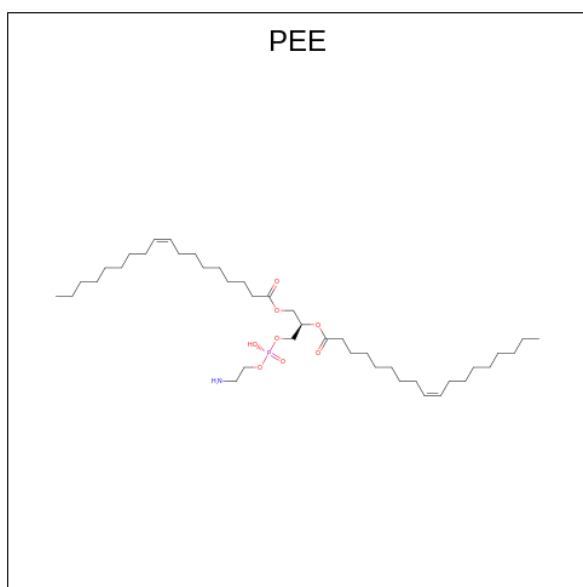
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
51	M	1	4	2	2	0
51	O	1	4	2	2	0

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

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

- Molecule 53 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



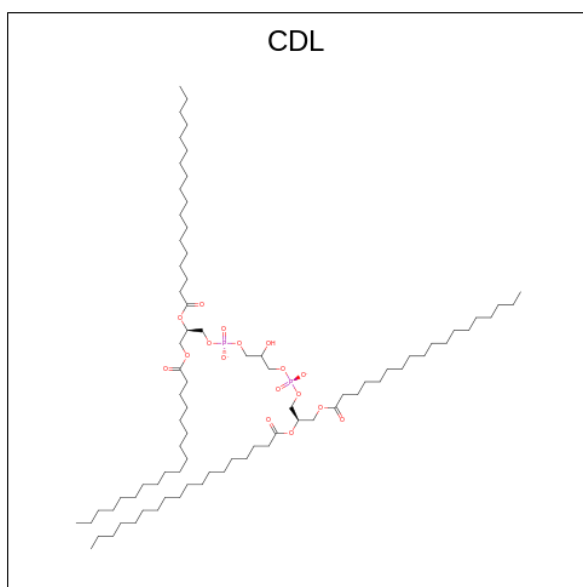


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	Q	1	47	37	1	8	1	0
53	Q	1	51	41	1	8	1	0
53	j	1	47	37	1	8	1	0
53	j	1	51	41	1	8	1	0
53	l	1	46	36	1	8	1	0
53	l	1	46	36	1	8	1	0
53	m	1	41	31	1	8	1	0
53	r	1	51	41	1	8	1	0

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

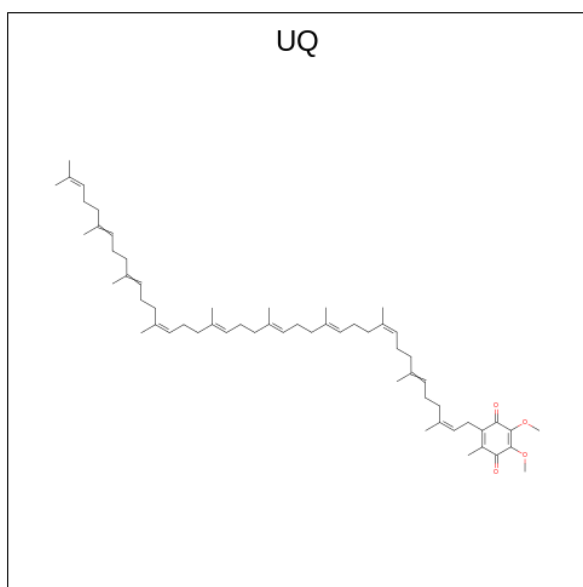
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	T	1	1	1	0

- Molecule 55 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



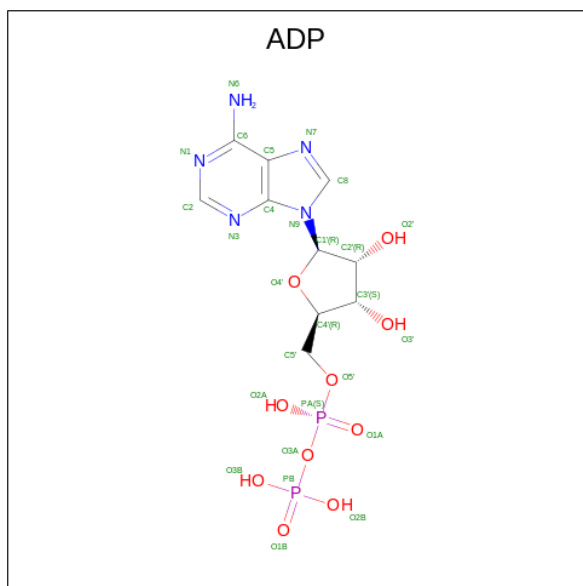
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
55	V	1	71	52	17	2	0
55	a	1	91	72	17	2	0
55	g	1	100	81	17	2	0
55	i	1	66	47	17	2	0
55	l	1	100	81	17	2	0

- Molecule 56 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
56	s	1	Total	C	O	0
			28	24	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

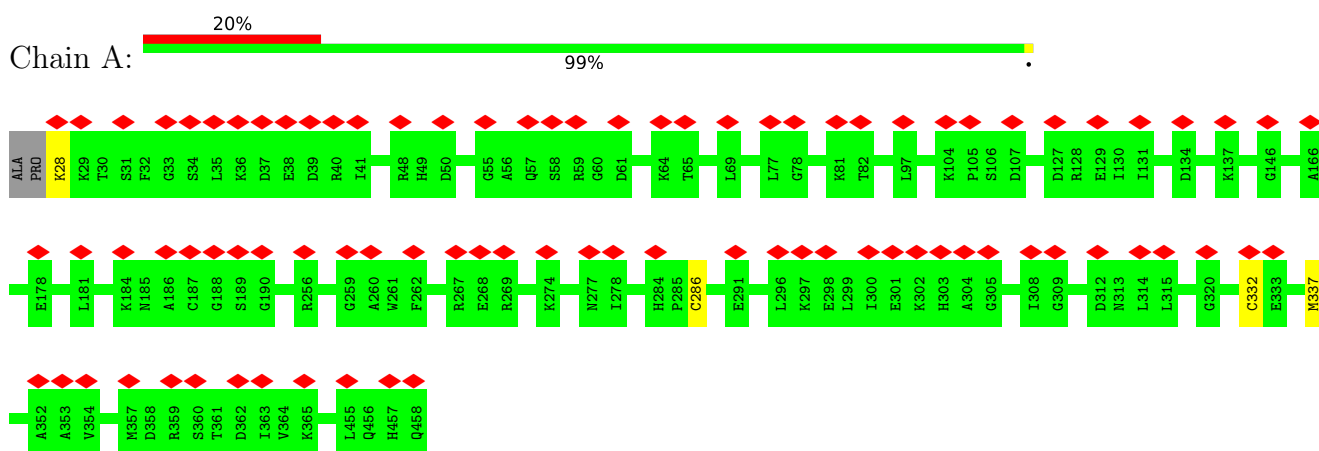


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

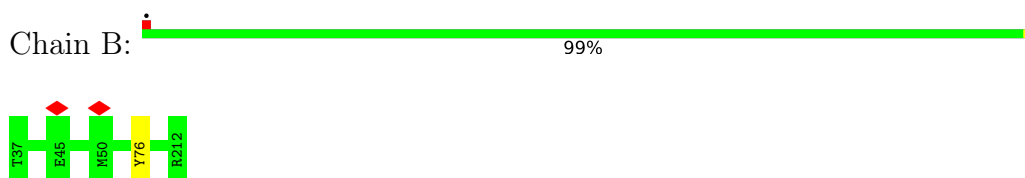
### 3 Residue-property plots [i](#)

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

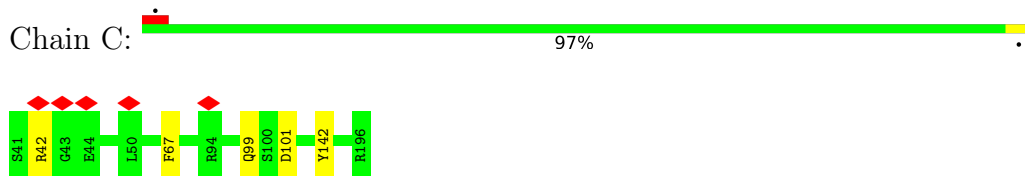
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



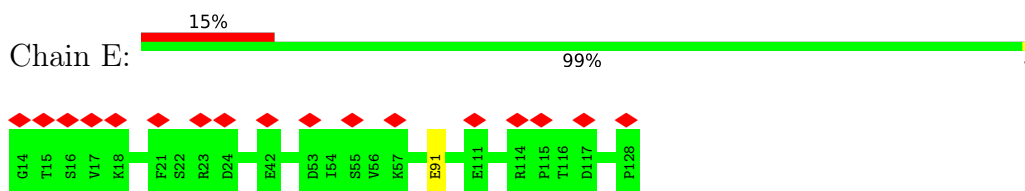
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



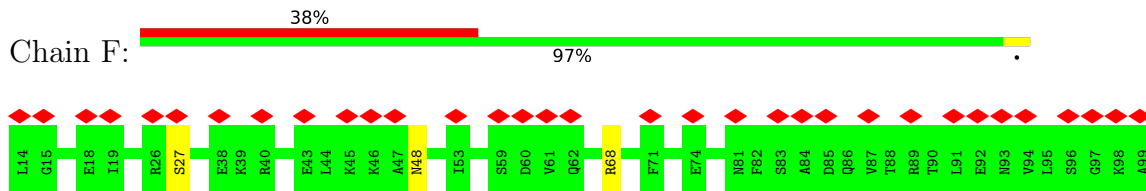
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



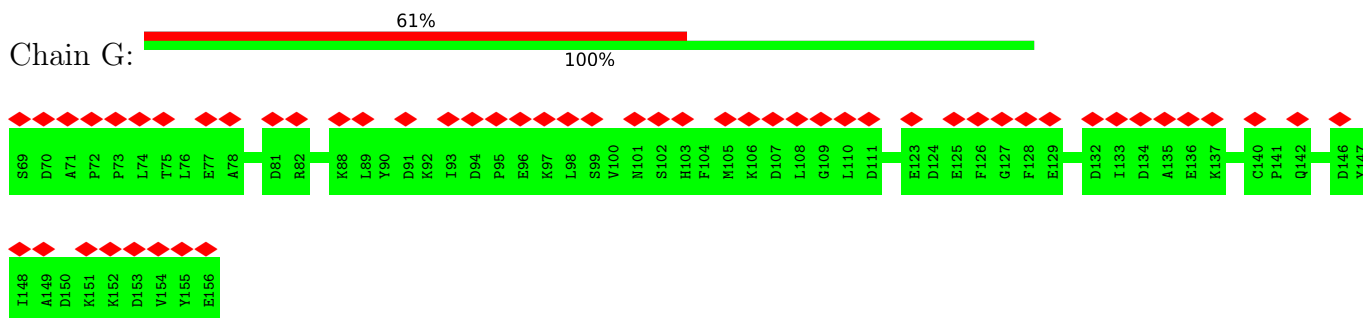
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



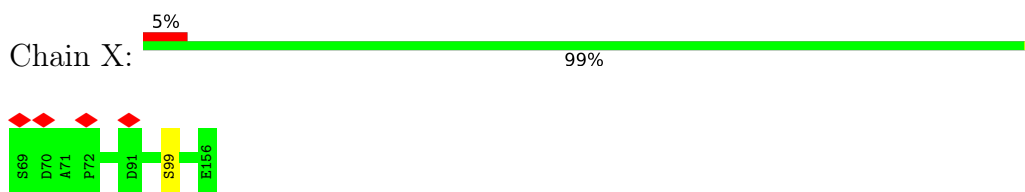
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



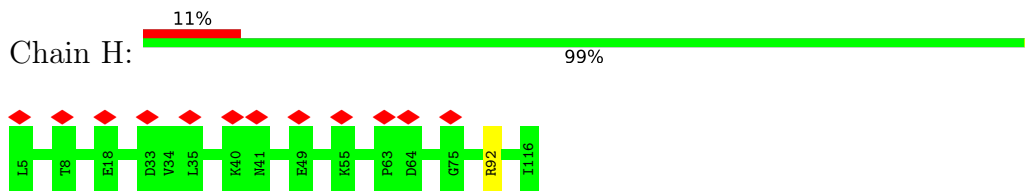
- Molecule 6: Acyl carrier protein



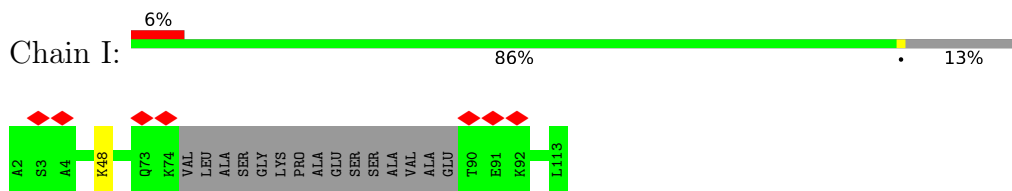
- Molecule 6: Acyl carrier protein



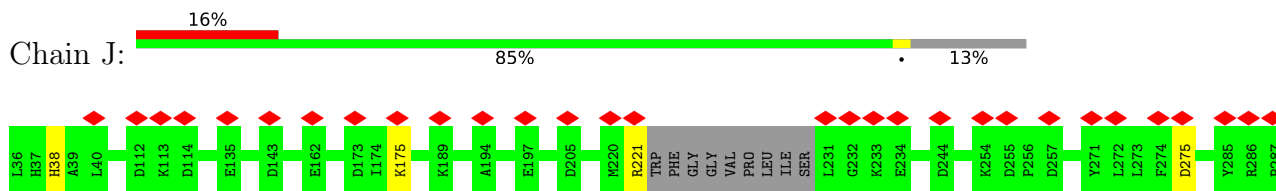
- Molecule 7: Complex I subunit B13

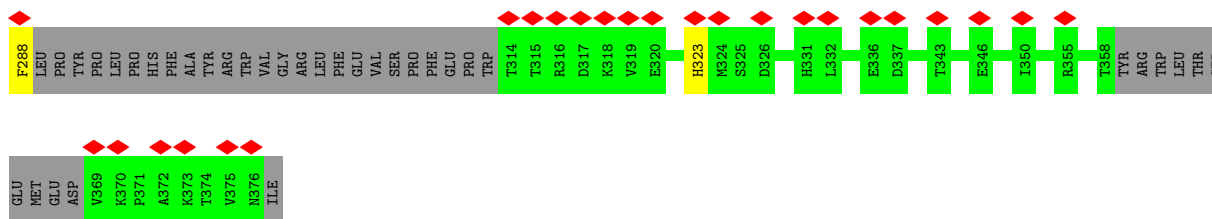


- Molecule 8: Complex I-B14.5a

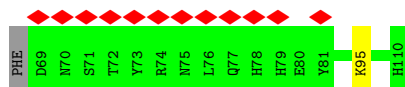


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

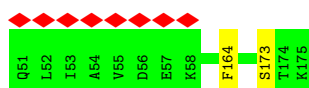




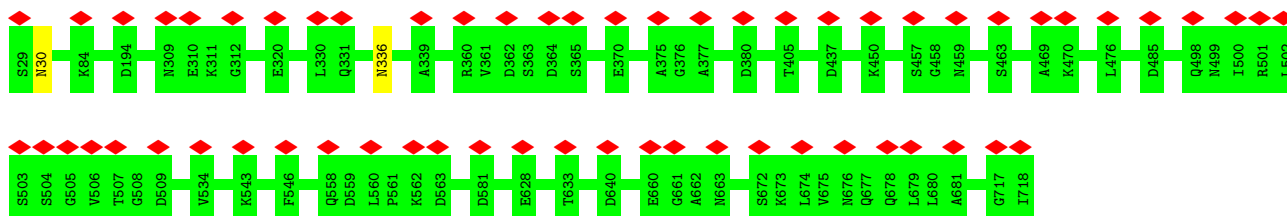
- Molecule 10: Complex I-9kD



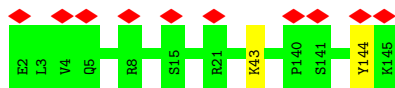
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



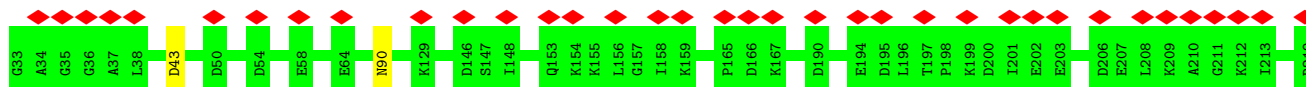
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

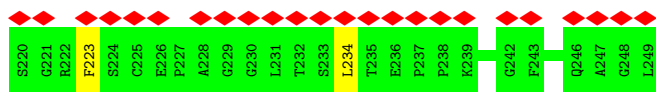


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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





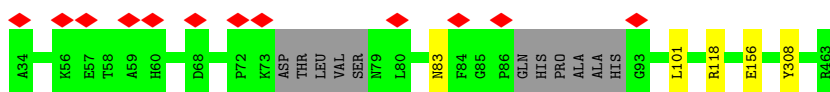
- Molecule 15: Complex I-30kD

Chain P: 97%



- Molecule 16: Complex I-49kD

Chain Q: 96%



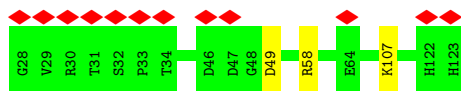
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 100%



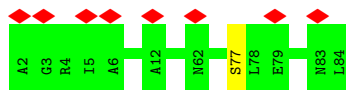
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 12% 97%



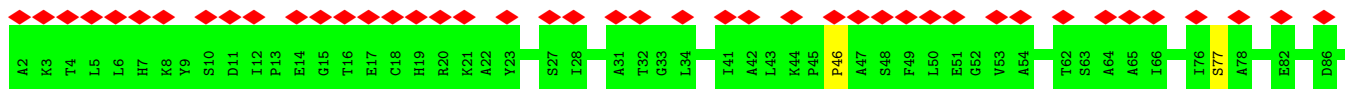
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

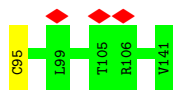
Chain U: 10% 99%



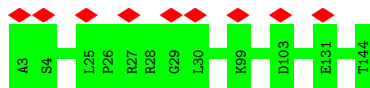
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 33% 98%

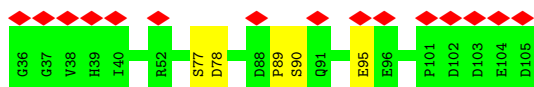
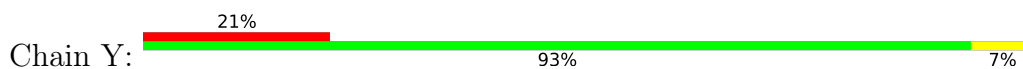




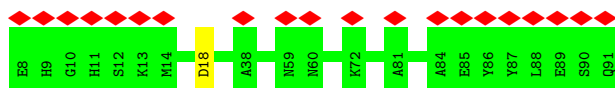
- Molecule 21: Complex I-B16.6



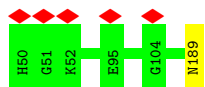
- Molecule 22: Complex I-AGGG



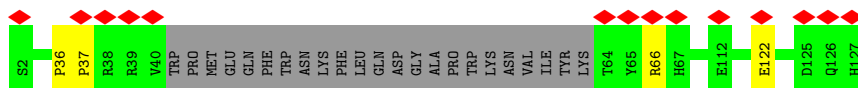
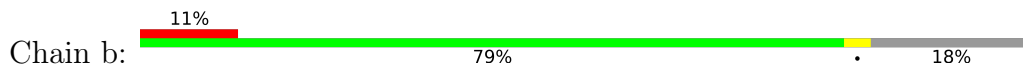
- Molecule 23: Complex I-B12



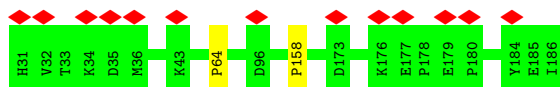
- Molecule 24: Complex I-SGDH



- Molecule 25: Complex I-B17

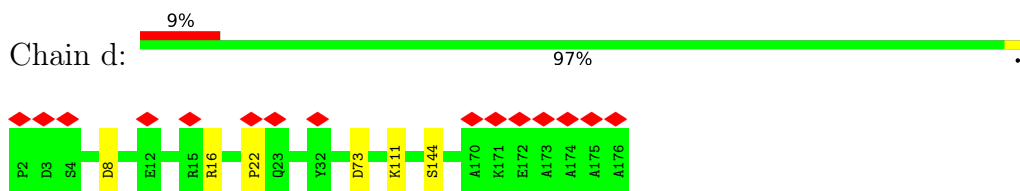


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

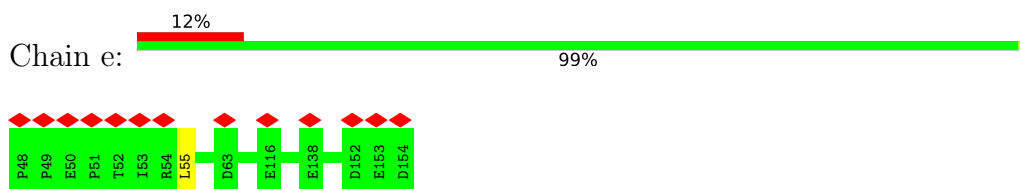




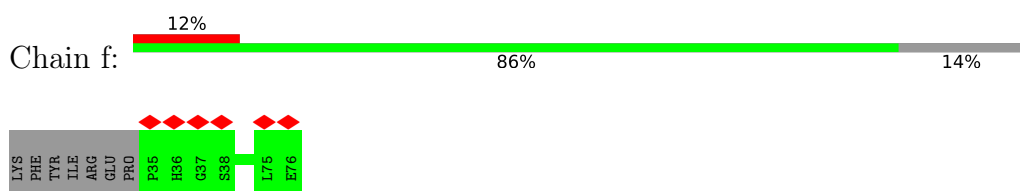
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



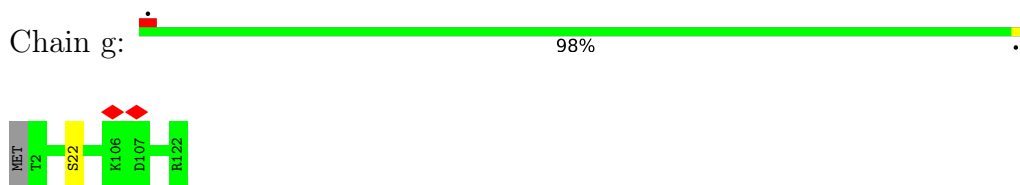
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



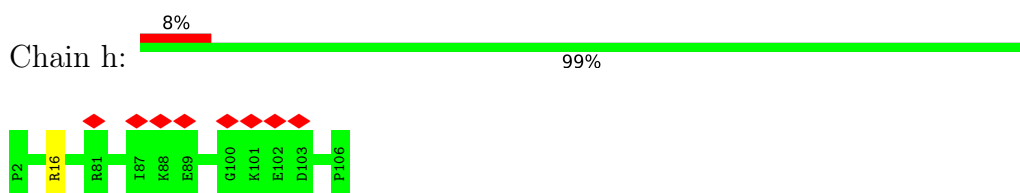
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



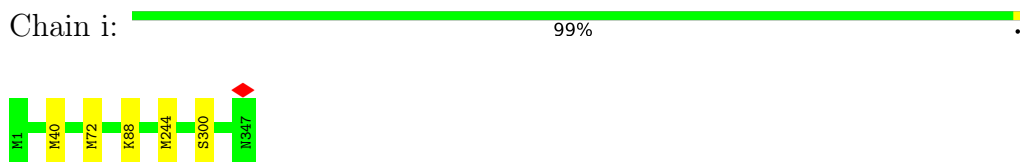
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



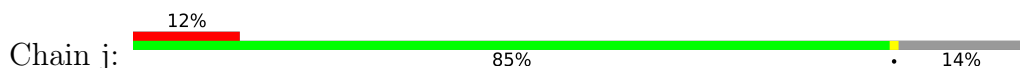
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

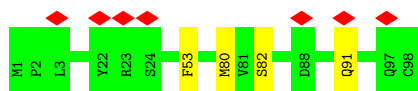


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

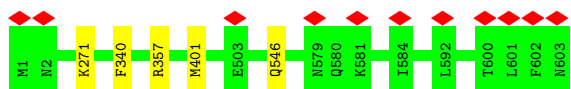




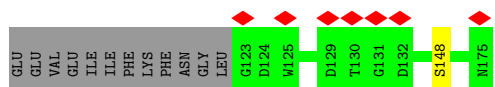
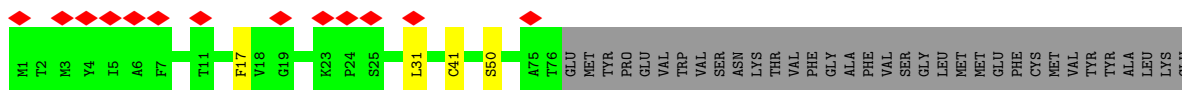
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



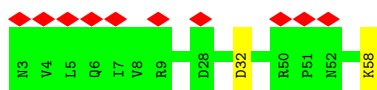
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



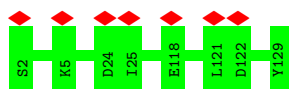
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



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

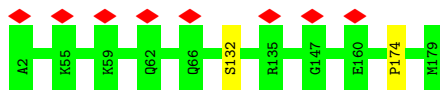


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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

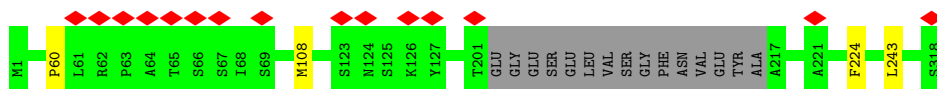
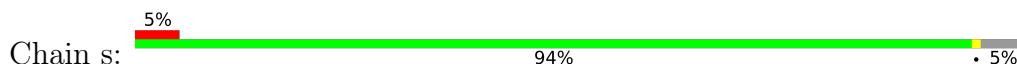




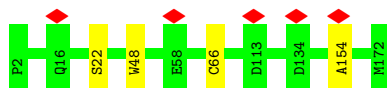
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



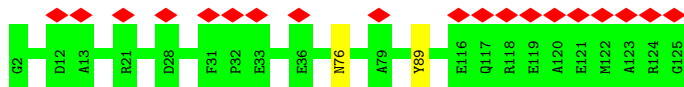
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



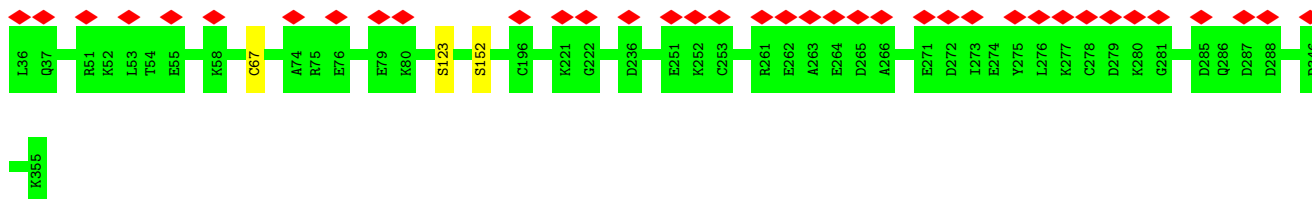
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



- 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	42665	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	0.219	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0296	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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: SF4, FES, NAI, 8Q1, UQ, PLX, NDP, ADP, FMN, ZN, PEE, 2MR, CDL, MG

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	0.26	0/3374	0.51	0/4559
2	B	0.26	0/1443	0.51	0/1952
3	C	0.26	0/1279	0.53	0/1730
4	E	0.26	0/995	0.53	0/1340
5	F	0.26	0/702	0.54	0/945
6	G	0.27	0/697	0.48	0/945
6	X	0.24	0/708	0.42	0/959
7	H	0.24	0/929	0.44	0/1258
8	I	0.25	0/798	0.55	0/1079
9	J	0.25	0/2404	0.51	0/3246
10	K	0.23	0/365	0.48	0/493
11	L	0.24	0/1039	0.50	0/1403
12	M	0.25	0/5383	0.50	0/7294
13	N	0.24	0/1245	0.52	0/1694
14	O	0.27	0/1711	0.50	0/2328
15	P	0.26	0/1789	0.52	0/2436
16	Q	0.27	0/3451	0.53	1/4672 (0.0%)
17	S	0.26	0/582	0.52	0/783
18	T	0.26	0/755	0.55	0/1018
19	U	0.26	0/664	0.46	0/912
20	V	0.26	0/1035	0.45	0/1403
21	W	0.26	0/1204	0.48	0/1624
22	Y	0.27	0/613	0.52	0/840
23	Z	0.24	0/695	0.44	0/939
24	a	0.26	0/1199	0.49	0/1623
25	b	0.25	0/894	0.53	0/1218
26	c	0.27	0/1363	0.53	0/1865
27	d	0.25	0/1490	0.49	0/2010
28	e	0.26	0/916	0.48	0/1246
29	f	0.25	0/350	0.45	0/473
30	g	0.27	0/1027	0.49	0/1390
31	h	0.25	0/889	0.50	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.25	0/2770	0.45	0/3765
33	j	0.27	0/818	0.49	0/1116
34	k	0.26	0/759	0.44	0/1029
35	l	0.27	0/4910	0.46	0/6678
36	m	0.30	0/970	0.48	0/1316
37	n	0.25	0/485	0.55	1/656 (0.2%)
38	o	0.26	0/1088	0.51	0/1476
39	p	0.26	0/1584	0.52	0/2147
40	r	0.26	0/3723	0.46	1/5078 (0.0%)
41	s	0.28	0/2464	0.51	2/3369 (0.1%)
42	u	0.24	0/1424	0.48	0/1923
43	v	0.29	0/1040	0.57	0/1397
44	w	0.25	0/2642	0.49	0/3580
All	All	0.26	0/66665	0.50	5/90397 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	101	LEU	CB-CG-CD1	-5.97	100.85	111.00
41	s	108	MET	CA-CB-CG	5.75	123.08	113.30
41	s	60	PRO	CA-N-CD	-5.33	104.04	111.50
37	n	32	ASP	CB-CG-OD1	5.04	122.84	118.30
40	r	367	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
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%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/342 (84%)	274 (95%)	14 (5%)	1 (0%)	41	73
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	661 (96%)	27 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	57
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	90 (91%)	7 (7%)	2 (2%)	7	31
26	c	154/156 (99%)	142 (92%)	11 (7%)	1 (1%)	25	59
27	d	173/175 (99%)	168 (97%)	4 (2%)	1 (1%)	25	59
28	e	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
33	j	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
35	l	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
36	m	125/175 (71%)	111 (89%)	14 (11%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
39	p	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	25	59
40	r	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
41	s	299/318 (94%)	284 (95%)	15 (5%)	0	100	100
42	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	25	59
43	v	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	304 (96%)	13 (4%)	1 (0%)	41	73
All	All	8029/8322 (96%)	7679 (96%)	341 (4%)	9 (0%)	54	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	u	154	ALA
9	J	38	HIS
27	d	22	PRO
44	w	123	SER
25	b	37	PRO
25	b	36	PRO
20	V	46	PRO
26	c	64	PRO
39	p	174	PRO

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

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

The Analysed column shows the number of residues for which the sidechain conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/346 (98%)	336 (99%)	4 (1%)	71	88
2	B	151/151 (100%)	150 (99%)	1 (1%)	84	93
3	C	132/132 (100%)	127 (96%)	5 (4%)	33	66
4	E	107/107 (100%)	106 (99%)	1 (1%)	78	91
5	F	76/76 (100%)	73 (96%)	3 (4%)	32	65
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	77/81 (95%)	76 (99%)	1 (1%)	69	87
7	H	99/99 (100%)	98 (99%)	1 (1%)	76	90
8	I	87/97 (90%)	86 (99%)	1 (1%)	73	89
9	J	253/296 (86%)	248 (98%)	5 (2%)	55	80
10	K	41/42 (98%)	40 (98%)	1 (2%)	49	76
11	L	113/113 (100%)	111 (98%)	2 (2%)	59	82
12	M	579/580 (100%)	577 (100%)	2 (0%)	92	96
13	N	130/130 (100%)	128 (98%)	2 (2%)	65	85
14	O	183/183 (100%)	179 (98%)	4 (2%)	52	78
15	P	190/190 (100%)	184 (97%)	6 (3%)	39	69
16	Q	361/370 (98%)	358 (99%)	3 (1%)	81	92
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	76 (96%)	3 (4%)	33	66
19	U	69/69 (100%)	68 (99%)	1 (1%)	67	86
20	V	99/101 (98%)	97 (98%)	2 (2%)	55	80
21	W	123/123 (100%)	123 (100%)	0	100	100
22	Y	59/63 (94%)	54 (92%)	5 (8%)	10	37
23	Z	65/65 (100%)	64 (98%)	1 (2%)	65	85
24	a	122/122 (100%)	121 (99%)	1 (1%)	81	92
25	b	96/119 (81%)	94 (98%)	2 (2%)	53	79
26	c	139/141 (99%)	138 (99%)	1 (1%)	84	93
27	d	154/155 (99%)	149 (97%)	5 (3%)	39	69
28	e	99/99 (100%)	98 (99%)	1 (1%)	76	90
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	107/109 (98%)	106 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	h	93/93 (100%)	92 (99%)	1 (1%)	73	89
32	i	310/311 (100%)	305 (98%)	5 (2%)	62	84
33	j	87/100 (87%)	86 (99%)	1 (1%)	73	89
34	k	85/85 (100%)	81 (95%)	4 (5%)	26	59
35	l	535/537 (100%)	530 (99%)	5 (1%)	78	91
36	m	98/141 (70%)	93 (95%)	5 (5%)	24	56
37	n	52/53 (98%)	51 (98%)	1 (2%)	57	81
38	o	112/113 (99%)	112 (100%)	0	100	100
39	p	157/159 (99%)	156 (99%)	1 (1%)	86	94
40	r	410/410 (100%)	408 (100%)	2 (0%)	88	94
41	s	263/275 (96%)	261 (99%)	2 (1%)	81	92
42	u	150/153 (98%)	147 (98%)	3 (2%)	55	80
43	v	102/111 (92%)	100 (98%)	2 (2%)	55	80
44	w	281/283 (99%)	279 (99%)	2 (1%)	84	93
All	All	7033/7246 (97%)	6934 (99%)	99 (1%)	68	86

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	286	CYS
1	A	332	CYS
1	A	337	MET
2	B	76	TYR
3	C	42	ARG
3	C	67	PHE
3	C	99	GLN
3	C	101	ASP
3	C	142	TYR
4	E	91	GLU
5	F	27	SER
5	F	48	ASN
5	F	68	ARG
7	H	92	ARG
8	I	48	LYS
9	J	175	LYS
9	J	221	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	J	275	ASP
9	J	288	PHE
9	J	323	HIS
10	K	95	LYS
11	L	164	PHE
11	L	173	SER
12	M	30	ASN
12	M	336	ASN
13	N	43	LYS
13	N	144	TYR
14	O	43	ASP
14	O	90	ASN
14	O	223	PHE
14	O	234	LEU
15	P	91	ASP
15	P	102	ASP
15	P	110	SER
15	P	139	SER
15	P	213	ASP
15	P	231	ARG
16	Q	83	ASN
16	Q	156	GLU
16	Q	308	TYR
18	T	49	ASP
18	T	58	ARG
18	T	107	LYS
19	U	77	SER
20	V	77	SER
20	V	95	CYS
6	X	99	SER
22	Y	77	SER
22	Y	78	ASP
22	Y	89	PRO
22	Y	90	SER
22	Y	95	GLU
23	Z	18	ASP
24	a	189	ASN
25	b	66	ARG
25	b	122	GLU
26	c	158	PRO
27	d	8	ASP
27	d	16	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	d	73	ASP
27	d	111	LYS
27	d	144	SER
28	e	55	LEU
30	g	22	SER
31	h	16	ARG
32	i	40	MET
32	i	72	MET
32	i	88	LYS
32	i	244	MET
32	i	300	SER
33	j	22	PHE
34	k	53	PHE
34	k	80	MET
34	k	82	SER
34	k	91	GLN
35	l	271	LYS
35	l	340	PHE
35	l	357	ARG
35	l	401	MET
35	l	546	GLN
36	m	17	PHE
36	m	31	LEU
36	m	41	CYS
36	m	50	SER
36	m	148	SER
37	n	58	LYS
39	p	132	SER
40	r	304	GLN
40	r	410	MET
41	s	224	PHE
41	s	243	LEU
42	u	22	SER
42	u	48	TRP
42	u	66	CYS
43	v	76	ASN
43	v	89	TYR
44	w	67	CYS
44	w	152	SER

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	441	HIS
8	I	29	GLN
12	M	278	HIS
12	M	464	GLN
12	M	666	GLN
15	P	181	HIS
16	Q	234	GLN
22	Y	46	GLN
25	b	14	GLN
27	d	124	ASN
42	u	99	HIS

### 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	1.97	1 (10%)	5,13,15	5.96	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.67	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	12.07	130.54	119.48
16	Q	118	2MR	CD-NE-CZ	4.70	132.21	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.03	130.57	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	PLX	C	302	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
49	8Q1	X	201	-	31,34,34	1.67	6 (19%)	40,43,43	1.50	5 (12%)
53	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	8Q1	G	201	-	31,34,34	1.73	6 (19%)	40,43,43	1.61	6 (15%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.21	8 (16%)
48	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.63	1 (1%)
53	PEE	Q	501	-	46,46,50	1.19	6 (13%)	49,51,55	1.02	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
56	UQ	s	401	-	28,28,63	3.26	8 (28%)	34,37,79	2.92	10 (29%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.44	4 (13%)
53	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.96	2 (4%)
53	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.97	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
55	CDL	g	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
55	CDL	i	401	-	65,65,99	1.29	9 (13%)	71,77,111	0.99	4 (5%)
50	NDP	J	401	-	45,52,52	4.58	20 (44%)	53,80,80	1.98	8 (15%)
53	PEE	j	201	-	46,46,50	1.22	6 (13%)	49,51,55	0.93	2 (4%)
48	PLX	j	203	-	51,51,51	1.16	4 (7%)	55,59,59	0.58	1 (1%)
55	CDL	a	201	-	90,90,99	1.13	8 (8%)	96,102,111	0.94	5 (5%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
47	NAI	A	503	-	42,48,48	4.95	19 (45%)	47,73,73	1.32	7 (14%)
53	PEE	Q	502	-	50,50,50	1.17	6 (12%)	53,55,55	1.06	2 (3%)
53	PEE	l	702	-	45,45,50	1.22	6 (13%)	48,50,55	1.01	2 (4%)
55	CDL	l	701	-	99,99,99	1.08	9 (9%)	105,111,111	0.85	4 (3%)
55	CDL	V	201	-	70,70,99	1.22	8 (11%)	76,82,111	0.97	4 (5%)
53	PEE	j	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
51	FES	O	301	14	0,4,4	-	-	-	-	-
51	FES	M	803	12	0,4,4	-	-	-	-	-
48	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.68	1 (1%)
45	SF4	C	301	16,3	0,12,12	-	-	-	-	-
48	PLX	r	503	-	51,51,51	1.14	5 (9%)	55,59,59	0.59	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
48	PLX	C	302	-	-	24/55/55/55	-
49	8Q1	X	201	-	-	20/41/41/41	-
53	PEE	r	501	-	-	23/54/54/54	-
49	8Q1	G	201	-	-	21/41/41/41	-
45	SF4	B	302	2	-	-	0/6/5/5
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
48	PLX	a	202	-	-	21/55/55/55	-
53	PEE	Q	501	-	-	25/50/50/54	-
56	UQ	s	401	-	-	8/21/45/87	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
57	ADP	w	401	-	-	4/12/32/32	0/3/3/3
53	PEE	l	703	-	-	26/49/49/54	-
51	FES	O	301	14	-	-	0/1/1/1
53	PEE	m	201	-	-	20/44/44/54	-
45	SF4	A	501	1	-	-	0/6/5/5
55	CDL	g	202	-	-	67/110/110/110	-
55	CDL	i	401	-	-	42/76/76/110	-
53	PEE	j	201	-	-	25/50/50/54	-
50	NDP	J	401	-	-	8/30/77/77	0/4/5/5
48	PLX	j	203	-	-	28/55/55/55	-
55	CDL	a	201	-	-	41/101/101/110	-
45	SF4	M	801	12	-	-	0/6/5/5
47	NAI	A	503	-	-	8/25/72/72	0/5/5/5
53	PEE	Q	502	-	-	23/54/54/54	-
53	PEE	l	702	-	-	25/49/49/54	-
55	CDL	l	701	-	-	63/110/110/110	-
55	CDL	V	201	-	-	47/81/81/110	-
53	PEE	j	202	-	-	24/54/54/54	-
48	PLX	r	502	-	-	26/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
51	FES	M	803	12	-	-	0/1/1/1
48	PLX	g	201	-	-	25/55/55/55	-
45	SF4	C	301	16,3	-	-	0/6/5/5
48	PLX	r	503	-	-	33/55/55/55	-

All (180) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.36	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.36	1.30	1.53
50	J	401	NDP	C3B-C2B	-12.84	1.24	1.52
50	J	401	NDP	C6N-C5N	12.52	1.55	1.33
50	J	401	NDP	O4D-C4D	10.68	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.11	1.27	1.53
50	J	401	NDP	C3D-C4D	-9.80	1.28	1.53
56	s	401	UQ	C13-C14	9.20	1.55	1.33
56	s	401	UQ	C8-C9	8.88	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.81	1.30	1.53
50	J	401	NDP	O4B-C1B	8.39	1.52	1.41
56	s	401	UQ	C18-C19	8.25	1.56	1.32
47	A	503	NAI	O4B-C4B	-8.19	1.26	1.45
50	J	401	NDP	O4B-C4B	-7.87	1.27	1.45
57	w	401	ADP	O4'-C4'	7.74	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.62	1.29	1.53
50	J	401	NDP	C2N-C3N	7.50	1.55	1.34
47	A	503	NAI	O4D-C4D	7.12	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.88	1.31	1.41
47	A	503	NAI	C2D-C3D	5.91	1.69	1.53
47	A	503	NAI	C7N-N7N	5.75	1.48	1.33
50	J	401	NDP	P2B-O2B	5.66	1.70	1.59
49	G	201	8Q1	C34-N36	5.56	1.45	1.33
50	J	401	NDP	C3B-C4B	5.47	1.67	1.53
49	G	201	8Q1	C39-N41	5.46	1.45	1.33
47	A	503	NAI	O4D-C1D	5.43	1.54	1.42
49	X	201	8Q1	C34-N36	5.42	1.45	1.33
49	X	201	8Q1	C39-N41	5.34	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.11	1.39	1.49
50	J	401	NDP	C6N-N1N	5.04	1.49	1.37
50	J	401	NDP	O4D-C1D	-4.89	1.30	1.42
47	A	503	NAI	O2B-C2B	4.55	1.53	1.43
50	J	401	NDP	C7N-N7N	4.21	1.44	1.33
50	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
50	J	401	NDP	C6A-N6A	4.07	1.48	1.34
46	A	502	FMN	C4A-N5	3.94	1.38	1.30
47	A	503	NAI	C6N-C5N	3.93	1.40	1.33
53	Q	502	PEE	C18-C19	3.78	1.53	1.31
57	w	401	ADP	C6-N6	3.77	1.47	1.34
53	j	201	PEE	C18-C19	3.76	1.53	1.31
53	l	702	PEE	C18-C19	3.75	1.53	1.31
53	j	202	PEE	C18-C19	3.74	1.53	1.31
53	r	501	PEE	C18-C19	3.73	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	m	201	PEE	C18-C19	3.73	1.53	1.31
53	l	703	PEE	C18-C19	3.72	1.53	1.31
53	Q	501	PEE	C18-C19	3.71	1.53	1.31
53	j	201	PEE	C39-C38	3.68	1.53	1.31
53	r	501	PEE	C39-C38	3.66	1.53	1.31
53	l	702	PEE	C39-C38	3.65	1.53	1.31
53	j	202	PEE	C39-C38	3.65	1.52	1.31
53	Q	502	PEE	C39-C38	3.65	1.52	1.31
53	l	703	PEE	C39-C38	3.64	1.52	1.31
53	Q	501	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C6A-N6A	3.62	1.47	1.34
47	A	503	NAI	C7N-C3N	3.59	1.56	1.48
55	V	201	CDL	OA8-CA7	3.55	1.43	1.33
55	i	401	CDL	OA8-CA7	3.52	1.43	1.33
55	l	701	CDL	OA8-CA7	3.38	1.43	1.33
55	a	201	CDL	OA8-CA7	3.38	1.43	1.33
55	g	202	CDL	OA8-CA7	3.37	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.37	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.36	1.40	1.48
50	J	401	NDP	C7N-C3N	3.11	1.55	1.48
50	J	401	NDP	O3D-C3D	3.10	1.50	1.43
57	w	401	ADP	O3'-C3'	3.10	1.50	1.43
55	a	201	CDL	OB6-CB5	3.10	1.43	1.34
55	l	701	CDL	OB6-CB5	3.06	1.42	1.34
55	i	401	CDL	OB6-CB5	3.06	1.42	1.34
55	g	202	CDL	OB6-CB5	3.05	1.42	1.34
55	i	401	CDL	OB8-CB7	3.04	1.42	1.33
55	i	401	CDL	OA6-CA5	3.01	1.42	1.34
55	V	201	CDL	OB6-CB5	3.01	1.42	1.34
55	l	701	CDL	OB8-CB7	3.00	1.42	1.33
55	V	201	CDL	OB8-CB7	2.97	1.42	1.33
55	V	201	CDL	OA6-CA5	2.97	1.42	1.34
55	l	701	CDL	OA6-CA5	2.95	1.42	1.34
55	a	201	CDL	OA6-CA5	2.95	1.42	1.34
55	g	202	CDL	OA6-CA5	2.95	1.42	1.34
55	a	201	CDL	OB8-CB7	2.95	1.41	1.33
55	g	202	CDL	OB8-CB7	2.93	1.41	1.33
48	C	302	PLX	O6-C4	-2.78	1.40	1.44
48	r	503	PLX	O6-C4	-2.73	1.41	1.44
48	g	201	PLX	O6-C4	-2.70	1.41	1.44
56	s	401	UQ	C6-C1	2.66	1.54	1.46
48	a	202	PLX	O6-C4	-2.61	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	l	703	PEE	O3-C30	2.53	1.40	1.33
53	l	702	PEE	O3-C30	2.51	1.40	1.33
46	A	502	FMN	C10-N1	2.51	1.38	1.33
48	j	203	PLX	O6-C4	-2.50	1.41	1.44
53	j	201	PEE	O3-C30	2.50	1.40	1.33
53	r	501	PEE	O3-C30	2.49	1.40	1.33
53	r	501	PEE	O2-C2	-2.47	1.40	1.46
48	j	203	PLX	C7-C6	2.47	1.56	1.50
53	Q	501	PEE	O3-C30	2.47	1.40	1.33
55	g	202	CDL	OA6-CA4	-2.47	1.40	1.46
47	A	503	NAI	PN-O5D	2.46	1.69	1.59
53	l	703	PEE	O2-C2	-2.45	1.40	1.46
53	j	202	PEE	O3-C30	2.44	1.40	1.33
50	J	401	NDP	O2B-C2B	2.44	1.53	1.44
49	G	201	8Q1	C1-S44	2.43	1.82	1.76
55	a	201	CDL	OA6-CA4	-2.43	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.43	1.37	1.43
53	Q	501	PEE	O2-C2	-2.42	1.40	1.46
53	m	201	PEE	O3-C30	2.42	1.40	1.33
50	J	401	NDP	C2D-C3D	2.42	1.60	1.53
53	m	201	PEE	O2-C10	2.41	1.41	1.34
53	Q	502	PEE	O3-C30	2.40	1.40	1.33
47	A	503	NAI	C5B-C4B	2.39	1.59	1.51
55	V	201	CDL	OA6-CA4	-2.38	1.40	1.46
53	l	702	PEE	O2-C10	2.37	1.41	1.34
53	j	202	PEE	O2-C2	-2.37	1.40	1.46
48	r	502	PLX	C7-C6	2.37	1.55	1.50
53	j	201	PEE	O2-C2	-2.37	1.40	1.46
55	i	401	CDL	OA6-CA4	-2.35	1.40	1.46
53	j	201	PEE	O2-C10	2.35	1.40	1.34
53	j	202	PEE	O2-C10	2.35	1.40	1.34
49	X	201	8Q1	C1-S44	2.35	1.81	1.76
55	l	701	CDL	OA6-CA4	-2.34	1.40	1.46
56	s	401	UQ	O4-C4	-2.34	1.18	1.23
48	g	201	PLX	C7-C6	2.33	1.55	1.50
49	G	201	8Q1	C6-C1	2.33	1.53	1.50
53	Q	502	PEE	O2-C10	2.32	1.40	1.34
48	r	502	PLX	O6-C4	-2.29	1.41	1.44
53	Q	502	PEE	O2-C2	-2.29	1.40	1.46
49	G	201	8Q1	O40-C39	-2.27	1.18	1.23
56	s	401	UQ	C7-C8	2.26	1.53	1.50
48	r	503	PLX	C7-C6	2.26	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	a	202	PLX	C7-C6	2.26	1.55	1.50
53	m	201	PEE	O2-C2	-2.25	1.41	1.46
55	i	401	CDL	PB2-OB5	2.25	1.68	1.59
53	l	702	PEE	O2-C2	-2.25	1.41	1.46
48	C	302	PLX	C7-C6	2.24	1.55	1.50
48	r	502	PLX	P1-O4	2.23	1.68	1.59
55	V	201	CDL	PB2-OB2	2.22	1.68	1.59
55	g	202	CDL	PB2-OB2	2.22	1.68	1.59
53	l	703	PEE	O2-C10	2.21	1.40	1.34
53	Q	501	PEE	O2-C10	2.21	1.40	1.34
49	G	201	8Q1	O35-C34	-2.21	1.19	1.23
55	l	701	CDL	OB6-CB4	-2.21	1.41	1.46
53	r	501	PEE	O2-C10	2.21	1.40	1.34
55	g	202	CDL	PB2-OB5	2.19	1.68	1.59
55	i	401	CDL	PB2-OB2	2.19	1.68	1.59
49	X	201	8Q1	O35-C34	-2.19	1.19	1.23
48	j	203	PLX	P1-O4	2.18	1.68	1.59
53	Q	502	PEE	O3-C3	-2.17	1.40	1.45
55	V	201	CDL	OB6-CB4	-2.16	1.41	1.46
55	a	201	CDL	PB2-OB2	2.15	1.68	1.59
53	m	201	PEE	O3-C3	-2.15	1.40	1.45
53	j	202	PEE	O3-C3	-2.15	1.40	1.45
55	l	701	CDL	PB2-OB2	2.14	1.68	1.59
49	X	201	8Q1	O40-C39	-2.14	1.18	1.23
55	V	201	CDL	PB2-OB5	2.13	1.67	1.59
55	i	401	CDL	OB6-CB4	-2.13	1.41	1.46
48	C	302	PLX	P1-O4	2.12	1.67	1.59
48	a	202	PLX	P1-O4	2.12	1.67	1.59
56	s	401	UQ	O1-C1	-2.12	1.18	1.23
48	r	502	PLX	P1-O1	2.11	1.67	1.59
55	a	201	CDL	PB2-OB5	2.11	1.67	1.59
55	l	701	CDL	PB2-OB5	2.11	1.67	1.59
50	J	401	NDP	PA-O5B	2.11	1.67	1.59
55	g	202	CDL	OB6-CB4	-2.10	1.41	1.46
55	a	201	CDL	OB6-CB4	-2.09	1.41	1.46
49	X	201	8Q1	C6-C1	2.09	1.53	1.50
50	J	401	NDP	O7N-C7N	-2.08	1.19	1.24
48	r	503	PLX	P1-O4	2.07	1.67	1.59
48	j	203	PLX	P1-O1	2.07	1.67	1.59
48	g	201	PLX	P1-O4	2.06	1.67	1.59
53	r	501	PEE	O3-C3	-2.06	1.40	1.45
53	Q	501	PEE	O3-C3	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C2N-C3N	2.05	1.40	1.34
48	a	202	PLX	P1-O1	2.05	1.67	1.59
55	i	401	CDL	C11-CA5	2.05	1.56	1.50
48	C	302	PLX	P1-O1	2.03	1.67	1.59
53	l	702	PEE	O3-C3	-2.03	1.40	1.45
56	s	401	UQ	O3-CM3	-2.03	1.40	1.45
55	l	701	CDL	C11-CA5	2.03	1.56	1.50
48	r	503	PLX	P1-O1	2.03	1.67	1.59
53	j	201	PEE	O3-C3	-2.02	1.40	1.45
48	r	503	PLX	C1-C2	2.02	1.57	1.51
53	l	703	PEE	O3-C3	-2.01	1.40	1.45

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-10.49	109.33	126.79
50	J	401	NDP	C3N-C2N-N1N	-7.76	112.02	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.85	109.72	121.11
49	G	201	8Q1	C6-C1-S44	6.18	120.65	113.46
56	s	401	UQ	C12-C13-C14	-6.10	112.96	127.66
49	X	201	8Q1	C6-C1-S44	5.67	120.05	113.46
50	J	401	NDP	C1D-N1N-C6N	-5.67	108.62	120.83
56	s	401	UQ	C11-C9-C8	-5.19	110.62	121.12
56	s	401	UQ	C10-C9-C8	-5.06	110.70	123.68
53	Q	502	PEE	O2-C10-C11	4.50	121.19	111.50
57	w	401	ADP	N3-C2-N1	-4.47	121.69	128.68
55	a	201	CDL	OA6-CA5-C11	4.45	121.08	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.34	121.89	128.68
56	s	401	UQ	C17-C18-C19	-4.16	113.52	127.75
56	s	401	UQ	C15-C14-C13	-4.11	113.13	123.68
55	V	201	CDL	OB6-CB5-C51	4.08	120.30	111.50
55	g	202	CDL	OB6-CB5-C51	4.08	120.28	111.50
56	s	401	UQ	C16-C14-C13	-4.07	112.89	121.12
50	J	401	NDP	N3A-C2A-N1A	-4.06	122.34	128.68
55	l	701	CDL	OA6-CA5-C11	4.05	120.22	111.50
53	l	702	PEE	O2-C10-C11	4.01	120.15	111.50
53	m	201	PEE	O2-C10-C11	3.98	120.09	111.50
55	i	401	CDL	OB6-CB5-C51	3.98	120.07	111.50
53	Q	501	PEE	O2-C10-C11	3.96	120.04	111.50
53	j	202	PEE	O2-C10-C11	3.92	119.94	111.50
55	a	201	CDL	OB6-CB5-C51	3.91	119.92	111.50
55	i	401	CDL	OA6-CA5-C11	3.82	119.74	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G	201	8Q1	C37-C38-C39	3.72	118.56	112.36
53	r	501	PEE	O2-C10-C11	3.70	119.47	111.50
55	g	202	CDL	OA6-CA5-C11	3.69	119.45	111.50
53	j	201	PEE	O2-C10-C11	3.64	119.36	111.50
55	l	701	CDL	OB6-CB5-C51	3.63	119.33	111.50
49	G	201	8Q1	O4-C1-C6	-3.62	119.71	123.99
53	l	703	PEE	O2-C10-C11	3.62	119.30	111.50
49	X	201	8Q1	O4-C1-C6	-3.52	119.84	123.99
56	s	401	UQ	C21-C19-C18	-3.24	113.29	122.65
55	V	201	CDL	OA6-CA5-C11	3.21	119.76	110.80
46	A	502	FMN	C4-N3-C2	-3.05	120.02	125.64
56	s	401	UQ	C20-C19-C18	-3.04	113.85	122.65
57	w	401	ADP	O4'-C1'-C2'	-2.94	102.63	106.93
53	Q	502	PEE	O3-C30-C31	2.92	121.06	111.91
47	A	503	NAI	PN-O3-PA	-2.91	122.84	132.83
53	l	702	PEE	O3-C30-C31	2.88	120.94	111.91
57	w	401	ADP	PA-O3A-PB	-2.87	122.96	132.83
53	r	501	PEE	O3-C30-C31	2.81	120.72	111.91
55	V	201	CDL	OA8-CA7-C31	2.81	120.72	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.75	103.40	109.47
55	i	401	CDL	OA8-CA7-C31	2.70	120.39	111.91
53	l	703	PEE	O3-C30-C31	2.65	120.21	111.91
50	J	401	NDP	C2B-C3B-C4B	2.64	107.73	101.99
47	A	503	NAI	C4A-C5A-N7A	-2.63	106.66	109.40
46	A	502	FMN	C4A-C4-N3	2.63	119.86	113.19
48	g	201	PLX	C1A-N1-C1	2.60	120.56	109.92
47	A	503	NAI	C3B-C2B-C1B	2.59	104.88	100.98
55	V	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
55	i	401	CDL	OB8-CB7-C71	2.56	119.95	111.91
53	Q	501	PEE	O3-C30-C31	2.56	119.94	111.91
55	a	201	CDL	OB8-CB7-C71	2.55	119.90	111.91
53	j	201	PEE	O3-C30-C31	2.54	119.89	111.91
47	A	503	NAI	C2D-C3D-C4D	2.54	107.57	102.64
48	r	503	PLX	C1A-N1-C1	2.52	120.24	109.92
55	g	202	CDL	OB8-CB7-C71	2.52	119.83	111.91
55	g	202	CDL	OA8-CA7-C31	2.51	119.78	111.91
49	X	201	8Q1	C38-C39-N41	2.50	120.63	116.42
53	j	202	PEE	O3-C30-C31	2.50	119.74	111.91
53	m	201	PEE	O3-C30-C31	2.49	119.74	111.91
55	l	701	CDL	OB8-CB7-C71	2.49	119.72	111.91
55	l	701	CDL	OA8-CA7-C31	2.49	119.72	111.91
46	A	502	FMN	O4-C4-C4A	-2.47	120.04	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C4A-C10-N10	2.46	120.08	116.48
48	a	202	PLX	C1A-N1-C1	2.45	119.94	109.92
49	G	201	8Q1	C43-S44-C1	2.39	109.32	101.87
47	A	503	NAI	C3D-C2D-C1D	2.36	105.91	101.43
49	X	201	8Q1	C38-C37-N36	-2.36	107.14	111.90
50	J	401	NDP	PN-O3-PA	-2.34	124.81	132.83
55	a	201	CDL	OA8-CA7-C31	2.32	119.19	111.91
48	C	302	PLX	C1A-N1-C1	2.32	119.39	109.92
48	j	203	PLX	C1A-N1-C1	2.31	119.37	109.92
48	r	502	PLX	C1A-N1-C1	2.30	119.32	109.92
49	G	201	8Q1	O4-C1-S44	-2.29	119.63	122.61
46	A	502	FMN	C10-C4A-N5	-2.28	120.03	124.86
49	X	201	8Q1	C43-S44-C1	2.27	108.94	101.87
46	A	502	FMN	C9A-C5A-N5	-2.26	119.98	122.43
50	J	401	NDP	C4A-C5A-N7A	-2.23	107.08	109.40
49	G	201	8Q1	C38-C39-N41	2.20	120.12	116.42
56	s	401	UQ	CM5-C5-C6	-2.18	120.84	124.40
46	A	502	FMN	C4A-C10-N1	-2.13	119.78	124.73
55	a	201	CDL	CA4-OA6-CA5	-2.12	112.56	117.79
46	A	502	FMN	C5A-C9A-N10	2.12	120.14	117.95
50	J	401	NDP	C2D-C3D-C4D	2.04	106.61	102.64
57	w	401	ADP	C4-C5-N7	-2.01	107.30	109.40

There are no chirality outliers.

All (685) 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	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PLX	O4-C3-C4-O6
48	C	302	PLX	C3-O4-P1-O1
48	C	302	PLX	C3-O4-P1-O2
48	C	302	PLX	C3-O4-P1-O3
48	a	202	PLX	O7-C6-C7-C8
48	a	202	PLX	C25-C24-O8-C5
48	g	201	PLX	O7-C6-C7-C8
48	g	201	PLX	O7-C6-O6-C4
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
48	j	203	PLX	O7-C6-C7-C8
48	j	203	PLX	O7-C6-O6-C4
48	j	203	PLX	C25-C24-O8-C5
48	j	203	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	C3-O4-P1-O1
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
48	r	503	PLX	C25-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
49	G	201	8Q1	C1-C6-C7-C8
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-O33
49	G	201	8Q1	N41-C42-C43-S44
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	O27-C28-C29-C32
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
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	C5B-O5B-PA-O1A
50	J	401	NDP	C5B-O5B-PA-O3
50	J	401	NDP	C2N-C3N-C7N-N7N
53	Q	501	PEE	C11-C10-O2-C2
53	Q	501	PEE	C4-O4P-P-O1P
53	Q	502	PEE	O4P-C4-C5-N
53	j	201	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
53	j	201	PEE	C4-O4P-P-O1P
53	j	201	PEE	O4P-C4-C5-N
53	j	202	PEE	C17-C18-C19-C20
53	j	202	PEE	C1-O3P-P-O1P
53	l	702	PEE	C11-C10-O2-C2
53	l	702	PEE	C4-O4P-P-O2P
53	l	702	PEE	C4-O4P-P-O1P
53	l	703	PEE	C1-O3P-P-O1P
53	m	201	PEE	C11-C10-O2-C2
55	V	201	CDL	OA9-CA7-OA8-CA6
55	V	201	CDL	C31-CA7-OA8-CA6
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2
55	a	201	CDL	CA3-OA5-PA1-OA3
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	OA5-CA3-CA4-OA6
55	a	201	CDL	CB3-OB5-PB2-OB3
55	g	202	CDL	CB2-C1-CA2-OA2
55	g	202	CDL	CA2-OA2-PA1-OA3
55	g	202	CDL	CA2-OA2-PA1-OA4
55	g	202	CDL	CA3-OA5-PA1-OA3
55	g	202	CDL	CA3-OA5-PA1-OA4
55	g	202	CDL	C51-CB5-OB6-CB4
55	i	401	CDL	CA2-OA2-PA1-OA5
55	i	401	CDL	CA3-OA5-PA1-OA3
55	i	401	CDL	CA3-OA5-PA1-OA4
55	i	401	CDL	CB2-OB2-PB2-OB3
55	i	401	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	O1-C1-CB2-OB2
55	l	701	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	701	CDL	CA3-OA5-PA1-OA2
55	l	701	CDL	CA3-OA5-PA1-OA3
55	l	701	CDL	CA3-OA5-PA1-OA4
55	l	701	CDL	OA6-CA4-CA6-OA8
55	l	701	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C10
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
53	Q	501	PEE	O4-C10-O2-C2
53	l	702	PEE	O4-C10-O2-C2
53	m	201	PEE	O4-C10-O2-C2
55	g	202	CDL	OB7-CB5-OB6-CB4
55	i	401	CDL	OA9-CA7-OA8-CA6
55	l	701	CDL	C71-CB7-OB8-CB6
56	s	401	UQ	C17-C18-C19-C21
53	l	702	PEE	C31-C30-O3-C3
53	l	703	PEE	C31-C30-O3-C3
53	m	201	PEE	C31-C30-O3-C3
55	g	202	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C31-CA7-OA8-CA6
53	Q	502	PEE	C37-C38-C39-C40
53	l	703	PEE	C37-C38-C39-C40
53	r	501	PEE	C17-C18-C19-C20
56	s	401	UQ	C7-C8-C9-C10
53	l	703	PEE	O5-C30-O3-C3
55	g	202	CDL	OB9-CB7-OB8-CB6
55	l	701	CDL	O1-C1-CA2-OA2
53	m	201	PEE	O5-C30-O3-C3
55	l	701	CDL	OB9-CB7-OB8-CB6
48	j	203	PLX	C28-C29-C30-C31
55	l	701	CDL	C11-C12-C13-C14
50	J	401	NDP	C2D-C1D-N1N-C6N
48	C	302	PLX	C28-C29-C30-C31
53	l	702	PEE	O5-C30-O3-C3
48	j	203	PLX	C15-C16-C17-C18
48	r	502	PLX	C9-C10-C11-C12
48	r	503	PLX	C12-C13-C14-C15
50	J	401	NDP	O4B-C4B-C5B-O5B
48	r	502	PLX	C30-C31-C32-C33
55	g	202	CDL	C36-C37-C38-C39
55	l	701	CDL	C59-C60-C61-C62
55	l	701	CDL	C35-C36-C37-C38
53	m	201	PEE	C33-C34-C35-C36
55	V	201	CDL	C60-C61-C62-C63
55	V	201	CDL	CA2-C1-CB2-OB2
53	j	202	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C31-C32-C33-C34
53	j	202	PEE	O5-C30-O3-C3
48	j	203	PLX	C34-C35-C36-C37
55	V	201	CDL	C74-C75-C76-C77
55	V	201	CDL	O1-C1-CB2-OB2
55	l	701	CDL	CB7-C71-C72-C73
55	g	202	CDL	C74-C75-C76-C77
53	j	202	PEE	C11-C10-O2-C2
53	m	201	PEE	C13-C14-C15-C16
55	i	401	CDL	CB7-C71-C72-C73
55	i	401	CDL	OB9-CB7-OB8-CB6
48	g	201	PLX	C7-C8-C9-C10
55	g	202	CDL	CB5-C51-C52-C53
55	g	202	CDL	CB7-C71-C72-C73
55	i	401	CDL	CA7-C31-C32-C33
55	a	201	CDL	CA7-C31-C32-C33
55	a	201	CDL	OB9-CB7-OB8-CB6
55	g	202	CDL	C78-C79-C80-C81
55	V	201	CDL	O1-C1-CA2-OA2
55	g	202	CDL	O1-C1-CA2-OA2
55	i	401	CDL	O1-C1-CA2-OA2
55	l	701	CDL	C39-C40-C41-C42
53	j	202	PEE	C30-C31-C32-C33
55	g	202	CDL	CA7-C31-C32-C33
53	Q	501	PEE	C17-C18-C19-C20
48	a	202	PLX	C29-C30-C31-C32
53	Q	501	PEE	C22-C23-C24-C25
48	r	502	PLX	C3-O4-P1-O1
53	j	201	PEE	C1-O3P-P-O4P
53	l	702	PEE	C4-O4P-P-O3P
53	m	201	PEE	C4-O4P-P-O3P
53	r	501	PEE	C1-O3P-P-O4P
55	V	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB2
55	g	202	CDL	CA2-OA2-PA1-OA5
55	g	202	CDL	CA3-OA5-PA1-OA2
55	g	202	CDL	CB2-OB2-PB2-OB5
55	g	202	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CA3-OA5-PA1-OA2
55	i	401	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	CB3-OB5-PB2-OB2
56	s	401	UQ	C12-C13-C14-C15
55	g	202	CDL	C76-C77-C78-C79
55	V	201	CDL	CB2-C1-CA2-OA2
55	i	401	CDL	CB2-C1-CA2-OA2
53	j	202	PEE	O4-C10-O2-C2
53	r	501	PEE	C41-C42-C43-C44
48	a	202	PLX	O6-C6-C7-C8
53	Q	502	PEE	C12-C13-C14-C15
48	g	201	PLX	C30-C31-C32-C33
53	r	501	PEE	C12-C13-C14-C15
53	j	201	PEE	C11-C10-O2-C2
48	C	302	PLX	C17-C18-C19-C20
48	j	203	PLX	C27-C28-C29-C30
48	r	502	PLX	C16-C17-C18-C19
48	r	503	PLX	C16-C17-C18-C19
48	r	503	PLX	C25-C26-C27-C28
53	Q	502	PEE	C14-C15-C16-C17
55	i	401	CDL	C36-C37-C38-C39
49	X	201	8Q1	O27-C28-C29-C30
49	X	201	8Q1	O27-C28-C29-C31
48	C	302	PLX	C33-C34-C35-C36
48	a	202	PLX	C28-C29-C30-C31
48	a	202	PLX	C31-C32-C33-C34
48	g	201	PLX	C33-C34-C35-C36
48	j	203	PLX	C14-C15-C16-C17
48	r	502	PLX	C27-C28-C29-C30
49	G	201	8Q1	C7-C8-C9-C10
53	j	201	PEE	C14-C15-C16-C17
55	V	201	CDL	C55-C56-C57-C58
55	a	201	CDL	C17-C18-C19-C20
53	j	201	PEE	O4-C10-O2-C2
53	r	501	PEE	C10-C11-C12-C13
46	A	502	FMN	O2'-C2'-C3'-C4'
53	m	201	PEE	C11-C12-C13-C14
55	a	201	CDL	C37-C38-C39-C40
48	g	201	PLX	C14-C15-C16-C17
53	Q	501	PEE	C32-C33-C34-C35
53	j	202	PEE	C40-C41-C42-C43
55	V	201	CDL	C52-C53-C54-C55
48	C	302	PLX	C7-C8-C9-C10
48	g	201	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
55	g	202	CDL	C17-C18-C19-C20
48	j	203	PLX	C25-C26-C27-C28
55	a	201	CDL	C22-C23-C24-C25
48	a	202	PLX	C11-C10-C9-C8
48	g	201	PLX	C25-C26-C27-C28
48	j	203	PLX	C12-C13-C14-C15
48	r	502	PLX	C7-C8-C9-C10
49	X	201	8Q1	C10-C11-C12-C13
53	j	201	PEE	C32-C33-C34-C35
53	j	202	PEE	C21-C22-C23-C24
55	V	201	CDL	C59-C60-C61-C62
55	g	202	CDL	C73-C74-C75-C76
53	Q	502	PEE	C32-C33-C34-C35
53	Q	502	PEE	C33-C34-C35-C36
55	i	401	CDL	C11-C12-C13-C14
48	g	201	PLX	C32-C33-C34-C35
48	r	503	PLX	C29-C30-C31-C32
53	r	501	PEE	C13-C14-C15-C16
55	g	202	CDL	C55-C56-C57-C58
53	Q	501	PEE	C19-C20-C21-C22
53	j	201	PEE	C15-C16-C17-C18
53	l	702	PEE	C19-C20-C21-C22
53	j	201	PEE	C30-C31-C32-C33
48	j	203	PLX	C10-C11-C12-C13
48	j	203	PLX	C7-C8-C9-C10
48	r	503	PLX	C9-C10-C11-C12
48	r	503	PLX	C33-C34-C35-C36
53	j	201	PEE	C13-C14-C15-C16
53	j	201	PEE	C33-C34-C35-C36
53	l	703	PEE	C33-C34-C35-C36
53	r	501	PEE	C31-C32-C33-C34
55	V	201	CDL	C62-C63-C64-C65
55	g	202	CDL	C75-C76-C77-C78
55	l	701	CDL	C73-C74-C75-C76
49	G	201	8Q1	C11-C12-C13-C14
53	m	201	PEE	C31-C32-C33-C34
55	a	201	CDL	C11-C12-C13-C14
53	r	501	PEE	O4P-C4-C5-N
48	C	302	PLX	C25-C26-C27-C28
48	C	302	PLX	C27-C28-C29-C30
48	g	201	PLX	C28-C29-C30-C31
48	r	502	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
53	l	702	PEE	C31-C32-C33-C34
55	a	201	CDL	C71-C72-C73-C74
48	g	201	PLX	C27-C28-C29-C30
48	r	503	PLX	C27-C28-C29-C30
48	r	503	PLX	C28-C29-C30-C31
53	l	703	PEE	C39-C40-C41-C42
55	g	202	CDL	C71-C72-C73-C74
55	l	701	CDL	C40-C41-C42-C43
55	V	201	CDL	C56-C57-C58-C59
53	Q	502	PEE	C34-C35-C36-C37
55	i	401	CDL	C71-C72-C73-C74
55	a	201	CDL	C32-C33-C34-C35
55	l	701	CDL	C72-C73-C74-C75
53	l	703	PEE	C17-C18-C19-C20
48	C	302	PLX	C16-C17-C18-C19
53	Q	501	PEE	C10-C11-C12-C13
48	a	202	PLX	C26-C27-C28-C29
48	C	302	PLX	O7-C6-C7-C8
48	a	202	PLX	C14-C15-C16-C17
48	j	203	PLX	C26-C27-C28-C29
55	l	701	CDL	C37-C38-C39-C40
55	V	201	CDL	CA7-C31-C32-C33
55	i	401	CDL	C52-C53-C54-C55
55	g	202	CDL	CA5-C11-C12-C13
55	a	201	CDL	C31-C32-C33-C34
48	C	302	PLX	C14-C15-C16-C17
53	r	501	PEE	C11-C12-C13-C14
55	a	201	CDL	C75-C76-C77-C78
55	g	202	CDL	C33-C34-C35-C36
55	i	401	CDL	C32-C33-C34-C35
53	j	202	PEE	C41-C42-C43-C44
55	l	701	CDL	C55-C56-C57-C58
53	l	702	PEE	C30-C31-C32-C33
48	C	302	PLX	C13-C14-C15-C16
53	l	702	PEE	C14-C15-C16-C17
55	g	202	CDL	C62-C63-C64-C65
53	Q	501	PEE	C31-C30-O3-C3
55	g	202	CDL	C31-CA7-OA8-CA6
48	C	302	PLX	C26-C27-C28-C29
55	g	202	CDL	C43-C44-C45-C46
53	l	703	PEE	C12-C13-C14-C15
53	Q	502	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C35-C36-C37-C38
48	a	202	PLX	C13-C14-C15-C16
53	j	202	PEE	C22-C23-C24-C25
55	g	202	CDL	C59-C60-C61-C62
55	l	701	CDL	C52-C53-C54-C55
55	l	701	CDL	C75-C76-C77-C78
48	C	302	PLX	C11-C12-C13-C14
48	g	201	PLX	C10-C11-C12-C13
48	r	503	PLX	C13-C14-C15-C16
48	r	502	PLX	C12-C13-C14-C15
49	G	201	8Q1	C12-C13-C14-C15
55	V	201	CDL	C54-C55-C56-C57
55	a	201	CDL	CB5-C51-C52-C53
53	Q	502	PEE	C11-C10-O2-C2
53	l	703	PEE	C11-C10-O2-C2
55	V	201	CDL	C11-CA5-OA6-CA4
55	V	201	CDL	C51-CB5-OB6-CB4
53	l	702	PEE	O3P-C1-C2-O2
48	a	202	PLX	C25-C26-C27-C28
55	g	202	CDL	C42-C43-C44-C45
55	g	202	CDL	C52-C53-C54-C55
55	V	201	CDL	OA7-CA5-OA6-CA4
55	i	401	CDL	CB5-C51-C52-C53
55	V	201	CDL	C84-C85-C86-C87
55	g	202	CDL	C35-C36-C37-C38
55	g	202	CDL	OB6-CB4-CB6-OB8
53	r	501	PEE	C20-C21-C22-C23
55	g	202	CDL	C41-C42-C43-C44
48	a	202	PLX	C15-C16-C17-C18
49	X	201	8Q1	C11-C10-C9-C8
46	A	502	FMN	O2'-C2'-C3'-O3'
48	r	502	PLX	C10-C11-C12-C13
55	V	201	CDL	C64-C65-C66-C67
55	l	701	CDL	C14-C15-C16-C17
48	r	503	PLX	C14-C15-C16-C17
53	Q	501	PEE	O5-C30-O3-C3
55	g	202	CDL	OA9-CA7-OA8-CA6
53	l	703	PEE	O4-C10-O2-C2
53	j	201	PEE	C42-C43-C44-C45
53	Q	501	PEE	C18-C19-C20-C21
53	j	202	PEE	C1-O3P-P-O4P
53	l	703	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
55	i	401	CDL	C74-C75-C76-C77
48	C	302	PLX	O4-C3-C4-C5
53	Q	502	PEE	O3P-C1-C2-C3
55	a	201	CDL	OA5-CA3-CA4-CA6
55	l	701	CDL	C77-C78-C79-C80
55	l	701	CDL	CB5-C51-C52-C53
55	a	201	CDL	C34-C35-C36-C37
53	Q	502	PEE	C20-C21-C22-C23
55	g	202	CDL	C37-C38-C39-C40
53	Q	502	PEE	C39-C40-C41-C42
55	i	401	CDL	CA5-C11-C12-C13
49	G	201	8Q1	C11-C10-C9-C8
48	g	201	PLX	C16-C17-C18-C19
55	V	201	CDL	C58-C59-C60-C61
55	g	202	CDL	C56-C57-C58-C59
48	a	202	PLX	C3-C4-C5-O8
48	g	201	PLX	C3-C4-C5-O8
48	j	203	PLX	C3-C4-C5-O8
48	r	503	PLX	C3-C4-C5-O8
53	Q	501	PEE	C1-C2-C3-O3
53	l	703	PEE	C1-C2-C3-O3
55	g	202	CDL	CB3-CB4-CB6-OB8
55	V	201	CDL	C77-C78-C79-C80
55	g	202	CDL	C11-C12-C13-C14
48	r	502	PLX	C15-C16-C17-C18
48	r	503	PLX	C18-C19-C20-C21
53	Q	501	PEE	C35-C36-C37-C38
53	Q	502	PEE	C15-C16-C17-C18
48	C	302	PLX	C9-C10-C11-C12
48	r	502	PLX	C31-C32-C33-C34
53	Q	501	PEE	C21-C22-C23-C24
55	l	701	CDL	C64-C65-C66-C67
55	a	201	CDL	C60-C61-C62-C63
55	i	401	CDL	C33-C34-C35-C36
55	i	401	CDL	C35-C36-C37-C38
53	j	202	PEE	C36-C37-C38-C39
49	G	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C7-C8-C9-C10
55	V	201	CDL	OB5-CB3-CB4-OB6
53	Q	502	PEE	C17-C18-C19-C20
48	g	201	PLX	C13-C14-C15-C16
53	Q	501	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	C78-C79-C80-C81
48	j	203	PLX	C33-C34-C35-C36
55	i	401	CDL	C15-C16-C17-C18
48	r	503	PLX	O6-C4-C5-O8
55	g	202	CDL	OA6-CA4-CA6-OA8
55	i	401	CDL	OB6-CB4-CB6-OB8
53	l	702	PEE	C23-C24-C25-C26
48	j	203	PLX	C13-C14-C15-C16
48	j	203	PLX	C9-C10-C11-C12
53	r	501	PEE	C22-C23-C24-C25
55	g	202	CDL	C83-C84-C85-C86
55	V	201	CDL	OB7-CB5-OB6-CB4
55	i	401	CDL	C75-C76-C77-C78
48	a	202	PLX	C7-C8-C9-C10
48	r	503	PLX	C31-C32-C33-C34
53	l	703	PEE	C13-C14-C15-C16
53	Q	502	PEE	C30-C31-C32-C33
53	l	702	PEE	O3P-C1-C2-C3
55	g	202	CDL	C14-C15-C16-C17
55	g	202	CDL	C64-C65-C66-C67
55	a	201	CDL	C59-C60-C61-C62
55	g	202	CDL	C20-C21-C22-C23
53	l	703	PEE	C16-C17-C18-C19
48	r	502	PLX	C33-C34-C35-C36
53	r	501	PEE	C1-C2-C3-O3
55	g	202	CDL	CA3-CA4-CA6-OA8
55	l	701	CDL	CA3-CA4-CA6-OA8
55	l	701	CDL	CB3-CB4-CB6-OB8
53	j	201	PEE	C37-C38-C39-C40
48	r	502	PLX	C18-C19-C20-C21
53	l	702	PEE	C32-C33-C34-C35
48	j	203	PLX	C3-O4-P1-O1
48	r	503	PLX	C5-C4-O6-C6
53	j	201	PEE	C4-O4P-P-O3P
53	l	703	PEE	C1-O3P-P-O4P
55	V	201	CDL	CA2-OA2-PA1-OA5
47	A	503	NAI	C2D-C1D-N1N-C2N
53	Q	502	PEE	C22-C23-C24-C25
55	g	202	CDL	C31-C32-C33-C34
48	r	503	PLX	C36-C37-C38-C39
53	Q	502	PEE	O3P-C1-C2-O2
48	r	502	PLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C26-C27-C28-C29
55	i	401	CDL	C14-C15-C16-C17
48	g	201	PLX	O6-C4-C5-O8
55	V	201	CDL	OB6-CB4-CB6-OB8
53	r	501	PEE	C11-C10-O2-C2
55	l	701	CDL	CB2-C1-CA2-OA2
48	g	201	PLX	C9-C10-C11-C12
48	r	502	PLX	C13-C14-C15-C16
55	a	201	CDL	C52-C53-C54-C55
53	m	201	PEE	C20-C21-C22-C23
55	l	701	CDL	C62-C63-C64-C65
48	g	201	PLX	C11-C12-C13-C14
49	G	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	O4-C1-S44-C43
53	l	703	PEE	C30-C31-C32-C33
53	r	501	PEE	O4-C10-O2-C2
55	a	201	CDL	C11-CA5-OA6-CA4
53	j	202	PEE	C32-C33-C34-C35
48	r	503	PLX	O8-C24-C25-C26
53	Q	501	PEE	O3P-C1-C2-C3
55	l	701	CDL	OA5-CA3-CA4-CA6
53	r	501	PEE	C36-C37-C38-C39
48	a	202	PLX	C30-C31-C32-C33
48	C	302	PLX	C11-C10-C9-C8
55	l	701	CDL	C82-C83-C84-C85
50	J	401	NDP	C3B-C4B-C5B-O5B
53	Q	502	PEE	C31-C30-O3-C3
48	g	201	PLX	C36-C37-C38-C39
55	a	201	CDL	C33-C34-C35-C36
53	j	202	PEE	C38-C39-C40-C41
53	l	703	PEE	C18-C19-C20-C21
49	G	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
53	m	201	PEE	C3-C2-O2-C10
55	l	701	CDL	C34-C35-C36-C37
49	G	201	8Q1	N36-C37-C38-C39
48	j	203	PLX	C7-C6-O6-C4
48	r	502	PLX	C3-C4-C5-O8
53	Q	501	PEE	C2-C1-O3P-P
55	l	701	CDL	C44-C45-C46-C47
55	i	401	CDL	OA5-CA3-CA4-OA6
55	l	701	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	C31-C29-C32-C34
55	l	701	CDL	C60-C61-C62-C63
53	r	501	PEE	O2-C2-C3-O3
53	m	201	PEE	O3-C30-C31-C32
55	a	201	CDL	C73-C74-C75-C76
47	A	503	NAI	C5B-O5B-PA-O3
48	r	503	PLX	C10-C11-C12-C13
55	a	201	CDL	OA7-CA5-OA6-CA4
55	l	701	CDL	C78-C79-C80-C81
55	i	401	CDL	CB3-OB5-PB2-OB2
55	g	202	CDL	C23-C24-C25-C26
55	l	701	CDL	C51-C52-C53-C54
55	l	701	CDL	C54-C55-C56-C57
55	g	202	CDL	CB4-CB3-OB5-PB2
56	s	401	UQ	C12-C11-C9-C8
46	A	502	FMN	C3'-C4'-C5'-O5'
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C3-O4-P1-O3
53	j	201	PEE	C1-O3P-P-O2P
53	j	201	PEE	C4-O4P-P-O2P
53	j	202	PEE	C1-O3P-P-O2P
53	m	201	PEE	C4-O4P-P-O2P
53	m	201	PEE	C4-O4P-P-O1P
53	r	501	PEE	C1-O3P-P-O2P
53	r	501	PEE	C1-O3P-P-O1P
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB4
55	g	202	CDL	CB2-OB2-PB2-OB3
55	g	202	CDL	CB2-OB2-PB2-OB4
55	g	202	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CB2-OB2-PB2-OB3
57	w	401	ADP	C5'-O5'-PA-O1A
55	g	202	CDL	OB5-CB3-CB4-CB6
55	i	401	CDL	OA5-CA3-CA4-CA6
53	j	201	PEE	C17-C18-C19-C20
53	Q	502	PEE	O5-C30-O3-C3
55	V	201	CDL	C81-C82-C83-C84
53	Q	501	PEE	C39-C40-C41-C42
53	j	201	PEE	C39-C40-C41-C42
55	g	202	CDL	C34-C35-C36-C37
55	l	701	CDL	C12-C13-C14-C15
47	A	503	NAI	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
48	g	201	PLX	O4-C3-C4-O6
55	g	202	CDL	OB5-CB3-CB4-OB6
55	l	701	CDL	OA5-CA3-CA4-OA6
48	r	503	PLX	C2-C1-N1-C1A
47	A	503	NAI	C2D-C1D-N1N-C6N
48	C	302	PLX	N1-C1-C2-O1
50	J	401	NDP	C2N-C3N-C7N-O7N
55	i	401	CDL	CA3-CA4-CA6-OA8
48	a	202	PLX	O6-C4-C5-O8
48	j	203	PLX	O6-C4-C5-O8
53	l	703	PEE	O2-C2-C3-O3
55	i	401	CDL	OA6-CA4-CA6-OA8
55	i	401	CDL	C73-C74-C75-C76
48	a	202	PLX	C10-C11-C12-C13
53	l	702	PEE	C21-C22-C23-C24
55	a	201	CDL	C16-C17-C18-C19
55	l	701	CDL	C32-C33-C34-C35
48	C	302	PLX	C18-C19-C20-C21
55	g	202	CDL	C61-C62-C63-C64
55	a	201	CDL	C24-C25-C26-C27
53	l	702	PEE	C20-C21-C22-C23
55	l	701	CDL	C17-C18-C19-C20
48	g	201	PLX	O4-C3-C4-C5
48	j	203	PLX	O4-C3-C4-C5
55	V	201	CDL	OB5-CB3-CB4-CB6
48	r	503	PLX	C17-C18-C19-C20
53	Q	501	PEE	C14-C15-C16-C17
46	A	502	FMN	C5'-O5'-P-O1P
48	r	502	PLX	C14-C15-C16-C17
55	i	401	CDL	C13-C14-C15-C16
55	l	701	CDL	C31-C32-C33-C34
48	j	203	PLX	O4-C3-C4-O6
48	r	503	PLX	C2-C1-N1-C1C
47	A	503	NAI	O4D-C1D-N1N-C2N
55	l	701	CDL	C58-C59-C60-C61
48	r	502	PLX	O6-C4-C5-O8
53	Q	501	PEE	O2-C2-C3-O3
49	G	201	8Q1	C6-C7-C8-C9
53	Q	501	PEE	C24-C25-C26-C27
53	r	501	PEE	C24-C25-C26-C27
48	a	202	PLX	C2-O1-P1-O4
55	V	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
55	g	202	CDL	C60-C61-C62-C63
49	G	201	8Q1	C30-C29-C32-O33
53	Q	502	PEE	C21-C22-C23-C24
55	i	401	CDL	CB3-CB4-CB6-OB8
55	l	701	CDL	C56-C57-C58-C59
53	j	201	PEE	C44-C45-C46-C47
48	r	503	PLX	C2-C1-N1-C1B
55	V	201	CDL	C75-C76-C77-C78
55	a	201	CDL	C57-C58-C59-C60
48	a	202	PLX	C11-C12-C13-C14
48	C	302	PLX	C31-C32-C33-C34
55	a	201	CDL	C54-C55-C56-C57
53	j	202	PEE	C37-C38-C39-C40
55	g	202	CDL	C82-C83-C84-C85
53	j	201	PEE	C18-C19-C20-C21
56	s	401	UQ	C14-C16-C17-C18
55	V	201	CDL	C82-C83-C84-C85
53	Q	502	PEE	C13-C14-C15-C16
55	l	701	CDL	C15-C16-C17-C18
53	m	201	PEE	C24-C25-C26-C27
48	r	503	PLX	C24-C25-C26-C27
55	a	201	CDL	C44-C45-C46-C47
48	j	203	PLX	O6-C6-C7-C8
48	j	203	PLX	O8-C24-C25-C26
55	V	201	CDL	C12-C11-CA5-OA7
57	w	401	ADP	C4'-C5'-O5'-PA
48	j	203	PLX	C35-C36-C37-C38
55	l	701	CDL	C23-C24-C25-C26
49	G	201	8Q1	C9-C10-C11-C12
53	j	201	PEE	C1-C2-C3-O3
55	a	201	CDL	C43-C44-C45-C46
49	G	201	8Q1	O27-C28-C29-C30
48	r	503	PLX	C7-C8-C9-C10
53	l	703	PEE	C32-C33-C34-C35
53	j	202	PEE	C24-C25-C26-C27
53	Q	501	PEE	C38-C39-C40-C41
55	V	201	CDL	C12-C11-CA5-OA6
55	i	401	CDL	C37-C38-C39-C40
55	a	201	CDL	C41-C42-C43-C44
53	Q	501	PEE	O3P-C1-C2-O2
53	r	501	PEE	C18-C19-C20-C21
55	l	701	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	C71-C72-C73-C74
55	V	201	CDL	C83-C84-C85-C86
55	g	202	CDL	C44-C45-C46-C47
48	r	503	PLX	C11-C12-C13-C14
55	l	701	CDL	C79-C80-C81-C82
53	m	201	PEE	C17-C18-C19-C20
53	j	202	PEE	C31-C32-C33-C34
53	m	201	PEE	C32-C33-C34-C35
53	l	703	PEE	C22-C23-C24-C25
48	a	202	PLX	C19-C20-C21-C22
55	l	701	CDL	C63-C64-C65-C66
50	J	401	NDP	PN-O3-PA-O1A
55	V	201	CDL	OB9-CB7-OB8-CB6
55	V	201	CDL	CB3-CB4-CB6-OB8
55	V	201	CDL	CB7-C71-C72-C73
47	A	503	NAI	O4D-C1D-N1N-C6N
53	l	702	PEE	C16-C17-C18-C19
53	l	703	PEE	C10-C11-C12-C13
53	j	202	PEE	C23-C24-C25-C26
48	C	302	PLX	O8-C24-C25-C26
48	g	201	PLX	O8-C24-C25-C26
48	a	202	PLX	C27-C28-C29-C30
56	s	401	UQ	C9-C11-C12-C13
53	l	703	PEE	O4P-C4-C5-N
48	j	203	PLX	C31-C32-C33-C34
48	r	502	PLX	C4-C3-O4-P1
55	i	401	CDL	CA4-CA3-OA5-PA1
53	j	202	PEE	C44-C45-C46-C47
55	V	201	CDL	C71-CB7-OB8-CB6
48	r	502	PLX	C11-C12-C13-C14
53	l	702	PEE	C13-C14-C15-C16
49	G	201	8Q1	O27-C28-C29-C31
48	C	302	PLX	C30-C31-C32-C33
55	l	701	CDL	C32-C31-CA7-OA8
53	j	201	PEE	C38-C39-C40-C41
53	l	702	PEE	C36-C37-C38-C39
53	l	703	PEE	C38-C39-C40-C41
53	m	201	PEE	C16-C17-C18-C19
55	l	701	CDL	C33-C34-C35-C36
55	V	201	CDL	C71-C72-C73-C74
55	V	201	CDL	C32-C31-CA7-OA8
53	Q	501	PEE	C36-C37-C38-C39

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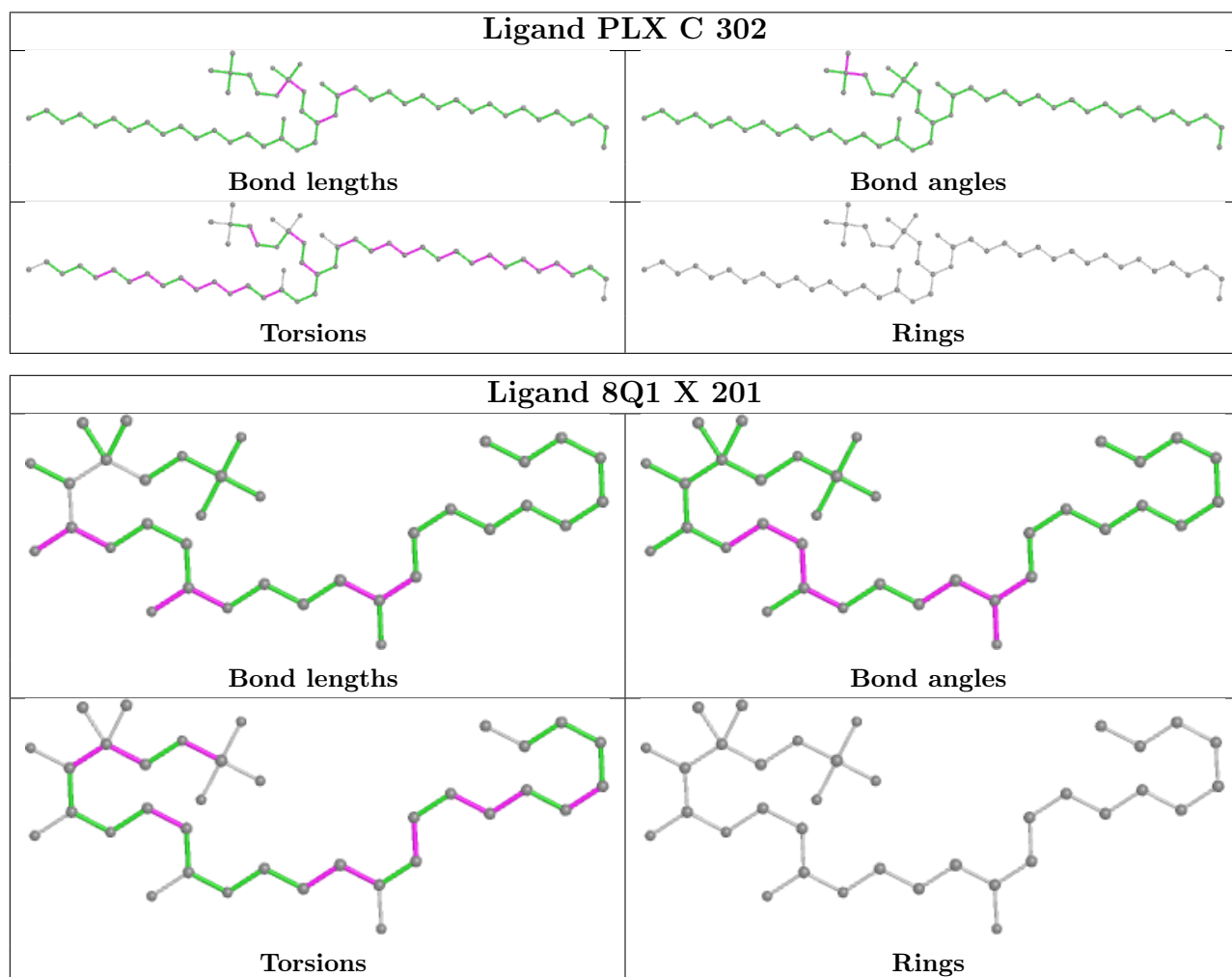
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Mol	Chain	Res	Type	Atoms
53	Q	502	PEE	C18-C19-C20-C21
53	j	201	PEE	C16-C17-C18-C19
53	Q	501	PEE	C15-C16-C17-C18
53	l	702	PEE	C1-C2-C3-O3
55	g	202	CDL	C52-C51-CB5-OB6
48	g	201	PLX	C18-C19-C20-C21
53	m	201	PEE	C18-C19-C20-C21
53	r	501	PEE	C32-C33-C34-C35
53	l	702	PEE	C22-C23-C24-C25
53	j	202	PEE	O2-C10-C11-C12
53	l	702	PEE	O2-C2-C3-O3
55	g	202	CDL	C81-C82-C83-C84
55	a	201	CDL	C15-C16-C17-C18
53	j	201	PEE	C36-C37-C38-C39
47	A	503	NAI	O4D-C4D-C5D-O5D
55	V	201	CDL	C32-C31-CA7-OA9
53	Q	502	PEE	C42-C43-C44-C45
53	r	501	PEE	C40-C41-C42-C43
55	g	202	CDL	C52-C51-CB5-OB7
55	a	201	CDL	CB3-CB4-CB6-OB8
53	j	202	PEE	O4-C10-C11-C12
53	l	702	PEE	O2-C10-C11-C12
55	l	701	CDL	C32-C31-CA7-OA9
48	j	203	PLX	C3-O4-P1-O3
53	r	501	PEE	C4-O4P-P-O1P
55	V	201	CDL	CA3-OA5-PA1-OA3
55	V	201	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CA2-OA2-PA1-OA4
55	i	401	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	OB6-CB4-CB6-OB8
55	g	202	CDL	C80-C81-C82-C83
53	l	703	PEE	C5-C4-O4P-P
53	l	703	PEE	O3-C30-C31-C32
55	g	202	CDL	C72-C71-CB7-OB8
55	l	701	CDL	C12-C11-CA5-OA6
53	l	702	PEE	O4-C10-C11-C12
53	m	201	PEE	C12-C13-C14-C15
55	g	202	CDL	C72-C71-CB7-OB9
53	l	703	PEE	O2-C10-C11-C12
53	j	202	PEE	C16-C17-C18-C19

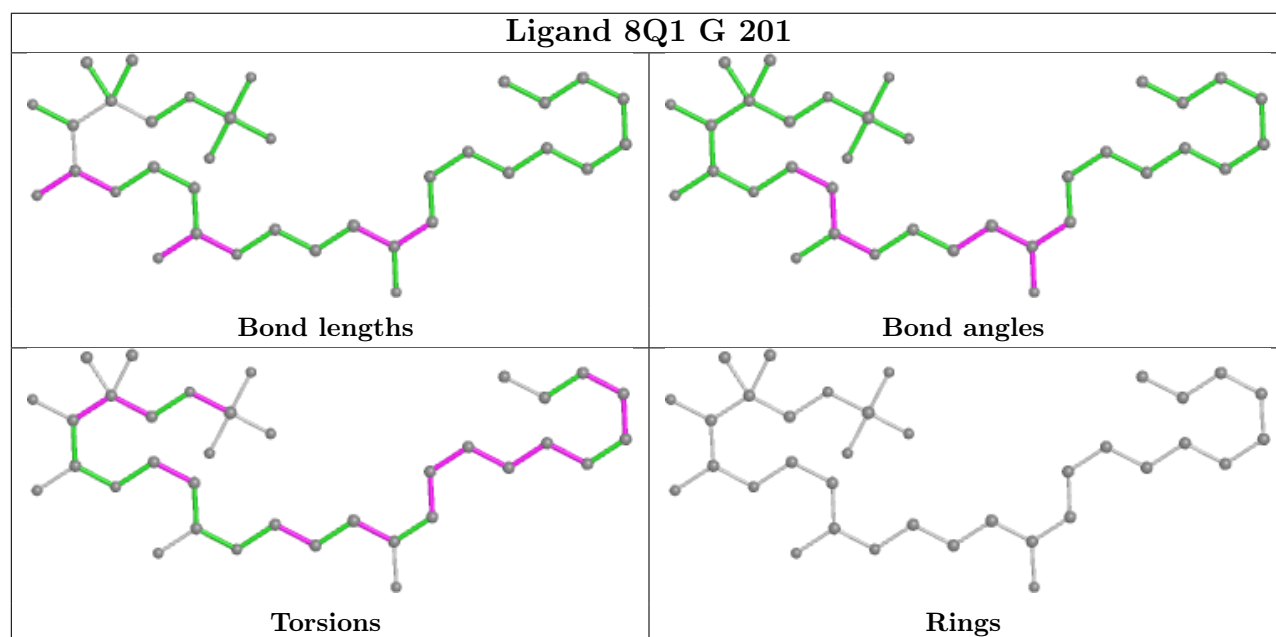
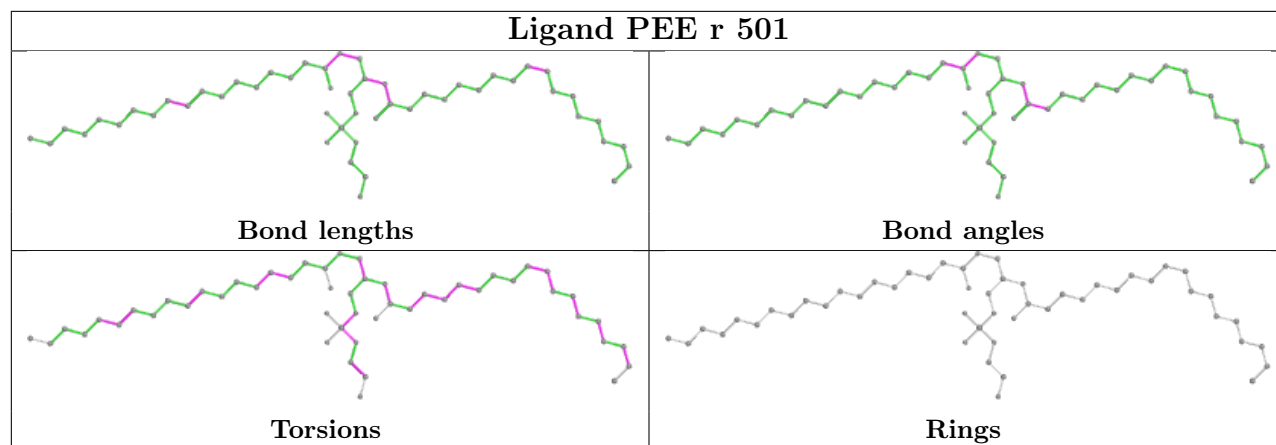
There are no ring outliers.

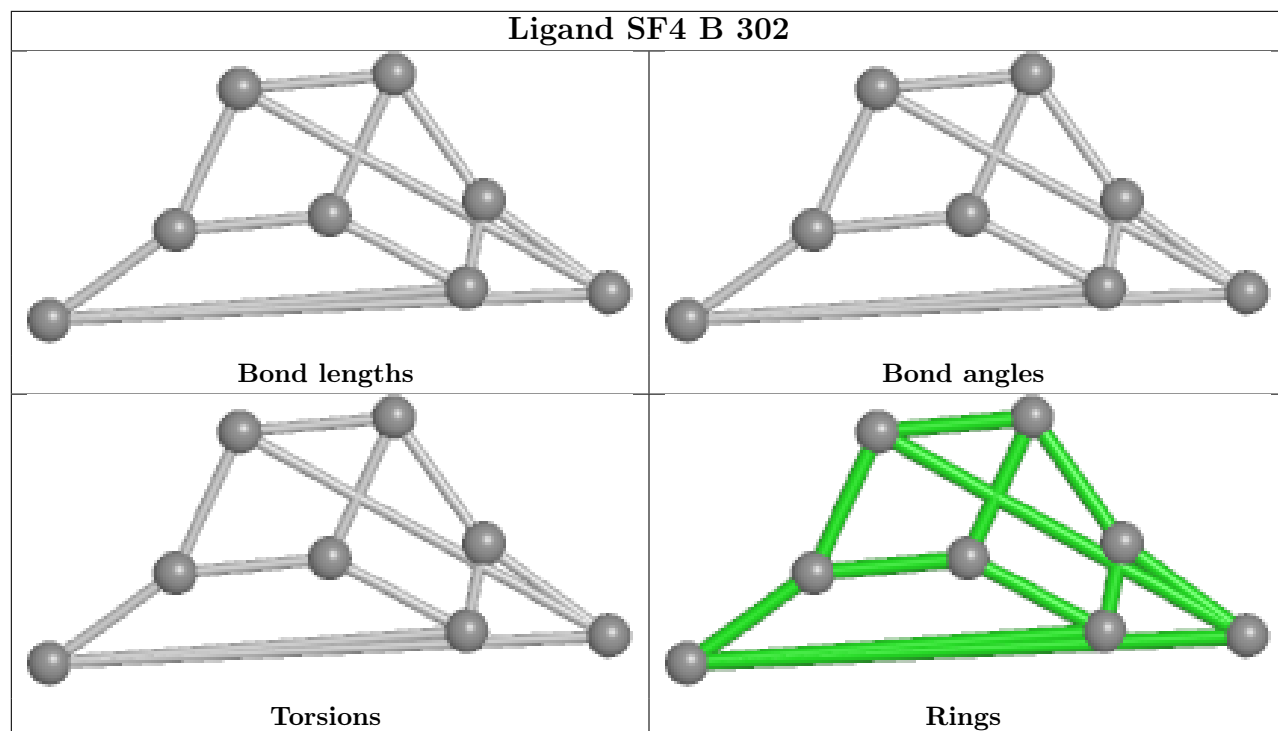
No monomer is involved in short contacts.

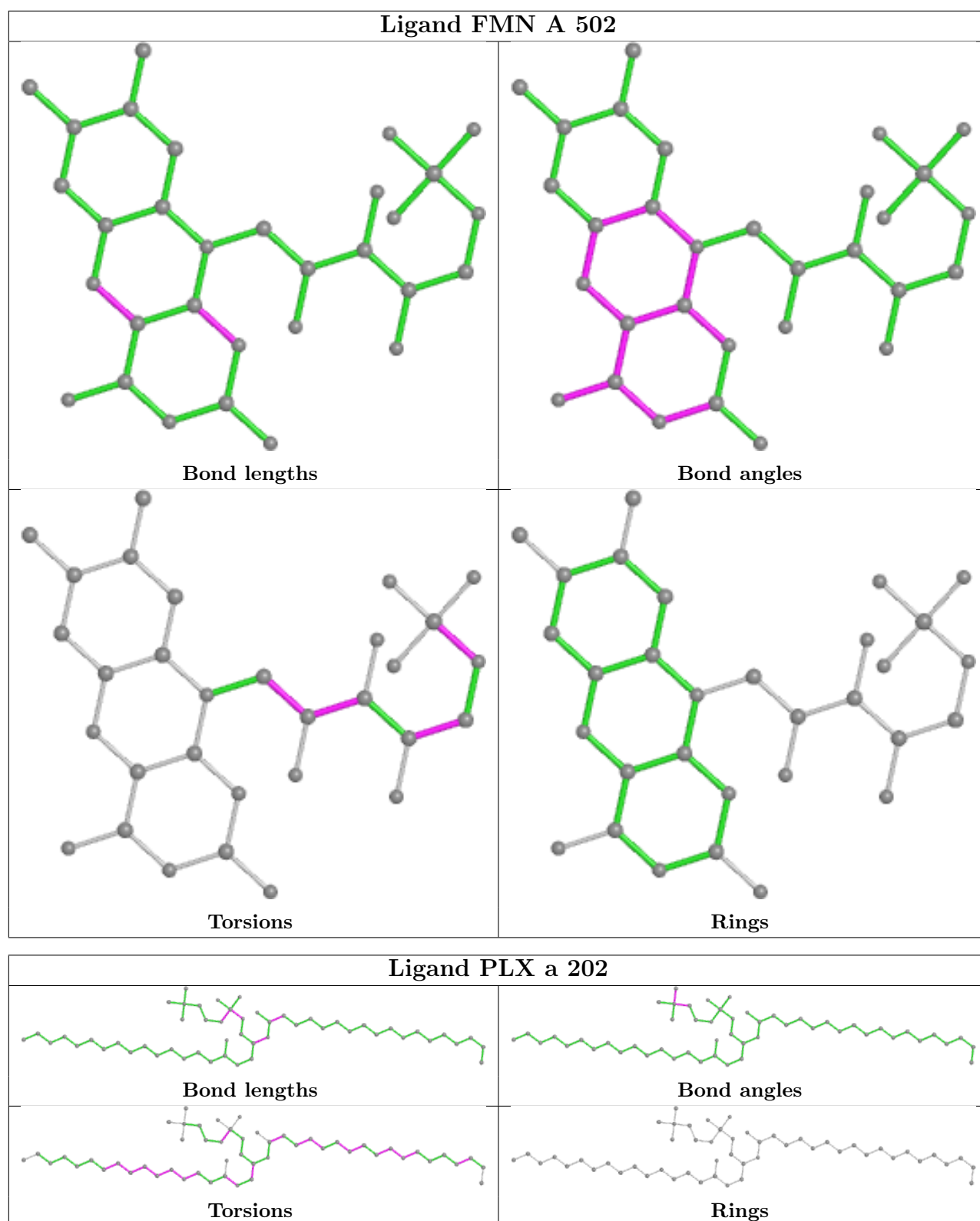
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

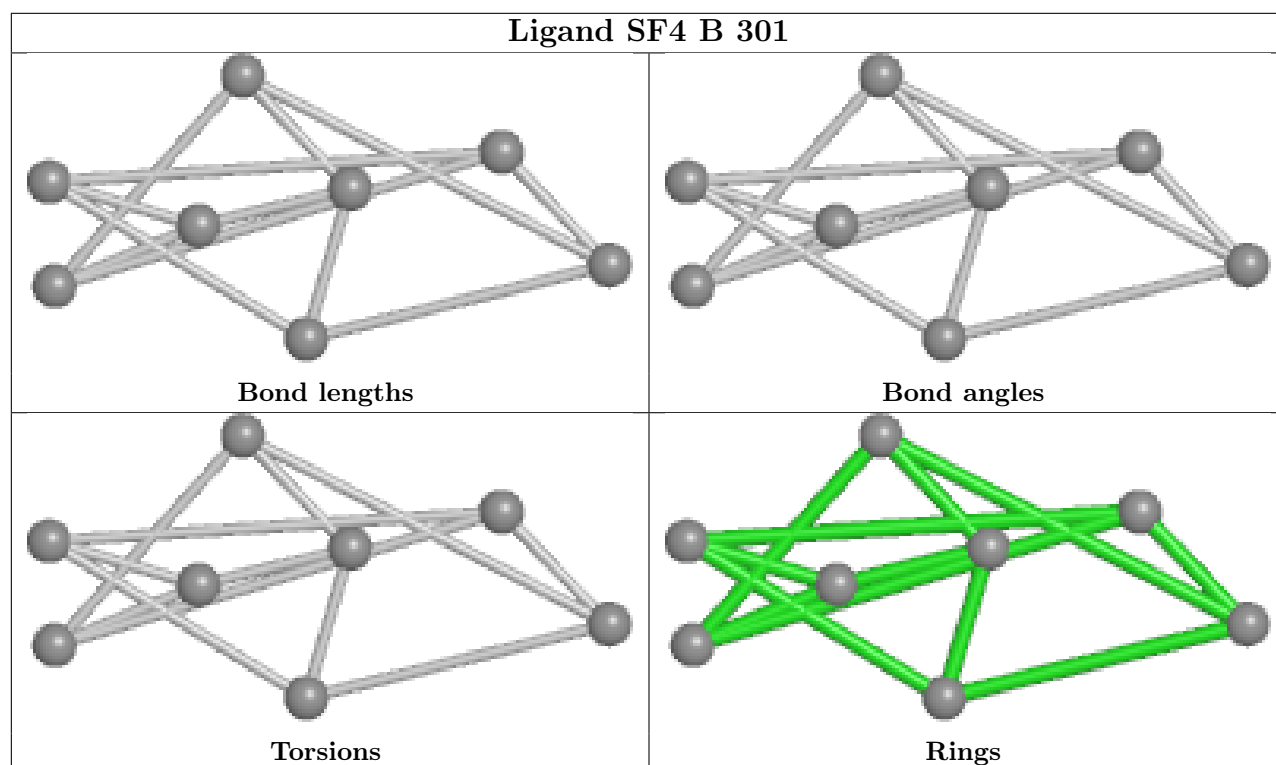
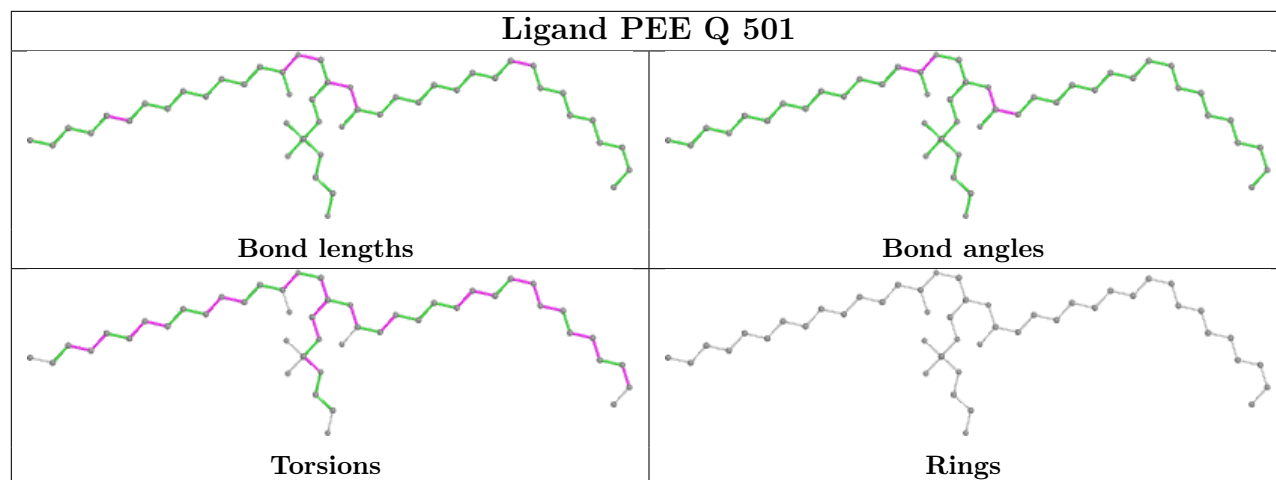


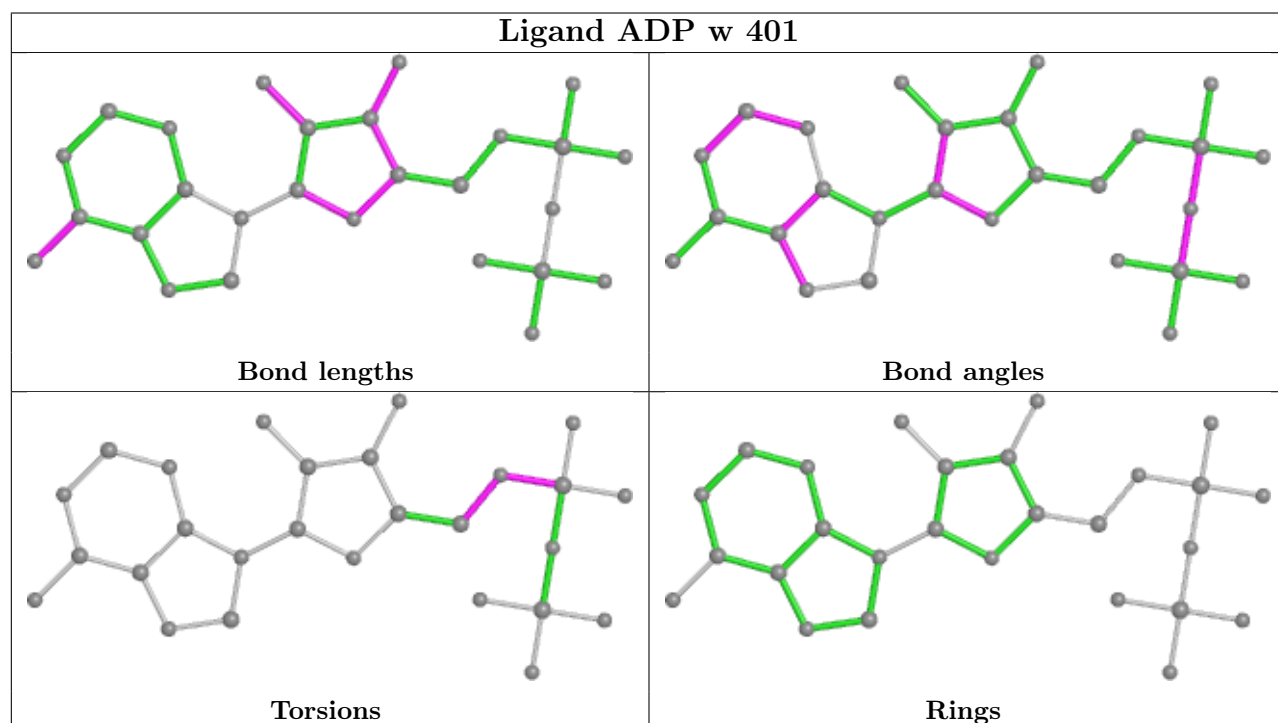
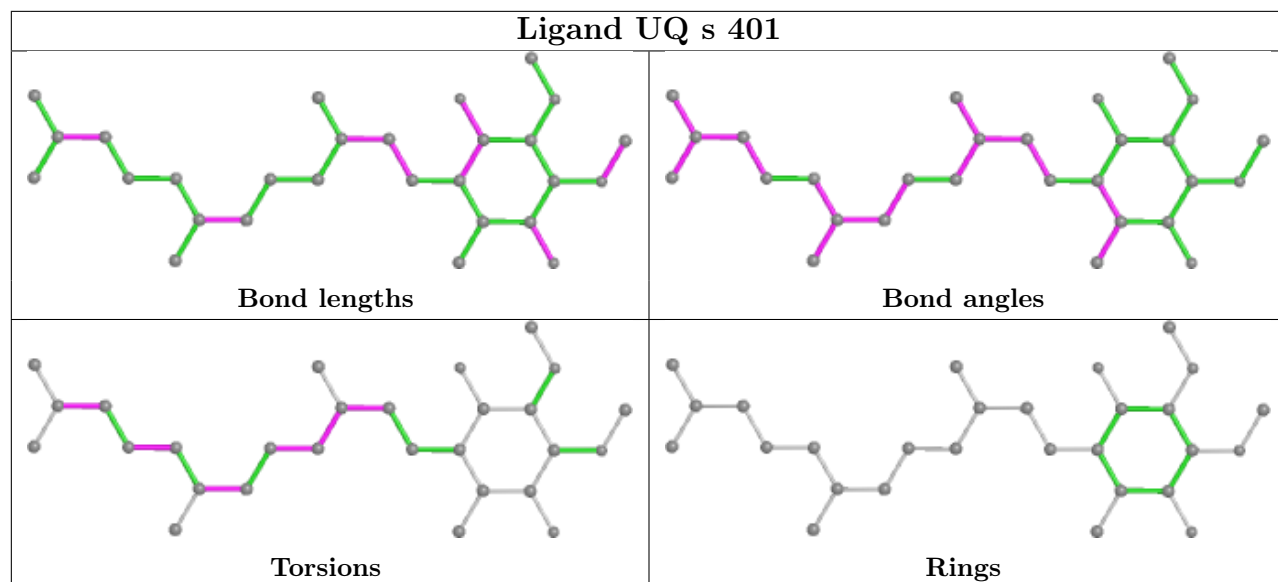


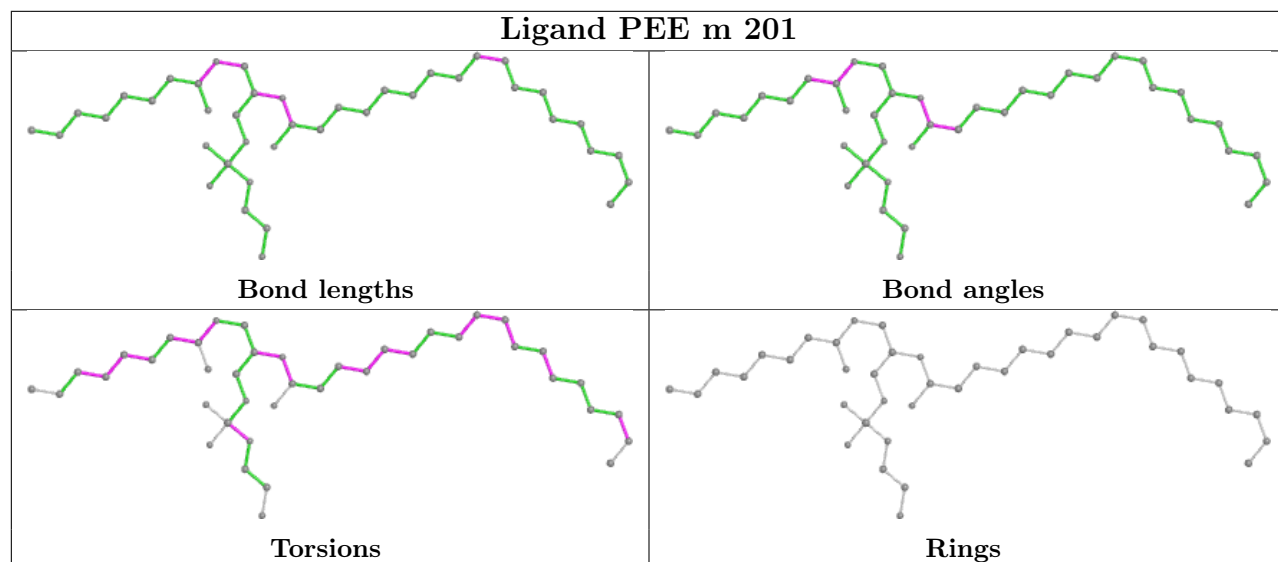
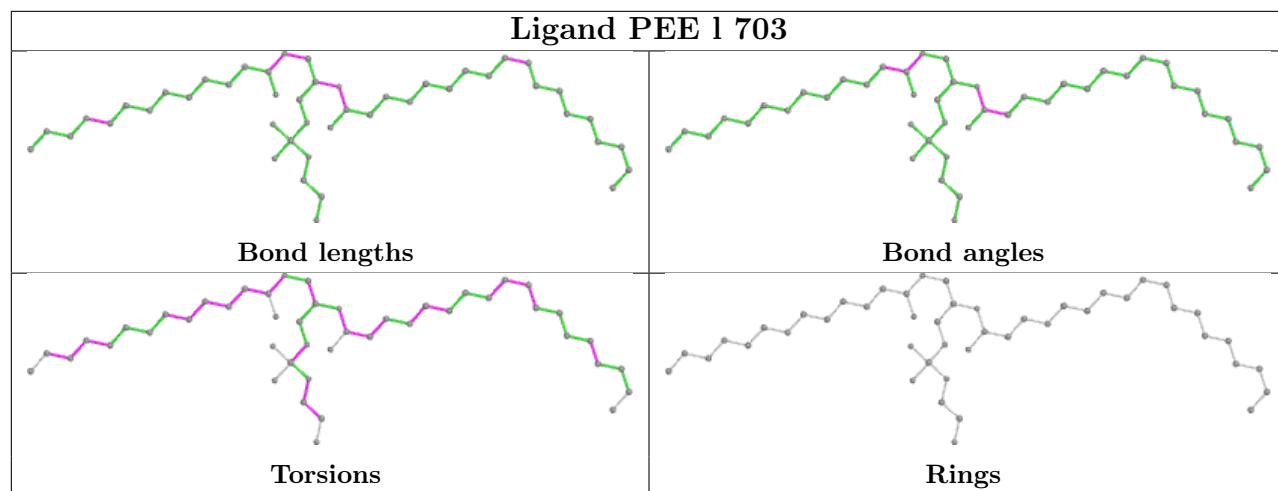


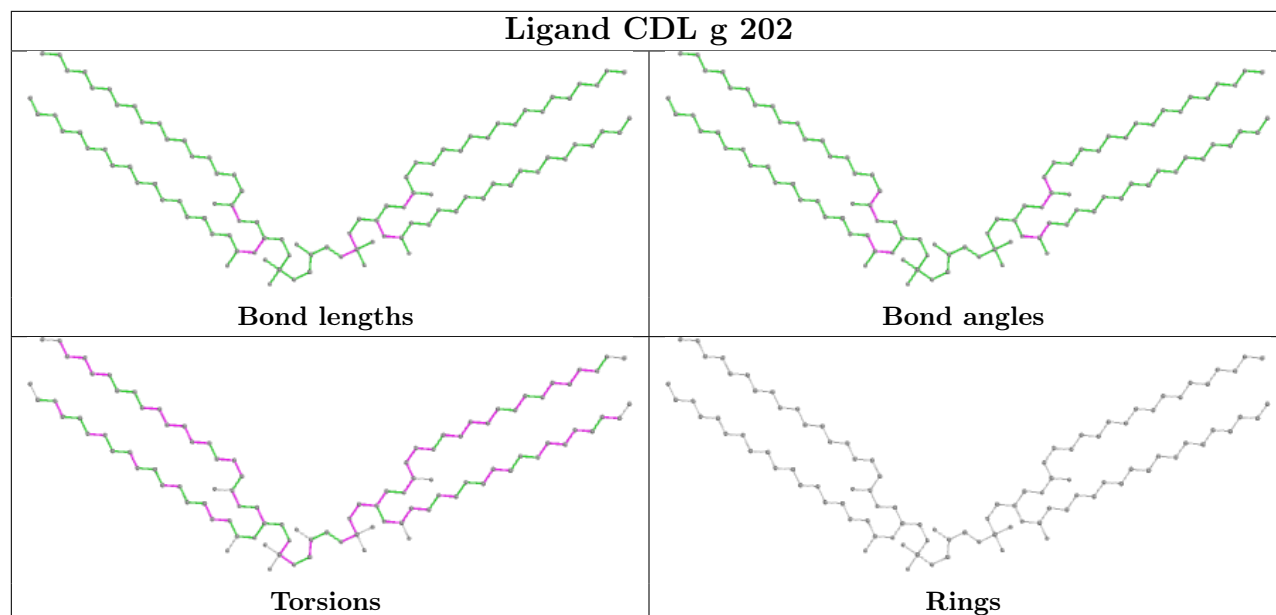
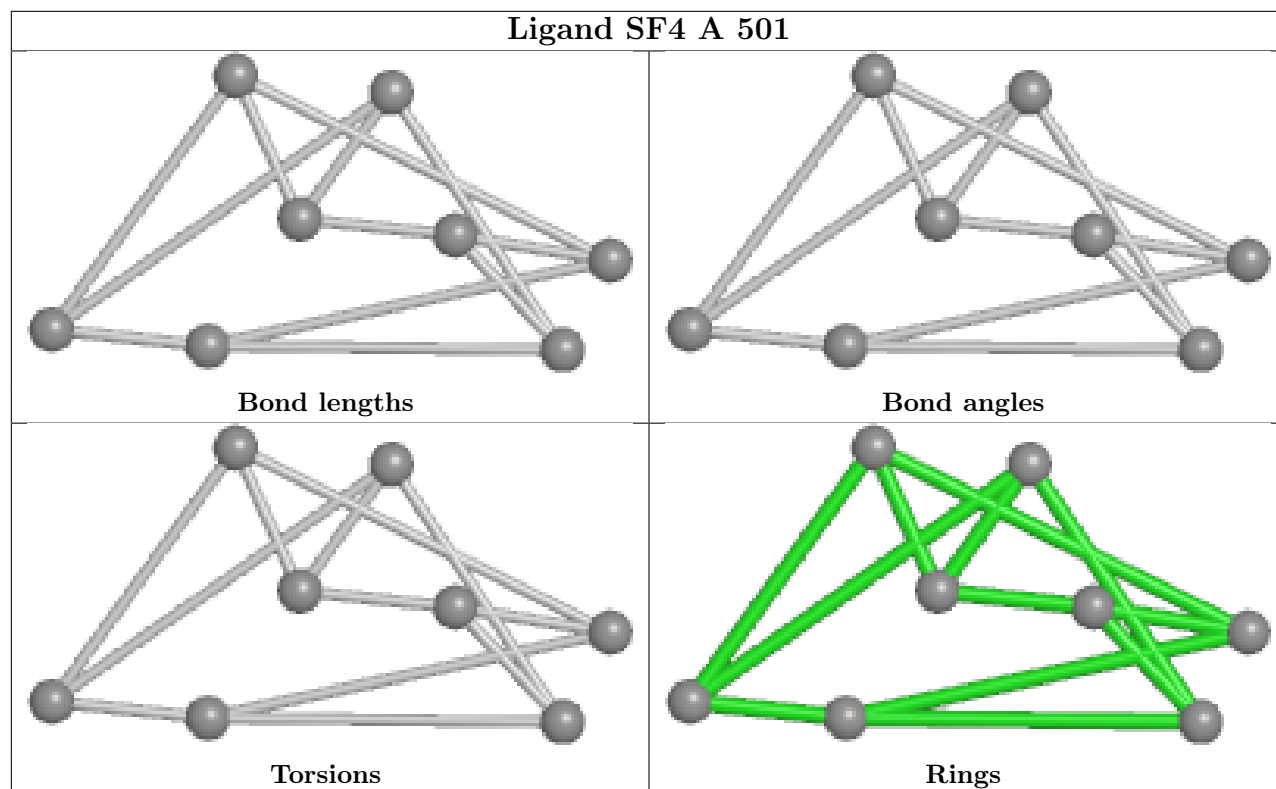


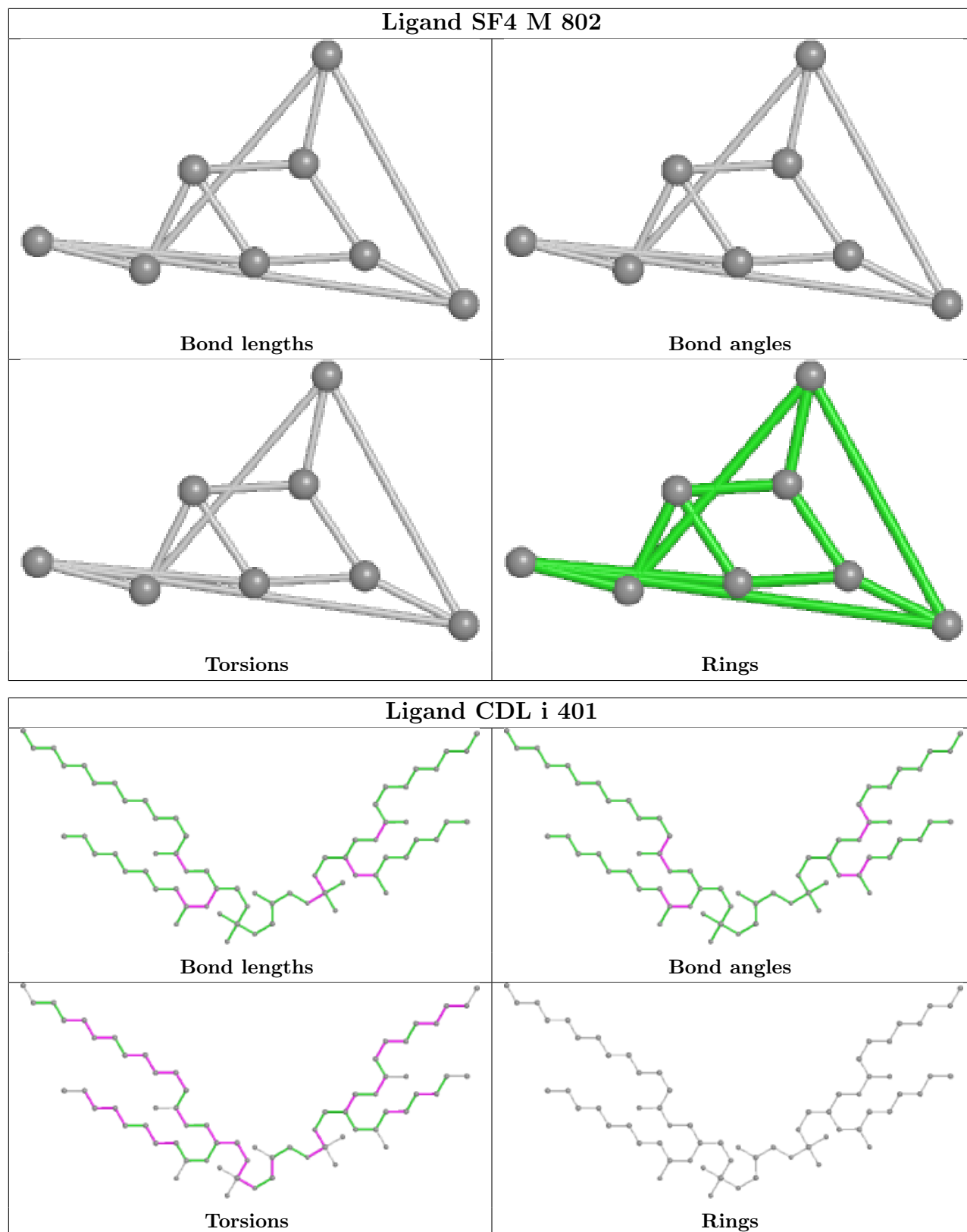




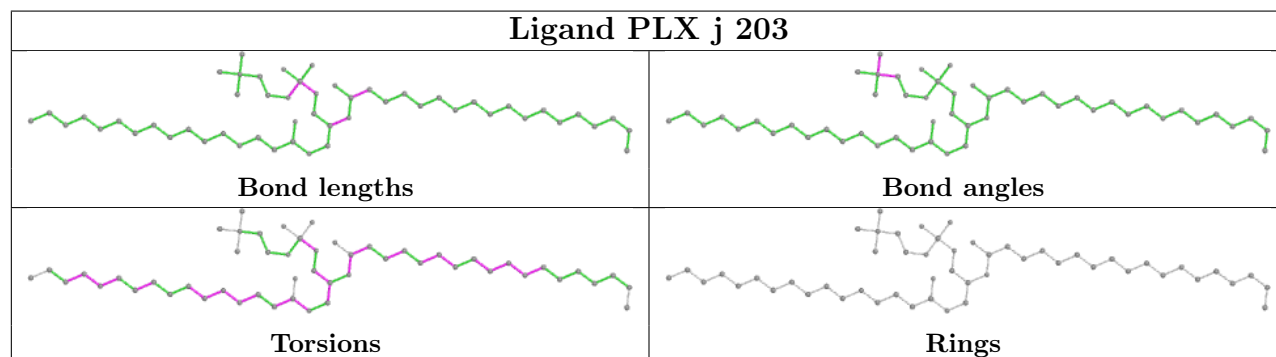
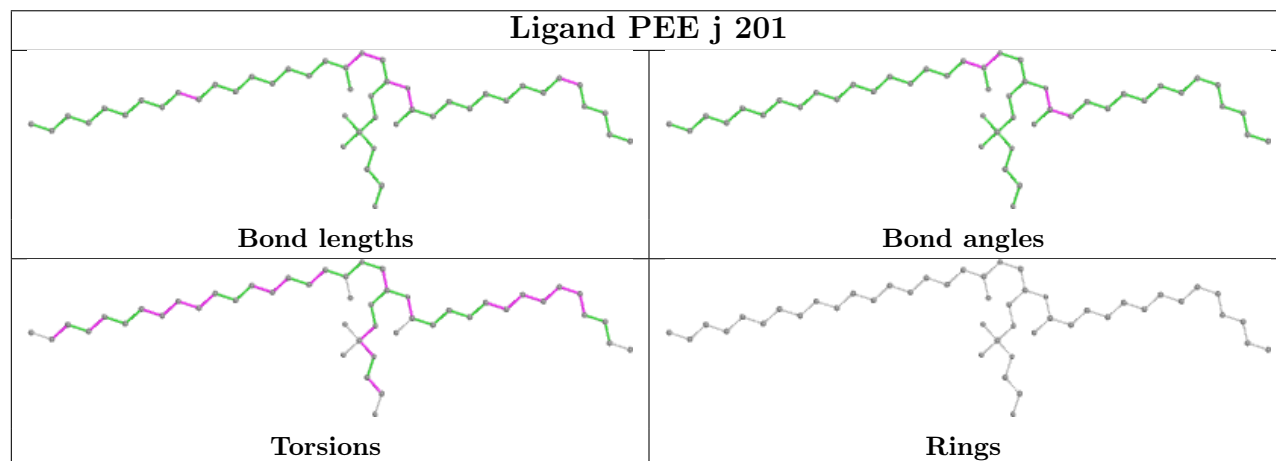
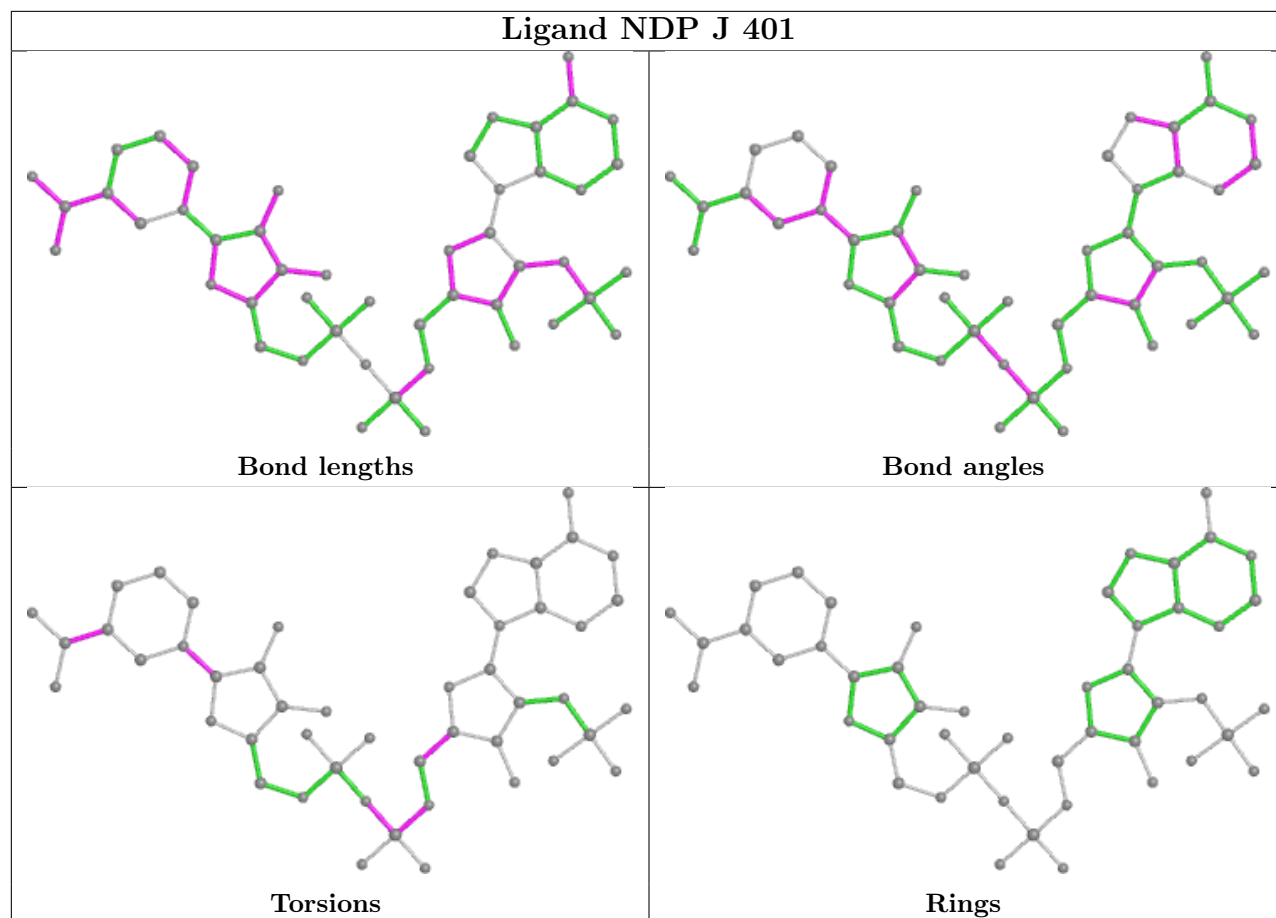


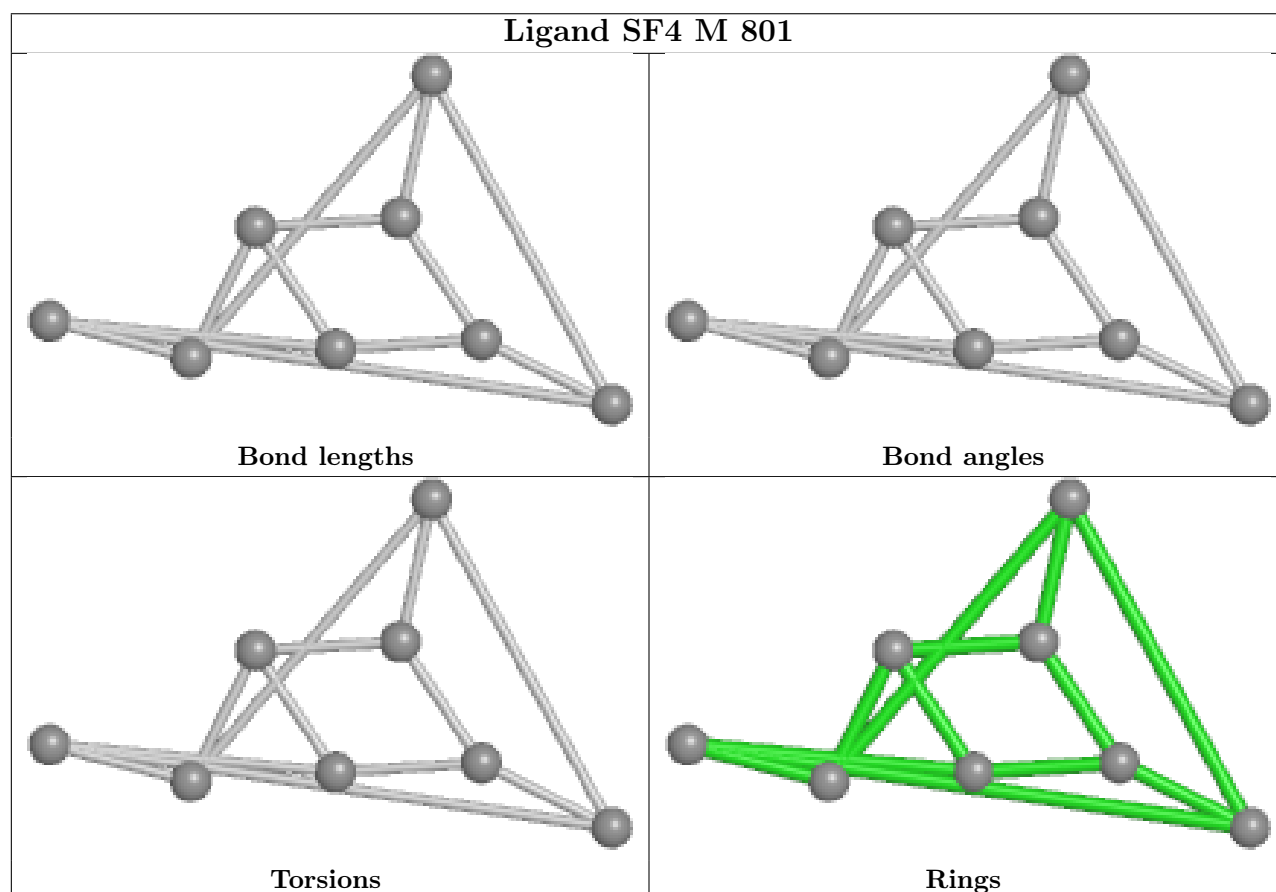
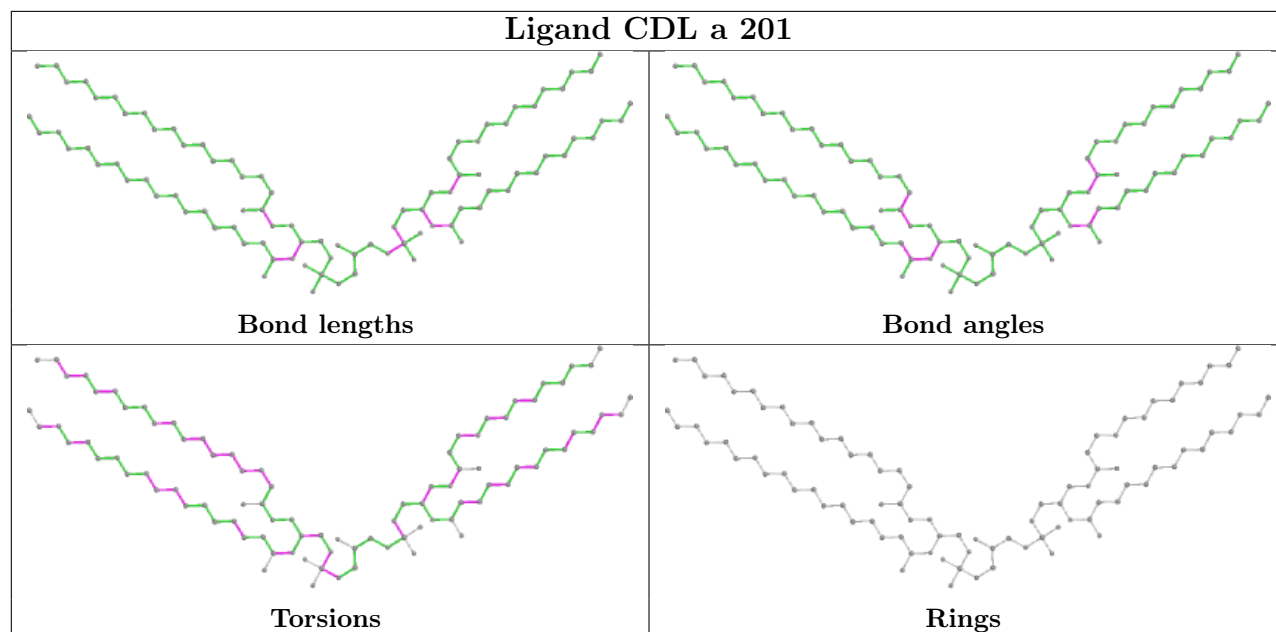


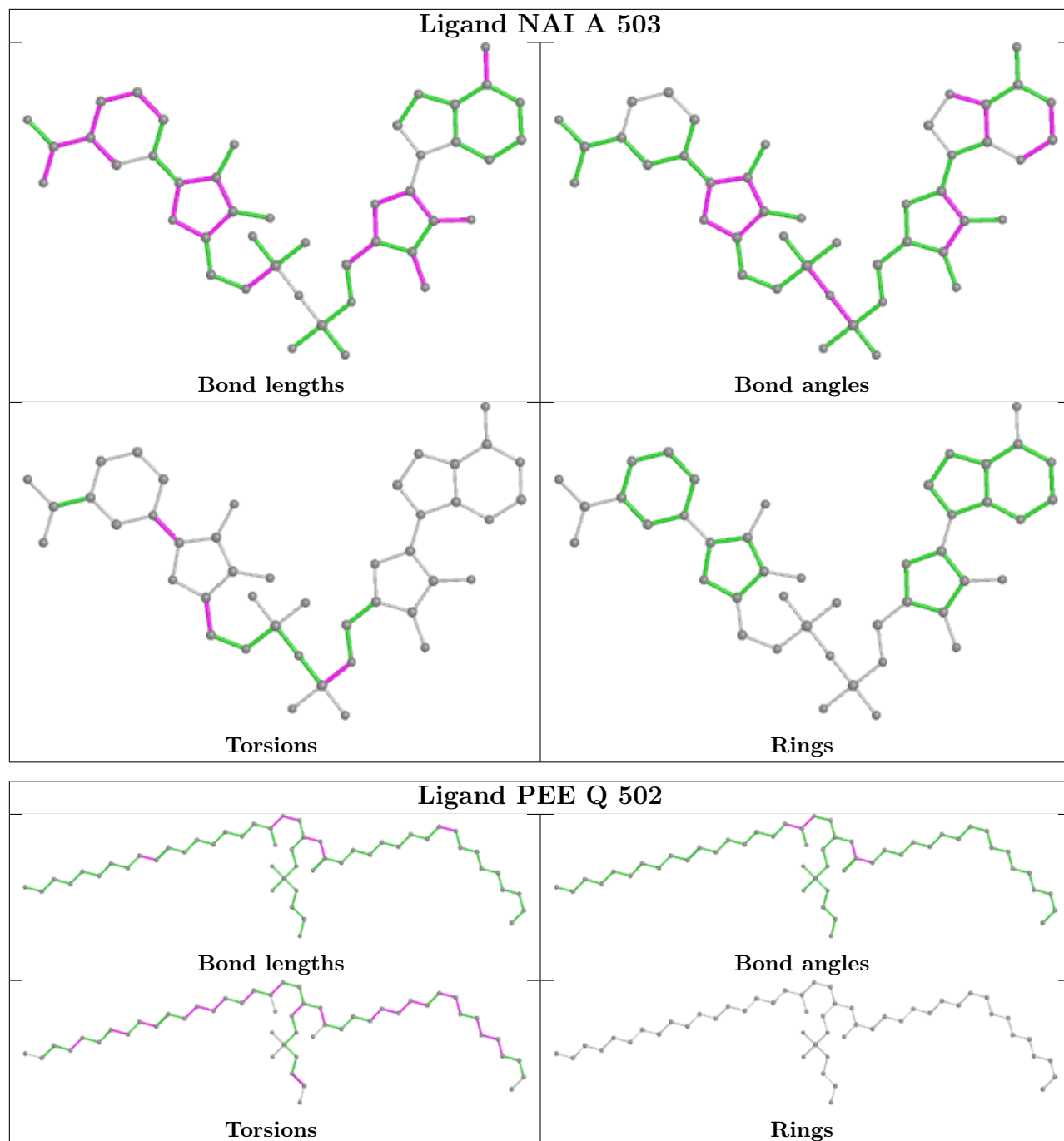


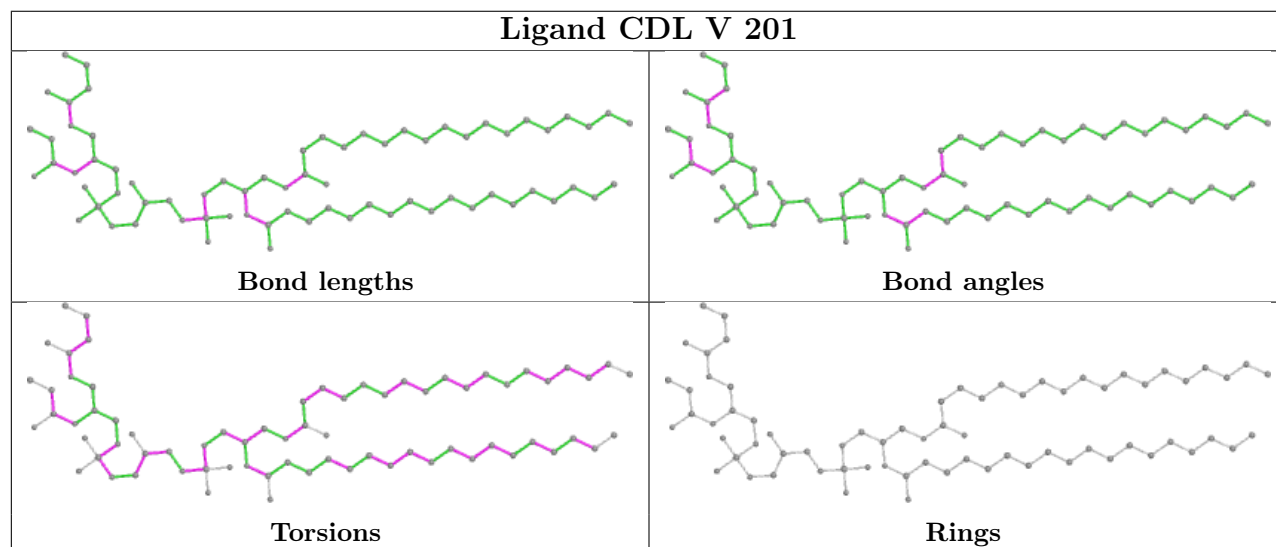
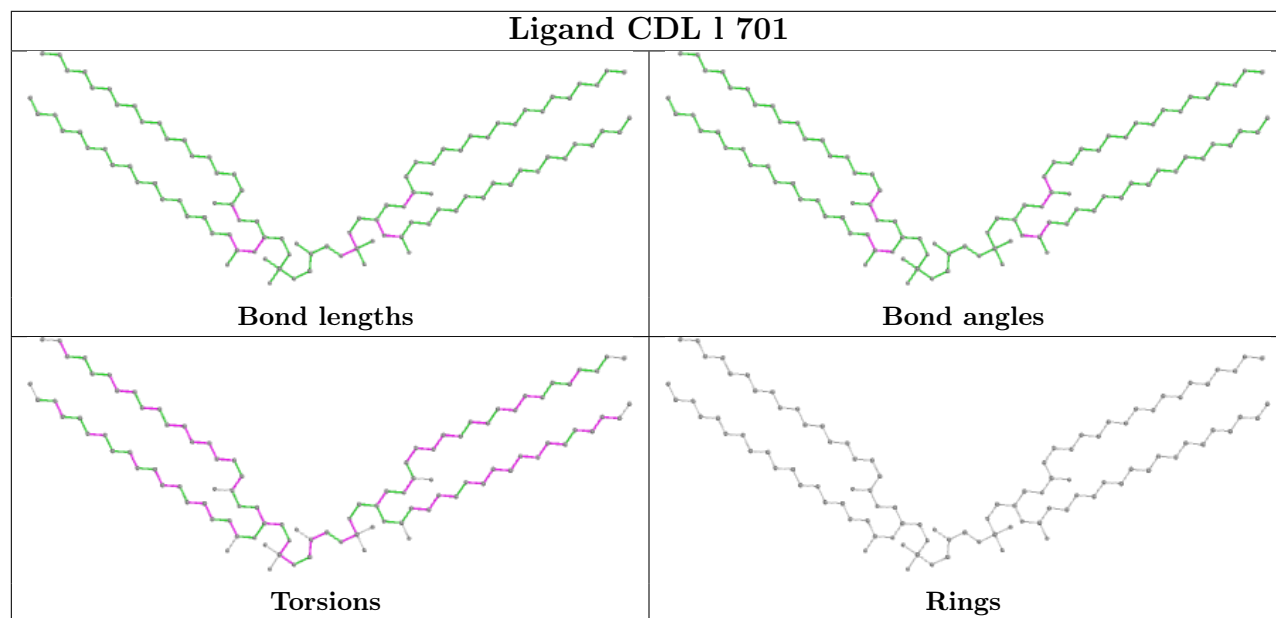
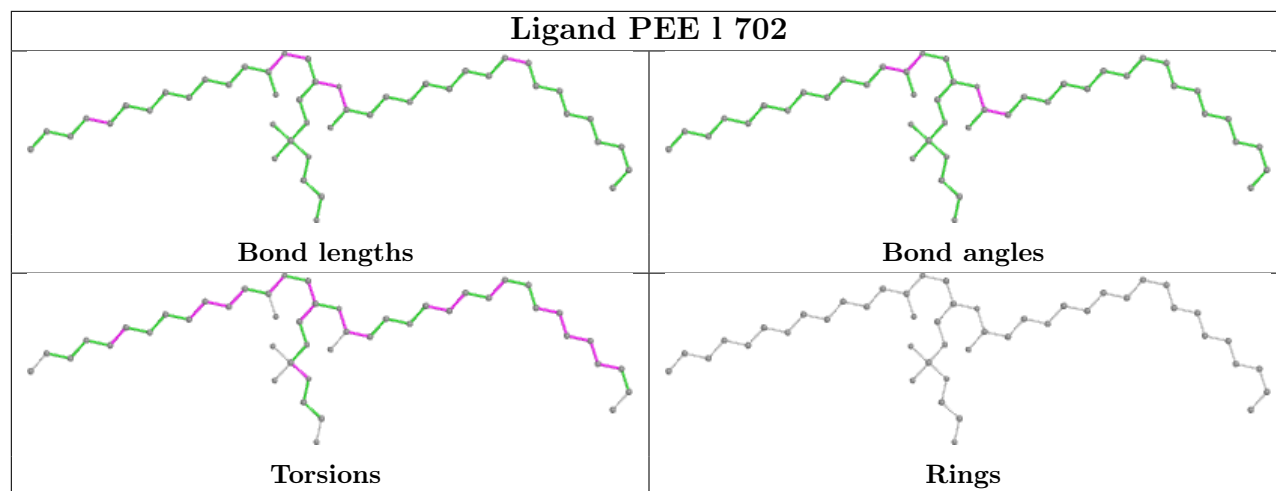


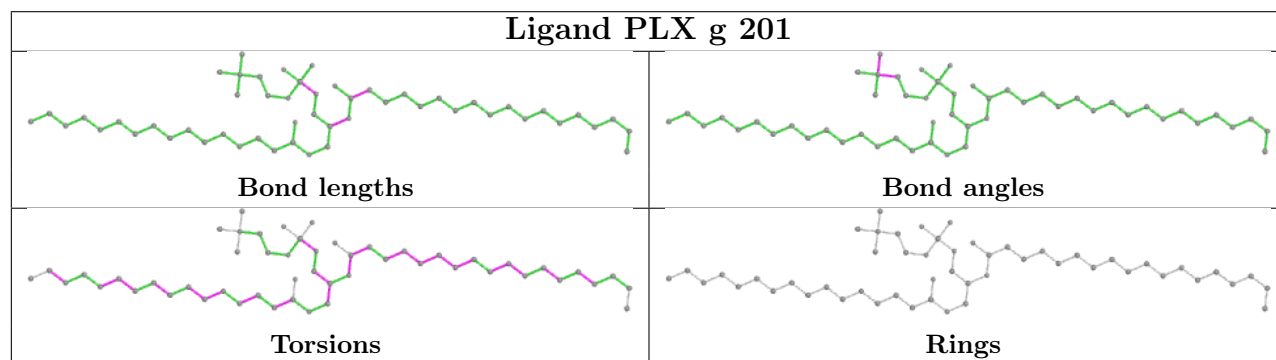
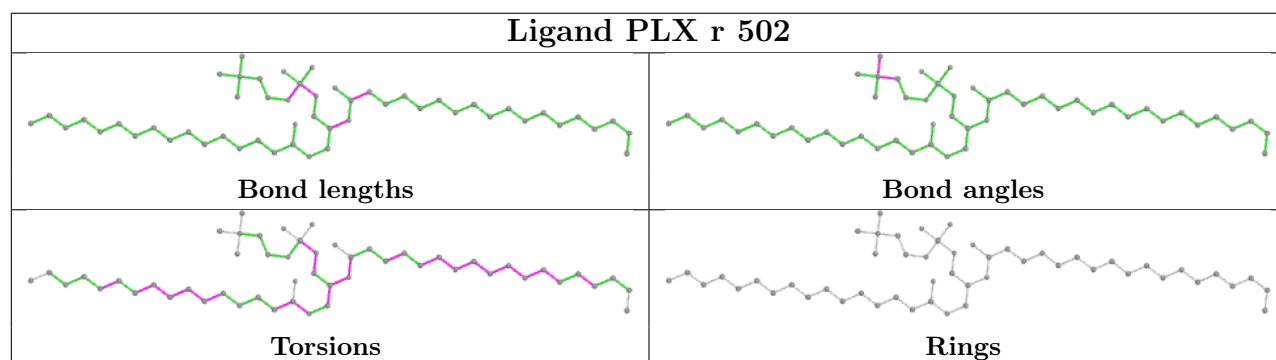
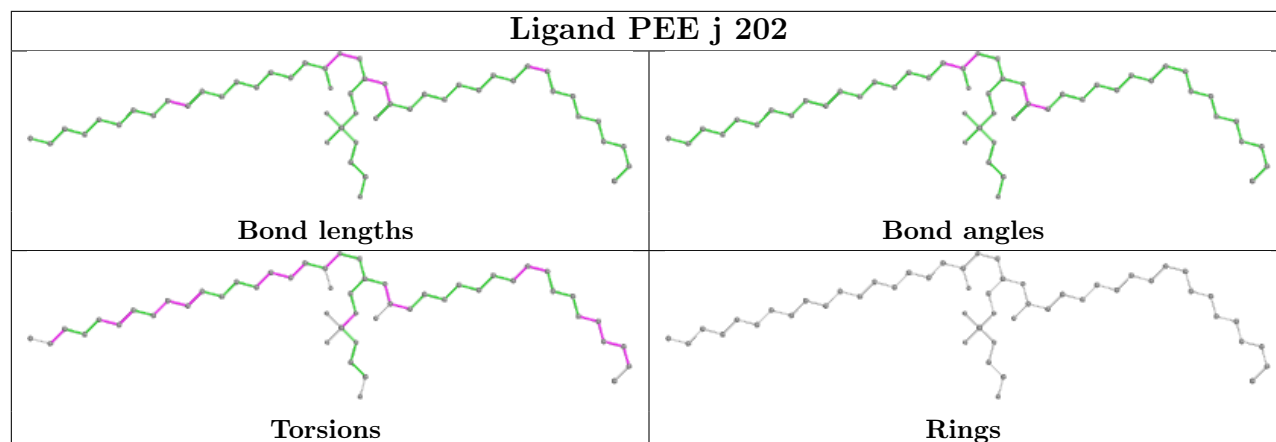


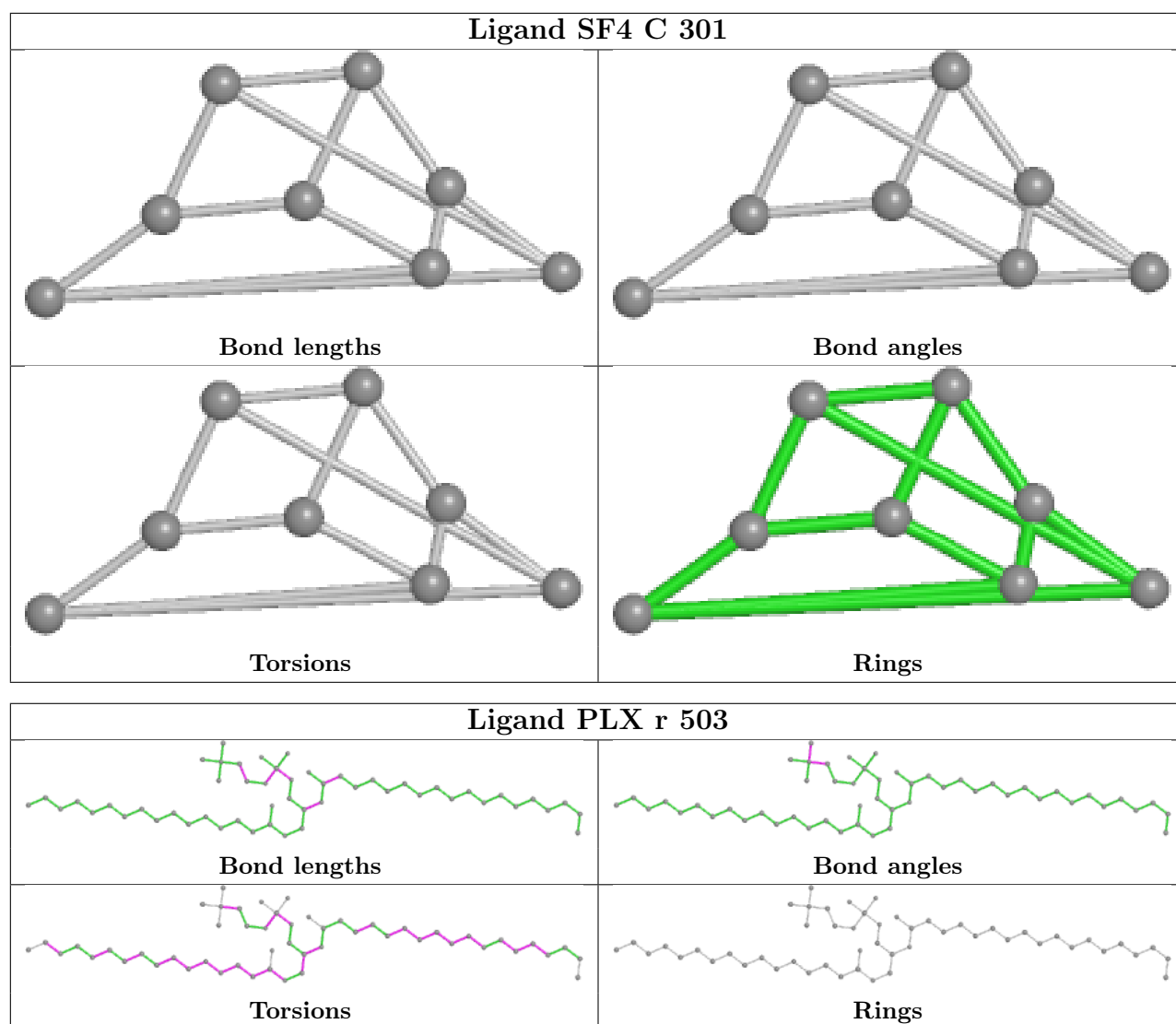












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

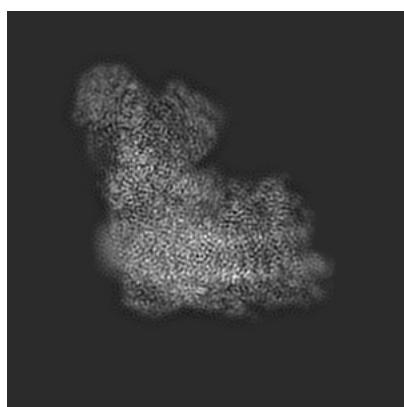
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32307. These allow visual inspection of the internal detail of the map and identification of artifacts.

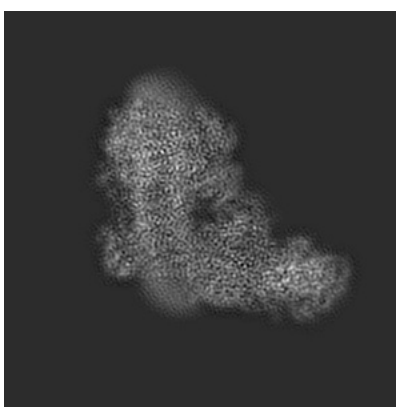
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

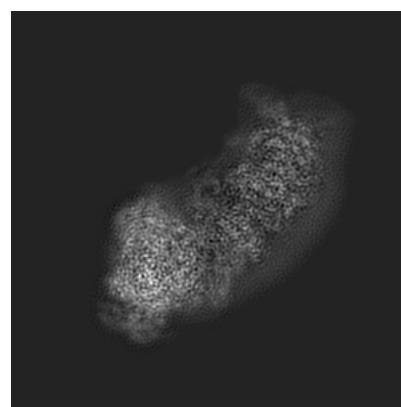
#### 6.1.1 Primary map



X



Y

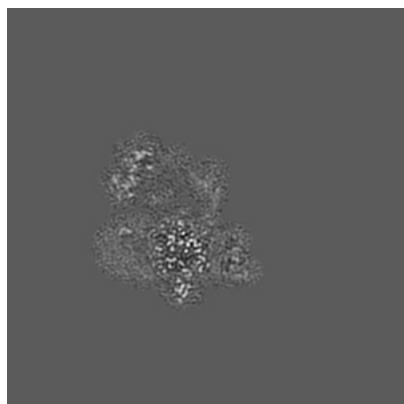


Z

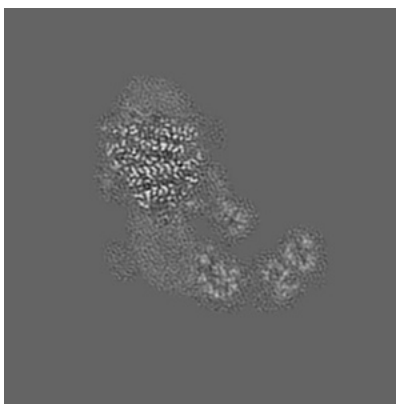
The images above show the map projected in three orthogonal directions.

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

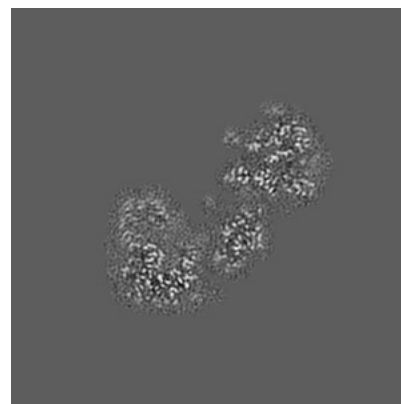
#### 6.2.1 Primary map



X Index: 152



Y Index: 152

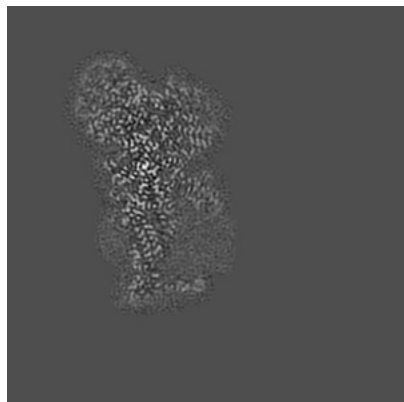


Z Index: 152

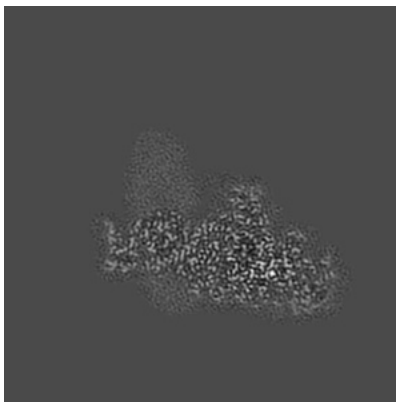
The images above show central slices of the map in three orthogonal directions.

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

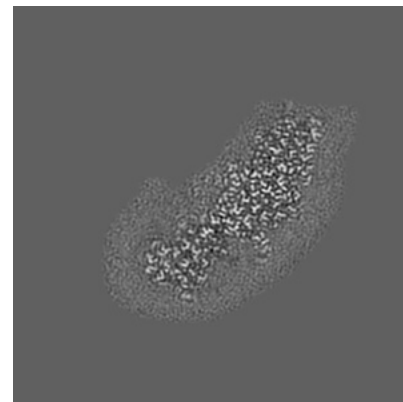
### 6.3.1 Primary map



X Index: 105



Y Index: 98

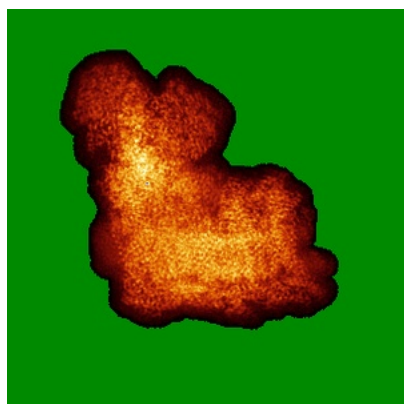


Z Index: 127

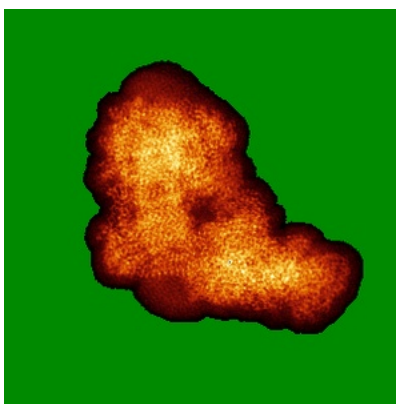
The images above show the largest variance slices of the map in three orthogonal directions.

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

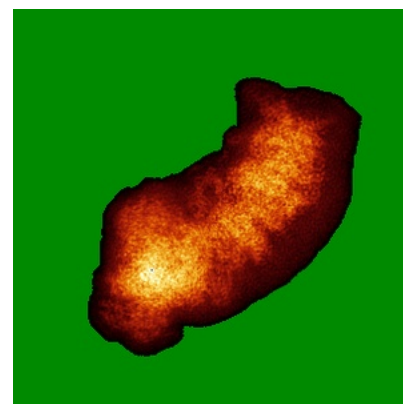
### 6.4.1 Primary map



X



Y



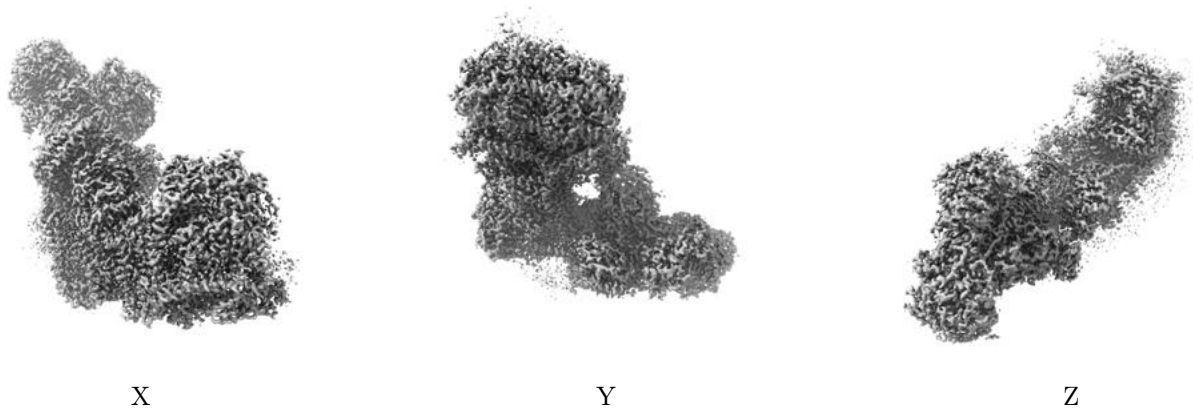
Z

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 0.0296. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

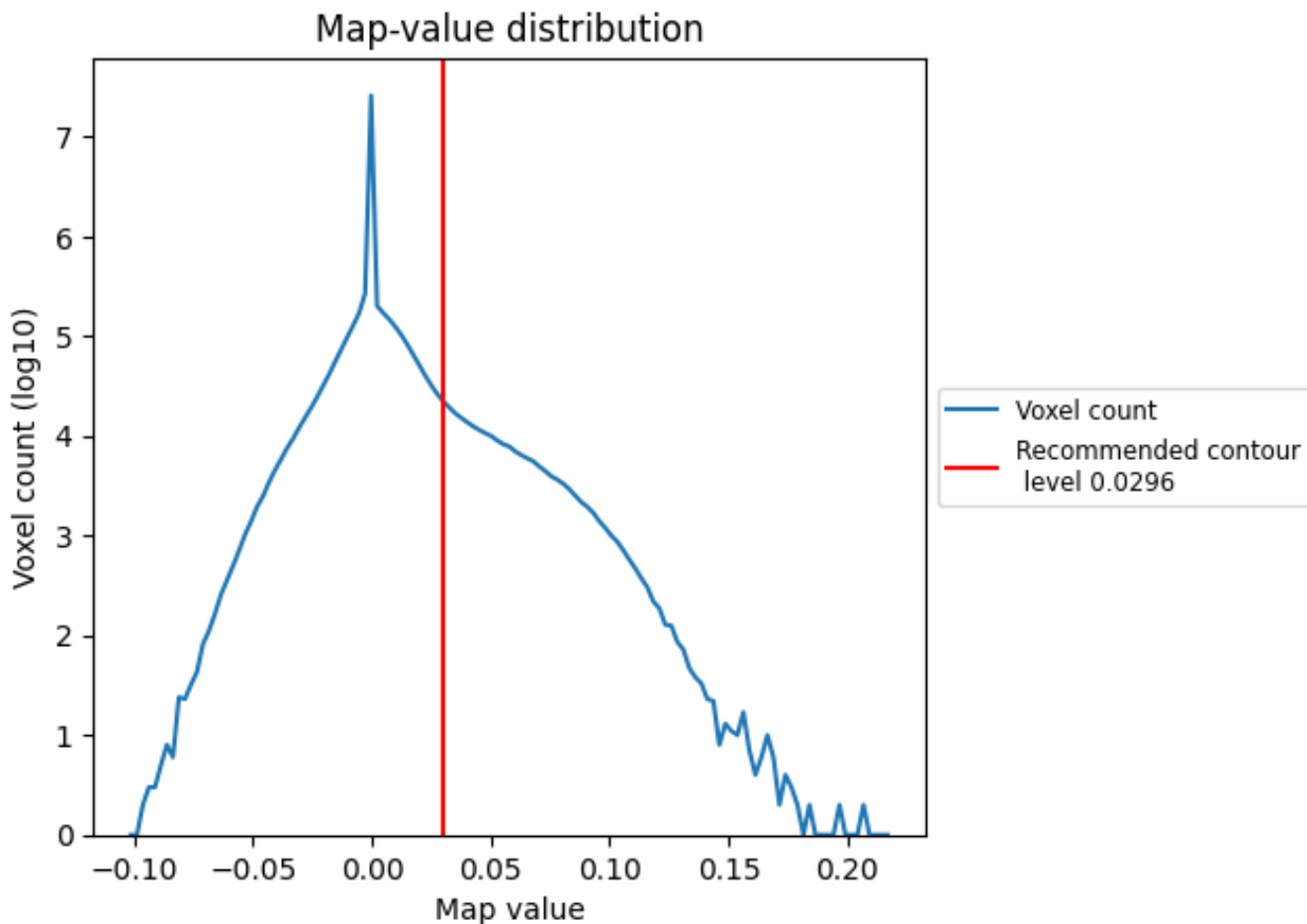
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

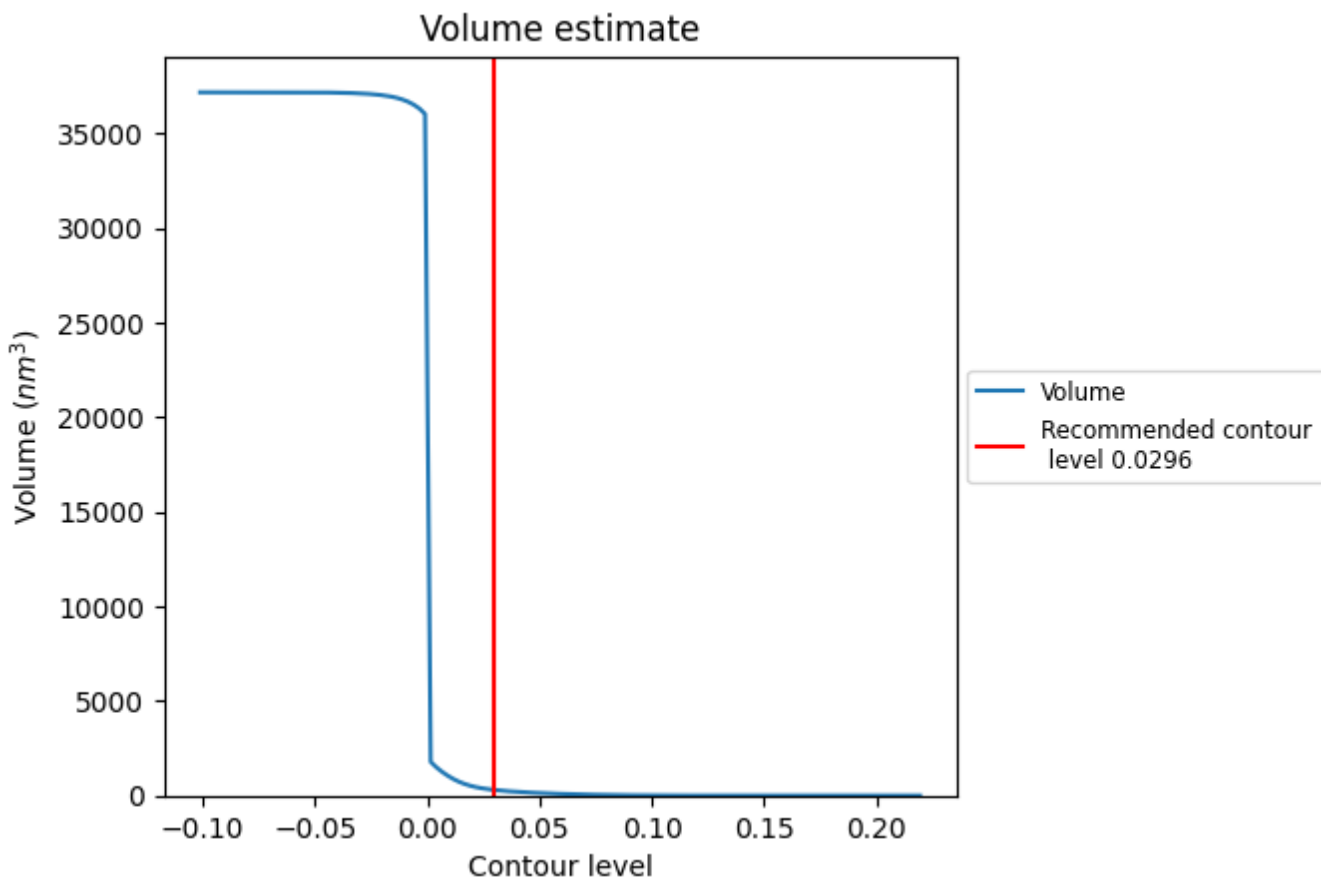
This section contains the results of statistical analysis of the map.

### 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.

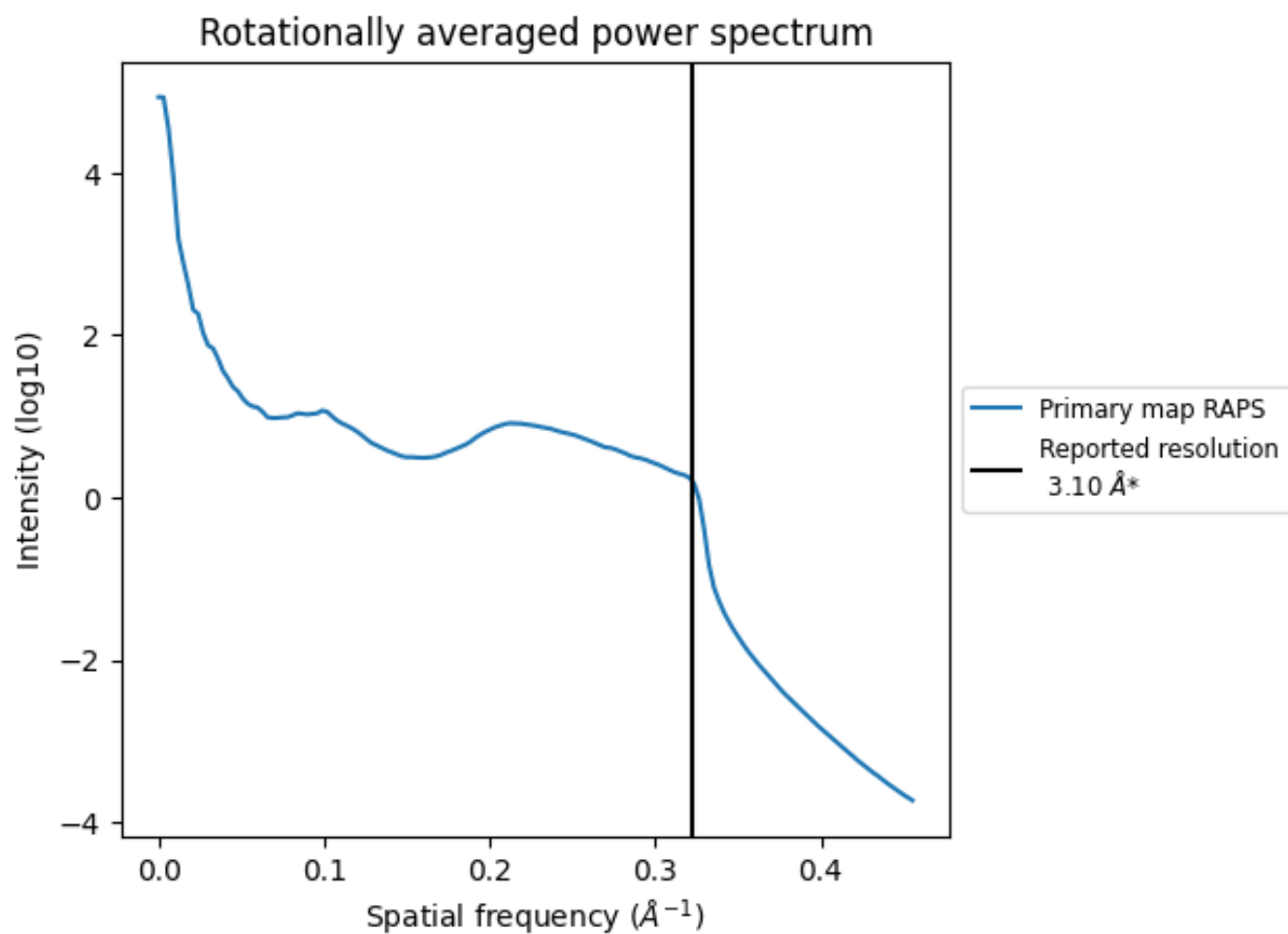
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 300 nm<sup>3</sup>; this corresponds to an approximate mass of 271 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 0.323 Å<sup>-1</sup>

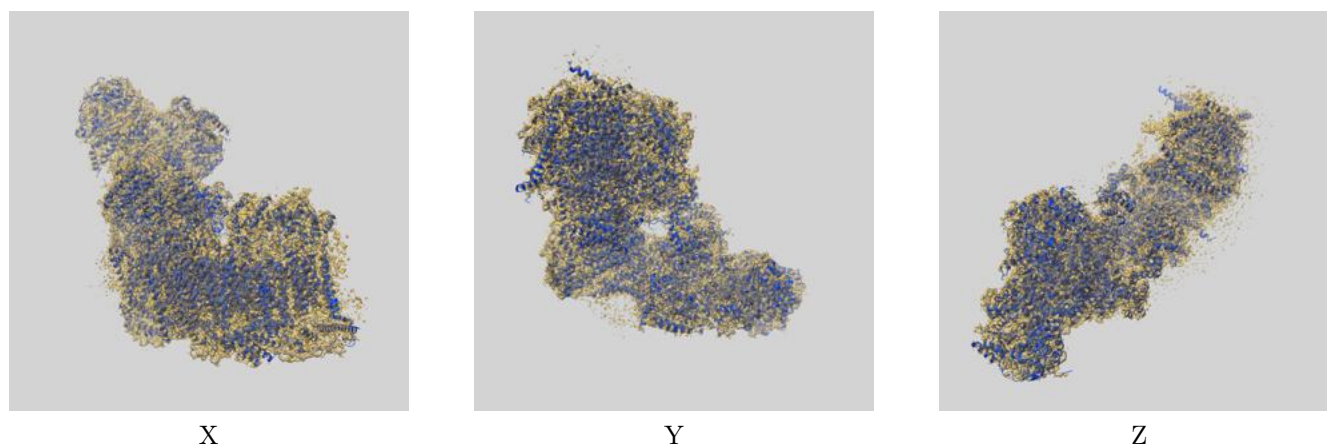
## 8 Fourier-Shell correlation

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

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

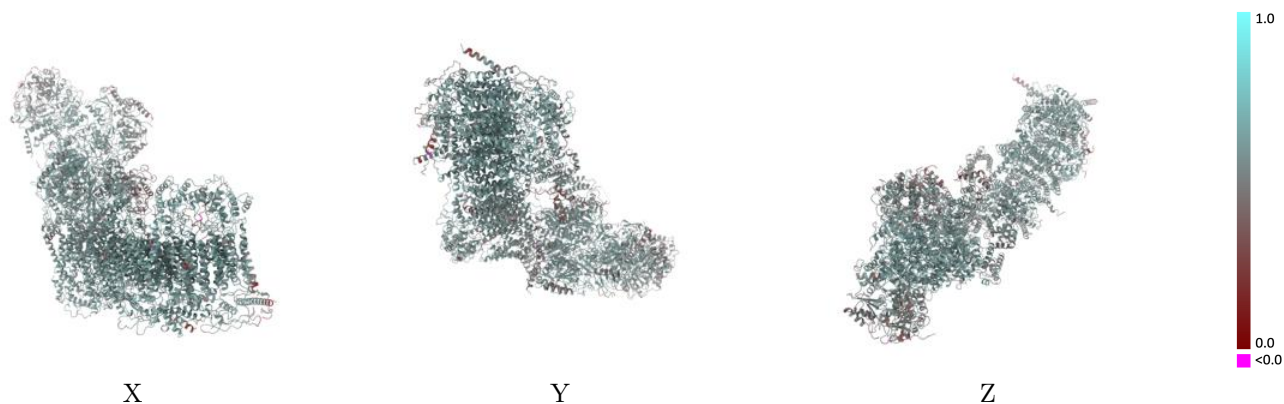
This section contains information regarding the fit between EMDB map EMD-32307 and PDB model 7W4L. Per-residue inclusion information can be found in section 3 on page 20.

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



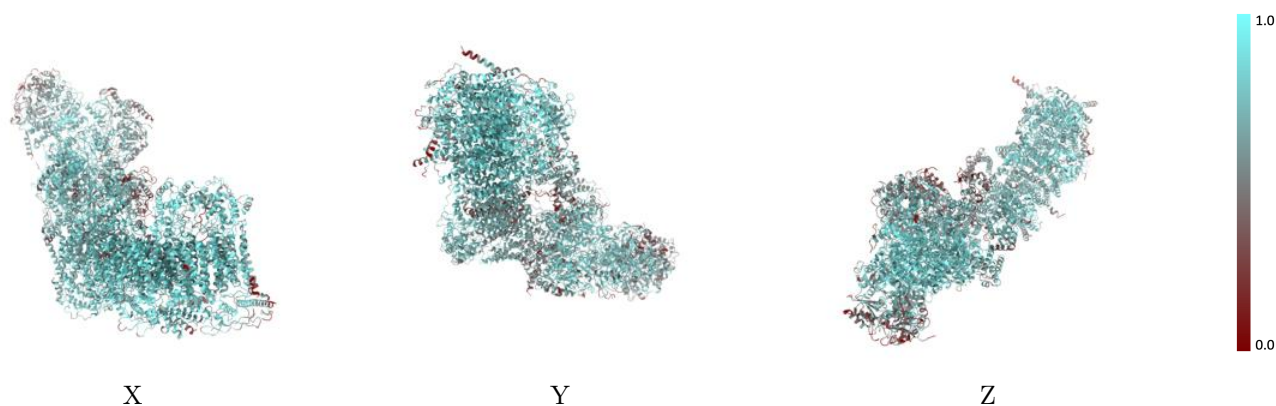
The images above show the 3D surface view of the map at the recommended contour level 0.0296 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



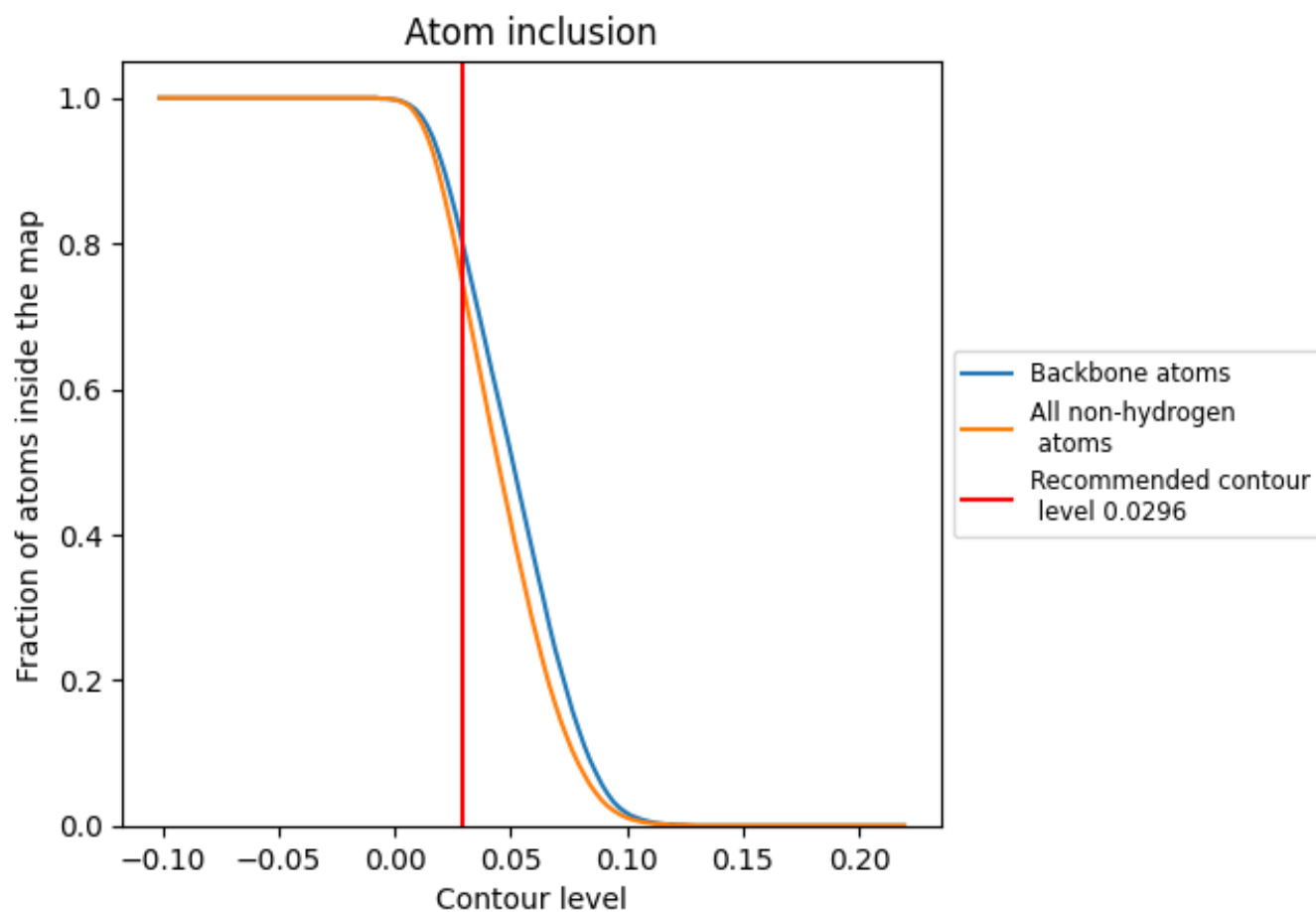
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0296).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0296) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5650
A	 0.6120	 0.5170
B	 0.8870	 0.6130
C	 0.8270	 0.5960
E	 0.6920	 0.5630
F	 0.4910	 0.4760
G	 0.3620	 0.3940
H	 0.6650	 0.5350
I	 0.7350	 0.5670
J	 0.6160	 0.5250
K	 0.5410	 0.4980
L	 0.7870	 0.5800
M	 0.7370	 0.5640
N	 0.7640	 0.5830
O	 0.5720	 0.5030
P	 0.8530	 0.6030
Q	 0.8420	 0.6060
S	 0.8140	 0.5880
T	 0.7330	 0.5800
U	 0.7280	 0.5610
V	 0.5260	 0.5160
W	 0.7560	 0.5700
X	 0.7260	 0.5480
Y	 0.6450	 0.5380
Z	 0.5990	 0.5020
a	 0.7820	 0.5900
b	 0.6800	 0.5330
c	 0.7780	 0.5750
d	 0.7440	 0.5590
e	 0.7040	 0.5550
f	 0.6290	 0.5240
g	 0.7750	 0.5810
h	 0.7640	 0.5720
i	 0.8500	 0.6050
j	 0.6200	 0.5370



*Continued on next page...*

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Chain	Atom inclusion	Q-score
k	 0.7220	 0.5720
l	 0.8050	 0.5930
m	 0.6870	 0.5470
n	 0.6650	 0.5450
o	 0.7700	 0.5850
p	 0.7840	 0.5750
r	 0.8580	 0.6060
s	 0.7900	 0.5770
u	 0.7700	 0.5730
v	 0.6850	 0.5290
w	 0.7040	 0.5500