



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 06:35 PM JST

PDB ID : 7W1P
EMDB ID : EMD-32254
Title : Deactive state CI from Q10-NADH dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-19
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

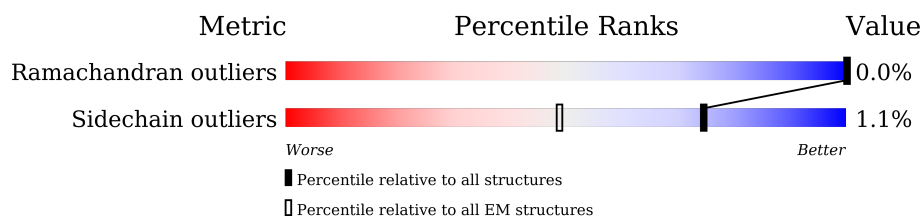
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

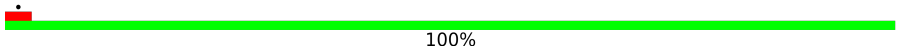
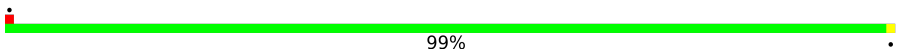
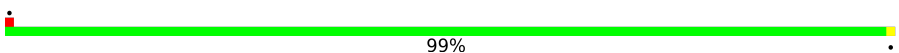
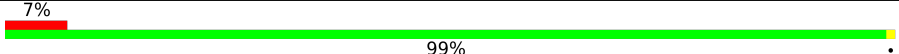
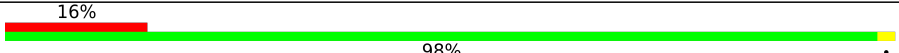
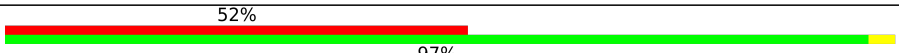
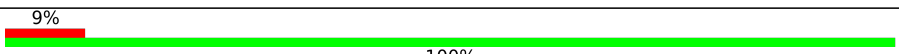
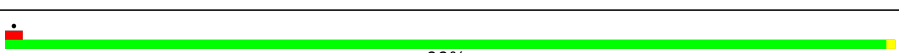
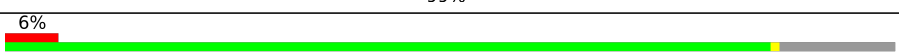
The reported resolution of this entry is 3.10 Å.

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.



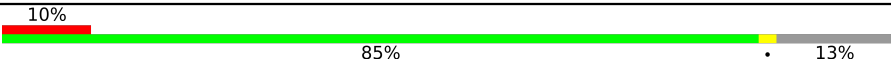
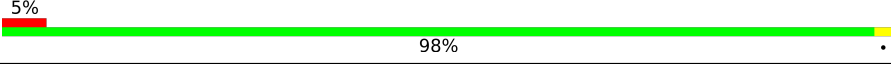
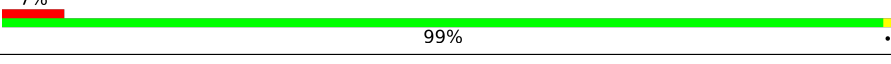
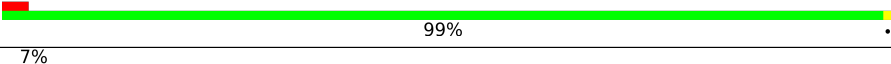
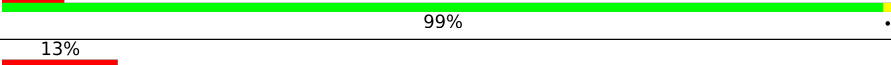
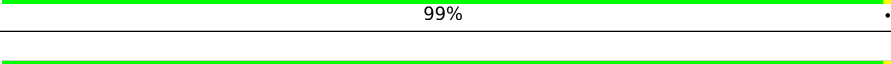
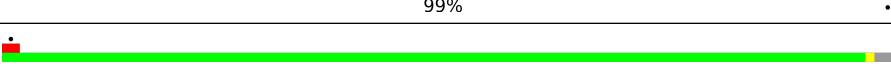
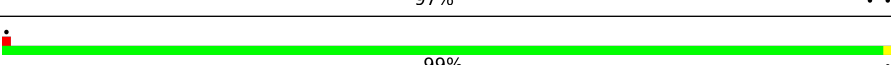
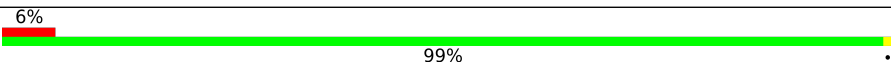
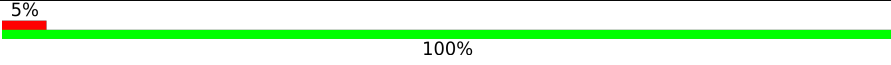
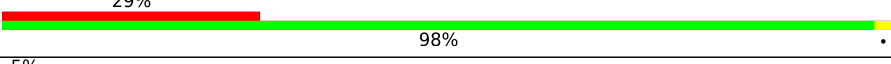
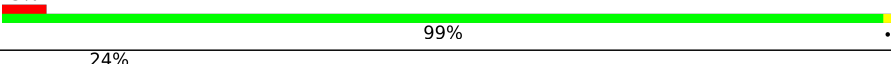
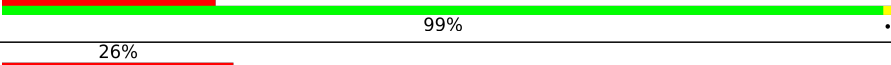
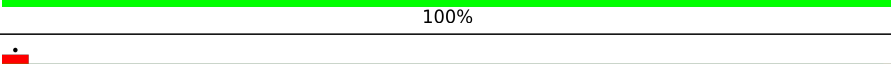
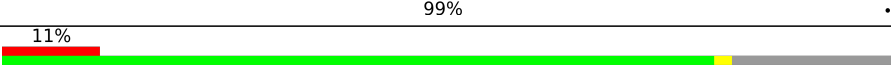
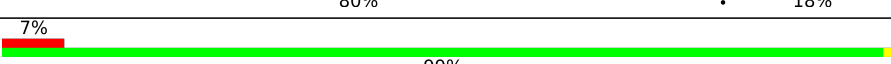
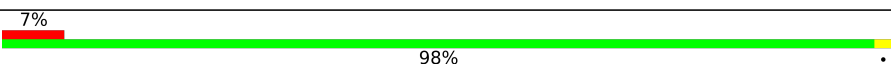
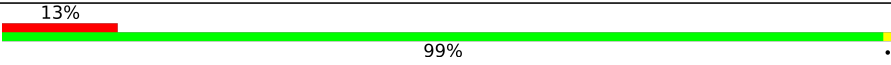
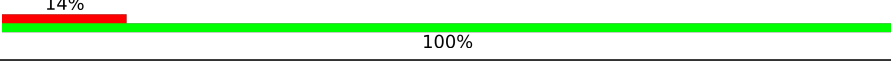
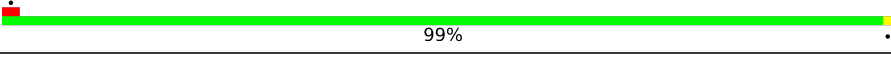
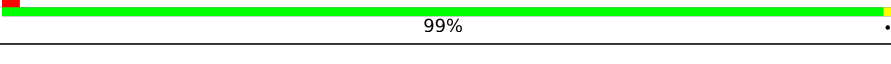
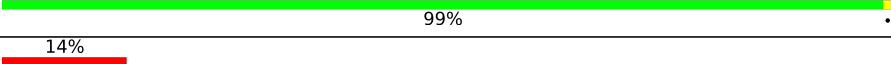
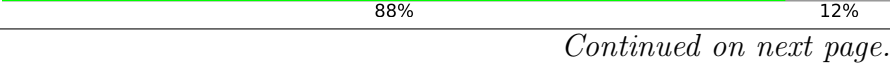


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	 100%
2	B	176	 99%
3	C	156	 99%
4	E	115	 7% 99%
5	F	86	 16% 98%
6	G	88	 52% 97%
6	X	88	 9% 100%
7	H	112	 99%
8	I	112	 6% 86% 13%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			699	449	103	142	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
			2359	1514	421	416	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
			5292	3319	922	1012	39		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	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
			879	573	158	147	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1530	980	279	263	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1012	633	188	182	9		

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

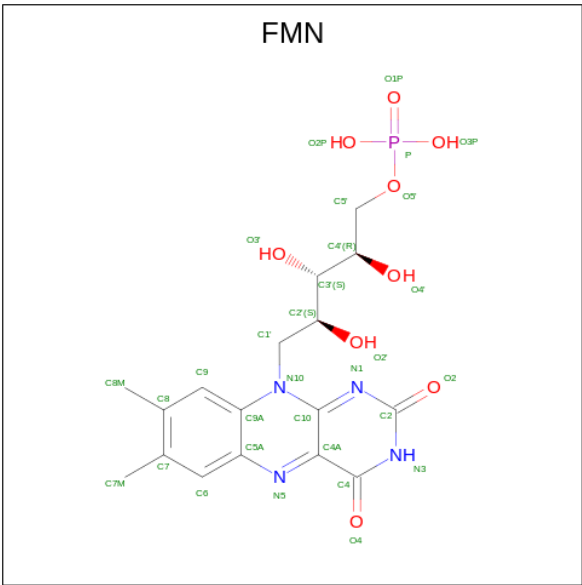
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2583	1646	437	491	9		

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



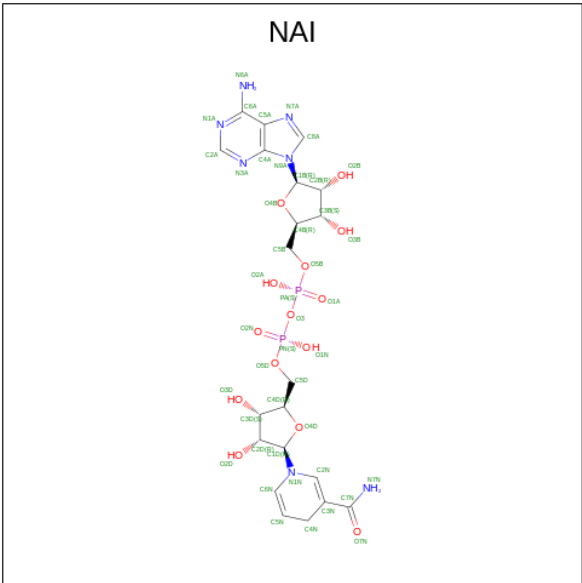
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			16	8	8	
45	B	1	Total	Fe	S	0
			16	8	8	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			16	8	8	
45	M	1	Total	Fe	S	0
			16	8	8	

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



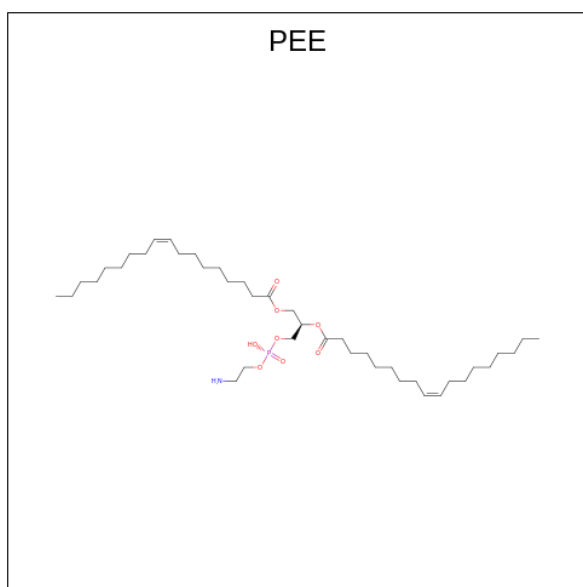
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



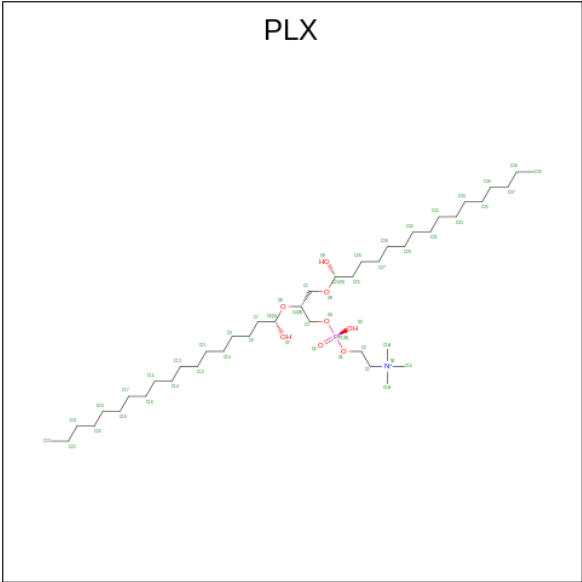
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			92	72	2	16	2	
48	l	1	Total	C	N	O	P	0
			92	72	2	16	2	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



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

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



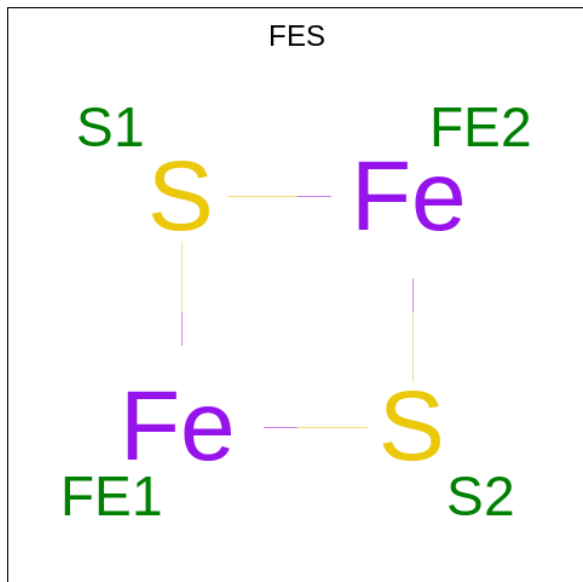
Mol	Chain	Residues	Atoms						AltCon
50	G	1	Total 35	C 23	N 2	O 8	P 1	S 1	0
50	X	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

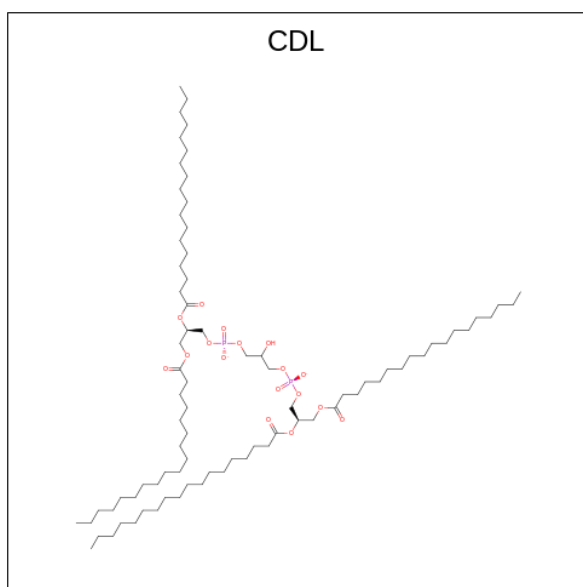


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

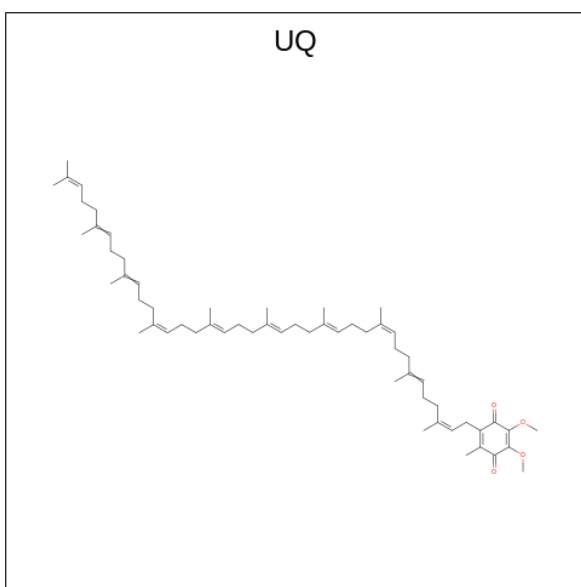


Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			51	32	17	2	
54	V	1	Total	C	O	P	0
			162	124	34	4	
54	V	1	Total	C	O	P	0
			162	124	34	4	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	g	1	Total	C	O	P	0
			97	78	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	l	1	Total	C	O	P	0
			199	161	34	4	
54	l	1	Total	C	O	P	0
			199	161	34	4	
54	u	1	Total	C	O	P	0
			78	59	17	2	

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

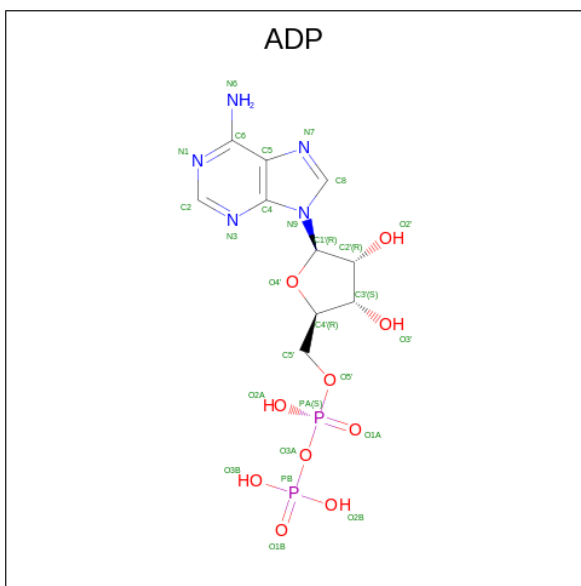
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄) (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: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

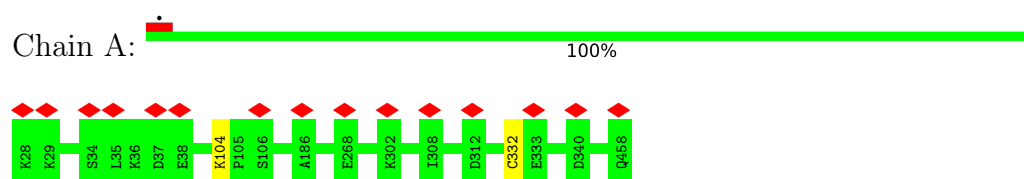


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

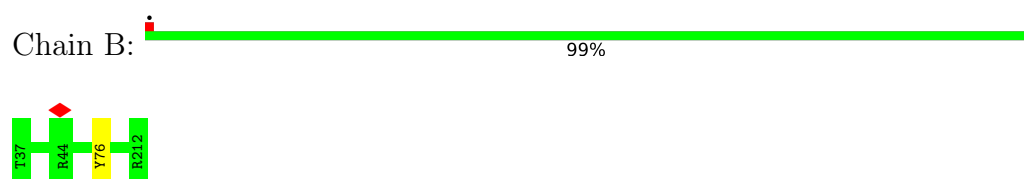
3 Residue-property plots [i](#)

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

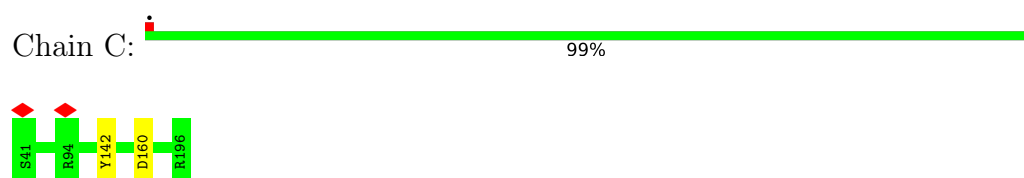
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



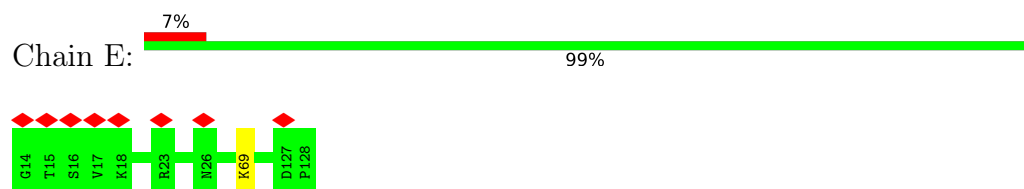
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



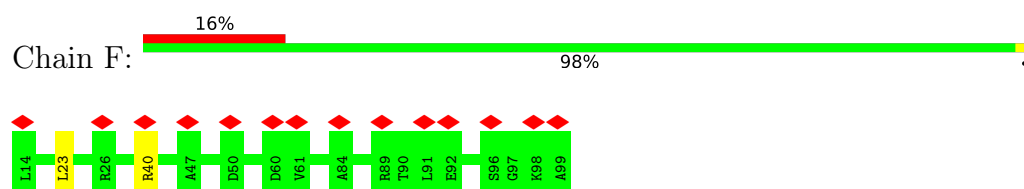
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



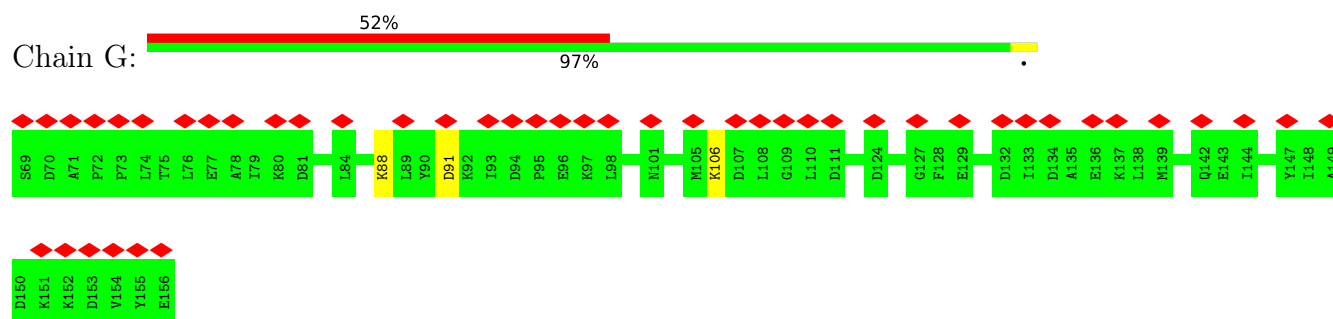
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



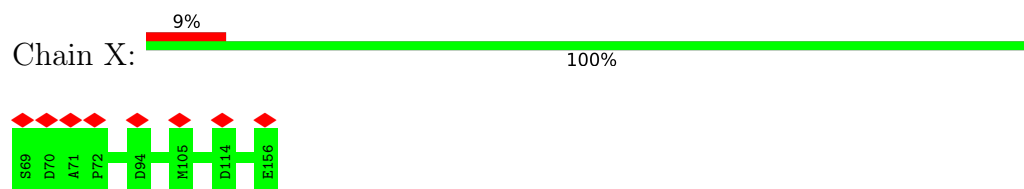
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



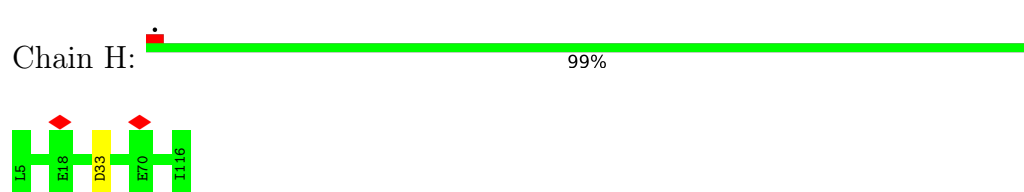
- Molecule 6: Acyl carrier protein



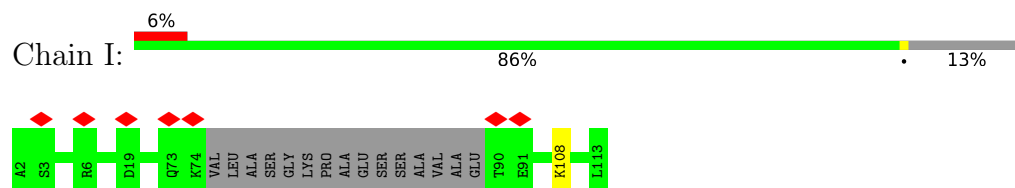
- Molecule 6: Acyl carrier protein



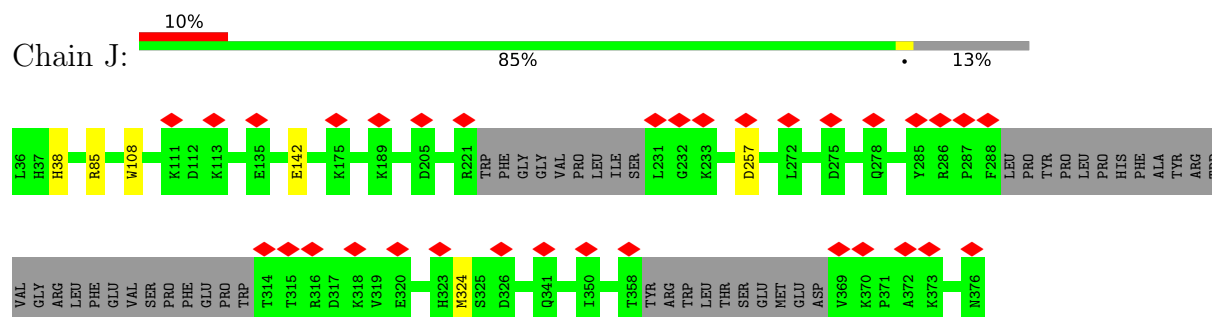
- Molecule 7: Complex I subunit B13



- Molecule 8: Complex I-B14.5a

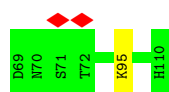


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

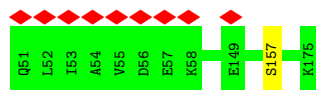


- Molecule 10: Complex I-9kD

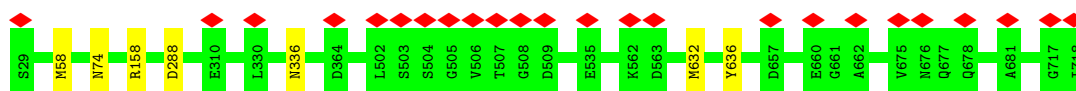




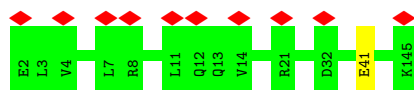
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



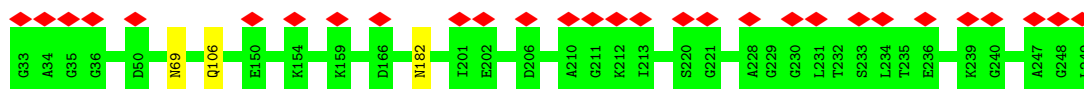
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



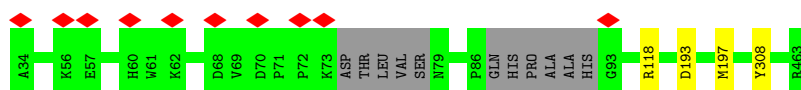
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD

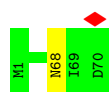


- Molecule 16: Complex I-49kD



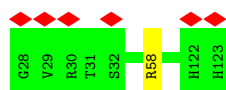
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  99%



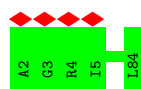
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  99%



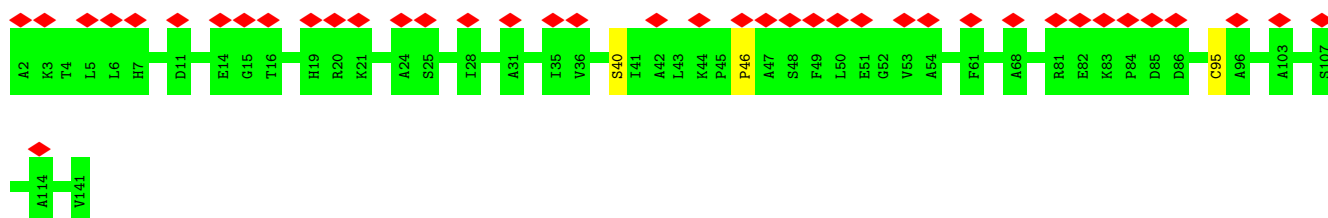
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  100%



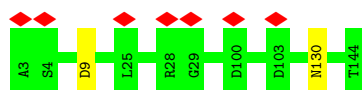
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  98%



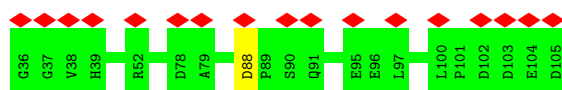
- Molecule 21: Complex I-B16.6

Chain W:  99%



- Molecule 22: Complex I-AGGG

Chain Y:  99%

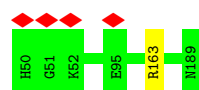


- Molecule 23: Complex I-B12

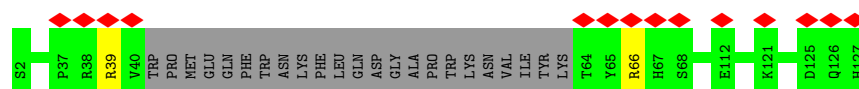
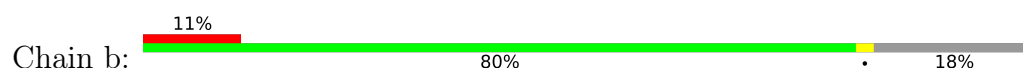
Chain Z:  100%



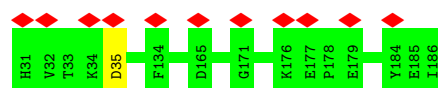
- Molecule 24: Complex I-SGDH



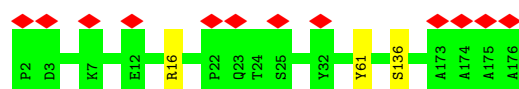
- Molecule 25: Complex I-B17



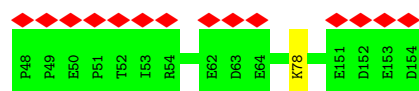
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



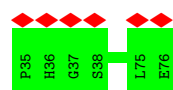
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

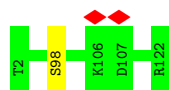


- Molecule 29: Complex I-KFYI



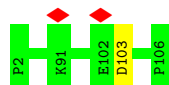
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  99%



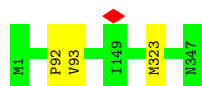
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  99%




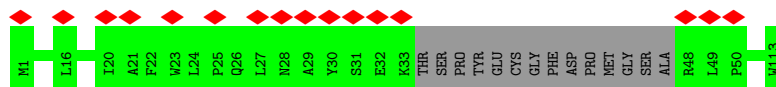
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  99%



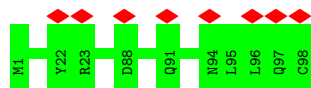
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  14% 88% 12%



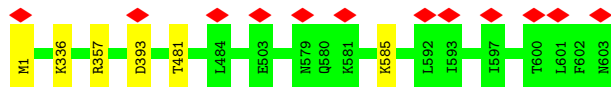
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  8% 100%




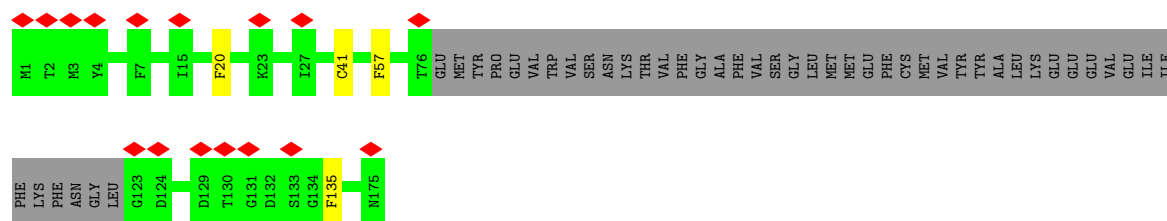
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  99%

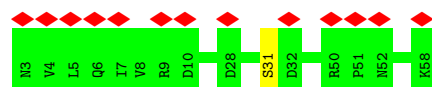


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

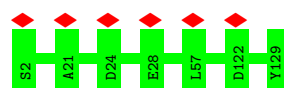
Chain m:  9% 71% 26%



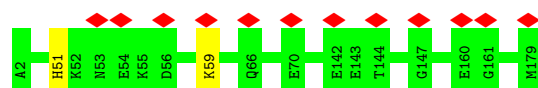
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



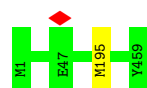
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



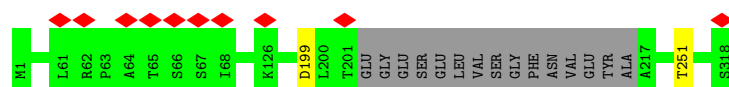
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

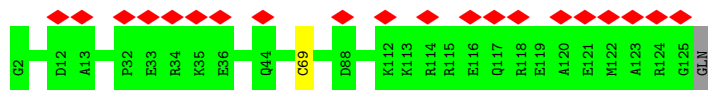


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

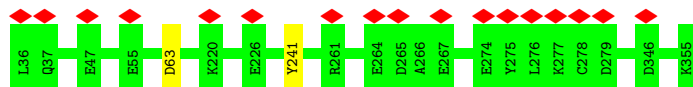




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0272	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/3393	0.49	0/4584
2	B	0.26	0/1443	0.49	0/1952
3	C	0.27	0/1279	0.51	0/1730
4	E	0.25	0/995	0.53	0/1340
5	F	0.25	0/702	0.55	0/945
6	G	0.25	0/705	0.49	0/956
6	X	0.24	0/711	0.44	0/963
7	H	0.24	0/929	0.45	0/1258
8	I	0.25	0/798	0.53	0/1079
9	J	0.25	0/2411	0.49	0/3254
10	K	0.24	0/365	0.49	0/493
11	L	0.24	0/1039	0.49	0/1403
12	M	0.25	0/5380	0.49	0/7290
13	N	0.25	0/1245	0.51	0/1694
14	O	0.25	0/1711	0.48	0/2328
15	P	0.26	0/1789	0.50	0/2436
16	Q	0.26	0/3451	0.48	0/4672
17	S	0.26	0/582	0.48	0/783
18	T	0.25	0/755	0.50	0/1018
19	U	0.24	0/664	0.44	0/912
20	V	0.25	0/1042	0.47	0/1411
21	W	0.27	0/1198	0.50	0/1617
22	Y	0.24	0/626	0.46	0/857
23	Z	0.24	0/695	0.50	0/939
24	a	0.26	0/1199	0.47	0/1623
25	b	0.25	0/906	0.51	0/1232
26	c	0.25	0/1371	0.44	0/1875
27	d	0.26	0/1494	0.53	0/2015
28	e	0.26	0/916	0.50	0/1246
29	f	0.25	0/350	0.45	0/473
30	g	0.27	0/1031	0.48	0/1394
31	h	0.25	0/889	0.48	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.25	0/2773	0.44	0/3768
33	j	0.26	0/819	0.51	0/1117
34	k	0.25	0/759	0.42	0/1029
35	l	0.26	0/4914	0.44	0/6683
36	m	0.26	0/973	0.47	0/1320
37	n	0.24	0/491	0.50	0/663
38	o	0.27	0/1092	0.50	0/1481
39	p	0.26	0/1586	0.52	0/2150
40	r	0.25	0/3723	0.44	0/5078
41	s	0.26	0/2464	0.44	0/3369
42	u	0.24	0/1436	0.48	0/1938
43	v	0.26	0/1036	0.52	0/1393
44	w	0.25	0/2643	0.46	0/3580
All	All	0.25	0/66773	0.48	0/90531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	414 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	101 (92%)	9 (8%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	277 (96%)	11 (4%)	1 (0%)	41	73
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	674 (98%)	14 (2%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (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%)	64 (94%)	4 (6%)	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%)	130 (94%)	7 (5%)	1 (1%)	22	57
21	W	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
22	Y	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	326 (94%)	17 (5%)	2 (1%)	25	59
33	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	k	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
35	l	601/603 (100%)	574 (96%)	27 (4%)	0	100	100
36	m	125/175 (71%)	113 (90%)	12 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	165 (94%)	11 (6%)	0	100	100
40	r	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
41	s	299/318 (94%)	288 (96%)	11 (4%)	0	100	100
42	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	302 (95%)	16 (5%)	0	100	100
All	All	8029/8309 (97%)	7717 (96%)	308 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	i	93	VAL
9	J	38	HIS
32	i	92	PRO
20	V	46	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	343 (99%)	2 (1%)	86	94
2	B	151/151 (100%)	150 (99%)	1 (1%)	84	93
3	C	132/132 (100%)	130 (98%)	2 (2%)	65	85
4	E	107/107 (100%)	106 (99%)	1 (1%)	78	91
5	F	76/76 (100%)	74 (97%)	2 (3%)	46	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	76/81 (94%)	73 (96%)	3 (4%)	32	65
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	99/99 (100%)	98 (99%)	1 (1%)	76	90
8	I	87/97 (90%)	86 (99%)	1 (1%)	73	89
9	J	255/295 (86%)	250 (98%)	5 (2%)	55	80
10	K	41/41 (100%)	40 (98%)	1 (2%)	49	76
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	91
12	M	578/580 (100%)	571 (99%)	7 (1%)	71	88
13	N	130/130 (100%)	129 (99%)	1 (1%)	81	92
14	O	183/183 (100%)	180 (98%)	3 (2%)	62	84
15	P	190/190 (100%)	188 (99%)	2 (1%)	73	89
16	Q	361/370 (98%)	358 (99%)	3 (1%)	81	92
17	S	58/58 (100%)	57 (98%)	1 (2%)	60	83
18	T	79/79 (100%)	78 (99%)	1 (1%)	69	87
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	99 (98%)	2 (2%)	55	80
21	W	122/123 (99%)	120 (98%)	2 (2%)	62	84
22	Y	63/63 (100%)	62 (98%)	1 (2%)	62	84
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	121 (99%)	1 (1%)	81	92
25	b	98/119 (82%)	96 (98%)	2 (2%)	55	80
26	c	141/141 (100%)	140 (99%)	1 (1%)	84	93
27	d	155/155 (100%)	152 (98%)	3 (2%)	57	81
28	e	99/99 (100%)	98 (99%)	1 (1%)	76	90
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	91
31	h	93/93 (100%)	92 (99%)	1 (1%)	73	89
32	i	311/311 (100%)	310 (100%)	1 (0%)	92	96
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/537 (100%)	531 (99%)	6 (1%)	73	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	m	99/141 (70%)	95 (96%)	4 (4%)	31	65
37	n	53/53 (100%)	52 (98%)	1 (2%)	57	81
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	158/159 (99%)	156 (99%)	2 (1%)	69	87
40	r	410/410 (100%)	409 (100%)	1 (0%)	93	97
41	s	263/275 (96%)	261 (99%)	2 (1%)	81	92
42	u	153/153 (100%)	148 (97%)	5 (3%)	38	69
43	v	101/112 (90%)	100 (99%)	1 (1%)	76	90
44	w	281/283 (99%)	279 (99%)	2 (1%)	84	93
All	All	7061/7235 (98%)	6983 (99%)	78 (1%)	74	89

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	332	CYS
2	B	76	TYR
3	C	142	TYR
3	C	160	ASP
4	E	69	LYS
5	F	23	LEU
5	F	40	ARG
6	G	88	LYS
6	G	91	ASP
6	G	106	LYS
7	H	33	ASP
8	I	108	LYS
9	J	85	ARG
9	J	108	TRP
9	J	142	GLU
9	J	257	ASP
9	J	324	MET
10	K	95	LYS
11	L	157	SER
12	M	58	MET
12	M	74	ASN
12	M	158	ARG
12	M	288	ASP
12	M	336	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	632	MET
12	M	636	TYR
13	N	41	GLU
14	O	69	ASN
14	O	106	GLN
14	O	182	ASN
15	P	91	ASP
15	P	231	ARG
16	Q	193	ASP
16	Q	197	MET
16	Q	308	TYR
17	S	68	ASN
18	T	58	ARG
20	V	40	SER
20	V	95	CYS
21	W	9	ASP
21	W	130	ASN
22	Y	88	ASP
24	a	163	ARG
25	b	39	ARG
25	b	66	ARG
26	c	35	ASP
27	d	16	ARG
27	d	61	TYR
27	d	136	SER
28	e	78	LYS
30	g	98	SER
31	h	103	ASP
32	i	323	MET
35	l	1	MET
35	l	336	LYS
35	l	357	ARG
35	l	393	ASP
35	l	481	THR
35	l	585	LYS
36	m	20	PHE
36	m	41	CYS
36	m	57	PHE
36	m	135	PHE
37	n	31	SER
39	p	51	HIS
39	p	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	r	195	MET
41	s	199	ASP
41	s	251	THR
42	u	66	CYS
42	u	88	CYS
42	u	100	CYS
42	u	113	ASP
42	u	121	ASP
43	v	69	CYS
44	w	63	ASP
44	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	451	GLN
12	M	336	ASN
14	O	133	GLN
16	Q	83	ASN
25	b	14	GLN
32	i	49	ASN
34	k	50	ASN
38	o	75	ASN
38	o	79	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.12	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	5.65	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	12.57	131.00	119.48
16	Q	118	2MR	CD-NE-CZ	4.52	131.87	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.90	130.28	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 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.57	1 (1%)
48	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	1.00	2 (4%)
56	UQ	s	401	-	28,28,63	3.27	8 (28%)	34,37,79	2.74	10 (29%)
50	8Q1	X	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.50	6 (15%)
48	PEE	Q	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
47	NAI	A	503	-	42,48,48	4.94	18 (42%)	47,73,73	1.32	7 (14%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.97	2 (4%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
49	PLX	l	701	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
48	PEE	C	302	-	35,35,50	1.20	5 (14%)	38,40,55	0.98	2 (5%)
54	CDL	V	202	-	67,67,99	1.25	8 (11%)	73,79,111	1.02	4 (5%)
54	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	1.02	4 (5%)
48	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
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%)
50	8Q1	G	201	6	31,34,34	1.71	6 (19%)	40,43,43	1.58	7 (17%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	V	203	-	39,39,50	1.31	6 (15%)	41,44,55	1.02	2 (4%)
52	FES	O	301	14	0,4,4	-	-	-	-	-
54	CDL	N	201	-	50,50,99	1.40	8 (16%)	56,62,111	1.17	4 (7%)
54	CDL	g	202	-	96,96,99	1.10	8 (8%)	102,108,111	0.88	4 (3%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
48	PEE	l	705	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
54	CDL	l	702	-	98,98,99	1.09	8 (8%)	104,110,111	0.89	4 (3%)
54	CDL	a	201	-	90,90,99	1.13	8 (8%)	96,102,111	0.90	4 (4%)
54	CDL	l	703	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
54	CDL	u	201	-	77,77,99	1.20	8 (10%)	83,89,111	0.95	4 (4%)
49	PLX	g	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	FES	M	803	12	0,4,4	-	-	-		
57	ADP	w	401	-	24,29,29	3.11	6 (25%)	29,45,45	1.42	5 (17%)
48	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.99	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
51	NDP	J	401	-	45,52,52	4.58	20 (44%)	53,80,80	1.94	6 (11%)
45	SF4	C	301	3,16	0,12,12	-	-	-		
54	CDL	V	201	-	93,93,99	1.11	9 (9%)	99,105,111	0.87	4 (4%)
49	PLX	C	303	-	51,51,51	1.14	3 (5%)	55,59,59	0.60	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
49	PLX	a	202	-	-	22/55/55/55	-
48	PEE	i	402	-	-	25/50/50/54	-
56	UQ	s	401	-	-	9/21/45/87	0/1/1/1
50	8Q1	X	201	6	-	19/41/41/41	-
48	PEE	Q	501	-	-	24/54/54/54	-
45	SF4	M	801	12	-	-	0/6/5/5
47	NAI	A	503	-	-	9/25/72/72	0/5/5/5
48	PEE	l	704	-	-	24/49/49/54	-
49	PLX	j	202	-	-	25/55/55/55	-
49	PLX	l	701	-	-	30/55/55/55	-
48	PEE	C	302	-	-	18/39/39/54	-
54	CDL	V	202	-	-	43/78/78/110	-
54	CDL	i	401	-	-	44/76/76/110	-
48	PEE	j	201	-	-	30/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
54	CDL	N	201	-	-	36/61/61/110	-
50	8Q1	G	201	6	-	16/41/41/41	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	V	203	-	-	22/43/43/54	-
45	SF4	B	302	2	-	-	0/6/5/5
52	FES	O	301	14	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CDL	g	202	-	-	64/107/107/110	-
48	PEE	r	501	-	-	27/54/54/54	-
48	PEE	l	705	-	-	22/49/49/54	-
54	CDL	l	702	-	-	50/109/109/110	-
54	CDL	a	201	-	-	44/101/101/110	-
54	CDL	l	703	-	-	60/110/110/110	-
54	CDL	u	201	-	-	44/88/88/110	-
49	PLX	g	201	-	-	20/55/55/55	-
52	FES	M	803	12	-	-	0/1/1/1
57	ADP	w	401	-	-	5/12/32/32	0/3/3/3
48	PEE	m	201	-	-	19/44/44/54	-
45	SF4	A	501	1	-	-	0/6/5/5
51	NDP	J	401	-	-	10/30/77/77	0/4/5/5
54	CDL	V	201	-	-	54/104/104/110	-
45	SF4	C	301	3,16	-	-	0/6/5/5
49	PLX	C	303	-	-	31/55/55/55	-

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.16	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.47	1.30	1.53
51	J	401	NDP	C3B-C2B	-13.01	1.23	1.52
51	J	401	NDP	C6N-C5N	12.41	1.55	1.33
51	J	401	NDP	O4D-C4D	10.72	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.22	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.79	1.28	1.53
56	s	401	UQ	C13-C14	9.29	1.55	1.33
56	s	401	UQ	C8-C9	8.89	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.85	1.30	1.53
51	J	401	NDP	O4B-C1B	8.57	1.53	1.41
47	A	503	NAI	O4B-C4B	-8.26	1.26	1.45
56	s	401	UQ	C18-C19	8.25	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.82	1.27	1.45
57	w	401	ADP	O4'-C4'	7.68	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.54	1.29	1.53
51	J	401	NDP	C2N-C3N	7.44	1.55	1.34
47	A	503	NAI	O4D-C4D	6.94	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.87	1.31	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C2D-C3D	5.93	1.69	1.53
47	A	503	NAI	C7N-N7N	5.76	1.48	1.33
51	J	401	NDP	P2B-O2B	5.63	1.69	1.59
47	A	503	NAI	O4D-C1D	5.56	1.55	1.42
50	G	201	8Q1	C34-N36	5.45	1.45	1.33
50	X	201	8Q1	C34-N36	5.45	1.45	1.33
51	J	401	NDP	C3B-C4B	5.37	1.66	1.53
50	X	201	8Q1	C39-N41	5.36	1.45	1.33
50	G	201	8Q1	C39-N41	5.35	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.07	1.40	1.49
51	J	401	NDP	O4D-C1D	-4.90	1.30	1.42
51	J	401	NDP	C6N-N1N	4.86	1.49	1.37
47	A	503	NAI	O2B-C2B	4.58	1.53	1.43
51	J	401	NDP	C7N-N7N	4.17	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.16	1.33	1.43
51	J	401	NDP	C6A-N6A	4.12	1.49	1.34
47	A	503	NAI	C6N-C5N	3.94	1.40	1.33
57	w	401	ADP	C6-N6	3.82	1.48	1.34
46	A	502	FMN	C4A-N5	3.82	1.38	1.30
48	V	203	PEE	C18-C19	3.75	1.53	1.31
48	Q	501	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.74	1.53	1.31
48	m	201	PEE	C18-C19	3.73	1.53	1.31
48	l	704	PEE	C18-C19	3.72	1.53	1.31
48	j	201	PEE	C18-C19	3.71	1.53	1.31
48	i	402	PEE	C18-C19	3.71	1.53	1.31
48	l	705	PEE	C18-C19	3.70	1.53	1.31
48	r	501	PEE	C39-C38	3.66	1.53	1.31
48	V	203	PEE	C39-C38	3.66	1.53	1.31
48	l	704	PEE	C39-C38	3.65	1.53	1.31
48	i	402	PEE	C39-C38	3.65	1.52	1.31
48	l	705	PEE	C39-C38	3.65	1.52	1.31
48	j	201	PEE	C39-C38	3.65	1.52	1.31
48	C	302	PEE	C39-C38	3.65	1.52	1.31
48	Q	501	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C6A-N6A	3.60	1.47	1.34
47	A	503	NAI	C7N-C3N	3.58	1.56	1.48
54	l	703	CDL	OA8-CA7	3.50	1.43	1.33
54	i	401	CDL	OA8-CA7	3.49	1.43	1.33
54	V	201	CDL	OA8-CA7	3.45	1.43	1.33
54	g	202	CDL	OA8-CA7	3.42	1.43	1.33
54	a	201	CDL	OA8-CA7	3.41	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	u	201	CDL	OA8-CA7	3.41	1.43	1.33
54	N	201	CDL	OA8-CA7	3.40	1.43	1.33
54	V	202	CDL	OA8-CA7	3.40	1.43	1.33
54	l	702	CDL	OA8-CA7	3.40	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.32	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.30	1.40	1.48
54	N	201	CDL	OA6-CA5	3.15	1.43	1.34
57	w	401	ADP	O3'-C3'	3.12	1.50	1.43
51	J	401	NDP	O3D-C3D	3.08	1.50	1.43
54	g	202	CDL	OB6-CB5	3.06	1.43	1.34
54	V	201	CDL	OA6-CA5	3.06	1.42	1.34
54	a	201	CDL	OB6-CB5	3.04	1.42	1.34
54	N	201	CDL	OB8-CB7	3.03	1.42	1.33
54	i	401	CDL	OB6-CB5	3.02	1.42	1.34
51	J	401	NDP	C7N-C3N	3.02	1.55	1.48
54	V	202	CDL	OB8-CB7	3.02	1.42	1.33
54	u	201	CDL	OB8-CB7	3.02	1.42	1.33
54	i	401	CDL	OB8-CB7	3.01	1.42	1.33
54	a	201	CDL	OB8-CB7	3.01	1.42	1.33
54	l	702	CDL	OB6-CB5	3.01	1.42	1.34
54	l	702	CDL	OB8-CB7	3.00	1.42	1.33
54	u	201	CDL	OB6-CB5	2.99	1.42	1.34
54	l	703	CDL	OB8-CB7	2.99	1.42	1.33
54	V	202	CDL	OA6-CA5	2.99	1.42	1.34
54	a	201	CDL	OA6-CA5	2.99	1.42	1.34
54	g	202	CDL	OB8-CB7	2.98	1.42	1.33
54	V	201	CDL	OB8-CB7	2.98	1.42	1.33
54	N	201	CDL	OB6-CB5	2.98	1.42	1.34
54	l	703	CDL	OB6-CB5	2.97	1.42	1.34
54	l	703	CDL	OA6-CA5	2.96	1.42	1.34
54	g	202	CDL	OA6-CA5	2.95	1.42	1.34
54	i	401	CDL	OA6-CA5	2.94	1.42	1.34
54	V	202	CDL	OB6-CB5	2.93	1.42	1.34
54	V	201	CDL	OB6-CB5	2.93	1.42	1.34
54	l	702	CDL	OA6-CA5	2.93	1.42	1.34
54	u	201	CDL	OA6-CA5	2.91	1.42	1.34
49	l	701	PLX	O6-C4	-2.76	1.40	1.44
49	C	303	PLX	O6-C4	-2.75	1.40	1.44
49	g	201	PLX	O6-C4	-2.71	1.41	1.44
49	a	202	PLX	O6-C4	-2.68	1.41	1.44
56	s	401	UQ	C6-C1	2.62	1.54	1.46
49	j	202	PLX	O6-C4	-2.55	1.41	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	705	PEE	O3-C30	2.52	1.40	1.33
46	A	502	FMN	C10-N1	2.50	1.38	1.33
48	V	203	PEE	O3-C30	2.48	1.40	1.33
48	Q	501	PEE	O3-C30	2.47	1.40	1.33
48	r	501	PEE	O3-C30	2.46	1.40	1.33
48	l	704	PEE	O2-C2	-2.46	1.40	1.46
48	C	302	PEE	O3-C30	2.46	1.40	1.33
54	u	201	CDL	OA6-CA4	-2.45	1.40	1.46
48	r	501	PEE	O2-C2	-2.45	1.40	1.46
48	i	402	PEE	O2-C2	-2.45	1.40	1.46
54	l	702	CDL	OA6-CA4	-2.45	1.40	1.46
48	l	704	PEE	O3-C30	2.44	1.40	1.33
47	A	503	NAI	PN-O5D	2.44	1.69	1.59
48	j	201	PEE	O3-C30	2.44	1.40	1.33
48	i	402	PEE	O3-C30	2.44	1.40	1.33
51	J	401	NDP	O2B-C2B	2.43	1.52	1.44
47	A	503	NAI	O3B-C3B	-2.43	1.37	1.43
50	G	201	8Q1	C1-S44	2.43	1.82	1.76
54	a	201	CDL	OA6-CA4	-2.43	1.40	1.46
48	j	201	PEE	O2-C2	-2.40	1.40	1.46
48	C	302	PEE	O2-C2	-2.40	1.40	1.46
54	g	202	CDL	OA6-CA4	-2.40	1.40	1.46
48	m	201	PEE	O3-C30	2.39	1.40	1.33
49	a	202	PLX	C7-C6	2.39	1.55	1.50
50	X	201	8Q1	C1-S44	2.38	1.81	1.76
54	V	202	CDL	OA6-CA4	-2.38	1.40	1.46
48	Q	501	PEE	O2-C2	-2.37	1.40	1.46
48	V	203	PEE	O2-C2	-2.36	1.40	1.46
49	g	201	PLX	C7-C6	2.36	1.55	1.50
54	l	703	CDL	OA6-CA4	-2.35	1.40	1.46
49	j	202	PLX	C7-C6	2.35	1.55	1.50
54	i	401	CDL	OA6-CA4	-2.35	1.40	1.46
48	l	705	PEE	O2-C2	-2.34	1.40	1.46
50	G	201	8Q1	O40-C39	-2.34	1.18	1.23
51	J	401	NDP	C2D-C3D	2.33	1.59	1.53
48	m	201	PEE	O2-C10	2.32	1.40	1.34
50	G	201	8Q1	C6-C1	2.32	1.53	1.50
48	m	201	PEE	O2-C2	-2.31	1.40	1.46
49	l	701	PLX	C7-C6	2.31	1.55	1.50
48	C	302	PEE	O2-C10	2.29	1.40	1.34
48	Q	501	PEE	O2-C10	2.29	1.40	1.34
47	A	503	NAI	C5B-C4B	2.29	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	303	PLX	C7-C6	2.29	1.55	1.50
48	l	705	PEE	O2-C10	2.28	1.40	1.34
48	l	704	PEE	O2-C10	2.26	1.40	1.34
48	j	201	PEE	O2-C10	2.26	1.40	1.34
48	V	203	PEE	O2-C10	2.25	1.40	1.34
48	i	402	PEE	O2-C10	2.24	1.40	1.34
50	X	201	8Q1	C6-C1	2.24	1.53	1.50
50	X	201	8Q1	O35-C34	-2.23	1.19	1.23
54	u	201	CDL	PB2-OB2	2.23	1.68	1.59
54	V	201	CDL	PB2-OB2	2.22	1.68	1.59
50	X	201	8Q1	O40-C39	-2.22	1.18	1.23
54	V	202	CDL	PB2-OB2	2.22	1.68	1.59
54	V	201	CDL	OB6-CB4	-2.22	1.41	1.46
56	s	401	UQ	O4-C4	-2.22	1.18	1.23
54	i	401	CDL	PB2-OB2	2.21	1.68	1.59
50	G	201	8Q1	O35-C34	-2.21	1.19	1.23
54	l	703	CDL	OB6-CB4	-2.21	1.41	1.46
54	l	702	CDL	PB2-OB5	2.20	1.68	1.59
54	g	202	CDL	PB2-OB2	2.20	1.68	1.59
54	i	401	CDL	PB2-OB5	2.20	1.68	1.59
48	l	704	PEE	O3-C3	-2.19	1.40	1.45
54	l	703	CDL	PB2-OB2	2.19	1.68	1.59
54	a	201	CDL	PB2-OB2	2.19	1.68	1.59
54	l	702	CDL	PB2-OB2	2.19	1.68	1.59
54	V	202	CDL	PB2-OB5	2.18	1.68	1.59
54	V	202	CDL	OB6-CB4	-2.18	1.41	1.46
56	s	401	UQ	C7-C8	2.18	1.53	1.50
54	N	201	CDL	PB2-OB5	2.18	1.68	1.59
54	g	202	CDL	PB2-OB5	2.18	1.68	1.59
54	u	201	CDL	PB2-OB5	2.17	1.68	1.59
48	r	501	PEE	O2-C10	2.17	1.40	1.34
54	V	201	CDL	PB2-OB5	2.16	1.68	1.59
54	i	401	CDL	OB6-CB4	-2.16	1.41	1.46
54	u	201	CDL	OB6-CB4	-2.16	1.41	1.46
54	a	201	CDL	PB2-OB5	2.15	1.68	1.59
54	l	702	CDL	OB6-CB4	-2.15	1.41	1.46
49	a	202	PLX	P1-O4	2.15	1.68	1.59
54	N	201	CDL	PB2-OB2	2.15	1.68	1.59
54	l	703	CDL	PB2-OB5	2.15	1.68	1.59
49	j	202	PLX	P1-O4	2.14	1.68	1.59
48	m	201	PEE	O3-C3	-2.14	1.40	1.45
51	J	401	NDP	PA-O5B	2.14	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	a	201	CDL	OB6-CB4	-2.13	1.41	1.46
49	g	201	PLX	P1-O4	2.13	1.67	1.59
48	r	501	PEE	O3-C3	-2.12	1.40	1.45
54	N	201	CDL	OB6-CB4	-2.11	1.41	1.46
49	C	303	PLX	P1-O4	2.11	1.67	1.59
51	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
49	l	701	PLX	P1-O4	2.10	1.67	1.59
48	j	201	PEE	O3-C3	-2.10	1.40	1.45
48	C	302	PEE	O3-C3	-2.10	1.40	1.45
54	V	201	CDL	OA6-CA4	-2.09	1.41	1.46
48	V	203	PEE	O3-C3	-2.09	1.40	1.45
49	a	202	PLX	P1-O1	2.09	1.67	1.59
48	Q	501	PEE	O3-C3	-2.09	1.40	1.45
49	j	202	PLX	P1-O1	2.08	1.67	1.59
54	N	201	CDL	OA6-CA4	-2.07	1.41	1.46
56	s	401	UQ	O1-C1	-2.06	1.18	1.23
54	g	202	CDL	OB6-CB4	-2.04	1.41	1.46
48	l	705	PEE	O3-C3	-2.03	1.40	1.45
54	V	201	CDL	C11-CA5	2.03	1.56	1.50
48	i	402	PEE	O3-C3	-2.03	1.40	1.45
56	s	401	UQ	O3-CM3	-2.03	1.40	1.45
49	g	201	PLX	P1-O1	2.02	1.67	1.59
49	l	701	PLX	P1-O1	2.00	1.67	1.59

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-9.34	111.24	126.79
51	J	401	NDP	C3N-C2N-N1N	-7.57	112.29	123.10
51	J	401	NDP	C1D-N1N-C2N	-7.12	109.26	121.11
50	G	201	8Q1	C6-C1-S44	5.89	120.32	113.46
50	X	201	8Q1	C6-C1-S44	5.82	120.23	113.46
56	s	401	UQ	C12-C13-C14	-5.81	113.68	127.66
51	J	401	NDP	C1D-N1N-C6N	-5.36	109.28	120.83
56	s	401	UQ	C11-C9-C8	-4.70	111.61	121.12
56	s	401	UQ	C10-C9-C8	-4.68	111.68	123.68
57	w	401	ADP	N3-C2-N1	-4.49	121.67	128.68
47	A	503	NAI	N3A-C2A-N1A	-4.35	121.88	128.68
56	s	401	UQ	C17-C18-C19	-4.11	113.69	127.75
54	N	201	CDL	OA6-CA5-C11	4.11	120.36	111.50
51	J	401	NDP	N3A-C2A-N1A	-4.10	122.27	128.68
54	N	201	CDL	OB6-CB5-C51	4.10	120.34	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	i	401	CDL	OB6-CB5-C51	4.07	120.26	111.50
48	m	201	PEE	O2-C10-C11	4.04	120.21	111.50
54	a	201	CDL	OA6-CA5-C11	4.03	120.19	111.50
54	g	202	CDL	OB6-CB5-C51	4.02	120.16	111.50
54	V	202	CDL	OA6-CA5-C11	4.01	120.14	111.50
54	l	702	CDL	OA6-CA5-C11	4.00	120.13	111.50
54	l	703	CDL	OA6-CA5-C11	4.00	120.12	111.50
54	i	401	CDL	OA6-CA5-C11	3.99	120.11	111.50
54	l	702	CDL	OB6-CB5-C51	3.99	120.09	111.50
54	V	202	CDL	OB6-CB5-C51	3.99	120.09	111.50
54	a	201	CDL	OB6-CB5-C51	3.98	120.08	111.50
48	r	501	PEE	O2-C10-C11	3.96	120.03	111.50
48	V	203	PEE	O2-C10-C11	3.95	120.02	111.50
48	l	705	PEE	O2-C10-C11	3.95	120.00	111.50
54	g	202	CDL	OA6-CA5-C11	3.94	120.00	111.50
48	Q	501	PEE	O2-C10-C11	3.94	119.99	111.50
48	i	402	PEE	O2-C10-C11	3.93	119.97	111.50
54	u	201	CDL	OB6-CB5-C51	3.91	119.94	111.50
56	s	401	UQ	C15-C14-C13	-3.89	113.69	123.68
54	u	201	CDL	OA6-CA5-C11	3.85	119.80	111.50
48	j	201	PEE	O2-C10-C11	3.85	119.80	111.50
54	l	703	CDL	OB6-CB5-C51	3.85	119.79	111.50
54	V	201	CDL	OA6-CA5-C11	3.83	119.75	111.50
56	s	401	UQ	C16-C14-C13	-3.82	113.39	121.12
54	V	201	CDL	OB6-CB5-C51	3.74	119.56	111.50
48	l	704	PEE	O2-C10-C11	3.70	119.47	111.50
50	G	201	8Q1	O4-C1-C6	-3.36	120.02	123.99
48	C	302	PEE	O2-C10-C11	3.36	120.16	110.80
56	s	401	UQ	C21-C19-C18	-3.33	113.03	122.65
50	X	201	8Q1	O4-C1-C6	-3.31	120.08	123.99
47	A	503	NAI	C3D-C2D-C1D	3.23	107.56	101.43
50	G	201	8Q1	C37-C38-C39	3.18	117.65	112.36
46	A	502	FMN	C4-N3-C2	-3.11	119.89	125.64
56	s	401	UQ	C20-C19-C18	-3.08	113.76	122.65
54	V	201	CDL	OB8-CB7-C71	2.90	121.00	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.76	103.38	109.47
48	Q	501	PEE	O3-C30-C31	2.75	120.55	111.91
47	A	503	NAI	C2D-C3D-C4D	2.74	107.96	102.64
48	r	501	PEE	O3-C30-C31	2.73	120.48	111.91
54	N	201	CDL	OA8-CA7-C31	2.73	120.47	111.91
50	X	201	8Q1	C37-C38-C39	2.73	116.90	112.36
48	i	402	PEE	O3-C30-C31	2.70	120.39	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	l	705	PEE	O3-C30-C31	2.70	120.39	111.91
54	V	202	CDL	OB8-CB7-C71	2.70	120.39	111.91
54	i	401	CDL	OA8-CA7-C31	2.69	120.36	111.91
54	N	201	CDL	OB8-CB7-C71	2.66	120.24	111.91
54	a	201	CDL	OB8-CB7-C71	2.65	120.24	111.91
54	l	702	CDL	OB8-CB7-C71	2.65	120.23	111.91
54	u	201	CDL	OB8-CB7-C71	2.64	120.19	111.91
54	g	202	CDL	OA8-CA7-C31	2.63	120.15	111.91
46	A	502	FMN	C4A-C4-N3	2.61	119.82	113.19
54	u	201	CDL	OA8-CA7-C31	2.61	120.09	111.91
54	g	202	CDL	OB8-CB7-C71	2.61	120.08	111.91
56	s	401	UQ	CM5-C5-C6	-2.60	120.15	124.40
57	w	401	ADP	PA-O3A-PB	-2.59	123.93	132.83
48	l	704	PEE	O3-C30-C31	2.59	120.04	111.91
48	j	201	PEE	O3-C30-C31	2.59	120.03	111.91
54	l	702	CDL	OA8-CA7-C31	2.59	120.03	111.91
54	i	401	CDL	OB8-CB7-C71	2.58	120.02	111.91
49	l	701	PLX	C1A-N1-C1	2.58	120.46	109.92
54	l	703	CDL	OB8-CB7-C71	2.57	119.99	111.91
54	a	201	CDL	OA8-CA7-C31	2.57	119.98	111.91
54	l	703	CDL	OA8-CA7-C31	2.56	119.94	111.91
48	V	203	PEE	O3-C30-C31	2.55	119.90	111.91
48	C	302	PEE	O3-C30-C31	2.54	119.87	111.91
54	V	201	CDL	OA8-CA7-C31	2.53	119.86	111.91
50	G	201	8Q1	C38-C39-N41	2.53	120.69	116.42
51	J	401	NDP	PN-O3-PA	-2.52	124.18	132.83
54	V	202	CDL	OA8-CA7-C31	2.51	119.78	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.49	106.80	109.40
47	A	503	NAI	PN-O3-PA	-2.49	124.29	132.83
48	m	201	PEE	O3-C30-C31	2.48	119.69	111.91
46	A	502	FMN	O4-C4-C4A	-2.47	120.06	126.60
47	A	503	NAI	C3B-C2B-C1B	2.45	104.67	100.98
46	A	502	FMN	C4A-C10-N10	2.43	120.04	116.48
49	j	202	PLX	C1A-N1-C1	2.38	119.66	109.92
51	J	401	NDP	C4A-C5A-N7A	-2.37	106.93	109.40
49	g	201	PLX	C1A-N1-C1	2.33	119.43	109.92
49	a	202	PLX	C1A-N1-C1	2.30	119.31	109.92
50	G	201	8Q1	O4-C1-S44	-2.27	119.66	122.61
50	X	201	8Q1	O4-C1-S44	-2.26	119.68	122.61
50	G	201	8Q1	C43-S44-C1	2.25	108.88	101.87
46	A	502	FMN	C4A-C10-N1	-2.22	119.59	124.73
50	X	201	8Q1	C43-S44-C1	2.21	108.77	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	O4'-C1'-C2'	-2.21	103.69	106.93
49	C	303	PLX	C1A-N1-C1	2.19	118.89	109.92
50	X	201	8Q1	C38-C39-N41	2.18	120.09	116.42
46	A	502	FMN	C10-C4A-N5	-2.17	120.25	124.86
46	A	502	FMN	C9A-C5A-N5	-2.17	120.08	122.43
57	w	401	ADP	C3'-C2'-C1'	2.11	104.16	100.98
46	A	502	FMN	C5A-C9A-N10	2.08	120.10	117.95
57	w	401	ADP	C2'-C3'-C4'	2.03	106.59	102.64
50	G	201	8Q1	C42-N41-C39	-2.02	119.09	122.84

There are no chirality outliers.

All (852) 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	C3D-C4D-C5D-O5D
48	Q	501	PEE	C1-O3P-P-O1P
48	V	203	PEE	C18-C19-C20-C21
48	V	203	PEE	C11-C10-O2-C2
48	V	203	PEE	O3P-C1-C2-O2
48	V	203	PEE	C1-O3P-P-O2P
48	V	203	PEE	C1-O3P-P-O1P
48	V	203	PEE	C1-O3P-P-O4P
48	V	203	PEE	C4-O4P-P-O1P
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	O4-C10-O2-C2
48	j	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	O3P-C1-C2-O2
48	l	705	PEE	C37-C38-C39-C40
48	m	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	O4-C3-C4-O6
49	C	303	PLX	C3-O4-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	O9-C24-O8-C5
49	C	303	PLX	O9-C24-C25-C26
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C5-C4-O6-C6
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	N1-C1-C2-O1
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C25-C24-O8-C5
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O7-C6-O6-C4
49	l	701	PLX	O7-C6-C7-C8
49	l	701	PLX	O7-C6-O6-C4
49	l	701	PLX	C3-O4-P1-O2
49	l	701	PLX	C2-O1-P1-O4
49	l	701	PLX	C2-O1-P1-O2
49	l	701	PLX	C2-O1-P1-O3
49	l	701	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
51	J	401	NDP	C2N-C3N-C7N-N7N
54	N	201	CDL	CA2-OA2-PA1-OA3
54	N	201	CDL	CA2-OA2-PA1-OA4
54	N	201	CDL	CA2-OA2-PA1-OA5
54	N	201	CDL	C11-CA5-OA6-CA4
54	N	201	CDL	CB2-OB2-PB2-OB3
54	N	201	CDL	CB2-OB2-PB2-OB4
54	N	201	CDL	CB3-OB5-PB2-OB3
54	V	201	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	V	201	CDL	CA3-OA5-PA1-OA2
54	V	201	CDL	CA3-OA5-PA1-OA3
54	V	201	CDL	CA3-OA5-PA1-OA4
54	V	201	CDL	CB2-OB2-PB2-OB3
54	V	201	CDL	CB3-OB5-PB2-OB3
54	V	201	CDL	CB3-OB5-PB2-OB4
54	V	202	CDL	CA2-C1-CB2-OB2
54	V	202	CDL	CA2-OA2-PA1-OA4
54	V	202	CDL	CA3-OA5-PA1-OA3
54	V	202	CDL	OA6-CA4-CA6-OA8
54	V	202	CDL	CB3-OB5-PB2-OB3
54	V	202	CDL	CB3-OB5-PB2-OB4
54	V	202	CDL	OB5-CB3-CB4-OB6
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	OA5-CA3-CA4-OA6
54	a	201	CDL	CB2-OB2-PB2-OB3
54	g	202	CDL	CB2-C1-CA2-OA2
54	g	202	CDL	CA2-OA2-PA1-OA3
54	g	202	CDL	CA2-OA2-PA1-OA4
54	g	202	CDL	OA6-CA4-CA6-OA8
54	g	202	CDL	CB2-OB2-PB2-OB3
54	g	202	CDL	CB3-OB5-PB2-OB2
54	g	202	CDL	CB3-OB5-PB2-OB3
54	g	202	CDL	CB3-OB5-PB2-OB4
54	g	202	CDL	C51-CB5-OB6-CB4
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	OA9-CA7-OA8-CA6
54	i	401	CDL	CB3-OB5-PB2-OB3
54	l	702	CDL	O1-C1-CA2-OA2
54	l	702	CDL	CA2-OA2-PA1-OA3
54	l	702	CDL	CB2-OB2-PB2-OB4
54	l	702	CDL	CB3-OB5-PB2-OB3
54	l	702	CDL	CB3-OB5-PB2-OB4
54	l	703	CDL	O1-C1-CA2-OA2
54	l	703	CDL	CA2-OA2-PA1-OA3
54	l	703	CDL	CA2-OA2-PA1-OA4
54	l	703	CDL	CA2-OA2-PA1-OA5
54	l	703	CDL	CA3-OA5-PA1-OA2
54	l	703	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	l	703	CDL	CB2-OB2-PB2-OB4
54	l	703	CDL	CB2-OB2-PB2-OB5
54	l	703	CDL	OB6-CB4-CB6-OB8
54	u	201	CDL	CB2-C1-CA2-OA2
54	u	201	CDL	CA2-OA2-PA1-OA5
54	u	201	CDL	CB2-OB2-PB2-OB3
54	u	201	CDL	CB3-OB5-PB2-OB3
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C10
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C14-C16-C17-C18
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
54	i	401	CDL	C31-CA7-OA8-CA6
56	s	401	UQ	C17-C18-C19-C21
54	l	702	CDL	OA9-CA7-OA8-CA6
48	V	203	PEE	O4-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
54	N	201	CDL	OA7-CA5-OA6-CA4
54	g	202	CDL	OB7-CB5-OB6-CB4
54	g	202	CDL	C71-CB7-OB8-CB6
54	l	702	CDL	C31-CA7-OA8-CA6
56	s	401	UQ	C13-C14-C16-C17
49	C	303	PLX	C28-C29-C30-C31
54	l	703	CDL	C11-C12-C13-C14
48	l	704	PEE	C31-C30-O3-C3
48	l	705	PEE	C31-C30-O3-C3
48	Q	501	PEE	C37-C38-C39-C40
48	V	203	PEE	C17-C18-C19-C20
54	V	201	CDL	C59-C60-C61-C62
54	l	702	CDL	C32-C33-C34-C35
56	s	401	UQ	C7-C8-C9-C10
54	V	201	CDL	OA7-CA5-OA6-CA4
48	l	705	PEE	O5-C30-O3-C3
54	g	202	CDL	OB9-CB7-OB8-CB6
54	N	201	CDL	O1-C1-CB2-OB2
54	V	201	CDL	O1-C1-CA2-OA2
54	l	702	CDL	O1-C1-CB2-OB2
54	u	201	CDL	O1-C1-CA2-OA2
54	u	201	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	l	703	CDL	C71-CB7-OB8-CB6
48	j	201	PEE	C11-C10-O2-C2
48	r	501	PEE	C11-C10-O2-C2
54	V	201	CDL	C11-CA5-OA6-CA4
49	g	201	PLX	C7-C8-C9-C10
54	V	201	CDL	C11-C12-C13-C14
54	l	702	CDL	C55-C56-C57-C58
54	l	703	CDL	C54-C55-C56-C57
46	A	502	FMN	O2'-C2'-C3'-O3'
54	l	703	CDL	C59-C60-C61-C62
47	A	503	NAI	O4D-C4D-C5D-O5D
51	J	401	NDP	O4D-C4D-C5D-O5D
46	A	502	FMN	O2'-C2'-C3'-C4'
48	V	203	PEE	C11-C12-C13-C14
49	l	701	PLX	C30-C31-C32-C33
54	u	201	CDL	C71-C72-C73-C74
48	l	704	PEE	O5-C30-O3-C3
54	V	201	CDL	C62-C63-C64-C65
54	l	703	CDL	OB9-CB7-OB8-CB6
49	j	202	PLX	C28-C29-C30-C31
54	l	703	CDL	C35-C36-C37-C38
48	C	302	PEE	C37-C38-C39-C40
54	V	202	CDL	C51-CB5-OB6-CB4
54	a	201	CDL	C31-C32-C33-C34
54	i	401	CDL	C31-C32-C33-C34
54	N	201	CDL	CA2-C1-CB2-OB2
54	a	201	CDL	CA2-C1-CB2-OB2
54	l	702	CDL	CB2-C1-CA2-OA2
54	l	702	CDL	CA2-C1-CB2-OB2
54	l	703	CDL	CB2-C1-CA2-OA2
54	u	201	CDL	CA2-C1-CB2-OB2
48	r	501	PEE	O4-C10-O2-C2
54	l	703	CDL	C39-C40-C41-C42
54	V	201	CDL	C32-C33-C34-C35
54	g	202	CDL	C13-C14-C15-C16
54	l	702	CDL	C58-C59-C60-C61
54	g	202	CDL	CB5-C51-C52-C53
54	l	702	CDL	CB7-C71-C72-C73
54	i	401	CDL	OB6-CB4-CB6-OB8
54	N	201	CDL	CA7-C31-C32-C33
51	J	401	NDP	C2D-C1D-N1N-C6N
48	V	203	PEE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C30-C31-C32-C33
54	a	201	CDL	CA5-C11-C12-C13
48	i	402	PEE	C17-C18-C19-C20
48	l	704	PEE	C37-C38-C39-C40
54	u	201	CDL	C75-C76-C77-C78
48	r	501	PEE	C10-C11-C12-C13
54	a	201	CDL	CA7-C31-C32-C33
54	g	202	CDL	CB7-C71-C72-C73
54	i	401	CDL	CA5-C11-C12-C13
54	i	401	CDL	CA7-C31-C32-C33
54	i	401	CDL	CB7-C71-C72-C73
54	l	702	CDL	CA7-C31-C32-C33
54	l	702	CDL	CB5-C51-C52-C53
54	l	703	CDL	CB5-C51-C52-C53
54	l	703	CDL	CB7-C71-C72-C73
54	u	201	CDL	CB5-C51-C52-C53
51	J	401	NDP	C3D-C4D-C5D-O5D
48	Q	501	PEE	C31-C30-O3-C3
48	m	201	PEE	C31-C30-O3-C3
54	V	201	CDL	C34-C35-C36-C37
49	l	701	PLX	C2-C1-N1-C1C
49	l	701	PLX	C2-C1-N1-C1A
54	g	202	CDL	CA5-C11-C12-C13
54	u	201	CDL	CA5-C11-C12-C13
54	V	202	CDL	C32-C33-C34-C35
56	s	401	UQ	C9-C11-C12-C13
49	l	701	PLX	C12-C13-C14-C15
54	u	201	CDL	CB7-C71-C72-C73
48	i	402	PEE	C11-C12-C13-C14
54	V	201	CDL	O1-C1-CB2-OB2
54	a	201	CDL	O1-C1-CA2-OA2
54	a	201	CDL	O1-C1-CB2-OB2
54	g	202	CDL	O1-C1-CA2-OA2
54	i	401	CDL	O1-C1-CA2-OA2
48	V	203	PEE	C4-O4P-P-O3P
48	i	402	PEE	C4-O4P-P-O3P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	l	704	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
49	a	202	PLX	C2-O1-P1-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C3-O4-P1-O1
54	N	201	CDL	CA3-OA5-PA1-OA2
54	N	201	CDL	CB2-OB2-PB2-OB5
54	N	201	CDL	CB3-OB5-PB2-OB2
54	V	201	CDL	CB2-OB2-PB2-OB5
54	V	201	CDL	CB3-OB5-PB2-OB2
54	V	202	CDL	CA2-OA2-PA1-OA5
54	V	202	CDL	CA3-OA5-PA1-OA2
54	V	202	CDL	CB3-OB5-PB2-OB2
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CB2-OB2-PB2-OB5
54	g	202	CDL	CA2-OA2-PA1-OA5
54	l	702	CDL	CB2-OB2-PB2-OB5
54	l	702	CDL	CB3-OB5-PB2-OB2
54	l	703	CDL	CB3-OB5-PB2-OB2
54	V	201	CDL	C31-CA7-OA8-CA6
54	V	202	CDL	C71-CB7-OB8-CB6
54	a	201	CDL	CB2-C1-CA2-OA2
54	i	401	CDL	CB2-C1-CA2-OA2
54	V	202	CDL	OB7-CB5-OB6-CB4
48	m	201	PEE	C13-C14-C15-C16
54	N	201	CDL	CB5-C51-C52-C53
49	j	202	PLX	C12-C13-C14-C15
48	C	302	PEE	C11-C10-O2-C2
48	r	501	PEE	C12-C13-C14-C15
49	C	303	PLX	C17-C18-C19-C20
49	a	202	PLX	C7-C8-C9-C10
49	g	201	PLX	C11-C10-C9-C8
49	j	202	PLX	C25-C26-C27-C28
50	X	201	8Q1	C9-C10-C11-C12
54	N	201	CDL	C11-C12-C13-C14
54	g	202	CDL	C55-C56-C57-C58
54	l	702	CDL	C75-C76-C77-C78
54	u	201	CDL	C57-C58-C59-C60
48	r	501	PEE	C42-C43-C44-C45
49	C	303	PLX	C16-C17-C18-C19
49	j	202	PLX	C10-C11-C12-C13
54	V	201	CDL	C52-C53-C54-C55
54	a	201	CDL	C37-C38-C39-C40
54	g	202	CDL	C73-C74-C75-C76
54	l	703	CDL	C60-C61-C62-C63
48	C	302	PEE	O4-C10-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	705	PEE	C33-C34-C35-C36
54	g	202	CDL	C43-C44-C45-C46
54	i	401	CDL	C11-C12-C13-C14
48	Q	501	PEE	O5-C30-O3-C3
48	l	704	PEE	C31-C32-C33-C34
49	j	202	PLX	C7-C8-C9-C10
54	a	201	CDL	C73-C74-C75-C76
54	g	202	CDL	C41-C42-C43-C44
54	l	703	CDL	C72-C73-C74-C75
54	V	202	CDL	O1-C1-CB2-OB2
49	g	201	PLX	C27-C28-C29-C30
54	a	201	CDL	C75-C76-C77-C78
54	g	202	CDL	C36-C37-C38-C39
54	l	702	CDL	C73-C74-C75-C76
54	l	703	CDL	C55-C56-C57-C58
54	N	201	CDL	CB7-C71-C72-C73
54	l	703	CDL	OA6-CA4-CA6-OA8
49	l	701	PLX	C31-C32-C33-C34
49	l	701	PLX	C33-C34-C35-C36
54	V	202	CDL	C75-C76-C77-C78
54	a	201	CDL	C17-C18-C19-C20
54	l	702	CDL	C79-C80-C81-C82
49	g	201	PLX	C33-C34-C35-C36
54	l	703	CDL	C37-C38-C39-C40
48	Q	501	PEE	C21-C22-C23-C24
48	V	203	PEE	C32-C33-C34-C35
49	C	303	PLX	C35-C36-C37-C38
49	a	202	PLX	C11-C12-C13-C14
49	l	701	PLX	C7-C8-C9-C10
49	l	701	PLX	C25-C26-C27-C28
54	V	202	CDL	C83-C84-C85-C86
54	a	201	CDL	C71-C72-C73-C74
54	g	202	CDL	C75-C76-C77-C78
54	l	703	CDL	C14-C15-C16-C17
54	l	703	CDL	C57-C58-C59-C60
48	m	201	PEE	O5-C30-O3-C3
49	C	303	PLX	C33-C34-C35-C36
54	u	201	CDL	C14-C15-C16-C17
48	m	201	PEE	C11-C10-O2-C2
48	r	501	PEE	C20-C21-C22-C23
54	l	702	CDL	C56-C57-C58-C59
48	Q	501	PEE	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	Q	501	PEE	C20-C21-C22-C23
54	g	202	CDL	C62-C63-C64-C65
54	g	202	CDL	C71-C72-C73-C74
54	g	202	CDL	C74-C75-C76-C77
54	i	401	CDL	C52-C53-C54-C55
48	V	203	PEE	C13-C14-C15-C16
48	l	704	PEE	C21-C22-C23-C24
49	C	303	PLX	C30-C31-C32-C33
48	l	705	PEE	O4P-C4-C5-N
48	C	302	PEE	C33-C34-C35-C36
48	l	705	PEE	C22-C23-C24-C25
54	a	201	CDL	C32-C33-C34-C35
54	V	202	CDL	OB9-CB7-OB8-CB6
48	Q	501	PEE	C14-C15-C16-C17
54	V	201	CDL	C55-C56-C57-C58
54	a	201	CDL	C34-C35-C36-C37
54	l	702	CDL	C35-C36-C37-C38
54	l	702	CDL	C37-C38-C39-C40
54	l	703	CDL	C62-C63-C64-C65
49	g	201	PLX	C28-C29-C30-C31
49	j	202	PLX	C13-C14-C15-C16
49	l	701	PLX	C15-C16-C17-C18
54	g	202	CDL	C60-C61-C62-C63
54	u	201	CDL	C54-C55-C56-C57
54	V	201	CDL	OA9-CA7-OA8-CA6
54	l	702	CDL	C82-C83-C84-C85
48	j	201	PEE	C41-C42-C43-C44
54	l	703	CDL	C40-C41-C42-C43
54	g	202	CDL	C37-C38-C39-C40
54	l	702	CDL	C11-CA5-OA6-CA4
49	C	303	PLX	C31-C32-C33-C34
54	V	201	CDL	C35-C36-C37-C38
48	i	402	PEE	C34-C35-C36-C37
49	C	303	PLX	C11-C12-C13-C14
54	u	201	CDL	CA7-C31-C32-C33
48	l	704	PEE	C15-C16-C17-C18
54	V	202	CDL	CB7-C71-C72-C73
54	V	202	CDL	C31-CA7-OA8-CA6
49	a	202	PLX	C12-C13-C14-C15
48	l	705	PEE	C31-C32-C33-C34
49	C	303	PLX	C7-C8-C9-C10
49	l	701	PLX	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	m	201	PEE	O4-C10-O2-C2
54	l	702	CDL	OA7-CA5-OA6-CA4
48	j	201	PEE	C21-C22-C23-C24
49	g	201	PLX	C9-C10-C11-C12
49	j	202	PLX	C27-C28-C29-C30
49	l	701	PLX	C32-C33-C34-C35
54	V	202	CDL	C56-C57-C58-C59
48	i	402	PEE	C14-C15-C16-C17
48	l	705	PEE	C13-C14-C15-C16
54	V	201	CDL	C71-CB7-OB8-CB6
54	l	702	CDL	C51-CB5-OB6-CB4
48	r	501	PEE	C23-C24-C25-C26
49	g	201	PLX	C32-C33-C34-C35
54	V	201	CDL	C14-C15-C16-C17
49	l	701	PLX	C11-C12-C13-C14
54	g	202	CDL	C17-C18-C19-C20
54	g	202	CDL	C35-C36-C37-C38
54	l	702	CDL	C81-C82-C83-C84
48	i	402	PEE	C19-C20-C21-C22
48	j	201	PEE	C19-C20-C21-C22
48	m	201	PEE	C19-C20-C21-C22
48	j	201	PEE	C30-C31-C32-C33
54	g	202	CDL	CA7-C31-C32-C33
48	C	302	PEE	C42-C43-C44-C45
49	j	202	PLX	C34-C35-C36-C37
54	V	201	CDL	C41-C42-C43-C44
54	V	201	CDL	C37-C38-C39-C40
54	l	702	CDL	C11-C12-C13-C14
54	l	703	CDL	C33-C34-C35-C36
49	C	303	PLX	C13-C14-C15-C16
54	a	201	CDL	C21-C22-C23-C24
54	i	401	CDL	C36-C37-C38-C39
48	l	704	PEE	C11-C12-C13-C14
49	a	202	PLX	C19-C20-C21-C22
54	u	201	CDL	C52-C53-C54-C55
54	N	201	CDL	C51-CB5-OB6-CB4
54	V	201	CDL	C51-CB5-OB6-CB4
54	u	201	CDL	C11-CA5-OA6-CA4
48	Q	501	PEE	C33-C34-C35-C36
49	C	303	PLX	C15-C16-C17-C18
49	g	201	PLX	C10-C11-C12-C13
49	j	202	PLX	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	l	701	PLX	C10-C11-C12-C13
54	i	401	CDL	C32-C33-C34-C35
48	j	201	PEE	C36-C37-C38-C39
54	N	201	CDL	OB7-CB5-OB6-CB4
54	V	201	CDL	OB7-CB5-OB6-CB4
54	l	702	CDL	OB7-CB5-OB6-CB4
54	u	201	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C30-C31-C32-C33
49	l	701	PLX	C28-C29-C30-C31
54	l	702	CDL	C20-C21-C22-C23
54	V	202	CDL	OB6-CB4-CB6-OB8
49	l	701	PLX	C2-C1-N1-C1B
54	V	201	CDL	C51-C52-C53-C54
48	V	203	PEE	C35-C36-C37-C38
48	Q	501	PEE	C17-C18-C19-C20
48	i	402	PEE	C13-C14-C15-C16
48	i	402	PEE	C31-C32-C33-C34
49	j	202	PLX	C30-C31-C32-C33
48	i	402	PEE	C32-C33-C34-C35
50	G	201	8Q1	C7-C8-C9-C10
54	u	201	CDL	C58-C59-C60-C61
54	V	201	CDL	OB9-CB7-OB8-CB6
54	V	202	CDL	OA9-CA7-OA8-CA6
48	l	705	PEE	O4-C10-O2-C2
48	l	705	PEE	C11-C10-O2-C2
54	u	201	CDL	C17-C18-C19-C20
48	r	501	PEE	C36-C37-C38-C39
48	r	501	PEE	C1-O3P-P-O4P
54	i	401	CDL	CB3-OB5-PB2-OB2
54	u	201	CDL	CB2-OB2-PB2-OB5
54	u	201	CDL	CB3-OB5-PB2-OB2
49	j	202	PLX	C9-C10-C11-C12
54	l	702	CDL	C54-C55-C56-C57
49	C	303	PLX	O4-C3-C4-C5
54	a	201	CDL	OA5-CA3-CA4-CA6
54	i	401	CDL	OB5-CB3-CB4-CB6
54	g	202	CDL	C31-C32-C33-C34
54	a	201	CDL	CB5-C51-C52-C53
49	C	303	PLX	C25-C26-C27-C28
54	a	201	CDL	C59-C60-C61-C62
48	Q	501	PEE	C15-C16-C17-C18
48	Q	501	PEE	C42-C43-C44-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	V	201	CDL	CB2-C1-CA2-OA2
49	C	303	PLX	C9-C10-C11-C12
48	i	402	PEE	C18-C19-C20-C21
48	m	201	PEE	C33-C34-C35-C36
49	a	202	PLX	C28-C29-C30-C31
49	g	201	PLX	C13-C14-C15-C16
54	V	201	CDL	C74-C75-C76-C77
54	i	401	CDL	C11-CA5-OA6-CA4
48	V	203	PEE	C31-C32-C33-C34
48	V	203	PEE	C33-C34-C35-C36
54	l	703	CDL	C56-C57-C58-C59
48	C	302	PEE	C1-C2-C3-O3
48	i	402	PEE	C1-C2-C3-O3
48	l	705	PEE	C1-C2-C3-O3
48	m	201	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
48	r	501	PEE	C41-C42-C43-C44
49	l	701	PLX	C3-C4-C5-O8
54	V	201	CDL	CA3-CA4-CA6-OA8
54	V	202	CDL	CB3-CB4-CB6-OB8
54	g	202	CDL	CA3-CA4-CA6-OA8
54	g	202	CDL	C11-C12-C13-C14
54	i	401	CDL	CB3-CB4-CB6-OB8
54	i	401	CDL	C73-C74-C75-C76
54	l	703	CDL	CA3-CA4-CA6-OA8
54	l	703	CDL	CB3-CB4-CB6-OB8
54	l	703	CDL	C31-C32-C33-C34
54	l	703	CDL	C64-C65-C66-C67
49	C	303	PLX	C11-C10-C9-C8
54	V	202	CDL	C55-C56-C57-C58
49	g	201	PLX	C25-C26-C27-C28
54	i	401	CDL	C13-C14-C15-C16
49	a	202	PLX	O6-C6-C7-C8
49	a	202	PLX	C25-C26-C27-C28
48	C	302	PEE	C39-C40-C41-C42
48	Q	501	PEE	C39-C40-C41-C42
48	i	402	PEE	C35-C36-C37-C38
48	C	302	PEE	C32-C33-C34-C35
49	a	202	PLX	C34-C35-C36-C37
48	Q	501	PEE	C34-C35-C36-C37
54	l	702	CDL	C84-C85-C86-C87
48	Q	501	PEE	C44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	N	201	CDL	CA6-CA4-OA6-CA5
54	V	201	CDL	CA6-CA4-OA6-CA5
48	C	302	PEE	C43-C44-C45-C46
50	G	201	8Q1	C28-O27-P24-O3
48	j	201	PEE	C31-C30-O3-C3
54	a	201	CDL	C71-CB7-OB8-CB6
54	l	702	CDL	OA5-CA3-CA4-OA6
48	l	704	PEE	C30-C31-C32-C33
54	i	401	CDL	C71-C72-C73-C74
48	r	501	PEE	C24-C25-C26-C27
54	u	201	CDL	C13-C14-C15-C16
49	C	303	PLX	O6-C4-C5-O8
48	r	501	PEE	C13-C14-C15-C16
50	X	201	8Q1	C31-C29-C32-O33
48	Q	501	PEE	C32-C33-C34-C35
54	a	201	CDL	C76-C77-C78-C79
54	l	702	CDL	C52-C53-C54-C55
54	l	703	CDL	C58-C59-C60-C61
48	l	704	PEE	C24-C25-C26-C27
49	a	202	PLX	C33-C34-C35-C36
54	N	201	CDL	C52-C53-C54-C55
54	a	201	CDL	C74-C75-C76-C77
54	u	201	CDL	C55-C56-C57-C58
54	l	702	CDL	C71-CB7-OB8-CB6
48	i	402	PEE	C24-C25-C26-C27
49	a	202	PLX	C30-C31-C32-C33
54	g	202	CDL	C76-C77-C78-C79
48	l	705	PEE	C32-C33-C34-C35
54	i	401	CDL	C14-C15-C16-C17
48	r	501	PEE	C11-C12-C13-C14
54	V	201	CDL	C54-C55-C56-C57
48	V	203	PEE	O3P-C1-C2-C3
48	l	704	PEE	O3P-C1-C2-C3
54	V	201	CDL	OA5-CA3-CA4-CA6
54	V	202	CDL	OA5-CA3-CA4-CA6
54	i	401	CDL	OA5-CA3-CA4-CA6
54	l	702	CDL	OA5-CA3-CA4-CA6
54	V	202	CDL	C74-C75-C76-C77
54	l	702	CDL	C33-C34-C35-C36
49	C	303	PLX	C14-C15-C16-C17
54	g	202	CDL	C59-C60-C61-C62
54	i	401	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	i	401	CDL	CB5-C51-C52-C53
54	l	703	CDL	C81-C82-C83-C84
54	N	201	CDL	C71-C72-C73-C74
54	l	703	CDL	C15-C16-C17-C18
49	j	202	PLX	C3-C4-C5-O8
54	V	202	CDL	CA3-CA4-CA6-OA8
54	g	202	CDL	C33-C34-C35-C36
54	V	202	CDL	CA7-C31-C32-C33
48	r	501	PEE	C17-C18-C19-C20
54	l	702	CDL	C13-C14-C15-C16
54	l	703	CDL	C41-C42-C43-C44
54	l	703	CDL	C74-C75-C76-C77
54	a	201	CDL	OB9-CB7-OB8-CB6
48	Q	501	PEE	C11-C10-O2-C2
49	C	303	PLX	C36-C37-C38-C39
49	l	701	PLX	C5-C4-O6-C6
54	l	702	CDL	CA2-OA2-PA1-OA5
48	r	501	PEE	O3P-C1-C2-O2
54	V	202	CDL	OA5-CA3-CA4-OA6
54	g	202	CDL	OB5-CB3-CB4-OB6
54	i	401	CDL	OA5-CA3-CA4-OA6
54	i	401	CDL	OB5-CB3-CB4-OB6
54	i	401	CDL	OA7-CA5-OA6-CA4
54	N	201	CDL	C31-CA7-OA8-CA6
48	j	201	PEE	O5-C30-O3-C3
49	g	201	PLX	C16-C17-C18-C19
54	V	202	CDL	C84-C85-C86-C87
48	r	501	PEE	O2-C2-C3-O3
49	j	202	PLX	O6-C4-C5-O8
49	a	202	PLX	C10-C11-C12-C13
54	u	201	CDL	C11-C12-C13-C14
48	l	705	PEE	C11-C12-C13-C14
54	l	702	CDL	OB9-CB7-OB8-CB6
48	i	402	PEE	C22-C23-C24-C25
54	g	202	CDL	C20-C21-C22-C23
54	V	201	CDL	C64-C65-C66-C67
48	i	402	PEE	C2-C1-O3P-P
54	N	201	CDL	C31-C32-C33-C34
48	j	201	PEE	C32-C33-C34-C35
49	a	202	PLX	C15-C16-C17-C18
50	X	201	8Q1	O4-C1-S44-C43
48	Q	501	PEE	O4-C10-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	g	202	CDL	C51-C52-C53-C54
48	l	705	PEE	C23-C24-C25-C26
47	A	503	NAI	PN-O3-PA-O5B
49	C	303	PLX	O8-C24-C25-C26
49	l	701	PLX	O8-C24-C25-C26
48	Q	501	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
49	j	202	PLX	O4-C3-C4-C5
54	N	201	CDL	OA5-CA3-CA4-CA6
54	N	201	CDL	OB5-CB3-CB4-CB6
54	V	202	CDL	OB5-CB3-CB4-CB6
54	g	202	CDL	OB5-CB3-CB4-CB6
54	l	703	CDL	O1-C1-CB2-OB2
48	l	705	PEE	C16-C17-C18-C19
54	g	202	CDL	C12-C13-C14-C15
54	u	201	CDL	C31-CA7-OA8-CA6
49	j	202	PLX	C33-C34-C35-C36
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	C28-O27-P24-O1
48	l	705	PEE	C10-C11-C12-C13
49	g	201	PLX	C12-C13-C14-C15
50	X	201	8Q1	C6-C1-S44-C43
54	l	703	CDL	C53-C54-C55-C56
54	V	202	CDL	C82-C83-C84-C85
54	N	201	CDL	OA9-CA7-OA8-CA6
54	l	702	CDL	C71-C72-C73-C74
48	Q	501	PEE	O3P-C1-C2-O2
48	j	201	PEE	O3P-C1-C2-O2
54	N	201	CDL	OA5-CA3-CA4-OA6
54	N	201	CDL	OB5-CB3-CB4-OB6
54	V	201	CDL	OA5-CA3-CA4-OA6
48	j	201	PEE	C22-C23-C24-C25
54	l	703	CDL	C32-C33-C34-C35
54	i	401	CDL	C37-C38-C39-C40
54	l	703	CDL	CA7-C31-C32-C33
50	G	201	8Q1	C11-C10-C9-C8
54	i	401	CDL	OB9-CB7-OB8-CB6
54	i	401	CDL	C34-C35-C36-C37
48	l	705	PEE	O2-C2-C3-O3
49	l	701	PLX	O6-C4-C5-O8
54	V	201	CDL	OA6-CA4-CA6-OA8
54	g	202	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	A	503	NAI	C5D-O5D-PN-O3
51	J	401	NDP	C2B-O2B-P2B-O3X
48	m	201	PEE	C20-C21-C22-C23
50	X	201	8Q1	C7-C8-C9-C10
54	V	201	CDL	C71-C72-C73-C74
54	u	201	CDL	C60-C61-C62-C63
54	l	703	CDL	C43-C44-C45-C46
54	u	201	CDL	OA9-CA7-OA8-CA6
49	j	202	PLX	C15-C16-C17-C18
54	l	703	CDL	C44-C45-C46-C47
50	G	201	8Q1	C12-C13-C14-C15
54	N	201	CDL	C71-CB7-OB8-CB6
54	V	201	CDL	C44-C45-C46-C47
54	a	201	CDL	C15-C16-C17-C18
48	C	302	PEE	C1-O3P-P-O4P
49	l	701	PLX	C3-O4-P1-O1
54	i	401	CDL	CB2-OB2-PB2-OB5
54	l	703	CDL	C12-C13-C14-C15
47	A	503	NAI	C2D-C1D-N1N-C2N
50	G	201	8Q1	C6-C7-C8-C9
54	V	201	CDL	C39-C40-C41-C42
54	V	201	CDL	CB4-CB3-OB5-PB2
54	u	201	CDL	CB4-CB3-OB5-PB2
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O1P
48	V	203	PEE	C4-O4P-P-O2P
48	i	402	PEE	C4-O4P-P-O2P
48	i	402	PEE	C4-O4P-P-O1P
48	j	201	PEE	C1-O3P-P-O2P
48	l	704	PEE	C4-O4P-P-O2P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C4-O4P-P-O2P
54	N	201	CDL	CA3-OA5-PA1-OA4
54	N	201	CDL	CB3-OB5-PB2-OB4
54	V	201	CDL	CB2-OB2-PB2-OB4
54	V	202	CDL	CA2-OA2-PA1-OA3
54	V	202	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB3
54	i	401	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	i	401	CDL	CB3-OB5-PB2-OB4
54	l	703	CDL	CA3-OA5-PA1-OA4
54	l	703	CDL	CB3-OB5-PB2-OB3
54	l	703	CDL	CB3-OB5-PB2-OB4
54	u	201	CDL	CB2-OB2-PB2-OB4
54	u	201	CDL	CB3-OB5-PB2-OB4
54	l	703	CDL	OA5-CA3-CA4-CA6
54	g	202	CDL	C64-C65-C66-C67
50	G	201	8Q1	C11-C12-C13-C14
54	N	201	CDL	OB9-CB7-OB8-CB6
54	g	202	CDL	C72-C73-C74-C75
49	a	202	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
49	l	701	PLX	C25-C24-O8-C5
48	j	201	PEE	C34-C35-C36-C37
54	V	201	CDL	C57-C58-C59-C60
54	l	702	CDL	C36-C37-C38-C39
48	l	705	PEE	C14-C15-C16-C17
54	i	401	CDL	C15-C16-C17-C18
54	g	202	CDL	C31-CA7-OA8-CA6
54	g	202	CDL	OA5-CA3-CA4-OA6
54	l	703	CDL	OA5-CA3-CA4-OA6
54	i	401	CDL	C33-C34-C35-C36
48	j	201	PEE	C23-C24-C25-C26
54	l	703	CDL	C52-C53-C54-C55
49	j	202	PLX	C24-C25-C26-C27
49	C	303	PLX	N1-C1-C2-O1
51	J	401	NDP	C2N-C3N-C7N-O7N
54	u	201	CDL	CA3-CA4-CA6-OA8
48	l	704	PEE	O2-C2-C3-O3
48	m	201	PEE	O2-C2-C3-O3
54	u	201	CDL	OA6-CA4-CA6-OA8
54	V	201	CDL	C58-C59-C60-C61
48	V	203	PEE	C2-C1-O3P-P
54	V	202	CDL	C32-C31-CA7-OA8
49	C	303	PLX	O6-C6-C7-C8
54	g	202	CDL	OA9-CA7-OA8-CA6
54	V	201	CDL	C32-C31-CA7-OA8
48	l	705	PEE	C18-C19-C20-C21
47	A	503	NAI	O4D-C1D-N1N-C2N
51	J	401	NDP	O4D-C1D-N1N-C6N
48	Q	501	PEE	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
54	g	202	CDL	C78-C79-C80-C81
48	j	201	PEE	O3P-C1-C2-C3
54	l	702	CDL	C51-C52-C53-C54
48	i	402	PEE	C38-C39-C40-C41
50	X	201	8Q1	C28-O27-P24-O3
49	j	202	PLX	O4-C3-C4-O6
48	j	201	PEE	C24-C25-C26-C27
56	s	401	UQ	C12-C11-C9-C8
54	g	202	CDL	C80-C81-C82-C83
48	C	302	PEE	O2-C2-C3-O3
48	i	402	PEE	O2-C2-C3-O3
48	Q	501	PEE	C1-O3P-P-O4P
49	a	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C3-O4-P1-O1
54	V	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CB3-OB5-PB2-OB2
48	m	201	PEE	C22-C23-C24-C25
54	V	201	CDL	C31-C32-C33-C34
48	l	704	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
54	V	202	CDL	C51-C52-C53-C54
48	Q	501	PEE	C13-C14-C15-C16
54	g	202	CDL	C63-C64-C65-C66
49	l	701	PLX	C11-C10-C9-C8
48	l	704	PEE	C2-C1-O3P-P
54	g	202	CDL	CB4-CB3-OB5-PB2
54	V	201	CDL	C13-C14-C15-C16
48	C	302	PEE	C38-C39-C40-C41
48	V	203	PEE	C38-C39-C40-C41
48	l	704	PEE	C16-C17-C18-C19
48	l	705	PEE	C38-C39-C40-C41
48	j	201	PEE	C44-C45-C46-C47
54	a	201	CDL	C60-C61-C62-C63
48	j	201	PEE	C38-C39-C40-C41
48	i	402	PEE	O3P-C1-C2-C3
54	g	202	CDL	OA5-CA3-CA4-CA6
54	a	201	CDL	C14-C15-C16-C17
54	g	202	CDL	C44-C45-C46-C47
54	g	202	CDL	C56-C57-C58-C59
48	l	704	PEE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	l	702	CDL	C39-C40-C41-C42
54	l	702	CDL	C59-C60-C61-C62
50	X	201	8Q1	N41-C42-C43-S44
54	a	201	CDL	C22-C23-C24-C25
48	l	704	PEE	C12-C13-C14-C15
54	g	202	CDL	CB3-CB4-CB6-OB8
50	X	201	8Q1	O27-C28-C29-C30
48	l	704	PEE	C19-C20-C21-C22
54	g	202	CDL	C40-C41-C42-C43
47	A	503	NAI	C2D-C1D-N1N-C6N
54	g	202	CDL	C15-C16-C17-C18
54	a	201	CDL	OB5-CB3-CB4-CB6
48	i	402	PEE	C21-C22-C23-C24
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C9-C10-C11-C12
54	V	201	CDL	CA7-C31-C32-C33
49	a	202	PLX	C14-C15-C16-C17
54	a	201	CDL	C55-C56-C57-C58
48	m	201	PEE	C17-C18-C19-C20
54	V	202	CDL	CB2-C1-CA2-OA2
54	l	703	CDL	C82-C83-C84-C85
49	g	201	PLX	C36-C37-C38-C39
51	J	401	NDP	PN-O3-PA-O1A
54	V	202	CDL	C33-C34-C35-C36
54	l	703	CDL	C42-C43-C44-C45
54	V	202	CDL	C12-C11-CA5-OA6
48	V	203	PEE	C16-C17-C18-C19
54	g	202	CDL	C57-C58-C59-C60
48	i	402	PEE	C36-C37-C38-C39
48	m	201	PEE	C16-C17-C18-C19
49	g	201	PLX	O8-C24-C25-C26
49	j	202	PLX	O6-C6-C7-C8
48	m	201	PEE	O3-C30-C31-C32
48	Q	501	PEE	C18-C19-C20-C21
48	r	501	PEE	C38-C39-C40-C41
48	j	201	PEE	O2-C10-C11-C12
54	u	201	CDL	C72-C71-CB7-OB8
54	u	201	CDL	OB9-CB7-OB8-CB6
54	V	201	CDL	C12-C13-C14-C15
49	C	303	PLX	C32-C33-C34-C35
48	m	201	PEE	C18-C19-C20-C21
48	r	501	PEE	C44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	i	402	PEE	C30-C31-C32-C33
48	l	704	PEE	C36-C37-C38-C39
54	V	202	CDL	C72-C73-C74-C75
47	A	503	NAI	O4D-C1D-N1N-C6N
54	a	201	CDL	C12-C13-C14-C15
48	C	302	PEE	O3-C30-C31-C32
50	G	201	8Q1	N36-C37-C38-C39
48	j	201	PEE	C40-C41-C42-C43
48	l	705	PEE	C34-C35-C36-C37
48	m	201	PEE	C23-C24-C25-C26
54	u	201	CDL	C19-C20-C21-C22
54	l	703	CDL	C34-C35-C36-C37
57	w	401	ADP	O4'-C4'-C5'-O5'
57	w	401	ADP	C3'-C4'-C5'-O5'
48	C	302	PEE	C41-C42-C43-C44
50	X	201	8Q1	C31-C29-C32-C34
54	N	201	CDL	C72-C71-CB7-OB8
54	l	702	CDL	C61-C62-C63-C64
54	l	703	CDL	C32-C31-CA7-OA8
54	i	401	CDL	OA6-CA4-CA6-OA8
49	l	701	PLX	C24-C25-C26-C27
48	m	201	PEE	C12-C13-C14-C15
48	r	501	PEE	C14-C15-C16-C17
49	a	202	PLX	O9-C24-C25-C26
54	u	201	CDL	C71-CB7-OB8-CB6
54	a	201	CDL	C52-C53-C54-C55
54	g	202	CDL	C61-C62-C63-C64
49	j	202	PLX	C31-C32-C33-C34
54	l	703	CDL	C12-C11-CA5-OA6
54	g	202	CDL	C52-C51-CB5-OB6
54	a	201	CDL	C43-C44-C45-C46
54	l	702	CDL	C12-C11-CA5-OA6
54	i	401	CDL	CA2-C1-CB2-OB2
48	C	302	PEE	O5-C30-C31-C32
54	N	201	CDL	C72-C71-CB7-OB9
54	i	401	CDL	CA3-CA4-CA6-OA8
48	j	201	PEE	C12-C13-C14-C15
54	V	202	CDL	C76-C77-C78-C79
48	j	201	PEE	O4-C10-C11-C12
47	A	503	NAI	C5D-O5D-PN-O1N
48	m	201	PEE	C1-O3P-P-O1P
49	C	303	PLX	C2-O1-P1-O3

Continued on next page...

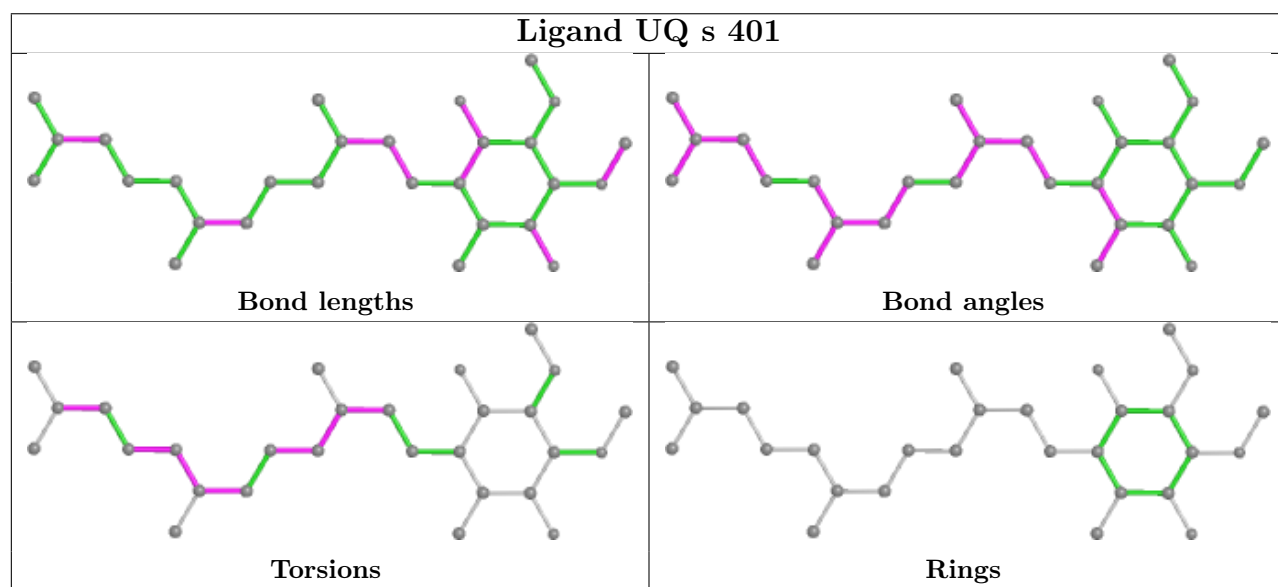
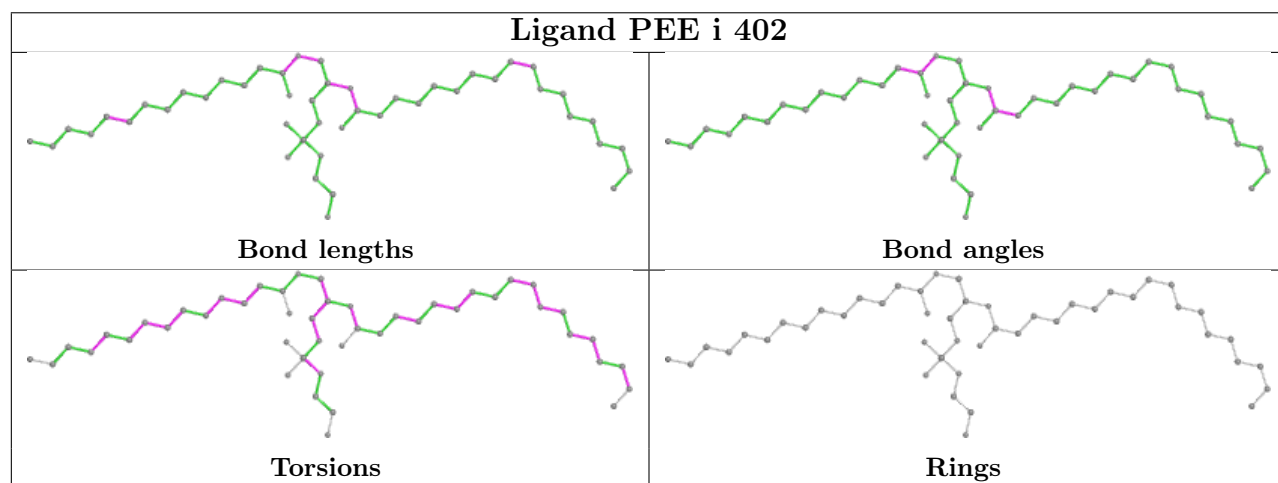
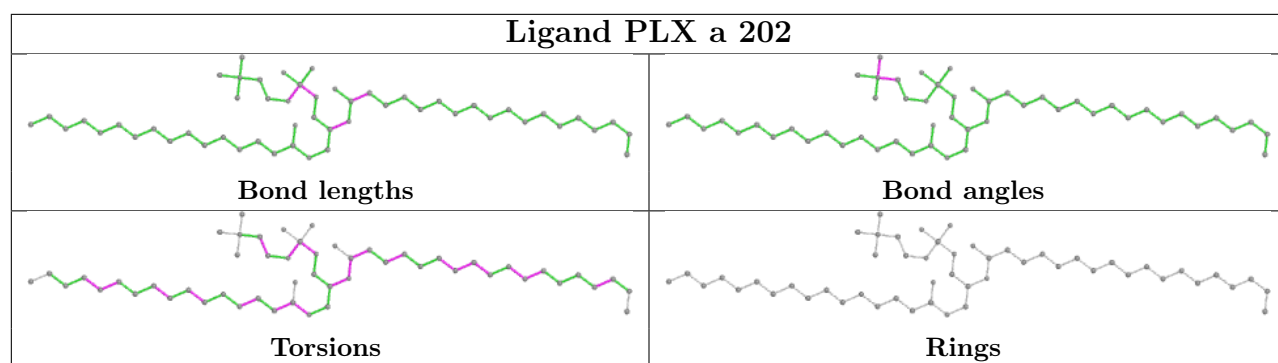
Continued from previous page...

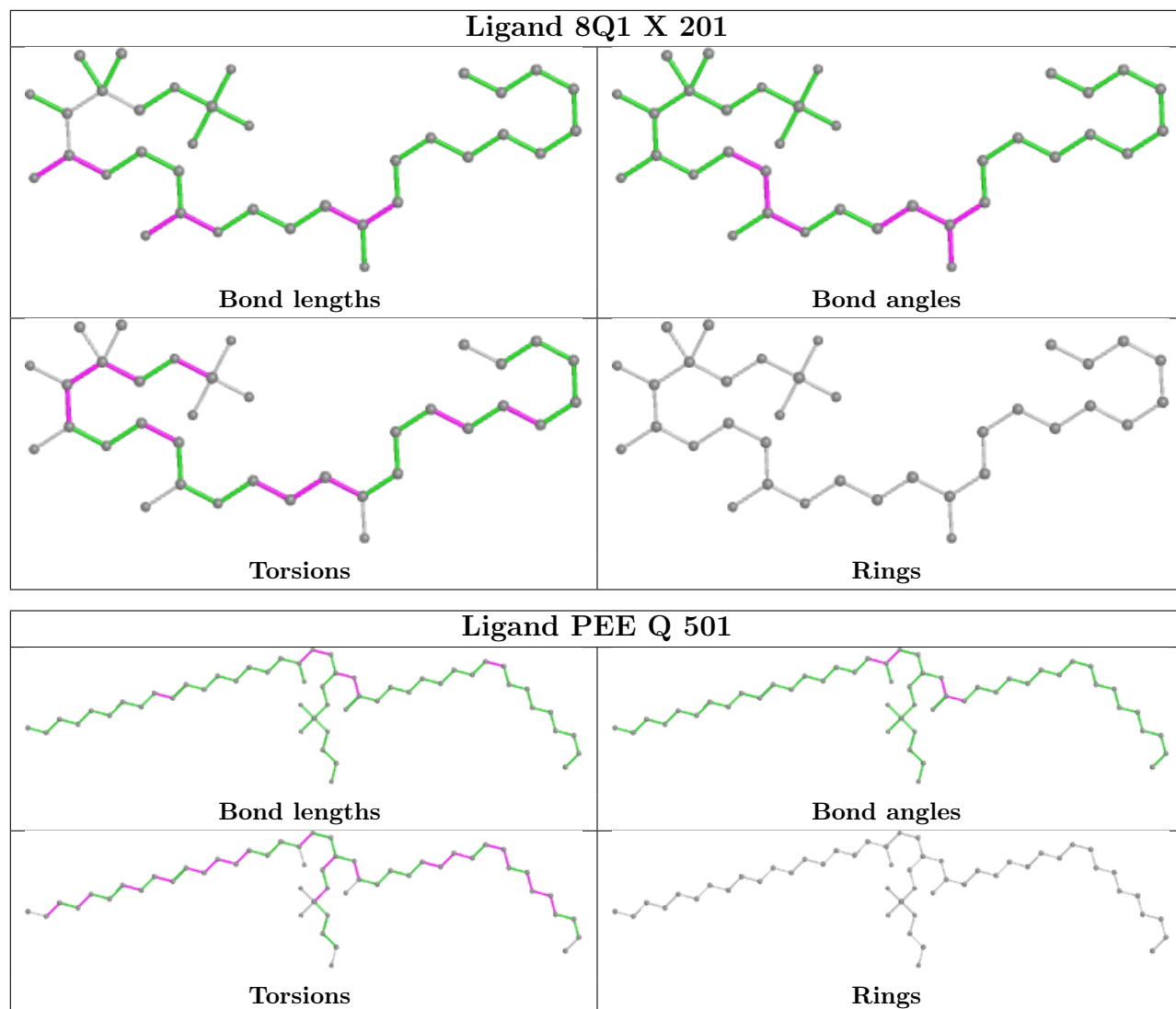
Mol	Chain	Res	Type	Atoms
51	J	401	NDP	C5D-O5D-PN-O1N
54	a	201	CDL	CB3-OB5-PB2-OB3
54	u	201	CDL	CA2-OA2-PA1-OA4
54	u	201	CDL	CA3-OA5-PA1-OA3
51	J	401	NDP	O4B-C4B-C5B-O5B
54	u	201	CDL	C72-C71-CB7-OB9
48	C	302	PEE	O5-C30-O3-C3
54	a	201	CDL	C72-C73-C74-C75
54	N	201	CDL	C52-C51-CB5-OB6
54	u	201	CDL	C22-C23-C24-C25
54	l	703	CDL	C12-C11-CA5-OA7
54	V	202	CDL	C78-C79-C80-C81
48	j	201	PEE	C5-C4-O4P-P
50	X	201	8Q1	C29-C32-C34-O35
54	l	703	CDL	C32-C31-CA7-OA9
54	g	202	CDL	C12-C11-CA5-OA6
49	j	202	PLX	C35-C36-C37-C38
54	a	201	CDL	C41-C42-C43-C44
54	i	401	CDL	C53-C54-C55-C56
54	l	702	CDL	C12-C11-CA5-OA7
54	u	201	CDL	C12-C11-CA5-OA7
48	l	705	PEE	O3-C30-C31-C32
54	u	201	CDL	C12-C11-CA5-OA6
54	g	202	CDL	C52-C51-CB5-OB7
48	l	704	PEE	C38-C39-C40-C41
54	V	201	CDL	C52-C51-CB5-OB6

There are no ring outliers.

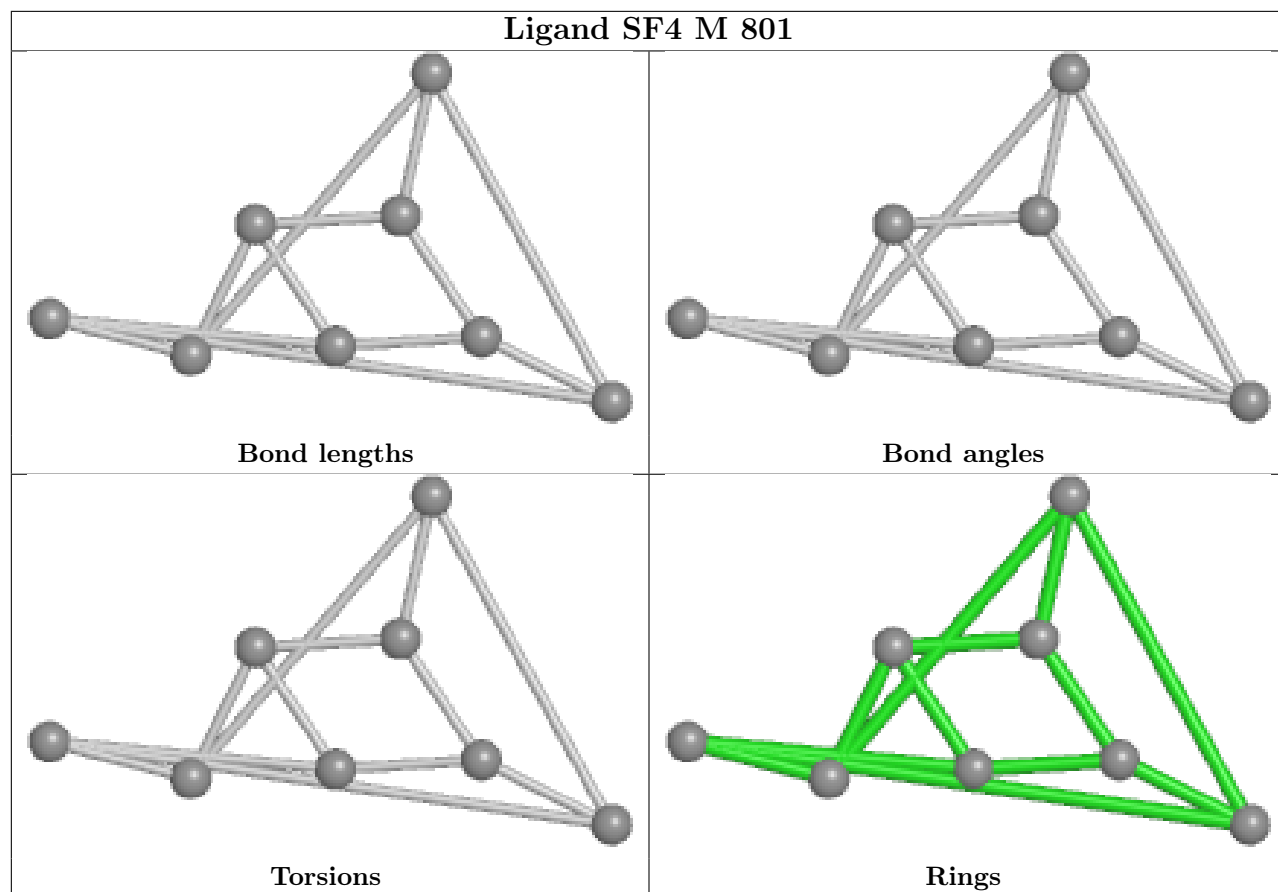
No monomer is involved in short contacts.

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

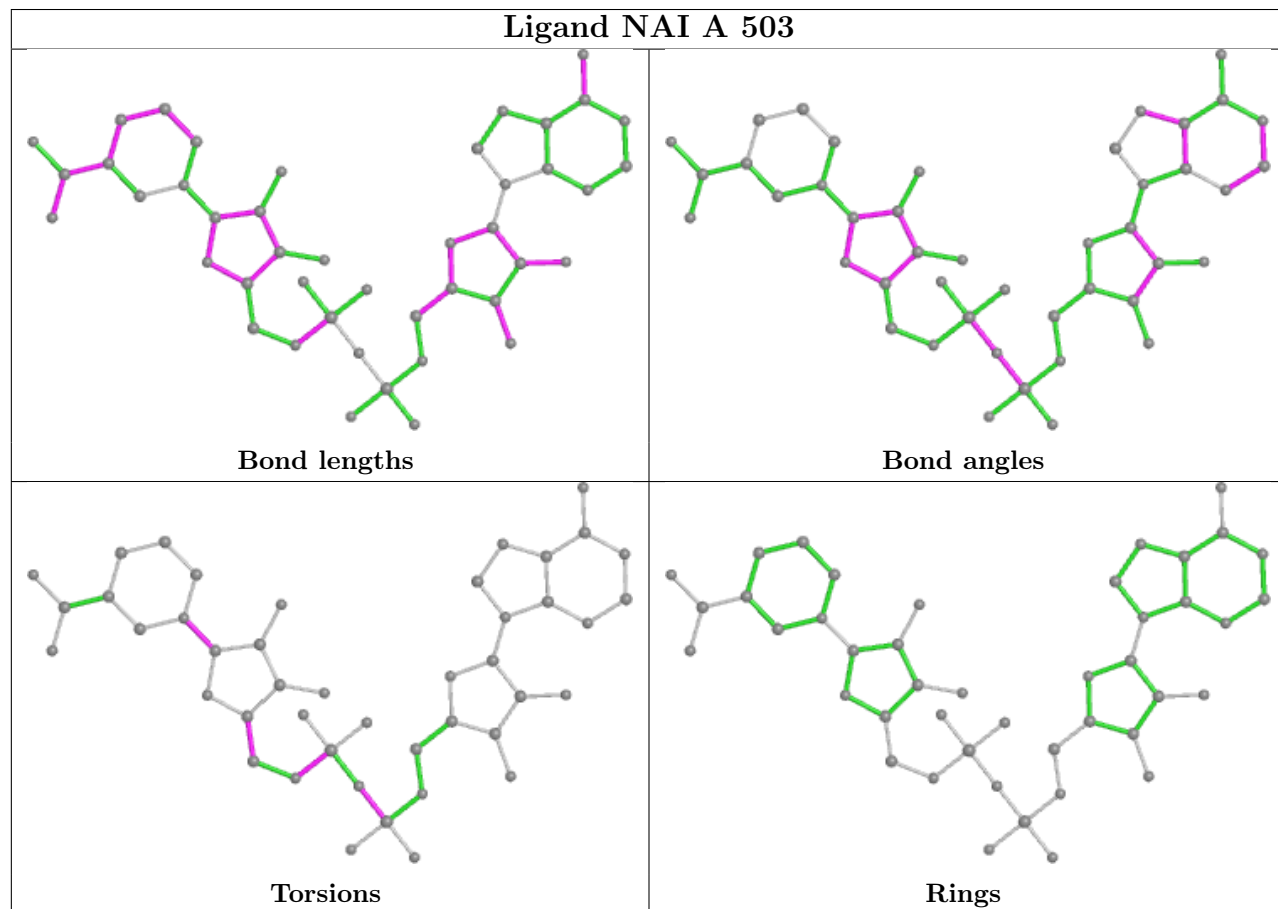


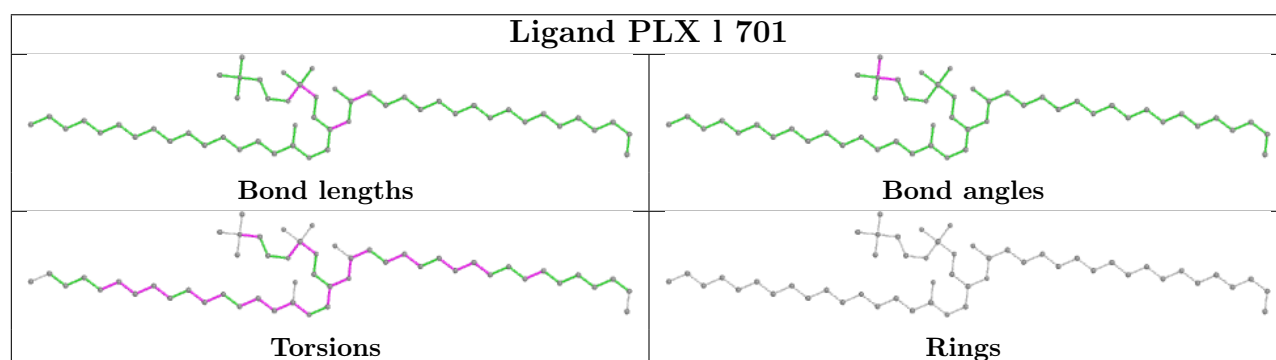
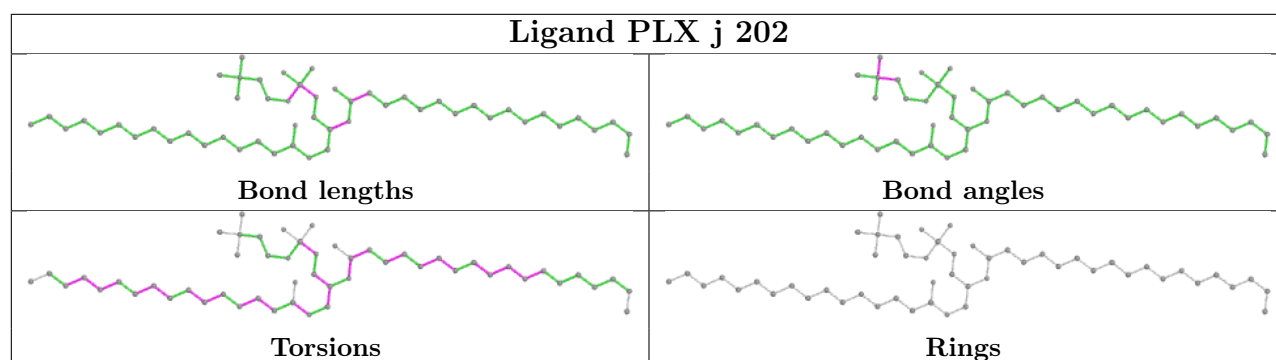
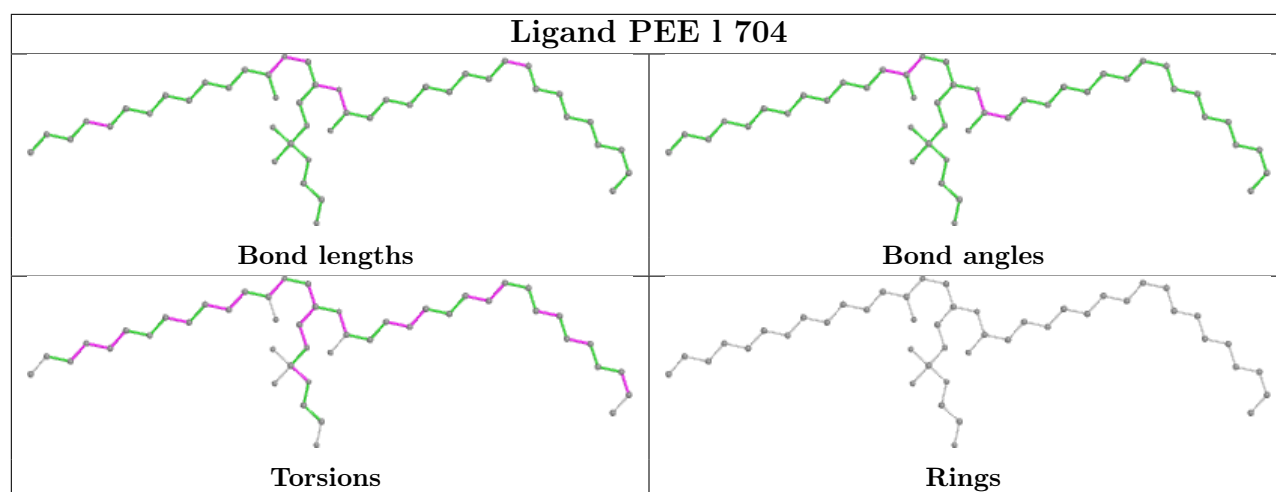


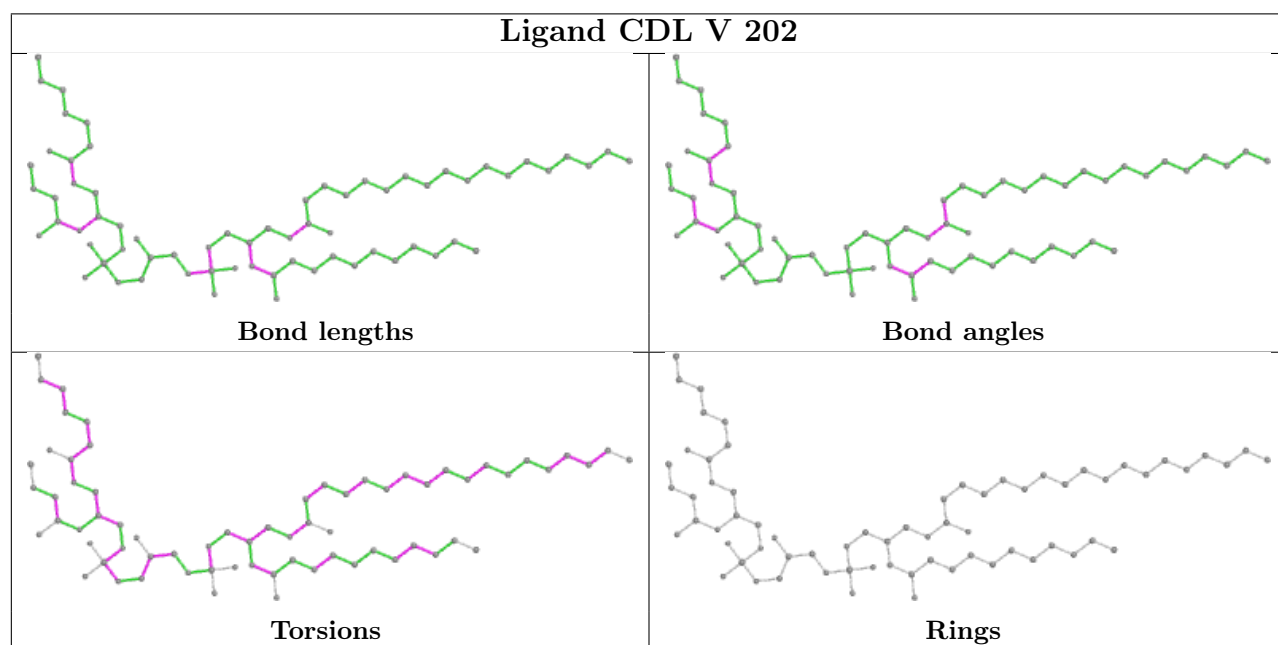
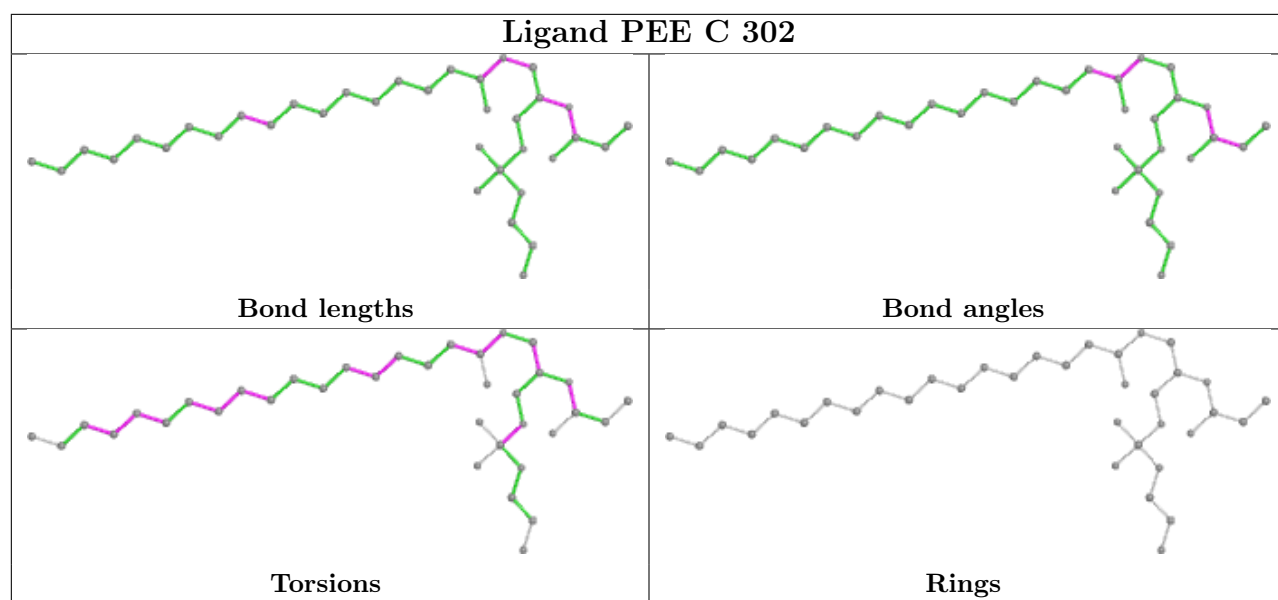
Ligand SF4 M 801

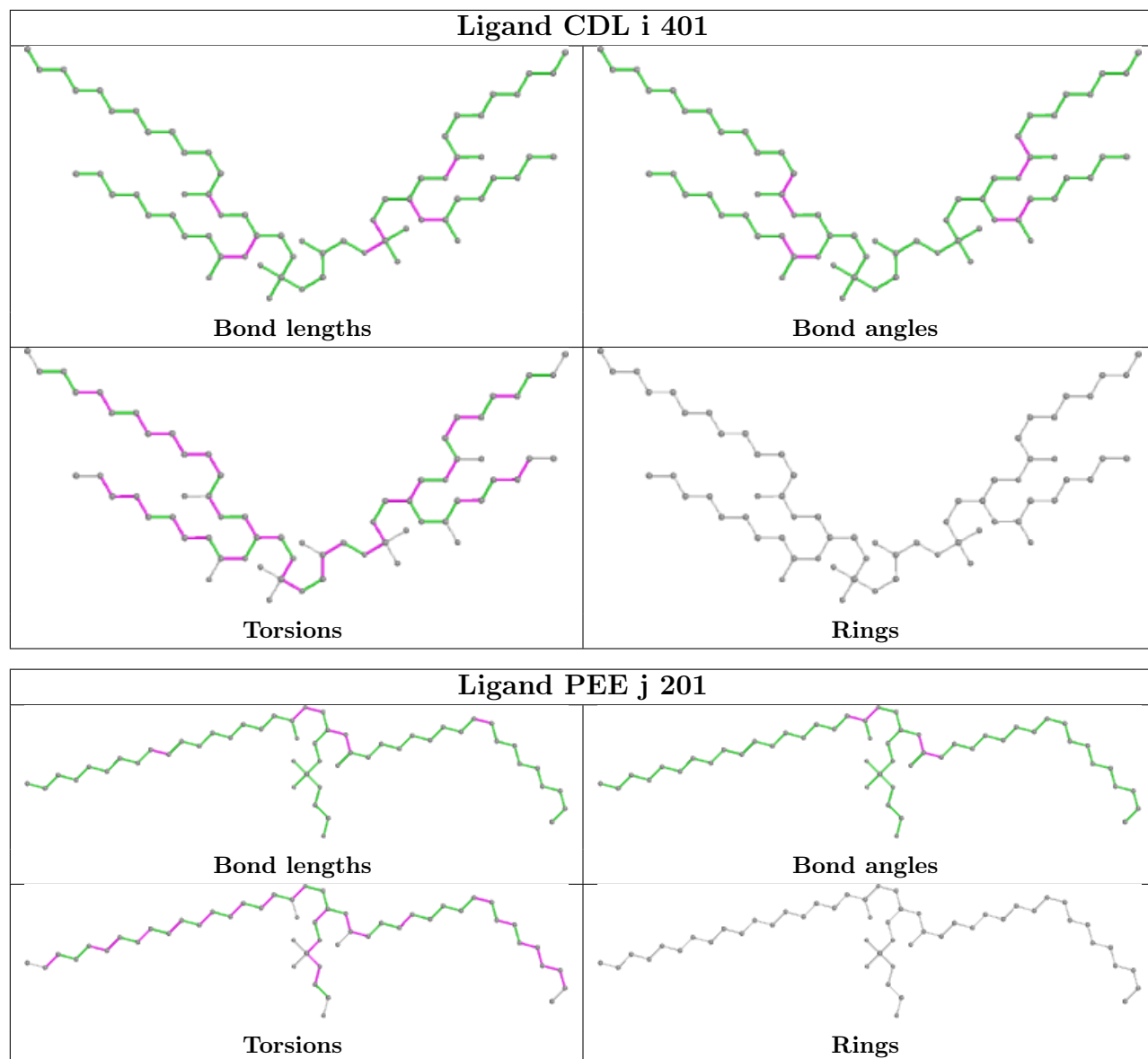


Ligand NAI A 503

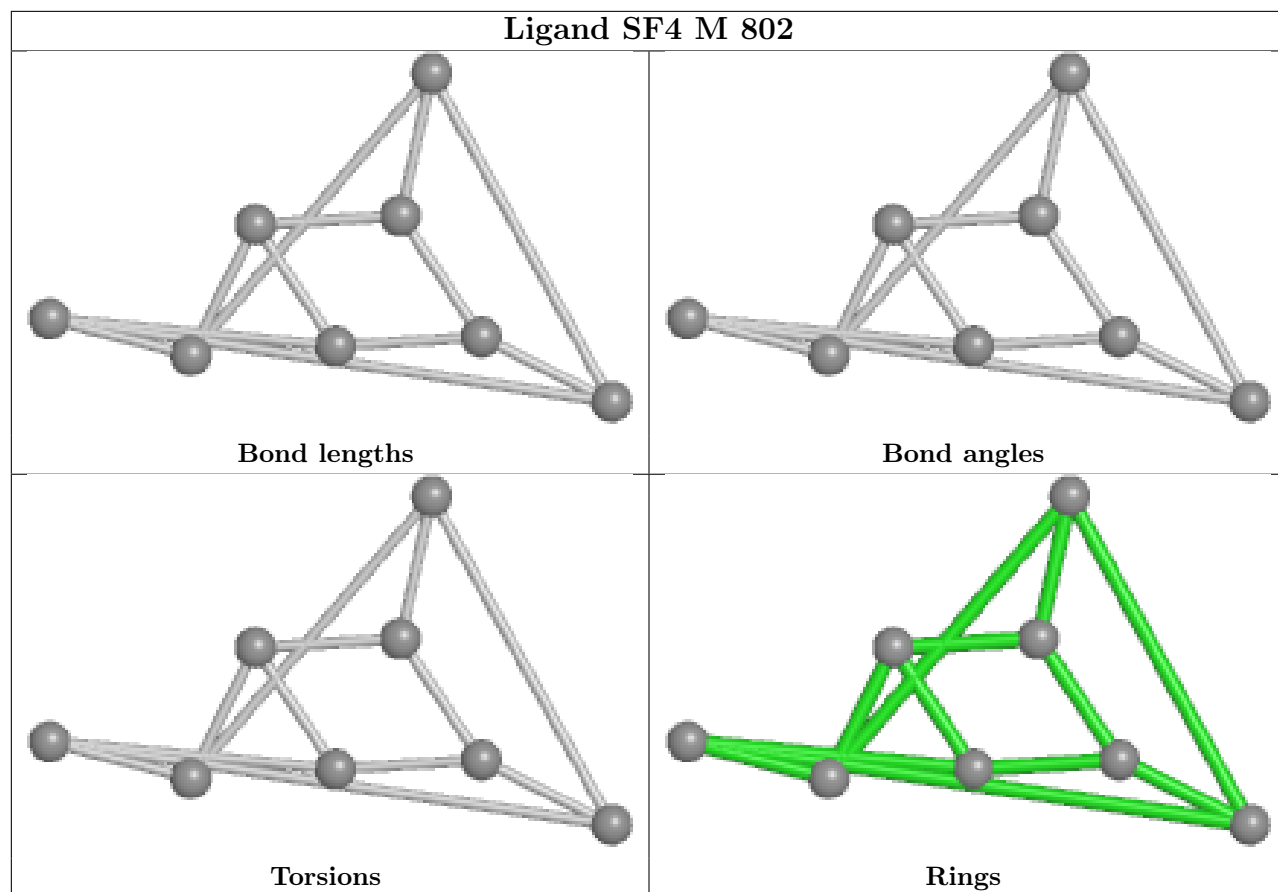




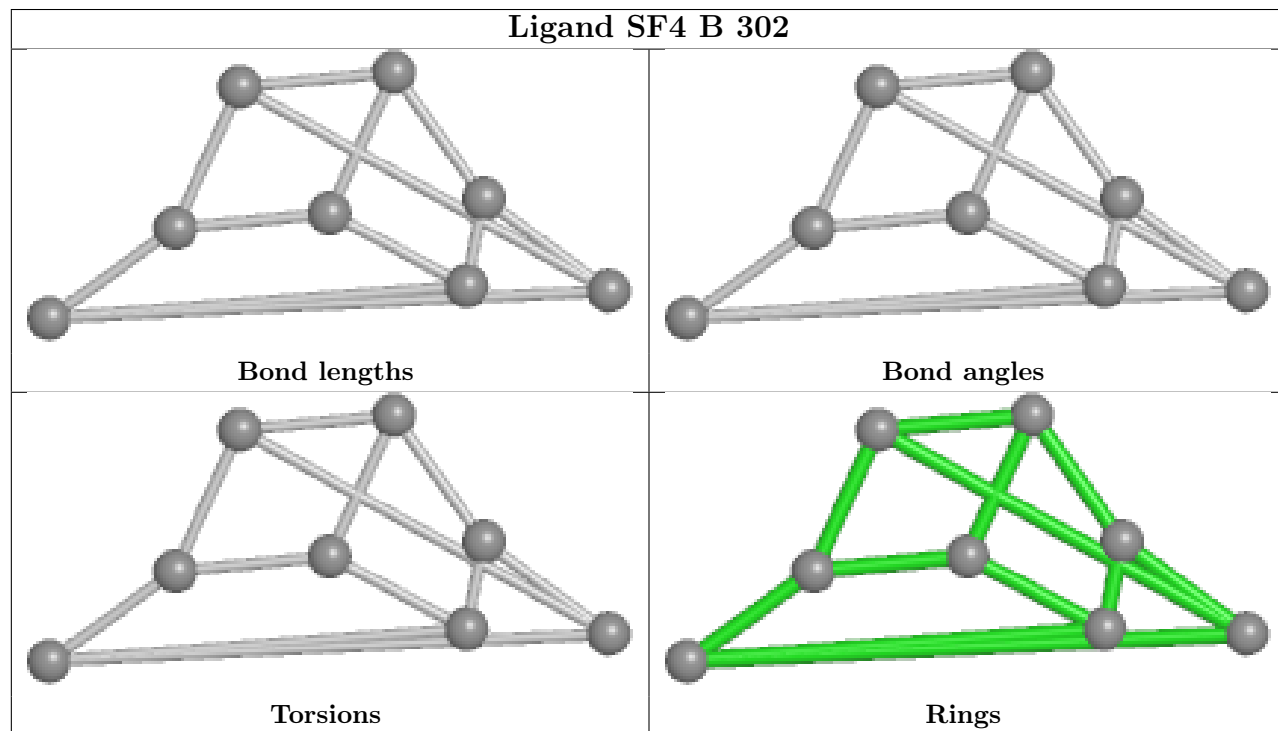


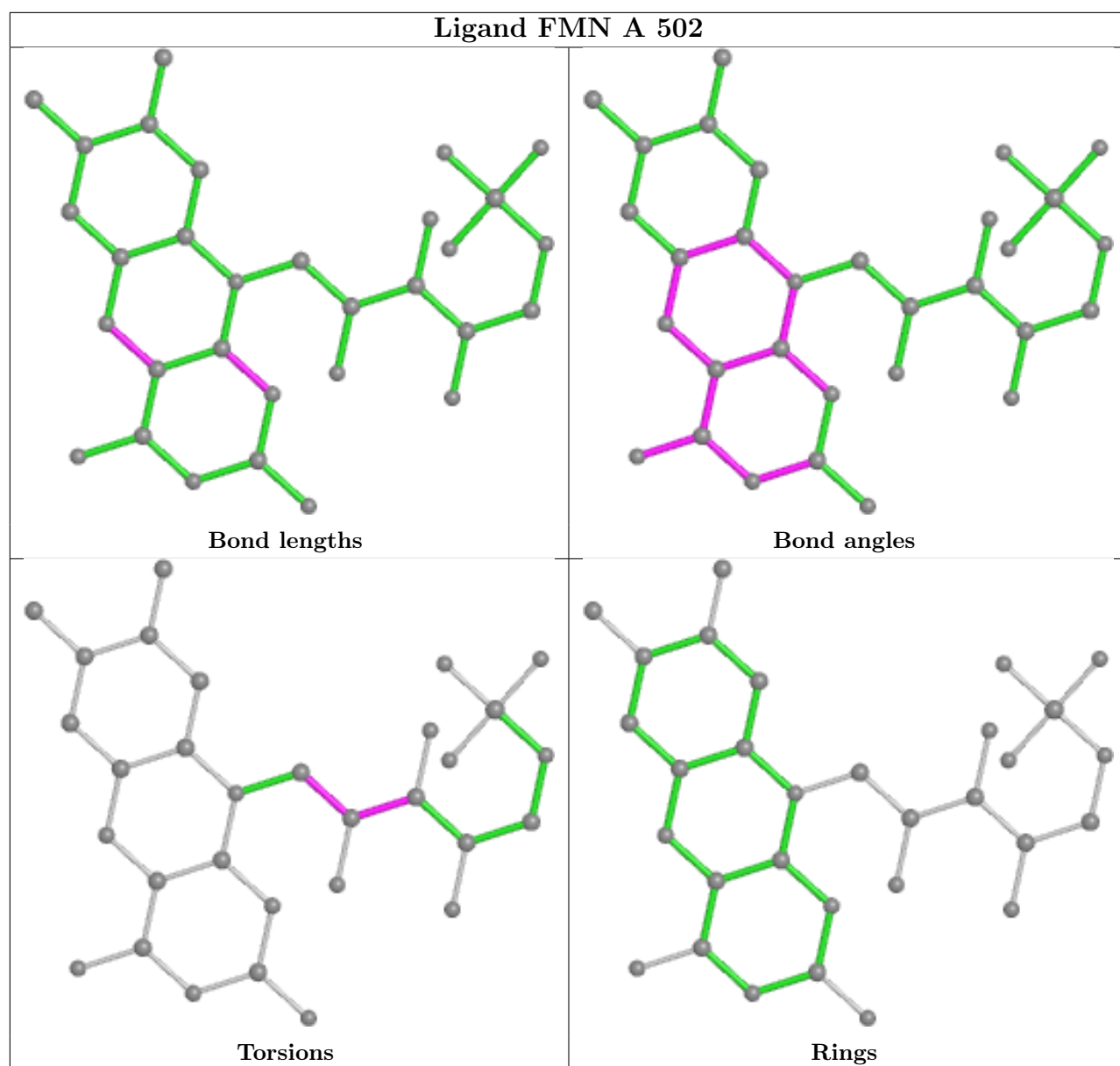


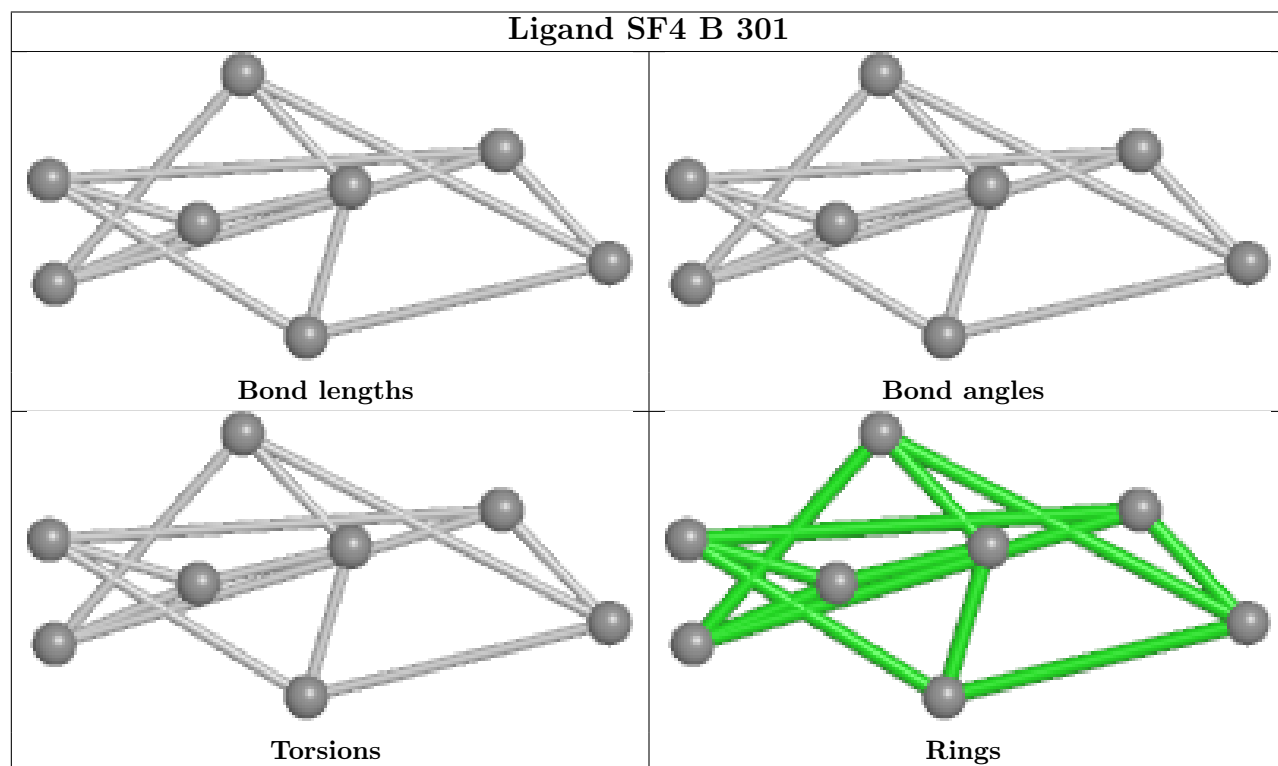
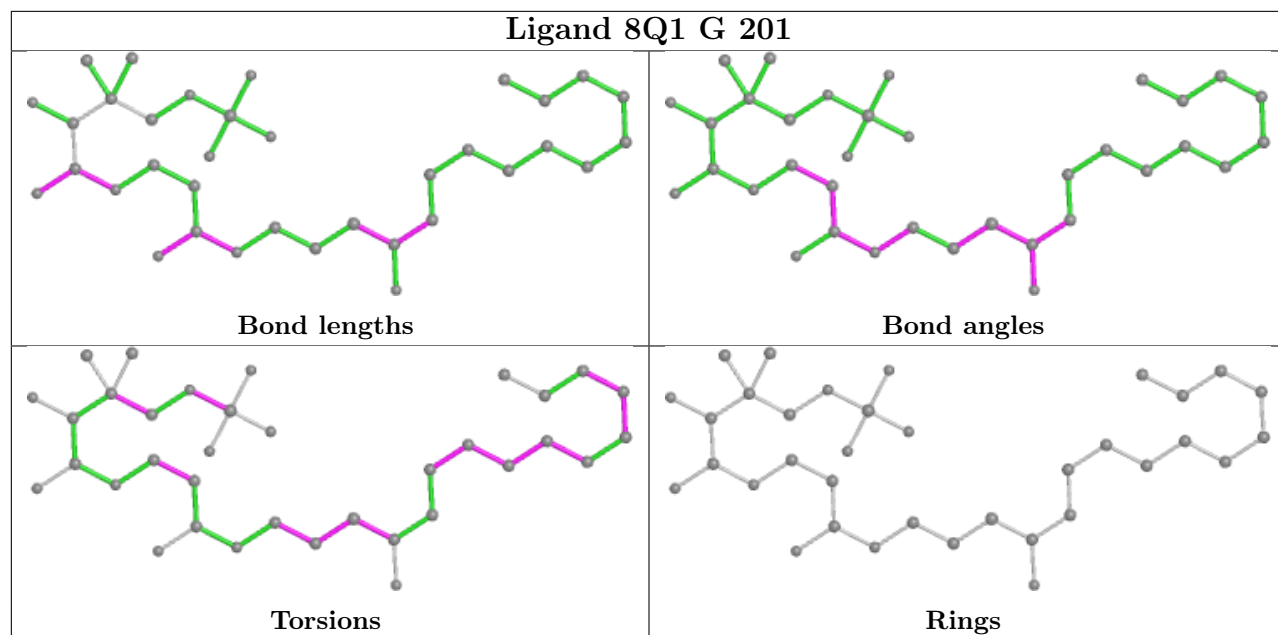
Ligand SF4 M 802



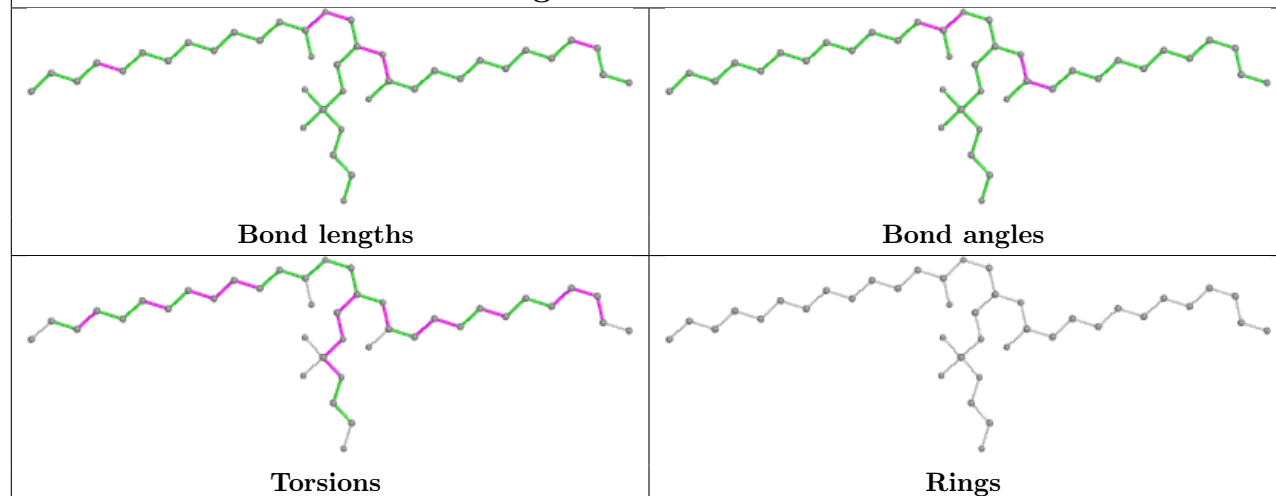
Ligand SF4 B 302



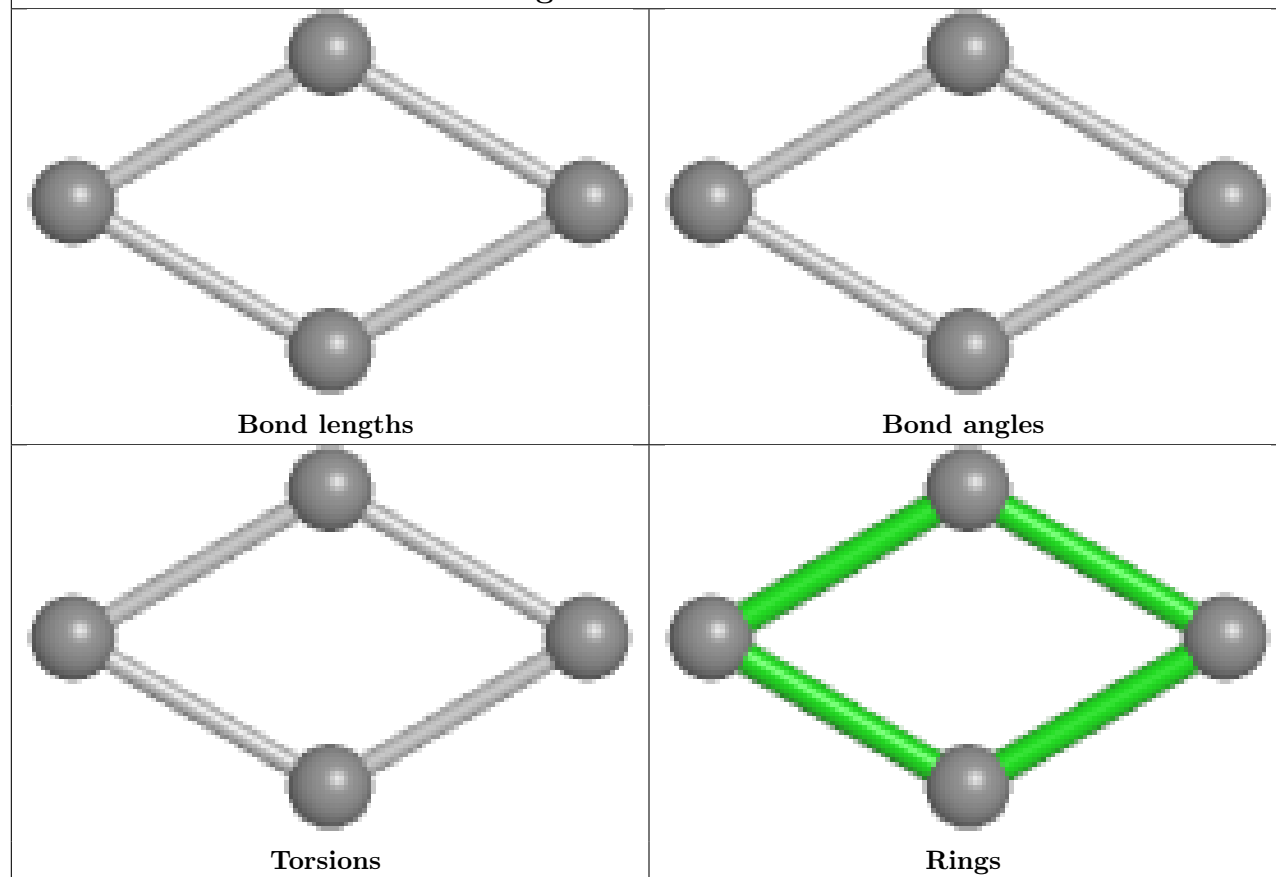


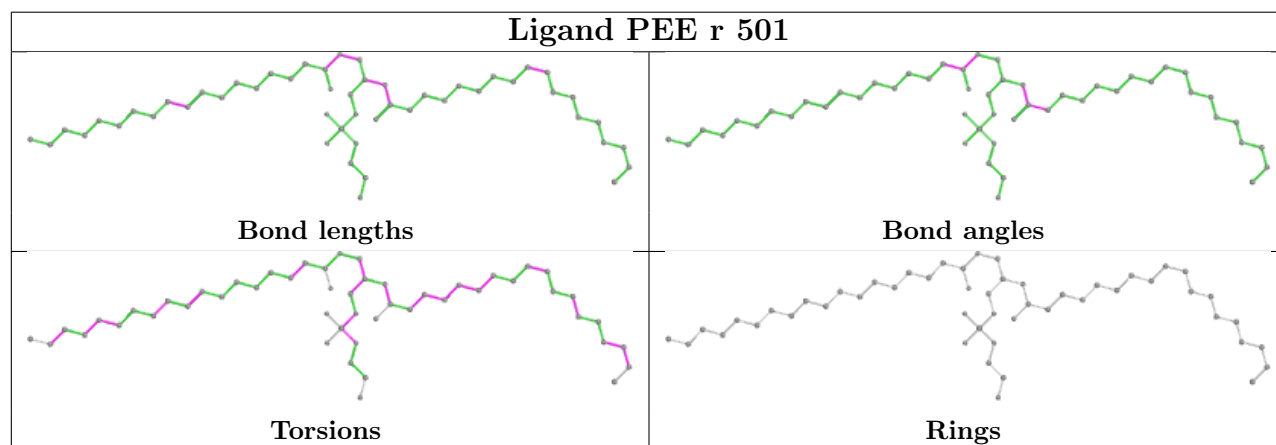
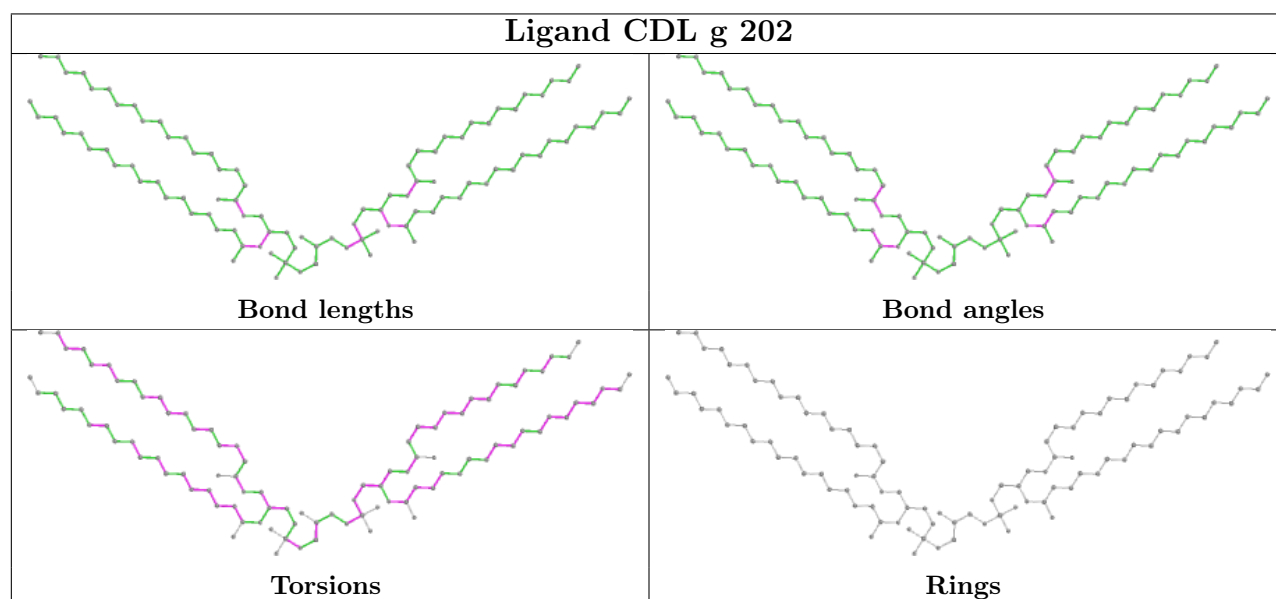
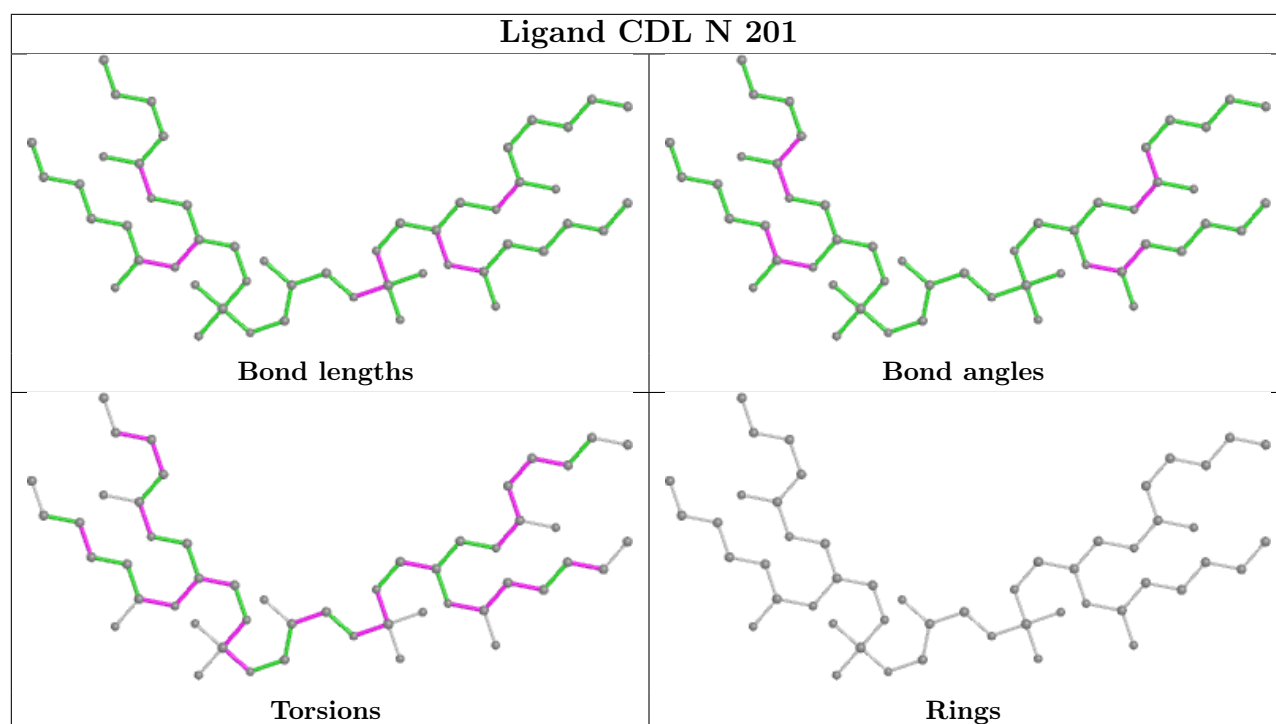


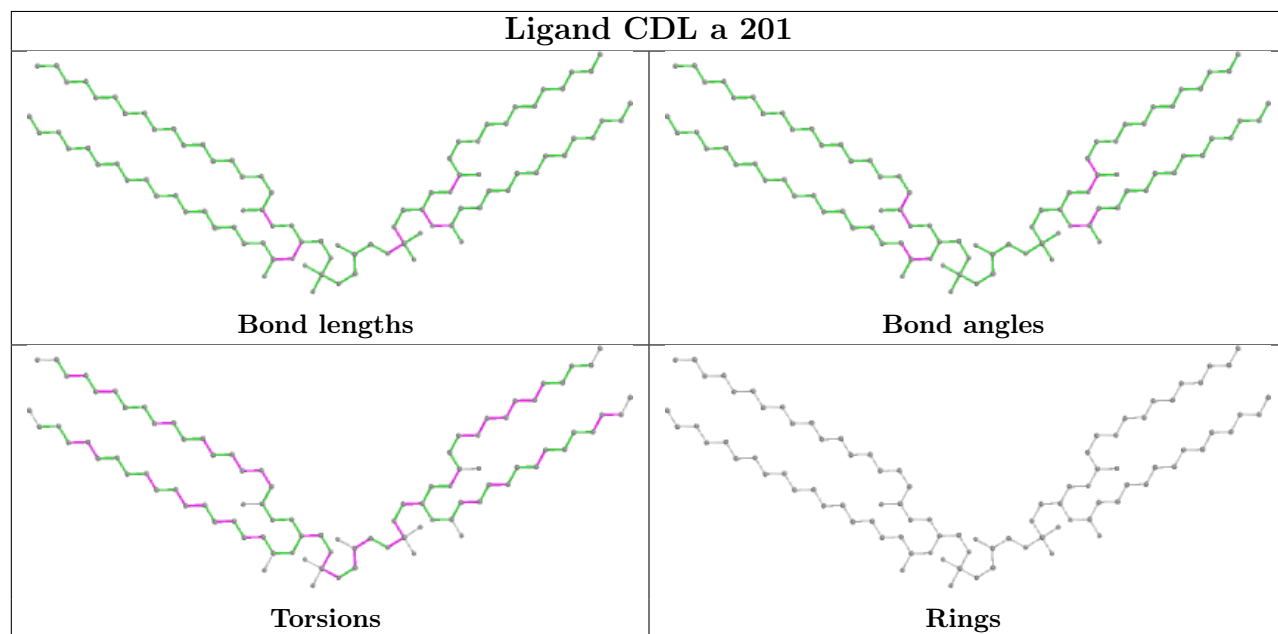
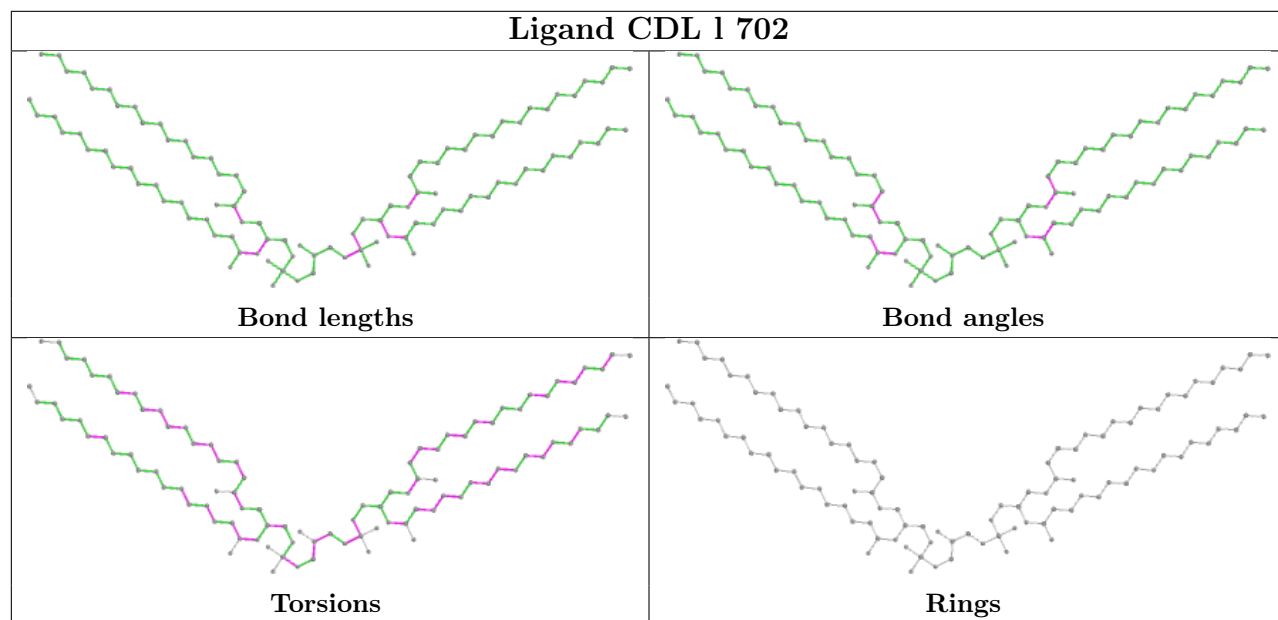
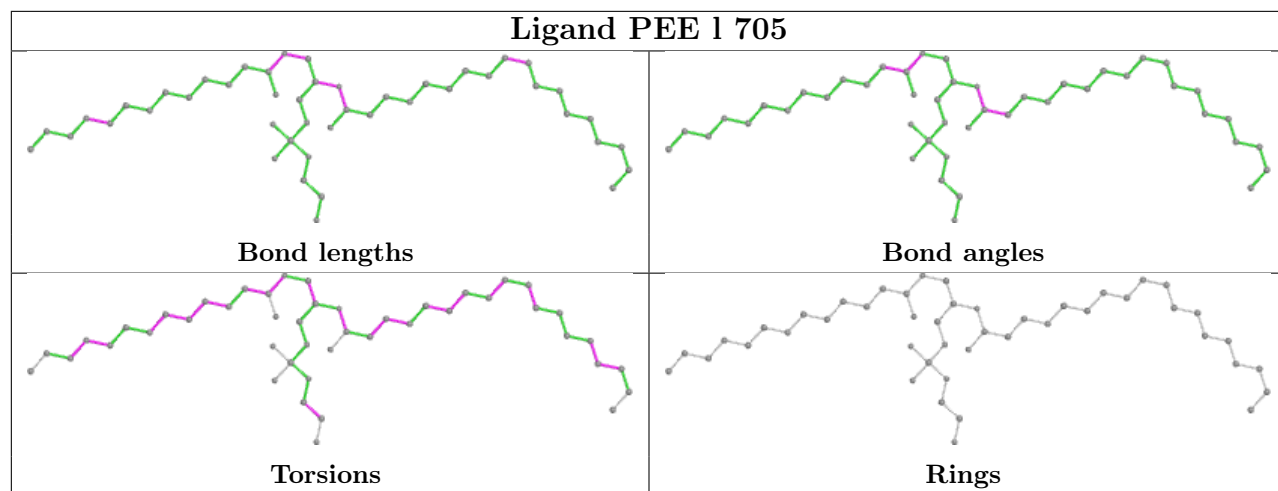
Ligand PEE V 203

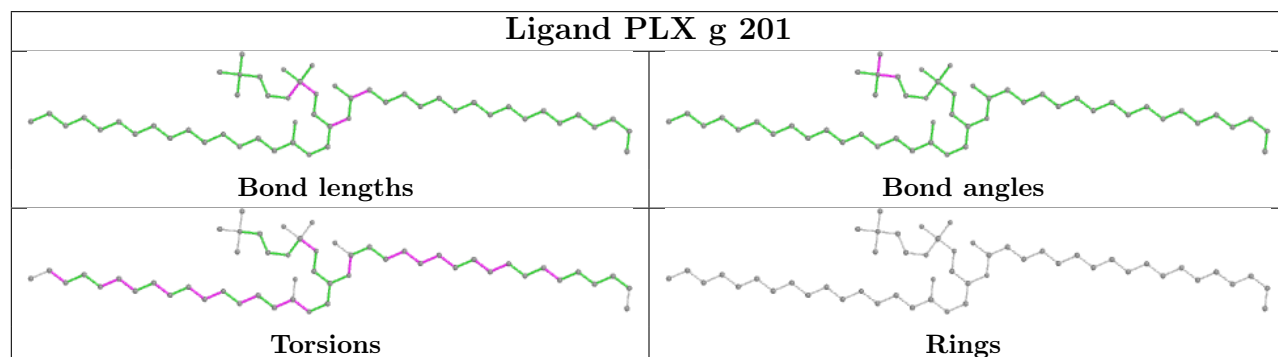
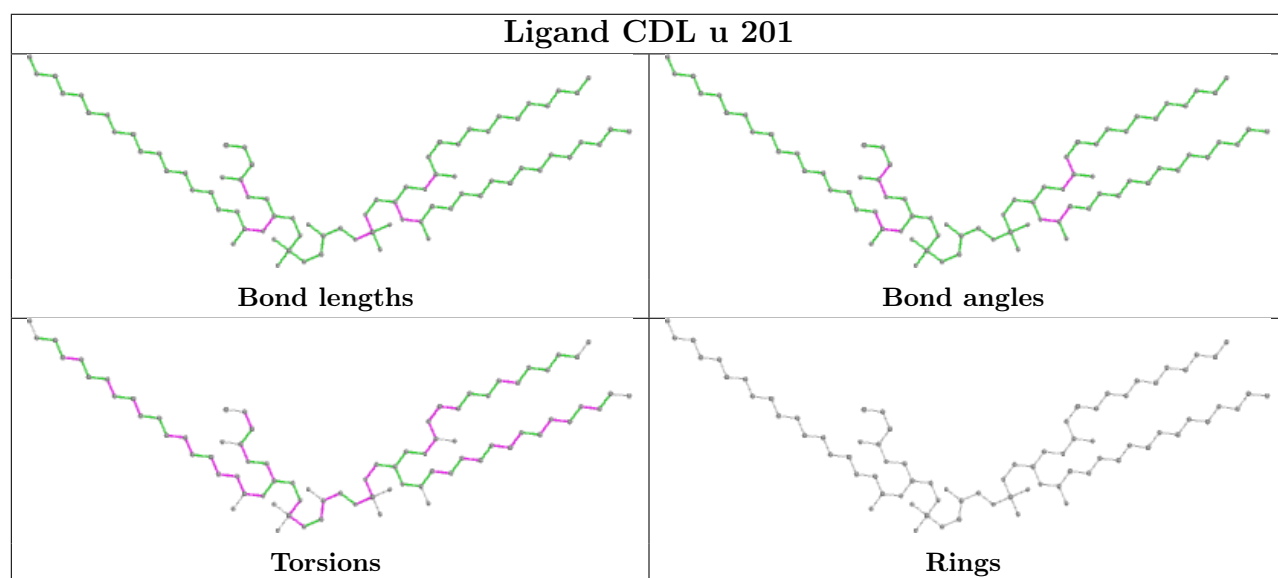
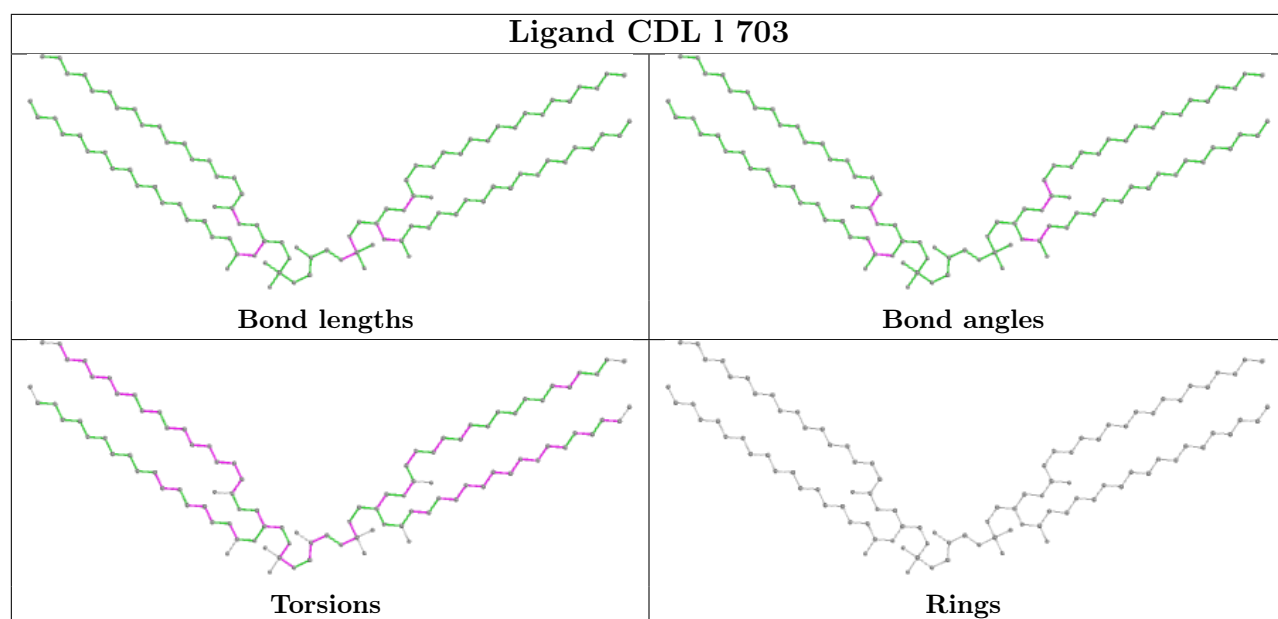


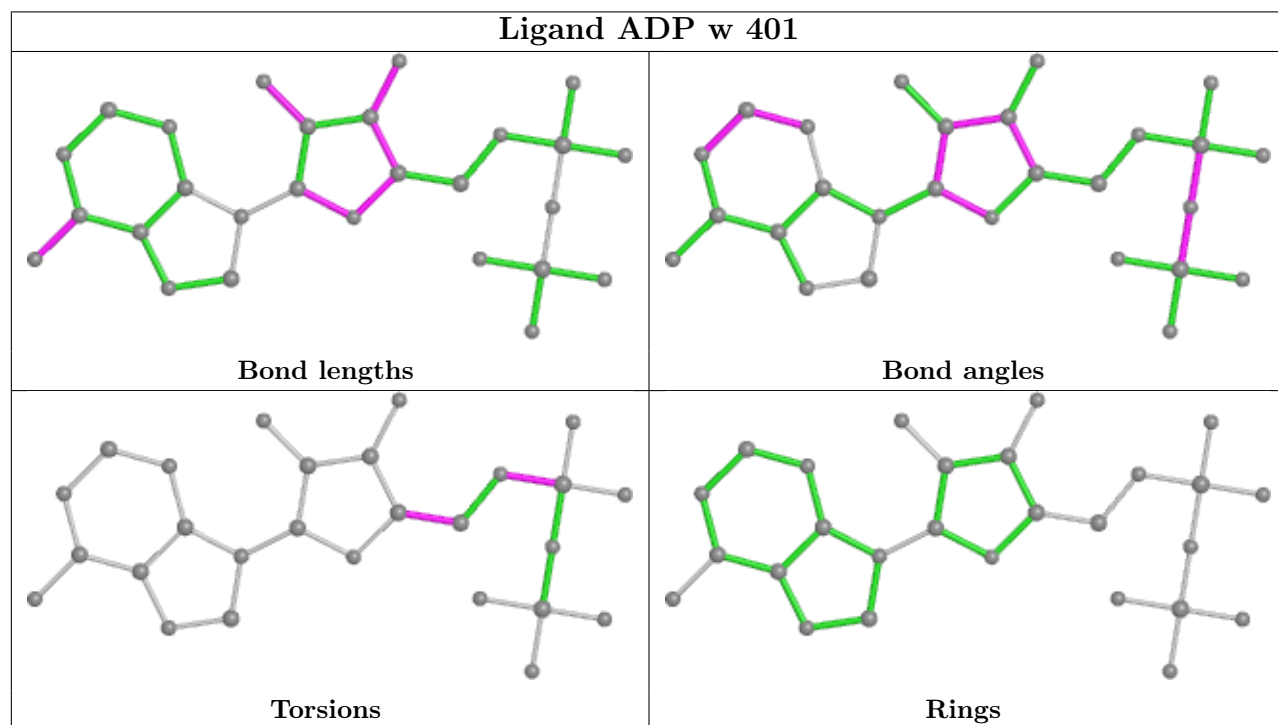
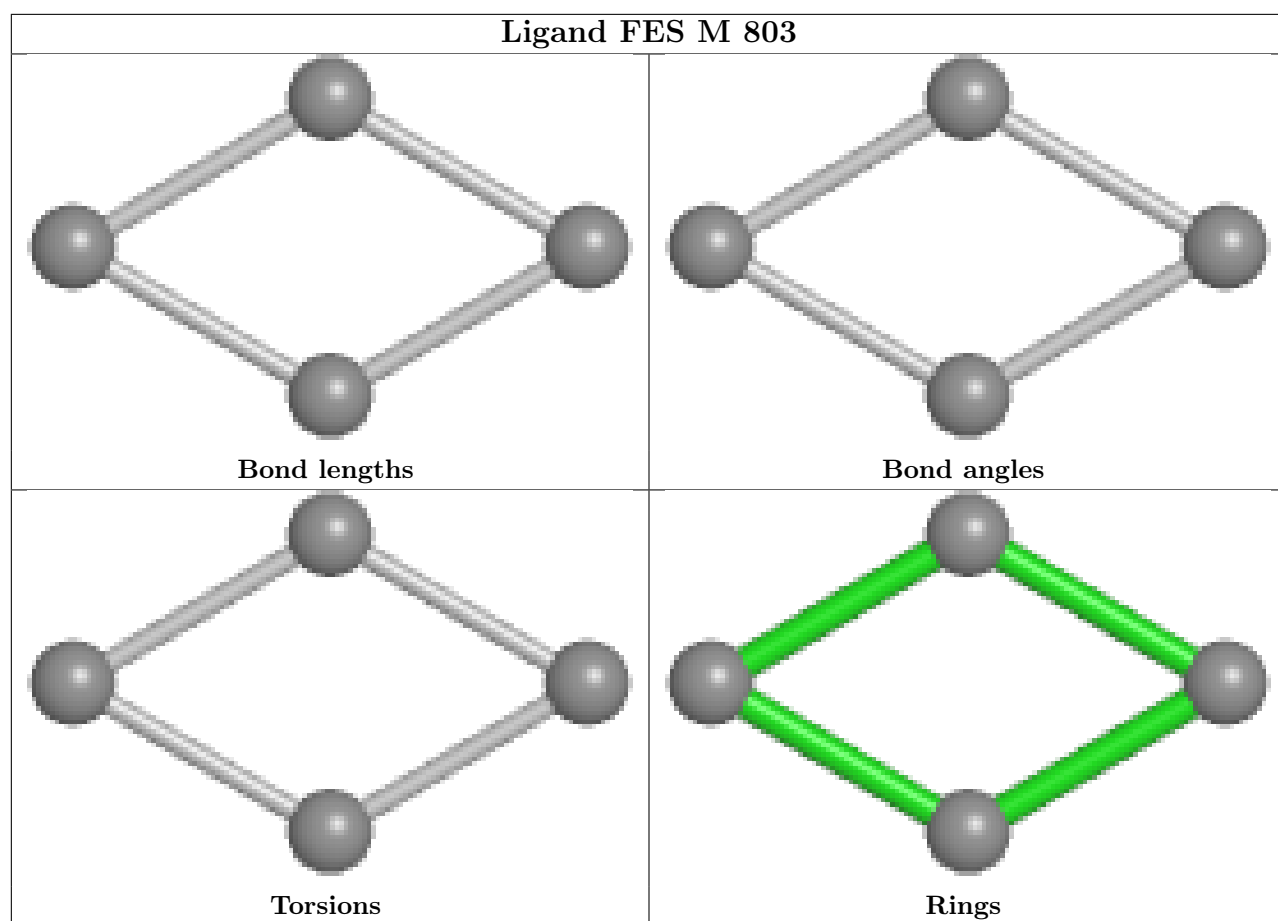
Ligand FES O 301

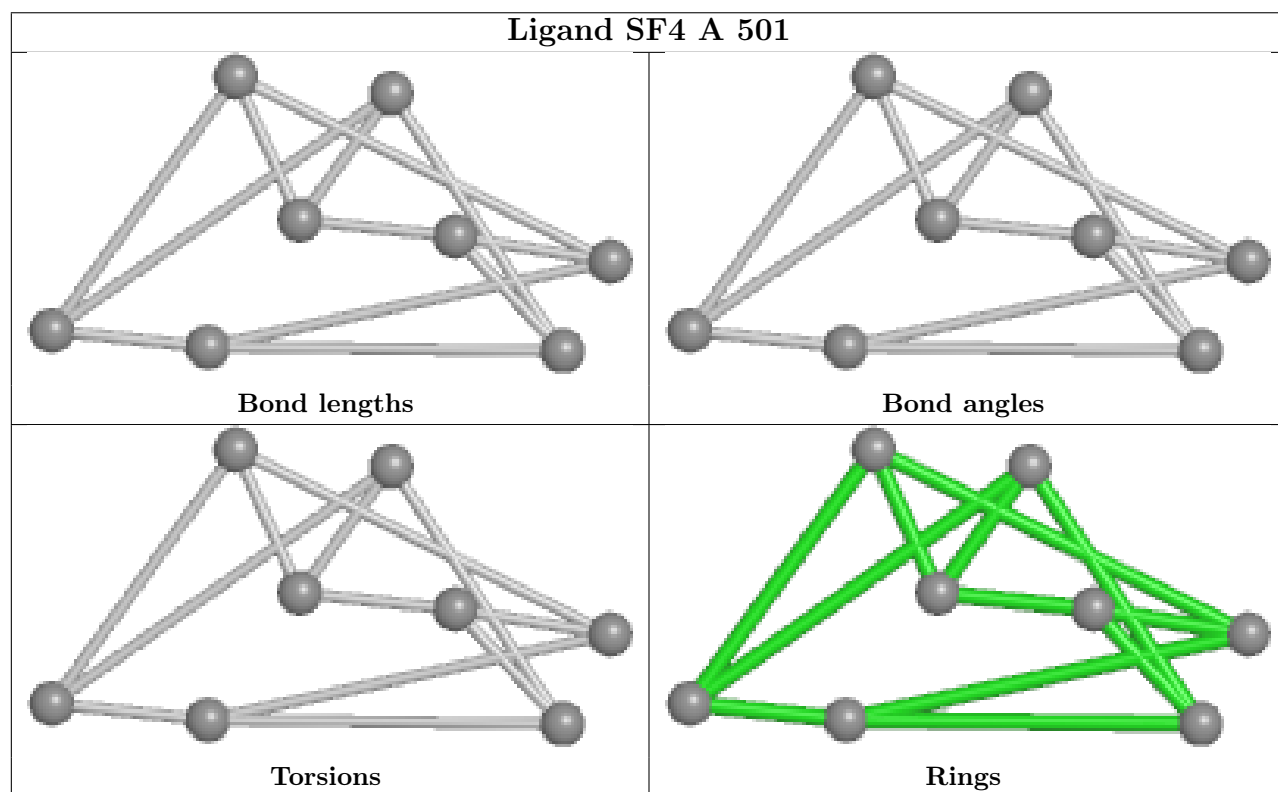
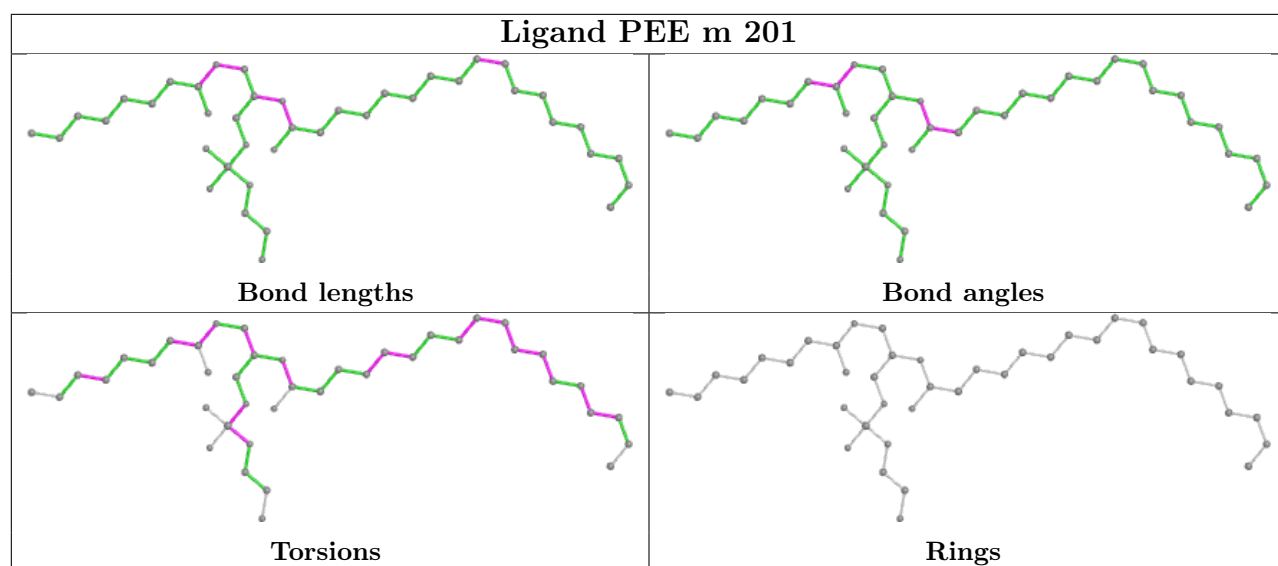




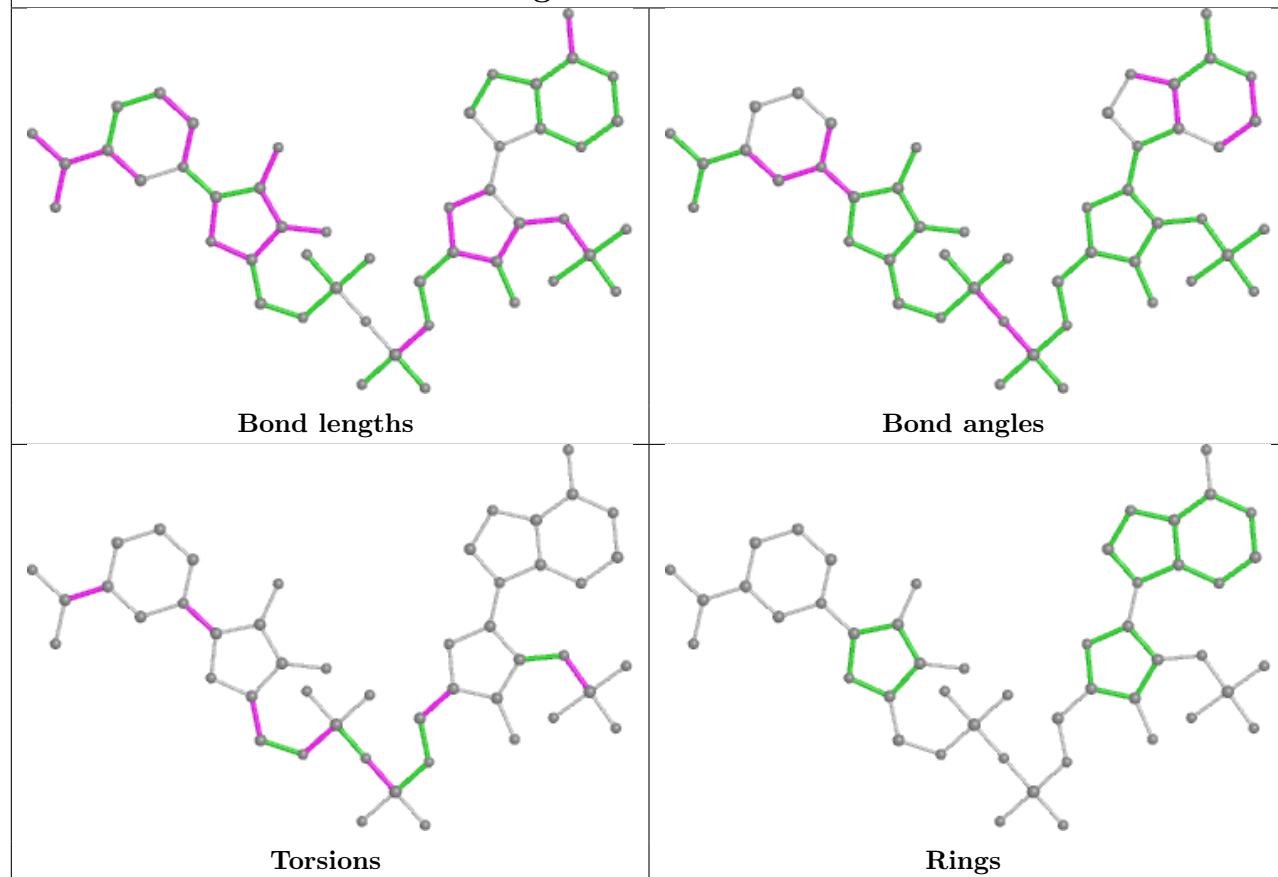




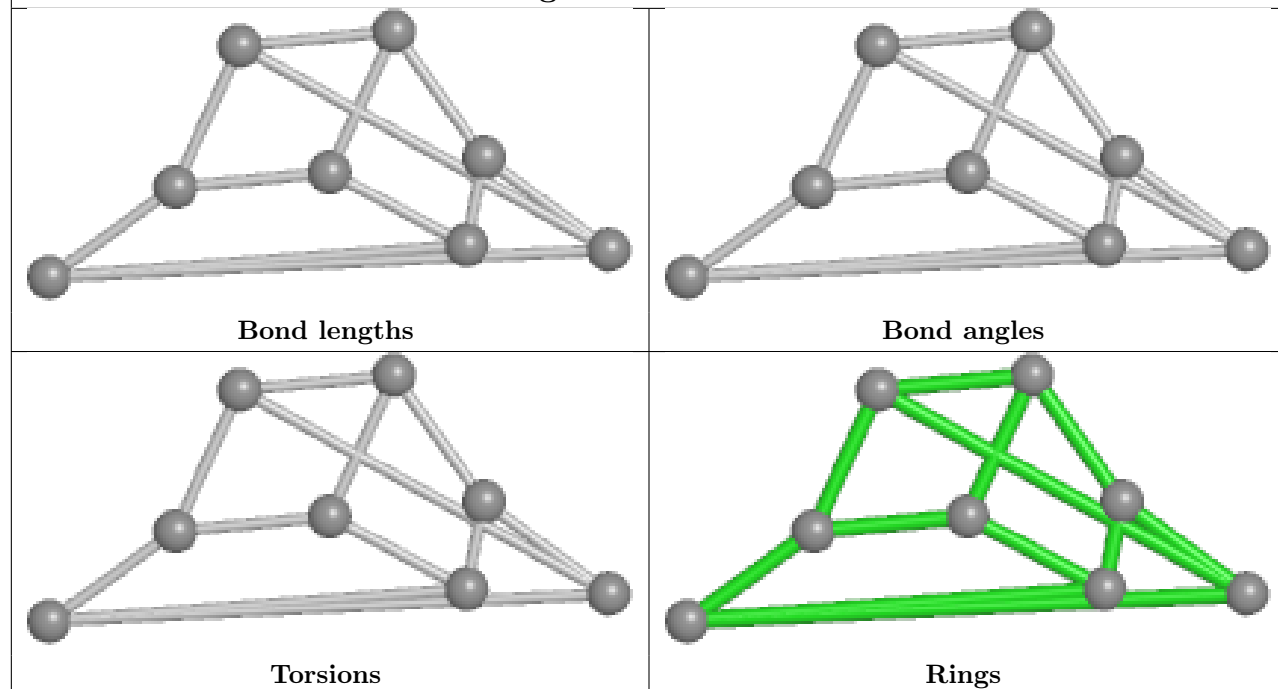


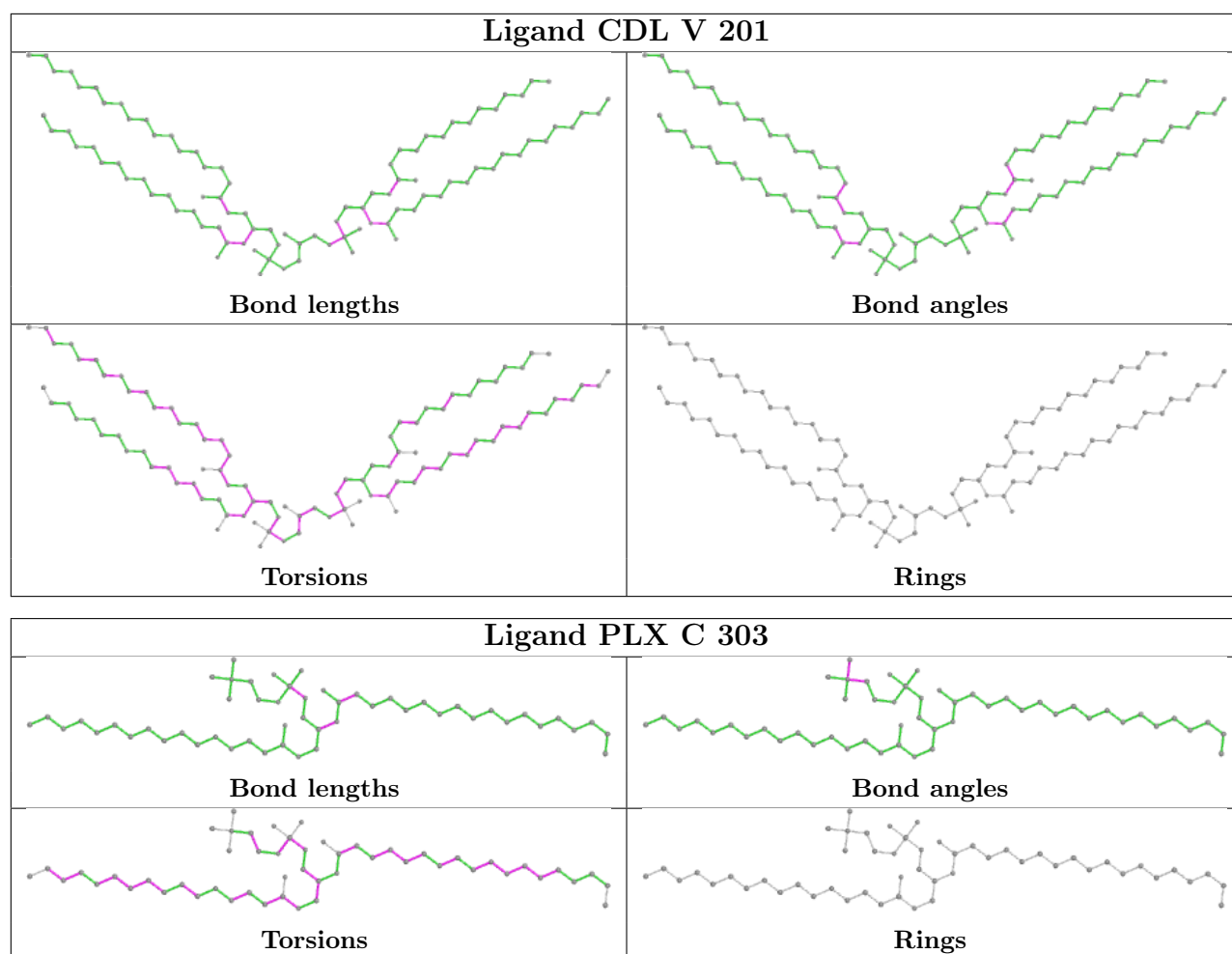


Ligand NDP J 401



Ligand SF4 C 301





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.

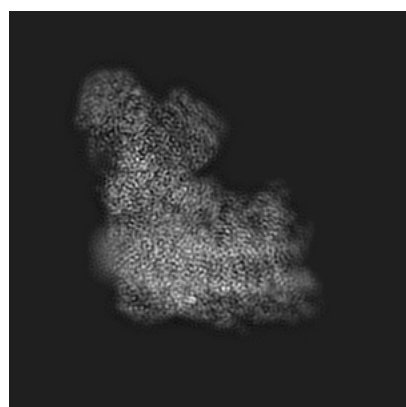
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32254. These allow visual inspection of the internal detail of the map and identification of artifacts.

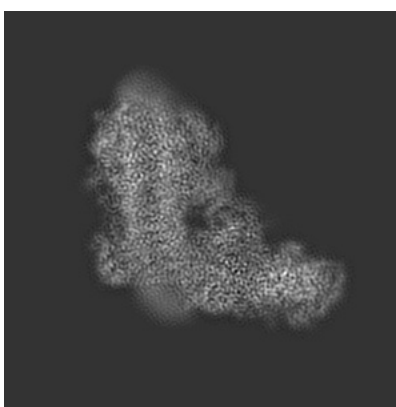
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

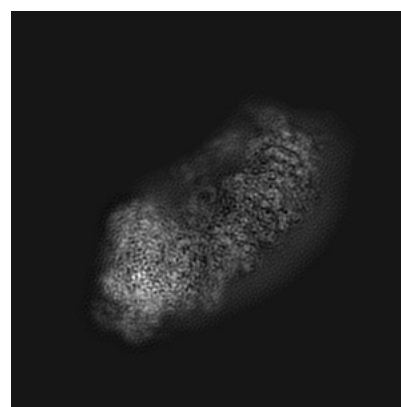
6.1.1 Primary map



X



Y

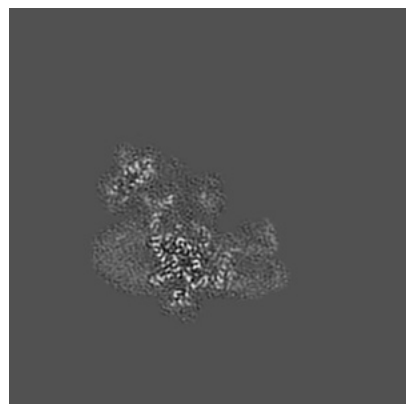


Z

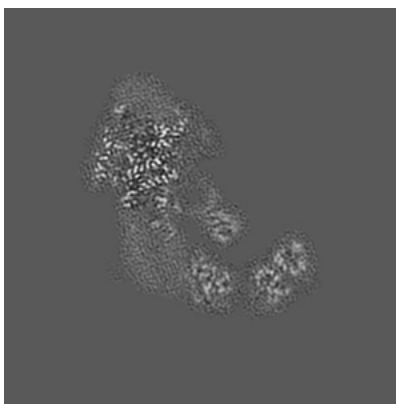
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

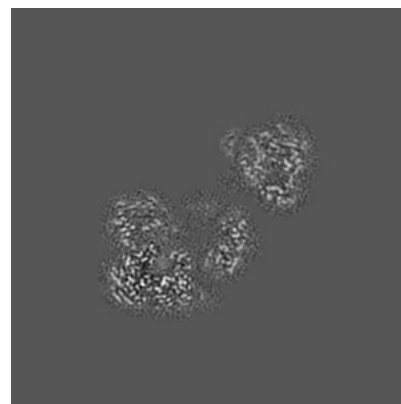
6.2.1 Primary map



X Index: 155



Y Index: 155

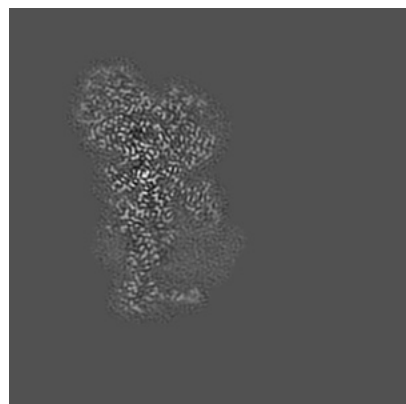


Z Index: 155

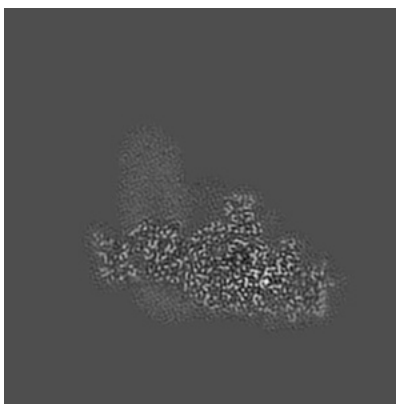
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

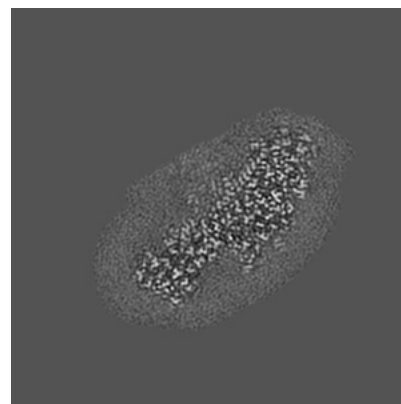
6.3.1 Primary map



X Index: 102



Y Index: 99

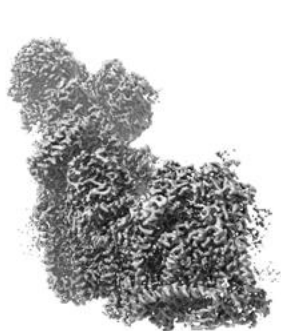


Z Index: 121

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0272. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

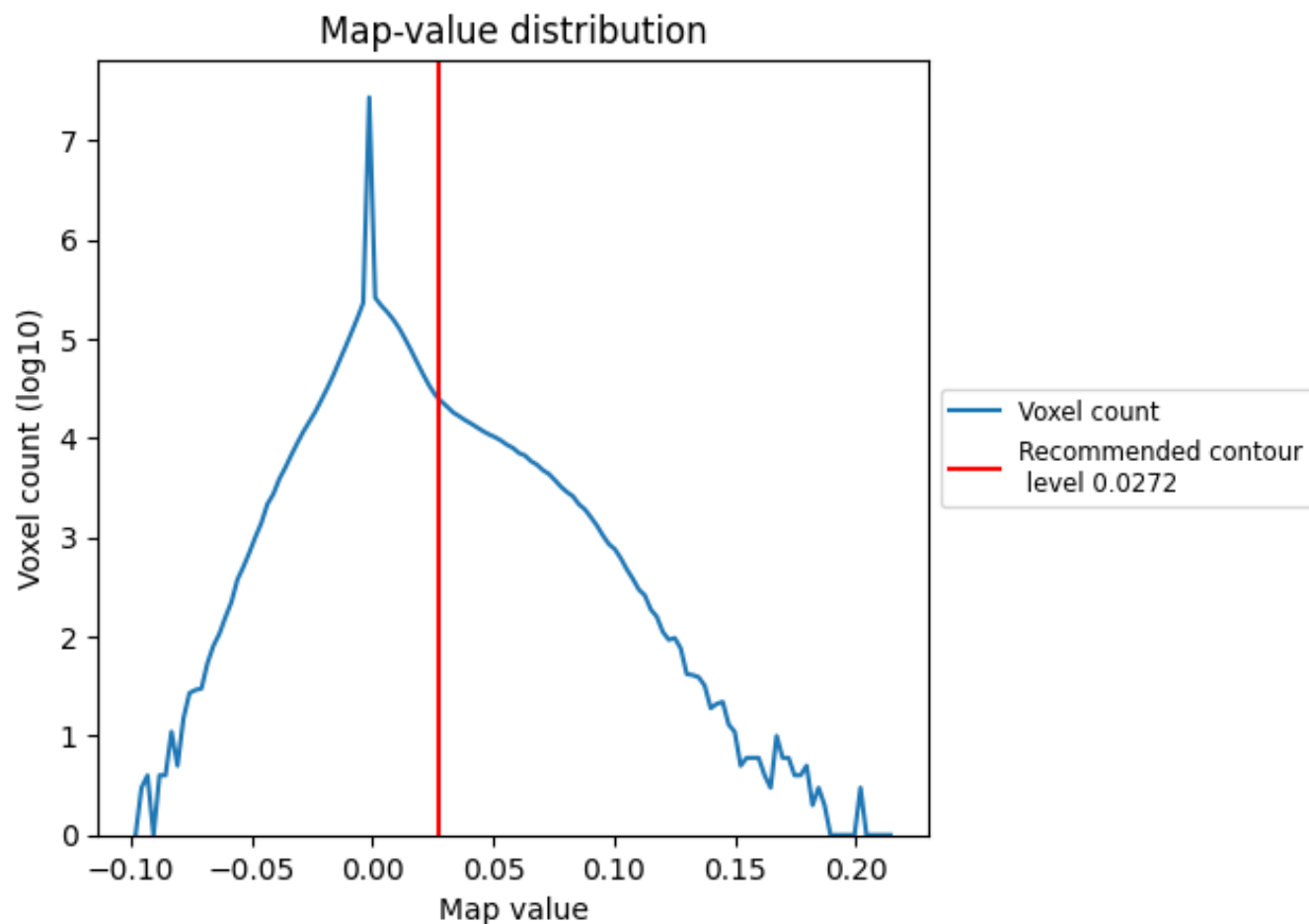
6.5 Mask visualisation

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

7 Map analysis [i](#)

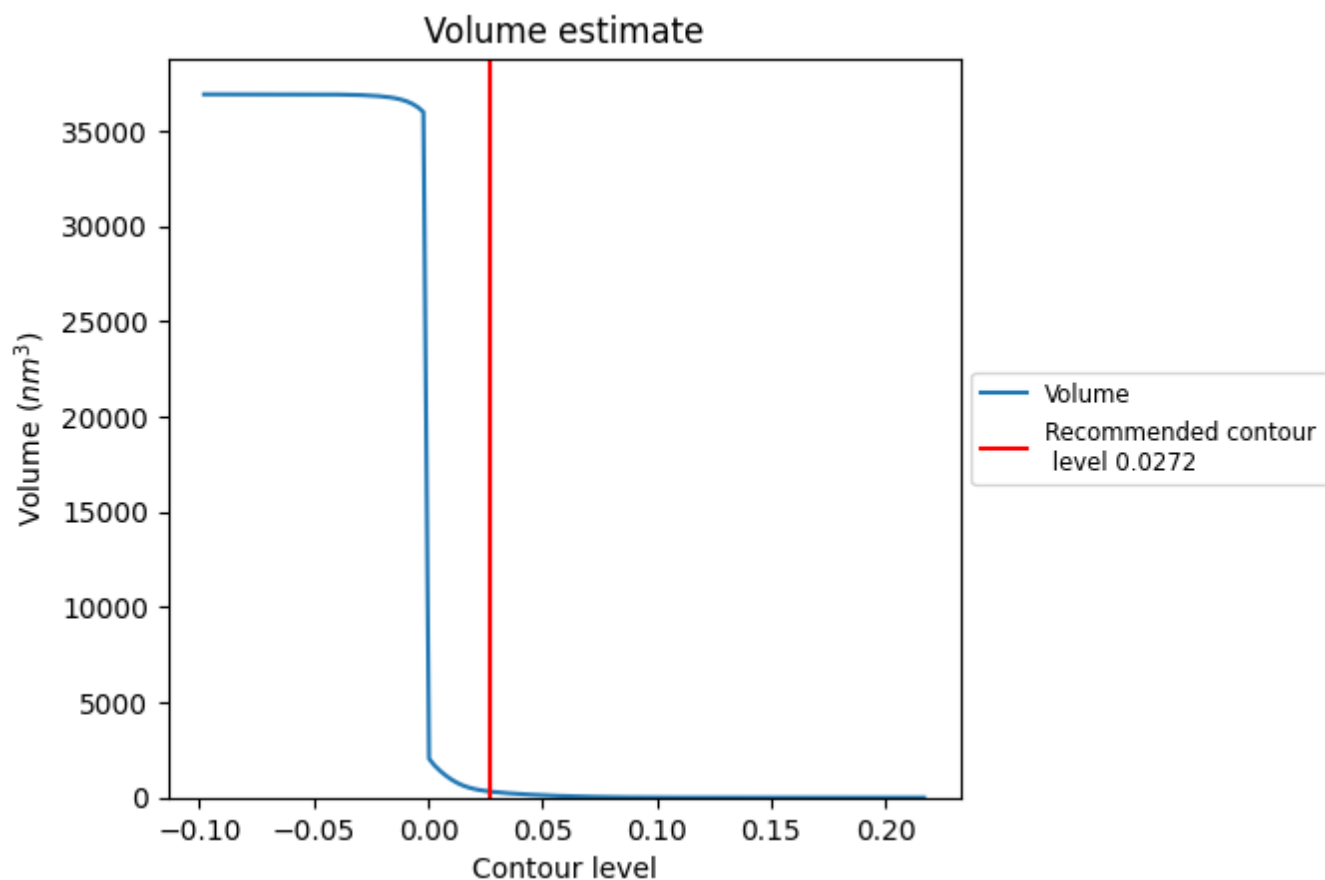
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

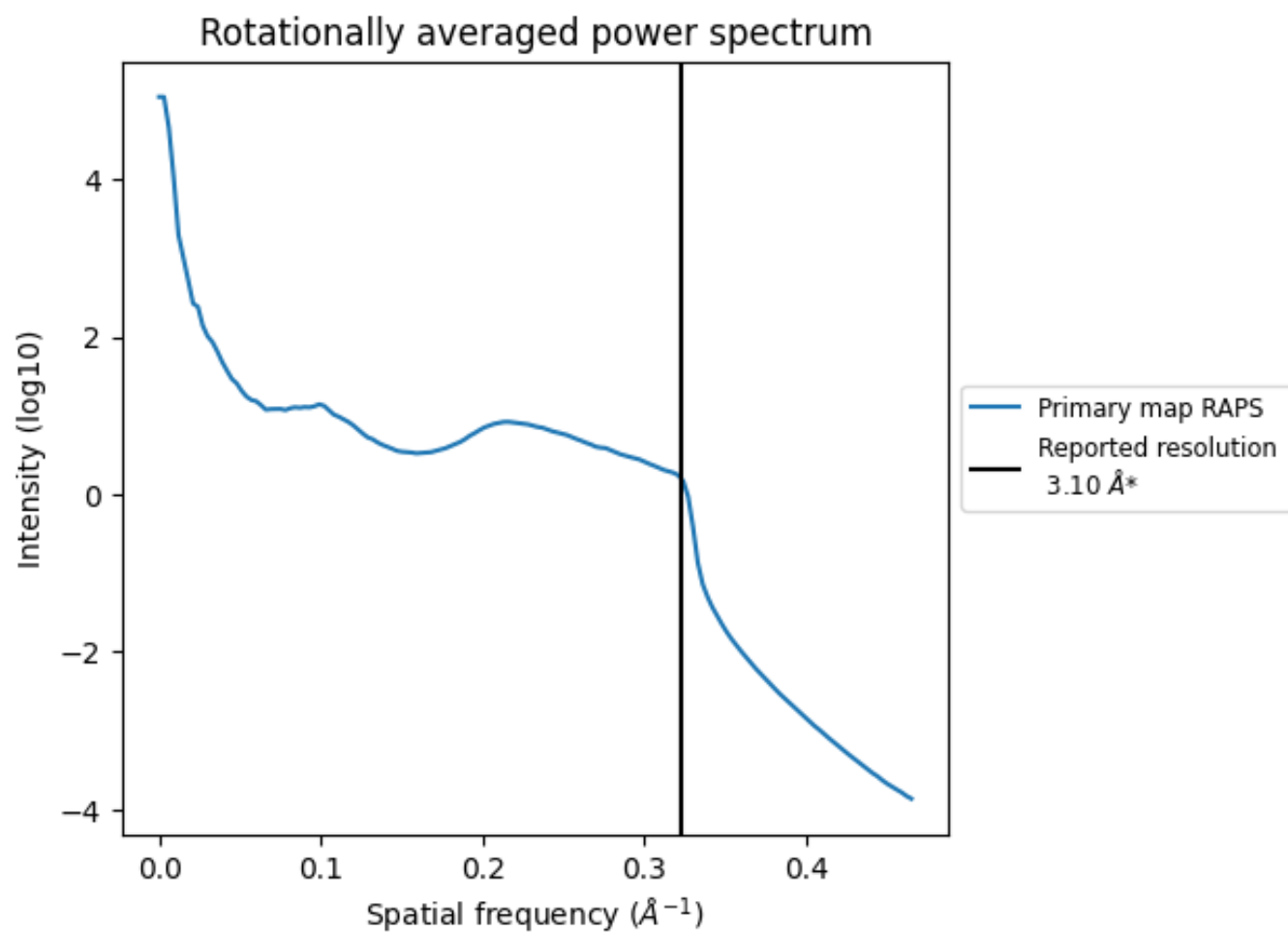
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; this corresponds to an approximate mass of 285 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

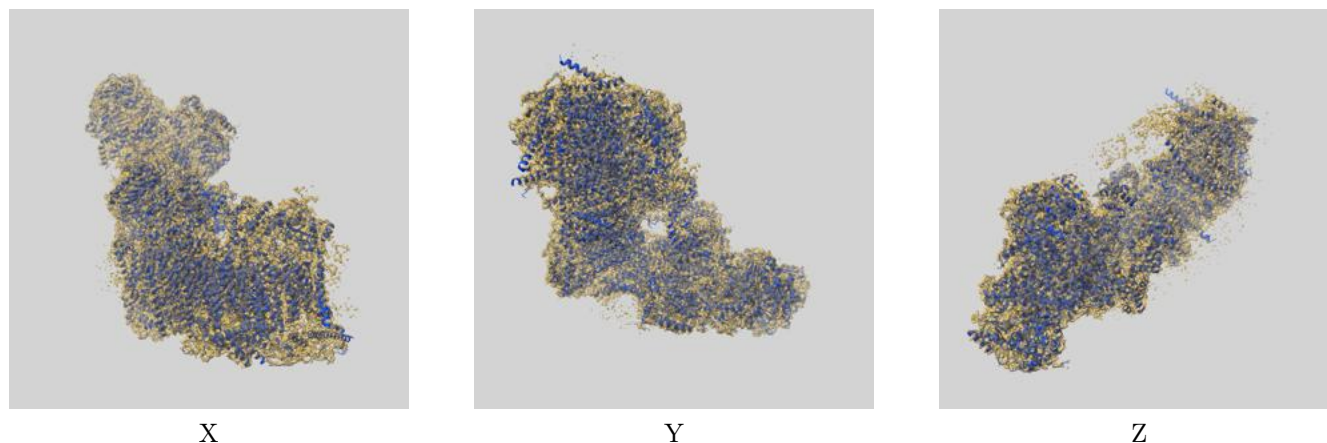
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

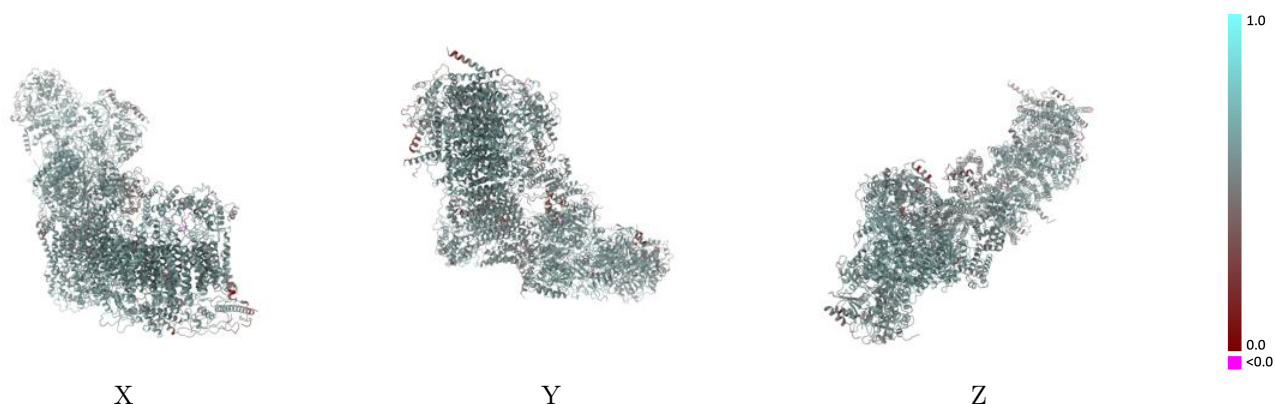
This section contains information regarding the fit between EMDB map EMD-32254 and PDB model 7W1P. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



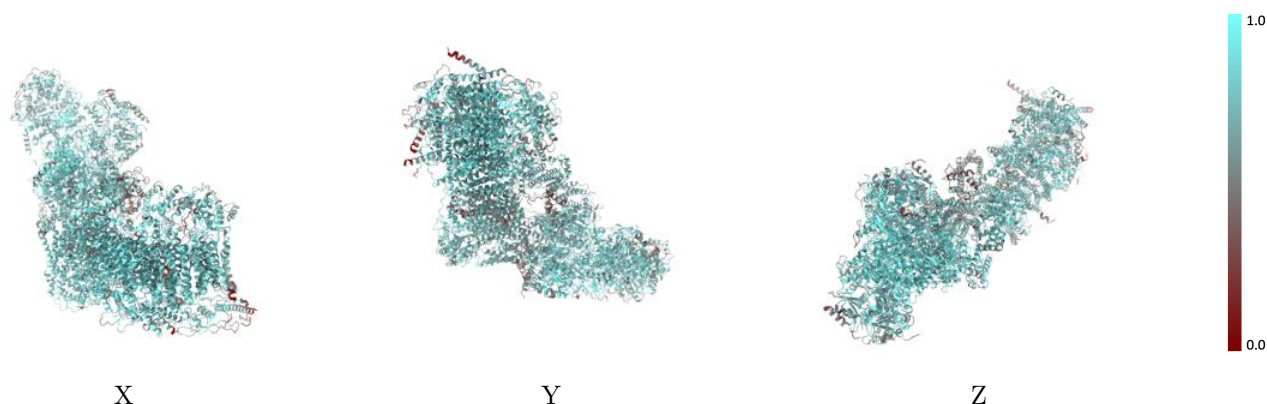
The images above show the 3D surface view of the map at the recommended contour level 0.0272 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



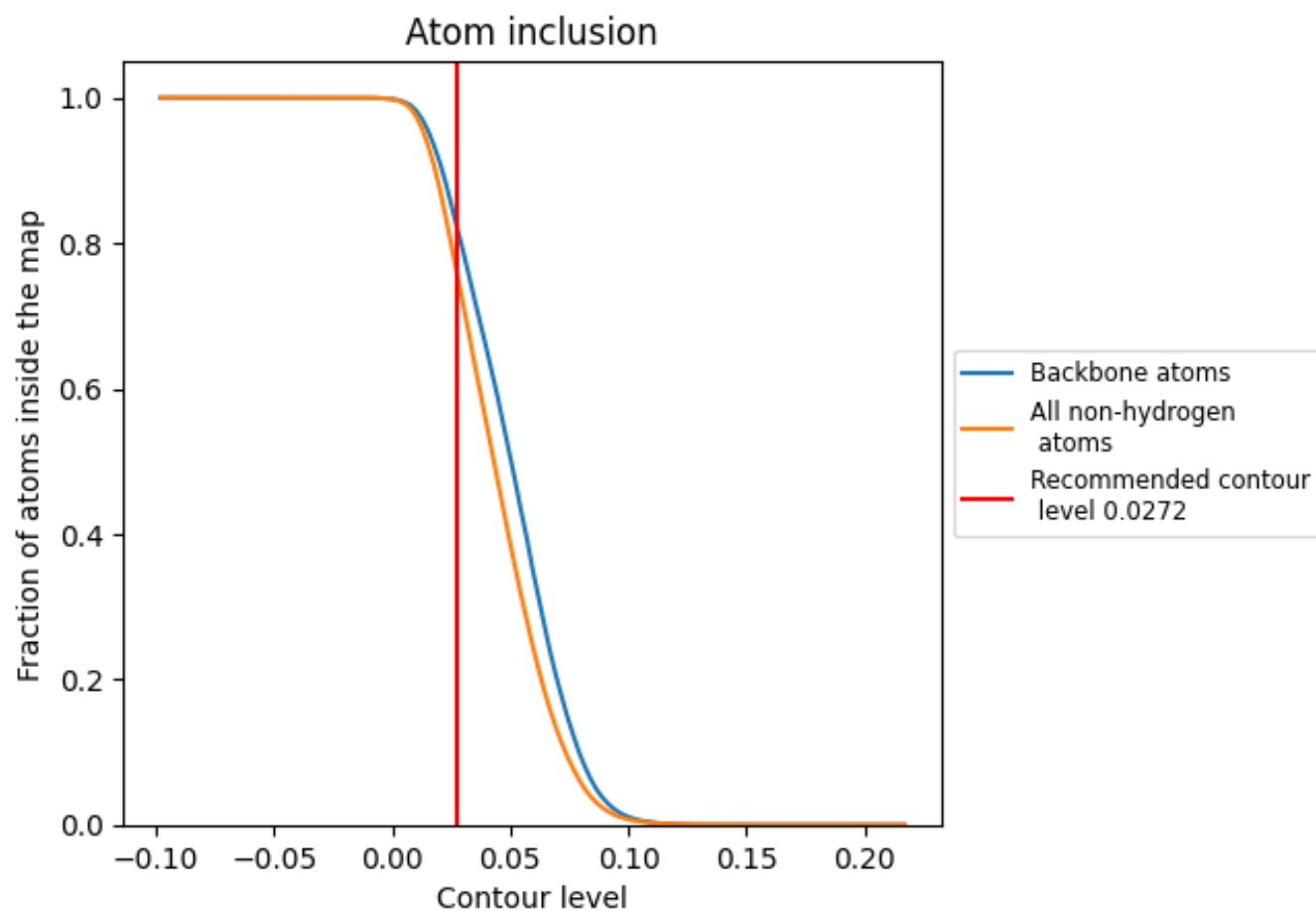
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0272).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.0272) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7635	 0.5680
A	 0.7503	 0.5550
B	 0.9158	 0.6130
C	 0.8557	 0.6010
E	 0.7495	 0.5680
F	 0.6339	 0.4950
G	 0.4321	 0.4210
H	 0.7464	 0.5580
I	 0.7606	 0.5700
J	 0.7305	 0.5510
K	 0.7122	 0.5550
L	 0.8018	 0.5880
M	 0.8114	 0.5830
N	 0.7722	 0.5820
O	 0.6776	 0.5310
P	 0.8912	 0.6130
Q	 0.8560	 0.6050
S	 0.8427	 0.5810
T	 0.8075	 0.5900
U	 0.7933	 0.5570
V	 0.4572	 0.5000
W	 0.7966	 0.5760
X	 0.6703	 0.5360
Y	 0.6239	 0.5100
Z	 0.5532	 0.4730
a	 0.7592	 0.5770
b	 0.6678	 0.5290
c	 0.7498	 0.5690
d	 0.7258	 0.5500
e	 0.7031	 0.5430
f	 0.6587	 0.5340
g	 0.7853	 0.5860
h	 0.7813	 0.5740
i	 0.8335	 0.5960
j	 0.6480	 0.5480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7197	 0.5640
l	 0.7643	 0.5760
m	 0.6983	 0.5520
n	 0.6616	 0.5410
o	 0.7376	 0.5590
p	 0.7536	 0.5600
r	 0.8500	 0.6000
s	 0.8064	 0.5810
u	 0.7798	 0.5810
v	 0.6544	 0.5110
w	 0.7515	 0.5600